iChemLabs

The Future of Scientific Software

ChemDoodle® v12.12 User Guide



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Contents

LIST OF FIGURES ii

LIST OF TABLES x

1 INTRODUCTION 2

2 CHEMDOODLE BASICS 21

3 WIDGETS 67

4 DRAWING CHEMICAL STRUCTURES 103

5 INORGANIC COMPOUNDS AND COMPLEXES 141

6 ADVANCED STRUCTURES 154

7 QUERY STRUCTURES 165

8 REACTIONS 173

9 SPECTRA 210

10 SHAPES 222

11 ICHEMLABS ART 261

12 CONTENT MANAGEMENT TOOLS 271

13 STYLES 298

14 CHEMINFORMATICS 320

15 IUPAC NAMING 365

16 STEREOCHEMISTRY 395

17 SHARING INFORMATION 416

APPENDICES 460

INDEX 483

List of Figures

1.1 On Apple Silicon Macs, you should use the faster Apple Silicon build of ChemDoodle . . . 8
1.2 You cannot run the Apple Silicon build of ChemDoodle on an Intel Mac . . . 8
1.3 Digital signature for Windows . . . 10
1.4 Apple notarization verification on macOS, press Open . . . 11
1.5 The Update Available Window . . . 16
2.1 ChemDoodle Graphical User Interface . . . 23
2.2 The Doodle Board . . . 24
2.3 Tab Tray . . . 25
2.4 Undisplayed Tabs . . . 25
2.5 List of Undisplayed Tabs . . . 25
2.6 Formatting Toolbar . . . 39
2.7 Content Toolbar . . . 39
2.8 Chemistry Toolbar . . . 40
2.9 Document Toolbar . . . 41
2.10 Drawing toolbar in attached and detached mode . . . 42
2.11 Labels Palette . . . 43
2.12 Common Labels Palette . . . 43
2.13 Bonds Palette . . . 43
2.14 Rings Palette . . . 44
2.15 Carbon Chain Toolbar . . . 45
2.16 Macromolecular Tools . . . 45
2.17 Chemical Attributes Palette . . . 46
2.18 Orbitals Palette . . . 47
2.19 Arrows Palette . . . 47
2.20 Shapes Palette . . . 48
2.21 Brackets Palette . . . 49
2.22 Polylines Toolbar . . . 50
2.23 Controls Settings . . . 52
2.24 Operating system cursor differences . . . 57
2.25 Creating a New Formatted Document . . . 60
2.26 Input a custom document rendering scale. . . . 62
2.27 The file chooser on Windows . . . 63
2.28 The file chooser on Linux . . . 63
2.29 The file chooser on macOS . . . 64
2.30 ChemDoodle's macOS Quick Look plugin . . . 65
3.1 Widget Menu . . . 69
3.2 Widget Button and Drawer . . . 70
3.3 Widget Window Components . . . 71
3.4 Widget Expansion . . . 72
3.5 Elemental Analysis Widget . . . 74
3.6 Data output from the Elemental Analysis Widget . . . 75
3.7 History Widget . . . 76
3.8 Line Notation Pad Widget . . . 77
3.9 MolGrabber Widget . . . 79
3.10 Multiplet Tool Widget . . . 83
3.11 Multiplet Input Parameters . . . 84
3.12 Multiplet Real-Time Sliders . . . 84

3.13 Multiplet Settings . . . 85
3.14 NMR Simulation Widget . . . 86
3.15 NMR Simulation Settings . . . 87
3.16 In-depth Simulation Information . . . 88
3.17 Properties Widget Interface . . . 89
3.18 Search Widget Interface . . . 91
3.19 Search Settings for the Search Widget . . . 93
3.20 Statistics Widget . . . 94
3.21 Symbols Widget . . . 95
3.22 Symbol Preview . . . 95
3.23 The Unicode Character Selector . . . 96
3.24 Templates Widget . . . 97
3.25 TLC Canvas Widget . . . 99
3.26 Format Spot Window . . . 101
4.1 Customizing menu accelerators . . . 106
4.2 Customizing tool shortcuts . . . 107
4.3 Listing all available shortcuts for reference . . . 108
4.4 Hovered Objects . . . 108
4.5 Trailing Carbon Atom . . . 109
4.6 A Hovered Atom . . . 110
4.7 A Selected Atom . . . 110
4.8 Hidden carbon labels are shown. . . . 112
4.9 Default Atom Label Format Bar . . . 113
4.10 Stacked atom label tokens . . . 114
4.11 A few cases where subtoken alignment for a terminal label will produce different graphics . . . 114
4.12 Sulfur hexachloride with subtoken alignment on and off . . . 115
4.13 Applying a custom format to an atom label . . . 115
4.14 New Bond Placement Preview . . . 117
4.15 Connecting a bond between two existing atoms . . . 118
4.16 A Hovered Bond . . . 118
4.17 A Selected Bond . . . 118
4.18 Carbon Chains . . . 120
4.19 New Ring Placement Preview . . . 122
4.20 New Template Placement Preview . . . 125
4.21 Updating an existing template . . . 128
4.22 Various types of attributes . . . 129
4.23 A Hovered Attribute . . . 129
4.24 A Selected Attribute . . . 129
4.25 Auto-layout of attributes in a complex figure . . . 130
4.26 A Charge Attribute . . . 131
4.27 Different dashes used for representing a negative charge . . . 132
4.28 A Symbol Attribute . . . 132
4.29 Incremental Attributes for an IUPAC Ring Block . . . 133
4.30 Nitrogen atom attribute . . . 134
4.31 Using the Add Attribute window . . . 135
4.32 Carbon-13 Isotope . . . 135
4.33 Nuclear Notation . . . 136
4.34 Using the Script Merge feature . . . 137
4.35 Orbital and Anchors . . . 137
5.1 An explicit zero-order connection in a sodium chloride representation . . . 142
5.2 A dative bond from ammonia to borane . . . 143
5.3 An η^6 haptic bond between a benzene ring and a chromium atom . . . 144
5.4 A multi-center attachment added to a benzene ring . . . 144
5.5 Hovering over a multi-center attachment reveals its associated atoms . . . 144
5.6 A benzene multi-center attachment connected to chromium by a single bond . . . 145
5.7 Ionic models of the pentadienyl anion . . . 146
5.8 An η^5 haptic connection between a delocalized pentadienyl anion and a manganese cation . . . 146

5.9 A haptic bond from a tropylium ring in the CSD entry PEVHUT . . . 147
5.10 An allyl ligand . . . 148
5.11 The uncharged, unconnected allyl drawing is interpreted as C_3H_6 . . . 148
5.12 The delocalized η^3-allyl ligand is correctly understood when participating in a covalent haptic bond . . . 148
5.13 The uncharged, unconnected Cp drawing is interpreted as C_5H_6 . . . 149
5.14 The delocalized Cp ligand is correctly understood when participating in a covalent haptic bond . . . 149
5.15 Ionic models of diamminesilver(I) . . . 150
5.16 Single N–Ag bonds result in a different chemical structure . . . 150
5.17 The ionic representation of ferrocene. . . . 151
5.18 The covalent representation of ferrocene. . . . 151
5.19 An inconsistent ferrocene representation produced by mixing the ionic and covalent models. . . . 151
5.20 Lithium aluminum hydride . . . 152
5.21 A covalent representation of Zeise's salt. . . . 152
5.22 An ionic representation of Zeise's salt. . . . 152
6.1 A sample structure image from ChemDoodle 3D . . . 155
6.2 Perspective drawings from 3D coordinates . . . 156
6.3 Sample Perspective Drawings . . . 157
6.4 Aromatic Ring Circle (Rotated Perspective) . . . 157
6.5 Aromatic Ring Circles Mold to any Shape. . . . 157
6.6 Cyclopentadienyl anion rings in the Templates widget. . . . 158
6.7 Flip perspective ring templates for more orientations. . . . 158
6.8 Pseudo 3D . . . 159
6.9 Lewis Dot Structures . . . 160
6.10 Carbon Nanotube Geometry . . . 161
6.11 Building a Prismane Geometry . . . 162
6.12 A Half-completed Newman Projection . . . 162
6.13 A Completed Newman Projection . . . 163
6.14 A Wrapped Sequence for Crambin . . . 163
7.1 A query structure . . . 166
7.2 Query Interface . . . 169
7.3 The interface to define a query variable, in this case the atom identity variable . . . 169
8.1 Arrow palette in the Drawing toolbar . . . 175
8.2 Arrow Shape and Anchors . . . 176
8.3 Reaction interpretation . . . 182
8.4 Edit Reaction Window . . . 183
8.5 A mechanism drawn with electron pushers . . . 184
8.6 The result of the mechanism diagram is automatically generated . . . 184
8.7 The result of the mechanism diagram cannot be represented . . . 184
8.8 Cutting an aspirin molecule to build a retrosynthetic reaction . . . 185
8.9 The results of cutting an aspirin molecule to build a retrosynthetic reaction . . . 185
8.10 Reaction Styles . . . 186
8.11 A Stacked Wide Reaction . . . 187
8.12 A warning is shown if the atom mapping is between two atoms within the same structure . . . 188
8.13 A warning is shown if two atom mappings include the same atoms . . . 188
8.14 A warning is shown if the atom mapping is between two reactants or two products of a built reaction . . . 188
8.15 The Balance Equation Window . . . 190
8.16 A Balanced Equation . . . 191
8.17 ChemDoodle can deduce oxidation states and correctly balance redox reactions. . . . 192
8.18 You may manually define oxidation state values in unclear cases. . . . 193
8.19 An example stoichiometry form for an organic reaction . . . 194
8.20 The Create Stoichiometry Table Window . . . 197
8.21 Hovering an editable cell in a stoichiometry form with the Text for Atoms and Captions tool . . . 199
8.22 Editing a stoichiometry form entry . . . 199
8.23 Suspicious results are flagged in the stoichiometry form . . . 201
8.24 Stoichiometry example: calculating expected mass of product . . . 202
8.25 Reaction to produce 2-chloropropane . . . 203
8.26 Stoichiometry example: calculating required mass of reactants . . . 203

8.27 Determining the percentage yield of a reaction . . . 204
8.28 Stoichiometry example: calculating required mass of reactants . . . 204
8.29 Stoichiometry example: determining the limiting reagent using experimental fields . . . 205
8.30 Stoichiometry example: determining the limiting reagent using theoretical fields . . . 206
8.31 The multistep synthesis of acetaminophen . . . 207
8.32 A partially drawn reaction . . . 207
8.33 Stoichiometry warning for an unbalancable reaction . . . 207
8.34 Stoichiometry example: partial stoichiometry . . . 208
9.1 An NMR Spectrum Loaded from a JCAMP File . . . 211
9.2 An IR Spectrum Loaded from a JCAMP File . . . 212
9.3 An MS Spectrum Loaded from a JCAMP File . . . 212
9.4 Sample NTUPLES input from a JCAMP File . . . 213
9.5 ChemDoodle could not obtain any data from the JCAMP file. . . . 213
9.6 Fragmenting an aspirin molecule . . . 216
9.7 The results of fragmenting an aspirin molecule . . . 216
9.8 Hovering Over a Spectrum to Display its Anchor Points . . . 217
9.9 The Spectrum Edit Window . . . 218
9.10 A Grid Displayed Over a Spectrum . . . 219
9.11 An Integration Line Calculated Over an NMR Multiplet . . . 220
10.1 Control Anchors . . . 226
10.2 Corner/Edge Anchors . . . 226
10.3 Line Shape and Anchors . . . 228
10.4 Arc Shape and Anchors . . . 229
10.5 Rectangle Shape and Anchors . . . 230
10.6 Oval Shape and Anchors . . . 231
10.7 Bracket Shape and Anchors . . . 232
10.8 Pen and Polyline Control Points . . . 233
10.9 Bézier Control Points . . . 234
10.10 Closed vs. open Bézier curves . . . 236
10.11 Ruler Shape and Anchors . . . 237
10.12 Table Shape and Anchors . . . 239
10.13 Defining a table by the number of rows and columns . . . 240
10.14 Highlighting a Table Row . . . 240
10.15 Highlighting a Table Column . . . 241
10.16 Fitting a Table to Contents . . . 242
10.17 Highlighting a Table Cell . . . 242
10.18 A Highlighted Table Cell for Label Editing . . . 243
10.19 Styling a Table Cell . . . 244
10.20 A Hovered Label . . . 246
10.21 Editing a label . . . 246
10.22 An Updating Label . . . 248
10.23 The interface for adding updating labels . . . 249
10.24 An atom mapping for the acylation of benzene . . . 250
10.25 A hovered atom mapping . . . 250
10.26 Three different types of electron pushing arrows . . . 251
10.27 A hovered electron pusher . . . 251
10.28 Electron pusher shapes will automatically start from radical and electron pair attributes, when applicable. 252
10.29 Toggling a bond-to-atom electron pair pusher to the opposite side of the bond . . . 253
10.30 A molecule with highlight shapes . . . 254
10.31 A hovered highlight . . . 254
10.32 Colored in rings using highlights . . . 255
10.33 A structure containing a repeat unit . . . 256
10.34 A hovered repeat unit . . . 256
10.35 A text field appears to edit the repeat unit display value . . . 256
10.36 Flipping a repeat unit in a ring . . . 257
10.37 Some styles will have no effect if the repeat unit is invalid . . . 258
10.38 Different methods for rendering repeat unit brackets . . . 258

11.1 Sample iChemLabs Art . . . 263
11.2 The Glassware Clipart Window . . . 264
11.3 A Glassware Setup with Altered Colors . . . 265
11.4 A Beaker with and without Solution . . . 266
11.5 Glassware Figure with Tubing . . . 267
11.6 The BioArt Window . . . 268
12.1 Selected Content . . . 273
12.2 Scaling a individual bond . . . 280
12.3 Off-page Content . . . 283
12.4 Intersecting Bonds . . . 283
12.5 ChemDoodle can automatically layer your bonds for you by inferring *z*-order from wedges. . . . 285
12.6 The Quick Colors Palette . . . 290
12.7 Advanced Colors Window . . . 291
12.8 Advanced Colors Icon . . . 292
12.9 The HSB/RGB Color Chooser . . . 293
12.10 The Pinwheel Color Chooser . . . 294
12.11 The Recent Colors Chooser . . . 295
12.12 Defining a custom color set for elements . . . 296
13.1 Styles Window . . . 300
13.2 Choose options for exporting a style sheet . . . 301
13.3 On/Off Choice . . . 303
13.4 Single Option Choice . . . 303
13.5 Drop Down Choice . . . 304
13.6 Number Slider . . . 304
13.7 Color Button . . . 304
13.8 Complete Font . . . 304
13.9 Anti-aliasing . . . 315
13.10 Stroke Control . . . 318
14.1 ChemDoodle's References List . . . 323
14.2 Condensed vs. Expanded Chemical Structures . . . 325
14.3 Abbreviations in chemical labels . . . 325
14.4 Single bond order in a chemical label . . . 326
14.5 Double bond order in a chemical label . . . 326
14.6 Triple bond order in a chemical label . . . 326
14.7 Quadruple bond order in a chemical label . . . 326
14.8 Charge symbols in chemical labels . . . 326
14.9 A charge symbol in a chemical label following hydrogen is applied to the atom the hydrogen is attached to. 327
14.10 A charge symbol in a chemical label applied to the next element . . . 327
14.11 A charge symbol followed by the number 2 (input as "+2") is understood and rendered as a "2+" charge. . . . 327
14.12 Multiple charge symbols (in this case "++") is understood as a +2 charge. . . . 327
14.13 Hydrogen counts explicitly defined in chemical labels will be enforced . . . 327
14.14 A period character (.) is used to denote fragmentation . . . 328
14.15 A space ( ) and bullet (•) character pair is used to denote fragmentation . . . 328
14.16 ChemDoodle understands the connection between the nitrogen and chlorine atoms is an implied fragmentation . . . 328
14.17 ChemDoodle expands a molecular formula to an isomer all-atom model. . . . 328
14.18 Linear notation in chemical labels . . . 329
14.19 Multiplicity in chemical labels . . . 329
14.20 Repetition in chemical labels . . . 330
14.21 Two bonds connected to a chemical label of a repeating unit will be attached at both ends of the expanded structure. . . . 330
14.22 Chemical warnings as rendered on atoms . . . 332
14.23 Explanations for chemical warnings . . . 332
14.24 Chemical Warnings . . . 333
14.25 No chemical warnings found . . . 333
14.26 Deduce Covalent Bonds Window . . . 338
14.27 The Interactive Periodic Table . . . 342

14.28 Focusing on a classification . . . 343
14.29 Element Format . . . 343
14.30 States of Matter Display . . . 344
14.31 Additional information for carbon . . . 344
14.32 How the Elemental Analysis widget handles an isotope with no mass data . . . 345
14.33 Generating a mass parent peak for a chemical structure including an isotope with no mass data will show this error . . . 345
14.34 Options for the Highlight Functional Groups function. . . . 346
14.35 Functional groups for the structure of aspirin are automatically highlighted. . . . 347
14.36 Hydrogens Added as Atoms . . . 350
14.37 Hydrogens Added as Text . . . 350
14.38 Repeat units are automatically interpreted . . . 351
14.39 Examples of invalid repeat unit values . . . 352
14.40 Repeat values of 0 cut out the contained substructure . . . 352
14.41 A stereo bond can start a repeat unit as long as the closing bond is a single bond . . . 352
14.42 Repeat unit on a substructure where both ends are double bonds . . . 353
14.43 Repeat unit bond ends must have the same bond order . . . 353
14.44 A trimer of nylon 6/6 drawn with 3 repeat units, 2 of which are embedded in the third . . . 353
14.45 You may mix condensed labels with repeat units . . . 353
14.46 Partially intersecting repeat units are invalid . . . 354
14.47 Exactly overlapping repeat units are invalid . . . 354
14.48 An embedded repeat unit that shares one bond with the outer repeat unit is valid . . . 354
14.49 There are two directions for a repeat unit in a ring . . . 354
14.50 Examples of ambiguous repeat units . . . 355
14.51 Repeat units are possible in fused ring systems . . . 355
14.52 Expanding a repeat unit . . . 356
14.53 Expanding a ring based repeat unit . . . 356
14.54 Invalid repeat units cannot be expanded . . . 356
14.55 Inner repeat units must be expanded before outer repeat units . . . 357
14.56 Aromatic Representations . . . 357
14.57 Showing aromatic and anti-aromatic electron counts . . . 358
14.58 A Kekulé model of imidazole . . . 358
14.59 A delocalized imidazole ring . . . 359
14.60 Rendering conjugated chain resonance lines as a curve . . . 359
14.61 Conjugated Curve Sharpness . . . 359
14.62 Kekulizing a Single Bond Frame to Generate Corannulene . . . 360
14.63 Kekulizing the Aromatic Rings in the Resonance Model for Viagra . . . 360
14.64 Different ring sets for cubane . . . 361
14.65 The Hanser ring set for cubane . . . 361
14.66 A generated text description for 1-propanol with low sophistication . . . 362
15.1 IUPAC naming of various structures with covalent bond types . . . 369
15.2 IUPAC naming of stereocenters . . . 369
15.3 IUPAC naming of various structures with zero order bonds . . . 369
15.4 IUPAC naming will work on both Kekulé and delocalized structures . . . 370
15.5 IUPAC naming of various structures with dative bonds . . . 370
15.6 Only a single additive center may be defined per structure . . . 371
15.7 The directionality of dative bonds is important . . . 371
15.8 A dative bond in this context does not make any sense and this structure cannot be named . . . 371
15.9 ChemDoodle may automatically employ additive nomenclature, depending on the structure . . . 372
15.10 Both the additive and substitutive name may be equally desirable . . . 372
15.11 You may expand the additive scope so ChemDoodle will more likely name structures via additive nomenclature 372
15.12 Dative bonds and explicit charges may be used to manually define additive centers . . . 373
15.13 Bond type choice is very important for neutral ligands . . . 373
15.14 Alkyl groups will be named as neutral substituents in additive centers when single covalent bonds are used 373
15.15 IUPAC naming of various radicals by ChemDoodle . . . 374
15.16 IUPAC naming of various ionic structures by ChemDoodle . . . 375
15.17 A warning is displayed describing why a name cannot be parsed . . . 376

15.18 A warning is displayed describing why a name cannot be generated . . . 376
15.19 The Enter IUPAC Name window . . . 377
15.20 The Traditional IUPAC name and the Attempted PIN will be shown in a window . . . 378
15.21 Generating a name from multiple components, such as this ionic compound . . . 379
15.22 The interface for adding an IUPAC updating label . . . 380
15.23 An updating label displaying an IUPAC name . . . 380
15.24 An auto-updating label to show the IUPAC name for multiple components connected with zero order bonds 381
15.25 A formatted IUPAC name converted into unicode plain text . . . 381
15.26 Showing IUPAC locants can help clarify main chains . . . 382
15.27 Complex IUPAC names with specifically numbered base systems are elucidated . . . 382
15.28 IUPAC naming options in the Settings window . . . 383
16.1 The same structure evaluated for stereochemical features using both IUPAC and MDL/BIOVIA specifications 397
16.2 Examples of incorrectly drawn tetrahedral geometries . . . 398
16.3 Examples of incorrectly drawn rectangular geometries . . . 398
16.4 An example of a Fischer projection evaluated in ChemDoodle . . . 399
16.5 Example Haworth projections evaluated in ChemDoodle . . . 400
16.6 A chair projection and its inversion evaluated in ChemDoodle . . . 400
16.7 Axial (a) and equitorial (e) substituents . . . 401
16.8 Wedge types for chair projection substituents . . . 401
16.9 ChemDoodle expertly assigns CIP descriptors, as validated by the Hanson validation suite . . . 403
16.10 Thorough CIP rule handling . . . 404
16.11 An odd numbered cumulene system with an (E) configuration . . . 405
16.12 An allene stereocenter with a (M) configuration . . . 405
16.13 An atropisomer with a (P) configuration . . . 406
16.14 The CIP configurations for this structure would take a very long time to resolve and may likely lockup your computer, so they are skipped . . . 406
16.15 Using a wavy or ambiguous double bond will mark a stereochemical feature as undefined . . . 407
16.16 Absolute enhanced stereochemistry is defined by default, designating only a single enantiomer . . . 410
16.17 “Or” enhanced stereochemistry defines the current enantiomer or the opposite configuration . . . 410
16.18 “And” enhanced stereochemistry defines the current enantiomer and the opposite configuration . . . 410
16.19 Enhanced stereochemistry, using “or” operators on two separate chiral centers in two separate groups, representing all 4 stereoisomers . . . 411
16.20 Enhanced stereochemistry, using “or” operators on two separate chiral centers in the same group, representing only a pair of diastereomers . . . 412
16.21 Enhanced stereochemistry, using “and” operators on two separate chiral centers in two separate groups, representing all 4 stereoisomers . . . 412
16.22 Enhanced stereochemistry, using “and” operators on two separate chiral centers in the same group, representing only a pair of diastereomers . . . 413
16.23 Prompt for enhanced stereochemistry grouping number . . . 413
17.1 Copy Settings . . . 420
17.2 Raster Image vs. Vector Image . . . 421
17.3 Paste Special Window . . . 423
17.4 Excluding file types from the Save As file choosers . . . 425
17.5 When saving a file, an individualized output settings window will be presented, in this case for PNG image output . . . 426
17.6 File Annotations Window . . . 429
17.7 Chemical File Conversion Utility . . . 430
17.8 Chemistry Format Options . . . 431
17.9 An Activated ChemDoodle Embedded Object (Microsoft Word) . . . 437
17.10 OLE Server Installation Corruption . . . 438
17.11 Round-trip Editing: Workaround for iWork Applications . . . 439
17.12 PDF Round-trip Editing has been Blocked . . . 440
17.13 Registered ChemDoodle extension for LibreOffice . . . 441
17.14 The menu item used to insert OLE Objects in LibreOffice . . . 442
17.15 Selecting ChemDoodle Embedded Object to insert in LibreOffice . . . 442
17.16 Use the Paste Special menu item on Windows to paste a traditional Windows OLE object . . . 443
17.17 Select “ChemDoodle OLE” . . . 443

17.18 Missing ChemDoodle Document and Image Data . . . 444
17.19 Missing ChemDoodle Document . . . 444
17.20 Missing Image Data . . . 444
17.21 Corrupted ChemDoodle Document . . . 444
17.22 ChemDoodle reads in chemical files in a pixel-perfect manner . . . 446
17.23 In this image, ChemDoodle on macOS recovers complex chemical figures pasted from ChemDraw into Microsoft Word on Windows. . . . 447
17.24 Window to select a Microsoft Office file to recover chemical data from. . . . 448
17.25 Recovered chemical figures from a Microsoft Powerpoint file. . . . 448
17.26 Image Sizing . . . 451
17.27 Custom sized image with unscaled contents, leading to cutoff . . . 451
17.28 Previewing the image size . . . 452
17.29 Image Format Options . . . 453
17.30 Recovering a chemical drawing from an image. The recovered drawing may be further edited or used as input to a chemistry function. . . . 456
17.31 No chemical drawings were recovered from the input image. . . . 456
A.1 The SciFinder-n query window . . . 463
A.2 Logging into SciFinder-n . . . 464
A.3 Setting up a proxy for SciFinder-n . . . 465
A.4 The Google Patents query window . . . 466
A.5 The GSRS query window . . . 467
A.6 Advanced settings for the GSRS instance . . . 468
A.7 The LabArchives post window . . . 469
A.8 Authenticating your LabArchives account . . . 469
A.9 The PubChem query window . . . 472
B.1 Generate ChemDoodle Web Component Window . . . 474
B.2 Previewing the Web Component . . . 475
C.1 Contact Customer Service Menu Item . . . 479

List of Tables

1.1 Typographical Conventions . . . 5
2.1 Elements of ChemDoodle GUI . . . 23
2.2 Available Widgets . . . 51
2.3 Mouse Cursors . . . 56
3.1 Widgets . . . 73
3.2 Line Notation Pad Widget Buttons . . . 78
3.3 MolGrabber Widget Buttons . . . 80
3.4 Multiplet Widget Buttons . . . 83
3.5 NMR Simulation Widget Buttons . . . 86
3.6 Search Widget Buttons . . . 92
3.7 Template Widget Buttons . . . 98
3.8 TLC Plate Widget Buttons . . . 100
4.1 Customizing Formatting . . . 116
5.1 Charges and electron counts in aromatic ring models . . . 147
7.1 Attribute Variable Types . . . 167
7.2 Atom Attribute Variables . . . 168
7.3 Bond Attribute Variables . . . 168
7.4 Atom Query Variable Icons . . . 170
7.5 Bond Query Variable Icons . . . 170
10.1 Available Custom Shapes . . . 233
12.1 Extended SMARTS Atomic Primitives . . . 275
12.2 Extended SMARTS Bond Primitives . . . 276
16.1 Situations where stereochemical configurations cannot be forced . . . 409
17.1 File Option Types . . . 431

CHAPTER 1

Introduction

Contents

1.1 About ChemDoodle **4**

1.2 What's new in ChemDoodle 12.12 . . . . . **4**

1.3 About this manual **5**
- 1.3.1 Typographical conventions 5
- 1.3.2 How to use this manual 5

1.4 Additional information **6**

1.5 Installation and system requirements **7**
- 1.5.1 Installation vs. Activation 7
- 1.5.2 Microsoft Windows system requirements 7
  - 1.5.2.1 Silent installation 7
- 1.5.3 Apple macOS system requirements 7
  - 1.5.3.1 Mac processors 8
- 1.5.4 Linux system requirements 8
  - 1.5.4.1 Resolving taskbar icon issues on GNOME with Dash to Panel 9
- 1.5.5 High-DPI screens 10
  - 1.5.5.1 Manually defining the scale factor on Linux (and Windows) 10

1.6 Operating system security features **10**
- 1.6.1 Windows 10
- 1.6.2 macOS 11

1.7 Multiple users on a single computer **11**
- 1.7.1 Windows 11
- 1.7.2 macOS 11
- 1.7.3 Linux 11

1.8 ChemDoodle folders **13**
- 1.8.1 Installation folder 13
  - 1.8.1.1 Application and file icons 13
- 1.8.2 Settings folder 14

1.9 Socket communications **14**

1.10 File type associations **14**
- 1.10.1 Windows 14
- 1.10.2 macOS 15
- 1.10.3 Linux 15

1.11 Program activation **15**
- 1.11.1 User licenses 15
- 1.11.2 Site licenses 15
- 1.11.3 Connection issues 16
  - 1.11.3.1 Firewall issues 16
  - 1.11.3.2 Proxy issues 16

1.12 Updating ChemDoodle **16**
- 1.12.1 Windows administrator privileges 17
- 1.12.2 Skipping updates 17

1.13 Moving your activated copy to a new computer **17**

1.14 Preparing for a system restore **18**

1.15 Restricted use versions **18**

1.15.1 Free trial 18

1.16 Unauthorized use **19**

1.17 Ownership **19**

1.18 Attributions **19**

1.19 Referencing **19**

1.1 About ChemDoodle

ChemDoodle is a desktop software tool for drawing chemical structures, diagrams and figures. It is a richly featured, multi-platform (Windows, macOS, Linux) graphical user interface containing many features for working with scientific information and graphics.

ChemDoodle is integrated with the following iChemLabs Products:

ChemDoodle 3D - A desktop software tool for creating 3D scientific graphics and molecular modeling.
https://www.chemdoodle.com/3d

ChemDoodle Web Components - A pure Javascript chemical graphics and cheminformatics library.
https://web.chemdoodle.com

ChemDoodle Mobile - A companion mobile app to the desktop software.
https://mobile.chemdoodle.com

1.2 What's new in ChemDoodle 12.12

iChemLabs is continuously developing ChemDoodle and version 12.12 includes significant new features and improvements.

For a complete version history, visit the following url:
https://www.ichemlabs.com/support/version-history?product=ChemDoodle

If you would like to see new features added, please do reach out to us: https://www.ichemlabs.com/contact-us?tab=support

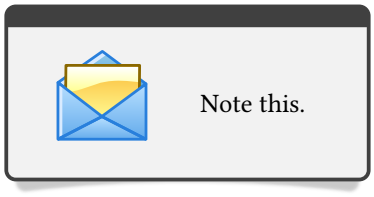
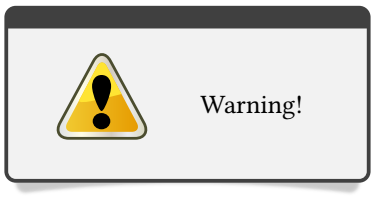
1.3 About this manual

This User Guide contains information for the ChemDoodle application for the Windows, macOS and Linux operating systems. It assumes you are familiar with the basics of your operating system. If necessary, please review your operating system manual before using ChemDoodle.

1.3.1 Typographical conventions

The following typographical conventions are used in this manual:

Table 1.1: Typographical Conventions

Item	Convention	Example
Toolbar buttons, prompt titles, and other interface components	Bold	Select the **Clear** button or type in the text field titled **Filename**
Series of menu items in a specific order	Menu icons	File ⟩ New means from the **File** menu, choose the **New** menu item
Keyboard input	Key icons	To undo an action, press ctrl + Z (Note that on macOS, the ctrl key refers to the cmd/⌘ key)
Figure/Table captions	Italic	*Figure 1.4: The Doodle Board*
Folder and File locations	Monospace	In the `ChemDoodleSettings` folder
Product Names	Dark Gray	ChemDoodle works on Windows, macOS and Linux
Internal link within the document	Dark Green	In the ADDITIONAL INFORMATION section
External link to the internet	Underlined Blue	https://www.chemdoodle.com
Optional additional information	Note icon box	
Caution! / Warning!	Warn icon box	

1.3.2 How to use this manual

It is not necessary to read this entire manual before proceeding to use ChemDoodle; however, it is recommended that you skim the TABLE OF CONTENTS and read this INTRODUCTION chapter. Once you have the program installed, read ChemDoodle BASICS. Subsequent chapters can be consulted as questions arise during use of the program. This user's guide can be found by clicking on Help ⟩ User Guide in the application menu at the top of the program screen.

1.4 Additional information

Additional information about ChemDoodle and its use and related software can be found by following any of the links in the table below.

ChemDoodle Help Pages	https://www.ichemlabs.com/knowledgebase
ChemDoodle	https://www.chemdoodle.com
ChemDoodle 3D	https://www.chemdoodle.com/3d
ChemScribble	https://www.chemscribble.com
ChemDoodle Web Components	https://web.chemdoodle.com
ChemDoodle Mobile	https://mobile.chemdoodle.com
iChemLabs Customer Support	https://www.ichemlabs.com/contact-us?tab=support
iChemLabs Sales	https://www.ichemlabs.com/contact-us
iChemLabs Website	https://www.ichemlabs.com

You can also discover information about ChemDoodle and iChemLabs on social media.

iChemLabs on X (formerly Twitter)	https://www.x.com/ichemlabs
iChemLabs on Instagram	https://www.instagram.com/ichemlabs/
ChemDoodle on Facebook	https://www.facebook.com/Chemdoodle/
iChemLabs Youtube Channel	https://www.youtube.com/user/ichemlabs
iChemLabs on LinkedIn	https://www.linkedin.com/company/ichemlabs

1.5 Installation and system requirements

1.5.1 Installation vs. Activation

Using ChemDoodle requires two setup steps:

- Installation
- Activation

Installation of ChemDoodle should be done by a system administrator (or yourself if you control the computer), and will make ChemDoodle available to some or all users on your machine or network. The administrator should install ChemDoodle, but **SHOULD NOT** activate ChemDoodle on the administrator account.

Activation (see PROGRAM ACTIVATION) of ChemDoodle is done per user, by the user, and will allow that user to use ChemDoodle in accordance with the license. Activation is done when the user opens ChemDoodle the first time after accepting the user license.



ChemDoodle is a Java based application. A Java runtime environment (JRE) is bundled into the ChemDoodle application as required by Oracle best practices. So while you do not have to install Java to run ChemDoodle, you may still see system warnings and messages about allowing Java to run to use ChemDoodle. Accept these prompts.

1.5.2 Microsoft Windows system requirements

- Windows 10/11+
- A 64 bit (x86_64) processor is required
- A minimum of 1GB of memory, 2GB recommended

1.5.2.1 Silent installation

The ChemDoodle installer on Windows is an NSIS installer that can be run silently.

1. Open a command prompt with administrator privileges.
2. Run the following NSIS command. Note that NSIS flags are case sensitive.

   <location of downloaded installer>\ChemDoodle-windows-<version>.exe /S

When run in silent mode, the installer will create a log file in the `Temp` directory. This is typically located here, where "<username>" is replaced by the current user's name: `C:\Users\<username>\AppData\Local\Temp`

The name of the log file will be the following, where "<version>" is replaced by the current version of the application being installed: `ChemDoodle-<version>-install.log`



For best results, remove the previous installation before installing an update. It is safe to simply just delete the `C:\Program Files\ChemDoodle` folder.

1.5.3 Apple macOS system requirements

- macOS 11+ (Big Sur, Monterey, Ventura, Sonoma, Sequoia, Tahoe or more recent)
- A 64 bit (x86_64 or Apple Silicon) processor is required

- A minimum of 1GB of memory, 2GB recommended

1.5.3.1 Mac processors

There are currently two main types of Mac processors, the legacy Intel chips, and the newer Apple Silicon chips. Apple Silicon chips may also be referred to as ARM, aarch64 or Apple M series chips (M1, M1 Max, M1 Ultra, M2, etc.). All contemporary Macs are created with Apple Silicon chips, but some older Macs will require Intel compatible software.

iChemLabs provides two builds for the ChemDoodle application, **Intel** and **Apple Silicon**. If you are using a legacy Intel Mac, then download the **Intel** build of ChemDoodle. If you are using a Mac with an Apple Silicon chip, then download the **Apple Silicon** build of ChemDoodle.

If you are unsure what processor is in your Mac, then download and install the **Intel** build of ChemDoodle. The **Intel** build will work on both processor types, however it will run via emulation on Apple Silicon Macs using a program called Rosetta 2. ChemDoodle will automatically detect the processor type and notify you to choose the better **Apple Silicon** build instead, if possible, as shown in Figure 1.1. Again, the **Intel** build of ChemDoodle will run on both Mac processor types, but the **Apple Silicon** build of ChemDoodle will run natively, and therefore much faster, on Apple Silicon Macs.

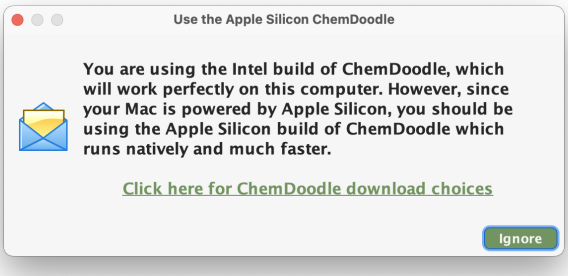


Figure 1.1: *On Apple Silicon Macs, you should use the faster Apple Silicon build of ChemDoodle*

If you try to open the **Apple Silicon** build of ChemDoodle on an Intel Mac, you will see the following error (Figure 1.2). Please install the **Intel** build of ChemDoodle instead.

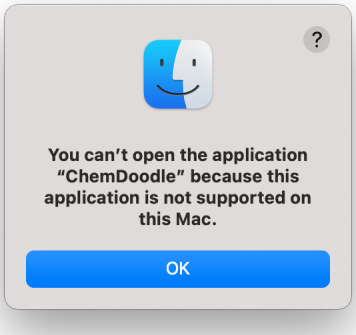


Figure 1.2: *You cannot run the Apple Silicon build of ChemDoodle on an Intel Mac*

1.5.4 Linux system requirements

- Any version of Linux (we test with Mint, Fedora, Debian and OpenSUSE Linux)
- A 64 bit (x86_64) processor is required

- Any working GUI, although we recommend and test with GNOME
- A minimum of 1GB of memory, 2GB recommended

1.5.4.1 Resolving taskbar icon issues on GNOME with Dash to Panel

On some Linux systems with the GNOME desktop and the Dash to Panel extension, users may notice the ChemDoodle icon does not appear correctly on the taskbar. Instead, a generic icon is shown, and the application may not group properly or behave like a traditional taskbar window.

This issue occurs because the GNOME Shell extension cannot associate the running ChemDoodle window with its `.desktop` launcher file, due to a mismatch in internal window properties.

Cause

Linux desktop environments like GNOME use a window property called `WM_CLASS` to match running applications to their `.desktop` files. If this does not match what is expected, the system shows a generic icon or treats the window as a separate, unidentified process.

By default, ChemDoodle is launched using a shell script, which starts the Java runtime. Without further configuration, the window class is not explicitly defined and may not match the entry in the `.desktop` file.



This issue **does not affect** users on KDE, Cinnamon, or other desktop environments that do not depend on `StartupWMClass`.

Solution

This issue can be resolved by ensuring that your system's `ChemDoodle.desktop` file includes a `StartupWMClass` entry that matches the internal window class name used by the Java application.

Step-by-Step Fix

1. **Locate your `ChemDoodle.desktop` file**, typically found in one of the following locations:
   - Per-user installation: `~/.local/share/applications/ChemDoodle.desktop`
   - System-wide installation: `/usr/share/applications/ChemDoodle.desktop`
2. **Open the file in a text editor** (e.g., gedit, nano, or Vim). For example:

   ```
   gedit ~/.local/share/applications/ChemDoodle.desktop
   ```
3. **Add the following line** to the bottom of the `[Desktop Entry]` section:

   ```
   StartupWMClass=gui-twod-ChemDoodleLauncher
   ```

   Your updated `.desktop` file should look similar to this (make sure to replace [PATH TO INSTALLATION FOLDER] with the path to the ChemDoodle installation folder):

   ```
   [Desktop Entry]
   Version=1.0
   Name=ChemDoodle
   GenericName=ChemDoodle
   Comment=2D Chemical Drawing, Publishing and Informatics
   Exec=[PATH TO INSTALLATION FOLDER]/ChemDoodle
   Icon=[PATH TO INSTALLATION FOLDER]/ChemDoodle/resources/ChemDoodle.png
   Terminal=false
   Type=Application
   Categories=Science;Chemistry;Graphics;Office;
   StartupWMClass=gui-twod-ChemDoodleLauncher
   ```

4. **Save the file** and restart GNOME Shell or log out and log back in to see the changes take effect.

   Alternatively, press `Alt+F2`, type `r`, and hit `Enter` to reload GNOME Shell (on X11 sessions only).

1.5.5 High-DPI screens

ChemDoodle is able to detect the resolution of your screen and scale its interface accordingly. High-DPI screens are fully supported for Windows and Linux. Retina displays are fully supported for macOS.

1.5.5.1 Manually defining the scale factor on Linux (and Windows)

Some Linux builds may not provide Java with an optimal DPI scaling factor. In these cases, you must manually define the scale factor. To define a high-DPI scaling factor for ChemDoodle on Linux distributions, add the following line to the JVM parameters in the ChemDoodle initialization file (`ChemDoodle.ini` file located in the root of the `ChemDoodle` installation folder on Linux, please see APPENDIX: TECHNICAL SUPPORT for further instructions to locate and modify this file):

-Dsun.java2d.uiScale=2.0

You may also need to set the *XRender* JVM parameter to true for high-DPI scaling to work properly on Linux:

-Dsun.java2d.xrender=true

Please note that your Linux machine may not support the *XRender* pipeline, and if high-DPI scaling requires *XRender* for your build, you will not be able to scale the application on your build.

You may also define the *-Dsun.java2d.uiScale* parameter on Windows to change the application scaling factor (if you want even larger buttons and text, for instance), but this parameter will not behave as expected on macOS as macOS has a lower level scaling system that will conflict with this parameter.

Values of "1.5" and "2.0" are optimal for the *-Dsun.java2d.uiScale* parameter. Note on Linux platforms, only whole number based values are supported by Java.

1.6 Operating system security features

iChemLabs signs its applications given best practices by the operating system vendors. You may still see some warning messages when starting ChemDoodle. This section lists common installation information regarding the built-in operating system security features.

1.6.1 Windows

ChemDoodle (and its installer) is signed for Windows platforms with a code signing authority. You should see that the publisher is iChemLabs when viewing the certificate. You may still see questions when running or downloading the installer, especially from Windows SmartScreen, but they should only be questions and not warnings or errors. Just allow or deny the desired capabilities and continue to run ChemDoodle.

You can view the certificate by right-clicking on the application *EXE* or the installer and selecting the Properties item. Under the **Digital Signatures** tab, you should see the iChemLabs signature as shown in Figure 1.3.

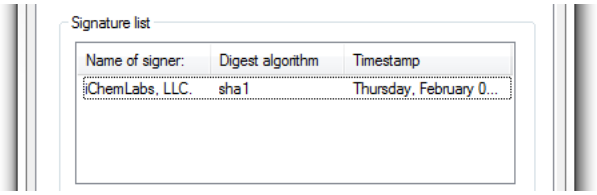


Figure 1.3: *Digital signature for Windows*

1.6.2 macOS

ChemDoodle is notarized by Apple for security, which can be detected on macOS Catalina or more recent. You can verify the notarization is correct, as macOS will display the message in Figure 1.4 upon opening the application for the first time after downloading it. Apple verifies "Apple checked it for malicious software and none was detected". Press the **Open** button to continue.

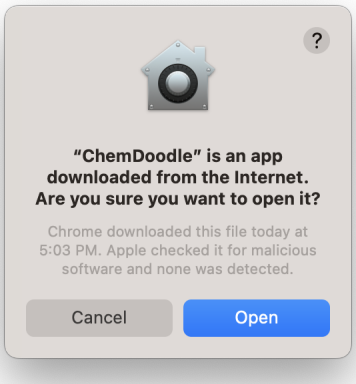


Figure 1.4: *Apple notarization verification on macOS, press Open*

1.7 Multiple users on a single computer

Several users can set up licenses for ChemDoodle on a single computer if all users have separate operating system accounts. Each named user account will have its own private preferences and settings files for customizing ChemDoodle. Each account that wishes to use ChemDoodle must be licensed. Licensing is executed by inputting a license code (see PROGRAM ACTIVATION). Instructions for installing ChemDoodle for multiple users are operating-system-dependent and specifics for each operating system are given in the following subsections.

1.7.1 Windows

During the installation, keep the install folder in `C:\Program Files\`. All users will be able to execute ChemDoodle from within this folder.

There will be periodic updates to ChemDoodle. ChemDoodle requires administrator privileges to update. Updates are performed only once on a given computer; all users then have access to the updated program.

1.7.2 macOS

During the installation, drag the `ChemDoodle` folder to the `/Applications` folder as instructed. All users will be able to execute ChemDoodle from within this folder.

There will be periodic updates to ChemDoodle. Only superusers are able to update ChemDoodle. Updates are performed only once on a given computer; all users then have access to the updated program.

1.7.3 Linux

Run the Linux *BIN* in a folder that all users have rights to execute binaries from. After the installation, verify that all users that will be using ChemDoodle have the necessary permissions to do so.

There will be periodic updates to ChemDoodle. You may want to restrict write privileges to the `ChemDoodle` installation folder to a single user. This user will then need to update ChemDoodle as root on the computer. This only needs to be done once for the computer, and all users will then have access to the updated program.

1.8 ChemDoodle folders

There are two main parent folders that the ChemDoodle application uses: the main `ChemDoodle` installation folder and the `ChemDoodleSettings` folder.

1.8.1 Installation folder

The contents of the main `ChemDoodle` installation folder are specified in the table below:

Name	Type	Description of Contents
`ChemDoodle` application	Program	`ChemDoodle.exe` on Windows, `ChemDoodle.app` on macOS, or the `ChemDoodle` shell script on Linux
`config` directory	Folder	Various configuration files, such as `proxy.config`, for setting ChemDoodle to use your proxy. It also contains the site license configuration file for site licenses.
`docs` directory	Folder	Documentation, such as this user guide.
`external` directory	Folder	Required packages that ChemDoodle needs to start up and run properly. Any licenses associated with these packages are also provided.
`jre` directory	Folder	This folder contains the Oracle JRE that ChemDoodle runs on. Do not alter or edit this JRE. This folder is not present in the macOS distribution of ChemDoodle.
`resources` directory	Folder	Native application icons, product images and other resources such as the auto-updater, native plugins and the ChemDoodle Web Components library.
`ChemDoodle.jar`	File	Executable Java jar of ChemDoodle. **This jar is not meant to be run directly.** This jar is not present in the macOS distribution of ChemDoodle.
`ChemDoodle.ini` (initialization file)	File	Contains parameters for the Java virtual machine. On Windows, this file is named `ChemDoodle.vmoptions`. This file is found in the application package of the macOS distribution of ChemDoodle. Please see APPENDIX: TECHNICAL SUPPORT for instructions to modify this file.



Do not remove or alter the contents of the ChemDoodle installation folder or unexpected behavior may occur or the software will most likely not run. To move the application, you must move the entire `ChemDoodle` folder or reinstall the application in a different location.

1.8.1.1 Application and file icons

You may wish to associate file icons and application icons with ChemDoodle if ChemDoodle does not already do this for you, such as on Linux. In the `resources` folder in the main `ChemDoodle` installation folder, operating system-specific graphics will be provided for ChemDoodle and recognized chemical file types. Use your operating system's documentation to associate those icons with the application and file types.

1.8.2 Settings folder

The ChemDoodleSettings folder can be found in the operating system's standard Documents folder. The location of the standard operating system Documents folder for the different platforms on which ChemDoodle runs are indicated below:

Windows	C:\Users\[username]\My Documents
macOS	/Users/[username]/Documents
Linux	/Users/[username]/Documents

You may change the location of the settings folder by editing the config/application.config file in the main installation ChemDoodle folder. Make sure you know what you are doing if you edit this file! Set the value for the "user_settings_folder" element to the absolute path of the folder where you would like ChemDoodle settings to be stored. A value of "!" means that the default behavior will occur. Be sure to move any of the contents from the previous settings folder location if you want to continue to use them.

1.9 Socket communications

ChemDoodle hosts communications through a private socket on your OS user account. This is essential for communicating between iChemLabs applications, for instance when viewing a chemical structure drawn in ChemDoodle 2D in 3D through ChemDoodle 3D. This is also essential for working with 3rd party applications, such as SciFinder.

The specific socket reserved for ChemDoodle is accessible through port 42501.

You may change the socket communication port used by editing the config/application.config file in the main installation ChemDoodle folder. Make sure you know what you are doing if you edit this file! Set the value for the "communication_port" element to the desired port you would like communications to pipe through. A value of "!" means that the default port will be used. You may also block communications to ChemDoodle in any way you see fit, but keep in mind any inter-application features will no longer work.

1.10 File type associations

File type associations link a certain file type, usually by what extension it has, to opening in a specific program. This is useful when opening a chemical file in ChemDoodle. You should also see a ChemDoodle file type icon on files that are associated with ChemDoodle, allowing you to quickly recognize these files. Certain operating systems even include additional functionality for associated file types, such as showing a preview using the Quick Look plugin on macOS. The process for setting this up ranges from manual to automatic, depending on which operating system you are installing on. The following sections detail how file type associations are registered on each platform.

Of course, file type associations only refer to how the operating system determines which application to use to open files of a certain type. System associations do not affect which files ChemDoodle can open, and any supported files can still be manually opened by dragging the file from the file system onto ChemDoodle or by using the File » Open... menu item, regardless of file type associations.

1.10.1 Windows

File type associations on Windows are defined in the system registry. ChemDoodle will programmatically edit the registry when it is being activated and when ChemDoodle detects it has been updated. However, the registry can only be edited when ChemDoodle has administrator privileges. If ChemDoodle does not have administrator privileges, then ChemDoodle will not edit the registry and therefore file type associations will not be set up. You can learn more about Windows administrator privileges in the WINDOWS ADMINISTRATOR PRIVILEGES section below.

That being said, ChemDoodle will allow you to manually control the file type associations within the software at any time, given ChemDoodle has been run with administrator privileges. This is helpful if you did not properly do this during installation.

To do so, select the Help » Register Filetype Associations menu item. This menu item is only present on Windows. In the window that appears, you will be able to see all the possible file types that can be registered to ChemDoodle. Follow the instructions and press the **Continue** button to register the file type associations.



You can also unassign filetype associations using this interface, however, this will only remove the file type from being associated with ChemDoodle; it will not assign the file type to a different application.

1.10.2 macOS

macOS file type associations are defined in the application's properties list, and are automatically handled when ChemDoodle is installed. On macOS, ChemDoodle will assert itself as the default editing tool for all primary ChemDoodle file types. For all other file types, such as the *MDL MOLFile* format, ChemDoodle assigns itself the "Alternate" role which informs macOS that it can handle that file, but is not the official editor of that file type, allowing another application to be the primary handler. This of course could refer to file types that have no official editor on macOS, and then your system may default to opening these types in ChemDoodle.

1.10.3 Linux

File type associations will need to be manually assigned on Linux. The process for this may vary between the flavors of Linux. Please consult the operating system manual or a Linux administrator to set up file type associations. File type icon images can be found in the `resources` folder of the `ChemDoodle` installation folder.

1.11 Program activation

1.11.1 User licenses

Activation occurs when a purchased license code is used to associate a license with the ChemDoodle application for a given user account.

Activation is achieved in one of two ways: (1) the license code is entered in the activation screen after first opening ChemDoodle and accepting the license (the activation screen is accessed before a trial is started or after a trial has completed), or (2) the user clicks on the Purchase » Activate ChemDoodle... menu item while a trial is active and enters the license code.

The license code may be manually typed into the activation form or copied and pasted (in its entirety) from the receipt into the form. Once activated with a purchased license, all restrictions from the trial are removed.

Activation requires an active internet connection. Our server is sent the license code, which is then validated and grants permission to create the license file. There are no exceptions to the internet activation.

1.11.2 Site licenses

For a site license, each member of the site will receive his/her own unique license code to activate ChemDoodle on personal computers (see USER LICENSES above). An additional campus configuration capability which will allow use without individual activation by any users that log into campus computers is also provided. Campus configurations are set up globally for a ChemDoodle installation and are typically done by IT staff at the institution owning the site license.

To configure ChemDoodle for campus use, place the provided `site_license.config` file in the `config` subfolder inside the `ChemDoodle` installation folder. Do this wherever you install ChemDoodle on campus. Then no matter where you open ChemDoodle on campus, if a configured ChemDoodle is used, ChemDoodle will open without activation. This procedure works on Windows, macOS and Linux.

Individual license codes can be obtained by the user by inputting their institution affiliated email address into the site license form on the iChemLabs website:

https://www.ichemlabs.com/support/request-site-code/

1.11.3 Connection issues

Connectivity issues may arise during activation. These are most likely to occur in corporate environments and are usually related to a firewall or proxy server.

1.11.3.1 Firewall issues

If your firewall blocks internet connections from Java applications, then ChemDoodle will not be allowed to connect to the internet. An administrator should set up a special exception to allow ChemDoodle to connect to the internet, at least for activation. There are no exceptions to our activation procedure.

ChemDoodle connects to the iChemLabs server via **HTTPS**, port **443**, at the following origin: **https://www.ichemlabs.com**

1.11.3.2 Proxy issues

If you use a proxy to access the internet, ChemDoodle will use the default system proxy information to connect to the internet. If that fails, then you will need to manually define the proxy settings in the `proxy.config` file that can be found in the `config` folder in the `ChemDoodle` installation folder.

1.12 Updating ChemDoodle

ChemDoodle will automatically check for official updates when it is opened. If an update is available, you will see an **Update Available** window appear listing all the changes introduced by the update as shown in Figure 1.5. Just click the **Update** button to proceed. Press the **Cancel** button to decline the update, but be reminded of it the next time you open the software. If you press the **Skip this Version** button, the update will be declined, and you will no longer be notified about this update. However, you may always manually check for updates by selecting the Help › Check For Updates menu item, and the latest update information will be shown, even if you skipped the update.

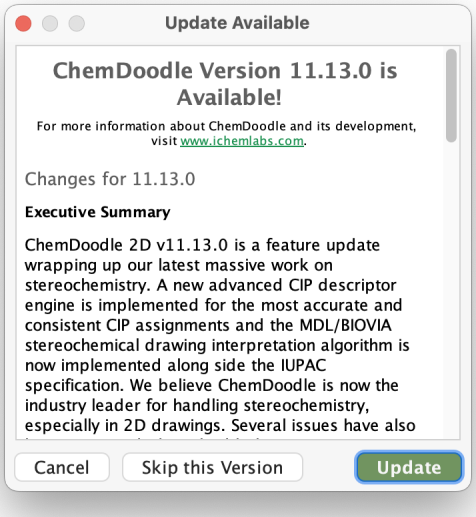


Figure 1.5: *The Update Available Window*

After you click the **Update** button, the download page showing the latest version of ChemDoodle will appear in your default browser. Make sure to first close and uninstall your current version of ChemDoodle before installing the new version. You will not need to activate again.

To disable automatically checking for updates on load, in the **Settings** window under the **Online** tab, deselect the **Automatically Check for Updates when Loading** option. Even if you disable this option, you may still manually check for updates by using the Help 〉 Check For Updates menu item.



You must have administrator privileges to update ChemDoodle. If you see a message stating that you cannot update because you do not have the necessary permissions, please double check that you ran ChemDoodle as administrator (on Windows for instance) or contact your system administrator to help you.

1.12.1 Windows administrator privileges

A common issue on Windows Vista/7+ is to enable administrator privileges for ChemDoodle to update. If ChemDoodle states that you do not have the necessary administrator privileges on these platforms, perform the following steps:

1. Exit ChemDoodle.
2. Locate the ChemDoodle icon (shortcut or actual executable).
3. Right-click on the icon and select Run as administrator.
4. Accept the security request.

You will then be able to update ChemDoodle.

If this process does not work, you will need to consult with a system administrator to update ChemDoodle.

1.12.2 Skipping updates

If you wish to skip the current update, when the **Update Available** window is displayed, just select the **Skip this Version** button as shown in Figure 1.5. You will no longer be notified that this update is available. You will still be notified of subsequent updates, which you may also skip.

To obtain an update that was skipped, select the Help 〉 Check For Updates menu item.

1.13 Moving your activated copy to a new computer

At some point, you may want to switch to a different computer. Your purchased ChemDoodle license code is restricted by the number of computers ChemDoodle is activated on, as determined by your license. Therefore, we provide you the ability to deactivate ChemDoodle and reactivate it on a new computer. To begin, just click the Help 〉 Deactivate ChemDoodle menu item.



When deactivating ChemDoodle and switching to a new computer, your custom preferences and other user settings will be lost. If you have settings files (templates, chemical style sheets), those can be copied to the new `ChemDoodleSettings` folder that will appear after ChemDoodle is activated on the new computer.

Once the deactivation procedure has begun, it cannot be cancelled. Make sure you record your license code, which will be displayed in the **Details** section of the deactivation confirmation message, so you can use it again. You should also have a record of your code from the email receipt you received upon purchasing it.

Once you accept the confirmation message, ChemDoodle will close and your copy will be deactivated. You may now use your license code to activate ChemDoodle on a new computer.



The deactivation function is to be used for permanent transference of licenses only. It is not to be used for circumventing license activation restrictions. If you purchase a new computer and need to move your license to that new computer from the old one, this is the function to use. But if you need to use ChemDoodle on multiple computers, please purchase the appropriate license for that many computers and do not use this function to continuously switch licenses between those computers. The deactivation function is limited to a certain number of executions for a given license.

1.14 Preparing for a system restore

If you do anything to your system that will remove or eliminate the ChemDoodle license file, such as performing a system restore or installing your operating system from scratch, you will need to first deactivate your copy of ChemDoodle. Instructions for deactivating ChemDoodle can be found in the previous section, MOVING YOUR ACTIVATED COPY TO A NEW COMPUTER.

1.15 Restricted use versions

1.15.1 Free trial

A free trial may be initiated by clicking the **Free Trial** button on the activation screen when ChemDoodle is opened. Trials will remain active for 14 days and cannot be renewed. Once you have activated a trial for ChemDoodle on your user account, you will not be able to activate any further trials of ChemDoodle until a new major version of ChemDoodle is released. So if you started a trial for ChemDoodle version 1, for instance, you will be able to start a new trial of ChemDoodle when version 2 is released, but not version 1.1.

The trial is intended to provide the user with access to the application for evaluation purposes only. Output from the trial will contain watermarks and should not be used for other purposes.

Free trials are subject to the following restrictions:

- Documents show a watermark at the top and will render a background texture.
- The **Save...**, **Save as Image...**, **Save Selection as Image...** and **Convert...** functions are disabled.
- Only images and ChemDoodle data can be pasted from ChemDoodle.
- IUPAC naming is disabled for structures with 10 or more atoms. This should be sufficient for evaluation.
- All copied and printed content will contain a watermark.
- Templates cannot be saved.
- ChemDoodle Web Components cannot be previewed or generated.

1.16 Unauthorized use

Using ChemDoodle to output the Laboratory/Glassware graphics or the BioArt graphics for the sole purpose of publishing, selling, or distributing them individually or as a set is forbidden.

1.17 Ownership

Copyright for the output from this software belongs to the author of said content (the licensee of this software).

1.18 Attributions

Attribution of graphics and output to ChemDoodle is appreciated, but not required.

1.19 Referencing

ChemDoodle can be referenced in publications. In the window that appears after selecting the Help 〉 References menu item, a copyable reference template is provided for your use. In this window, you can also find published reviews of ChemDoodle, which are found in the references tree in the **Reviews of iChemLabs Software** section.

CHAPTER 2

ChemDoodle Basics

Contents

2.1 Overview **23**

2.2 The ChemDoodle graphical user interface **23**
2.2.1 Doodle board 24
2.2.1.1 Ruler guides 24
2.2.1.2 Scrollbars 24
2.2.1.3 Tab tray 25
2.2.2 Application menu bar 26
2.2.2.1 ChemDoodle menu 26
2.2.2.2 File menu 27
2.2.2.3 Edit menu 28
2.2.2.4 View menu 30
2.2.2.5 Content menu 31
2.2.2.6 Structure menu 33
2.2.2.7 Reaction menu 36
2.2.2.8 Spectrum menu 36
2.2.2.9 Window menu 36
2.2.2.10 Purchase menu 37
2.2.2.11 Help menu 37
2.2.3 Toolbars 39
2.2.3.1 Formatting toolbar 39
2.2.3.2 Content toolbar 39
2.2.3.3 Chemistry toolbar 40
2.2.3.4 Document toolbar 41
2.2.4 Drawing toolbar and palettes 41
2.2.4.1 Text input palette 42
2.2.4.2 Elemental labels palette 43
2.2.4.3 Bonds palette 43
2.2.4.4 Rings palette 44
2.2.4.5 Chain palette 45
2.2.4.6 Macromolecular palette 45
2.2.4.7 Chemical attribute palette 46
2.2.4.8 Orbitals palette 47
2.2.4.9 Arrows palette 47
2.2.4.10 Shapes palette 48
2.2.4.11 Brackets palette 49
2.2.4.12 Table tool 49
2.2.4.13 Pen palette 50
2.2.4.14 Ruler tool 50
2.2.4.15 iChemLabs Vector Art 50
2.2.5 Styles and settings buttons 50
2.2.6 Widgets and the widget menu 50
2.2.7 The workspace 51
2.2.7.1 Resizing the application window 51
2.2.7.2 Resetting to the default workspace 52
2.2.7.3 Reverting to the last saved workspace 52
2.2.7.4 Saving the current workspace 52

2.3 Interface settings **52**
2.3.1 Controls Settings 53
2.3.1.1 Drawing controls 53

2.3.1.2 Selection controls . . . 54
2.3.1.3 3D rotation controls . . . 54
2.3.2 Appearance settings . . . 54
2.3.2.1 Fonts . . . 54
2.3.2.2 Colors . . . 54
2.3.2.3 Interface . . . 55
2.3.2.4 Decorations . . . 55
2.3.2.5 Other settings . . . 55
2.3.3 Mouse cursors . . . 56
2.3.3.1 Customizing the drawing cursor . . . 57
2.3.3.2 Operating system cursor differences . . . 57
2.3.3.3 Other cursor customizations . . . 57

2.4 Accessibility . . . 58
2.4.1 Colors . . . 58
2.4.2 Sizes . . . 58
2.4.3 Left handed mode for cursors . . . 58
2.4.4 Menu item and toolbar shortcuts . . . 58
2.4.5 Single click mode . . . 58

2.5 Documents . . . 59
2.5.1 Opening a document . . . 59
2.5.2 Creating a document . . . 59
2.5.3 Changing document size . . . 60
2.5.4 Changing the number of pages in the document . . . 60
2.5.5 Reversing actions . . . 61
2.5.6 Discard recent changes to a document . . . 61
2.5.7 Saving documents . . . 61
2.5.8 Autosaving . . . 61
2.5.9 Rendering scale . . . 61
2.5.9.1 Defining the current scale . . . 61
2.5.9.2 Using the document bar . . . 61
2.5.9.3 Keyboard shortcuts . . . 62
2.5.9.4 Using the mouse . . . 62

2.6 File chooser . . . 63
2.6.1 File chooser previews . . . 63
2.6.2 macOS Quick Look plugin . . . 64
2.6.3 File chooser types . . . 65

2.1 Overview

This chapter is going to introduce the new user to the ChemDoodle user interface. It covers the following topics:

- What are the various parts of the interface?
- What functions the menu items perform.
- What functions the buttons perform.
- How to interpret the mouse cursor icons.
- How to open files and create new documents.
- How to save files and the autosave system.
- How to customize the interface.

2.2 The ChemDoodle graphical user interface

Although the Windows, macOS and Linux versions of the ChemDoodle graphical user interface (GUI) differ slightly, the main elements of the GUI are consistent across platforms. The common elements of the GUI are shown in Figure 2.1.

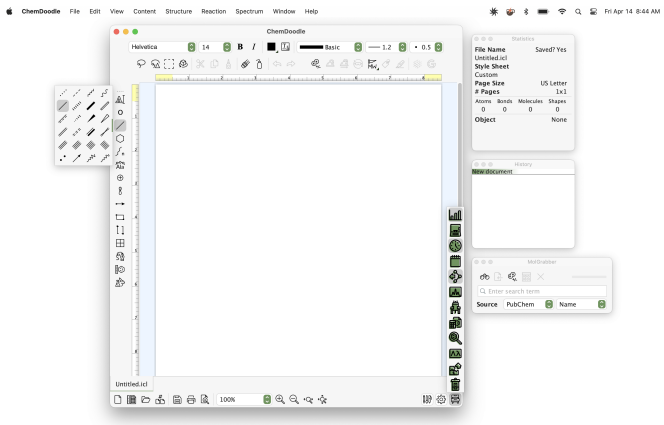


Figure 2.1: *ChemDoodle Graphical User Interface*

ChemDoodle's functions are accessed through interaction with several types of interface components as indicated in Table 2.1 below.

Table 2.1:

	Component	Description
Elements of ChemDoodle GUI	**Doodle Board**	The main drawing window: DOODLE BOARD
	Menus	Core application functions: APPLICATION MENU BAR
	Toolbars and Palettes	Quickly access functions and modify how mouse gestures interact with the Doodle Board: TOOLBARS
	Widgets	Mini applications within ChemDoodle that provide specific functionality: WIDGETS

2.2.1 Doodle board

The **Doodle Board** is the main drawing window and contains all of the documents you create and edit. You may use mouse and keyboard gestures to interact with the **Doodle Board** and to draw your figures. Figure 2.2 displays the main components of the **Doodle Board**.

2.2.1.1 Ruler guides

There are two rulers aligned with the currently displayed document on the **Doodle Board**. The ruler to the left of the document allows for vertical measurements and the ruler to the top of the document allows for horizontal measurements.

When the document rendering scale is changed, the ruler scale will also change to match the new dimensions. When the scrollbars are used to focus on a different area of the document, the rulers will also scroll to match the new location.

The ruler displays full ticks at each inch, half-ticks at each half-inch, and quarter-ticks every eighth of an inch. The ruler units can be set to metric mode for centimeter ticks instead of inches by changing the **Ruler Mode** setting in the **Settings** window under the **Appearance** tab in the **Other Settings** section.

Several colored ticks and areas are also present on the rulers for visual feedback as described below. These feedback tips can be disabled in the **Settings** window under the **Appearance** tab.

- **Margin Areas** - Margins are highlighted in a yellow color.
- **Mouse Pointer Ticks** - Mouse pointer locations are ticked on the rules with a red color.
- **Selection Dimension Area** - Marks the bounds of the currently selected content. This is denoted by a dual-toned amber area. This inner darker area corresponds to the internal coordinates of the content, while the outer lighter area denotes the additional dimensions containing the visual bounds. For example, the darker area will denote the bounding box given the atom coordinates, while the lighter area includes the dimensions of the labels for those atoms.

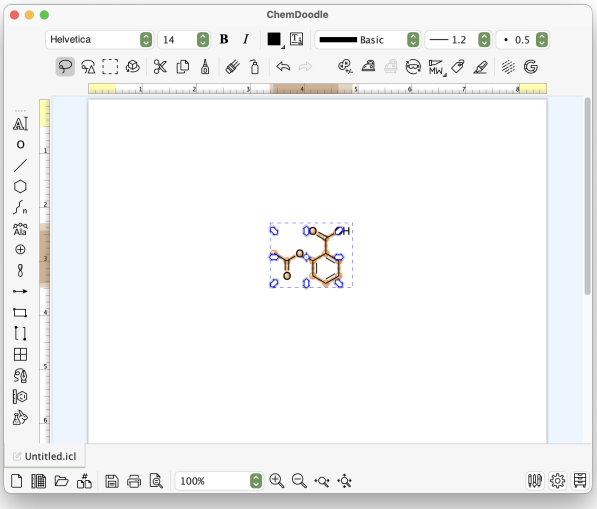


Figure 2.2: *The Doodle Board*

2.2.1.2 Scrollbars

Scrollbars will appear to the right and bottom of the document if the height and width, respectively, of the document are too large to fit on the **Doodle Board**. You can click and drag the scroll bars to change which area of the document is displayed on the **Doodle Board**. You can also use the mouse or trackpad scroll gesture to translate the view.



If the alt key is held down while vertical scrolling over the current document, the document scale will be altered instead.

2.2.1.3 Tab tray

The **Doodle Board** stores all drawing content and organizes it into documents that can be saved as files or images. Each document has a corresponding tab, located at the bottom of the **Doodle Board** in the tab tray. When a tab is pressed, the corresponding document will be selected and viewed. This allows you to manage a large number of files at once, without having to manage a large number of windows.

The number of tabs present in the tab tray will change depending on how many documents are open. If only a single document is present, then only one tab is displayed and will be selected. Selected tabs are bordered on the bottom with the application color (see Figure 2.3a). When multiple documents are open, multiple tabs will be displayed in the tab tray. The tab corresponding to the document currently being edited will be selected (see Figure 2.3b).



(a) *Single Tab* (b) *Multiple Tabs*

Figure 2.3: *Tab Tray*

If there are more tabs than can fit in the tab tray, not all the tabs will be displayed in the tray. Only the most recently viewed tabs will be displayed. Left and right chevrons to the left and right of the tabs will be present if tabs exist in that direction. Clicking on each chevron will allow you to traverse the tabs in that direction (see Figure 2.4). If there are no tabs to the left or right of the current view, then the corresponding chevron will not be shown.



Figure 2.4: *Undisplayed Tabs*

You may also click on the upward pointing chevron to open a popup menu that lists all undisplayed tabs (see Figure 2.5). Click on an item in the list to select that tab and document.

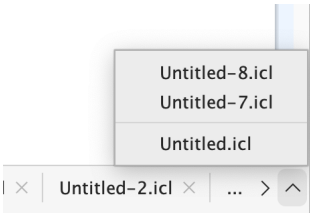


Figure 2.5: *List of Undisplayed Tabs*

The name of the file is displayed on the tab. If the name is too long, it may be cropped and appended with an ellipsis (...). You may also see an icon ( ) to the left of the document name in the tab. This icon notifies you changes have been made to the document since the last change, and you should save the file to commit those changes.

Tab specific functions that can be accessed by right-clicking on any given tab are:

- **Close** - Close the tab you are right-clicking on. This option is only enabled if multiple tabs are present.

- **Close Documents to the Left** - Close all of the documents to the left of the tab you are right-clicking on. This option is only enabled if tabs exist to the left of the tab you are right-clicking on.
- **Close Documents to the Right** - Close all of the documents to the right of the tab you are right-clicking on. This option is only enabled if tabs exist to the right of the tab you are right-clicking on.
- **Close Other Documents** - Close the other tabs, but leave the tab you are right-clicking on. This option is only enabled if multiple tabs are present.
- **New Document** - Create a new document and tab.
- **Duplicate** - Create a new document and tab, duplicating the content in the tab you are right-clicking on.
- **Restore** - If the corresponding document was created by opening a file, then this function will be enabled, allowing you to revert all of your changes and reload the file from the last save.

2.2.2 Application menu bar

Menus are located on the top of the ChemDoodle application. On macOS, the ChemDoodle menu bar is displayed as the screen menu bar. Use the Window > Edit Shortcuts... to view and edit keyboard shortcuts, as well as output a reference document.

There are 9 menus in the menu bar (10 on macOS), not including the **Purchase** menu that is present during the free trial:

- **ChemDoodle** - This is a macOS specific menu bar and contains access to several macOS specific tasks as well as the **About**, **Settings** and **Quit** menu items.
- **File** - This menu handles all input and output of data, as well as file specific functions such as **Annotations...**. You also have access to your iChemLabs account through this menu and the **Quit** menu item is located here on non-macOS platforms.
- **Edit** - Standard global document functions are located here including **Cut**, **Copy** and **Paste**.
- **View** - Functions for changing how documents are shown are located here as well as access to the elemental and chemical data provided with ChemDoodle. The dynamic periodic table is also accessible through this menu.
- **Content** - Contains all non-chemical functions for editing content in the current document.
- **Structure** - Contains all functions related to editing and analyzing molecules.
- **Reaction** - Contains all functions related to editing and analyzing reactions.
- **Spectrum** - Contains all functions related to editing and analyzing spectra.
- **Window** - Manage your workspace and the entire ChemDoodle application window.
- **Purchase** - This menu is only present during the free trial and when a subscription license is expiring and provides functions for purchasing and activating licenses for ChemDoodle.
- **Help** - This menu contains several functions to access this user guide, list references, contact customer service and other common help items.

2.2.2.1 ChemDoodle menu

This is a macOS specific menu bar and provides access to several macOS specific tasks as well as the **About**, **Settings** and **Quit** menu items.

- **About ChemDoodle**[1] - Display information about ChemDoodle, your license code and your license.
- **Settings...**[2] - Open the Settings window to edit ChemDoodle application settings.
- **Services** - Standard macOS submenu that will likely be empty.
- **Hide ChemDoodle** - Hide the ChemDoodle application.
- **Hide Others** - Hide other applications.

[1] This menu item is in the **Help** menu on Windows and Linux.
[2] This menu item is in the **Edit** menu on Windows and Linux.

- **Show All** - Show all hidden applications.
- **Quit ChemDoodle**[3] - Quit the ChemDoodle application.

2.2.2.2 File menu

- **New** - Add a new blank document to the **Doodle Board**.
- **New Formatted Document...** - Add a new blank formatted document to the **Doodle Board**.
- **Open...** - Open a recognized chemical file that you locate with a file chooser.
- **Open Recent** > - The 10 most recently opened chemical files are listed here. Click a file to open it.
- **Insert Image...** - Add a recognized image file to the current document that you locate with a file chooser.
- **Recover from Image...** - This function will recover chemical structures from chemical images for further editing. Chemical structures are rebuilt from the input pixels with no chemical data embedded.
- **Recover from MS Office File...** - Search Microsoft Office documents for embedded chemical figures inserted for round-trip editing from chemical software and recover the original chemical information for further editing.
- **Convert...** - Displays a window to convert chemical files to different chemical file types that ChemDoodle interprets. Nothing is loaded to the **Doodle Board**, as output is written directly to a new file that is created.
- **Close** - Close the current document. This function is only enabled if two or more documents are present.
- **Close Others** - Close all but the current document. This function is only enabled if two or more documents are present.
- **Restore** - Restores a file from its last save. This function will only be enabled for files that have been previously saved or were opened from a preexisting file.
- **Annotations** - Associate annotations with the current document or view previously set annotations.
- **Save** - Saves the current file with the present save settings determined when opening the file or by previously saving it.
- **Save As...** - Saves the current document as a new file or overwrites an existing file.
- **Save As Image...** - Save the current document as an image. Several bitmap and vector image types are supported.
- **Save Selection As Image...** - Saves the currently selected objects as an image. Several bitmap and vector image types are supported. This menu item is disabled if no objects are selected.
- **Generate Web Component...** - Generate a **ChemDoodle Web Component**. An entire window will appear for you to define and edit the **ChemDoodle Web Component**, as well as preview and generate the Javascript for it. More information on this feature is covered in APPENDIX: CHEMDOODLE WEB COMPONENTS.
- **Interfaces** > - This submenu provides access to third party interfaces, including ChemExper, LabArchives, and SciFinder.
  - **ChemDoodle 3D** - Functions for communicating with ChemDoodle 3D. You must have ChemDoodle 3D installed on your computer to use these functions.
    - **View Molecule in 3D** - Load your molecule in ChemDoodle 3D, where hydrogens will be automatically added and 3D coordinates will be automatically generated.
    - **Bind Molecule in 3D** - Load your molecule in ChemDoodle 3D. This creates a direct link with ChemDoodle where changes to the structure in ChemDoodle will be reflected in the structure shown in ChemDoodle 3D.
  - **ChemExper** - Functions for communicating with ChemExper.
    - **Substructure Match** - Find chemical suppliers for the selected structure by substructure search.
    - **Exact Match** - Find chemical suppliers for the selected structure by exact match.
  - **Google Patents** - Functions for communicating with Google Patents.
    - **Exact** - Show the Google Patents interface in ChemDoodle to initiate an exact search of the selected content.

[3] This menu item is in the **File** menu on Windows and Linux and is listed as **Exit ChemDoodle**.

    - **Substructure** - Show the Google Patents interface in ChemDoodle to initiate a substructure search of the selected content.
    - **Similarity** - Show the Google Patents interface in ChemDoodle to initiate a similarity search of the selected content.
  - **GSRS** - Functions for communicating with GSRS databases.
    - **Substructure** - Show the GSRS interface in ChemDoodle to initiate a substructure search of the selected content.
    - **Exact** - Show the GSRS interface in ChemDoodle to initiate an exact search of the selected content.
    - **Flex** - Show the GSRS interface in ChemDoodle to initiate a flex search of the selected content.
    - **Similarity** - Show the GSRS interface in ChemDoodle to initiate a similarity search of the selected content.
  - **LabArchives** - Functions for communicating with LabArchives.
    - **Post Selected Content** - Post the selected content to your LabArchives account.
  - **precisionFDA** - Functions for communicating with the precisionFDA system.
    - **UNIISearch** - Perform a UNIISearch into the precisionFDA system.
  - **PubChem** - Functions for communicating with PubChem database.
    - **Exact** - Show the PubChem interface in ChemDoodle to initiate an exact search of the selected content.
    - **Similarity** - Show the PubChem interface in ChemDoodle to initiate a similarity search of the selected content.
    - **Substructure** - Show the PubChem interface in ChemDoodle to initiate a substructure search of the selected content.
    - **Superstructure** - Show the PubChem interface in ChemDoodle to initiate a superstructure search of the selected content.
    - **3D Similarity** - Show the PubChem interface in ChemDoodle to initiate a 3D similarity search of the selected content.
  - **SciFinder-n** - Functions for communicating with SciFinder-n.
    - **Substances** - Show the SciFinder-n interface in ChemDoodle to initiate a substances search of the selected content.
    - **Reactions** - Show the SciFinder-n interface in ChemDoodle to initiate a reactions search of the selected content.
    - **References** - Show the SciFinder-n interface in ChemDoodle to initiate a references search of the selected content.
    - **Suppliers** - Show the SciFinder-n interface in ChemDoodle to initiate a suppliers search of the selected content.
- **Page Setup...** - Display the operating system specific window for selecting initial print settings.
- **Print Preview** - View the current document in its entirety on the screen as it would appear on a printed page.
- **Print...** - Print the current document.
- **Exit**[4] - Exits ChemDoodle.

2.2.2.3 Edit menu

- **Undo** - Undo the last action.
- **Redo** - Redo the last undone action.
- **Cut** - Copy the selected objects to the system clipboard in addition to removing them from the document.

[4] On macOS this menu item is listed as **Quit ChemDoodle** and is found in the **ChemDoodle** menu.

- **Copy** - Copy the selected objects to the system clipboard.
- **Copy As** > - Contains convenience functions for quickly placing specific data on the system clipboard as text and as a chemical to be transferred to a range of 3rd party applications that use that data type. This submenu is only enabled if content is selected.
  - **ChemDoodle JSON** - Place *ChemDoodle JSON* for the currently selected content on the system clipboard as text and as chemical data.
  - **Chemical Markup Language** - Place *CML* for the currently selected content on the system clipboard as text and as chemical data.
  - **Daylight SMILES** - Place a SMILES string for the currently selected content on the system clipboard as text and as chemical datal.
  - **iChemLabs ChemDoodle Document** - Place *iChemLabs ChemDoodle Document* XML for the currently selected content on the system clipboard as text and as chemical data.
  - **IUPAC InChI** - Place an *InChI* string for the currently selected content on the system clipboard as text and as chemical data.
  - **MDL MOLFile** - Place a complete molfile for the currently selected content on the system clipboard as text and as chemical data.
  - **Tripos SLN** - Place a SLN string for the currently selected content on the system clipboard as text and as chemical data.
- **Paste** - Paste the system clipboard data of highest priority into the document.
- **Paste and Match Style** - Paste the system clipboard data of highest priority into the document and match the style to the current style sheet.
- **Paste Text as Chemical** > - Pastes the current text on the clipboard, interpreted as chemical data, as any of the options provided in the submenu.
  - **Beilstein ROSDAL** - Paste *ROSDAL* text as a chemical structure.
  - **ChemDoodle JSON** - Paste *ChemDoodle JSON* text as a chemical structure.
  - **Daylight SMILES** - Paste *SMILES* text as a chemical structure.
  - **IUPAC InChI** - Paste *InChI* text as a chemical structure.
  - **Tripos SLN** - Paste *SLN* text as a chemical structure.
  - **XYZ-Like Data** - Paste text as a chemical, interpreted from a text blob where *XYZ*-like data is parseable.
  - **IUPAC Name** - Paste *IUPAC* name text as a chemical structure.
  - **Guess Chemical Format** - Paste text as chemical, where the format is guessed from the content. If the data is ambiguous or a parsing issue occurs, an appropriate message will be displayed.
- **Paste Special...** - Lists all data that ChemDoodle can interpret from the system clipboard. You may then choose the data of choice to be pasted into the document. This function is useful, for instance, when you would like to paste SMILES string text instead of a structure into the document. A structure has higher priority than text.
- **Delete** - Remove the currently selected content from the current document.
- **Clear** - Remove all content from the current document.
- **Number of Pages...** - Change the number of pages in the document. You can change the number of pages arranged in rows and columns.
- **Resize Document...** - Resize the current document. You may also change the page margins in the **Styles** window under the **Pages** tab.
- **Conform Document...** - Conform all objects in the current document to a selected style sheet. This function will also change all fonts and scale all objects if you choose to do so.

- **Remember Style Sheet...** - Save the current styles of the workspace to the default style sheet. New unformatted documents will open with these settings.
- **Export Style Sheet...** - Export the current styles to a ChemDoodle Style Sheet file in the `ChemDoodleSettings/styleSheets` folder.
- **Purge Clipboard** - This function clears the system clipboard.
- **Purge History** - This function clears the undo/redo history, which will reset the **History** widget. This may be convenient if the action list gets so long that it becomes unmanageable and causes memory issues, or if you would like to prevent yourself from undoing past a certain action.
- **Settings...**[5] - Open the **Settings** window to edit ChemDoodle application settings.

2.2.2.4 View menu

- **Hide Warnings** - Hide all the warnings in the document.
- **Drawing Aids** > - Display various guides to help when drawing figures.
  - **Atoms** > - Display guides associated with atoms.
    - **Show Circular Guidelines** - Display circular guides around atoms with radii equal to the current bond length document setting.
    - **Show Orthogonal Guidelines** - Display vertical and horizontal guidelines that intersect through the atom for aiding in alignment tasks.
  - **Bonds** > - Display guides associated with bonds.
    - **Show Parallel Guidelines** - Display a line that goes through the bonds to extrapolate where they point to.
  - **Rings** > - Display guides associated with rings.
    - **Color in Rings** - Color in rings with a color associated with the size of the ring.
  - **Molecules** > - Display guides associated with molecules.
    - **Show Bounds** - Draw rectangular bounding guides around molecules to show their visual bounds.
    - **Show Orthogonal Guidelines** - Displays vertical and horizontal guidelines that intersect through the center of the molecule for aiding in alignment tasks.
  - **Background** > - Displays guides associated with the page.
    - **Show Crosshair** - Displays a crosshair.
    - **Grid** > - Displays grids.
      - **Every Quarter-Inch** - Displays a grid with quarter-inch spacing.
      - **Every Half-Inch** - Displays a grid with half-inch spacing.
      - **Every Inch** - Displays a grid with inch spacing.
      - **Every Centimeter** - Displays a grid with centimeter spacing.
    - **Show Margin Guidelines** - Displays a rectangular region that specifies the printable area of the page.
  - **Switch Off All Drawing Aids** - Turn off all currently enabled drawing aids.
- **Unique IDs** > - Associates ID attributes with objects.
  - **On Atoms** > - Associate IDs with atoms.
    - **Incremental** - Associate incremental IDs with atoms. The atoms are numbered in chronological order from time of creation.
    - **Morgan Indices** - Associate Morgan indices with atoms.

[5] This menu item is in the ChemDoodle menu on macOS.

    - **IUPAC Locants** - Associate atoms with their respective IUPAC locant designation; this is the index they are defined in an IUPAC name.
  - **On Bonds** > - Associate IDs with bonds.
    - **Incremental** - Associate incremental IDs with bonds. The bonds are numbered in chronological order from time of creation.

- **Elemental Data** - View the entire elemental database packaged in ChemDoodle that is used for all calculations and cheminformatics functions. The data is displayed in a dynamic table.
- **Ionization Energies** - View ionization energies of the elements in a dynamic table. This data is part of ChemDoodle's elemental database.
- **Isotopes** - View isotope data for the elements in a dynamic table. This data is part of ChemDoodle's elemental database.
- **Interactive Periodic Table** - View an interactive periodic table that can be customized and printed. You may also use its dynamic features to create nice demonstrations.
- **Actual Size** - Negate any zoom effects.
- **Current Selection** - Center the current selection on the **Doodle Board**. This function is useful if the document perspective is zoomed in and it is difficult to locate selected content.
- **Zoom Out** - Zoom out and decrease the document scale, you may also use the drop down selection provided in the **Files + Formatting** toolbar.
- **Zoom In** - Zoom in and increase the document scale, you may also use the drop down selection provided in the **Files + Formatting** toolbar.

2.2.2.5 Content menu

- **Select** > - Contains various tools for selecting content.
  - **All** - Select all content in the current document.
  - **Inverse** - Select all content in the current document that isn't currently selected while deselecting all content in the current document that is currently selected.
  - **Next Molecule** - Select the next molecule in the document. This function will traverse chronologically through the molecules in the current document based on the time they were drawn. If a molecule isn't currently selected, it will first select the last molecule drawn.
  - **Previous Molecule** - Select the previous molecule in the document. This function will traverse in reverse chronological order through the molecules in the current document based on the time they were drawn. If a molecule isn't currently selected, it will first select the last molecule drawn.
  - **Next Shape** - Select the next shape in the document. This function will traverse chronologically through the shapes in the current document based on the time they were drawn. If a shape isn't currently selected, it will first select the last shape drawn.
  - **Previous Shape** - Select the previous shape in the document. This function will traverse in reverse chronological order through the shapes in the current document based on the time they were drawn. If a shape isn't currently selected, it will first select the last shape drawn.
  - **SMARTS...** - A text field will appear. Type in the desired SMARTS pattern here and then click the Accept button. Any content in the current document that matches the SMARTS pattern will be selected.
- **Deselect** - Deselect all content that is currently selected. This function is only enabled if content is currently selected.
- **Reselect** - Reselect the last content that was selected. This function is only enabled if no content is currently selected. This function may not work as expected when content is removed. For instance, if you selected content and then deleted it, then pressing reselect will have no action because the content to be reselected no longer exists.
- **Center** > - Contains various functions for centering content.
  - **All on Page** - Center all content on the page.

  - **Selection on Page** - Center only the currently selected content on the page.
  - **Selection Horizontally** - Horizontally center only the currently selected content.
  - **Selection Vertically** - Vertically center only the currently selected content.
- **Flip** > - Contains functions for flipping selected content.
  - **Horizontally** - Flip the currently selected content horizontally over its midpoint.
  - **Vertically** - Flip the currently selected content vertically over its midpoint.
- **Rotate** > - Contains various functions for rotating selected content.
  - **90° CW** - Rotate selected content clockwise by 90 degrees.
  - **90° CCW** - Rotate selected content counterclockwise by 90 degrees.
  - **180°** - Rotate selected content by 180 degrees.
  - **Arbitrary...** - Rotate selected content by an arbitrary angle that you input.
- **Scale...** - Scale the currently selected objects. You will be presented with a window to set various options to define how the content will be scaled. You can even choose to scale all molecules individually, to set them all to a common bond length for instance.
- **Align Bond** > - Contains functions for aligning a single selected bond, rotating the molecule it is contained in. This function is enabled when only a single bond is selected.
  - **Up** - Align bond *up*.
  - **Right** - Align bond *right*.
  - **Down** - Align bond *down*.
  - **Left** - Align bond *left*.
- **Flip Bond Orientation** - Flip the orientation of the bond. This switches the start and end atoms of the bond. Non-symmetrical bonds will face the other direction.
- **Torsion Bond** - Flip the orientation of atoms and bonds connected to the bond, as if the bond was rotating on its own axis.
- **Scale Bond...** - Scale the currently selected bond. This function is enabled when only a single bond is selected. You will be presented with a window to set various options to define how the bond will be scaled.
- **Align** > - Contains functions for aligning selected content.
  - **Left Edges** - Align all selected content by the left edges of their visual bounds.
  - **Centers Vertically** - Align all selected content by the horizontal centers of their visual bounds.
  - **Right Edges** - Align all selected content by the right edges of their visual bounds.
  - **Top Edges** - Align all selected content by the top edges of their visual bounds.
  - **Centers Horizontally** - Align all selected content by the vertical centers of their visual bounds.
  - **Bottom Edges** - Align all selected content by the bottom edges of their visual bounds.
- **Distribute** > - Contains functions for distributing selected content.
  - **Horizontally on Page** - Distribute selected content horizontally on the page such that they are evenly distributed based on their visual bounds and fit within the page margins.
  - **Vertically on Page** - Distribute selected content vertically on the page such that they are evenly distributed based on their visual bounds and fit within the page margins.
  - **Horizontally by Buffer Space...** - Distribute selected content horizontally on the page such that they are evenly distributed based on their visual bounds by a value that you input.

  - **Vertically by Buffer Space...** - Distribute selected content vertically on the page such that they are evenly distributed based on their visual bounds by a value that you input.
- **Grid All on Page...** - A numeric field will appear. Select the number of columns or rows to place the content in, and ChemDoodle will then align all content in a grid with that many rows or columns.
- **Stack All on Page** - Stack all content on the page. Stacking will place all content within the page margins based on their visual bounds. Stacking proceeds by placing content from left to right, and then top to bottom, on the page using a small buffer space.
- **Group** - Group the currently selected content into a single shape. Single items in grouped content cannot be edited and transformations will affect the entire group as a whole. Groups can also be grouped into larger groups.
- **Ungroup** - Ungroup grouped content. Ungrouping is not recursive, so if the group being ungrouped contains a group, then that inner group will remain grouped.
- **Join** - If two atoms are selected, then they will be joined into a single atom, and their bonds will all point to the new joined atom. If selected atoms were part of two discrete molecules, then one molecule is translated to the other. If two bonds are selected, then they will be joined together, and all bonds connected to the selected bonds will connect to the new joined bond. Two bonds within the same molecule cannot be joined. One molecule will be translated and rotated to the other to aesthetically display the new joined molecule. This function is disabled in all other cases.
- **Flatten** - This function will change all z-coordinates of selected atoms to zero, thereby flattening 3D structures.
- **Frame** > - Contains various functions for surrounding selected content with shapes based on their visual bounds.
  - **Chevrons** - Surround selected content with chevrons based on the content's visual bounds.
  - **Curly Brackets** - Surround selected content with curly brackets based on the content's visual bounds.
  - **Parentheses** - Surround selected content with parentheses based on the content's visual bounds.
  - **Rectangle** - Surround selected content with a rectangle based on the content's visual bounds.
  - **Square Brackets** - Surround selected content with square brackets based on the content's visual bounds.
- **Highlight** - Highlight the selected chemical structures. The **Styles** window for the created highlight will be displayed for immediate edit.
- **Measure** > - Contains various functions for measuring selected content.
  - **Diagonal** - Place one ruler object diagonally over selected content based on its visual bounds to measure its diagonal. You can change the units of the ruler object.
  - **Width and Height** - Place two ruler objects, one vertically to the left and one horizontally below selected content based on its visual bounds to measure its width and height. You can change the units of the ruler object.
- **Edit Styles...** - The **Styles** window will appear allowing you to edit the style sheet for the current document.
- **Conform to Current Styles** - Conform all currently selected objects to the current style sheet of the document, including scaling and changing fonts.

2.2.2.6 Structure menu

- **Add/Remove Hydrogens** > - Contains functions for adding hydrogens to structures. Settings for defining how hydrogens will be added to structures can be set in the **Styles** window under the **Atoms** tab.
  - **All** - Add hydrogens to all structures in the current document.
  - **From Selection** - Add hydrogens only to the currently selected
- **Add Attribute...** - Add an attribute to the selected object. This will only be enabled if a single atom or bond is selected.
- **Atom Properties** > - Automatically determine certain atom properties from the existing molecular structure.
  - **Place Formal Charges** - Calculate and assign formal charges on selected atoms.
  - **Place Lone Pairs** - Calculate and place lone pairs on selected atoms.
- **Place Formal Charges** - Will place formal charges on selected atoms based on their valency.

- **Place Lone Pairs** - Will place the appropriate number of lone pairs on the selected atoms.
- **Deduce Covalent Bonds...** - This function will deduce covalent bonds and bond orders in structures based on atomic 3D distances and the covalent radii present in ChemDoodle's elemental database. A window will appear with further options. This function is very useful for working with files that may not contain explicit topology, such as PDB or XYZ files.
- **Remove Selected Bonds** - This function will remove all selected bonds, leaving the constituent atoms.
- **Saturate** - This function will change the bond orders of all selected bonds to the single bond order.
- **Kekulize** - This function will convert a delocalized substructure (defined with resonance bonds) or a single bond skeleton to a Kekulé structure with the most delocalized area.
- **Delocalize** - Converts a Kekulé structure to the delocalized equivalent.
- **Graph Reduction** > - Contains several functions for reducing the underlying graph data structures that represent the selected structures. This is ideal for extracting information about small molecule building blocks for drug discovery purposes.
  - **Reduce 0° (Lone)** - This function will remove all 0 degree nodes, so all lone atoms will be removed.
  - **Reduce 1° (Terminals)** - This function will remove all 1 degree nodes, so all terminal atoms will be removed.
  - **Repeatedly Reduce 1° (Terminals)** - This function will repeatedly remove all 1 degree nodes until none remain, so all isolated chains will be removed.
  - **Reduce 1° + 0°** - This function will remove all 0 and 1 degree nodes, so all lone and terminal atoms will be removed.
  - **Reduce 2° (Chains)** - This function will remove all 2 degree nodes, so all inner chain atoms will be removed.
  - **Reduce 2° + 1° + 0°** - This function will remove all 0, 1 and 2 degree nodes, so all lone, terminal and chain (including non-isolated chains) atoms will be removed.
- **Add Breakers** > - Contains several functions for adding atom and bond breakers.
  - **On Atoms** - Add a breaker to each selected atom.
  - **On Bonds** - Add a breaker to each selected bond.
- **Auto-Collapse to Labels** - Have ChemDoodle automatically collapse your selected structure using condensed label rules and the defined abbreviations library.
- **Collapse to Label** - A label field will appear, input the text and styling you wish to display for the collapsed fragment and close the text input. The selected fragment will be replaced by the newly created collapsed label.
- **Expand Labels** - Will expand all complex atom labels to their all-atom equivalents.
- **Highlight Functional Groups** - For each selected structure, any functional groups will be highlighted and a corresponding table will appear below the structure stating which functional groups are present and the associated color of the highlights.
- **Rings** > - Contains several functions for defining ring sets in selected structures. If a highly overlapping figure results, just stack the content for a cleaner layout.
  - **Explode Smallest Set of Smallest Rings** - Explode out the smallest set of smallest rings (SSSR) for selected structures. The SSSR is the standard for defining ring sets in flat 2D structures.
  - **Explode Euler Facet Rings** - Explode out the Euler facet rings for selected structures. The Euler facet ring set is better than the SSSR at defining essential rings in 2D depictions of 3D structures.
  - **Explode Hanser (All) Rings** - Explode every last graph cycle in selected structures.
- **Stereochemistry** > - Contains several functions for deducing the stereochemistry of selected structures.
  - **Assign All (CIP)** - Finds and assigns all recognized stereocenters based on CIP rules.
  - **Assign R/S (CIP)** - Finds and assigns CIP stereochemistry to chiral centers.
  - **Assign E/Z (CIP)** - Finds and assigns CIP stereochemistry to double bonds.

  - **Assign M/P (CIP)** - Finds and assigns CIP stereochemistry to axial centers.
  - **Assign cis/trans** - Finds and assigns cis/trans stereochemistry to applicable double bonds.
  - **Remove Assignments** - Removes any attributes for stereochemical assignments present in the selection.
- **Attach Updating Label** - A window will appear with a drop down to select which description to set to the label attached to selected molecules. These labels will update as you edit the associated molecule.
- **Auto-layer Bonds by Wedges** - This function will automatically layer bonds based on the wedges within a structure so overlaps appear properly.
- **Clean** > - Contains various functions for optimizing and beautifying selected structures.
  - **Reset Attributes** - Reset all user defined attribute placements, so that they are again automatically placed by ChemDoodle.
  - **Beautify Structure Drawing** - The Clark depiction algorithm (which is a stochastic build) is performed on your selected structures to clean them in 2D.
  - **Build 3D Model (NIH Cactus)** - This function will use the Cactus service from the NIH to build a 3D molecule based on templates. This function is very fast, but requires an internet connection.
  - **Universal Force Field Minimization** - Generate 3D coordinates for your selected structure by minimizing a Universal Force Field (UFF) function.
  - **Distance Geometry Embedding (3D)** - Distance geometry is used on the bond distance matrix of the selected structures to embed them in 3D. This is great for highly connected structures like buckyballs or adamantane and will produce suitable 3D coordinates for figures. It will not work very well on less connected structures like chains.
- **Create Lewis Dot Structure** - This function will create Lewis Dot Structure models from any selected molecules.
- **Descriptors** > - Contains various functions that will display the named descriptor for the first of the selected molecules. See CHEMINFORMATICS for further details and the full list of descriptors.
  - **Last Chosen** - This menu item is a placeholder that will remember the last chosen descriptor for easy repeat access.
  - **Constitutional** > - Contains any constitutional descriptors; descriptors that are defined by the chemical makeup of the molecule.
  - **Topological** > - Contains any topological descriptors; descriptors that are defined by the bond connectivity of the molecule.
  - **Physicochemical** > - Contains any physicochemical descriptors; descriptors that are defined by physics or chemistry of the molecule.
  - **ADME Filters** > - Contains descriptors that assess bioactivity.
- **Generate Line Notation** > - Contains functions for generating line notations of selected structures.
  - **Daylight SMILES** - Generates simplified molecular input line entry specification (SMILES).
  - **Tripos SLN** - Generates Sybyl Line Notation (SLN).
  - **IUPAC InChI** - Generates the international chemical identifier (InChI).
  - **Beilstein ROSDAL** - Generates the representation of organic structure descriptions arranged linearly (ROSDAL).
- **Parse IUPAC Name...** - A form will appear. Type or paste in a valid IUPAC name and the structure will be generated and inserted into the current document.
- **Structure to IUPAC Name** - Generates the IUPAC name for the selected structure, which can then be pasted into the document or to the system clipboard.
- **Generate Text Description** - Generates a text description of the selected content with various sophistication levels.
- **Abbreviations** > - Contains functions for maintaining ChemDoodle's abbreviations database.
  - **Add New...** - Pops up a window to add a new abbreviation to ChemDoodle's abbreviations database.

  - **Manage Recognized...** - Pops up a window to add, edit and delete abbreviations from ChemDoodle's abbreviations database.

2.2.2.7 Reaction menu

- **Clean** - Clean the selected reaction. The reaction must first be defined using the **Build Implied Reaction** or **Edit Reaction...** functions. This function will align and distribute the reaction as well as beautify the reaction arrow. Settings to control how reactions are cleaned can be set in the **Styles** window under the **Reactions** tab.
- **Sprout** - Generates a reaction template from a selected structure or group of structures, including creating a reaction arrow, assigning the selected structures as reactants, and copying these structures to the products side as products.
- **Show Electron Pusher Result** - Given a drawn mechanism with pusher shapes, the result of the pusher arrows will be shown in a built reaction with the mechanism structure(s) as the reactant(s).
- **Build Implied Reaction** - When an arrow and structures are selected, this function will become enabled. All selected structures with midpoints to the left of the arrow midpoint become reactants while all selected structures with midpoints to the right of the arrow midpoint become products.
- **Edit Reaction...** - Will open up a window showing all the structures in the current document. Click and drag structures from the document tray to the reactant and product trays to explicitly define the reaction. This function is enabled when an arrow is selected.
- **Dissolve Reactions** - Will dissociate any selected reaction data structures.
- **Balance Reaction...** - Balance a drawn reaction in the document. If no reaction is selected, a window will appear to allow you to input a reaction equation to be balanced.
- **Stoichiometry...** - Generate a form to perform stoichiometry calculations for a selected reaction. If no reaction is selected, a window will appear to allow you to input a reaction equation to create a stoichiometry table from.

2.2.2.8 Spectrum menu

- **View XY Data** - View the XY plot data of the first selected spectrum. You can copy and paste this data into other programs, like Excel.
- **Edit Perspective...** - Will open up a window showing several tools for editing the spectrum view and axis. Once closed, the spectrum in the document will update.
- **Expand Perspective** - Will expand the spectrum perspective to view the entire domain and range of the plot. This function is enabled when a spectrum is selected.
- **Generate** > - Contains various functions for generating and simulating spectra.
  - ^{1}**H NMR** - Generates a proton nuclear magnetic resonance spectrum of the first selected structure.
  - ^{13}**C NMR** - Generates a carbon-13 nuclear magnetic resonance spectrum of the first selected structure.
  - **Mass Parent Peak** - Generates a mass parent peak from the mass spectrum of the first selected structure. This will show the magnitude of the parent ion and the isotopic distribution.

2.2.2.9 Window menu

- **Minimize** - Iconify the main ChemDoodle window to the dock or system tray. ChemDoodle's menu bar will remain focused on macOS.
- **Zoom** - Expand the ChemDoodle window to fill the entire screen without overlapping any docks or system trays.
- **Select Tab Right** - This function is enabled if there are one or more tabs present in the tab tray. This function will select the tab to the right of the currently selected tab. If the currently selected tab it the rightmost tab, then the first tab is selected.
- **Select Tab Left** - This function is enabled if there are one or more tabs present in the tab tray. This function will select the tab to the left of the currently selected tab. If the currently selected tab it the leftmost tab, then the last tab is selected.
- **Edit Shortcuts...** - The shortcut editor will appear to define menu item and toolbar keyboard shortcuts.

- **Show/Hide Dialogs** - Toggle the visibility of all other ChemDoodle windows besides the main window.
- **Widgets** > - Controls which widgets are visible on the screen. Widgets are fully described in WIDGETS.
  - **Statistics**
  - **Elemental Analysis**
  - **History**
  - **Line Notation Pad**
  - **MolGrabber**
  - **Multiplet Tool**
  - **NMR Simulation**
  - **Properties**
  - **Search**
  - **Symbols**
  - **Templates**
  - **TLC Canvas**
- **Close All Widgets** - Close all currently open widgets.
- **Collect Windows** - Collect all of ChemDoodle's windows around the main window.
- **Default Workspace** - Return the configuration of windows within the main ChemDoodle window to the default layout.
- **Revert Workspace** - Revert the ChemDoodle workspace to the last saved workspace.
- **Save Workspace** - Save the current configuration of the windows within the main ChemDoodle window. This also saves file chooser paths and other workspace settings. This command is executed automatically when ChemDoodle is closed.

2.2.2.10 Purchase menu

The **Purchase** menu is only present during the trial or when a subscription license is expiring.

- **Activate ChemDoodle** - Displays the activation form to input a purchased license code and generate the license for the ChemDoodle application.
- **Buy a License Code** - Opens the default internet browser to the purchase page of the iChemLabs website.

2.2.2.11 Help menu

- **About ChemDoodle**[6] - Displays information about ChemDoodle, your license code and your license expiration, if any.
- **User Guide** - View this user guide in the program most appropriate for opening *PDF* files.
- **Quick Start Guide** - Provides a basic overview of program functionality. By default the Quick Start Guide appears at startup.
- **References** - View an organized list of references for the data and algorithms used in ChemDoodle. You can use this list to assess ChemDoodle's quality.
- **View User License** - View the user license that you accepted when you activated ChemDoodle.
- **Deactivate ChemDoodle** - ChemDoodle can only be used on the number of computers determined in your license. To switch from one computer to another, use this function first. This function is also useful if you need to reinstall your operating system.
- **Contact Customer Service** - Open the iChemLabs customer support form and fill in the appropriate fields. This is the quickest and easiest way to contact iChemLabs customer service.

[6] This menu item is in the ChemDoodle menu on macOS.

- **iChemLabs Newsfeed** - View the iChemLabs newsfeed *RSS*.
- **Check for Updates** - Check for updates to ChemDoodle. If any are found, you will see the changes listed and you will be requested to update ChemDoodle. If allowed, ChemDoodle will automatically update itself. There is no need to redownload or reinstall ChemDoodle for updates.
- **Register Filetype Associations** - Manage file type associations for ChemDoodle on Windows. This menu item is only present on Windows.

2.2.3 Toolbars

The main toolbars for editing content are located at the top of the ChemDoodle window (see Figure 2.1). The first row contains the formatting toolbar. The second row contains the content and chemistry toolbars.

2.2.3.1 Formatting toolbar

The formatting toolbar includes controls for defining the fonts, colors and strokes of the objects in your document.

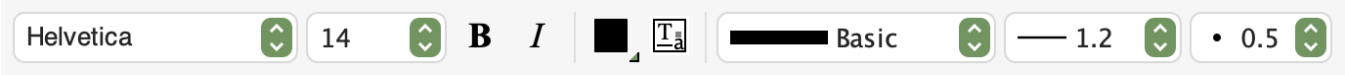
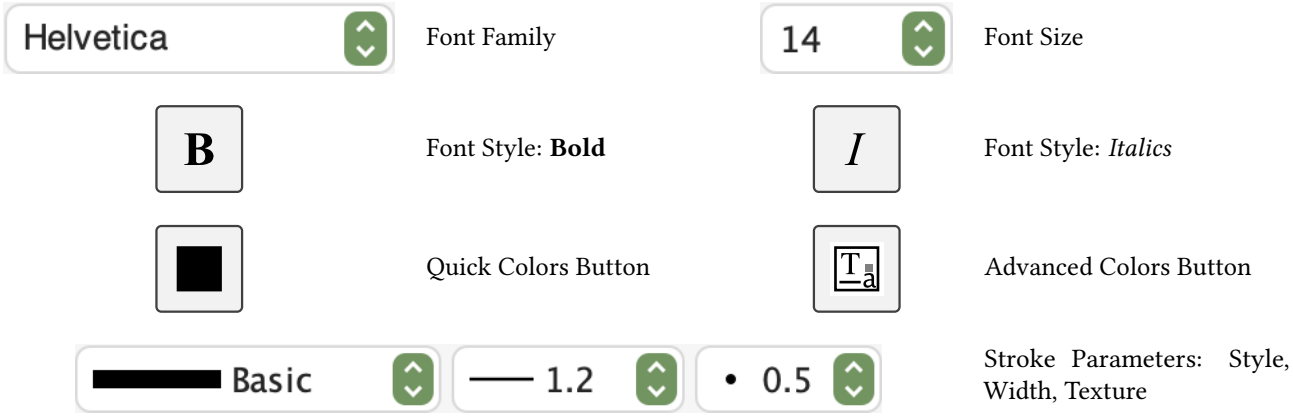


Figure 2.6: *Formatting Toolbar*



2.2.3.2 Content toolbar

The content toolbar includes tools for selecting and generically editing the objects in the document.



Figure 2.7: *Content Toolbar*


Lasso Selection Tools


Lasso Shapes Only Selection Tool


Rectangular Marquee Selection Tool


Rotate in 3D


Cut


Copy


Paste


Erase Content


Clear Current Document


Undo


Redo

2.2.3.3 Chemistry toolbar

The chemistry toolbar includes tools for working with and editing chemical data in your document.

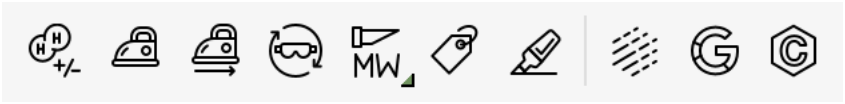


Figure 2.8: *Chemistry Toolbar*


Add/Remove Hydrogen


Optimize Structures in 2D


Clean Reaction


Conform Selection to Current Style Sheet


Fragmentation Tools


Attach Auto-updating Labels


Structure Highlighter


SciFinder-n


Google Patents


PubChem

2.2.3.4 Document toolbar

The document toolbar is located at the bottom of the **Doodle Board** and includes functions for working with files, documents and tabs.



Figure 2.9: *Document Toolbar*


Create a new blank document


Print preview


Create a new blank formatted document



Document Scale


Open a file


Zoom In


Change number of pages


Zoom Out


Save a file


Fit to Width

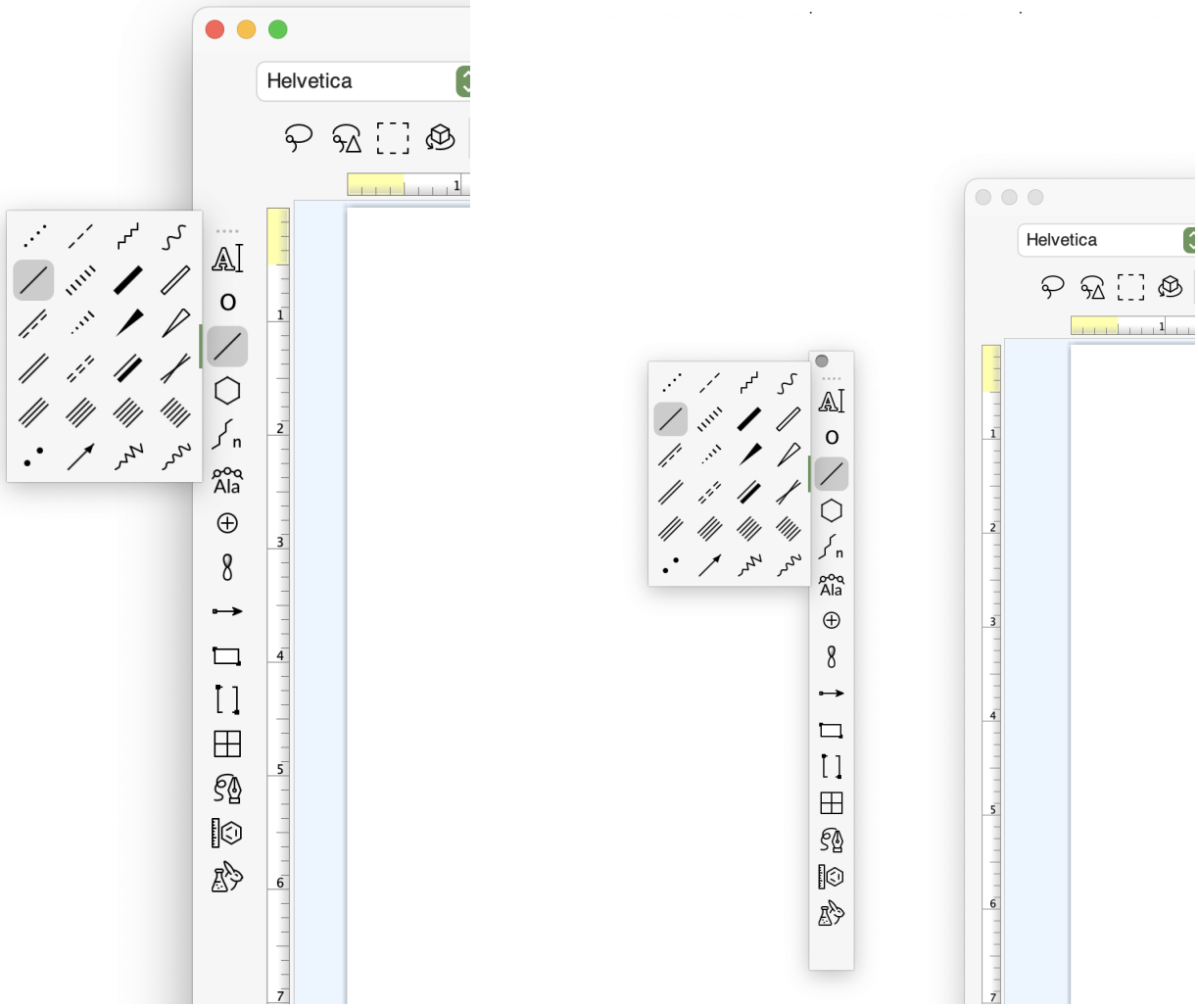

Print document


Fit to Window

2.2.4 Drawing toolbar and palettes

The **Drawing Toolbar** and palettes are located on the left hand side of the main window and contain tools for drawing on the document. Many buttons in the **Drawing Toolbar** represent a group of drawing tools. When you click on the button, several options will appear in a palette. The option that is chosen becomes the default tool for that button.

This toolbar can be detached and moved to the desired position while working by pressing the mouse down and dragging on the drag anchor at the top of this toolbar as shown in Figures 2.10.



(a) *Attached drawing toolbar* (b) *Detached drawing toolbar*

Figure 2.10: *Drawing toolbar in attached and detached mode*

2.2.4.1 Text input palette

Text for Atoms and Captions



When selected, will allow you to click on any atom and open a text field. Enter desired text in the text field and then click on the page or press the escape key to close the text field, thus setting the selected atom's label to the contents of the text field.

This tool will also allow the creation of labels (non-chemical text). Simply click on an empty space in the document to create a label with the default caption font, type and format your text and then press the escape key to set the label. Click on a label with this tool to edit the label.

Set Query to Atom or Bond



When selected, will allow you to click on any atom or bond and open a query field for that object. Enter the desired query or use the query toolbar to set the query and press the escape key to set the query. Query structures are covered in the QUERY STRUCTURES chapter.

2.2.4.2 Elemental labels palette

Click on the element label to see a full periodic table. Select an element label to set or attach it to any atom in the drawing.

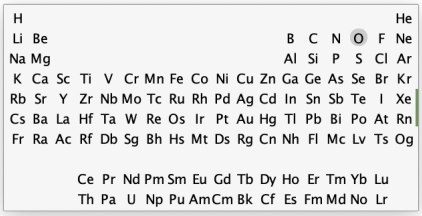


Figure 2.11: *Labels Palette*

Right click on the elemental labels button to see the common labels palette as shown in Figure 2.12.

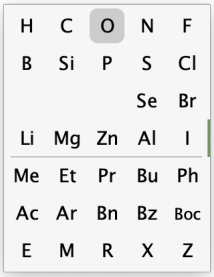
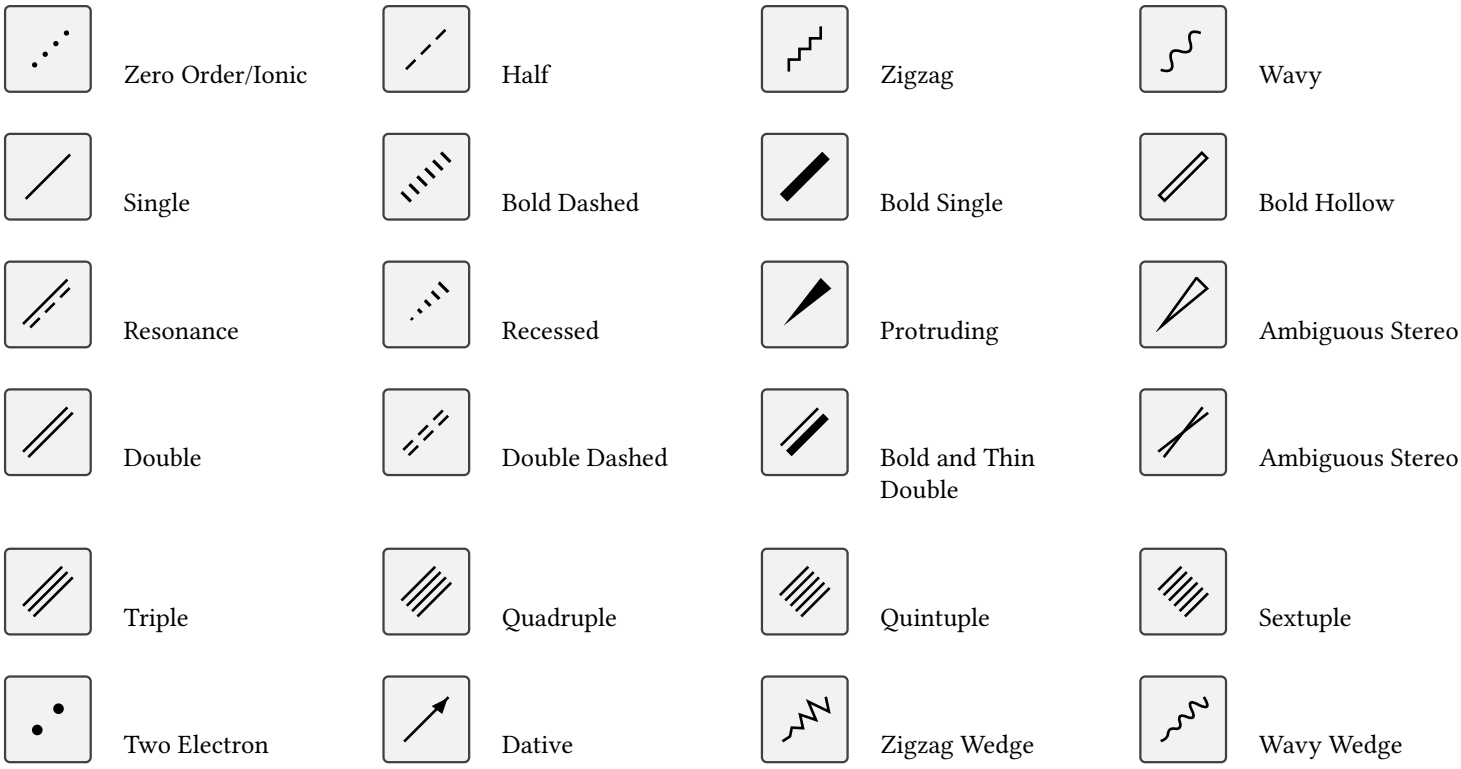


Figure 2.12: *Common Labels Palette*

2.2.4.3 Bonds palette



Figure 2.13: *Bonds Palette*



To place bonds of a specified type, click on the desired type of bond and the drawing mode will change to place a bond of that type. Clicking on a hovered bond will change that bond's current bond type to the selected bond type.

The single bond order will add to other bond orders by default. So clicking on a single bond will change it to a double bond, clicking on a double bond will change it to a triple bond, etc. Clicking on a triple bond will change it to a single bond. Clicking on decorated bond orders (protruding, ambiguous double, etc.) will convert it to a single bond before incrementing it. To stop single bond orders from adding to bonds, you can set the single bond behavior to always override other bond orders in the **Settings** window under the **Controls** tab.

2.2.4.4 Rings palette



Figure 2.14: *Rings Palette*


Cyclopropane ring


Cyclobutane ring


Cyclopentane ring


Cyclohexane ring


Cycloheptane ring


Cyclooctane ring


Cyclobutadiene ring


Cyclopentadiene ring


Benzene ring


Cycloheptatriene ring


Cyclohexane Chair Conformer 1


Cyclohexane Chair Conformer 2



Arbitrary Ring Size Tool



Arbitrary Crown Size Tool

2.2.4.5 Chain palette



Figure 2.15: *Carbon Chain Toolbar*



Linear Carbon Chain Tool



Fischer Projection Carbon Chain Tool



Freeform Carbon Chain Tool

2.2.4.6 Macromolecular palette



Figure 2.16: *Macromolecular Tools*



Three Letter Amino Acid Sequence Tool


Carbon Nanotube Builder


Prism Builder

2.2.4.7 Chemical attribute palette



Figure 2.17: *Chemical Attributes Palette*


Increase Charge


Decrease Charge



Add Positive Dipole



Add Negative Dipole


Add Electron Pair


Add Single Electron


Add Radical Cation


Add Radical Anion


Add Electron Pair (Bar)

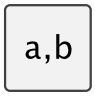

Add Asterisk/Undefined Stereocenter



Number Incrementals



Roman Numeral Incrementals



Letter Incrementals



Greek Letter Incrementals

2.2.4.8 Orbitals palette

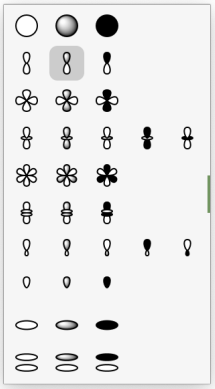


Figure 2.18: *Orbitals Palette*


Atomic s orbital


Atomic $p_{x|y|z}$ orbital


Atomic $d_{xz|yz|xy|x^2-y^2}$ orbital


Atomic d_{z^2} orbital


Atomic $f_{xz^2|xy^2|x(x^2-3y^2)|y(3x^2-y^2)}$ orbital


Atomic f_z^3 orbital


Hybrid sp^3 orbital


Hybrid sp lobe orbital


Bonding σ orbital


Bonding π orbital

2.2.4.9 Arrows palette

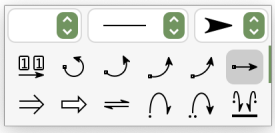


Figure 2.19: *Arrows Palette*

The top row of the arrows palette consists of three drop-down menus specifying the starting arrow style, the connector style between arrows and the ending arrow style.



Starting arrow style



Connector style between arrows



Ending arrow style



The set of buttons to the left allows you to place an arrow in the document at a given preset angle. The preset angles, from left to right, are 270°, 180°, 120°, 90° and 0°. At any time, you can change the arc angle of a placed arc to an arbitrary angle of your choice.



This set of buttons contains presets for common non-standard arrow types, such as retrosynthetic arrows. The arc angles of these arrows cannot be changed.



This set of buttons allows you to create electron pushers. These automatic shapes are defined by a to and from object and will automatically display based on the objects they are assigned to. See the SHAPES chapter for more information.



This is the atom mapping tool for creating associations between atoms. See the SHAPES chapter for more information.

2.2.4.10 Shapes palette

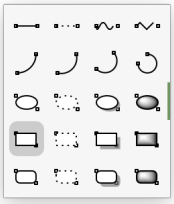


Figure 2.20: *Shapes Palette*


Straight line


Dashed line


Wavy line


Zigzag line


90° arc


120° arc


180° arc


270° arc


Plain oval


Dashed oval


Shadowed oval


Shaded oval


Plain rectangle


Dashed rectangle


Shadowed rectangle


Shaded rectangle


Plain rounded rectangle


Dashed rounded rectangle


Shadowed rounded rectangle


Shaded rounded rectangle

2.2.4.11 Brackets palette

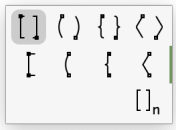


Figure 2.21: *Brackets Palette*


Square bracket set


Parenthesis set


Curly bracket set

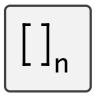

Chevron bracket set


Square individual bracket


Parenthesis individual bracket


Curly individual bracket


Chevron individual bracket


Dynamic brackets update to always fit content between two bonds

2.2.4.12 Table tool


A tool for building advanced tables.

2.2.4.13 Pen palette



Figure 2.22: *Polylines Toolbar*

 Pen Tool

 Custom Bezier Curve

 Polyline Tool

2.2.4.14 Ruler tool

 Measure content with a ruler object.

2.2.4.15 iChemLabs Vector Art

 Opens the laboratory glassware and BioArt vector art window to build diagrams with iChemLabs drawn art.

2.2.5 Styles and settings buttons

There are 3 buttons on the bottom right corner of the ChemDoodle window (see Figure 2.1). The first is the **Edit Styles** button, the second is the **Settings** button and the third is the **Widget Drawer** button. The **Widget Drawer** button is covered in the next sub-section.

Edit Styles



A window containing the definitions for the current document style sheet will appear when clicking this button. Edit the style sheet as desired to control the graphics in your document. More instruction on style sheets may be found in the STYLES chapter.

Settings



A window containing the settings for the ChemDoodle application will appear when clicking this button. Edit these settings to customize how the application works.

2.2.6 Widgets and the widget menu

Widgets are auxiliary applications that provide added functionality to ChemDoodle. Each widget has its own unique interface contained within a widget window. A widget window is a simple, movable and resizable window that contains the widget interface and two buttons in its top bar for closing and for maximizing/minimizing the widget. A comprehensive guide to the widgets and their use can be found in the WIDGETS chapter of this manual.

To hide or show the available widgets, select the **Widget Drawer**  in the lower right hand corner of the ChemDoodle window (see Figure 2.1). When the **Widget Drawer** is shown, the **Widget Drawer** button will change to an open drawer  . You can also use the Window > Widgets submenu to list and show widgets by name.

Table 2.2 briefly lists the widgets available in ChemDoodle.

Table 2.2: Available Widgets

Name	Description
Elemental Analysis	Calculates molecular masses, elemental analysis and isotopic distributions for structures
History	Provides full access to the undo/redo queue
Line Notation Pad	Generates and parses line notations and will also correct your input
MolGrabber	Search databases for chemical structures
Multiplet Tool	Simulate multiplets
NMR Simulation	Simulate nuclear magnetic resonance and associate peaks to nuclei as well as provide more thorough information about the spectrum and simulation
Properties	Calculates molecular descriptors
Search	Search your computer and attached storage devices for chemical structures
Statistics	Displays document and drawing statistics
Symbols	Quick access to chemically relevant symbols and the full unicode range
Templates	Organizes chemical structure templates for your use
TLC Canvas	Draw thin layer chromatography plates

2.2.7 The workspace

The ChemDoodle workspace consists of the application's windows and all interface elements contained within. You may freely place interface windows, select widgets (if available), change the document scale, select view options, etc., and your choices will be remembered for your next session. While this happens automatically, ChemDoodle also provides several functions for directly managing your workspace.

2.2.7.1 Resizing the application window

At any time, you may minimize and maximize the ChemDoodle application or resize it to your preference. You can use the operating system specific functions located in the top handle of the window, or by using functions in the Window menu.



A minimum screen resolution of 1280 by 800 pixels is recommended to optimally fit all of the components in ChemDoodle on the screen - smaller resolutions may experience some visual overlap!

The workspace will keep track of the size and location of ChemDoodle when it was last closed.

2.2.7.2 Resetting to the default workspace

To reset to the default workspace that was presented when ChemDoodle was first opened, select the Window ⟩ Default Workspace menu item.

2.2.7.3 Reverting to the last saved workspace

To revert to the last saved workspace select the Window ⟩ Revert Workspace menu item.

2.2.7.4 Saving the current workspace

To save the current workspace, which will override the last saved workspace, execute the following steps:

1. Organize the workspace as desired.
2. Select the Window ⟩ Save Workspace menu item.

The current workspace is now saved and can be reverted to.



Upon closing, ChemDoodle will automatically save your current workspace and when it is opened again the workspace will look exactly as it did when it was closed, overriding your previously saved workspace. Therefore, you may wish to revert the workspace to your saved workspace before exiting ChemDoodle.

2.3 Interface settings

In addition to being a very powerful application for your chemical data, ChemDoodle is readily customizable. ChemDoodle provides many settings for changing the way it looks, how it works, and what it does. To access the interface settings, open the **Settings** window by selecting the Edit ⟩ Settings... menu item (in the ChemDoodle menu on macOS). Then select the tab section on the left for the category of setting you wish to adjust. For instance, we chose the **Controls** tab  in Figure 2.23.

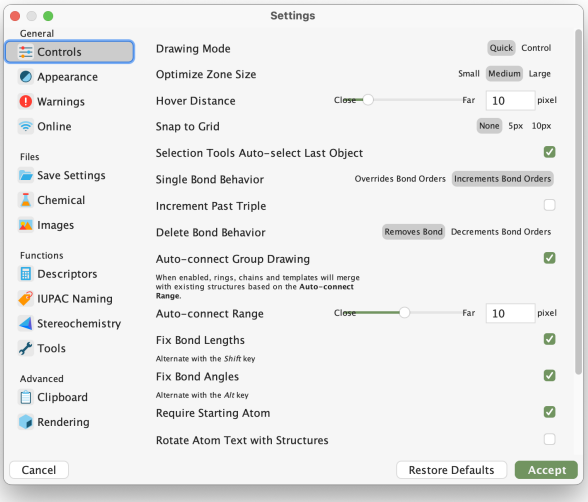


Figure 2.23: *Controls Settings*

2.3.1 Controls Settings

2.3.1.1 Drawing controls

Default Tool The default tool is the tool activated when ChemDoodle is opened or when a tab for a blank document is selected. You may choose between "Single Bond" for quickly drawing molecules or "Lasso" for the selection tool.

Drawing Mode There are two drawing modes, Quick and Control. Quick mode is the default, and actions are performed by pressing down with the mouse, dragging to set the tool, and then releasing the mouse to finish the action. In Control mode, the same action is achieved by clicking the mouse once, moving the mouse to set the tool and then clicking again to complete the action.

Snap to Grid By default, coordinates for all objects can be placed anywhere. However, you can set a 5-pixel or 10-pixel grid for objects to snap to.

Hover Distance The hover distance controls how close the mouse pointer must be to an object for it to be considered hovered. The default is 10 pixels, but it can be made more sensitive or more pinpoint.

Optimize Zone Size The Optimize Zone is a special component in ChemDoodle for placing bonds in the optimal position around atoms. It appears as a blue circle when placing bonds and other molecule fragments. To use the Optimize Zone, just place the mouse pointer in the blue circle. The bond or fragment being placed will automatically be oriented in the most optimal position. You can change the size of the optimize zone to be Small, Medium or Large. It is Medium by default.

Require Starting Atom ☑ Many chemical sketchers have the bond as the smallest building block. ChemDoodle uses atoms as the smallest building blocks, and all drawing functions require a starting atom. You can disable this requirement and allow new bonds to be placed with a single mouse click.

Rotate Atom Text with Structures ☑ By default, text does not rotate when you rotate structures. This setting enables atom text rotation when structures are rotated.

Bonds are Focusable ☑ If you are working only with atoms or you don't want to touch bonds, disabling this setting will make editing easier. When disabled, bonds cannot be hovered or selected.

Single Bond Behavior By default, single bonds will increment bond orders. So using the **Single** bond tool, if you click on a single bond it will become a double bond and so forth. However, you can change this behavior to instead override bond orders so any bonds clicked on with the **Single** bond tool become single bonds.

Increment Past Triple ☑ By default, when the **Increment Bond Orders** option under **Single Bond Behavior** is disabled, bonds will not be incremented past triple bonds, instead falling back to being single bonds again. When this option is enabled, bonds can be incremented all the way to sextuple bonds before becoming single bonds again.

Delete Bond Behavior By default, using delete functions when a bond is hovered will remove that bond entirely. However, you can change this behavior to instead decrement bond orders.

Fix Bond Lengths ☑ This option is enabled by default and fixes the bond lengths of the drawing tools. You can quickly modify this setting when drawing by holding down the shift key.

Fix Bond Angles ☑ This option is enabled by default and fixes the bond angles of the drawing tools. You can quickly modify this setting when drawing by holding down the alt key.

Bond Angle Increment Choose between 15° or 30° as the bond angle increment when drawing using fixed angles outside of the Optimize Zone.

Auto-connect Group Drawing ☑ This option is enabled by default and will have the atoms placed by ring and template tools automatically merge with any overlapping atoms present in the document. Note, you may also disable auto-connections when drawing groups by holding down the space key.

Auto-connect Range This value determines the distance at which group drawings will automatically merge and connect with nearby atoms.

Edit Shapes while Drawing Shapes When drawing shapes, you can use the same tool to edit shapes, without having to switch to a selection tool. By default, you can edit any shape type that is the **Same** type as the one you are currently drawing (you may edit other rectangles when drawing rectangles). You may change this setting to expand the range to editing **All** shapes or restrict it to editing **None**. The **None** choice is optimal if you have a very congested figure and want more control over precisely drawing shapes.

2.3.1.2 Selection controls

Auto-select Last Object ☑ This option is enabled by default and when enabled, the last object added to the document (molecule or shape) will be automatically selected if a corresponding selection tool is activated. Disable this and no selection will be automatically made when a selection tool is chosen.

Double Click on Atom/Bond When using a selection tool, this setting determines the action when a hovered atom or bond is double-clicked on. If **Select Full Structure** is selected, then the full molecule the atom or bond is a part of will become completely selected. If **Edit Object Styles** is selected, then the **Styles** window for the hovered object will appear for you to edit styles.

2.3.1.3 3D rotation controls

3D Rotation Mode When using the structure perspective tool, mouse movements will correspond to x- and y-axis movements during 3-D rotation. You can change this to correspond to a quaternion rotation if desired.

2.3.2 Appearance settings



Make sure to restart the ChemDoodle application after changing settings in this section.

Light/Dark Mode Switch between the light and dark mode appearances for the application.

2.3.2.1 Fonts

Application Font Family If you prefer a different font from the standard sans-serif font that ChemDoodle uses, you can change it here. This is also helpful if you need to switch to a different font that supports characters for another language.

Application Font Size If you prefer a different font size from the standard size that ChemDoodle uses, you can change it here. This is also helpful if you have trouble reading the labels in the program.

2.3.2.2 Colors

Application If you prefer a color other than the default green color, you can choose to change this here. Light, pale color choices are easiest on the eyes and are least distracting.

Highlight This color is used for hovered decorations and some selected highlights. It is pale brown by default.

Lasso This color is used for the selection anchors and other lasso decorations. It is a dark blue by default.

Guideline This color is used for the optional guidelines. It is a light gray by default.

Error This color is used to highlight errors and other problems. It is a brick red by default.

Icons Light This color is used to render enabled button icon images in "Light" mode.

Icons Light Disabled This color is used to render disabled button icon images in "Light" mode.

Icons Dark This color is used to render enabled button icon images in "Dark" mode.

Icons Dark Disabled This color is used to render disabled button icon images in "Dark" mode.

2.3.2.3 Interface

Default Document Scale Change this value to define what scale should be used to display new and opened documents. The default is **100%**.

Scrollbar Unit Increment Using this slider, you can make scroll and swipe gestures slower or faster. By default, the value is 16. Decreasing the value will make scrolling slower, while increasing the value will make scrolling faster.

2.3.2.4 Decorations

Show Drawing Measurements Statistics are rendered on the document when drawing to always show lengths and angles if **Always** is selected, or only if they are not fixed if **Unfixed** is selected, or never if **Never** is selected.

Show Transform Measurements ☑ When enabled, statistics are rendered to show how lasso functions alter your figures.

View Crawling Ants Effect When Lassoing ☑ When enabled, the lasso outline will exhibit a crawling ants effect.

View Mouse Position on Rulers ☑ When enabled, the mouse position will be ticked on the document's rulers in red.

View Selection Bounds on Rulers ☑ When enabled, the lasso selection will be highlighted on the document's rulers in amber.

View Margins on Rulers ☑ When enabled, the margin areas will be highlighted on the document's rulers in a yellow color.

Render Page Shadows ☑ When enabled, an aesthetically pleasing drop shadow is displayed under the document pages.

2.3.2.5 Other settings

Ruler Mode Set the interface rulers to either Metric or US mode.

Document Alignment Allows setting the alignment of documents in the main application window between Center and Left.

Hide Dialogs on Switching Applications ☑ Will hide all widgets and other windows when ChemDoodle is not the active application.

Widgets Update with Latest Drawing ☑ The **Properties** and **Elemental Analysis** widgets will update with the last modified molecule if no content is selected. The **Properties** widget will only update if a single molecule structure is present on the document.

2.3.3 Mouse cursors

The mouse pointer is context sensitive and will change when hovered over the document to display visual feedback about the current mouse gestures that can be performed. The different mouse cursors are described in Table 2.3.

Table 2.3: Mouse Cursors

Cursor	Function
	This pinpoints the exact location that your click will hit. This is the default drawing cursor. Clicking and dragging perform the usual functions.
	This is the text cursor and signifies that text can be typed with the keyboard or a text field or area can be initiated.
	This is the lasso cursor. Clicking and dragging will generate an outline following the drag path. All content within the drag path will be selected.
	This signifies that a single object may be selected.
	This means that content can be grabbed. Individual objects or selected content can be grabbed.
	This means that content has been grabbed and dragging gestures will perform appropriate actions.
	This cursor only appears when rotating structures in 3D. It means that content can be grabbed.
	This cursor only appears when rotating structures in 3D. It means that content has been grabbed and drag gestures will perform appropriate actions.
	This cursor signifies that resize actions can be performed by clicking and dragging. This cursor will also appear when translating the rotation anchor.
	This cursor signifies that rotation actions can be performed by clicking and dragging.
	This cursor is used in the eraser mode and notifies the user that clicks will remove hovered objects.
	This cursor specifies that a table row or column is the current focus of the action context. Right clicking will show table row and column specific actions. Some keyboard and tool shortcuts will affect table columns and rows directly.
	This cursor specifies that a separator for table rows or columns can be adjusted to control row or column spacing. Press the mouse down and drag to move the separator.

2.3.3.1 Customizing the drawing cursor

You can change the drawing cursor from the crosshair if you so choose. In the **Settings** window, under the **Appearance** tab in the **Cursors** section, change the **Drawing Cursor** choice to one of the cursors available. The following cursors can be used:


- The system mouse pointer.


- The system crosshair pointer. This is the default drawing cursor.


- A pencil cursor.


- A large circle cursor.


- A smaller circle cursor.

2.3.3.2 Operating system cursor differences

Each operating system has different cursors available to applications. ChemDoodle uses the system cursors for the crosshair, text and pointer cursors. So these cursors will appear different on different platforms. The rest of the cursors are custom built for ChemDoodle and will have the same shape on all operating systems. However, the colors will be different. On macOS, the cursors are black with a white border and a shadow. On Windows and Linux, the cursors are white with a black outline and no shadow. This is shown in Figure 2.24.



(a) *The open hand cursor on macOS*



(b) *The open hand cursor on Windows/Linux*

Figure 2.24: *Operating system cursor differences*

2.3.3.3 Other cursor customizations

You can customize a few other cusor options. In the **Settings** window, under the **Appearance** tab in the **Cursors** section, several options are listed:

- **Invert Colors** - Invert the colors of the cursors, so white becomes black and black becomes white.
- **Left Handed Mode (Flip Horizontally)** - The cursors will be flipped horizontally so that left handed users can feel more comfortable using them.
- **Render Shadow** - This option is only available on macOS. A shadow will be rendered under the cursor when this option is enabled as this is the natural rendering for macOS cursors.



These options will affect all cursors in ChemDoodle except for the default system cursors.

2.4 Accessibility

ChemDoodle is customizable with a focus on accessibility.

2.4.1 Colors

You can change the default rendering for colors, including the interface color in the **Settings** window in the **Appearance** tab. Those that are colorblind may wish to change some of these colors. The following colors can be changed:

- **Application** - This is the main color used by the interface to decorate windows and components. A pale color is recommended for best results.
- **Hovered** - This is the color used to signify that an object is hovered.
- **Selected** - This is the color used to signify that an object is selected.
- **Preview** - This color is used to preview drawing tool results when drawing figures.
- **Lasso** - This is the color used to render the selection tools and selections.
- **Lassoed Object Background** - This is the color rendered behind lassoed objects to differentiate them from not lassoed objects.
- **Guideline** - This color is used to render guidelines and other drawing aids, such as a background grid.
- **Error** - This color notifies the user that an error or warning is present.
- **Icons Light** - This color is used to render enabled button icon images in "Light" mode.
- **Icons Light Disabled** - This color is used to render disabled button icon images in "Light" mode.
- **Icons Dark** - This color is used to render enabled button icon images in "Dark" mode.
- **Icons Dark Disabled** - This color is used to render disabled button icon images in "Dark" mode.

2.4.2 Sizes

You can change the default family and sizes for interface fonts, if you find them difficult to read, in the **Settings** window in the **Appearance** tab.

2.4.3 Left handed mode for cursors

If you are left handed, you may find using **Left Handed Mode**, in the **Settings** window in the **Appearance** tab, is more comfortable for you to draw with.

2.4.4 Menu item and toolbar shortcuts

Any menu action and tool in ChemDoodle can be mapped to a keyboard shortcut of your choosing for improved access to essential functions. Use the Window > Edit Shortcuts... menu item to assign shortcuts. See the KEYBOARD SHORTCUTS section for more information.

2.4.5 Single click mode

Mouse based gestures for drawing objects, such as having to click drag the mouse to sprout a new bond, can instead be changed to a click-move-click based system. This is defined by the **Drawing Mode** setting the in **Settings** window under the **Controls** tab. Set the **Drawing Mode** setting to **Control**.

2.5 Documents

The main object created in ChemDoodle is a document. Each document represents one or more blank pages that chemical figures can be drawn on.

2.5.1 Opening a document

To open a document, select the File › Open... menu item, locate the file you would like to open with the file chooser that appears and click the **Open** button. You may also use the **Open** button  in the bottom toolbar.

ChemDoodle can read many file formats, and the default file type the file chooser searches for is a *ChemDoodle Document*. To allow other file types, click on the format drop down selection at the bottom of the file chooser and select the file type you would like to open. If you select the **All Files** type, ChemDoodle will automatically detect the file type you are opening if it has the correct extension. You can find a full list of the supported formats in the SHARING INFORMATION chapter.



Selecting **All Files** will allow you to select any file, including files that ChemDoodle cannot read. If such a file is chosen, you will see a file read error displayed. Otherwise, ChemDoodle will attempt to open the file by analyzing the file extension and file content to determine its type.

To open a recently opened document, expand the File › Open Recent submenu and select the file you would like to open. The ten most recently opened files are remembered.

2.5.2 Creating a document

You can create a new, blank document using the default chemical style sheet, or use a *ChemDoodle Style Sheet* file to create a new formatted document. To create a new blank document using the default style sheet, select the File › New menu item (or use the **New Document** button  in the **Document** toolbar). To create a new blank document using a predefined style sheet, select the File › New Formatted Document... menu item (or use the **New Formatted Document** button  in the **Document** toolbar).

ChemDoodle provides built-in *ChemDoodle Style Sheet* files. For example, the *ACS Document 1996* style is configured to create documents set with the bond lengths, bond width, spacing, and fonts used in the 2-column format of all **American Chemical Society** journals. Currently, ChemDoodle provides the following style sheets:

- ACS Document 1996
- Adv. Synth. Catal Document 20
- J. Chin. Chem. Soc. Document
- J. Het. Chem. Document
- J. Mol. Mod. Document (1 Column)
- J. Mol. Mod. Document (2 Column)
- Nature
- Phytomedicine Document
- RSC Document (1 Column)
- RSC Document (2 Column)
- Science of Synthesis Document
- SYNTHESIS, SYNLETT Document

- Verlag Helv. Chim. Acta Document
- Wiley Document

These style sheets are available when you create a new formatted document as is shown in Figure 2.25 below.

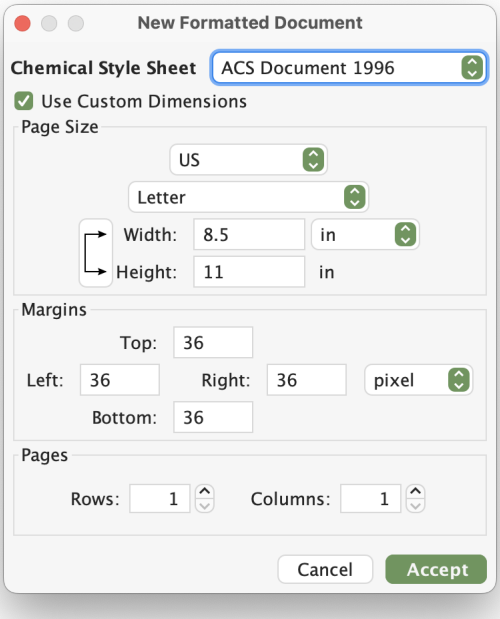


Figure 2.25: *Creating a New Formatted Document*

The style sheets are organized into three sections. The first contains just the default style sheet, the second contains all the built-in style sheets and the last contains custom style sheets. Select the style sheet that you prefer, override any custom dimensions if necessary, and then click the **Accept** button to create your new formatted document.

If you would like to modify the default document dimensions for the formatted document, select the **Use Custom Dimensions** checkbox and edit the appropriate fields.

2.5.3 Changing document size

To change the size of the current document, execute the following steps:

1. Choose the Edit ⟩ Resize Document... menu item.
2. Use the form to select a preset document size or manually type in the desired document dimensions.
3. Click the **Resize** button to resize the document.

2.5.4 Changing the number of pages in the document

To change the size of the current document, execute the following steps:

1. Choose the Edit ⟩ Number of Pages... menu item. You may also use the **Change Number of Pages** button  in the **Files** toolbar.
2. Use the form to define the number of rows and columns making up the document. The total number of pages will be equal to the number of rows times the number of columns.
3. Click the **Accept** button to change the number of pages.

2.5.5 Reversing actions

ChemDoodle keeps track of the actions you perform. You can reverse actions one at a time by selecting the Edit ⟩ Undo menu item (you may also use the **Undo** button  in the **Content** toolbar) then restore them with the Edit ⟩ Redo menu item (you may also use the **Redo** button  in the **Content** toolbar). Once you close your document, the undo queue is cleared.

More advanced undo/redo functionality is associated with the **History** widget; this is covered in the WIDGETS chapter.

2.5.6 Discard recent changes to a document

To retrieve the last saved version of a file without using **Undo** functions, select the File ⟩ Restore menu item. All changes made to the file since it was last saved are discarded and the saved version of the file will be reloaded.

2.5.7 Saving documents

To save your document as a file, select the Save or Save As... menu items from the File menu. Save (you may also use the **Save** button  in the bottom toolbar) will automatically save the document to the file it is associated with, while Save As... will allow you to save that document to a new location or overwrite another file. If there is no file associated with a document, the Save function is identical to the Save As... function.

When saving a new file or using the Save As... function, a file chooser will appear. Select the location to save the document to and type a preferred file name or accept the default name. You do not need to type in an extension. The extension will automatically be added and set to the file type extension selected at the bottom of the file chooser in the **Format** drop down.



Only the *ChemDoodle Document* can store your scene with 100% accuracy. Other file types, designed for other purposes, may not accurately or fully describe the objects and properties in ChemDoodle. A warning will pop up when saving to a file type other than a *ChemDoodle Document*. These warnings can be disabled in the **Settings** window under the **Chemical Files** tab.

After selecting the file type to be used, press the **Save** button to save your document as a file.

2.5.8 Autosaving

ChemDoodle will automatically save unsaved work for you at regular intervals. If your computer shuts off unexpectedly, the next time ChemDoodle opens, all autosaved content will be displayed. You can turn off autosaving in the **Settings** window under the **Save Settings** tab. You may also specify the autosave interval in the same section. The default autosave interval is five minutes.

2.5.9 Rendering scale

You may need to change the scale the document is rendered at depending on the situation. For instance, if you are working with a large document, you may want to decrease the scale to better view the content in its entirety. If you want to work on fine details of your figures, you may want to increase the scale to better see the content and for more precise control.

2.5.9.1 Defining the current scale

There are different methods to define the document scale, discussed in this section.

2.5.9.2 Using the document bar

The **Document** bar includes 5 controls for defining the document scale. First there are 4 buttons:

1.  **Zoom In** - increases the document scale.
2.  **Zoom Out** - decreases the document scale.
3.  **Fit to Width** - the document scale becomes dynamic and will optimize to fit the current width of the document or documents displayed by the interface.
4.  **Fit to Window** - the document scale becomes dynamic and will optimize to fully fit all documents displayed.

There is also a **Scale** interface drop down, allowing you to manually define the current scale or scale mode. The drop down has an **Other...** option, where upon selection, a prompt will appear (Figure 2.26) for you to input a custom document rendering scale. Input the scale you desire in the text field as a percentage (a 2x scale would be 200%) and press the **Accept** button to commit.

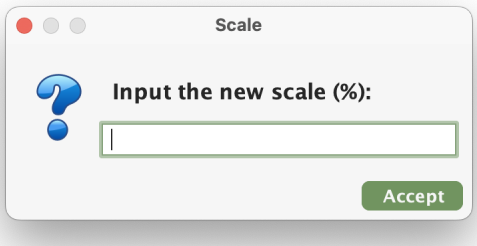


Figure 2.26: *Input a custom document rendering scale.*

2.5.9.3 Keyboard shortcuts

You may use the ctrl+= keyboard shortcut to increase the current scale level and you may use the ctrl+- keyboard shortcut to decrease the current scale level. Keyboard shortcuts may be changed, please see the KEYBOARD SHORTCUTS section for instructions.

2.5.9.4 Using the mouse

While holding down the ctrl key and using the mouse wheel or scroll gesture on a trackpad, the interface scale will be zoomed in or out (depending on the direction of the scroll). While zooming, ChemDoodle will attempt to keep the location in the document of last mouse position in the center of the display area.

2.6 File chooser

The file choosers that you use to open your files will closely resemble the standard file choosers of the operating system.

However, there are some enhancements. One addition is chemical file previews.

2.6.1 File chooser previews

On all operating systems, you will see a preview of chemical files that you select in file choosers. On Windows and Linux, the file chooser will show a preview of the entire document to the right as shown in Figures 2.27 and 2.28. If you place your mouse over the document preview, that part of the preview will be zoomed in for a closer inspection.

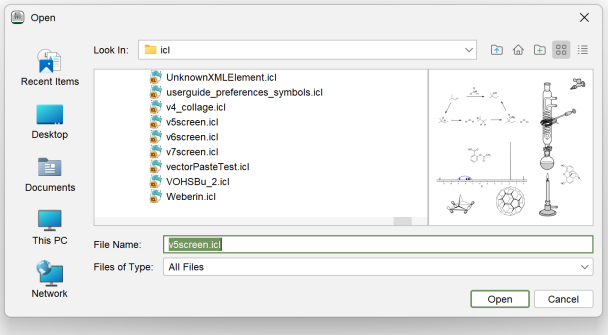


Figure 2.27: *The file chooser on Windows showing the file preview*

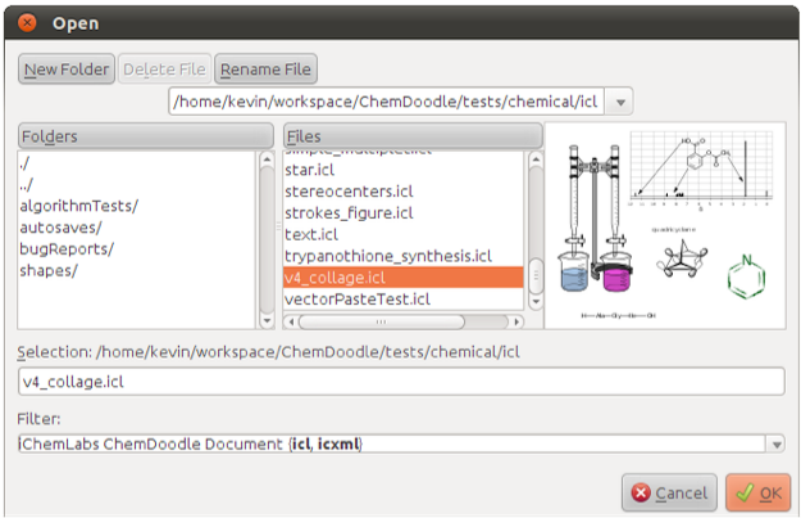


Figure 2.28: *The file chooser on Linux showing the file preview*

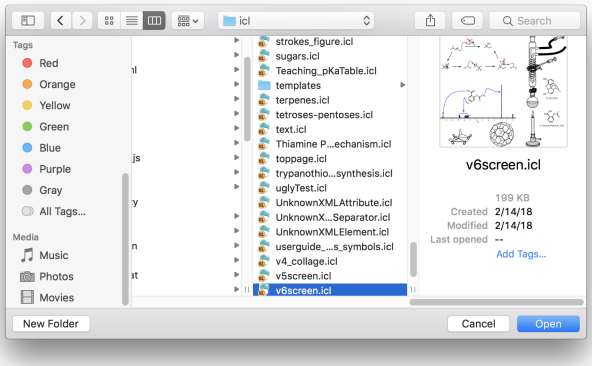


Figure 2.29: *The file chooser on macOS showing the file preview as expected for the native Finder window*

On macOS, a file preview will be given in certain views of the native Finder window as shown in Figure 2.29. A **Quick Look** plugin is also provided on macOS, for you to quickly preview any files ChemDoodle recognizes using Quick Look functionality in Finder.

2.6.2 macOS Quick Look plugin

Quick Look is a feature of the macOS platform that allows you to quickly preview files in Finder. ChemDoodle contains a Quick Look plugin to provide Quick Look previews for all the compatible chemical file types recognized by ChemDoodle.



On slower Macs, it may take up to 15 seconds to generate a preview for complex files.

To register the plugin with macOS, run the ChemDoodle application once. It may take a few minutes for the operating system to fully register the plugin.

To view a Quick Look preview in Finder for a compatible file, execute the following steps:

1. Locate the file you would like to see a Quick Look preview for.
2. Click on the file and press the space key, or right-click on the file and select the **Quick Look "filename"** menu item.

A preview will pop up in a preview window as shown in Figure 2.30. Previews will also appear in the side panel and **Get Info** windows for compatible file types.

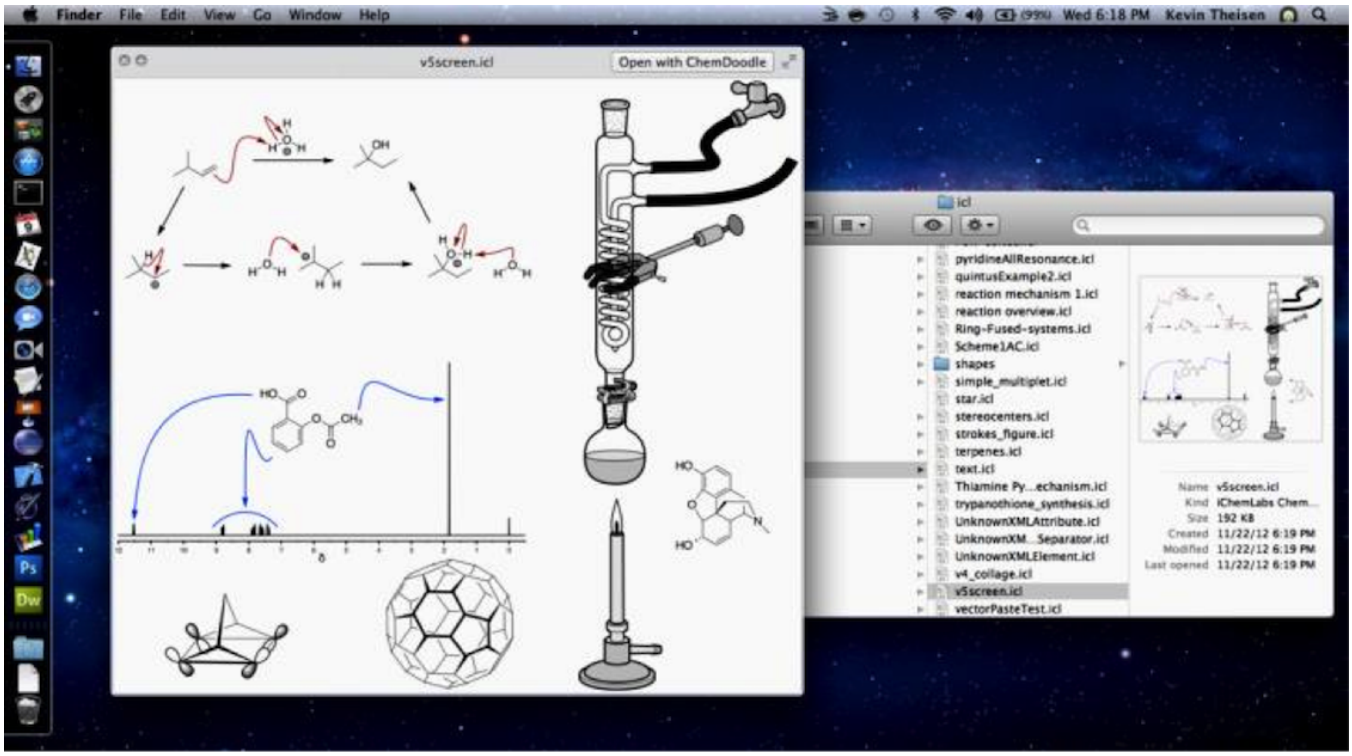


Figure 2.30: *ChemDoodle's macOS Quick Look plugin*

2.6.3 File chooser types

There are three file choosers available in ChemDoodle: **Java**, **Native**, and **Modern**.

- **Java** - this is the Java *JFileChooser* and is fully functional but will not have the same feel as the native system file chooser. File chooser previews are only visible in the Java file choosers on Windows and Linux. This is also the most compatible option if you are encountering technical difficulties.
- **Native** - this is the Java *FileDialog* and while native, it is missing a lot of features from the base system file chooser. The native file chooser requires a prerequisite step of choosing the output format first. There are known issues with the Java *FileDialog* and accessibility features of macOS.
- **Modern** - this is a custom native file chooser that bypasses Java. This option will offer the best functionality and feel when compared to the native system file chooser.

Regardless of the different experiences, you may use the one you like best. You control this by defining the **Filechooser Type** option in the **Settings** window, under the **Save Settings** tab in the **Filechooser Settings** section.

CHAPTER 3

Widgets

Contents

3.1 Overview **69**

3.2 What are widgets? **69**

3.3 Accessing widgets **69**
3.3.1 Widget menu 69
3.3.2 Widget Drawer 70

3.4 Widget windows **71**
3.4.1 Closing all widgets at once 71

3.5 Widget expansion **71**

3.6 Widget list **72**

3.7 Individual widgets **74**
3.7.1 Elemental analysis widget 74
3.7.1.1 Purpose 74
3.7.1.2 Interface 74
3.7.1.3 Outputting calculations to the document 74
3.7.1.4 Copying calculations to the system clipboard 75
3.7.2 History widget 76
3.7.2.1 Purpose 76
3.7.2.2 Interface 76
3.7.3 Line notation pad widget 77
3.7.3.1 Purpose 77
3.7.3.2 Interface 77
3.7.4 MolGrabber widget 79
3.7.4.1 Purpose 79
3.7.4.2 Interface 79
3.7.4.3 Directing to the Online Database 80
3.7.4.4 Database Notes 80
3.7.4.5 ChemExper Disclaimer 81
3.7.4.6 ChemSpider Disclaimer 81
3.7.4.7 PubChem User Requirements 81
3.7.5 Multiplet tool widget 83
3.7.5.1 Purpose 83
3.7.5.2 Interface 83
3.7.5.3 Simulating Multiplets 83
3.7.5.4 Setting up the Multiplet Figure 84
3.7.5.5 Editing Multiplets from the Doodle Board 85
3.7.5.6 Memory and Runtime Issues 85
3.7.6 NMR simulation widget 86
3.7.6.1 Purpose 86
3.7.6.2 Interface 86
3.7.6.3 Simulating NMR 86
3.7.6.4 Analyzing the Results 87
3.7.6.5 How NMR is Simulated 88
3.7.7 Properties widget 89
3.7.7.1 Purpose 89
3.7.7.2 Interface 89
3.7.8 Search widget 91

3.7.8.1 Purpose . . . 91
3.7.8.2 Interface . . . 91
3.7.8.3 Search Settings . . . 92
3.7.9 Statistics widget . . . 94
3.7.9.1 Purpose . . . 94
3.7.9.2 Interface . . . 94
3.7.10 Symbols widget . . . 95
3.7.10.1 Purpose . . . 95
3.7.10.2 Interface . . . 95
3.7.10.3 Expanded Unicode Range . . . 95
3.7.11 Templates widget . . . 97
3.7.11.1 Purpose . . . 97
3.7.11.2 Interface . . . 97
3.7.11.3 Using Templates . . . 98
3.7.12 TLC canvas widget . . . 99
3.7.12.1 Purpose . . . 99
3.7.12.2 Interface . . . 99
3.7.12.3 Drawing TLC Plates . . . 100
3.7.12.4 Editing TLC Plates from the Doodle Board . . . 101

3.1 Overview

This chapter is going to introduce the new user to widgets in ChemDoodle. It covers the following topics:

- What are widgets?
- How to control widget interfaces.
- Which widgets are available?
- The functions the widgets perform.

3.2 What are widgets?

Widgets are auxiliary applications providing added functionality to ChemDoodle. Each widget has its own unique interface contained within a widget window.

Essentially, each widget performs a very specific task that complements the functionality of ChemDoodle, but they are complex enough to have their own unique interface to maximize their utility.

3.3 Accessing widgets

Widgets can be accessed in two ways: (1) through the Window menu and (2) through the **Widget Drawer**.

3.3.1 Widget menu

The Window > Widgets submenu lists the available widgets by name as shown in Figure 3.1.

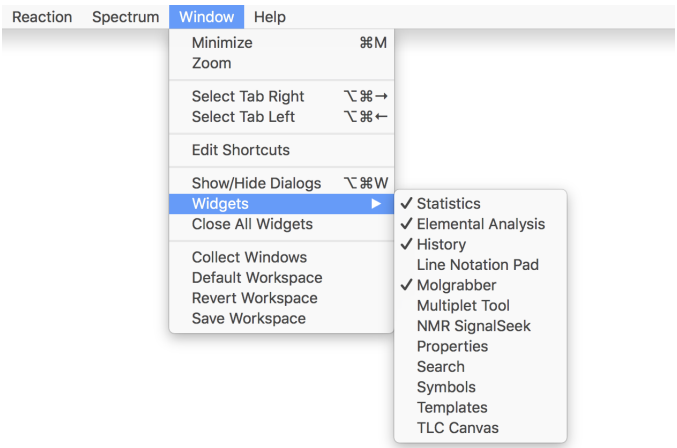


Figure 3.1: *Widget Menu*

Clicking on an unchecked menu item will show the corresponding widget. Clicking a checked menu item will hide the corresponding widget.

3.3.2 Widget Drawer

You may also hide or show the available widgets by selecting the **Widget Drawer**  in the lower right hand corner of the ChemDoodle window. The expanded drawer is shown in Figure 3.2.



Figure 3.2: *Widget Button and Drawer*

Clicking on an unselected widget icon will show the corresponding widget. Clicking a selected widget icon will hide the corresponding widget.

When the **Widget Drawer** is opened, the icon will change to an open drawer  . If you click on the **Widget Drawer** button while the drawer is shown, the drawer will be hidden.

3.4 Widget windows

A widget window is a simple, movable and resizable window that contains the widget interface and two buttons in its top bar[1] for controlling the widget as shown in Figure 3.3.

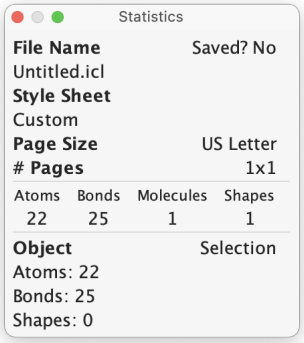


Figure 3.3: *Widget Window Components*

The top bar contains a button for maximizing the widget to fill the entire screen space. Clicking on this button again when the widget is maximized will return it to its original size. You can also use the drag anchors that appear when you move your mouse over the border of the widget window to resize widgets.

Clicking on the close button in the top bar will close the widget.

To move widgets, press and drag the top bar.

The entire functional widget interface is presented below the top bar.

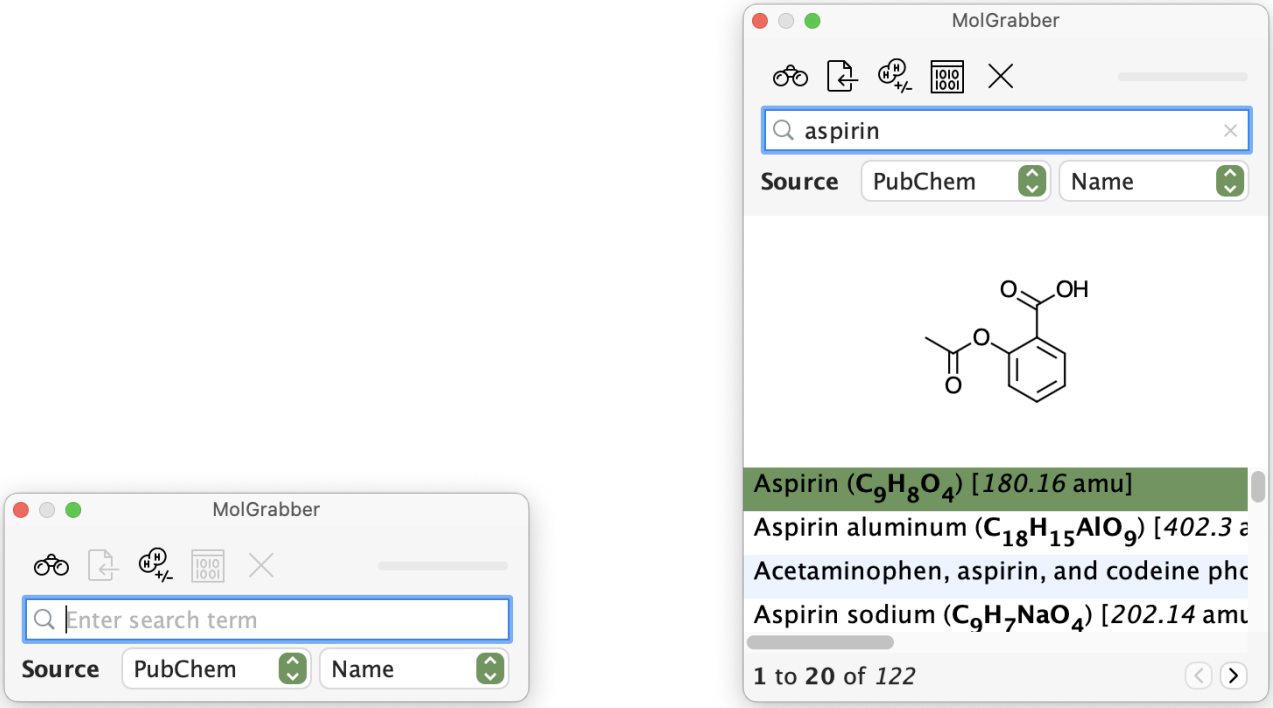
3.4.1 Closing all widgets at once

If you have many widgets open, you may desire to close them all quickly. Simply select the Window » Close All Widgets menu item to do this.

3.5 Widget expansion

Some widgets are initially in a collapsed state. Each collapsed widget will have some method to expand it. For example, the **MolGrabber** widget is initially collapsed. Type a search term in the text field and press the enter key to expand it as shown in Figure 3.4. Every collapsible widget will also have a **Collapse** button to collapse it.

[1] Widget window decorations (drag anchor, maximize/unmaximize button) have a slightly different appearance on each operating system.



(a) *Collapsed* ***MolGrabber*** *Widget*

(b) *Expanded* ***MolGrabber*** *Widget*

Figure 3.4: *Widget Expansion*

3.6 Widget list

There are currently 12 widgets provided in ChemDoodle: Brief descriptions are given in Table 3.1.

By default, the **Statistics**, **History** and **MolGrabber** widgets are shown when opening the software the first time. You can toggle which widgets are shown by using the Window 〉 Widgets menu or the **Widget Drawer**.

Table 3.1: Widgets

Name	Icon	Description
Statistics		Shows characteristics of the document, including atom, bond, and molecule counts.
Elemental Analysis		Calculates molecular masses, elemental analysis and isotopic distributions for structures.
History		Provides full access to the undo/redo stack.
Line Notation Pad		Generates and parses line notations and will also correct your input.
MolGrabber		Search databases for chemical structures and drag them into your document.
Multiplet Tool		Simulate and create advanced diagrams for multiplets.
NMR Simulation		Simulate nuclear magnetic resonance and associate peaks to nuclei as well as provide more thorough information about the spectrum and simulation.
Properties		Calculates molecular descriptors for selected and drawn molecules.
Search		Search your computer and attached storage devices for chemical structures.
Symbols		Quick access to chemically relevant symbols and the full unicode range.
Templates		Organizes chemical structure templates for your use.
TLC Canvas		Draw thin layer chromatography plates.

3.7 Individual widgets

3.7.1 Elemental analysis widget

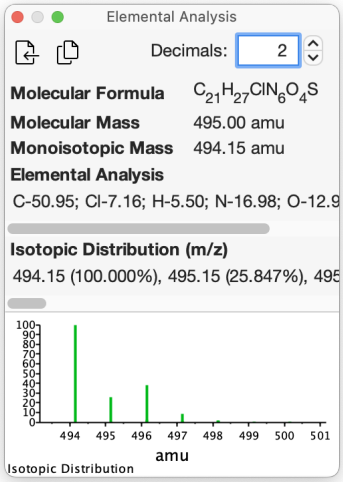


Figure 3.5: *Elemental Analysis Widget*

3.7.1.1 Purpose

This widget calculates formulas and masses, performs elemental analysis, and simulates isotopic distributions.

3.7.1.2 Interface

There are three controls at the top of the widget. An **Add to Document** button will create a table of the current data and insert it into the document. The next button is a **Copy to Clipboard** button which will copy all data to the system clipboard for pasting (the spectrum will not be included). These buttons will only be enabled if there is available data to be handled. A **Decimals** component on the right will allow you to control the resolution of the calculations between 1 to 5 decimal places.

The rest of the interface consists of a list of data (see Figure 3.5). From top to bottom, the molecular formula, molecular mass and monoisotopic mass are listed. The elemental analysis, where each element is shown with its percent composition, is listed next. The isotopic distribution, with mass values and intensities, is listed next. Finally an interactive spectrum of the isotopic distribution is presented. You may right-click on the formula and mass values and select the Copy menu item to copy the text value to the system clipboard. The **Elemental Analysis** and **Isotopic Distribution (m/z)** text contents are selectable and you may directly copy text contents from these components as well.

3.7.1.3 Outputting calculations to the document

You can output the current calculations to the document by pressing the **Add to Document** button on the top-left of the widget. This will create and insert an editable table into the current document as shown in Figure 3.6.

Molecular Formula	$C_{21}H_{27}ClN_6O_4S$
Molecular Mass	495.00 amu
Monoisotopic Mass	494.15 amu
Elemental Analysis	
C-50.95, Cl-7.16, H-5.50, N-16.98, O-12.93, S-6.48	
Isotopic Distribution (m/z)	
494.15 (100.000%), 495.15 (25.847%), 495.16 (0.311%), 496.14 (0.020%), 496.15 (37.998%), 496.16 (2.565%), 497.14 (0.800%), 497.15 (8.793%), 497.16 (0.392%), 498.14 (1.444%), 498.15 (1.468%), 498.16 (0.065%), 499.14 (0.033%), 499.15 (0.439%), 499.16 (0.070%), 500.14 (0.011%), 500.15 (0.053%), 500.16 (0.012%)	

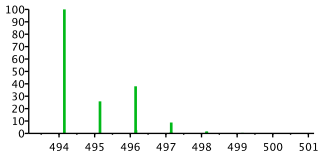


Figure 3.6: *Data output from the Elemental Analysis Widget*

3.7.1.4 Copying calculations to the system clipboard

You can copy the current calculations to the system clipboard by pressing the **Copy to Clipboard** button on the top-left of the widget. You may then paste the data into ChemDoodle or another application. The text data will appear as follows:

Molecular Formula = C21H27ClN6O4S
Molecular Mass = 495.00 amu
Monoisotopic Mass = 494.15 amu
Elemental Analysis = C-50.95; Cl-7.16; H-5.50; N-16.98; O-12.93; S-6.48
Isotopic Distribution (m/z) = 494.15 (100.000%), 495.15 (25.847%), 495.16 (0.311%), 496.14 (0.020%), 496.15 (37.998%), 496.16 (2.565%), 497.14 (0.800%), 497.15 (8.793%), 497.16 (0.392%), 498.14 (1.444%), 498.15 (1.468%), 498.16 (0.065%), 499.14 (0.033%), 499.15 (0.439%), 499.16 (0.070%), 500.14 (0.011%), 500.15 (0.053%), 500.16 (0.012%)

3.7.2 History widget

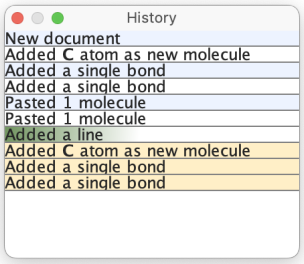


Figure 3.7: *History Widget*

3.7.2.1 Purpose

The **History** widget is an advanced undo/redo tool and provides access to the complete log of all actions performed since the document was created or opened. Click on a given action to jump back and forth to the document state when that action was performed.

3.7.2.2 Interface

The interface consists of a single list in a scrolling pane as shown in Figure 3.7. The current state of the document is signified with a green highlight over the left side of the latest action. Any actions performed earlier are undecorated and listed above the current state, while any actions that have been undone are highlighted in an amber color and are listed below the current state. By clicking on any actions above the current state, the document will revert back to that action, undoing all actions between the current state and the action clicked. By clicking on any actions below the current state, the document will redo all actions between the current state and the action clicked. Therefore, the **History** widget allows you to easily revert and restore any actions performed during the edit history of the document.

3.7.3 Line notation pad widget

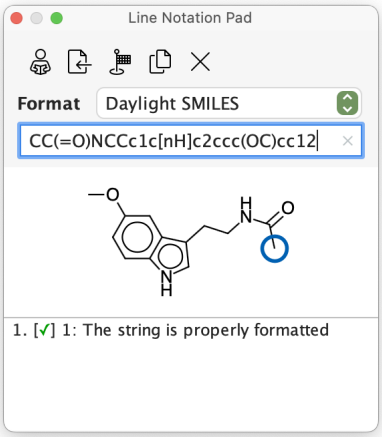


Figure 3.8: *Line Notation Pad Widget*

3.7.3.1 Purpose

The **Line Notation Pad** widget can interpret and generate *SMILES*, *SLN*, *InChI* and *ROSDAL* chemical line notation formats as well as convert between them with ease.

3.7.3.2 Interface

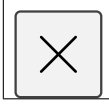
The interface for the **Line Notation Pad** widget is shown in Figure 3.8. The interface, from top to bottom, a row of buttons for performing various functions, consists of a **Format** drop-down menu, a **String** text field for inputting and outputting the line notation, the main structure panel and the input analysis list. Initially, the interface is collapsed. Type in a line notation in the **String** text field and press the enter key to expand it.

From the **Format** drop-down menu you can choose any of the line notations available to set the current line notation format. If content is present in the text field, then that content will be converted into the new format.

The **String** text field will display the generated line notation when a structure is dropped on the main structure panel. You may also explicitly type your line notation in this component and then press the enter key or the **Read Content** button to interpret it and display the corresponding structure in the main structure panel.

The buttons at the top of the widget perform functions as described in Table 3.2 below.

Table 3.2: Line Notation Pad Widget Buttons

Icon	Function	Description
	**Read Content**	Begins a search query using the search term input into the **Search** text field and restricts it to matching the field selected in the **Format** drop-down selections.
	**Add to the Doodle Board**	Places the current structure in the main structure panel onto the current document. Alternatively, you can click on the main structure panel and drag onto the document to place it.
	**Choose Start Point**	Allows you to click on an atom in the main structure panel to denote it as the start point for the generation of the line notation. If the line notation format is canonical or if such an option is set, then setting the starting point will have no effect.
	**Copy to System Clipboard as Text**	Copies the current text in the **String** text field onto the system clipboard as plain text. For MIME-type specific clipboard contents, set the appropriate options in the **Clipboard** tab of the **Settings** window, then copy from the **Doodle Board**.
	**Clear**	Clears the current contents and collapses the widget.

The main structure panel displays the structure associated with the line notation in the **String** text field. You can generate a line notation for a structure on the **Doodle Board** by selecting the structure and then by clicking and dragging that structure onto the main structure panel of the **Line Notation Pad** widget. Structures from the main drawing panel can also be dragged onto the **Doodle Board**.

The final component of the interface is a scrollable list. Any errors or warnings perceived when interpreting the line notation will be listed here. Use these suggestions to help correct malformed strings

3.7.4 MolGrabber widget

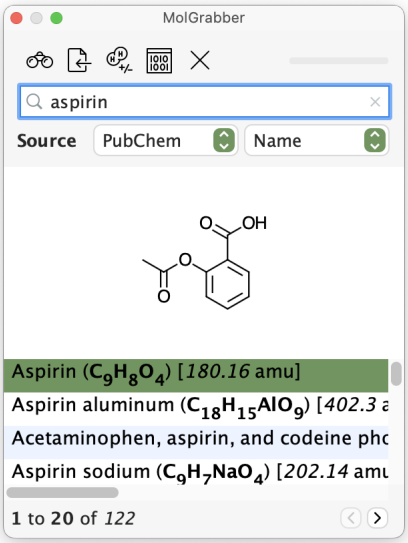


Figure 3.9: *MolGrabber Widget*

3.7.4.1 Purpose

MolGrabber is a web application for obtaining pre-drawn molecular structures and properties from online databases. The interface is shown in Figure 3.9. Currently, MolGrabber connects with the following databases:

- **ChemExper** - `http://www.chemexper.com/`
- **ChemSpider** - `http://www.chemspider.com/`
- **PubChem** - `https://pubchem.ncbi.nlm.nih.gov/`



Because MolGrabber connects to online databases, an active internet connection is required to use it.

3.7.4.2 Interface

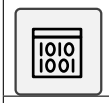
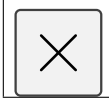
The interface for the **MolGrabber** widget consists of, from top to bottom, buttons for performing functions, a **Search** text field for inputting a search term, a **Source** drop-down selection for choosing the database to search through followed by a second drop-down selection to restrict the search, a progress bar to the top-right of these three components to notify you that a search is currently being performed, a main structure panel, a scrollable list to hold all search results and, at the bottom, statistics about the search result with traversal buttons for navigating through large numbers of results.

Initially, the interface is collapsed. Type a search term in the **Search** text field and press the enter or return key to expand it. This can be any search term that the associated database can handle. After pressing the enter or return key, the progress bar will activate to notify you it is performing the search. After the search completes, the progress spinner will deactivate, the results will populate the result list, and the first result will appear in the main structure panel.

The **Source** drop-down selection can be used to select which database to search. The second drop-down selection will restrict your search to a specific data field type supported by the database. Choose a specific field and the search will only match results in that field for the input search term.

The buttons on the top of the widget perform functions as described in Table 3.3 below.

Table 3.3: MolGrabber Widget Buttons

Icon	Function	Description
	**Search**	Begins a search query using the search term input into the **Search** text field and restricts it to matching the field selected in the **Source** drop-down selections.
	**Add to the Doodle Board**	Places the current structure in the main structure panel onto the current document. Alternatively, you can click on the main structure panel and drag onto the document to place it.
	**Show/Hide Hydrogen**	Adds and removes hydrogen atoms from the structure in the main structure panel based on the coordinates for the hydrogen atoms provided by the database. Some databases may not provide hydrogen coordinates and in those cases this function will have no effect.
	**Show Associated Data**	Displays all associated database data for the structure displayed in the main structure panel.
	**Clear**	Clears the current contents and collapses the widget.

The main structure panel will display the structure for the selected result. Once the desired structure is displayed on the main structure panel, it can be dragged and dropped onto the **Doodle Board**.

Below the main structure panel is the search result list. This list will display a maximum of 20 results with the following format for each entry:

Name (**Molecular Formula**) [*Molecular Mass amu*]

Click on any of the items in the list to display the corresponding structure in the main structure panel.

Below the search results is a label to inform you of which search results are presented in the current result set along with traversal buttons to navigate through large numbers of results. Press the left and right arrows to view the previous 20 and next 20 results respectively. If there are no previous or no next results, then the corresponding arrow will be disabled.



ChemSpider does not currently support pagination of results, so care must be taken with generic queries as they may return many, many results and may take a long time to complete.

3.7.4.3 Directing to the Online Database

After a molecule has been loaded, clicking on the **Show Associated Data** button will list associated data from that database. The top item will be the specific database ID as a hyperlink. The link will open up your default browser to the selected database's page for the current result.

3.7.4.4 Database Notes



ChemDoodle only provides an interface to the databases supported in the **MolGrabber** widget. It is important to be aware of any restrictions regarding copyrights, disclaimers and warranty information before using these databases.

3.7.4.5 ChemExper Disclaimer

https://www.chemexper.com/disclaimer.shtml

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The accuracy or reliability of the data is not guaranteed or warranted in any way and the Providers disclaim liability of any kind whatsoever, including, without limitation, liability for quality, performance, merchantability and fitness for a particular purpose arising out of the use, or inability to use the data.

3.7.4.6 ChemSpider Disclaimer

http://www.chemspider.com/Disclaimer.aspx

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Data

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Data on ChemSpider, including structures and spectra, are sourced also from individuals. In depositing these data to the ChemSpider website, these individuals undertake that they have the rights to do so, and that the rights do not reside with any third party.

3.7.4.7 PubChem User Requirements

https://pubchemdocs.ncbi.nlm.nih.gov/pug-rest

USAGE POLICY: Please note that PUG REST is not designed for very large volumes (millions) of requests. We ask that any script or application not make more than 5 requests per second, in order to avoid overloading the PubChem servers. To check additional request volume limitations, please read this document. If you have a large data set that you need to compute with, please contact us for help on optimizing your task, as there are likely more efficient ways to approach such bulk queries.

3.7.5 Multiplet tool widget

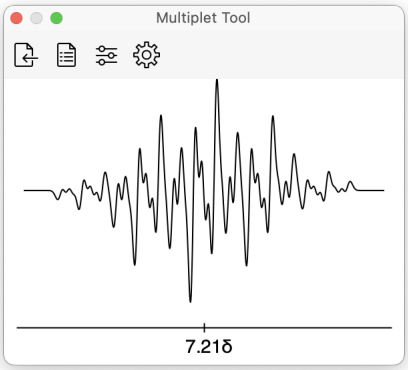


Figure 3.10: *Multiplet Tool Widget*

3.7.5.1 Purpose

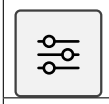
The **Multiplet Tool** widget is a comprehensive tool for generating multiplet trees, simulating signals and producing their figures. It is perfectly suited for simulating nuclear magnetic resonance (NMR) or electron paramagnetic resonance (EPR, aka ESR) signals. The interface is shown in Figure 3.10.

3.7.5.2 Interface

The interface for the **Multiplet Tool** widget consists of, from top to bottom, a row of buttons for performing various functions and the main multiplet panel.

Use the buttons to set up the simulation and layout of the multiplet. The buttons perform functions as described in Table 3.4.

Table 3.4: Multiplet Widget Buttons

Icon	Function	Description
	**Add to the Doodle Board**	Places the current multiplet from the main multiplet panel into the current document.
	**Input Parameters**	Pops up a window for you to define parameters for the simulation including the number of neighboring nuclei, their spin and coupling magnitude.
	**Real-Time Sliders**	Provides a window with sliders for each parameter. Changing the sliders will affect the simulation in real time.
	**Settings**	Displays a window to define how the simulation is performed and how the multiplet figure is laid out and displayed.

After completing your simulation, drag and drop the multiplet from the main multiplet panel onto the **Doodle Board**.

3.7.5.3 Simulating Multiplets

To simulate multiplets, define the parameters in the **Input Parameters** window that appears after clicking the **Input Parameters** button and then click the **Calculate** button as shown in Figure 3.11. Press the reset button in this window to reset all parameters.

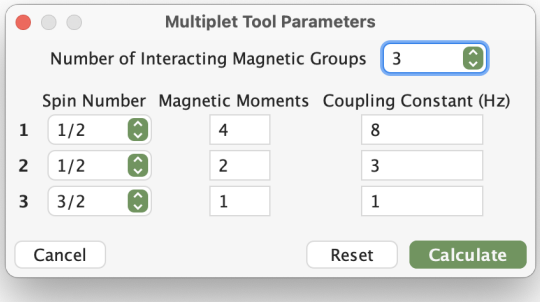


Figure 3.11: *Multiplet Input Parameters*

To tweak the input parameters to analyze their effect on the simulation, use the **Real-Time Sliders** button and change the values slowly in the window that appears as shown in Figure 3.12. When you are satisfied with the simulation, press the **Accept** button. The **Reset** button will reset the parameters to their initial values before the window was opened.

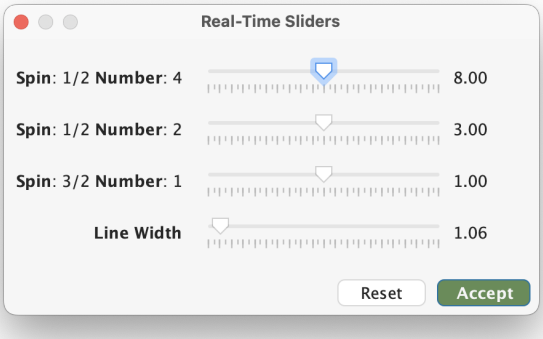


Figure 3.12: *Multiplet Real-Time Sliders*

3.7.5.4 Setting up the Multiplet Figure

To define how the simulation is performed and how the multiplet figure is displayed, click on the **Settings** button to display the **Multiplet Settings** window (see Figure 3.13).

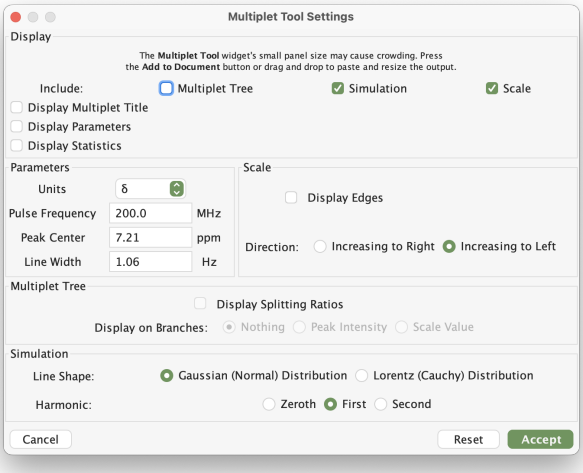


Figure 3.13: *Multiplet Settings*

3.7.5.5 Editing Multiplets from the Doodle Board

To edit a multiplet from the **Doodle Board**, select it and then drag and drop it onto the main multiplet panel in the **Multiplet Tool** widget. A copy will be made and can be edited using the **Multiplet Tool** widget. Add this new edited multiplet to the **Doodle Board** and delete the old one.

3.7.5.6 Memory and Runtime Issues

A nucleus of any spin may be used, including hypothetical spins, however more complex simulations require more memory and processor power leading to longer runtimes. Some extremely complex simulations may encounter memory issues.

3.7.6 NMR SIMULATION WIDGET

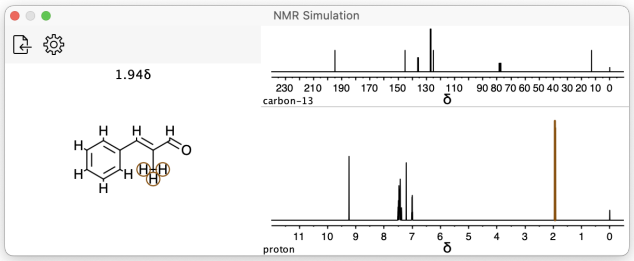


Figure 3.14: *NMR Simulation Widget*

3.7.6.1 PURPOSE

The **NMR Simulation** widget simulates ^{1}H and ^{13}C nuclear magnetic resonance and also associates peaks with nuclei. Full information about each simulation is provided for in-depth analysis.

3.7.6.2 INTERFACE

The interface for the **NMR Simulation** widget is shown in Figure 3.14. The interface consists of the main structure panel above which are two buttons for performing various functions, and to the right is a set of panels for displaying the simulated NMR spectra with ^{13}C displayed on top and ^{1}H displayed on the bottom.

The main structure panel displays the structure being analyzed and is interactive. The spectra are also interactive and display the simulation results. Use the buttons to set up the simulation and copy content to the **Doodle Board**. The buttons perform functions as described in Table 3.5.

Table 3.5: NMR Simulation Widget Buttons

Icon	Function	Description
	**Add to the Doodle Board**	Places both the simulated ^{1}H and ^{13}C spectra onto the current document.
	**Settings**	Displays a window to define how the simulation is performed.

3.7.6.3 SIMULATING NMR

To simulate NMR spectra for a structure, drag and drop that structure from the **Doodle Board** onto the **NMR Simulation** widget's main structure panel. Make sure to completely drag the desired structure out of the document window first, so a drag event is initiated, before dropping on the **NMR Simulation** widget. The ^{1}H and ^{13}C NMR spectra are instantly generated and displayed.

All variables for the simulation can be customized. To define the variables, click on the **Settings** button to display a window containing the parameters, as shown in Figure 3.15.

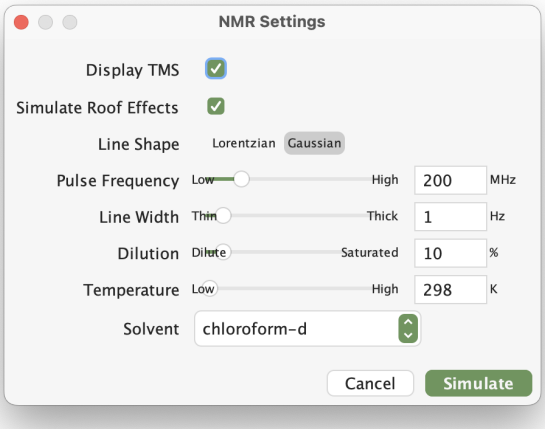


Figure 3.15: *NMR Simulation Settings*

When you are finished defining the variables, click the **Simulate** button to recalculate the spectra. Adjust these parameters to match an experimental spectrum for correlated figures on the **Doodle Board**. Settings include:

- **TMS** - Display or hide the reference peak.
- **Roof Effects** - Simulate roof effects.
- **Line Shape** - Lorentzian or Gaussian.
- **Pulse Frequency** - The spectrum resolution. The value is appropriate for ^{1}H NMR. ^{13}C NMR will be simulated to a resolution of a quarter of this value to remain consistent with experimental spectrometers.
- **Line Width** - Control the line width.
- **Dilution** - Affect the solvent/solute intensity ratio.
- **Temperature** - Change the simulation temperature.
- **Solvent** - Choose a solvent. Splitting is fully calculated with the appropriate spin of the nuclei (Deuterium has a spin of 1 and you will see this splitting correctly in the solvent peaks).

3.7.6.4 Analyzing the Results

The spectra are completely interactive. You can easily change the view of the spectrum by clicking and dragging to zoom in on the x-axis. Double clicking on the spectrum will revert it to the full view. Scrolling will change the scale of the y-axis.

Peaks and nuclei are hoverable. Hovering over a peak will highlight the corresponding nuclei and vice versa. The chemical shift of the nuclei is displayed above the structure in the main structure panel.

Clicking on a highlighted peak or nuclei set will display further data from the simulation, including the shift prediction, splitting nuclei and j-constant predictions as shown in Figure 3.16.

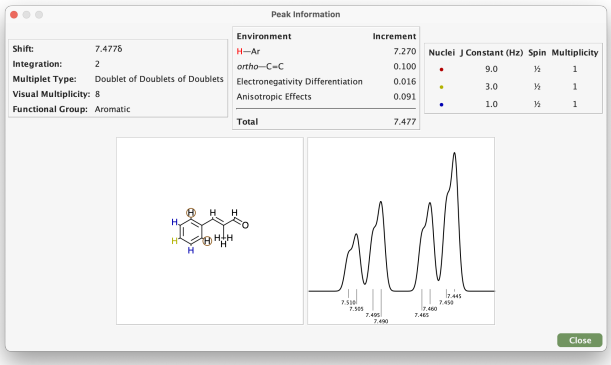


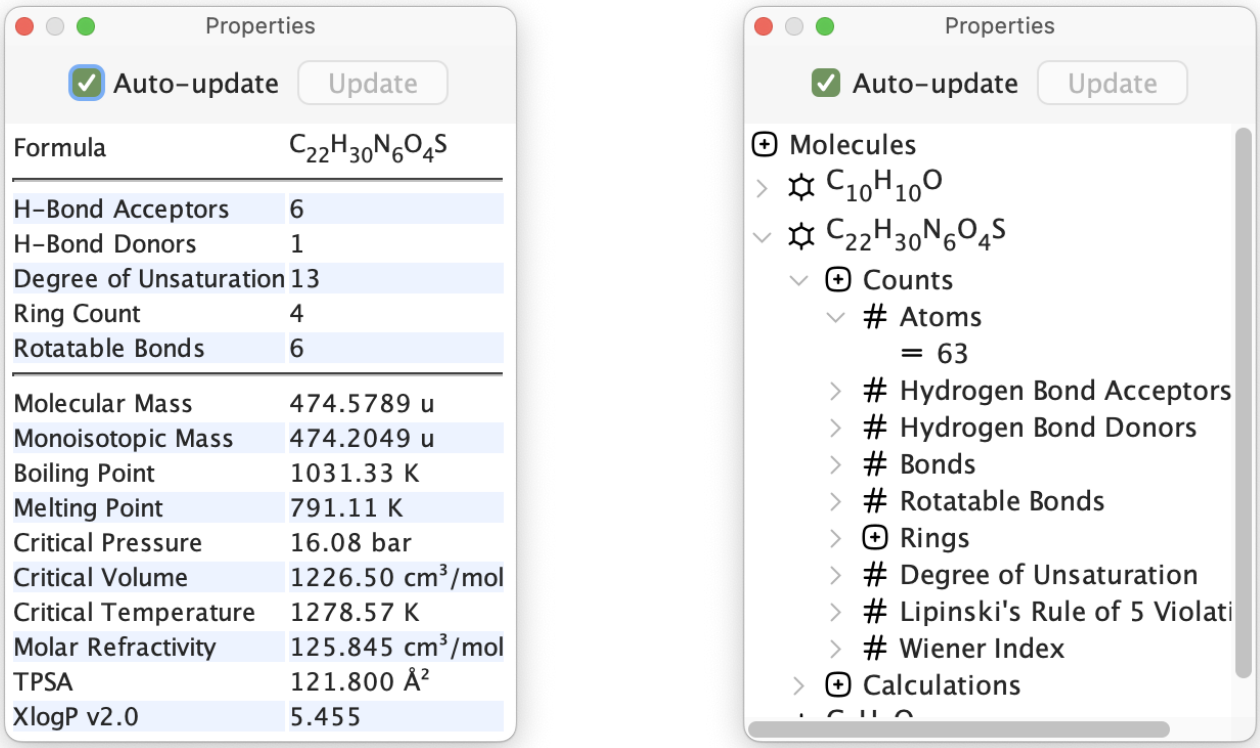
Figure 3.16: *In-depth Simulation Information*

The **NMR Simulation** widget is initially small to conserve space. But as with all widgets, you can resize or maximize them if you desire more interaction space.

3.7.6.5 How NMR is Simulated

The simulations in the **NMR Simulation** widget are based on empirical algorithms, with a database of incremental constants compiled from publications and some unpublished work. These references are listed by clicking the **References** menu item in the **Help** menu. Further information on the algorithms used to simulate NMR is provided in the SPECTRA chapter.

3.7.7 Properties widget



(a) *Single Molecule* (b) *Multiple Molecules*

Figure 3.17: *Properties Widget Interface*

3.7.7.1 Purpose

The **Properties** widget calculates and displays descriptors for molecules. There are two unique interfaces displayed by the **Properties** widget depending on the situation. First, make sure the **Properties** widget is open and visible. If only a single molecule is being drawn or if a single molecule is selected, a table will be displayed. Otherwise, a drop-down tree will be presented to show data for each of the selected molecules, if any. The **Properties** widget will automatically update to reflect any changes if the **Auto-update** box is checked. The interface displayed when a single molecule is being edited is shown in Figure 3.17a, and the interface displayed when multiple molecules are selected is shown in Figure 3.17b.

3.7.7.2 Interface

The interface consists of a checkbox and button at the top that control when the widget updates and the data component at the bottom which displays a table or drop-down tree depending on the situation.

The table is non-interactive and only displays the most important information. For multiple selected molecules, a tree will be displayed. To use the tree, click the arrow to the left of each item, or double click on the item to expand it.

When the **Auto-update** checkbox is selected, the **Properties** widget will refresh automatically when any content is changed. Deselect the checkbox to improve drawing performance when handling large molecules. When the **Auto-update** checkbox is deselected, the **Update** button will be enabled to manually control when the widget refreshes.

Currently, the **Properties** widget calculates the following properties for each molecule:

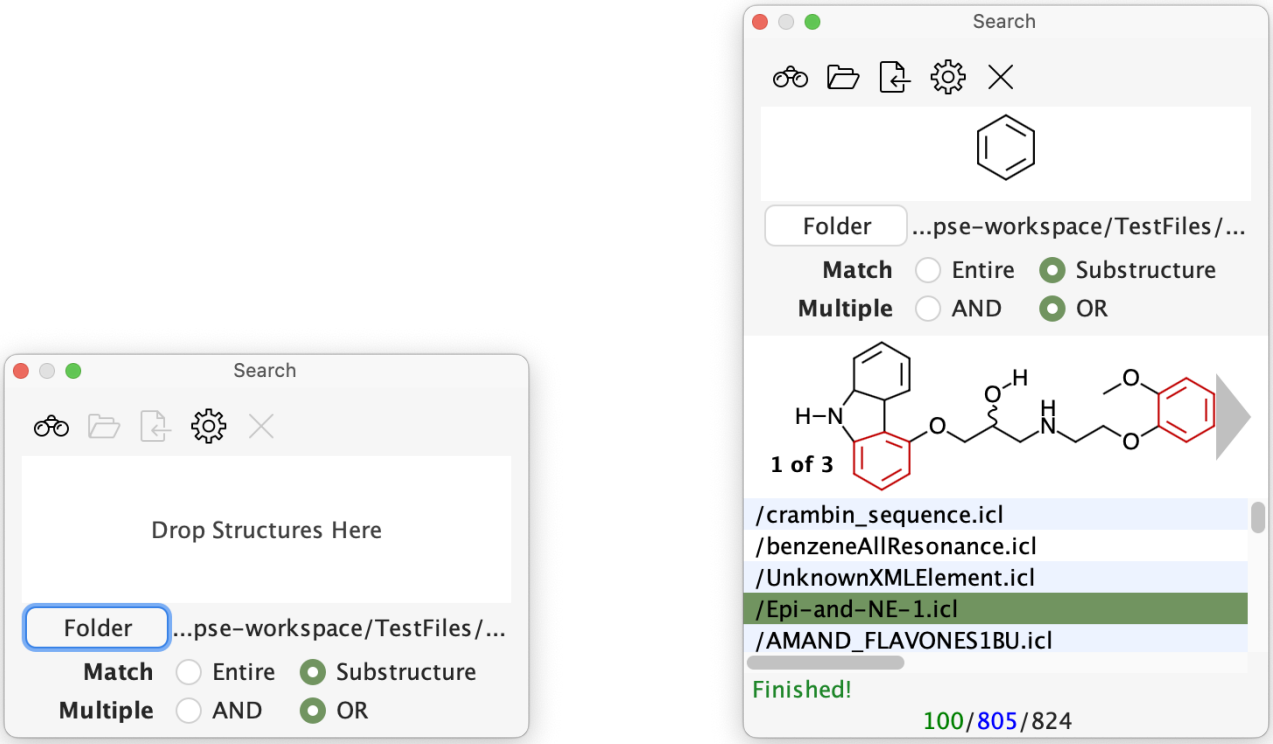
- Molecular Formula
  - Counts

        * Atoms
        * Bonds
        * Rings
            · Frèrejacque Number
            · All Rings
        * Hydrogen Bond Acceptors
        * Hydrogen Bond Donors
        * Degree of Unsaturation
        * Lipinski's Rule of 5 Violations
        * Wiener Index
    – Calculations
        * Molar Refractivity
        * Topological Polar Surface Area
        * XlogP v2.0
        * Mass
            · Molecular
            · Monoisotopic
            · Elemental Composition

To copy content from the **Properties** widget, right-click on any item and choose the **Copy** menu item.

It may take quite a few clicks to access information through the **Properties** widget. For quicker access to all molecular descriptors, use the Structure » Descriptors menu.

3.7.8 Search widget



(a) *Before a search* (b) *After a search*

Figure 3.18: *Search Widget Interface*

3.7.8.1 Purpose

The **Search** widget allows you to search your hard drive and any attached storage devices for chemical structures. The **Search** widget recognizes all formats that ChemDoodle understands, so you will be able to find the old files you thought you lost a long time ago and edit them in ChemDoodle.

3.7.8.2 Interface

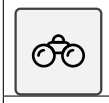
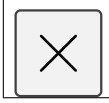
The **Search** widget interface is shown in Figure 3.18b. The interface consists of, from top to bottom, a row of buttons for various functions, a drop panel to drop the structures to be searched for and to notify you that a search is currently being performed, a **Folder** button to select the root directory of the search, **Match** and **Multiple** options to define how the search is performed, the main structure panel to view results, a list of search results and then labels to notify you of search progress.

The top section will allow you to select a root folder for the search. Click on the **Folder** button and use the file chooser that appears to select a folder. Be as exclusive as possible when choosing a root folder, as searching your entire hard drive can take a very long time and may cause memory issues. The **Match** and **Multiple** options will affect how the search is performed. Setting **Match** to **Entire** will guarantee that all results are exact matches of the query structures, while selecting **Substructure** will match any structures where the query structures are matched exactly or contained within larger structures. Setting **Multiple** to **AND** will ensure that all query structures are matched in a file for that file to be considered a result, while selecting **OR** will allow any matched query structure to qualify the file as a result.

Initially, the interface is collapsed (Figure 3.18a). Drag and drop a structure or group of structures from the **Doodle Board** onto the drop panel to expand it and set the query structure content. Make sure to completely drag the desired content out of the document window first, so a drag event is initiated, before dropping on the **Search** widget.

The buttons on the top of the widget perform functions as described in Table 3.6 below.

Table 3.6: Search Widget Buttons

Icon	Function	Description
	**Search**	Begins the search query using the query structure(s) dropped onto the **Search** widget's main panel with the specified search options.
	**Open**	Opens the currently selected document on the **Doodle Board**.
	**Add to the Document**	The **Add to Document** button adds the structure, without the highlighted red hit, to the document. In contrast, dragging the structure from the main structure panel and dropping it in the document yields the structure as shown in the main structure panel, with the highlighted red hit.
	**Settings**	Allows you to control search parameters and improve performance.
	**Clear**	Clears the current contents and collapses the widget.

While the search is being performed, a pulsing stop sign will become visible on the top panel to notify you of search progress. Clicking on the stop sign will terminate the search. At the bottom of the interface are two labels. The first label names the file currently being searched, and will display Finished! when completed. The second label displays statistics about the files searched from the onset of the search. The statistics have the following format:

Files Matched/Chemical Files Searched/Total Files Searched



Be careful with the search! Searching large numbers of files may cause ChemDoodle to run out of memory, causing ChemDoodle to respond slowly. Choose the root search folder and the search settings described in the next section with care.

Once the search is completed, all matched files will be listed in the results list. Click on any result to view all the structures in that file, one at a time, in the main structure panel. All hits are highlighted in red. If a file contains multiple structures, clicking the gray arrows appearing to the left and right of the structure will allow you to browse through them. The total number of structures in the file is noted at the bottom left of the main structure panel. Once you have found the structure you were looking for, drag and drop the structure from the main structure panel onto the **Doodle Board**. You can also use the **Open** button  at the top of the widget to open the entire file on the **Doodle Board**.

3.7.8.3 Search Settings

Search parameters can be defined by clicking on the **Settings** button  at the top of the widget. A window with the options will appear as shown in Figure 3.19.

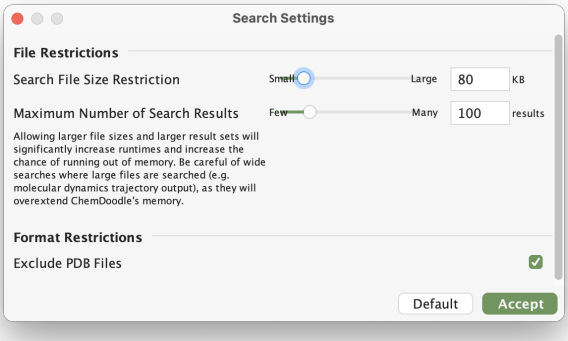


Figure 3.19: *Search Settings for the Search Widget*

There are currently three options:

1. **Search File Size Restriction** - This value determines the maximum file size that the **Search** widget will include in its search, to avoid memory issues.

2. **Maximum Number of Search Results** - This value will control the maximum number of search results. The search will continue until all the files in the selected root search folder are visited or when this maximum result value is reached. Keeping it low and providing smaller root search folders will avoid runtime and memory issues.

3. **Exclude PDB Files** - Many times, *PDB* files are very large and contain molecular dynamics trajectories or Monte Carlo distributions. To avoid all of these files and the subsequent runtime and memory issues, keep this option selected. If you need to search through *PDB* files, turn this option off.

3.7.9 Statistics widget

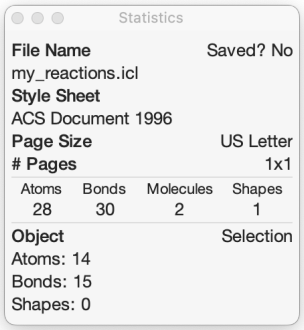


Figure 3.20: *Statistics Widget*

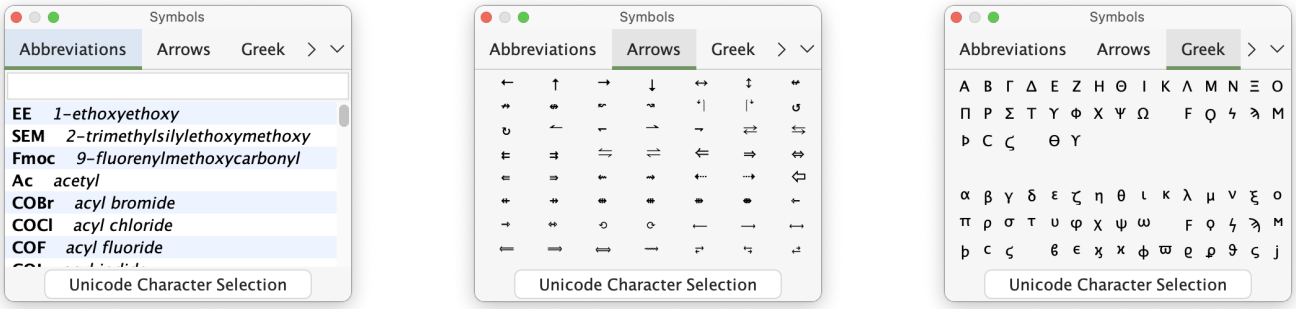
3.7.9.1 Purpose

The **Statistics** widget will display information about the current document and hovered or selected items. Use the widget to quickly gain insight into the state of your document and work.

3.7.9.2 Interface

The interface is separated into three sections as shown in Figure 3.20. The top section displays information about the document, the middle section displays information about the content, and the final section displays specific information about hovered or selected objects.

3.7.10 Symbols widget



(a) *Abbreviations Tab* (b) *Arrows Tab* (c) *Greek Letters Tab*

Figure 3.21: *Symbols Widget*

3.7.10.1 Purpose

The **Symbols** widget is a complement to the **Labels** toolbar. This widget contains an abbreviation library, arrows, Greek letters and many other symbols. A few selected tabs are shown in Figures 3.21.

3.7.10.2 Interface

The content in the **Symbols** widget is small and may be difficult to read. As can be seen in Figure 3.22, hovering over any symbol will show a larger preview at the top left hand corner of the widget. Hovering for a few seconds will also display a tooltip description.



Figure 3.22: *Symbol Preview*

When abbreviations are chosen, you may modify atoms as you would using the element label tools. Other symbols, such as arrows may not be used directly as atom labels. However, you can open up an atom label text field, and then press the symbol button to input the symbol. If you are modifying any text component, clicked symbols will be inserted into the component's content at the cursor position.

If you set an atom's label to one that is not recognized or parsed by ChemDoodle, an unrecognized warning will appear. You may dismiss this warning or edit the current list of abbreviations to allow unrecognized tokens by selecting the Structure 〉 Abbreviations 〉 Add New... menu item.

3.7.10.3 Expanded Unicode Range

All possible symbols available through unicode are accessible in the **Symbols** widget, even if they are not displayed immediately in the tab sets. Click the **Unicode Character Selection** button at the bottom of the widget to view the unicode character

selector shown in Figure 3.23.

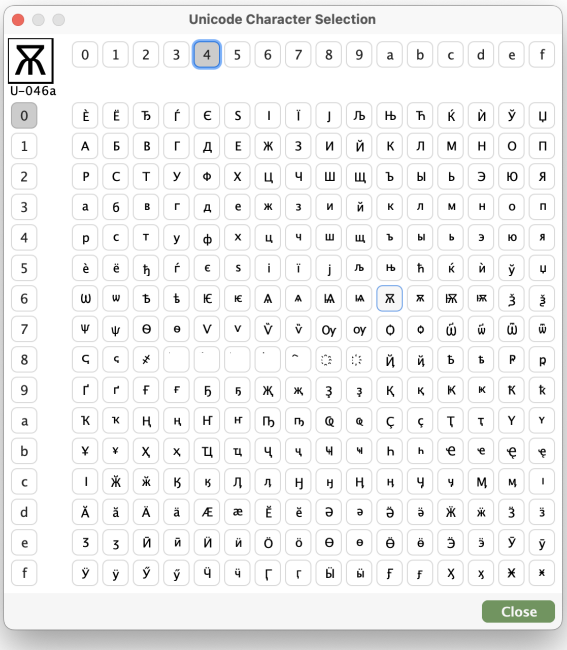


Figure 3.23: *The Unicode Character Selector*

Using hex, you can traverse the entire unicode range and easily insert any desired symbols into text components. Note that not all fonts will have character glyphs assigned to each hex value. In these cases, a blank space or empty rectangle will appear in your text component and in the unsupported symbol button.



Some programs use the Symbol font to display symbols. This is an archaic solution and the standard is to now use unicode characters, which ChemDoodle fully supports. ChemDoodle will try to recognize and correct such cases when reading in files from other programs.

3.7.11 Templates widget

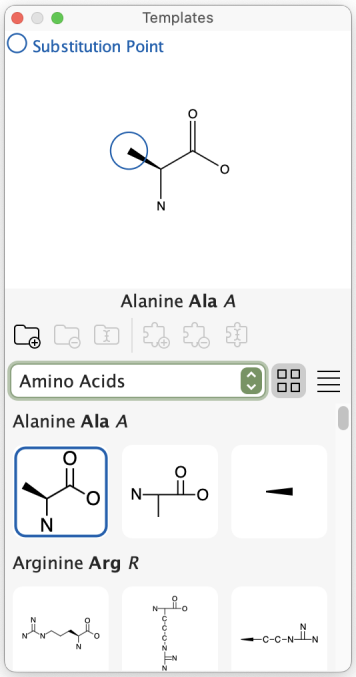


Figure 3.24: *Templates Widget*

3.7.11.1 Purpose

The **Templates** widget organizes your created templates along with predefined templates from iChemLabs and allows you to easily use them. The interface is shown in Figure 3.24.

3.7.11.2 Interface

The interface consists of, from top to bottom, a main structure panel, the name of the current template, a row of buttons for controlling the templates and template sets, a drop down selection for selecting a template set next to a choice to show how the templates are listed, and finally a scrollable list/tiles where you select a template.

The main structure panel displays the currently selected template. A default substitution atom will be defined, but you may change the substitution atom to another by clicking on a different atom. The substitution point is the atom that will be overlapped with the atom in the document the template is being connected to. Note that selecting the substitution point does not place the template into the document, you will still need to follow the directions in DRAWING CHEMICAL STRUCTURES to use the template.

The template group drop-down selection will allow you to select a set of templates to browse. After selecting a template set, the template list/tiles will populate with templates from that set. Choosing **Tile** will organize the templates as graphics, while choosing **List** will list the available templates as text items. Click on a template to display it in the main structure panel for use.

The buttons above the drop-down selection perform functions as described in Table 3.7 below.

Table 3.7: Template Widget Buttons

Icon	Function	Description
	**Create Template Set**	Adds a new template set after requesting a name for the set.
	**Remove Template Set**	Removes the currently selected template set and all of the templates contained in the set. This action cannot be undone. This function is not available for the predefined sets from iChemLabs.
	**Rename Template Set**	Prompts you for a new name to rename the currently selected template set. This function is not available for the predefined sets from iChemLabs.
	**Add Template**	Creates a new template from the current selection in the document and adds it to the currently selected template set. Templates may not be added to the predefined sets from iChemLabs.
	**Remove Template**	Removes the currently selected template from the template set. This action cannot be undone. Templates may not be removed from the predefined sets from iChemLabs.
	**Update Template**	Prompts you for a new name to rename the currently selected template. If there is currently a selection in the document, you will also be able to replace the current template data with the content selected in the document. Templates from the predefined sets from iChemLabs may not be updated.

3.7.11.3 Using Templates

Drawing with templates, creating and editing templates, and managing template sets is discussed in detail in DRAWING CHEMICAL STRUCTURES.

3.7.12 TLC CANVAS WIDGET

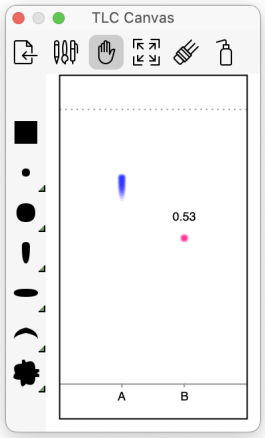


Figure 3.25: *TLC Canvas Widget*

3.7.12.1 PURPOSE

The **TLC Canvas** widget provides a tool for creating graphics of thin-layer chromatography (TLC) plates. The interface is shown in Figure 3.25.

3.7.12.2 INTERFACE

The interface consists of, from left to right, a column of buttons for spot types and the main TLC panel for drawing the TLC plate. Above them both are a row of buttons for performing various functions.

The top button in the spot type column sets the color of spots. Beneath the color button are six different shapes of spots:

- **Compact Spot** - a small dot
- **Expanded Spot** - a circle
- **Trailing Spot** - a small dot with a trail
- **Widened Spot** - an oval aligned horizontally
- **Crescent Spot** - a crescent shape with bowl facing downwards
- **Custom Spot** - a splatter shape that can be changed

Click on any of the spot types to set the drawing mode to place the spot.

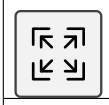
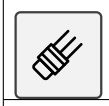
Each spot button is a group button. Expand the group button for more spot styles. For each spot there are three spot styles:

- **Solid Style** - Solid throughout
- **Empty Style** - Just a line border
- **Diffuse Style** - Gradient from the center to the edges

The main TLC panel contains the TLC plate being drawn. You can edit it using the controls at the top of the widget. When finished editing the TLC plate, use the **Add to Doodle Board** button  to place it on the **Doodle Board**.

The top button row contains function buttons to control how to edit the TLC plate. The buttons perform functions as described in the table below.

Table 3.8: TLC Plate Widget Buttons

Icon	Function	Description
	**Add to the Doodle Board**	Places the current TLC plate in the main TLC panel onto the current document.
	**Styles**	Pops up a window to edit the styles of the TLC plate.
	**Move**	Allows you to translate spots along their lanes and allows you to move the origin and solvent front.
	**Resize Spots**	Displays the anchor points for all spots and allows you to click and drag them to alter spot shapes.
	**Delete**	Allows you to remove spots by clicking on them and allows you to delete lanes by clicking on the lane tick at the origin.
	**Clear**	Removes all spots, leaves a single lane, and resets the origin and solvent front.

3.7.12.3 Drawing TLC Plates

There are 13 buttons associated with the TLC Canvas. The controls on the left are the simplest. The top button is the color of the spots; click it to choose a different color. The rest of the buttons in that column correspond to spot shapes. These are the compact, expanded, trailing, widened, crescent and custom spots, in that order. Click on a spot button, then hover over the TLC plate for a preview and R_f calculation. Once you are satisfied with a location, click to place the spot. You can create new lanes by placing spots in between or outside of the existing lanes.

These spot buttons are group buttons and more spot styles will appear when hovered. All of the spots can be initialized with a solid, hollow or gradient style. The gradient styled spots most closely represent actual spots.

Using the **Move** button  , you hover over spots to highlight them, and then click and drag to move them along their lanes. R_f values are displayed while you move spots. You may also click and drag the origin and solvent front to move them, preserving R_f values.

When spots are hovered, you can right click on them to open a popup menu with the following functions:

- **Duplicate Spot** - Will produce a duplicate spot of the hovered spot, underneath the hovered spot in the same lane.
- **Remove Spot** - Will delete the spot.
- **Format Spot...** - Opens the **Format Spot** window.

The Format Spot window will provide several options for precisely defining its color, style, display settings and position as shown in Figure 3.26.

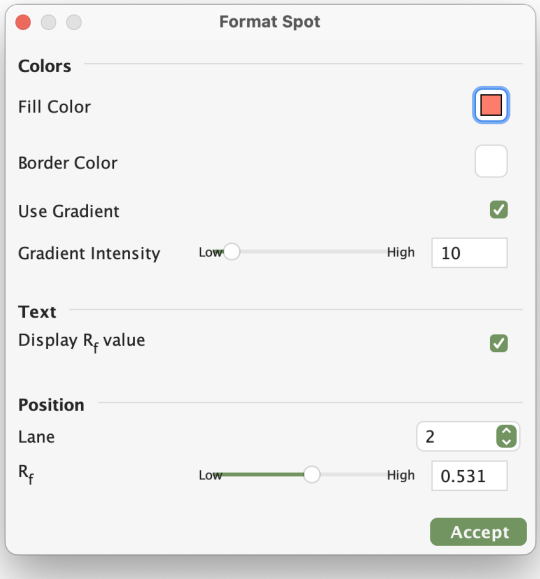


Figure 3.26: *Format Spot Window*

To resize and reshape spots on the TLC plate, use the **Resize Spots** button  . Hover over the control points that appear, and then click and drag to move them. All spots except the custom spot are defined by 4 control points. You may move all four to create different shapes. The custom spot is unique and is defined by eight control points. You may use custom spots to create much more complicated shapes.

To remove spots and lanes, use the **Delete** button  . Hover over spots to highlight them, then click to remove them. You may delete a lane by clicking its lane tick at the origin. Deleting a lane will also delete its contained spots. To clear and reset the entire TLC plate, click the **Clear** button  .

3.7.12.4 Editing TLC Plates from the Doodle Board

To edit a TLC plate from the **Doodle Board**, select it and then drag and drop it onto the main TLC panel in the **TLC Canvas** widget. Make sure to completely drag the TLC object out of the document window first, so a drag event is initiated, before dropping on the **TLC Canvas** widget. A copy will be made and can be edited. Add this new edited TLC plate to the **Doodle Board** and delete the old one.

CHAPTER 4

Drawing Chemical Structures

Contents

4.1 Overview . . . **106**

4.2 Keyboard shortcuts . . . **106**
- 4.2.1 Menu accelerators . . . 106
- 4.2.2 Tool shortcuts . . . 107
- 4.2.3 Drawing shortcuts . . . 107
- 4.2.4 Shortcut list . . . 107

4.3 Hovering . . . **108**

4.4 Cancelling drawing actions . . . **109**

4.5 Atoms . . . **109**
- 4.5.1 Placing carbon atoms . . . 109
- 4.5.2 Placing other elements . . . 109
- 4.5.3 Placing atoms with non-elemental labels . . . 109
- 4.5.4 Hovering atoms . . . 110
- 4.5.5 Selecting atoms . . . 110
- 4.5.6 Changing atom labels to other elements . . . 110
- 4.5.7 Sprouting bonds to labels . . . 111
- 4.5.8 Changing atom labels to non-elemental text . . . 111
- 4.5.9 Repeating the most recently typed atom label . . . 111
- 4.5.10 Moving an atom . . . 111
- 4.5.11 Deleting an atom . . . 111

4.6 Carbon labels . . . **112**
- 4.6.1 Terminal carbon labels . . . 112

4.7 Deuterium and Tritium labels . . . **113**

4.8 Chemical labels . . . **113**
- 4.8.1 Label toolbar . . . 113
- 4.8.2 Atom label token stacking . . . 113
- 4.8.3 Subtoken alignment . . . 114
- 4.8.4 Atom label orientation . . . 115
- 4.8.5 Formatting atom labels . . . 115

4.9 Bonds . . . **116**
- 4.9.1 Single bonds . . . 116
- 4.9.2 Placing bonds other than single bonds . . . 117
- 4.9.3 Optimize zone . . . 117
- 4.9.4 Placing bonds with fixed lengths and angles . . . 117
- 4.9.5 Placing bonds at non-fixed lengths . . . 117
- 4.9.6 Placing bonds at non-fixed angles . . . 117
- 4.9.7 Placing bonds at non-fixed lengths and non-fixed angles . . . 117
- 4.9.8 Connecting two atoms with a new bond . . . 118
- 4.9.9 Hovering bonds . . . 118
- 4.9.10 Selecting bonds . . . 118
- 4.9.11 Changing a bond type . . . 118
- 4.9.12 Changing selected bonds to single bonds . . . 119
- 4.9.13 Incrementing a bond order . . . 119
- 4.9.14 Deleting a bond . . . 119
- 4.9.15 Decrementing a bond order . . . 119

4.9.16 Deleting bonds around atoms . . . 119

4.10 Chains . . . **120**
4.10.1 Placing chains at fixed angles . . . 120
4.10.2 Placing chains at non-fixed angles . . . 120
4.10.3 Forcing the placement of chains vertically and horizontally . . . 121
4.10.4 Inverting linear chains . . . 121

4.11 Rings . . . **121**
4.11.1 Placing a ring . . . 121
4.11.2 Optimize zone . . . 122
4.11.3 Placing rings with fixed lengths and angles . . . 122
4.11.4 Placing rings at non-fixed lengths . . . 122
4.11.5 Placing rings at non-fixed angles . . . 122
4.11.6 Placing rings at non-fixed lengths and non-fixed angles . . . 122
4.11.7 Adding rings to bonds . . . 123
4.11.8 Adding rings of any size . . . 123
4.11.9 Adding crowns of any size . . . 123
4.11.10 Unsaturated ring fusing . . . 123

4.12 Templates . . . **124**
4.12.1 Selecting a template for use . . . 124
4.12.2 Placing a template . . . 125
4.12.3 Optimize zone . . . 125
4.12.4 Placing templates with fixed lengths and angles . . . 125
4.12.5 Placing templates at non-fixed lengths . . . 125
4.12.6 Placing templates at non-fixed angles . . . 125
4.12.7 Placing templates at non-fixed lengths and non-fixed angles . . . 126
4.12.8 Managing your templates . . . 126
4.12.8.1 Creating a template set . . . 126
4.12.8.2 Removing a template set . . . 126
4.12.8.3 Renaming a template set . . . 126
4.12.9 Adding a new template . . . 127
4.12.10 Removing a template . . . 127
4.12.11 Renaming a template . . . 127
4.12.12 Updating a template . . . 128

4.13 Attributes . . . **129**
4.13.1 Hovering attributes . . . 129
4.13.2 Selecting attributes . . . 129
4.13.3 Auto-placement of attributes . . . 129
4.13.3.1 Overriding the auto-placement . . . 130
4.13.3.2 Resetting the auto-placement . . . 130
4.13.4 Moving attributes . . . 130
4.13.5 Removing attributes . . . 131
4.13.6 Charges . . . 131
4.13.6.1 Adding charges . . . 131
4.13.6.2 Incrementing and decrementing charges . . . 131
4.13.6.3 Removing charges . . . 131
4.13.6.4 Placing circles around charges . . . 132
4.13.6.5 Negative charge symbol length . . . 132
4.13.7 Symbols . . . 132
4.13.7.1 Adding symbols . . . 133
4.13.8 Incrementals . . . 133
4.13.8.1 Adding incrementals . . . 134

4.13.8.2 Resetting the incrementation . . . 134
4.13.9 Custom attributes . . . 134
4.13.9.1 Adding custom attributes . . . 134
4.13.9.2 Editing custom attributes . . . 135

4.14 Isotopes . . . **135**
4.14.1 Setting published isotope mass numbers . . . 135
4.14.2 Setting arbitrary isotope mass numbers . . . 136
4.14.3 Removing mass numbers . . . 136

4.15 Nuclear Notation . . . **136**

4.16 Orbitals . . . **137**
4.16.1 Placing orbitals at fixed lengths and angles . . . 138
4.16.2 Placing orbitals at non-fixed lengths or angles . . . 138
4.16.3 Forcing orbitals to be drawn vertically and horizontally . . . 138
4.16.4 Moving orbitals . . . 138
4.16.5 Resizing orbitals . . . 138
4.16.6 Removing orbitals . . . 138

4.1 Overview

This chapter introduces the new user to the basic structure drawing tools within ChemDoodle. The topics covered in this chapter include:

- Atoms
- Chemical labels
- Bonds and bond orders
- Chains
- Rings
- Templates
- Attributes, including symbols, charges and isotope values
- Isotopes
- Orbitals

4.2 Keyboard shortcuts

4.2.1 Menu accelerators

You can use menu accelerators to quickly access menu item functionality using keyboard shortcuts. For instance pressing the ctrl + S keys (command + S on macOS) will attempt to save all content in the current document to your filesystem. While menu accelerators are assigned by default, you can edit them by selecting the Window > Edit Shortcuts menu item. An image of this interface is shown in Figure 4.1.

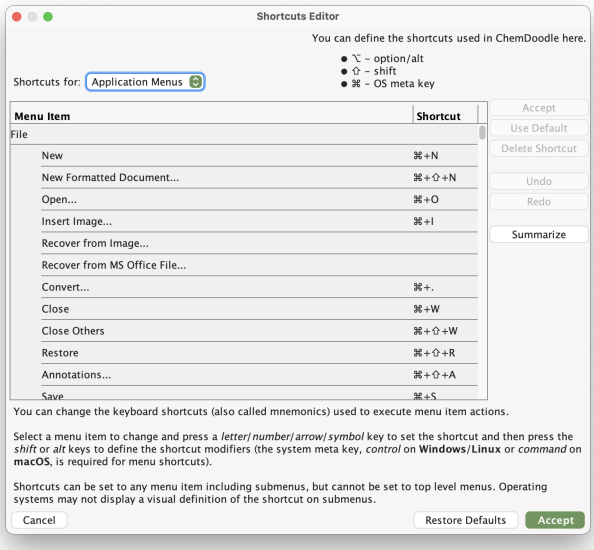


Figure 4.1: *Customizing menu accelerators*

4.2.2 Tool shortcuts

Many drawing tools are assigned tool shortcuts, which will change the drawing mode to that tool when the corresponding key is pressed. For instance, pressing the S key will change the drawing mode to the lasso tool for selection and editing. While tool shortcuts are assigned by default, you can edit them by selecting the Window > Edit Shortcuts menu item and then selecting **Shortcuts for: Tools** in the drop down. An image of this interface is shown in Figure 4.2.

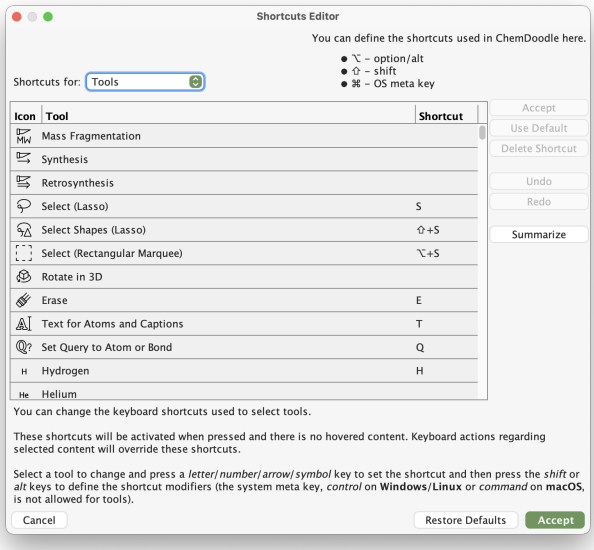


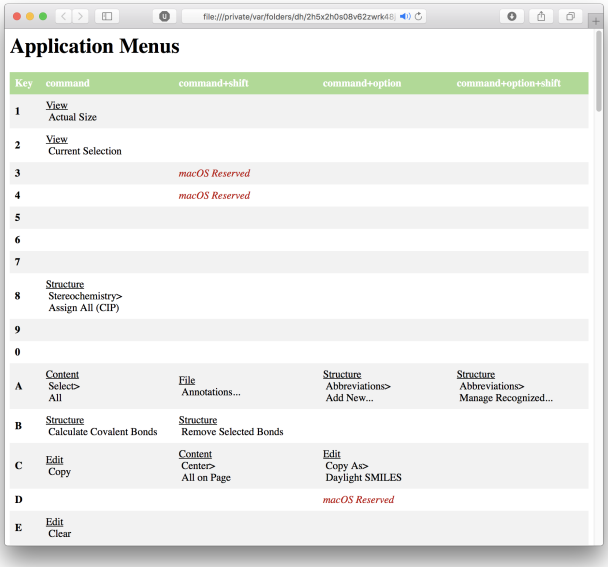
Figure 4.2: *Customizing tool shortcuts*

4.2.3 Drawing shortcuts

There are many keyboard shortcuts associated to specific content editing actions to help you draw structures quickly and efficiently. For instance, hovering a bond and pressing the 2 key will change that bond into a double bond. We will note these keyboard shortcuts when describing the different actions for drawing molecules in this chapter.

4.2.4 Shortcut list

A table of available menu accelerators and tool shortcuts, as assigned by default and by you, is provided by clicking the **Summarize** button in the **Shortcuts Editor** window shown in Figure 4.1. A webpage with tables for these shortcuts will appear in your default browser and can then be used directly for reference or printing as shown in Figure 4.3.



Application Menus

Key	command	command+shift	command+option	command+option+shift
1	View Actual Size			
2	View Current Selection			
3		*macOS Reserved*		
4		*macOS Reserved*		
5				
6				
7				
8	Structure Stereochemistry> Assign All (CIP)			
9				
0				
A	Content Select> All	File Annotations...	Structure Abbreviations> Add New...	Structure Abbreviations> Manage Recognized...
B	Structure Calculate Covalent Bonds	Structure Remove Selected Bonds		
C	Edit Copy	Content Center> All on Page	Edit Copy As> Daylight SMILES	
D			*macOS Reserved*	
E	Edit Clear			

Figure 4.3: *Listing all available shortcuts for reference*

4.3 Hovering

All objects in ChemDoodle can be hovered. This signifies that the focus is on this object and it can then be acted upon or selected for further edit. To hover an object simply move the mouse close enough to the object that an amber highlight encloses the object. See Figure 4.4 below for visual examples of hovering common structure components. Once an object is hovered, further actions pertaining to it can be performed.



(a) *A Hovered Atom*



(b) *A Hovered Bond*



(c) *A Hovered Attribute*

Figure 4.4: *Hovered Objects*

4.4 Cancelling drawing actions

If at any point when you see a preview of the results of the current drawing tool, and you wish to cancel the current drawing action, simply press the escape key to nullify the action, allowing you to release the mouse without making any changes.

4.5 Atoms

Atoms are the basic building blocks for chemical structures and are the basic building blocks in ChemDoodle. Before any other chemical objects can be drawn, an atom must be present as the starting point.

4.5.1 Placing carbon atoms

When you first open ChemDoodle, a gray dot follows your mouse pointer on the **Doodle Board** as shown in Figure 4.5.



Figure 4.5: *Trailing Carbon Atom*

To set a carbon atom at the current location of the mouse pointer, just click the mouse. After a carbon atom has been set structures can be grown from it.

At any time while drawing chemical structures, if there is no hovered atom to grow from, a carbon atom will trail your mouse and once placed can be used to grow a new structure.



More advanced users may find it inconvenient to always require a starting atom to draw structures. You can turn off this restriction in the **Settings** window under the **Controls** tab, by deselecting the **Require Starting Atom** checkbox. Clicks with the bond tools will then immediately place those bonds and rings, templates and chains will not require a starting atom.

4.5.2 Placing other elements

To place atoms with element symbols other than carbon, use the **Elemental Labels** palette. Just click on the desired element symbol and the mouse cursor will change to be that symbol with a small arrow in the bottom-left corner of the symbol. To place an atom of the selected element, click on any empty space in the document to create a new atom with that label at that location. If you click while hovering over an existing atom of a different element, then that atom's label will change to the currently selected element symbol.

4.5.3 Placing atoms with non-elemental labels

Lone chemically interpreted notations can be placed in the document. This is useful for quickly writing and parsing a molecular formula to calculate a molecular mass, for instance. See the CHEMICAL LABELS section for more information on parsing chemical notations. To do this, simply click within the document where you want the notation to go without anything hovered using the **Text for Atoms and Captions** tool A in the **Drawing** toolbar. Before setting the label, turn on chemical

interpretation by pressing the **Interpret Chemically** button CH_2 in the toolbar above the text field. Click elsewhere in the current document or press the Enter key (return on macOS) to close the text field and a new atom representing the chemically interpreted notation will be created.

You can also modify existing atoms into any chemical label you desire using the **Text for Atoms and Captions** tool A. When chosen, hover an existing atom and click on it to open an editable text field for that atom's label. Type the desired atom label text into the text field and then click elsewhere in the current document or press the Enter key (return on macOS) key to close the text field and set the atom to the typed text.

Note that if you use this tool without an atom being hovered or without selecting the **Interpret Chemically** button, a caption label will appear instead. This is a non-chemical label and is covered in the SHAPES chapter.

4.5.4 Hovering atoms

Atoms can be hovered with most tools in ChemDoodle. Exceptions include the shape tools, such as when drawing rectangles. Once an atom is hovered further relevant actions can be performed.



Figure 4.6: *A Hovered Atom*

4.5.5 Selecting atoms

To select an atom, first hover one and then press and hold the mouse down. The amber circle indicating hovering will turn into a blue circle. The blue circle is actually a special component called the **Optimize Zone**, which will be discussed in the BONDS section of this chapter.



Figure 4.7: *A Selected Atom*

To deselect atoms, just release the mouse.

4.5.6 Changing atom labels to other elements

To change an atom's label to another element symbol, use the **Elemental Labels** palette or the **Abbreviations** panel in the **Symbols** widget. Just click on the desired element symbol or abbreviation, and the mouse cursor will change to be that symbol with a small arrow at the bottom-left. Once you have hovered the atom with the label to be changed, just click to set the new label.

Additionally, when an atom is hovered, you can press any of the letter keys on the keyboard to cycle through the element symbols that begin with that letter. For instance, if you hover a carbon atom and press the N key, the atom's element will be changed to nitrogen.

If you press the space key while an atom is hovered, you will open the text field to edit the atom's label.

4.5.7 Sprouting bonds to labels

While placing labels using element symbols or other label tool presets, you will see an amber circle highlighting any atom you hover over. If you press the mouse down and drag the mouse cursor outside of the amber circle, the **Optimize Zone** (blue circle, see Figure 4.7) appears and you will sprout a new bond to the selected label in an optimal position. If you then drag the mouse cursor outside of the **Optimize Zone**, you will be able to place the sprouted atom to a location pointing towards your mouse. If you then move the mouse cursor back into the center of the **Optimize Zone**, the circle will revert back to a small amber highlight, and the function will revert back to modifying the label of that atom.

Sprouting the bond follows the same conventions as placing a new bond while using the **Optimize Zone**.

4.5.8 Changing atom labels to non-elemental text

To change an atom's label to any text you desire, click on the **Text for Atoms and Captions** tool  located on the **Drawing** toolbar. Then hover the atom with the label to be changed and click to open up its atom label text field. Type the desired atom label text into the text field and then click elsewhere on the **Doodle Board** or press the Enter key (return on macOS) to close the text field and set the new label. Additionally, you can hover the atom in any mode and then press the space key to open the atom label's text field.

4.5.9 Repeating the most recently typed atom label

To reuse a complex atom label for other atoms, hover the other atoms with labels to be changed and press the enter key. The hovered atom's label will be set to the most recently typed label.

You can also define the label text to be used when you press the enter key by opening up a previously typed atom label text field and then closing it.

4.5.10 Moving an atom

To move an atom, first select one of the selection tools discussed in CONTENT MANAGEMENT TOOLS. Make sure that no content is currently selected by emptying the lasso. Then execute the following steps:

1. Hover the atom to be moved.
2. Press the mouse down to select the atom.
3. Drag the mouse to move the atom.
4. Release the mouse to finish the move action.

If the atom is a terminal atom in a molecule, then the above instructions will move the atom and bond with fixed angles and lengths as described in the BONDS section of this chapter.

If the atom is part of a molecule and not a terminal atom, the above instructions will move that entire molecule. Hold down the shift key while executing the above instructions to move just the atom itself.

4.5.11 Deleting an atom

To delete an atom, select the **Erase** button  in the **Content** toolbar. Hover the atom to be deleted and click the mouse. You may also press the delete or backspace key when an atom is hovered to quickly remove it. All attached bonds will also be removed, leaving the adjacent atoms.

4.6 Carbon labels

By default, ChemDoodle draws skeleton figures where carbon labels are suppressed. However, it may be necessary to show the carbon label for various reasons and this can be done easily for each atom or globally for all atoms. To affect this globally, change the **Display Carbon Label** style for the document style sheet in the **Styles** window under the **Atoms** tab. To do this for a specific carbon atom, change the **Display Carbon Label** style in the atom's **Format** window.

The atom **Display Carbon Label** style has four options for displaying carbon labels:

- **Always** - always display the "C" for the carbon label.
- **On Lone and Hidden** - only display carbon labels on lone and hidden carbons.
- **On Hidden** - only display carbon labels on hidden carbons. (default)
- **Never** - never display "C" labels.

The default is **On Hidden** and only carbon atoms that are "hidden" between two bonds of the same bond order will have their label displayed as shown in Figure 4.8.

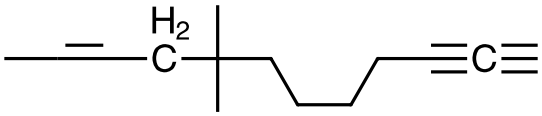


Figure 4.8: *Hidden carbon labels are shown.*

Lone carbons are disconnected atoms and have no bonds attached. In addition to manually changing the **Display Carbon Label** style, there is a quick method provided to show/hide carbon labels. To quickly show individual carbon labels, execute the following steps:

1. Hover the carbon atom with label to be shown.
2. Right-click on the atom and select the **Show Carbon Label** menu item.

To hide the carbon label execute the same steps, but instead select the **Hide Carbon Label** menu item.

4.6.1 Terminal carbon labels

You may prefer that all terminal carbon atoms will display labels. To show terminal carbon labels, check the **Show Terminal Labels** style in the **Carbons** section in the **Atoms** tab of the **Styles** window.

4.7 Deuterium and Tritium labels

A frequent need of chemists is to express isotopes of hydrogen in figures. The two most common are deuterium (^{2}H) and tritium (^{3}H). You can assign isotope mass values to atoms in ChemDoodle by following the instructions in the ISOTOPES section.

In addition to the mass value representations, both the *D* label for deuterium and the *T* label for tritium are recognized by ChemDoodle. The definitions for these abbreviations can be found (along with others) by using the **Symbols** widget which will aid you in inserting these symbols into labels. The **Symbols** widget is discussed in the WIDGETS chapter. You may also quickly write out your own labels including *D* and *T* using the **Text for Atoms and Captions** tool  .

4.8 Chemical labels

We previously described how to use the **Text for Atoms and Captions** tool  to assign any arbitrary text to an atom. This text is chemically interpreted; a label of *CH3* will be interpreted as one carbon atom with three hydrogen atoms attached to it. Much more advanced labels can be written and parsed. More information on chemical interpretation, and expanding these labels, is described in the CHEMINFORMATICS chapter.

In addition to chemical interpretation, the label will automatically be formatted for display; the *CH3* label will display as CH_3. Stacking will also be applied, so bond overlap with labels is kept to a minimum. You can override ChemDoodle's chemical interpretation and apply your own formatting to more advanced labels such as for rendering isopropyl groups (*i*Pr and ^{i}Pr) or adding indexes to carbon chain groups (R^{10}).

4.8.1 Label toolbar

When opening an atom label field, a format toolbar will appear above it containing several controls. The only enabled button will be the **Interpret Chemically** button, which is selected by default as shown in Figure 4.9.

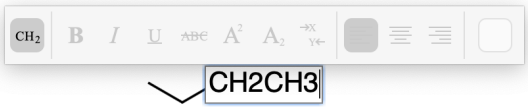


Figure 4.9: *Only **Interpret Chemically** button is enabled by default*

Without further editing, closing this label will assign an ethyl group to the atom and the text will be automatically formatted as CH_2CH_3.

4.8.2 Atom label token stacking

When labels are chemically interpreted, they will be split up into tokens that describe each discrete unit. For instance, NH will be split into (N)(H) and CCH2COOH will be split into (C)(CH2)(COOH). More about this is covered in the CHEMINFORMATICS chapter. ChemDoodle will automatically stack tokens in atom labels such that they overlap with surrounding bonds as little as possible, as shown in Figure 4.10.

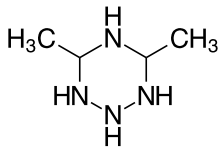


Figure 4.10: *Stacked atom label tokens with minimal bond overlapping*

By default, if not on a terminal atom, the second token and all subsequent tokens will be stacked to the next line. There are two styles for more precise control over this behavior: **Stack Lone/Terminal** and **Token Stacking**.



You can set this checkbox to determine if lone and terminal labels will also stack labels.

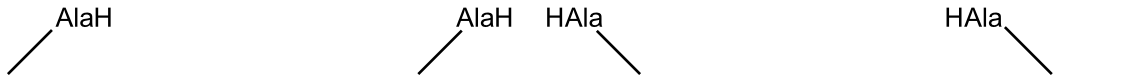


You can set this option to declare whether token stacking occurs for all individual tokens, for only the second token or never for any token.

In addition to the token behavior settings, you also have full control of the spacing between tokens. All of these settings are present in the **Styles** window in the **Atoms** tab under the **Labels** section. All styles are covered in detail in the STYLES chapter.

4.8.3 Subtoken alignment

Multicharacter tokens attached to bonds will be centered by either the entire token center, or by the edge character center. For instance, if your terminal label consists of a single "Ala" token, disabling this style will center the label around the center of the entire "Ala" string (close to the "l" character), regardless of orientation. If subtoken alignment is applied, the rendering will center the label around the starting "A" or ending "a" depending on whether the label is oriented to the left or the right. Please see Figure 4.11 for a demonstration. Multicharacter tokens directly attached to more than 1 bond may also be subaligned to a character depending on the style sheet.

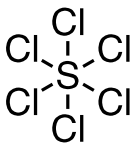


(a) *Left subtoken alignment* (b) *Center token alignment* (c) *Right subtoken alignment*

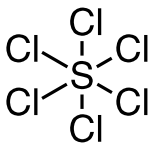
Figure 4.11: *A few cases where subtoken alignment for a terminal label will produce different graphics*

Subtoken alignment is applied by ChemDoodle as defined by the **Subtoken Alignment** style choice for atoms, present in the **Styles** window in the **Atoms** tab under the **Labels** section. You may choose to **Never** apply subtoken alignment, **Always** apply it to every atom label, apply it to **Only Terminal** atom labels or apply an **Optimized** algorithm. When in **Optimized** mode, ChemDoodle will strive to produce the best possible layout for the specific situation of each atom label.

Subtoken alignment will improve the layout of labels starting with longer length tokens by making the structure clearer and exposing more rendering of the bond lines. However, there are detriments to enabling this feature. Structures will appear asymmetrical as enabling subtoken alignment will most likely offset multi-character tokens. This asymmetry is most apparent when working with shorter bond lengths and larger font sizes. For instance, see Figure 4.12 for a clear example of how the symmetry of a sulfur hexachloride drawing is broken by enabling subtoken alignment. Therefore, we leave the choice to enable subtoken alignment to the user and **Never** is the default mode in ChemDoodle.



(a) *When tokens are centered, figures will appear symmetrical*



(b) *Subtoken alignment breaks symmetry*

Figure 4.12: *Sulfur hexachloride with subtoken alignment on and off*

4.8.4 Atom label orientation

By default, atom label tokens will orient themselves in the direction of least overlap with the rest of the structure. It may be necessary, on occasion, to force the label to orient in a specific direction. To do so, execute the following steps:

1. Hover the atom with label to orient.
2. Right-click on the atom and expand the Label Orientation submenu.
3. Choose the direction to orient the label. Choose **Auto** if you want ChemDoodle to automatically determine the best orientation.

4.8.5 Formatting atom labels



When chemical interpretation is disabled the label loses all chemical significance, and is not expandable or suitable for any chemical algorithms.

If a different formatting for the atom label is desired, just deselect the **Interpret Chemically** button and the formatting options will be enabled as shown in Figure 4.13.

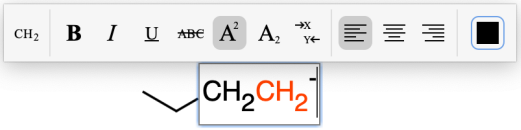


Figure 4.13: *Applying a custom format to an atom label*

Use the controls in the toolbar that appears above the atom label field to explicitly format the atom label. The formatting options that can be changed are listed in the table below. In the third column of the table are instructions of how to change each of the formatting options.

Table 4.1: Customizing Formatting

Button	Attribute	Control
B	**Bold**	Select the text to be bold and press the **Bold** button. The corresponding keyboard shortcut is ctrl + B.
I	*Italics*	Select the text to be italicized and press the **Italics** button. The corresponding keyboard shortcut is ctrl + I.
U	Underline	Select the text to be underlined and press the **Underline** button. The corresponding keyboard shortcut is ctrl + U.
ABC	~~Strikethrough~~	Select the text to display the strikethrough and press the **Strikethrough** button. The corresponding keyboard shortcut is ctrl + shift + X.
A^2	Superscript	Select the text to be superscript and press the **Superscript** button. The corresponding keyboard shortcut is ctrl + shift + =.
A_2	Subscript	Select the text to be subscript and press the **Subscript** button. The corresponding keyboard shortcut is ctrl + =.
→X Y←	Script Merge	Select the superscripted and subscripted text to be merged and press the **Merge Script** button. This is useful for atomic attributes, such as aligning an atomic mass and isotopic mass number vertically.
	Alignment	The entire label will be aligned according to the selection of the **Align Left**, **Align Center** or **Align Right** buttons.
	Color	Select the text to be colored and press the **Choose Color** button. Then select the desired color.
Helvetica	Font Family	Select the text to change the font family of and then use the font chooser in the **Formatting** toolbar to select the font.
14	Font Size	Select the text to change the font size of and then use the size chooser in the **Formatting** toolbar to select the font size.

4.9 Bonds

Bonds are the second most important building blocks in chemistry. Bonds in ChemDoodle are graphical connectors between atoms. There are many options for bond types and for defining how they look.

4.9.1 Single bonds

To place a single bond, click the **Single Bond** tool ( ) in the **Bonds** palette in the **Drawing Toolbar**. By default, this tool will be selected when ChemDoodle is opened. Then hover over an atom and press and hold the mouse down. A preview of the new bond and atom will be drawn as shown in Figure 4.14.

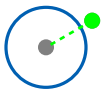


Figure 4.14: *New Bond Placement Preview*

Drag the mouse and use the techniques discussed in the following subsections to place the bond in the preferred orientation. Then release the mouse to set the bond.

4.9.2 Placing bonds other than single bonds

To place bond types other than single bonds, just click on the desired bond type in the **Bonds** palette. Then follow the instructions for placing a single bond.

4.9.3 Optimize zone

The **Optimize Zone** is a special component in ChemDoodle to help you place bonds in the optimal position around atoms. It is the blue circle that appears when placing bonds and other molecule fragments. To use the **Optimize Zone**, just place the mouse pointer in the blue circle. The bond or fragment being placed will then automatically be oriented in the most optimal position.

The **Optimize Zone** size can be changed in the **Settings** window under the **Controls** tab.

4.9.4 Placing bonds with fixed lengths and angles

By default, fixed lengths and fixed angles are enforced when drawing structures. To place a bond with these constraints, hover over an atom and press the mouse down with a bond tool. You will see the **Optimize Zone** appear.

Drag the mouse pointer out of the **Optimize Zone**. The new bond placement will now orient towards the mouse pointer.

The default fixed length is defined by the **Bond Length** style in the **Styles** window under the **Bonds** tab. Angles are fixed every 30° starting at 0°.

You can set whether fixed lengths and/or fixed angles are on by default in the **Settings** window under the **Controls** tab.

4.9.5 Placing bonds at non-fixed lengths

When placing bonds, fixed lengths will be enforced. To break from fixed lengths, hold down the shift key while placing the bond. This will alter the length even if the mouse pointer is inside of the **Optimize Zone**.

You may turn off fixed lengths in the **Settings** window under the **Controls** tab. In this case, the shift key will then enforce fixed lengths.

4.9.6 Placing bonds at non-fixed angles

When placing bonds, fixed angles will be enforced. To break from fixed angles, hold down the alt key while placing the bond. This will alter the angle even if the mouse pointer is inside of the **Optimize Zone**.

You may turn off fixed angles in the **Settings** window under the **Controls** tab. In this case, the alt key will then enforce fixed angles.

4.9.7 Placing bonds at non-fixed lengths and non-fixed angles

When placing bonds, fixed angles and fixed lengths will be enforced. To break from fixed lengths and fixed angles at the same time, hold down both the shift and alt keys while placing the bond. This will alter the length and angle even if the mouse

pointer is inside of the **Optimize Zone**.

You may turn off fixed lengths and fixed angles in the **Settings** window under the **Controls** tab. In this case, holding down both the shift and alt keys will enforce fixed lengths and angles.

4.9.8 Connecting two atoms with a new bond

If two atoms are already present in the document and you want to connect them with a bond, just initiate drawing a new bond from one atom and without releasing the mouse, drag over the second atom until it is highlighted with a red circle as shown in Figure 4.15. Then release the mouse and the new bond will be formed between those two atoms.

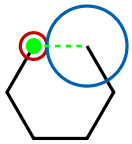


Figure 4.15: *Connecting a bond between two existing atoms*

To place a new atom directly on top of an existing atom without using the existing atom in the new bond, hold down the space key while placing the new atom and releasing the mouse button.

4.9.9 Hovering bonds

Bonds can be hovered with some tools in ChemDoodle. Once a bond is hovered further relevant actions can be performed.



Figure 4.16: *A Hovered Bond*

4.9.10 Selecting bonds

Bonds can only be selected when using the selection tools discussed in CONTENT MANAGEMENT TOOLS. To select bonds, first hover them and then press and hold the mouse down. The amber semicircles will turn a blue color, indicating that the bond has been selected.



Figure 4.17: *A Selected Bond*

4.9.11 Changing a bond type

To change a bond type, first select the bond type you would like to change the bond to in the **Bonds** palette. Then hover the bond with the type that you would like to change and click the mouse. The new bond type will override the old type.

You may also use the number keys to change bond types for hovered bonds. For instance, the 2 key will change a hovered bond to a double bond and the 3 key will change a hovered bond to a triple bond.

4.9.12 Changing selected bonds to single bonds

To change the bond types of a large number of bonds to all be single bonds, execute the following steps:

1. Select the bonds to be changed to single bonds using a selection tool as discussed in CONTENT MANAGEMENT TOOLS.
2. Click on the Structure » Saturate menu item.

4.9.13 Incrementing a bond order

When using the **Single Bond** tool, clicking on hovered bonds will not override other bond types. Instead the **Single Bond** tool will increment the bond order. For example, clicking on a double bond will change it to a triple bond and clicking on the triple bond will change it back to a single bond.

This functionality can be disabled so that the **Single Bond** tool overrides bond types in the **Settings** window under the **Controls** tab. Also under the **Controls** tab is the option to allow bonds to be incremented past triple; if this option is enabled, bonds will be incremented all the way up to sextuple bonds before reverting back to a single bond.

4.9.14 Deleting a bond

To delete a bond, select the **Erase** button  in the **Content** toolbar. Hover the bond to be deleted and click the mouse. You may also press the delete or backspace key when a bond is hovered to quickly remove it. The constituent atoms will remain.

4.9.15 Decrementing a bond order

By default, deleting a bond will remove that bond completely. You can change this behavior to instead decrement bond orders. You can enable this behavior in the **Settings** window under the **Controls** tab, by setting the **Delete Bond Behavior** setting to **Decrements Bond Orders**.

If you select **Decrements Bond Orders**, press the delete or backspace keys or use the **Eraser** tool  while a bond is hovered. A triple bond will change to a double bond, a double bond will change to a single bond, and a single bond will simply be removed.

4.9.16 Deleting bonds around atoms

To delete many bonds, but retain the atoms contained in the bonds, execute the following steps:

1. Select the bonds to be removed using a selection tool as discussed in CONTENT MANAGEMENT TOOLS.
2. Press the Structure » Remove Selected Bonds menu item.

All selected bonds will be removed, but their atoms will remain.

4.10 Chains

Chains are a group of carbon atoms, linked linearly by bonds. Three types of chains are provided in ChemDoodle:

Linear Chain 

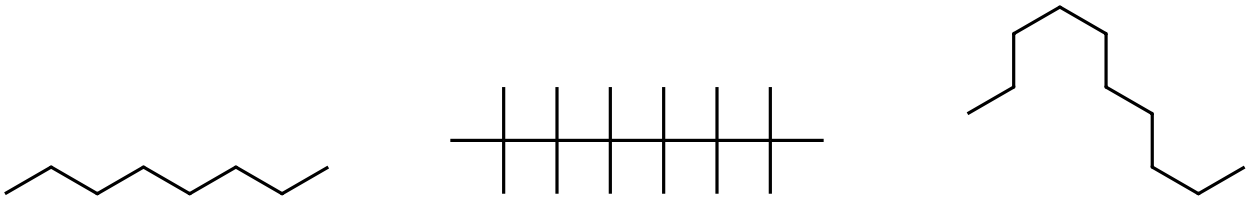
A consistent linear carbon chain, with all chain angles alternating at ±120° as shown in Figure 4.18a.

Fischer Projection Chain 

A straight carbon chain, with all chain angles at 180°. All non-terminal chain atoms also have two additional carbon atoms depicted perpendicular to the chain orientation as shown in Figure 4.18b.

Random Chain 

A carbon chain where all chain angles are at 120°, but the chain itself can deviate in any direction as shown in Figure 4.18c.



(a) *Linear* (b) *Fischer Projection* (c) *Random*

Figure 4.18: *Carbon Chains*

4.10.1 Placing chains at fixed angles

To place chains at fixed angles, execute the following steps:

1. Select a chain tool on the **Chains** palette using the **Chain Tool** group button ()
2. Choose a starting atom to sprout the chain from by hovering it. If you do not want to start the chain from any existing atoms, create an atom in a new place by clicking in the current document where no atoms are hovered.
3. Press and hold the mouse down on the hovered atom.
4. Drag the mouse to the desired length of the chain. When using the **Random** chain, drag the mouse in the outline of the chain you would like to draw and the chain will grow following that path.
5. Release the mouse to set the chain.

By default, the chains will be oriented at fixed angles every 15° starting at 0°. All bond lengths are defined by the **Bond Length** style in the **Styles** window under the **Bonds** tab.

4.10.2 Placing chains at non-fixed angles

To place chains at non-fixed angles, hold down the alt key while dragging the mouse when defining the chain to break from the fixed chain orientation angles.

4.10.3 Forcing the placement of chains vertically and horizontally

To place chains oriented vertically or horizontally, hold down the shift key while dragging the mouse when defining the chain. The chain preview will then automatically orient vertically or horizontally depending on the angle from the starting atom to the current mouse cursor position.

4.10.4 Inverting linear chains

Linear chains can be inverted by holding down the slash key / while placing. The preview will update accordingly.

4.11 Rings

Rings are chains of carbon atoms in which the last atom in the chain connects to the first.

Rings may contain bond types other than single bonds. Currently the following rings can be drawn quickly from the **Rings** palette, with additional ring choices in the **Templates** widget:


Cyclopropane ring


Cyclobutane ring


Cyclopentane ring


Cyclohexane ring


Cycloheptane ring


Cyclooctane ring


Cyclobutadiene ring


Cyclopentadiene ring


Benzene ring


Cycloheptatriene ring


Cyclohexane Chair Conformer 1


Cyclohexane Chair Conformer 2



Arbitrary Ring Size Tool



Arbitrary Crown Size Tool

4.11.1 Placing a ring

To place a ring execute the following steps:

1. Click the preferred ring tool in the **Rings** palette.
2. Hover over an atom and press the mouse down. A preview of the new ring will be drawn as shown in Figure 4.19.
3. Drag the mouse and use the techniques discussed in the following subsections to place the ring in the preferred orientation.

4. Release the mouse to set the ring.

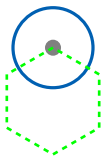


Figure 4.19: *New Ring Placement Preview*

4.11.2 Optimize zone

The **Optimize Zone** can be used to optimize ring placement as described earlier in the BONDS section of this chapter.

4.11.3 Placing rings with fixed lengths and angles

By default, fixed lengths and fixed angles are enforced when drawing rings. To place a ring within these constraints, hover over an atom and press and hold the mouse down with a ring tool. You will see the **Optimize Zone** appear.

Drag the mouse pointer out of the **Optimize Zone**. The new ring placement will now orient towards the mouse pointer.

The default fixed length is defined by the **Bond Length** style in the **Styles** window under the **Bonds** tab. Angles are fixed at 30° intervals starting with 0°.

You can specify whether fixed lengths and/or fixed angles are turned on by default in the **Settings** window under the **Controls** tab.

4.11.4 Placing rings at non-fixed lengths

When placing rings outside of the **Optimize Zone**, fixed lengths will be enforced. To break from fixed lengths, hold down the shift key while placing the ring. This will alter the lengths even if the mouse pointer is inside of the **Optimize Zone**.

You can turn off fixed lengths in the **Settings** window under the **Controls** tab. In this case, the shift key will then enforce fixed lengths.

4.11.5 Placing rings at non-fixed angles

When placing rings outside of the **Optimize Zone**, fixed angles will be enforced. To break from fixed angles, hold down the alt key while placing the ring. This will alter the angle even if the mouse pointer is inside of the **Optimize Zone**.

You can turn off fixed angles in the **Settings** window under the **Controls** tab. In this case, the alt key will then enforce fixed angles.

4.11.6 Placing rings at non-fixed lengths and non-fixed angles

When placing rings outside of the **Optimize Zone**, fixed angles and fixed lengths will be enforced. To break from fixed lengths and fixed angles at the same time, hold down both the shift and alt keys while placing the ring. This will alter the lengths and angle even if the mouse pointer is inside of the **Optimize Zone**.

You can turn off fixed lengths and fixed angles in the **Settings** window under the **Controls** tab. In this case, holding the shift and alt keys will then enforce fixed lengths and angles.

4.11.7 Adding Rings to Bonds

When adding rings to atoms, it is sometimes difficult to achieve an aesthetic fuse angle. To correct for this problem, add the ring to a bond instead of an atom. The ring will automatically align to the bond to which it is being added.

To add rings to bonds, execute the following steps:

1. Select a ring tool from the **Rings** palette.
2. Hover the bond to which a ring will be added.
3. Click and drag the mouse pointer to the side of the bond to which the ring should be added.
4. Release the mouse to set the ring.

When the mouse pointer is close to the bond the ring is sprouting from, ChemDoodle will automatically select the optimal side of the bond to add to.

4.11.8 Adding Rings of Any Size

To add rings of any size, perform the following steps:

1. Select the **Arbitrary Ring Size** tool  from the **Rings** palette.
2. Hover the atom or bond to which a ring will be added so that object is hovered.
3. Click and drag the mouse pointer in the direction you would like the ring added. A preview will show you the ring that will be set. Dragging the mouse pointer away from the start object expands the the ring size. Dragging the mouse pointer toward the start object decreases the ring size.
4. Holding down the alt key will break from standard angles if adding to an atom. Holding down the shift key will alternate double bonds in the placed ring.
5. Release the mouse to set the ring.

4.11.9 Adding Crowns of Any Size

To add crowns of any size, perform the following steps:

1. Select the **Arbitrary Crown Size** tool  from the **Rings** palette.
2. Hover the atom or bond to which a ring will be added so that object is hovered.
3. Click and drag the mouse pointer in the direction you would like the ring added. A preview will show you the ring that will be set. Dragging the mouse pointer away from the start object expands the the ring size. Dragging the mouse pointer toward the start object decreases the ring size.
4. Holding down the alt key will break from standard angles if adding to an atom. Holding down the shift key will add oxygens at the appropriate places to create a crown ether.
5. Release the mouse to set the ring.

4.11.10 Unsaturated Ring Fusing

When using unsaturated ring tools, such as the **Benzene** tool  , ChemDoodle will intelligently allocate the double bonds to maximize conjugation when those rings are fused together. This allows you to quickly build complex fused ring systems. Keep in mind that there may be cases where the only possibility for ChemDoodle to avoid overvalencing these systems is to exclude a double bond completely, so make sure to build ring blocks in a manner that allows for a completely conjugated system.

4.12 Templates

ChemDoodle contains a very advanced structure templates system. Several sets of predefined templates are already packaged with ChemDoodle and can be accessed through the **Templates** widget. Currently, the following template sets are provided:

- Amino Acids
- Cyclic Terpenes
- Cycloalkanes
- Diamondoids
- Fullerenes
- Metallocenes
- Nucleotides
- Other
- Platonic Solids
- Ring Conformers
- Rings (Cp-)
- Rings (Flu-)
- Rings (Ind-)
- Rings (Benzene)
- Rings (Tropylium)
- Rotational Conformations
- Stereochemical Configurations
- Sugars (Hexoses)
- Sugars (Other Monosaccharides)
- Vitamins

4.12.1 Selecting a template for use

The **Templates** widget organizes your templates and allows you to easily use them. Execute the following steps to select a template for use:

1. Activate the **Templates** widget by clicking on the **Templates** widget button.
2. Choose a template set from the drop-down menu.
3. The templates belonging to the selected set will populate the bottom portion of the widget. Click on a specific template to select it.
4. The selected template will be displayed at the top of the widget, rendered in the style sheet of the current document. A default substitution atom will be defined, but you may change the substitution atom to another by clicking on a different atom. The substitution point is the atom that will be overlapped with the atom in the document the template is being connected to.

Note this will not place the template into the document; please see the following sections for template placement instructions.

4.12.2 Placing a template

To place a template, select a template as described above and choose a substitution atom in the **Templates** widget. Then hover over the atom in your document to which you are attaching the template and press and hold the mouse down. A preview of the template will be depicted as in Figure 4.20.

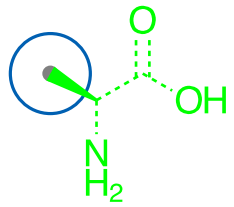


Figure 4.20: *New Template Placement Preview*

Drag the mouse and use the techniques discussed in the following subsections to place the template in the preferred orientation. Then release the mouse to set the template.

4.12.3 Optimize zone

The Optimize Zone can be used to optimize template placement as described in the BONDS section of this chapter.

4.12.4 Placing templates with fixed lengths and angles

By default, fixed widths and fixed angles are enforced when drawing structures. To place a template within these constraints, hover over an atom and press and hold the mouse down with a template selected. You will see the **Optimize Zone** appear. Drag the mouse pointer out of the **Optimize Zone**. The new template placement will now orient towards the mouse pointer.

The default fixed length is defined by the **Bond Length** style in the **Styles** window under the **Bonds** tab. Angles are fixed at 30° intervals starting at 0°.

You can set whether fixed lengths and/or fixed angles are on by default in the **Settings** window under the **Controls** tab.

4.12.5 Placing templates at non-fixed lengths

When placing templates outside of the **Optimize Zone**, fixed lengths will be enforced. To break from fixed lengths, hold down the shift key while placing the template. This will alter the length even if the mouse pointer is inside of the **Optimize Zone**.

You can turn off fixed lengths in the **Settings** window under the **Controls** tab. In this case, the shift key will then enforce fixed lengths.

4.12.6 Placing templates at non-fixed angles

When placing templates outside of the **Optimize Zone**, fixed angles will be enforced. To break from fixed angles, hold down the alt key while placing the template. This will alter the angle even if the mouse pointer is inside of the **Optimize Zone**.

You can turn off fixed angles in the **Settings** window under the **Controls** tab. In this case, the alt key will then enforce fixed angles.

4.12.7 Placing templates at non-fixed lengths and non-fixed angles

When placing templates outside of the **Optimize Zone**, fixed angles and fixed lengths will be enforced. To break from fixed lengths and fixed angles at the same time, hold down both the shift and alt keys while placing the template. This will alter the length and angle even if the mouse pointer is inside of the **Optimize Zone**.

You can turn off fixed lengths and fixed angles in the **Settings** window under the **Controls** tab. In this case, holding the shift and alt keys will then enforce fixed lengths and angles.

4.12.8 Managing your templates

You may create custom templates in ChemDoodle and organize them into custom template sets. These functions are facilitated using the buttons found above the template set drop-down select in the **Templates** widget. These buttons are context sensitive and will only be enabled when the function is possible.

In order to add your own templates, you must create your own template set, as you cannot add templates to the predefined template sets provided in ChemDoodle.

All of your templates are stored in files in the `templates` folder in the `ChemDoodleSettings` folder located in your operating system's standard `Documents` folder. You may distribute your template sets to other ChemDoodle users or place third party template sets in this folder to use them in ChemDoodle. If ChemDoodle is open when manually placing template set files in the `templates` folder, you must close and then restart ChemDoodle for these new template sets to be registered and usable.

4.12.8.1 Creating a template set

To create a new template set, which will store any number of templates, perform the following steps:

1. In the **Templates** widget, press the **Create Template Set**  button.
2. A text field will appear asking you for a name for this new template set. You must pick a name that is not the same as another template set.
3. Once you have entered a name for the new template set, press the **Accept** button.
4. This new template set will then be created and automatically selected in the **Templates** widget. However, it will be empty. Please see the sections below for managing individual templates within a set.

4.12.8.2 Removing a template set

To remove a template set, including all templates within the set, perform the following steps:

1. In the **Templates** widget, select the template set you wish to remove in the template set drop-down select. The predefined template sets in ChemDoodle may not be removed.
2. Press the **Remove Template Set**  button.
3. A question window will appear asking you to confirm the removal of this template set, which will remove the set and all contained templates. This action cannot be undone. If you are sure, press the **Yes** button.
4. The selected template set will be removed and the **Templates** widget will automatically select the first template set in the drop-down select.

4.12.8.3 Renaming a template set

To rename a template set, perform the following steps:

1. In the **Templates** widget, select the template set you wish to rename in the template set drop-down select. The predefined template sets in ChemDoodle may not be renamed.

2. Press the **Rename Template Set**  button.
3. A text field will appear asking you for the new name of this template set. You must pick a name that is not the same as another template set.
4. Once you have entered a name for the new template set, press the **Accept** button.
5. The template set will be renamed and the **Templates** widget will update to reflect the new name.

4.12.9 Adding a new template

To add a template into a template set in the **Templates** widget, execute the following steps:

1. Draw the desired template in the current document.
2. Select your drawn template with the selection tools discussed in CONTENT MANAGEMENT TOOLS. Templates in ChemDoodle may consist of both shapes and one or more chemical structures. A template *must* contain at least 1 atom.
3. In the **Templates** widget, select the template set you wish to add the new template to in the template set drop-down select. You may not add a template to the predefined template sets in ChemDoodle.
4. Press the **Add Template**  button.
5. A text field will appear asking you for a name for this new template. You must pick a name that is not the same as another template in the current set.
6. Once you have entered a name for the new template, press the **Accept** button.
7. This new template will then be created and automatically selected in the **Templates** widget.

4.12.10 Removing a template

To remove a template from a template set in the **Templates** widget, execute the following steps:

1. In the **Templates** widget, select the template set that contains the template you wish to remove in the template set drop-down select. You may not remove a template from the predefined template sets in ChemDoodle.
2. Of the available templates in the template set, click on and select the template you wish to remove.
3. Press the **Remove Template**  button.
4. A question window will appear asking you to confirm the removal of this template. This action cannot be undone. If you are sure, press the **Yes** button.
5. The selected template set will be removed and the **Templates** widget will automatically select the first template in the current set, or become blank if there are no remaining templates in the set.

4.12.11 Renaming a template

To rename a template from a template set in the **Templates** widget, execute the following steps:

1. In the **Templates** widget, select the template set that contains the template you wish to rename in the template set drop-down select. You may not rename a template from the predefined template sets in ChemDoodle.
2. Of the available templates in the template set, click on and select the template you wish to rename.
3. Press the **Update Template**  button.

4. A window will appear with a text field to change the name of the selected template, as shown in Figure 4.21. Type in the new template name. You must pick a name that is not the same as another template in the current set.
5. Once you have finished typing the new template name, press the **Update** button.
6. The template will be renamed and the **Templates** widget will update to reflect the new name.

4.12.12 Updating a template

To update a template from a template set in the **Templates** widget with a new drawing, execute the following steps:

1. Draw the new desired template in the current document.
2. Select your drawn template with the selection tools discussed in CONTENT MANAGEMENT TOOLS. Templates in ChemDoodle may consist of both shapes and one or more chemical structures. A template *must* contain at least 1 atom.
3. In the **Templates** widget, select the template set that contains the template you wish to update in the template set drop-down select. You may not update a template in the predefined template sets in ChemDoodle.
4. Of the available templates in the template set, click on and select the template you wish to update.
5. Press the **Update Template**  button.
6. A window will appear with a text field to change the name of the selected template, if you desire to, as shown in Figure 4.21. Underneath the text field, there will be a checkbox titled **Update template with current selection?**. Make sure this checkbox remains selected. If this checkbox is disabled, there is no selection in the current document.

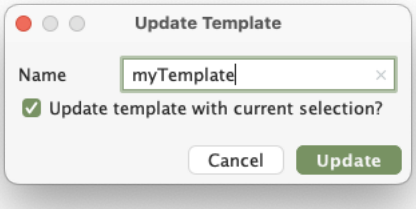


Figure 4.21: *Updating an existing template*

7. Press the **Update** button.
8. The template will be updated accordingly and the **Templates** widget will update to reflect the new drawing.

4.13 Attributes

Attributes are special objects in ChemDoodle that are associated with other chemical objects. These include charges, symbols, incrementals and custom attributes. Apart from the attributes you add, there are some attributes that ChemDoodle can add, such as stereochemical configurations and IUPAC locants. Attributes are both spatially and semantically linked to the chemical object that they describe. Any number of attributes can be added to a single chemical object.

Figure 4.22 demonstrates several different uses of attributes.

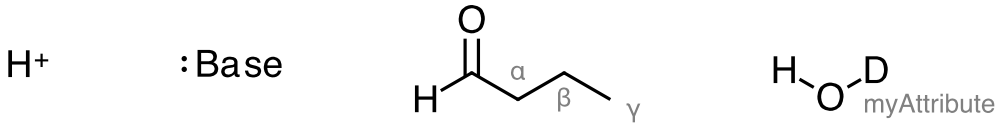


Figure 4.22: *Various types of attributes*

4.13.1 Hovering attributes

You can hover attributes by using any of the selection tools. First, make sure the current selection is empty and then move the mouse cursor close to the center of the attribute so that it is closer to the attribute than any other chemical objects. The attribute will then be defined as hovered and an amber circle will be rendered on top of it as shown in Figure 4.23.



Figure 4.23: *A Hovered Attribute*

To help identify which object the attribute describes, a transparent amber circle is drawn over that object (the nitrogen atom in Figure 4.23).

4.13.2 Selecting attributes

Attributes can only be selected when using tools that affect attributes. To select attributes, first hover them and then press and hold the mouse down. The amber circle indicating hovering will turn into a blue circle as shown in Figure 4.24.



Figure 4.24: *A Selected Attribute*

4.13.3 Auto-placement of attributes

ChemDoodle automatically places attributes on your structures for you. Simply add your attributes and they will automatically be placed with any existing attributes in an aesthetic manner. Charges are always placed on the top right, as if they were

typed and superscripted after the label. All other attributes will be distributed according to their environment and placed so they do not overlap with the label of the object they are attached to or other associated attributes. A complex figure with several automatically placed attributes is shown in Figure 4.25.

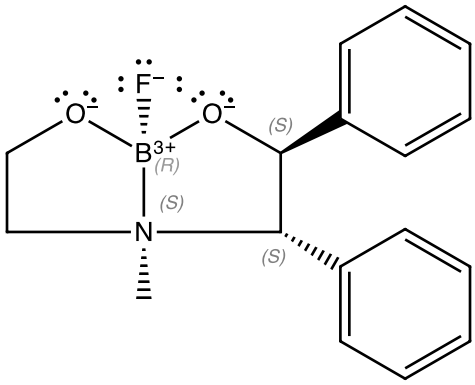


Figure 4.25: *Auto-layout of attributes in a complex figure*

4.13.3.1 Overriding the auto-placement

When placing attributes, a single click of any attribute tool will create them and they will be automatically placed around the object they are associated with. If you wish to quickly create attributes in a specific location, keep the mouse pressed down after creating the attribute using any attribute tool. Before releasing the mouse, drag your mouse to the location you desire the newly created attribute to be placed. Then release the mouse to set the location. If you hold down the shift key while placing attributes, locked distances will be released; if you hold down the alt key while placing attributes, locked angles will be released.

To manually override the layout of an attribute already present in your document, simply move it. This is covered in the MOVING ATTRIBUTES section below. Any other attributes associated with the same object will still be automatically placed unless you override them as well. Keep in mind, any other attributes that continue to be automatically placed will not consider the attributes you have manually placed.

4.13.3.2 Resetting the auto-placement

To reset any manually placed attribute to be automatically placed, just select the object the attributes are associated with that you wish to reset and press the Structure › Clean › Reset Attributes menu item. Cleaning structures will also reset attribute placements and revert them to be automatically placed. This can be done by selecting the structure and pressing the **Optimize Structures in 2D** button .

4.13.4 Moving attributes

To move attributes, execute the following steps:

1. Using a selection tool, hover the attribute to be moved.
2. Press and hold the mouse down to select the hovered attribute.
3. Drag the attribute to the new preferred location.
4. Release the mouse to set the new position.

Attributes are locked a certain distance from the object that they describe. This distance is specified by the **Optimal Distance** style in the **Styles** window under the **Attributes** tab. Change this to suit your needs.

Just as with moving terminal atoms, if you hold down the shift key while moving attributes, locked distances will be released; if you hold down the alt key while moving attributes, locked angles will be released.

4.13.5 Removing attributes

To remove an attribute, use the **Eraser** tool and click on the hovered attribute or hover the attribute with the selection tools and press the delete or backspace key.

4.13.6 Charges

Charges are attributes that can be associated with atoms as shown in Figure 4.26. Both positive and negative values can be used.



Figure 4.26: *A Charge Attribute*

4.13.6.1 Adding charges

To add charge to an atom, execute the following steps:

1. Select the **Increase Charge** (⊕) or **Decrease Charge** (⊖) tool in the **Attributes** palette.
2. Hover the atom to add charge to.
3. Press and hold the mouse down to add the charge.
4. If you prefer to have the charge placed elsewhere, then before releasing the mouse, drag the pointer to the desired location. This will work identically to placing bonds with the **Optimize Zone**. Hold down the shift key to break from standard lengths, and hold down the alt key to break from standard angles.
5. Release the mouse to set the charge.

The + and − keys on the keyboard can also be used to add a positive or negative charge to a hovered atom if no charge exists on that atom.

4.13.6.2 Incrementing and decrementing charges

To change the charge of an atom, execute the following steps:

1. Select the **Increase Charge** (⊕) or **Decrease Charge** (⊖) tools in the **Attributes** palette.
2. Hover the atom with the charge to be changed.
3. Click the mouse down to increment or decrement the charge.

The + and − keys on the keyboard can also be used to increment and decrement charge values when the associated atom is hovered.

4.13.6.3 Removing charges

Removing charges can be done in several ways:

- Decrement or increment the charge value to 0 using the **Increase Charge** (⊕) or **Decrease Charge** (⊖) tools.
- Select the **Eraser** tool and click on a hovered charge to remove it.
- Hover the charge using the selection tools and press the delete or backspace key.

4.13.6.4 Placing circles around charges

Circles can be placed around charges globally for the document, or individually for the charge attribute. Circles will only surround the charge symbol, and not any magnitude numbers.

To add circles around all charges in the document, execute the following steps:

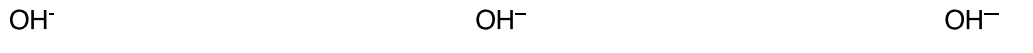
1. Select all the content in the document.
2. In the **Styles** window, select the **Attributes** tab.
3. In the **Charges** section, enable the **Surround with a Circle** option.

To add a circle to an individual charge attribute, execute the following steps:

1. Hover the charge that you would like to surround with a circle with a selection tool while nothing is selected.
2. Right-click on the hovered charge and select the Format Charge... menu item, or press the comma , key.
3. In the **Charges** section, enable the **Surround with a Circle** option.

4.13.6.5 Negative charge symbol length

When a minus symbol is written manually at the end of an atom label, ChemDoodle will interpret that symbol as a -1 negative charge associated with the atom. In many fonts, the minus symbol dash (-) is very short, and you may wish to make the negative charge more visible. So, you may instead input an "en dash" (–) or "em dash" (—) symbol instead of the minus symbol for a longer dash, as shown in Figure 4.27. This gives you control over the length of the dash used.



(a) *Minus Symbol Dash* (b) *en Dash* (c) *em Dash*

Figure 4.27: *Different dashes used for representing a negative charge*

When using the charge attribute tools described above, ChemDoodle will use an "en dash" symbol for the negative charge, by default.



Did you know? The "en dash" and "em dash" symbols are named after their lengths, the length of an "n" character and "m" character respectively from the font.

4.13.7 Symbols

Symbols are standard types of atom decorations that can be associated with atoms such as the radical cation symbol shown in Figure 4.28.



Figure 4.28: *A Symbol Attribute*

δ+ Add Positive Dipole

δ− Add Negative Dipole

•• Add Electron Pair

• Add Single Electron

•+ Add Radical Cation

•− Add Radical Anion

— Add Electron Pair (Bar)

* Add Asterisk/Undefined Stereocenter

4.13.7.1 Adding symbols

To add a symbol to an atom, execute the following steps:

1. Select the desired symbol tool in the **Attributes** palette.
2. Hover the atom to which the symbol is to be added.
3. Press the mouse down to add the symbol.
4. If you prefer to have the symbol placed elsewhere, then before releasing the mouse, drag the pointer to the desired location. This will work identically to placing bonds with the **Optimize Zone**. Hold down the shift key to break from standard lengths, and hold down the alt key to break from standard angles.
5. Release the mouse to set the symbol.

4.13.8 Incrementals

Incrementals are used for labeling atoms and/or bonds in an incremental fashion. For instance, the IUPAC numbering for a ring block is incrementally attributed and rendered in Figure 4.29.

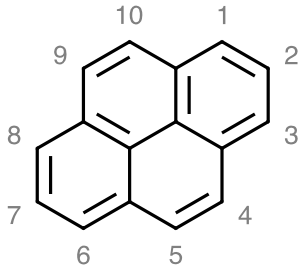


Figure 4.29: *Incremental Attributes for an IUPAC Ring Block*

1,2 Number Incrementals

I,II Roman Numeral Incrementals

a,b Letter Incrementals

α,β Greek Letter Incrementals

4.13.8.1 Adding incrementals

To add incremental attributes to a chemical structure, execute the following steps:

1. Select the desired incremental tool in the **Attributes** palette.
2. Hover the atom or bond to which the incremental is to be added.
3. Press the mouse down to add the incremental.
4. If you prefer to have the incremental placed elsewhere, then before releasing the mouse, drag the pointer to the desired location. This will work identically to placing bonds with the **Optimize Zone**. Hold down the shift key to break from standard lengths, and hold down the alt key to break from standard angles.
5. Release the mouse to set the incremental.
6. Repeat steps 2 through 5 until all parts of the structure are labelled as desired. The tool will automatically increment the incremental value with each placed attribute.

If you accidentally place an incremental on the wrong object, using the undo function will remove that attribute and decrement the incremental value so it can be used again.

Some incrementals have a final value (for instance letter incrementals end at "z"). Once you reach the end of the incremental values, the value will reset to the initial value and repeat.



When placing incrementals on atoms only, disabling the **Bonds are Focusable** setting in the **Settings** window under the **Controls** tab will make it easier to quickly place your incrementals.

4.13.8.2 Resetting the incrementation

To reset the incremental value to the first value, simply press again the button for the current incremental tool in the **Attributes** palette.

4.13.9 Custom attributes

In addition to the standard symbols provided in ChemDoodle, you can add your own text-based attributes as shown in Figure 4.30.



Figure 4.30: *Nitrogen atom attribute with "attribute" as the display text.*

4.13.9.1 Adding custom attributes

To add a custom attribute, execute the following steps:

1. Hover the atom to which the attribute is to be added.
2. Right-click on the hovered atom.
3. Select the Add Attribute... menu item. The **Add Attribute** window will appear as shown in Figure 4.31.
4. Type in the text to be displayed in the **Graphical Display** text field.
5. Type in an identifying name for the attribute in the **Metadata ID** text field. This value is used for the internal classification and is not rendered.

6. Press the **Add** button to set the attribute.

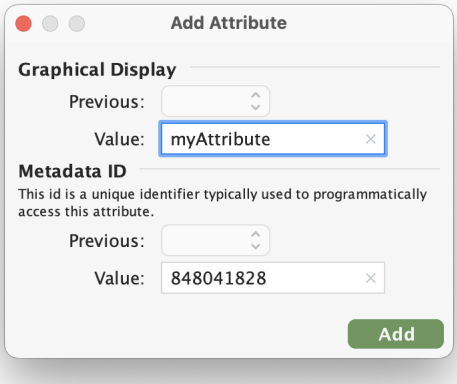


Figure 4.31: *Using the Add Attribute window*

ChemDoodle will keep track of a certain number of your previously used **Display** and **Name** values so you can quickly build semantic data.

4.13.9.2 Editing custom attributes

The display text and names of custom attributes can be edited at any time by executing the following steps:

1. Hover the attribute to be edited.
2. Right-click on the hovered attribute.
3. Press the Format Attribute… menu item. In the format window that appears, change the **Name** and **Display** text to the new values.
4. Click the **Accept** button to set the new text values.

4.14 Isotopes

Mass numbers can be associated to atoms with element symbols as their label to designate isotopes.

All mass numbers are displayed in superscript format to the left of element symbols as shown in Figure 4.32.

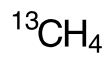


Figure 4.32: *Carbon-13 Isotope*

If you later change an atom's label and there is a mass number associated with that atom, then the mass number will be removed.

4.14.1 Setting published isotope mass numbers

To set a published mass number to an elemental atom, execute the following steps:

1. Hover the atom with the mass number to be set.

2. Right-click on the hovered atom.
3. Expand the Mass Number submenu.
4. Select any of the listed values to set the mass number of the isotope. The relative abundance of the isotope choice is displayed in parenthesis in each menu item, if available.

4.14.2 Setting arbitrary isotope mass numbers

To set an arbitrary mass number to an element atom, execute the following steps:

1. Hover the atom with the mass number to be set.
2. Right-click on the hovered atom.
3. Select the Mass Number ⟩ Other... menu item.
4. Type an integer value into the text field that appears.
5. Click the **Accept** button to set the mass number.

4.14.3 Removing mass numbers

To remove a mass number from an atom, execute the following steps:

1. Hover the atom with the mass number to be removed.
2. Right-click on the hovered atom.
3. Select the Mass Number ⟩ Remove Mass Number menu item to remove the mass number.

4.15 Nuclear Notation

Nuclear notations can be quickly typed in ChemDoodle due to a special feature called script merging. Chemistry often requires superscripts and subscripts to be vertically aligned for chemical significance. For instance, the mass number needs to be displayed above the atomic number to the left of the element label. Figure 4.33 shows off the results of script merging used in a label.



Figure 4.33: *Nuclear Notation*

In chemistry, the top left is reserved for the mass number, the bottom left is reserved for the atomic number, the top right is reserved for the charge, and the bottom right is reserved for either the number of neutrons or the multiplicity.

To use script merging, execute the following steps:

1. Click on the **Text for Atoms and Captions** tool AI located on the **Drawing** toolbar.
2. Start a new label by clicking on an empty area of the document.
3. Type in the label and set superscripts (A²) and subscripts (A₂).
4. Highlight the superscript and subscript pairs that are to be aligned vertically and press the **Script Merge** button →X Y←. A purple highlight will designate the merge as shown in Figure 4.34.

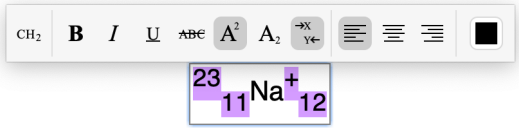


Figure 4.34: *Using the Script Merge feature*

5. Click elsewhere in the document or press the escape key to set the label.

4.16 Orbitals

2D graphics for various orbital shapes can be placed directly into the document or attached onto structures. Use them to show more detailed chemical figures. Each orbital shape has several different shading and fill styles.

The following orbital types are provided:


Atomic s orbital


Atomic $p_{x|y|z}$ orbital


Atomic $d_{xz|yz|xy|x^2-y^2}$ orbital


Atomic d_{z^2} orbital


Atomic $f_{xz^2|xy^2|x(x^2-3y^2)|y(3x^2-y^2)}$ orbital


Atomic f_{z^3} orbital


Hybrid sp^3 orbital


Hybrid sp lobe orbital


Bonding σ orbital


Bonding π orbital

Orbitals are defined by two anchor points as shown in Figure 4.35. The first anchor point defines the center of the orbital while the second anchor point defines the extent of the orbital. Orbitals are shapes in ChemDoodle and are not considered chemical objects. Additional functions for shapes, including orbitals, are covered in the SHAPES chapter.



Figure 4.35: *Orbital and Anchors*

4.16.1 Placing orbitals at fixed lengths and angles

To place an orbital, execute the following steps:

1. Select an orbital tool by clicking any **Orbital** button in the **Orbitals** palette in the **Drawing** toolbar.
2. Press and hold the mouse down on the current document to set the center of the orbital.
3. Drag the mouse to preview the placement of the extent of the orbital. A dotted green outline of the orbital will be shown.
4. Release the mouse to set the orbital.

In Step 2 of the above procedure, you may want to attach the orbital to an atom or bond center. ChemDoodle will automatically lock onto atoms and bonds when placing orbitals if the mouse pointer gets close enough to them. Once the atom or bond has been hovered, continue through Step 2 to place the orbital and set the center to be the atom or bond center.

4.16.2 Placing orbitals at non-fixed lengths or angles

To place orbitals at non-fixed lengths or angles, hold down the alt key while dragging the mouse when defining the orbital to break from the fixed lengths and angle orientations.

4.16.3 Forcing orbitals to be drawn vertically and horizontally

To place orbitals oriented vertically or horizontally at non-fixed lengths, hold down the shift key while dragging the mouse when defining the orbital. The orbital preview will then automatically orient vertically or horizontally depending on the angle from the start point to the current mouse cursor position.

4.16.4 Moving orbitals

To move orbitals, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the orbital so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in Figure 4.35 above.
2. Press and hold the mouse down and drag without selecting an anchor point to move the orbital.
3. Release the mouse to finish the edit.

4.16.5 Resizing orbitals

To resize orbitals, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the orbital so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in Figure 4.35 above.
2. Move the mouse pointer over one of the two end anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the orbital.
5. Release the mouse to finish the resize action.

4.16.6 Removing orbitals

Orbitals can be removed in a number of ways. You can do the following:

- Use the **Eraser** tool  to hover the mouse pointer over the orbital so the orbital anchor points are drawn. Then click with the mouse.
- Use a selection tool to hover the mouse pointer over the orbital so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in Figure 4.35 above. Then press the backspace or delete key.

CHAPTER 5

Inorganic Compounds and Complexes

Contents

5.1 Overview **142**

5.2 Choosing a bond representation **142**
- 5.2.1 Covalent bonds involving metals 142
- 5.2.2 Zero order/ionic bonds 142
  - 5.2.2.1 File format support 143
- 5.2.3 Dative bonds 143
  - 5.2.3.1 Reversing dative bond direction 143
  - 5.2.3.2 File format support 143
- 5.2.4 Haptic bonds and multi-center attachments 143
  - 5.2.4.1 Removing a multi-center attachment 145
  - 5.2.4.2 File format support 145

5.3 Models **146**
- 5.3.1 Ionic 146
  - 5.3.1.1 Delocalization considerations 146
  - 5.3.1.2 Charges in aromatic rings 147
- 5.3.2 Covalent 148
  - 5.3.2.1 Delocalization considerations 148

5.4 Limitations **149**
- 5.4.1 Cheminformatics functions 149
- 5.4.2 Aromatic π electron counts in haptic systems of covalent models 149

5.5 Examples **150**
- 5.5.1 Diamminesilver(I) 150
- 5.5.2 Ferrocene 150
- 5.5.3 Lithium aluminum hydride 152
- 5.5.4 Zeise's salt 152

5.1 Overview

The tools introduced in the DRAWING CHEMICAL STRUCTURES chapter can also be used to draw inorganic structures, including metal compounds and complexes. However, salts, coordination complexes and organometallic compounds often require additional control over connectivity, charges and implicit hydrogens. This chapter explains how to:

- Define zero-order or ionic bonds
- Define dative bonds
- Create haptic bonds using multi-center attachments
- Represent salts, ligands and counterions
- Use consistent ionic or covalent representations
- Ensure both excellent graphics and the integrity of the underlying chemical structure model
- Draw examples of common inorganic structures

5.2 Choosing a bond representation

When you are creating a metal-containing structure, choose a bond type according to the interaction and representation you intend to describe. The presence of a metal does not by itself determine the bond type.

While there are many bond types in ChemDoodle, the bond types described in this section are suitable for metal-containing structures, if not solely for them. A single complex may contain any combination of these bond types.

5.2.1 Covalent bonds involving metals

Covalent bonds (single, double, triple, quadruple) are often used in metal compounds, including representations of metal–carbon, metal–hydrogen and metal–metal bonds. These bonds contribute to the atoms' covalent valences and affect their implicit hydrogen counts accordingly.

5.2.2 Zero order/ionic bonds

A zero-order bond is an explicit connection assigned a bond order of 0. In ChemDoodle, it groups components without affecting covalent valences or associated implicit hydrogen counts. This is useful for associating ions and counterions, but the bond may be used to group any number or type of chemical structures. Components connected by zero-order bonds are treated as one structure for functions including formula generation, structure cleaning and separation into structures during file output.

You can use a zero-order bond by selecting the **Zero/Ionic** bond type button  in the **Bonds** palette of the **Drawing** toolbar.

Zero-order bonds are rendered as dotted lines. For example, a sodium chloride formula unit represented by Na^+ and Cl^- and connected by a zero-order bond is shown in Figure 5.1. The connection associates the ions.

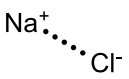


Figure 5.1: *An explicit zero-order connection in a sodium chloride representation*

5.2.2.1 File format support

The *ChemDoodle Document* format is the native filetype of the ChemDoodle application and will correctly store zero-order bonds.

Zero order bonds output in other file types are recorded with a bond order value of 0 where the format supports it. Some file formats explicitly allow a 0 bond order, while others may not. In files where it is not possible to define a 0 bond order, a single bond order will be defined instead. When loading files with zero bond orders into other applications, be wary those applications may not preserve bond order values of 0 on input.

5.2.3 Dative bonds

A dative bond, also called a coordinate bond, describes a bond in which the bonding electron pair is formally supplied by one partner. In ChemDoodle, dative bonds, like zero-order bonds, do not affect covalent valences or associated implicit hydrogen counts.

To draw a dative bond, select the **Dative** bond type button  in the **Bonds** palette of the **Drawing** toolbar. Draw the bond from the electron-pair donor toward the acceptor so the arrow points in the correct direction. For metal complexes, this usually means drawing from a ligand donor atom toward the metal.

In Figure 5.2, ammonia donates the nitrogen atom's lone pair to borane, completing the boron atom's octet.

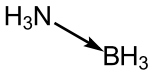


Figure 5.2: *A dative bond from ammonia to borane*

5.2.3.1 Reversing dative bond direction

To reverse an existing dative bond, hover over it and press the F key, or right-click on it and choose Flip Bond Orientation. Double check the direction after editing or importing a structure, since it carries information used by the cheminformatics engine.

5.2.3.2 File format support

ChemDoodle imports and exports dative bonds, including their direction, in the following chemistry file types:

- ACD/ChemSketch Document (*.sk2*)
- CambridgeSoft ChemDraw Exchange (*.cdx*)
- CambridgeSoft ChemDraw XML (*.cdxml*)
- ChemAxon Marvin Document (*.mrv*)
- iChemLabs ChemDoodle Document (*.icl*, *.icxml*)
- iChemLabs ChemDoodle 3D Scene (*.ic3*)
- iChemLabs ChemDoodle JSON (*.cwc.js*)
- MDL CT Files (both v2000 and v3000) (*.mol*, *.sdf*, *.rxn*, *.rdf*)

5.2.4 Haptic bonds and multi-center attachments

Haptic bonding describes the coordination of a metal to two or more contiguous atoms of a ligand. This delocalized interaction can be represented by a single connection in the drawing, simplifying the graphic.

For example, Figure 5.3 shows an η^6 haptic bond between a benzene ring, drawn using a perspective template, and a chromium atom. The single connection from the ring centroid to chromium represents coordination through all six carbon atoms. ChemDoodle treats the ring and chromium atom as parts of the same structure, and the **Elemental Analysis** widget therefore calculates the formula and mass of the combined structur

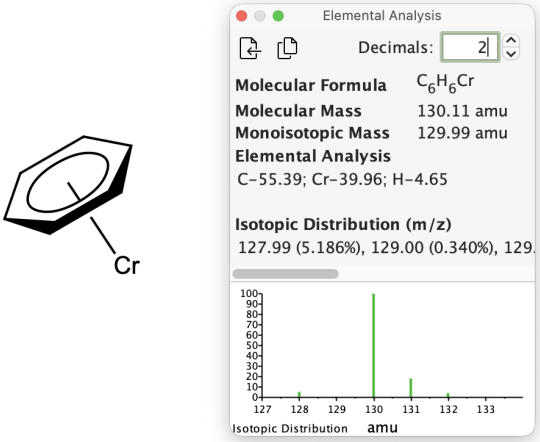


Figure 5.3: *An η^6 haptic bond between a benzene ring and a chromium atom*

Haptic bonds in ChemDoodle are created using multi-center attachments. To create a multi-center attachment:

1. Using a selection tool, select all atoms that will participate in the multi-center end of the haptic bond. At least two atoms must be selected, and all selected atoms must belong to the same molecular structure.
2. Execute the Structure » Add Multi-center Attachment menu item.

A multi-center attachment will appear at the centroid of the selected atoms. Until it is bonded to another atom, the attachment is displayed as an asterisk. Figure 5.4 shows a multi-center attachment created for a benzene ring.

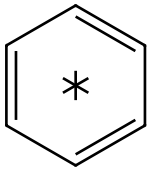


Figure 5.4: *A multi-center attachment added to a benzene ring*

The multi-center attachment represents all of its associated ligand atoms. When you hover over the attachment with a selection tool, temporary guide lines are displayed between the attachment and those atoms, as shown in Figure 5.5.

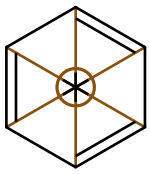


Figure 5.5: *Hovering over a multi-center attachment reveals its associated atoms*

A multi-center attachment can be selected, moved and deleted similarly to an atom. To complete a haptic bond, choose the bond type appropriate for your model and draw a bond between the attachment and the acceptor atom, which may be in the same or another structure. For example, Figure 5.6 shows a single bond to chromium. Once the bond is created, the asterisk is hidden, although the multi-center attachment remains part of the chemical model.

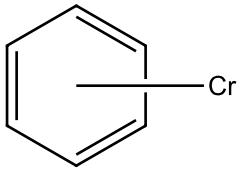


Figure 5.6: *A benzene multi-center attachment connected to chromium by a single bond*



As a shortcut, you may also select exactly one additional atom from a second, separate molecular structure before executing the Structure » Add Multi-center Attachment menu item. In this case, ChemDoodle automatically creates a bond between the new multi-center attachment and the selected isolated atom. If all selected atoms are neutral, a single bond is defined. If any selected atom is explicitly charged, a zero-order bond is defined instead.

5.2.4.1 Removing a multi-center attachment

To delete a multi-center attachment, select the **Erase** button  in the **Content** toolbar. Hover the multi-center attachment to be deleted and click the mouse. You may also press the delete or backspace key when a multi-center attachment is hovered to quickly remove it. All attached bonds will also be removed, leaving the adjacent atoms.

A multi-center attachment is automatically removed if any of its associated ligand atoms are deleted or if those ligand atoms become divided among separate molecular structures, which may occur when bonds are removed. Undoing the action that invalidated the attachment will restore it.

5.2.4.2 File format support

ChemDoodle imports and exports haptic bonds and multi-center attachments in the following chemistry file types:

- CambridgeSoft ChemDraw Exchange (*.cdx*)
- CambridgeSoft ChemDraw XML (*.cdxml*)
- ChemAxon Marvin Document (*.mrv*)
- iChemLabs ChemDoodle Document (*.icl*, *.icxml*)
- MDL CT Files (v3000 only) (*.mol*, *.sdf*, *.rxn*, *.rdf*)

5.3 Models

In ChemDoodle, one of the goals is to produce a beautiful picture to communicate our chemistry. But that does not mean sacrificing the underlying chemical data structure understood to the computer. It is important the underlying model is correct for communicating the chemical data to another program or user, or for various cheminformatics calculations, such as calculating a molecular mass. ChemDoodle's expert tools make it easy to build beautiful pictures that correctly communicate the underlying chemical structures.

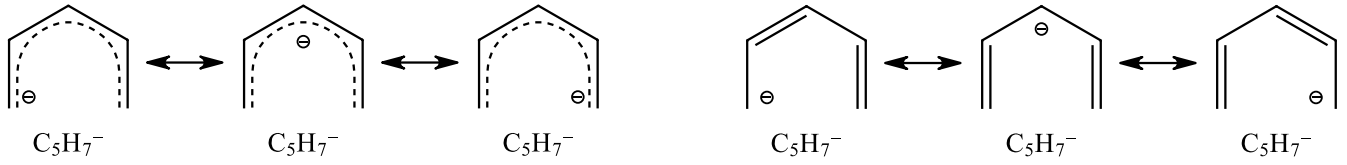
You may find one representation vs. another to be more appropriate for your work. These models may be used interchangeably, even within the same structure. For example, an ionic connection in one part of a structure may coexist with a covalent metal bond elsewhere.

5.3.1 Ionic

For metal–ligand connections in an ionic representation, assign formal charges explicitly and use zero-order or dative bonds. Use a dative bond when the drawing is intended to show electron-pair donation.

5.3.1.1 Delocalization considerations

Charged ligands may be drawn in delocalized form or as individual resonance contributors. In a delocalized drawing, place each formal charge on an atom consistent with a valid resonance contributor. Figure 5.7 compares charge locations in delocalized pentadienyl anions with the corresponding localized drawings.



(a) *Delocalized models of an η^5-pentadienyl anion* (b) *Individual resonance contributors for the η^5-pentadienyl anion*

Figure 5.7: *Ionic models of the pentadienyl anion*



Did you know ChemDoodle can render delocalization curves for conjugated chains, such as in Figure 5.7a? See the CONJUGATED CHAINS section of the CHEMINFORMATICS chapter for instructions.

These ligand representations may be used in haptic connections. For an ionic model, use a zero-order or dative bond from the multi-center attachment to the metal, as shown in Figure 5.8.

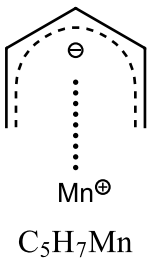
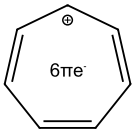
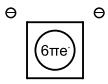
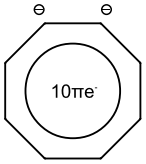


Figure 5.8: *An η^5 haptic connection between a delocalized pentadienyl anion and a manganese cation*

5.3.1.2 Charges in aromatic rings

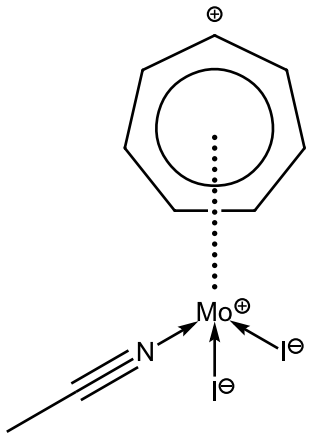
Charged aromatic rings also require explicit formal charges in an ionic model. For the cyclobutadiene and cyclooctatetraene dianions illustrated below, place a -1 charge on each of two consecutive atoms. Table 5.1 compares localized and delocalized representations of carbon-only aromatic rings with three through eight members. The number of π electrons displayed inside each ring is calculated by ChemDoodle and are unambiguous because the electrons are explicit in ionic models.

Table 5.1: *Charges and π-electron counts in the illustrated aromatic ring models.*

Ring	Cyclopropenyl cation	Cyclobutadiene dianion	Cyclopentadienyl anion	Benzene	Cycloheptatrienyl cation (tropylium)	Cyclooctatetraene dianion
Ring size	3	4	5	6	7	8
Net charge shown	$+1$	-2	-1	0	$+1$	-2
Molecular formula	$C_3H_3^+$	$C_4H_4^{2-}$	$C_5H_5^-$	C_6H_6	$C_7H_7^+$	$C_8H_8^{2-}$
Ring π electrons	2	6	6	6	6	10
n in $4n+2$	0	1	1	1	1	2
Full-ring hapticity	η^3	η^4	η^5	η^6	η^7	η^8
Localized						
Delocalized						

Charges and electron counts refer to the illustrated ring models, not to every metal complex containing a ring of that size. Full-ring hapticity applies only when all ring atoms coordinate to the same metal.

When creating a haptic bond to any of these rings for an ionic model, we recommend using a zero-order bond as shown in Figure 5.9.



$C_9H_{10}I_2MoN$

Figure 5.9: *A haptic bond from a tropylium ring in the CSD entry PEVHUT*

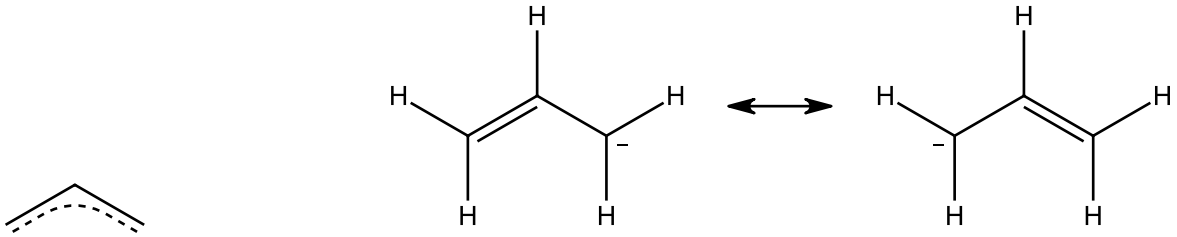
5.3.2 Covalent

In covalent models, the metal and ligand fragments are left neutral and covalent bonds are used for connections. For haptic systems, charges are typically implied by a delocalized ligand.

5.3.2.1 Delocalization considerations

In covalent models, a delocalized ligand may be drawn without an explicit charge because its intended valence interpretation depends on the haptic connection. Until that connection is created, the isolated ligand drawing may have a different implicit hydrogen count from the one intended.

For example, an allyl fragment may be drawn as a three-carbon chain with two resonance bonds. Figure 5.10 compares the uncharged drawing with the resonance contributors of the intended allyl anion.



(a) *An uncharged delocalized allyl drawing* (b) *Resonance contributors of the intended allyl anion*

Figure 5.10: *An η^3-allyl ligand*

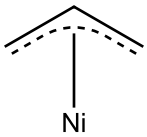
Without an explicit negative charge or a haptic connection, ChemDoodle interprets this drawing as C_3H_6, as shown in Figure 5.11. Valence completion produces an sp^3 carbon at one end of the chain, adding one more hydrogen than intended.



C_3H_6

Figure 5.11: *The uncharged, unconnected allyl drawing is interpreted as C_3H_6*

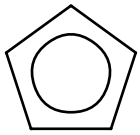
After the multi-center attachment representing the entire allyl ligand is connected to an acceptor with a single bond, ChemDoodle interprets the illustrated ligand as a C_3H_5 fragment, as shown in Figure 5.12.



C_3H_5Ni

Figure 5.12: *The delocalized η^3-allyl ligand is correctly understood when participating in a covalent haptic bond*

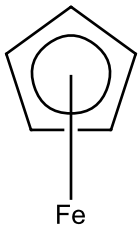
The same consideration applies to delocalized rings. An isolated, uncharged Cp drawing without an explicit radical does not specify the intended cyclopentadienyl fragment. In the example shown, ChemDoodle completes the valences with one sp^3 CH_2 group, giving C_5H_6 rather than C_5H_5. The displayed aromatic circle does not make this model aromatic.



C_5H_6

Figure 5.13: *The uncharged, unconnected Cp drawing is interpreted as C_5H_6*

After the multi-center attachment representing the entire Cp ligand is connected to an acceptor with a single bond, the illustrated ligand has the intended C_5H_5 composition, as shown in Figure 5.14.



C_5H_5Fe

Figure 5.14: *The delocalized Cp ligand is correctly understood when participating in a covalent haptic bond*

5.4 Limitations

5.4.1 Cheminformatics functions

Many cheminformatics algorithms are designed strictly for organic structures with traditional covalent bonds. For instance, creating a bond adjacency matrix would make little sense for a structure containing a haptic bond to a multi-center attachment. Check the documentation for the function you intend to use; successful formula or mass calculation does not establish that other calculations support the same representation.

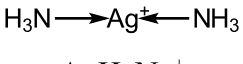
5.4.2 Aromatic π electron counts in haptic systems of covalent models

In the covalent haptic models illustrated here, ChemDoodle accounts for the attachment when determining implicit hydrogen counts. However, the calculated π-electron count for a delocalized aromatic ring may not be accurate or appropriate for that representation. If this count is important, use an ionic model with explicit ring charges that match the intended formal electron count.

5.5 Examples

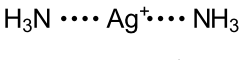
5.5.1 Diamminesilver(I)

Diamminesilver(I) can be represented as an ionic model, using either dative or zero-order bonds as shown in Figure 5.15.



$AgH_6N_2^+$
Diamminesilver(I)

(a) *Dative bonds showing electron-pair donation from nitrogen*



$AgH_6N_2^+$
Silver(I)—ammonia (1/2)

(b) *Zero-order bonds are used*

Figure 5.15: *Ionic models of diamminesilver(I)*

Although the molecular formulas are the same, the IUPAC names generated by ChemDoodle are different. The dative bonds convey donor–acceptor information, while zero-order bonds simply group the components together.

For this ionic representation in ChemDoodle, use dative or zero-order N–Ag bonds to preserve the intended NH_3 ligands. Ordinary single bonds change the implicit hydrogen counts: in Figure 5.16, the nitrogen atoms have NH_2 groups instead. The resulting formula, oxidation states, and chemical identity therefore differ from those of diamminesilver(I).



$AgH_4N_2^+$
Diamidosilver(III)

Figure 5.16: *Single N–Ag bonds result in a different chemical structure*

5.5.2 Ferrocene

The haptic interactions in ferrocene are modeled in ChemDoodle using multi-center attachments. Ferrocene may be represented using either the ionic or covalent electron-counting model. These are alternative formal representations of the same compound, not different forms of ferrocene.



Use **Metallocene** templates from the **Templates** widget to quickly build metallocene structures with perspective rings, such as ferrocene.

Ferrocene is a classic example of the 18-electron rule. This rule states that many stable transition-metal organometallic complexes have a total of 18 valence electrons supplied by the metal and its ligands. Although the rule has many exceptions, both accepted electron-counting methods assign 18 electrons to ferrocene:

- **Ionic model.** The iron center is represented as Fe^{2+} and each cyclopentadienyl ligand as $C_5H_5^-$. Fe^{2+} is a d^6 center and therefore contributes six electrons. Each η^5-cyclopentadienyl anion contributes six electrons:

  $$2(6\,e^-) + 6\,e^- = 18\,e^-$$

  In ChemDoodle, all formal charges must be assigned explicitly and the multi-center attachments are connected to iron using zero-order bonds.

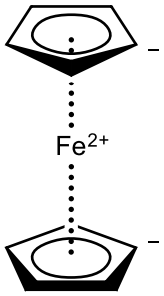


Figure 5.17: *The ionic representation of ferrocene.*

- **Covalent model.** In neutral-atom counting, iron contributes its eight group valence electrons. Each formally neutral cyclopentadienyl fragment ($C_5H_5^{\bullet}$) contributes five electrons:

  $$2(5\,e^-) + 8\,e^- = 18\,e^-$$

  In ChemDoodle, the iron and cyclopentadienyl fragments are left neutral and the multi-center attachments are connected to iron using single bonds.

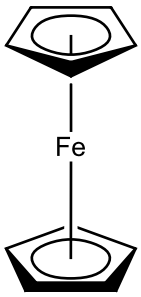


Figure 5.18: *The covalent representation of ferrocene.*

ChemDoodle accepts either representation, provided their formal charges and bond orders are used consistently. Changing only the charges or only the bond types can produce an unintended structure.

Figure 5.19 shows an invalid mixed representation in which neutral cyclopentadienyl fragments and a neutral iron center are connected using zero-order bonds. Because zero-order bonds do not satisfy the normal covalent valences, valence completion produces one sp^3 CH_2 atom in each five-membered ring. These atoms are consequently flagged with the warning "Unlikely constituent in resonance ring."

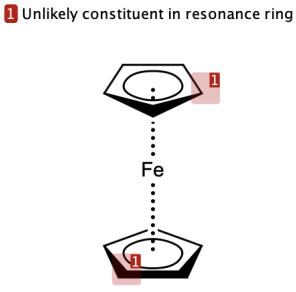
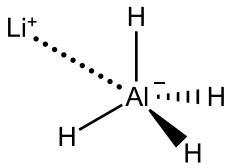


Figure 5.19: *An inconsistent ferrocene representation produced by mixing the ionic and covalent models.*

5.5.3 Lithium aluminum hydride

Lithium aluminum hydride combines covalent Al–H single bonds with a zero-order connection between Li^+ and the $[AlH_4]^-$ anion. Aluminum carries a formal charge of -1 in this single-bond representation. The grouped structure is neutral and has the formula $LiAlH_4$.



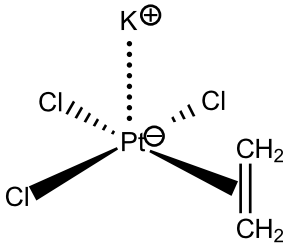
AlH_4Li

Figure 5.20: *Lithium aluminum hydride*

5.5.4 Zeise's salt

Zeise's salt illustrates covalent, dative, zero-order and haptic connections. The following drawings illustrate covalent and ionic models of the structure.

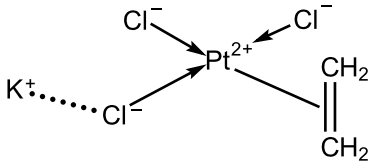
The covalent representation uses single bonds, drawn as wedges to show the square-planar geometry around platinum. A protruding bond type is used for the haptic connection to ethene. A zero-order bond connects the potassium atom to the platinum-containing component so that they are treated as one structure.



$C_2H_4Cl_3KPt$

Figure 5.21: *A covalent representation of Zeise's salt.*

In the ionic representation, assign a -1 charge to each chloride, $+1$ to potassium and $+2$ to platinum; ethene remains neutral. Draw dative bonds from the chloride atoms toward platinum to represent electron-pair donation. The K^+ counterion balances the net -1 charge of the $[PtCl_3(C_2H_4)]^-$ complex as a whole. Connect these components with a zero-order bond to group them without changing their explicit charges.



$C_2H_4Cl_3KPt$

Figure 5.22: *An ionic representation of Zeise's salt.*

In both representations, the molecular formula is correctly $C_2H_4Cl_3KPt$.

CHAPTER 6

Advanced Structures

Contents

6.1 Overview **155**

6.2 3D structures **155**
6.2.1 Perspective drawings 156
6.2.1.1 Starting from 3D coordinates 156
6.2.1.2 Partial structure manipulation 156
6.2.1.3 Manipulating aromatic ring circles 157
6.2.1.4 Perspective ring templates 157
6.2.2 Pseudo-3D graphics 158
6.2.3 ChemDoodle 3D integration 159

6.3 Lewis dot structures **160**
6.3.1 From drawn structures 160
6.3.2 Manually draw Lewis dot structures 160

6.4 Macromolecule builders **161**
6.4.1 Carbon nanotubes 161
6.4.2 Prismanes 161

6.5 Newman projections **162**

6.6 Sequence tool **163**

6.1 Overview

The previous chapter (DRAWING CHEMICAL STRUCTURES) introduced the tools necessary to build chemical structures. You can build any chemical structure imaginable with those tools. However, you may need to draw more advanced structures that will require more time and experience with ChemDoodle to draw efficiently. This chapter introduces the new user to techniques and tools within ChemDoodle for advanced structures. These include creating templates for structures such as Newman projections to using built-in ChemDoodle tools for drawing carbon nanotubes. The topics covered in this chapter include:

- 3D structures, including perspective and pseudo-3d graphics
- Lewis dot structures
- Carbon nanotubes, including armchair, zigzag and chiral variants
- Prisms
- Rings
- Newman projections
- Sequences

6.2 3D structures

The main ChemDoodle program is a tool for generating 2D graphics; to generate 3D graphics, you can use ChemDoodle 3D (https://www.chemdoodle.com/3d), which has its own user guide. Trying to do the same in ChemDoodle, with all of the bond types and atom labels showing, will result in very unclear figures. A sample image from ChemDoodle 3D is shown in Figure 6.1.

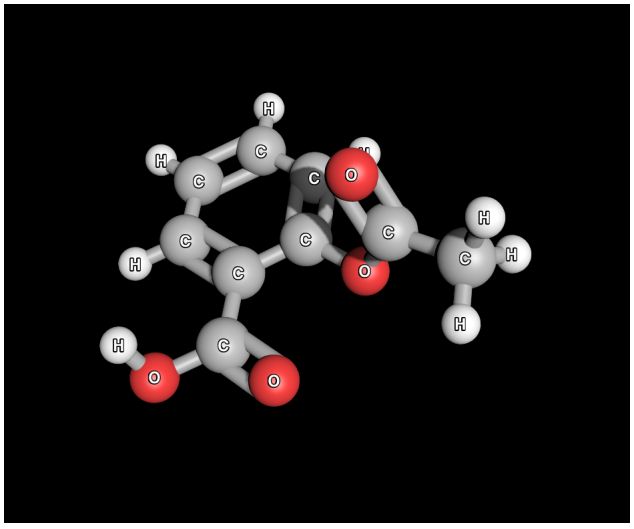


Figure 6.1: *A sample structure image from ChemDoodle 3D*

However, ChemDoodle does handle 3D input and all structures are represented internally by 3D coordinates. So you can create orthographic 2D scenes of your 3D data. Many users will take advantage of these features to create beautiful perspective drawings or pseudo-3D vector graphics. But these are advanced techniques and excellent results are more difficult to achieve. Techniques for doing so are described in this section.

6.2.1 Perspective drawings

ChemDoodle provides advanced algorithms for merging bond graphics. This makes it possible to create publication quality perspective drawings. A perspective drawing is a figure where the chemical structure is rendered as a flat 2D graphic, but segments of the structure are manipulated to give it a 3D appearance using bold and wedge bonds. There are two common ways for creating perspective drawings.

6.2.1.1 Starting from 3D coordinates

One method to create perspective drawings is as follows:

1. Load in a structure file with 3D coordinates. Alternatively, you can draw your molecule, select it and use one of the 3D coordinate options in the Structure » Clean submenu to generate 3D coordinates.
2. Select the 3D structure. Using the **Rotate in 3D** tool in the **Content** toolbar, rotate your structure so it is in the desired orientation.
3. Change the appropriate bonds to be their wedge and bold equivalents if they are in front of other bonds.
4. Adjust the positions of individual atoms as desired.

We use this technique to build a number of our templates that are perspective drawings, including cyclic terpenes and hexoses as shown in Figure 6.2.

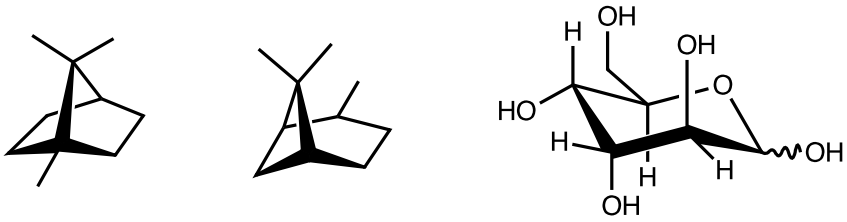


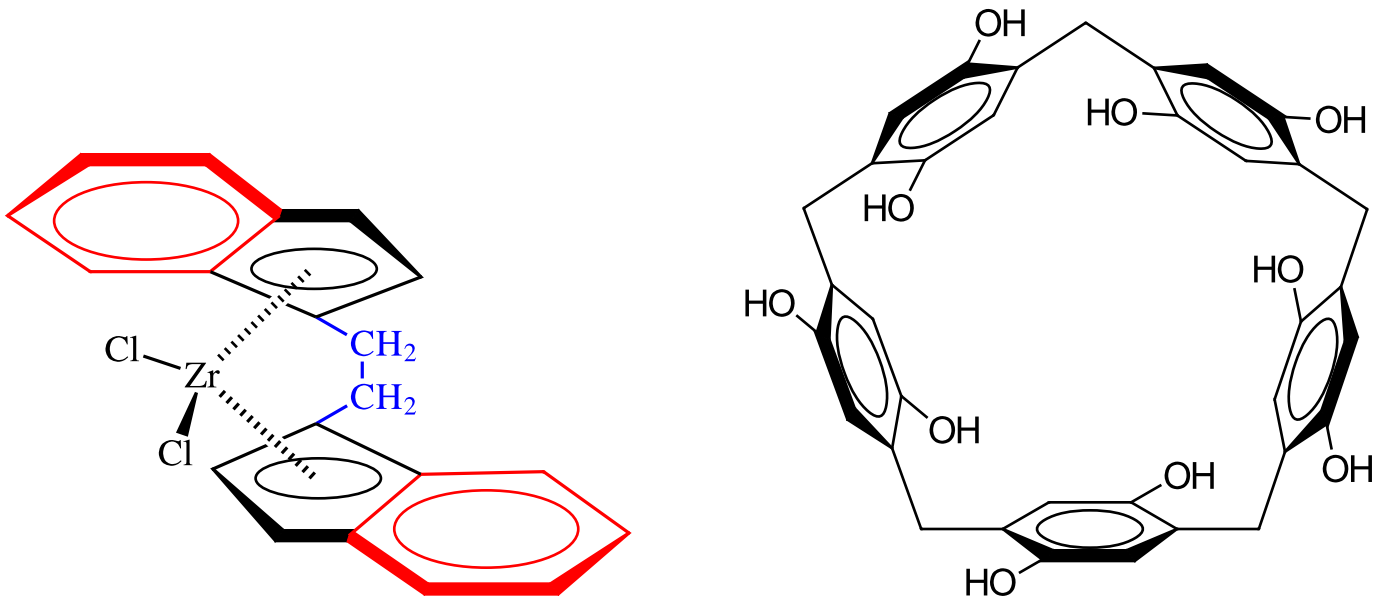
Figure 6.2: *Perspective drawings from 3D coordinates*

6.2.1.2 Partial structure manipulation

Another method to create perspective drawings involves only partial structure 3D manipulation:

1. Draw the structure as if it was flat. Parts of the structure that you wish to present in a perspective manner (such as rings) should be drawn separately.
2. Select the parts you wish to display in a perspective manner. Using the **Rotate in 3D** tool in the **Content** toolbar, rotate these pieces so they are drawn in the desired orientation.
3. Change the appropriate bonds to be their wedge and bold equivalents if they are in front of other bonds.
4. Adjust the positions of individual atoms as desired.
5. Attach these perspective parts to the rest of the flat structure.

Some examples of this technique can be seen in Figures 6.3.



(a) *Perspective drawing including connections to aromatic rings* (b) *Perspective drawing of Pillar[5]arene*

Figure 6.3: *Sample Perspective Drawings*

6.2.1.3 Manipulating aromatic ring circles

Aromatic ring circles are rendered by a special algorithm that molds to the shape of the aromatic ring in 3D. This allows you to easily create complex perspective figures using aromatic circles, as shown for various rotations of benzene in Figure 6.4.

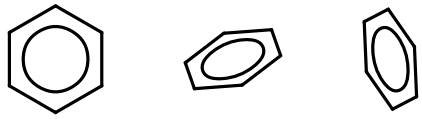


Figure 6.4: *The aromatic ring circle display for rotated perspective drawings*

Aromatic ring circles will even mold to nonplanar or warped rings as shown in Figure 6.5.



Figure 6.5: *Aromatic Ring Circles Mold to any Shape.*

6.2.1.4 Perspective ring templates

For quick drawing of structures with perspective rings, such as metallocenes, the following template sets are included in the **Templates** widget.

- **Rings (Cp-)** - Cyclopentadienyl anion rings
- **Rings (Flu-)** - Fluorenyl anion rings
- **Rings (Ind-)** -Indenyl anion rings
- **Rings (Benzene)** - Benzene rings
- **Rings (Tropylium)** - Tropylium cation rings

For more information on using templates in ChemDoodle, please see sections TEMPLATES WIDGET and TEMPLATES. To demonstrate, the **Rings (Cp)** set in the **Templates** widget is shown in Figure 6.6.

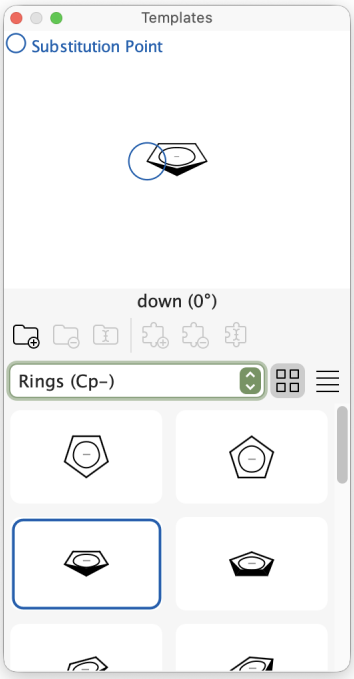


Figure 6.6: *Cyclopentadienyl anion rings in the Templates widget.*

These templates have 3D coordinates defined, so you may rotate them with the **Rotate in 3D** tool ( ). Additionally, perspective templates are only provided for a 90° rotation around the z-axis. Use the Content ⟩ Flip submenu items to get orientations in the other 3 quadrants (see Figure 6.7).



Figure 6.7: *Flip perspective ring templates for more orientations.*

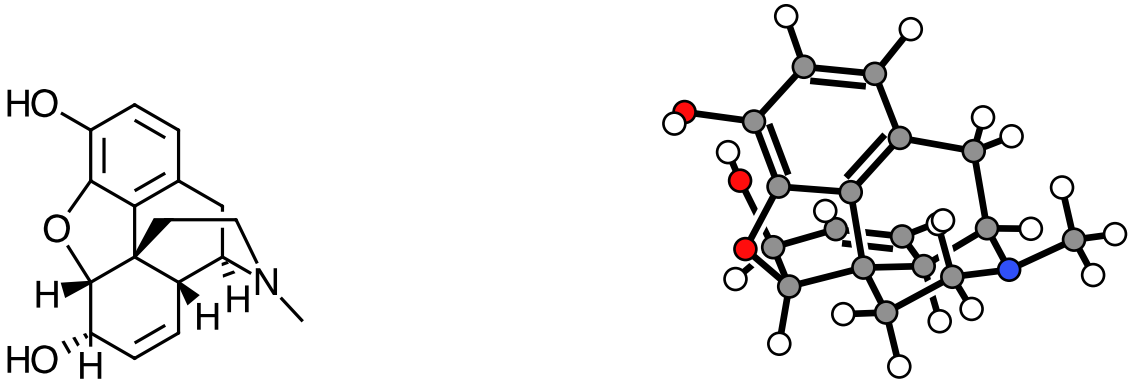
6.2.2 Pseudo-3D graphics

For high quality perspective 3D scenes, or other representations in three dimensions, use ChemDoodle 3D (https://www.chemdoodle.com/3d). If you must create 3D-like graphics in ChemDoodle, we recommend the following styling:

- Change all bonds to plain single bonds, and include double bonds if necessary.
- Change the styles to show all atoms as circles instead of as text labels. Change the radius accordingly for the size of your image.
- Change the styles to render atoms with their Jmol colors.
- Increase the bond thickness style.
- If you desire, change the styles to render bonds with a split color between their constituent atoms.
- Increase the bond overlap buffer style to clearly show bond overlaps.

Styles are covered thoroughly in the STYLES chapter.

After you are satisfied with the styling, rotate the structure as necessary to reduce overlapping components as much as possible. Only an orthographic projection can be achieved in ChemDoodle, you will need ChemDoodle 3D for 3D perspective projections. Example output and comparison to a perspective drawing of morphine (not to be confused with a 3D perspective projection) can be seen in Figures 6.8.



(a) *Perspective drawing of morphine*

(b) *Pseudo-3D rendering of morphine*

Figure 6.8: *Pseudo 3D*

6.2.3 ChemDoodle 3D integration

If you have both ChemDoodle and ChemDoodle 3D installed on your machine, you can use ChemDoodle to load or draw structures in real time in ChemDoodle 3D.

There are two menu items present for connecting to ChemDoodle 3D, found in the File › Interfaces › ChemDoodle 2D menu:

- View Molecule in 3D
- Bind Molecule in 3D

To use either of these methods, first make sure that ChemDoodle 3D is open and running on your computer.

To load an existing structure in/within/from ChemDoodle into ChemDoodle 3D, select it and use the File › Interfaces › ChemDoodle 2D › View Molecule in 3D menu item. The structure will then appear in ChemDoodle 3D, have hydrogens added and 3D coordinates generated. You may then edit the molecule in ChemDoodle 3D.

If you would like to build your molecule in real time in ChemDoodle 3D using ChemDoodle, start drawing a molecule in ChemDoodle and select it using any selection tool. Then use the File › Interfaces › ChemDoodle 2D › Bind Molecule in 3D menu item. Your molecule will then appear in ChemDoodle 3D. If you then continue to edit your molecule in ChemDoodle, you will see the corresponding structure in ChemDoodle 3D update as you edit.

6.3 Lewis dot structures

Lewis Dot Structures can be created manually or with a convenient function in the Structure menu.

6.3.1 From drawn structures

To quickly create a Lewis Dot Structure from a drawn molecule, execute the following steps:

1. Select the molecule you would like to generate a Lewis Dot Structure from.
2. Select the Structure > Create Lewis Dot Structure item.

The created Lewis Dot Structure will then appear below the selected structure. This function will work on the majority of structures and will automatically place lone pairs to satisfy the octet rule. Output of this function is show in Figure 6.9. You may wish to post edit these structures or change their scales for the optimal figures.

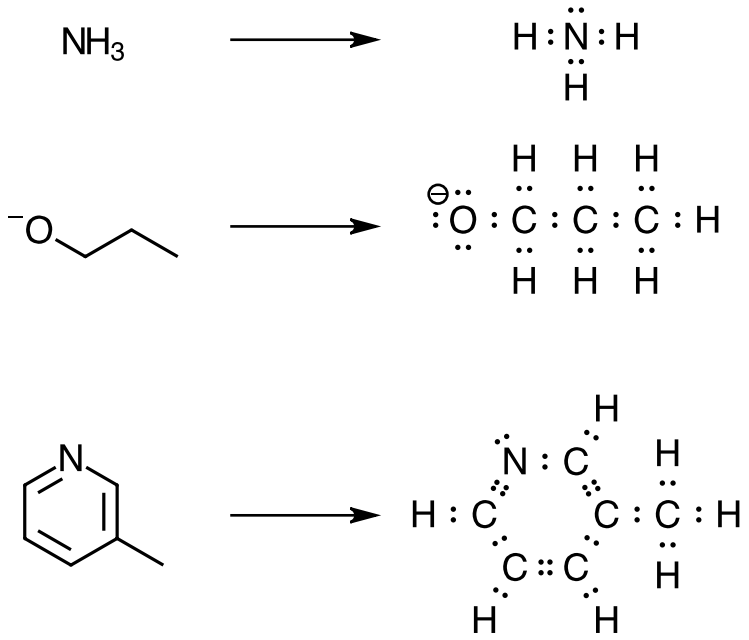


Figure 6.9: *ChemDoodle generates Lewis Dot Structures for drawn molecules.*

6.3.2 Manually draw Lewis dot structures

To manually create Lewis Dot Structures, you can modify a few options in ChemDoodle. Then as you draw, the tools will be optimized for Lewis Dot Structures and allow you to create them easily.

- **Bond Length** (Styles>Bonds>Settings) - Increase the bond length (30px recommended) to easily view double and triple bonds. You can also break from standard lengths when drawing for custom bond lengths.
- **Use Lewis Dot Style** (Styles>Bonds>Options) - Enable this option to change from rendering standard bond order bonds to their Lewis Dot Structure equivalent.
- **Show Implicit Hydrogens** (Styles>Atoms>Hydrogens) - While experienced chemists will want to see implicit hydrogens, they are not part of Lewis Dot Structures. Disable them and make sure to add all hydrogens explicitly.
- **Chain Angle** (Settings>Tools>Cleaning) - Set the chain angle to 180° to have the clean tool clean structures to 90° angles.

6.4 Macromolecule builders

ChemDoodle provides a few tools for building complex molecule geometries.

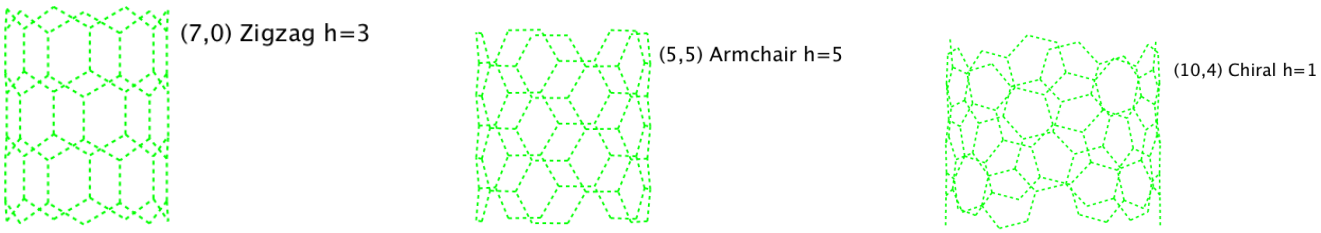
All structures generated by these tools are defined by 3D coordinates, so you can use the **Rotate in 3D** tool in the **Content** toolbar to change the orientation.

6.4.1 Carbon nanotubes

To create carbon nanotubes, select the **Carbon Nanotube Builder** tool in the **Macromolecular Tool** palette in the **Drawing** toolbar. You can then place a carbon nanotube by executing the following steps:

1. Press the mouse down in the current document where you would like the base of the carbon nanotube to sprout from.
2. While the mouse is pressed down, move the mouse horizontally to change the width of the carbon nanotube. The carbon nanotube will expand the number of rings present in the loop to fit a width that reaches the mouse pointer.
3. While the mouse is pressed down, move the mouse vertically to change the height of the carbon nanotube. The carbon nanotube will expand the number of loops present to fit a height that reaches the mouse pointer.
4. By default, zigzag geometries are created, hold down the shift key to create armchair geometries instead.
5. If you hold any of the number keys 1-9 down, you will be able to set the m value for the nanotube, allowing you to create chiral variants. The 0 key will set m equal to 10.
6. Release the mouse when you are satisfied with the current geometry to place it.

ChemDoodle will automatically place double bonds in the carbon nanotube. While using the tool to create carbon nanotubes, a preview will be displayed without double bonds to more easily view the output, and a description will be displayed to the bottom right of the mouse pointer stating whether the geometry is zigzag or armchair or other statistics about the geometry as shown in Figure 6.10.



(a) *Zigzag Carbon Nanotube Geometry* (b) *Armchair Carbon Nanotube Geometry* (c) *Chiral Carbon Nanotube Geometry*

Figure 6.10: *Carbon Nanotube Geometry*

Once set, double bonds will automatically be placed in the generated nanotube for you. You can select the nanotube and use the Structure > Saturate menu item to remove all double bonds, if desired.

6.4.2 Prismanes

To create prismanes, select the **Prismane Builder** tool in the **Macromolecular Tool** palette in the **Drawing** toolbar. You can then place a prismane by executing the following steps:

1. Press the mouse down in the current document where you would like the center of the prismane to be located.

2. While the mouse is pressed down, move the mouse horizontally to change the width of the prismane. The prismane will expand the number of rings present to fit a width that reaches the mouse pointer.
3. While the mouse is pressed down, move the mouse vertically to change the height of the prismane. The prismane will expand the number of levels present to fit a height that reaches the mouse pointer.
4. Release the mouse when you are satisfied with the current geometry to place it.

While using the tool to create prismanes, a preview will be displayed with a description to the bottom right of the mouse pointer stating statistics about the geometry as shown in Figure 6.11.

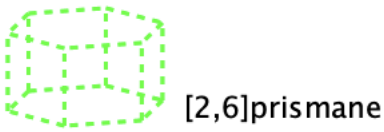


Figure 6.11: *Building a Prismane Geometry*

6.5 Newman projections



Starting with ChemDoodle v12.10, Newman projection templates are now included for use in the **Templates** widget in the **Rotational Conformations** template set. See the WIDGETS chapter for more information. If you wish to create Newman projection graphics from scratch, please follow the instructions in this section.

To build graphics for Newman projections, execute the following steps:

1. Draw a 2-methylpropane structure.
2. Hover the central atom and right-click.
3. Select the Format Atom... menu item.
4. In the **Elements** section, select the **Use Circles** checkbox, make sure **Coloring** is set to **Uniform** and **Radius Convention** is set to **Constant**, and then set the **Constant Radius** to the preferred size. You will now see a black circle appear over the central carbon.
5. In the same **Atom Styles** window, under the **Colors** section, change the **Text** color to white. You should now see a figure just like Figure 6.12.

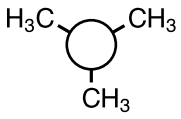


Figure 6.12: *A Half-completed Newman Projection*

6. Click on the **Accept** button to exit the **Atom Styles** window.
7. Draw a second 2-methylpropane structure.
8. Rotate the second structure to the desired torsion for the Newman Projection.

9. Using a selection tool, move the second drawn structure over the first to complete the Newman Projection.

You can then edit the terminal labels to display the structure desired as is shown in Figure 6.13. You may wish to save a copy of this structure as a file for later use.

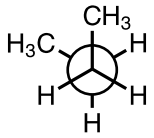


Figure 6.13: *A Completed Newman Projection*

6.6 Sequence tool

ChemDoodle provides a tool for generating sequence structures for common polymer types. The following polymer types are supported:

1. Three Letter Amino Acid Sequence

To generate sequences, use the **Three Letter Amino Acid Sequence** tool  from the **Macromolecular Tool** palette in the **Drawing** toolbar. To draw a sequence, execute the following steps:

1. Click on the current document where you want the sequence to originate from. The endpoints of the sequence will appear. For amino acid sequences, a water molecule will appear.
2. A single atom will be surrounded by a blue circle; this is the appending atom. All changes to the sequence append directly to this atom. You can hover over other atoms and click to set a different appending atom.
3. Use the keyboard to type the one letter hotkeys for the residues in the sequence set. For instance, pressing the A key will append an alanine residue, and pressing the R key will append an arginine residue.

Sequences will automatically wrap to stay within the margins of the current document as shown in Figure 6.14.

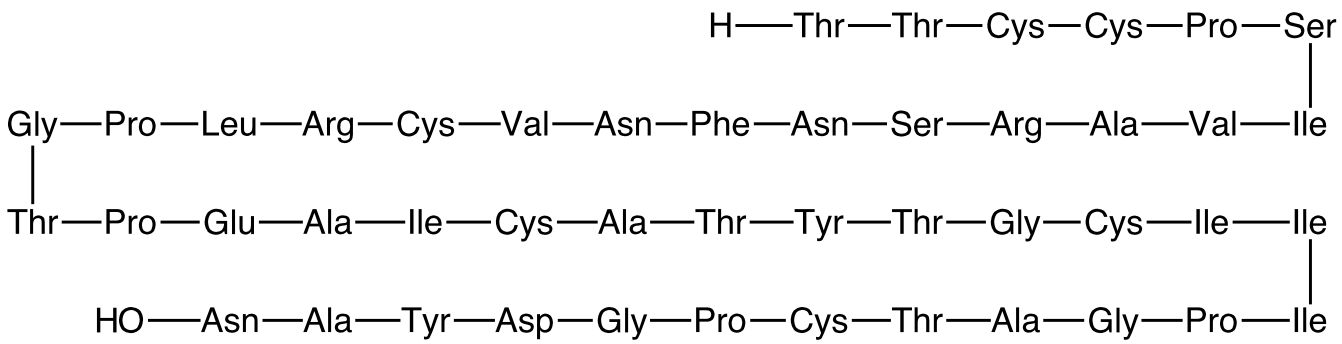


Figure 6.14: *A Wrapped Sequence for Crambin*

Use this tool to easily create macromolecular structures, and to quickly calculate properties such as weights and isotopic distributions.

CHAPTER 7

Query Structures

Contents

7.1 Overview **166**

7.2 What are query structures? **166**

7.3 Variables **167**
- 7.3.1 Atom variables 167
- 7.3.2 Bond variables 168
- 7.3.3 NOT operator 169

7.4 How to draw query structures **169**
- 7.4.1 Using the query interface to build queries 169
- 7.4.2 Manually typing a query 170
- 7.4.3 Setting the query 170

7.5 Uses of query structures **171**
- 7.5.1 Graphics 171
- 7.5.2 Search widget functionality 171
- 7.5.3 Private searching 171

7.6 Comparison to SMARTS **171**

7.1 Overview

In the DRAWING CHEMICAL STRUCTURES chapter, we discussed how to draw molecules. Each molecule is discrete and describes a single explicit structure. However, some tasks require the definition of a set of structures. For instance, if we need to do a database search for a group of molecules. This would mean having to draw all the structure possibilities to create a complete description of the set and running the search for each drawn structure. This can be very time consuming and prone to errors.

Query structures simplify this by defining a set of structures in a single drawing. You will define variables to the atoms and bonds and the structure will now represent all the possible combinations of these variables. While the graphic itself is a concise definition and can be used communicate the set of structures to other chemists, in ChemDoodle it is also interpreted as a data structure for performing more advanced computational tasks. Therefore these structures can be used for database searching, among other things.

This section introduces the new user to query structure features within ChemDoodle. It covers the following topics:

- What are query structures?
- How to build query structures in ChemDoodle.
- An overview of the query variables for atoms and bonds.
- How to use query structures.
- How does this relate to SMARTS?

7.2 What are query structures?

A query structure resembles other chemical structures, however various variables are set for the nodes (query atoms) and edges (query bonds) to define the possibilities allowed at those positions. For instance, in Figure 7.1, the query structure defines any molecule with a benzene ring where a halogen **[x]** is ortho to a saturated oxygen, sulfur or selenium atom and para to a 3 membered chain where the second bond is either a single or double bond and is contained in no rings.

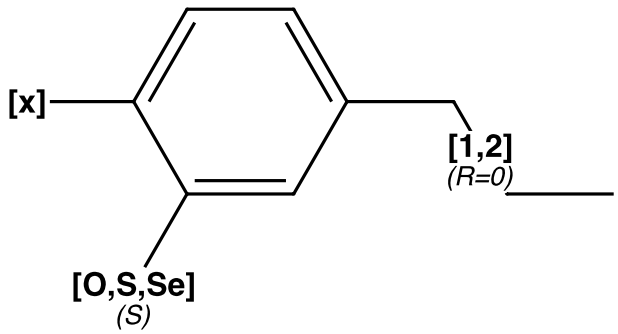


Figure 7.1: *A query structure*

A query structure is therefore a visual representation of a set of chemical structures. But it is also a computational construct, representing a graph data structure that software can use to also understand this set of chemical structures. For instance, let us consider a search of a molecule database. Structure matches will help to find molecules exactly as drawn, but users will also want to search for a range of results that fit some rules. To do this, ChemDoodle provides a query tool to create query structures. A user can set various properties to query atoms, such as element types, aromaticity and connectivity definitions. The same can be done for query bonds. The search then returns all results that fit those rules, allowing users to quickly discover a vast amount of desired information.

Note that query atoms and query bonds with no variables defined are defaulted to only representing their current definition. A carbon atom will be interpreted as a query atom that only matches carbon (**[C]**), while a single bond will be interpreted as a query bond that only matches single bonds (**[1]**).

7.3 Variables

There are two types of variables, *identity* variables and *attribute* variables. *Identity* variables define the entity type: element types for atoms and bond orders for bonds and are graphically represented in bold between square brackets. *Attribute* variables define all remaining criteria, such as the number of hydrogens on an atom or whether a bond is in a ring or not. *Attribute* variables are graphically represented in italics between parentheses below the *identity* variables.

Attribute variables are further categorized into several types as defined in Table 7.1 below. Each type corresponds to the type of data it matches and defines the match values.

Table 7.1: Attribute Variable Types

Type	Description	Value
Boolean	This datatype matches on a true/false basis, for instance declaring that a matched atom must be aromatic.	The value is implied at true. Use the not operator to force a false.
Integer	This datatype matches an integer or some range of values, for instance declaring that the atom's charge must be a certain value.	The value can be a specific integer value or an arbitrary range. For instance, users can define the charge to be -3, -1, or from 2-3.
Hash	This datatype matches a value that is mapped to some set of characters, for instance declaring that a matched atom's chirality must be either 'R' or 'S'.	The value is a character of the allowed values defined for the variable. For instance, for atom chirality, the allowed values are 'R', 'S' or 'A'.

7.3.1 Atom variables

The *identity* variables for query atoms define the allowed elemental values for matched atoms. The following values are allowed:

1. **Element Symbols** – H, C, N, Fe, Mn, U, etc. These are the element symbols from the periodic table and will match any atom of that element.
2. **Any** – The any wildcard, specified by a lowercase 'a' symbol, will match any atom label. This is the default.
3. **Non-hydrogen** – The non-hydrogen wildcard, specified by a lowercase 'r' symbol, will match any atom label except hydrogen.
4. **Heteroatom** – The heteroatom wildcard, specified by a lowercase 'q' symbol, will match any atom label except hydrogen or carbon.
5. **Halide** – The halide wildcard, specified by a lowercase 'x' symbol, will match any halogen symbol: F, Cl, Br, I, At.
6. **Metal** – The metal wildcard, specified by a lowercase 'm' symbol, will match any metal (transition metals, other metals).

The following query atom *attribute* variables are available:

Table 7.2: Atom Attribute Variables

Variable	Symbol	Datatype	Description
Aromaticity	**A**	Boolean	Matches any atom that is aromatic
Charge	**C**	Integer	Matches any atom with charge defined by range
Chirality	**@**	Hash	Matches any atom with CIP stereochemistry of 'R' or 'S', 'A' will match any stereocenter
Connectivity	**X**	Integer	Matches any atom with number of connections defined by range
Connectivity (No H)	**x**	Integer	Matches any atom with number of connections defined by range, not including any connections to hydrogen
Hydrogens	**H**	Integer	Matches any atom with number of connections to hydrogens defined by range, both implicit and explicit
Rings	**R**	Integer	Matches any atom contained in the number of rings defined by range (SSSR set)
Saturation	**S**	Boolean	Matches any atom that is saturated (connected to only single bonds)

Any combination of these *attribute* variables may be defined for a query atom, with or without the *identity* variable (the default is any element symbol). Combined with the *not* operator, very advanced queries are possible.

7.3.2 Bond variables

The *identity* variables for query bonds define the allowed bond type values for matched bonds. The following values are allowed:

1. **Positive Whole Numbers** – 0, 1, 2, 3, 4, and so on. These represent the standard zero, single, double, triple, quadruple and so forth bonds.
2. **Any** – The any wildcard, specified by a lowercase 'a' symbol, will match any bond type. This is the default.
3. **Half** – The half bond, specified by a lowercase 'h' symbol, will match any half bond, or 0.5 bond order bond (a single electron).
4. **Resonance** – The resonance bond, specified by a lowercase 'r' symbol, will match any resonance bond, or 1.5 bond order bond (delocalized).

A single variable, or any combination of variables is allowed for the *identity* definition.

The following query bond *attribute* variables are available:

Table 7.3: Bond Attribute Variables

Variable	Symbol	Datatype	Description
Aromaticity	**A**	Boolean	Matches any bond that is aromatic
Rings	**R**	Integer	Matches any bonds that are members of the number of rings defined by range (SSSR set)
Stereochemistry	**@**	Hash	Matches any bond with CIP stereochemistry of 'E' or 'Z', 'A' will match any stereocenter

Any combination of these *attribute* variables may be defined for a query bond, with or without the *identity* variable (the default is any bond type). Combined with the *not* operator, very advanced queries are possible.

7.3.3 NOT OPERATOR

The *not* operator inverts the query variable and is represented by an exclamation point (**!**) before the variable. Any variable, either identity or attribute, can be inverted. So for instance, a user can define to a query atom a saturated variable with the *not* operator to designate an unsaturated atom match.

7.4 HOW TO DRAW QUERY STRUCTURES

Use the **Set Query to Atom or Bond** button  to start query mode in ChemDoodle. The **Query** button can be found in the **Text Tools** tray at the top of the **Drawing** toolbar. Atoms and bonds can then be hovered. Select the atom or bond to define a query to and click the mouse. The query editor will appear for that object as shown in Figure 7.2. The interface for atoms is different from the interface for bonds.



(a) *Query Interface for Atoms* (b) *Query Interface for Bonds*

Figure 7.2: *Query Interface*

The button furthest to the right  removes the current query from the object. The button second from the right  cancels the current changes to the query or cancels the query if it is being initialized.

7.4.1 USING THE QUERY INTERFACE TO BUILD QUERIES

The buttons in the middle are the variables, starting with the identity definition and followed by all the attribute variables. Select one of the variables and a popup will appear above the query toolbar with an interface to set the available settings for that variable as shown in Figure 7.3.

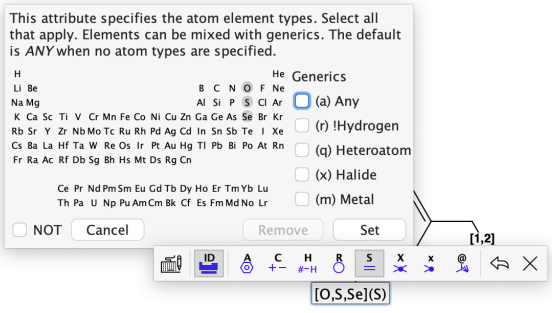


Figure 7.3: *The interface to define a query variable, in this case the atom identity variable*

Each variable can be set according to the rules defined in the VARIABLES section above and each interface will contain instructions for how to set the selected variable. Once defined, select the **Set** button to add the variable to the query. The **Cancel** button will cancel the current changes to the selected variable and close the variable interface, and the **Remove** button

will remove the selected variable from the query if it is currently there. Once added, the variable will appear in the text field below the query toolbar.

The meaning of the button icons for atom queries is listed in Table 7.4.

Table 7.4: Atom Query Variable Icons

Variable	Title	Variable Type
	Element Types	*identity*
	Aromaticity	*attribute*
	Charge	*attribute*
	Total Number of Attached Hydrogens	*attribute*
	Total Number of Rings	*attribute*
	Saturation	*attribute*
	Total Connectivity	*attribute*
	Total Connectivity Without Hydrogens	*attribute*
	Chirality	*attribute*

The meaning of the button icons for bond queries is listed in Table 7.5.

Table 7.5: Bond Query Variable Icons

Variable	Title	Variable Type
	Bond Order Types	*identity*
	Aromaticity	*attribute*
	Total Number Of Rings	*attribute*
	Stereochemistry	*attribute*

7.4.2 Manually typing a query

The button furthest to the left  allows you to manually type in the query specification. Advanced users may want to use this tool. If you are just beginning with the query structures in ChemDoodle, it is recommend that you first familiarize yourself with the query language by using the variable buttons as described above until you are comfortable with the scope and definitions allowed. No matter how you manually specify a correct query, ChemDoodle will automatically parse and standardize the query text for you when set. If incorrect text is included in a manually typed query, ChemDoodle will attempt to salvage the query by discarding uninterpretable parts of the text. If no part of the query can be salvaged, that input will be replaced with the default generic atom or bond query when set (**[a]** - "any" for both atoms and bonds).

7.4.3 Setting the query

Click anywhere else on the document or press the return or Enter key to set the query and any changes. You may also press the excape key to disregard your current changes.

7.5 Uses of query structures

Query structures can be used for a number of applications.

7.5.1 Graphics

Query structures can be copied and output as graphics just like other figures generated in ChemDoodle. This is useful for communicating sets of chemical structures.

7.5.2 Search widget functionality

Query structures can be used in the **Search** widget for a more advanced scan of your files. The **Search** widget is covered in detail in the WIDGETS chapter.

7.5.3 Private searching

Some companies and institutions use the ChemDoodle API to handle internal databases. Please contact your site system administrator for information on using ChemDoodle queries to search internal databases. Institutions that would like to implement the ChemDoodle query system for internal searching should contact iChemLabs: https://www.ichemlabs.com/contact-us

7.6 Comparison to SMARTS

You may be familiar with Daylight *SMARTS* which is related to Daylight *SMILES*. *SMARTS* stands for *SM*iles *AR*bitrary *T*arget *S*pecification and is defined by Daylight: http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html

SMARTS is another way of specifying a query structure and is thoroughly supported in ChemDoodle. However, currently *SMARTS* is only available in selecting content in your document by using the Content » Select » SMARTS... menu item. This is covered in detail in the CONTENT MANAGEMENT TOOLS chapter.

CHAPTER 8

Reactions

Contents

8.1 Overview **175**

8.2 Drawing arrows **175**
8.2.1 Drawing arrows at fixed angles 176
8.2.2 Drawing arrows at non-fixed angles 176
8.2.3 Forcing arrows to be drawn vertically and horizontally 176
8.2.4 Moving arrows 176
8.2.5 Resizing arrows 176
8.2.6 Changing arrow arc angles 177
8.2.7 Removing arrows 177

8.3 Arrow types **177**
8.3.1 Adding and removing arrowheads 177
8.3.2 Arrowhead styles 178
8.3.3 Customizing arrowheads 178
8.3.4 Changing arrowhead lengths and angles 179
8.3.5 Connector styles 179
8.3.6 Special arrow templates 179

8.4 Bezier arrows **180**
8.4.1 Electron Pushing Arrows 181

8.5 Building reactions **182**
8.5.1 Implicitly 182
8.5.2 Explicitly 182
8.5.3 Sprouting 183
8.5.4 Using electron pushers 183
8.5.5 Using fragmentation tools 184
8.5.6 Adding reaction conditions 185
8.5.7 Adding plus symbols 185
8.5.8 Additional text 186

8.6 Dissolving reactions **186**

8.7 Cleaning reactions **186**

8.8 Atom-to-atom mappings **187**
8.8.1 Assigning a mapping 187
8.8.2 Warnings 187
8.8.2.1 Mapping between atoms within same structure 188
8.8.2.2 Overlapping atom maps 188
8.8.2.3 Mapping is on one side of a reaction 188
8.8.3 File format support 189

8.9 Balancing reactions **189**
8.9.1 Drawn reactions 189
8.9.2 Reaction equations 189
8.9.2.1 Equation balancing instructions 190
8.9.2.2 Example equations 190
8.9.3 Output 191
8.9.4 Errors 191
8.9.5 Warnings 191
8.9.6 Redox reactions 192

8.10 Stoichiometry **194**
8.10.1 Definitions 194
8.10.1.1 Field explanations 195
8.10.1.2 Theoretical vs. experimental fields 196
8.10.1.3 Coefficients 196
8.10.1.4 Limiting component 196
8.10.2 Creating a stoichiometry form 196
8.10.2.1 From a drawn reaction 197
8.10.2.2 From a typed reaction equation 197
8.10.2.3 Relationship to a table shape 197
8.10.2.4 Releasing the stoichiometry form 198
8.10.3 Editing the stoichiometry form 198
8.10.3.1 Explicit vs. implicit entries 198
8.10.3.2 Default values 198
8.10.3.3 Defining and changing values 198
8.10.3.4 Clearing values 199
8.10.3.5 Changing units 200
8.10.3.6 Flagged results 200
8.10.4 Examples 202
8.10.4.1 Determining the expected amount of product from measured reactant values 202
8.10.4.2 Determining the required amount of reactant to produce a specific amount of product . 203
8.10.4.3 Calculating the percent yield of an experiment 204
8.10.4.4 Determining the limiting reagent for a reaction 205
8.10.4.5 Calculating partial stoichiometry using coefficients 207

8.1 Overview

Reactions can be drawn in ChemDoodle using structures and arrow shapes. Any type of reaction or mechanism can be drawn. ChemDoodle also contains tools for explicitly defining reactions for various purposes.

This section introduces the new user to reactions within ChemDoodle. It covers the following topics:

- How to draw reactions.
- How to draw mechanisms.
- What types of arrows can be drawn.
- How to build and define reactions and reaction schemes.
- How to edit reactions.
- How to clean reactions.
- How to balance reactions and chemical equations.
- How to perform stoichiometry calculations.

8.2 Drawing arrows

Arrows are essential in chemical graphics for many reasons, the most important being for reaction and mechanism diagrams. Arrows are so important that, in ChemDoodle, they have their own unique palette in the **Drawing** toolbar as shown in Figure 8.1.

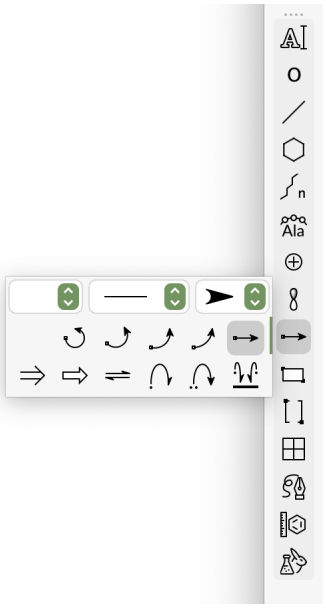


Figure 8.1: *Arrow palette in the Drawing toolbar*

These tools allow you to quickly draw various types of arrows, both straight and in arcs. Some special arrow type templates are also provided. Other types of paths, such as polylines and bezier curves can also be used for arrows, and they are discussed in the SHAPES chapter along with how to draw basic lines and arcs.

Essentially, arrow shapes are just path shapes with arrowheads. A hovered arrow shape is shown in Figure 8.2.

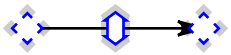


Figure 8.2: *Arrow Shape and Anchors*

8.2.1 Drawing arrows at fixed angles

To draw an arrow at fixed angles, execute the following steps:

1. Select the desired arrowheads and connector styles in the **Arrows** palette.
2. Click on the line or one of the arc angle buttons in the **Arrows** palette to enter the arrow placement mode.
3. Press the mouse down in the current document to set the start point of the arrow.
4. Drag the mouse to preview the placement of the end of the arrow.
5. Release the mouse to set the arrow.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

By default, arrows will be oriented at fixed angles every 15° starting at 0°.

8.2.2 Drawing arrows at non-fixed angles

To place arrows at non-fixed angles, break from the fixed orientation angles by holding down the alt key while dragging the mouse when defining the arrow.

8.2.3 Forcing arrows to be drawn vertically and horizontally

To place arrows oriented vertically or horizontally, hold down the shift key while dragging the mouse when defining the arrow. The arrow preview will then automatically orient vertically or horizontally depending on the angle from the start point to the current mouse cursor position.

8.2.4 Moving arrows

To move arrows, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the arrow so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in Figure 8.2.
2. Press the mouse down without selecting an anchor point and drag to move the arrow.
3. Release the mouse to finish the move action.

8.2.5 Resizing arrows

To resize arrows, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the arrow so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in Figure 8.2.
2. Move the mouse pointer over one of the two end anchor points so that anchor point is filled in with an amber color.

3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the arrow.
5. Release the mouse to finish the resize action.

8.2.6 Changing arrow arc angles

Arrow arc angles can be changed using the midpoint anchor. Choose a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the arrow so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in Figure 8.2.
2. Move the mouse pointer over the middle anchor point so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to change the arrow arc angle.
5. Release the mouse to set the new arrow arc angle.

While changing the angle of arrow arcs, the arrow arc angle will be displayed below the mouse cursor.



A few special arrow types, such as the retrosynthetic type, are always straight, and you will not be able to change the arc angles for these types.

8.2.7 Removing arrows

Arrows can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the arrow so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in Figure 8.2. Then press the backspace or delete key.
- Use the **Eraser** tool to hover the mouse pointer over the arrow so the arrow anchor points are drawn. Then click with the mouse.

8.3 Arrow types

Many different types of arrows can be easily created using the **Arrows** palette shown in Figure 8.1. This section briefly goes over the different styles and presets.

8.3.1 Adding and removing arrowheads

In the previous sections, we show how to use the **Arrows** palette to draw straight and arced arrows with arrowheads attached. However, arrows are simply path shapes with arrowheads on one or both ends. Arrowheads can be placed on several path shapes in ChemDoodle:

- Lines
- Arcs
- Pen paths
- Polylines

- Bezier Curves

Instructions for drawing these basic path shapes are provided in the SHAPES chapter. But once drawn, we can add or remove arrowheads. To add or remove arrowheads on a path shape, execute the following steps:

1. Hover the path shape you would like to add or remove arrowheads from.
2. Right-click on the path shape and select the **Format Shape...** menu item (Shape will be replaced with the name of the shape you are editing).
3. Scroll down to the **Arrows** section in the **Format Shape** window that appears.
4. In the **Arrow at Start** and **Arrow at End** sections, select or deselect the **Include** checkboxes to specify whether the arrowhead should be included or not.

For convenience, instead of opening the **Format Shape** window, you can easily toggle the display of arrowheads on the ends of objects that support arrowheads by hovering the object and pressing the left arrow [←] key (to toggle start) or right arrow [→] key (to toggle end).

8.3.2 Arrowhead styles

Arrowhead styles can be set to both the start and end of the arrow. Several arrowhead styles (half-heads) can be flipped over the arrow axis. The following arrowhead styles are provided:

- **Full Indented** -
- **Full** -
- **Unfilled Full Indented** -
- **Unfilled Full** -
- **Chevron** -
- **Half Indented** -
- **Half** -
- **Unfilled Half Indented** -
- **Unfilled Half** -
- **Hook** -

8.3.3 Customizing arrowheads

There are several settings that control how arrowheads are drawn:

- **Indented** - When selected, the back end of the arrow will be indented.
- **Filled** - When selected, the arrow will be filled in; otherwise it will be an outline.
- **Chevroned** - When selected, the arrow will be drawn as a simple chevron.
- **Length** - This setting controls the length of the arrow head along the line.
- **Angle** - This setting controls the angle of the arrow, from one side to the other.

These settings can be controlled in the **Format Shape...** window in the **Arrows** section.



If the arrowhead length is greater than 50% of the length of the line it is on, then the length will be decreased to 50% of the length of the line it is on.

8.3.4 Changing arrowhead lengths and angles

Both the arrowhead length and angle can be changed to match any look. To change the arrowhead length and angle, execute the following steps:

1. Hover the arrow containing the arrowhead to be edited.
2. Right-click on the arrow and select the **Format Shape...** menu item.
3. Scroll down to the **Arrows** section in the **Format Shape** window that appears.
4. In the **Arrow at Start** and **Arrow at End** sections, use the **Length** and **Angle** sliders to edit the arrowheads.

8.3.5 Connector styles

A connector is the line that connects the start and end arrows, if any. The following connector styles are provided:

- **Solid** -
- **Dashed** -
- **Wavy** -
- **Doubled** -
- **No Go (cross)** -
- **No Go (slash)** -
- **Rearrangement** -

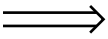
These settings can be controlled in the **Format Shape...** window under various section.

8.3.6 Special arrow templates

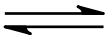
Many different types of arrows can be drawn from the **Arrows** palette. The following describes how these tools can be used to build common arrow types.

Reaction Arrow

A reaction arrow is the default style and is drawn with no start arrow, a **Full Indented** end arrow and a **Solid** connector.

Retrosynthetic Arrow 

A retrosynthetic arrow can be drawn with no start arrow, a **Chevron** end arrow and a **Doubled** connector. The default arrowhead angle and length is not aesthetic for this type of arrow, so use the **Retrosynthetic** preset  arrow button to quickly access this type.

Equilibrium Arrow 

An equilibrium arrow can be drawn with a **Half Indented** start arrow, a **Half Indented** end arrow and a **Doubled** connector. The double line spacing can be edited in the arrow's styles. Use the **Equilibrium** preset  arrow button to quickly access this type.

Resonance Arrow 

A resonance arrow can be drawn with a **Full Indented** start arrow, a **Full Indented** end arrow and a **Solid** connector.

Electron Pair Shift 

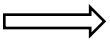
A shift of an electron pair can be drawn with no start arrow, a **Full Indented** end arrow and a **Solid** connector. Then select the appropriate arc angle for the figure.

Single Electron Shift 

A shift of a single electron can be drawn with no start arrow, a **Half Indented** end arrow and a **Solid** connector. Then select the appropriate arc angle for the figure.

Photon 

A photon can be drawn with a **Full** end arrow and a **Wavy** connector, but no start arrow.

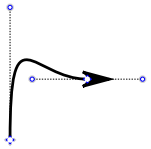
Bold 

A bold arrow can be drawn with no start arrow, an **Unfilled Full** end arrow and a **Doubled** connector. The default arrowhead angle and length is not aesthetic for this type of arrow, so use the **Bold** preset  arrow button to quickly access this type.

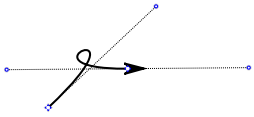
8.4 Bezier arrows

In addition to straight and arced arrows, some pretty complex arrow shapes may be drawn with the bezier tools. Bezier tools are described in the SHAPES chapter. The following are a few ideas. Just mimic the location of the control points to match them.

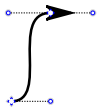
The Chute Arrow



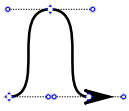
The Loop Arrow



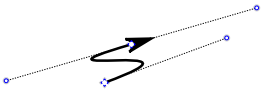
The Escalator Arrow



The Hump Arrow



The Zigzag Arrow



8.4.1 Electron Pushing Arrows

You can use bezier arrows to show electron movement. A full arrowhead describes the movement of 2 electrons, while a half arrowhead describes the movement of 1 electron. Instead of manually drawing these bezier arrows, you can use ChemDoodle's automatic electron pushing arrow shapes instead. See the SHAPES chapter for more information on automatic electron pushing arrows.

8.5 Building reactions

Reaction figures can be drawn by placing structures next to arrow shapes to describe reaction schemes. This method will create a visual diagram for the reaction, but underlying semantics will not exist. In other words, there is no formal definition of the reaction reactants or products. To address this, ChemDoodle provides a reaction building system with tools to implicitly and explicitly define reactions and reaction schemes.

After reactions have been defined, hovering over the reaction arrow will highlight any components as shown in Figure 8.3. Reactants will be outlined in a cyan rectangle with the word "reactant" above the rectangle. Products will be outlined in a magenta rectangle with the word "product" above the rectangle.

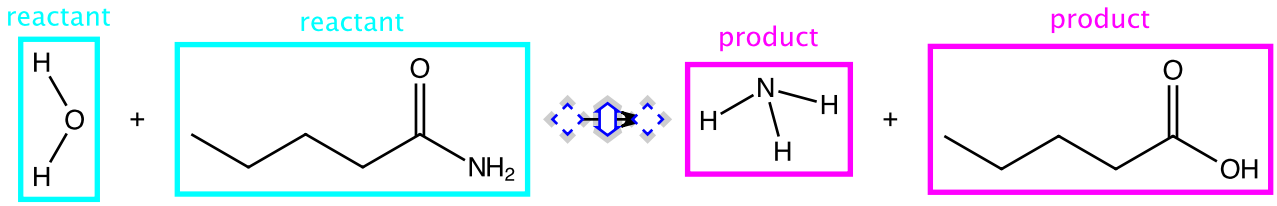


Figure 8.3: *Reaction interpretation*

This definition of the reaction is important for reaction functions in ChemDoodle and the visual feedback will describe how the reaction will be interpreted by the algorithms.

8.5.1 Implicitly

To implicitly define a reaction, execute the following steps:

1. Draw the arrow you would like to represent the reaction arrow.
2. Draw any reactants and place them to the *left* of the arrow shape.
3. Draw any products and place them to the *right* of the arrow shape.
4. Select the arrow shape and all reactants and products using the selection tools.
5. Press the Reaction ⟩ Build Implied Reaction menu item to define the reaction.

All structures with midpoints to the left of the arrow shape's midpoint will be defined as reactants in the reaction while all structures with midpoints to the right of the arrow shape's midpoint will be defined as products in the reaction.

8.5.2 Explicitly

To explicitly define a reaction, first select the arrow shape you would like to use to represent the reaction arrow using the selection tools. Then press the Reaction ⟩ Edit Reaction... menu item (you may also hover the arrow shape, right-click and select the Edit Reaction... menu item). Doing so opens the **Edit Reaction** window for the selected arrow, as shown in Figure 8.4.

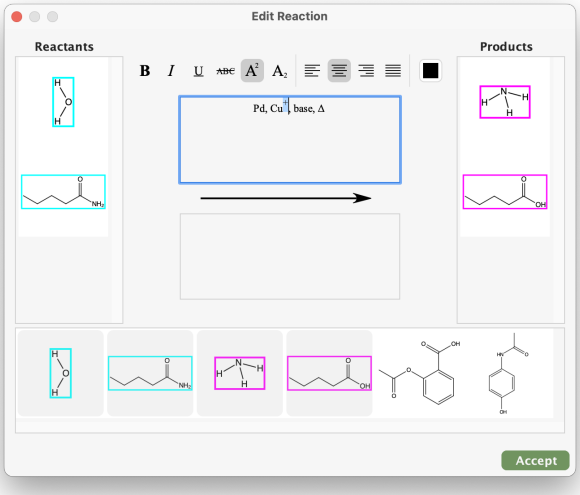


Figure 8.4: *Edit Reaction Window*

The **Edit Reaction** window is a drag and drop interface. All molecules in the current document are displayed in the bottom tray, while the left and right trays correspond to the constituent reactants and products respectively. If your selection contains any molecules, in addition to the arrow, then only those selected molecules and the molecules defined to the reaction will be present in the bottom tray. This is useful for limiting the number of molecules present in documents with many molecules.

Just drag and drop molecules from the bottom tray into the other two to set up the reaction. The corresponding molecule in the document will be highlighted when you hover over a molecule in this interface. Once a molecule has been placed, it will be grayed out in the bottom tray and no longer selectable. Molecules set as reactants will be outlined in a cyan color, while molecules set as products will be outlined in a magenta color. You can transfer a placed molecule between the products and reactants by dragging the molecule between the side trays. You can remove a molecule from the reaction completely by dragging and dropping it back into the bottom tray.

You can use the text areas above and below the arrow to set any text for the reaction. This text will be automatically adjusted and placed around the arrow in the document.

Press the **Accept** button in the **Edit Reaction** window to set the reaction.

8.5.3 Sprouting

You may begin creating a reaction by sprouting one from a selected molecule or a selection of a set of molecules. A reaction arrow will be created with all of the selected molecules defined as reactants. Copies of each reactant molecule will be placed in a product positions for the reaction, allowing you to quickly draw reaction figures. Perform the following steps to sprout a reaction from a selection of molecules:

1. Select the molecule or molecules you wish to sprout a reaction from.
2. Use the Reaction ⟩ Sprout menu item.

8.5.4 Using electron pushers

If you have a drawing of chemical structures participating in an electron pushing diagram, ChemDoodle will automatically generate the result for you in an explicit reaction. For example in the following Figure 8.5, a mechanism has been drawn using ELECTRON PUSHERS.

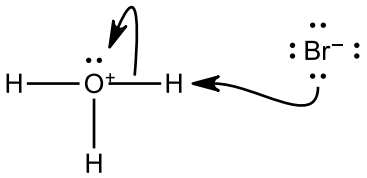


Figure 8.5: *A mechanism drawn with electron pushers*

To have ChemDoodle produce the result, please follow these steps.

1. Select all of the molecules and electron pusher shapes participating in the mechanism. If no electron pusher shapes are present or selected, this function will do nothing.
2. Use the Reaction › Show Electron Pusher Result menu item.

The result will be presented in an explicit reaction originating from the starting mechanism, as shown in the following Figure 8.6.

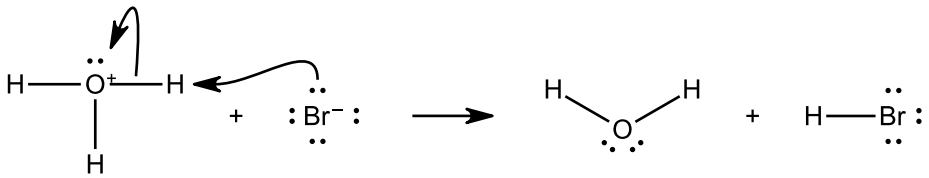


Figure 8.6: *The result of the mechanism diagram is automatically generated*

If the mechanism does not make sense, the result may not be representable in ChemDoodle. For instance, if you have 2 two-electron pusher arrows originating from a single bond, then the bond will be left in a bond order state of -1, which cannot be displayed. In these cases, ChemDoodle will display the error shown in Figure 8.7.

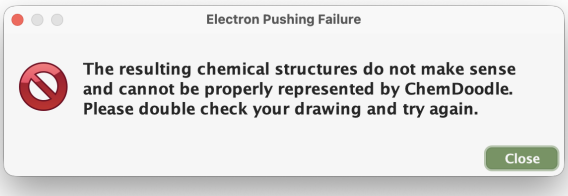


Figure 8.7: *The result of the mechanism diagram cannot be represented*

8.5.5 Using fragmentation tools

ChemDoodle contains convenient tools for building reactions based on bond breaking and formation. These tools can be found in the in the **Fragmentation Tools** group button in the **Content** toolbar.

Synthesis		The molecules will be fragmented and each fragment will be set as a reactant in a synthetic reaction leading to the original molecules.
Retrosynthesis		The molecules will be fragmented and each fragment will be set as a product in the retrosynthetic reaction starting from the original molecules.

To build a reaction from a molecule or group of molecules, execute the following steps:

1. Select the desired fragmentation tool in the **Content** toolbar.
2. Press the mouse down and drag through all of the bonds to be cut, defining how the reaction is to be formed. A green line will follow the mouse path as shown in Figure 8.8.

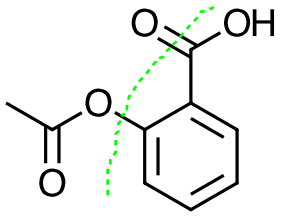


Figure 8.8: *Cutting an aspirin molecule to build a retrosynthetic reaction*

3. Release the mouse to complete the function. The appropriate reaction arrow will be added and fragments created to set up a new reaction as defined by the cut bonds. The results of such a cut for the **Retrosynthesis** tool is displayed in Figure 9.7.

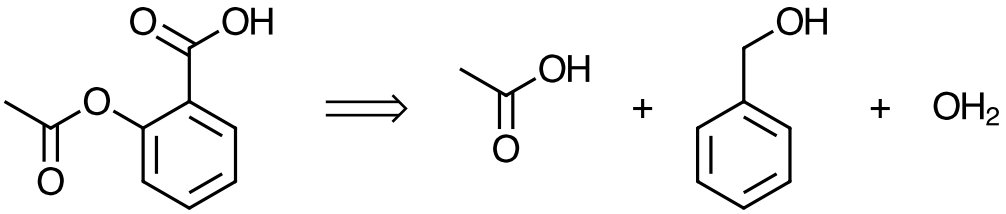


Figure 8.9: *The results of cutting an aspirin molecule to build a retrosynthetic reaction*

8.5.6 Adding reaction conditions

To add reaction conditions above and below the reaction arrow, first select the arrow shape you would like to add conditions to using the selection tools. Then press the Reaction ⟩ Edit Reaction... menu item to open the **Edit Reaction** window for the selected arrow.

The **Edit Reaction** window contains two text editors for adding text above and below the reaction arrow. Click on a text area and type to add text. You can format the text using the text formatting tools above the text areas.

Use the **Symbols** widget to input characters into the reaction condition text areas that are not present on the keyboard.

Press the **Accept** button in the **Edit Reaction** window to set the reaction.

8.5.7 Adding plus symbols

After building a reaction, plus symbols will automatically be added at the midpoints between the constituent reactants and products. This feature can be turned off in the **Styles** window under the **Reactions** tab as shown in Figure 8.10. Simply uncheck the **Automatically Place Pluses** option.

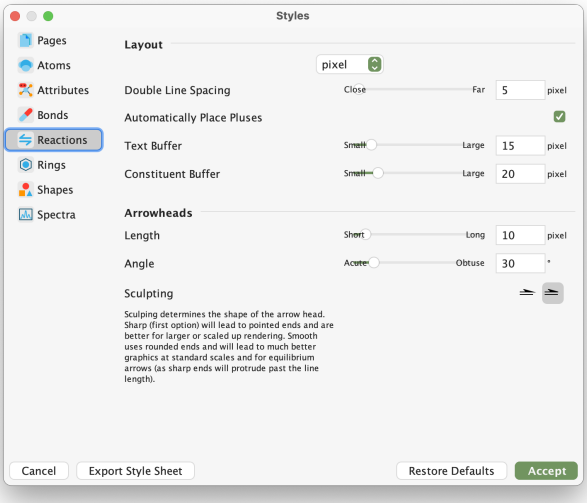


Figure 8.10: *Reaction Styles*

8.5.8 Additional text

If you want to add your own additional text to the reaction, use the **Text for Atoms and Captions** tool  in the **Drawing** toolbar and described in the SHAPES chapter.

8.6 Dissolving reactions

To dissolve a built reaction, select the arrow the reaction is defined by with a selection tool, then select the Reaction ⟩ Dissolve Reactions menu item.

8.7 Cleaning reactions

To clean a reaction, execute the following steps:

1. Define the reaction implicitly or explicitly using the instructions in the previous section.
2. Select the arrow shape of the reaction you would like to clean using the selection tools.
3. Press the Reaction ⟩ Clean menu item or press the **Clean Reaction** button  in the **Chemistry** toolbar.

The reaction arrow will be horizontally leveled and resized to its text adhering to the **Text Buffer** style. Then the reaction arrow and constituent molecules will be aligned according to their vertical centers and distributed horizontally with a buffer space. The entire reaction is then centered horizontally. If the reaction is too wide for the document, the reactants and arrow are then stacked above the products so that both groups are mutually centered as shown in Figure 8.11.

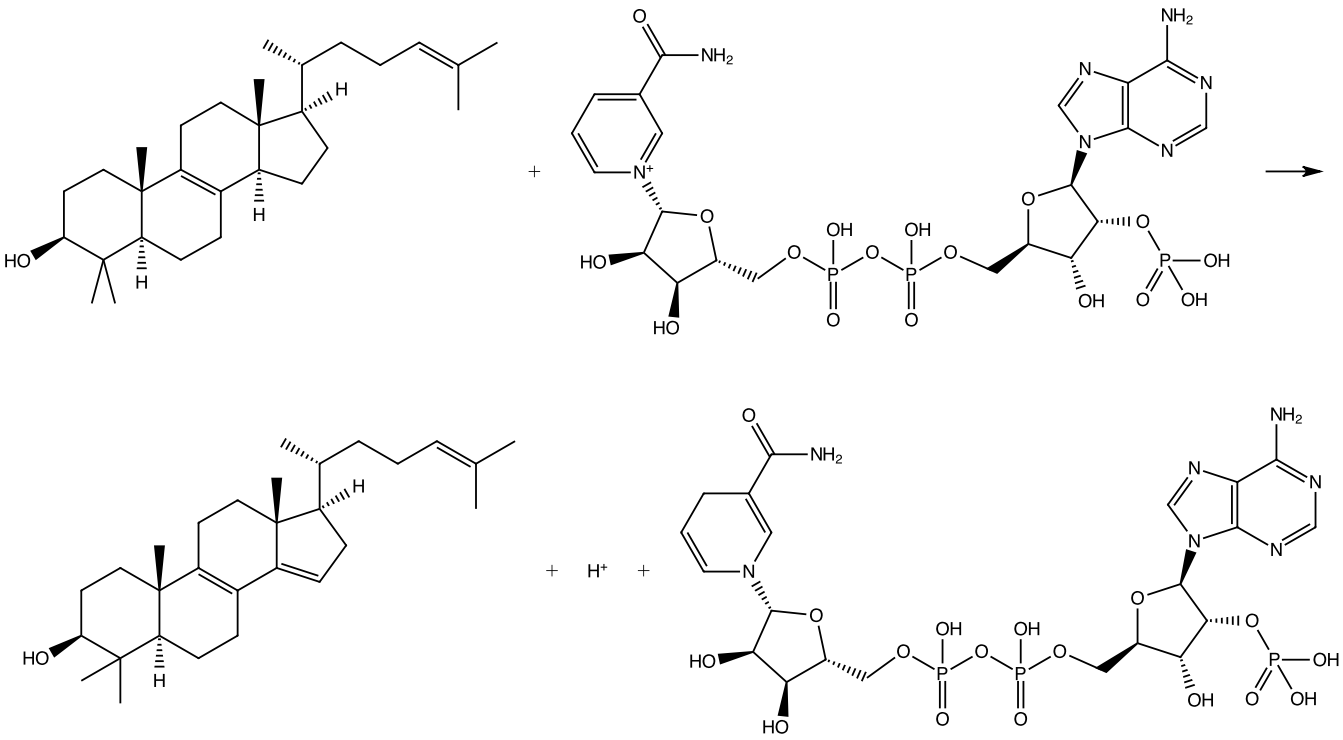


Figure 8.11: *A wide reaction that has been stacked.*

The settings for determining how reactions are laid out can be defined in the **Styles** window under the **Reactions** tab as shown in Figure 8.10 above.

You can adjust the double line spacing for equilibrium arrows, decide whether or not pluses should be automatically drawn, set the text buffer for conditions text and the buffer between constituent reaction objects. You can also set the default settings for arrowheads here.

ChemDoodle can clean multiple reactions at the same time, but currently can only properly clean discrete reactions. Cleaning complex reaction schemes with a given molecule defined in several different reactions may not produce desired results.

8.8 Atom-to-atom mappings

An atom mapping between any two atoms can serve a number of purposes. For instance, you may need to assign such associations in *ChemDoodle JSON* output for input into another function requiring that information to be explicitly defined. Most commonly, atom mappings are assigned for reaction processing.

8.8.1 Assigning a mapping

To manually assign atom mappings, you will use the **Atom Mapping** tool in the **Arrows** palette in the **Drawing** toolbar. Using this tool creates *Atom Mapping* shapes. Instructions are provided in the ATOM MAPPINGS section of the SHAPES chapter.

8.8.2 Warnings

The following warnings for atom mappings will be shown by ChemDoodle in your document. These warnings are simply to help you, and may be ignored. Please see the CHEMICAL WARNINGS section of the CHEMINFORMATICS chapter for more information on the warning system in ChemDoodle.

8.8.2.1 Mapping between atoms within same structure

This warning will appear if the atom mapping is between two atoms within the same structure as shown in Figure 8.12.

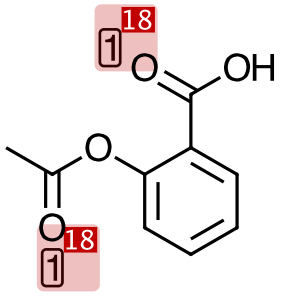


Figure 8.12: *A warning is shown if the atom mapping is between two atoms within the same structure*

8.8.2.2 Overlapping atom maps

This warning will appear when two or more atom mappings overlap by including the same atom or atoms as shown in Figure 8.13.

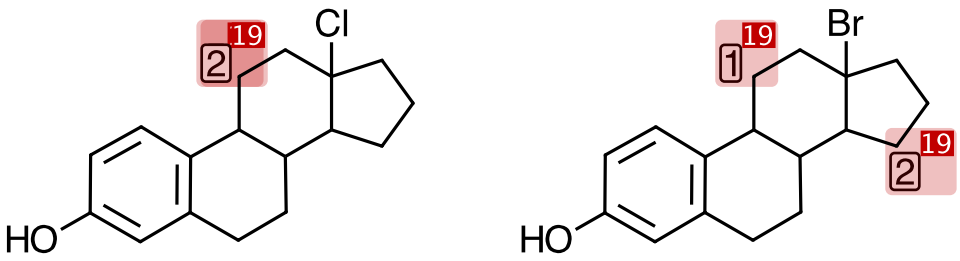


Figure 8.13: *A warning is shown if two atom mappings include the same atoms*

8.8.2.3 Mapping is on one side of a reaction

This warning will appear if the atom mapping exists within the scope of a reaction, but maps together two atoms on the same side of the reaction as shown in Figure 8.14.

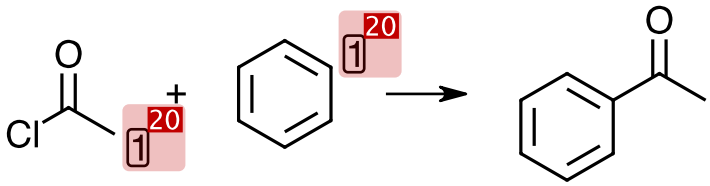


Figure 8.14: *A warning is shown if the atom mapping is between two reactants or two products of a built reaction*

8.8.3 File format support

ChemDoodle will input and output reaction atom-to-atom mapping information for the following chemistry file types:

- CambridgeSoft ChemDraw Exchange (*.cdx*)
- CambridgeSoft ChemDraw XML (*.cdxml*)
- ChemAxon Marvin Document (*.mrv*)
- Chemical Markup Language (*.cml*)
- Daylight SMILES (*.smi*, *.smiles*)
- iChemLabs ChemDoodle Document (*.icl*, *.icxml*)
- iChemLabs ChemDoodle JSON (*.cwc.js*)
- MDL RXNFiles (*.rxn*)



While ChemDoodle will always accurately input the atom mappings from these file formats, the numbers associated with each mapping may not be preserved. ChemDoodle will optimize the numbers once in the document to increment starting from 1.

8.9 Balancing reactions

Complete reactions can be balanced by ChemDoodle, either when drawn using structures and arrows, or typed as a reaction equation.

ChemDoodle will be able to balance any reaction equation that can be balanced. Drawn reactions will be converted into reaction equations. Keep in mind not all equations can be balanced, and some equations have an infinite number of irreducible solutions. In some cases, there may be a solution if a reactant is moved to the product side or a product moved to the reactant side. In these cases a negative number will be provided for the coefficient. If there is more information to convey, a message will be presented upon balancing.

8.9.1 Drawn reactions

If a complete reaction is drawn in the document, you may balance it by performing the following steps:

1. If the reaction has already been defined to the arrow, simply select the arrow. Otherwise, select the arrow and all reactants and products in their entirety.
2. Select the Reaction ⟩ Balance Reaction... menu item.
3. The balanced equation and component table will be output to the document and centered below the drawn reaction.

8.9.2 Reaction equations

If you would like to balance a written reaction equation, you may balance it by performing the following steps:

1. Make sure there is nothing selected in the document.
2. Select the Reaction ⟩ Balance Reaction... menu item. A window for balancing written equations will appear as shown in Figure 8.15.
3. Input your reaction equation into the text area, being sure to follow the formatting instructions.

4. Press the **Balance Equation** button when ready.
5. The balanced equation and component table will be output to the document.

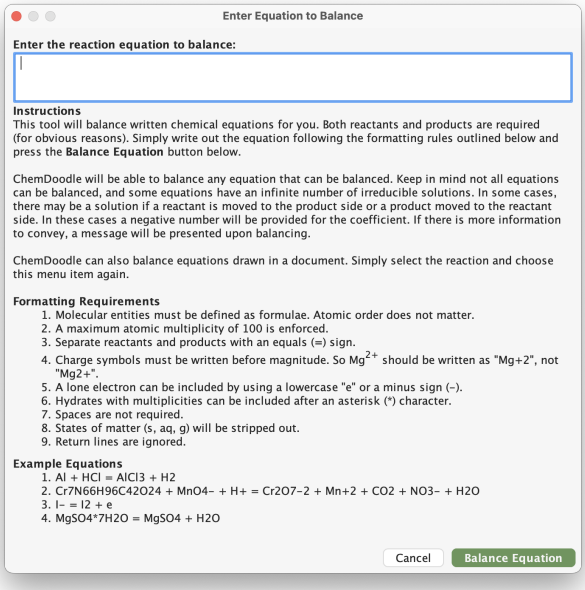


Figure 8.15: *Enter a written reaction equation to be balanced.*

8.9.2.1 Equation balancing instructions

This tool will balance written chemical equations for you. Both reactants and products are required (for obvious reasons). Simply write out the equation following the formatting rules outlined here.

Formatting Requirements

1. Molecular entities must be defined as formulae. Atomic order does not matter.
2. A maximum atomic multiplicity of 100 is enforced.
3. Separate reactants and products with an equals (=) sign.
4. Charge symbols must be written before magnitude. So Mg^{2+} should be written as “Mg+2”, not “Mg2+”.
5. A lone electron can be included by using a lowercase “e” or a minus sign (−).
6. Hydrates with multiplicities can be included after an asterisk (∗) character.
7. For redox reactions where element oxidation states cannot be deduced, specify them in curly braces ({}) after the element using Arabic or Roman numerals.
8. Spaces are not required.
9. States of matter (*s, aq, l, g*) will be stripped out.
10. Return lines are ignored.

8.9.2.2 Example equations

You can copy and paste these equations into the **Equation Balancing** window in ChemDoodle to try out this feature.

1. Al + HCl = AlCl3 + H2
2. Cr7N66H96C42O24 + MnO4- + H+ = Cr2O7-2 + Mn+2 + CO2 + NO3- + H2O
3. I- = I2 + e
4. MgSO4*7H2O = MgSO4 + H2O

8.9.3 Output

The output from this function consists of two editable shapes, a table and a label. The table will separate reactants and products into components, with the second row detailing the entities and the third row providing the associated coefficient. The label will render the complete balanced reaction equation, with coefficients and full formatting. Sample output is shown in Figure 8.16 for the input of the chemical equation presented in *Example 2* above.

Reactants				Products				
$Cr_7N_{66}H_{96}C_{42}O_{24}$	MnO_4^-	H^+		$Cr_2O_7^{2-}$	Mn^{2+}	CO_2	NO_3^-	H_2O
10	1176	2798		35	1176	420	660	1879

$$10Cr_7N_{66}H_{96}C_{42}O_{24} + 1176MnO_4^- + 2798H^+ = 35Cr_2O_7^{2-} + 1176Mn^{2+} + 420CO_2 + 660NO_3^- + 1879H_2O$$

Figure 8.16: *A table and label describing the balanced equation.*

Just like other labels, you can hover the balanced equation, right-click and select the Copy Text menu item to put the formatted text on the system clipboard for pasting into other applications such as word processing software.

8.9.4 Errors

Some input to this function may be invalid, leading to an error. In such cases, no results will be provided and you will need to edit the input to make it valid and possible to be balanced. The following error conditions may be encountered:

- **Reactants or products is empty.** - A drawn equation has defined reactants or products, but not both.
- **The same elements must be on both sides of the equation. [element] is missing on the [reactants/products] side.** - *e.g.* F = F + Cl
- **The same elements must be on both sides of the equation. At the very least, [element] is missing on the [reactants/products] side.** - *e.g.* F = Cl

The following errors can only be encountered for written chemical equations:

- **No equation defined. Missing equals (=) sign.** - *e.g.* CO2 + H2O
- **Error parsing reactants.** - Something on the reactants side caused an error.
- **Error parsing products.** - Something on the products side caused an error.
- **Unable to parse: [entity]** - The entity that could not be parsed as presented.
- **Hydrate is malformatted: [entity]** - The presented hydrate is malformatted.

8.9.5 Warnings

A warning may be presented in some cases, even though a solution is reached and the corresponding result is provided.

The following warning conditions may be encountered:

- **The input equation comprises [x] balanceable equations, yielding infinite irreducible combinations. A balanced solution with minimized positive integer coefficients has been deduced.** - ChemDoodle uses a unique proprietary algorithm to find the best possible balanced equation, where each component has the smallest positive integer coefficient when the equation is viewed as a whole.
- **Coefficients of negative value indicate molecular entities are on the wrong side of the input equation.** - *e.g.* C6H12O6 = O2 + CO2 + H2O, O2 should be a reactant
- **Coefficients of zero (0) indicate such molecular entities are not significant in the input equation.** - *e.g.* C2H6 + C6H12 + H2O = C6H12 + H2O, C2H6 should not be included

8.9.6 Redox reactions

Oxidation-reduction (redox) reactions can be tricky to balance by hand, but ChemDoodle can balance them for you. Redox equation balancing becomes more complicated when there are infinite irreducible combinations, as minimizing the coefficients to create a balance among the elements may not correctly balance the electrons exhanged in the half-reactions. For instance, consider this redox reaction:

H2S + KMnO4 + H2SO4 = S + K2SO4 + MnSO4 + H2O

Balancing this equation produces an infinite number of irreducible combinations. Minimizing the coefficients yields:

2H2S + 2KMnO4 + 2H2SO4 = 1S + 1K2SO4 + 2MnSO4 + 4H2O

All of the elements are balanced between the reactants and the products, but this result is incorrect. Oxidation states change between the reactants and the products for sulfur (-II and VI → 0 and VI) and manganese (VII → II). To correctly balance this equation, the change in oxidation states must be taken into account, balancing the electrons exhanged in the half-reactions as well as the elements. ChemDoodle is able to deduce oxidation states for most chemical species and therefore correctly balances this equation. The output in ChemDoodle is shown in Figure 8.17.

Reactants				Products			
H_2S	$KMnO_4$	H_2SO_4		S	K_2SO_4	$MnSO_4$	H_2O
5	2	3		5	1	2	8

$$5H_2S + 2KMnO_4 + 3H_2SO_4 = 5S + 1K_2SO_4 + 2MnSO_4 + 8H_2O$$

Figure 8.17: *ChemDoodle can deduce oxidation states and correctly balance redox reactions.*

There will be cases where ChemDoodle is not able to deduce the oxidation states of some or all of the elements in an equation. For instance, consider the equation from above, but we replace all oxygen atoms with selenium. Manganese, sulfur and selenium exhibit many oxidation states, and therefore ChemDoodle cannot deduce what the exact oxidation states are for each element in each compound:

H2S + KMnSe4 + H2SSe4 = S + K2SSe4 + MnSSe4 + H2Se

In such cases, the infinite irreducible combinations warning will appear with a balanced result and the following additional warning:

2H2S + 2KMnSe4 + 2H2SSe4 = 1S + 1K2SSe4 + 2MnSSe4 + 4H2Se

The input equation comprises 2 balanceable equations, yielding infinite irreducible combinations. A balanced solution with minimized positive integer coefficients has been deduced.
If this is a redox reaction, the result may not be correct, as ChemDoodle was unable to determine the oxidation state for Mn in KMnSe4.

You may manually define the oxidation state of an element of a compound in the equation by including the oxidation state value in curly braces immediately after that element symbol in the compound. You may use either Arabic numbers or Roman numerals. In this case, we can define the Se element oxidation states and the Mn in $MnSSe_4$ so the remaining elements may be deduced:

```
H2S + KMnSe{-2}4 + H2SSe{-2}4 = S + K2SSe{-2}4 + Mn{2}SSe{-2}4 + H2Se
```

The intended result is then produced by ChemDoodle in Figure 8.18.

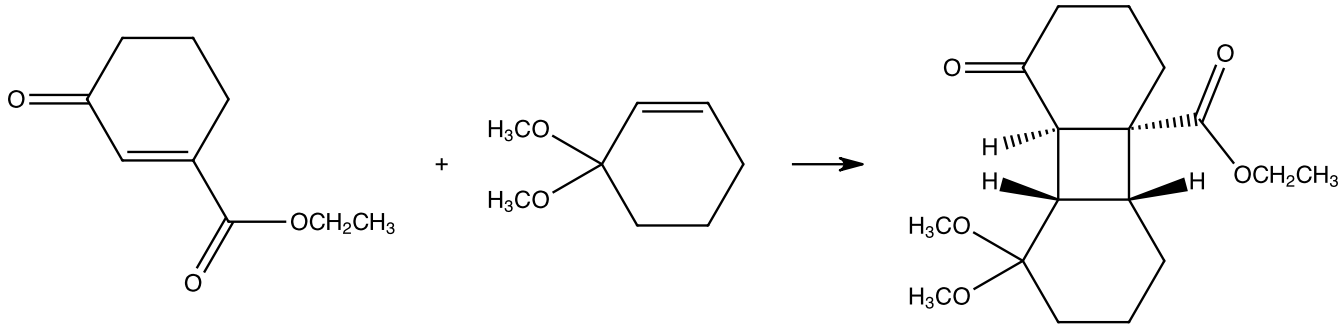
Reactants				**Products**			
H_2S	$KMnSe^{-II}_4$	$H_2SSe^{-II}_4$		S	$K_2SSe^{-II}_4$	$Mn^{II}SSe^{-II}_4$	H_2Se
5	2	3		5	1	2	8

$$5H_2S + 2KMnSe^{-II}_4 + 3H_2SSe^{-II}_4 = 5S + 1K_2SSe^{-II}_4 + 2Mn^{II}SSe^{-II}_4 + 8H_2Se$$

Figure 8.18: *You may manually define oxidation state values in unclear cases.*

8.10 Stoichiometry

The relationship between the relative quantities of substances taking part in a reaction or forming a compound is called stoichiometry. Given measured or theoretical information about your experiment, you may need to calculate different values for a reaction. For instance, you may need to know how many grams of a reactant is necessary, or what is the percent yield of the product. But doing these calculations by hand is time consuming and error prone. Instead, ChemDoodle includes an advanced stoichiometry form to quickly calculate many parameters of your reaction. The stoichiometry forms in ChemDoodle are self-calculating, chemically aware and will maintain proper balancing while editing. An example stoichiometry form is rendered for an organic reaction in Figure 8.19.



Reactants				*Products*	
Formula	$C_9H_{12}O_3$	$C_8H_{14}O_2$		Formula	$C_{17}H_{26}O_5$
Molecular Mass	**168.19amu**	**142.20amu**		Molecular Mass	**310.38amu**
Coefficients	***1***	***1***		Coefficients	***1***
Equivalents	1.00	2.25		Equivalents	0.871
Measured Mass	***45.21g***	***86.11g***		Measured Mass	***90.87g***
Purity (by mass)				Purity (by mass)	***72%***
Density				Output Mass	65.43g
Volume				Output Moles	0.211mol
Molarity				%Completion	***90%***
Reacting Mass	45.21g	38.22g		Expected Mass	75.09g
Reacting Moles	0.269mol	0.269mol		Expected Moles	0.242mol
Excess Mass	0.00g	47.89g		%Yield	87.13%

Figure 8.19: *An example stoichiometry form for an organic reaction*

8.10.1 Definitions

There are many terms used in this section to describe the stoichiometry form feature. The following terms are defined:

- **Table** - A table is the editable shape construct that organizes content in columns and rows.
- **Form** - A form is a table with a set of rules enforced on it, which may restrict your actions and allow for content to be automatically determined in parts of the table.
- **Field** - A field defines a row in the table and is a set of entries representing a specific concept of the reaction for all reactants, all products, or all components.

- **Entry** - An entry is an input or output for an individual component of the reaction in a single field, composed of both a value and a unit. Some entries may be unitless.
- **Value** - A value is the numeric portion of an entry.
- **Unit** - A unit provides physical context for the entry, and is the non-numeric portion of an entry. For instance, grams (*g*) and milliliters (*mL*) are units.

8.10.1.1 Field explanations

The following fields are presented in the stoichiometry form. Fields are specific to reactants or products, although many fields are shared by both reactants and products. Here is what each reactant field represents, along with its default unit and theoretical or experimental definition:

- **Formula** - *unitless, theoretical* - The molecular formula of the molecule, determined by drawn reaction.
- **Molecular Mass** - *amu, theoretical* - The molecular mass of the molecule, determined by drawn reaction.
- **Coefficients** - *unitless, experimental* - This value defines the stoichiometric ratio of this component to the other components in the reaction. Non-integer values are allowed, but a zero value is not allowed.
- **Equivalents** - *unitless, experimental* - The relative amount of this reactant compared to the limiting component. This value is expressed as the ratio of the moles of this component to its stoichiometric coefficient, divided by the corresponding quantity for the limiting component.
- **Measured Mass** - *g, experimental* - The is the measured mass of your substance from your experiment.
- **Purity (by mass)** - *%, experimental* - This is the purity of your substance.
- **Density** - *g/mL, experimental* - This is the density of of your substance in the form of matter your substance was observed in.
- **Volume** - *mL, experimental* - This is the volume of your substance in gas form or the volume of the solution containing your substance.
- **Molarity** - *mol/L, experimental* - This number defines how many moles of your substance are present in a liter of solution.
- **Reacting Mass** - *g, theoretical* - Once a limiting component is determined, this value is the theoretical mass of the reactant necessary to achieve the defined value of limiting component.
- **Reacting Moles** - *moles, theoretical* - Once a limiting component is determined, this value is the theoretical number of moles of the reactant necessary to achieve the defined value of limiting component.
- **Excess Mass** - *g, experimental* - This number is defined as the remaining mass after all of the reacting mass is used from the measured mass. It is whatever is leftover or unnecessary for your reaction.

Here is what each product field represents, along with its default unit and theoretical or experimental definition:

- **Formula** - *unitless, theoretical* - The molecular formula of the molecule, determined by drawn reaction.
- **Molecular Mass** - *amu, theoretical* - The molecular mass of the molecule, determined by drawn reaction.
- **Coefficients** - *unitless, experimental* - This value defines the stoichiometric ratio of this component to the other components in the reaction. Non-integer values are allowed, but a zero value is not allowed.
- **Equivalents** - *unitless, experimental* - The relative amount of this product compared to the limiting component. This value is expressed as the ratio of the moles of this component to its stoichiometric coefficient, divided by the corresponding quantity for the limiting component.
- **Measured Mass** - *g, experimental* - The is the measured mass of the substance resulting from your experiment.
- **Purity (by mass)** - *%, experimental* - This is the purity of your resulting substance.

- **Output Mass** - *g, experimental* - This is the measured amount of pure product recovered from your experiment.
- **Output Moles** - *moles, experimental* - This is the calculated amount of moles of the pure product recovered from your experiment.
- **%Completion** - *%, theoretical* - This value defines how far your reaction went to completion. This value is defined once for all products.
- **Expected Mass** - *g, theoretical* - Once a limiting component is determined, this value is the theoretical mass of the product produced as defined by the value of limiting component.
- **Expected Moles** - *moles, theoretical* - Once a limiting component is determined, this value is the theoretical number of moles of the product produced as defined by the value of limiting component.
- **%Yield** - *%, experimental* - The percent yield is defined as the total recovered mass of pure product from your experiment over the theoretical expected mass of the product.

8.10.1.2 Theoretical vs. experimental fields

There are two types of fields in the stoichiometry form, theoretical and experimental. Theoretical fields have a light gray background and are strictly defined by the assigned molecule or the ratios in the balanced equation (or the input equivalents) for the reaction. Experimental fields are determined based on observed or measured values from your experiment, and may or may not be dependent on entries input into other fields in the stoichiometry form.

Regardless, there is no need to be concerned by whether a field is theoretical or experimental, you simply just need to input your values and units into the correct entries in the stoichiometry form and everything else will be automatically taken care of for you.

8.10.1.3 Coefficients

Coefficients define the stoichiometric ratios between the components of the reaction. For balanceable reactions, ChemDoodle will automatically enforce stoichiometry and the **Coefficients** fields will be predefined with these values. If a reaction can not be balanced, for instance, the drawn reaction only contains the most important reactants and products and not the complete reaction, all entries for the **Coefficients** field will be defined to 1 by default.

You can override the stoichiometric ratios for any reaction by editing the **Coefficients** entries. Any non-zero positive value is allowed, including non-integer values. If you delete a **Coefficients** cell value, the cell will automatically be repopulated with the correct balanced coefficient or 1 if the reaction is not balanceable.

8.10.1.4 Limiting component

The limiting reagent for a reaction is the reagent that is completely converted into product. By adding more of the limiting reagent, theoretically, more product is produced, while increasing the amounts of other reagents does not affect the total amount of product produced.

Some programs may require you to define a limiting reagent for stoichiometry calculations. In ChemDoodle, the limiting component is automatically determined based on the input entries, and you do not need to worry about specifying a limiting reagent. ChemDoodle's stoichiometry form may even determine a product to be the limiting component: if you explicitly define the **Expected Mass** or **Expected Moles** for a product, then we know exactly how many moles of each reactant is necessary and all reactants may then have an **Excess Mass** calculated. This is very useful if you need to know the amount of waste for your experiment.

If you want to know which reagent is the limiting reagent using the stoichiometry form, make sure to define as many entries as possible in the form, and specifically define the **Measured Mass** entries. Any reagent with a calculated **Excess Mass** of *0*, or **Equivalents** value of *1*, is a limiting reagent.

8.10.2 Creating a stoichiometry form

Stoichiometry forms are generated from typed reaction equations or drawn reactions in your document. This section describes what a stoichiometry form is and the steps needed to create one.

8.10.2.1 From a drawn reaction

Perform the following steps to create a stoichiometry form from a drawn reaction:

1. Select the reactants, products and arrow you have drawn to represent your reaction. If you have already explicitly or implicitly defined a reaction, only the arrow needs to be selected.
2. Select the Reaction ▸ Stoichiometry... menu item and the generated stoichiometry form will appear below the reaction.

You may then use the **Text for Atoms and Captions** tool  in the **Drawing** toolbar to begin defining entries to the form.

8.10.2.2 From a typed reaction equation

Perform the following steps to create a stoichiometry form from a typed reaction equation:

1. Make sure there is nothing selected in the document.
2. Select the Reaction ▸ Stoichiometry... menu item. A window for your written equations will appear as shown in Figure 8.20.
3. Input your reaction equation into the text area, being sure to follow the formatting instructions. Note this typed equation should not contain coefficients and does not need to be balanceable. ChemDoodle will automatically balance the equation for the correct ratios, or default to 1:1 ratios using the **Equivalents** row.
4. Press the **Create Stoichiometry Table** button when ready.
5. The stoichiometry table will be output to the document.

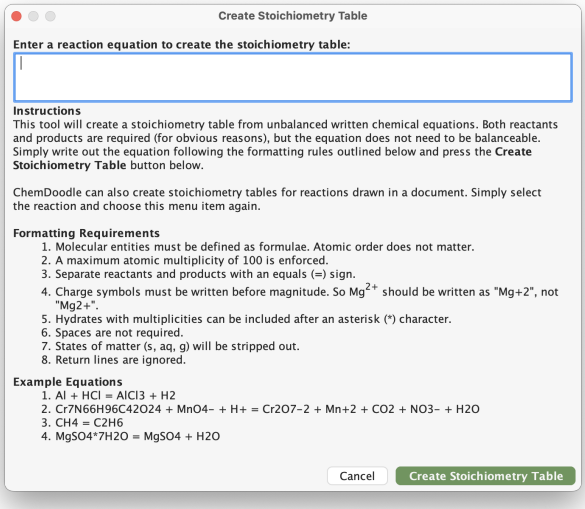


Figure 8.20: *Enter a written reaction equation to create a stoichiometry table.*

You may then use the **Text for Atoms and Captions** tool  in the **Drawing** toolbar to begin defining entries to the form.

8.10.2.3 Relationship to a table shape

A stoichiometry table is a common construct, typically taught in high school chemistry, where one value is converted into another using multipliers to convert units. The stoichiometry form in ChemDoodle is more complex as you can define various entries for your reaction, and other entries dependent on those you input will be instantly calculated.

In ChemDoodle, forms are a special type of table shape. See the SHAPES chapter for more information on table shapes. Forms can be edited just like tables, but with specific restrictions placed on editing.

The following restrictions are placed on stoichiometry forms:

- You may only edit the appropriate cells to input entries for the calculations. You cannot change any of the title cells.
- Only specific content can be defined to cells. Only number values and a unit can be defined to each entry.
- You cannot add or remove columns or rows.
- Content cannot be pasted into a cell.
- Only appropriate cells containing explicit entries can be cleared (using delete or cut functions). Implicit entries cannot be removed, as you will need to instead clear the cells containing the entries that lead to the calculation of the implicit entry. More on this in the EXPLICIT VS. IMPLICIT ENTRIES section.

8.10.2.4 Releasing the stoichiometry form

When you are done using the stoichiometry form, you may release the form and convert it to a standard table shape, which then can be edited as you desire with no restrictions. To do so, simply hover the stoichiometry form with a selection tool, right-click and select the Release Stoichiometry Form menu item.

Keep in mind that when you choose to release the stoichiometry form, the stoichiometry calculations based on the entries in the cells will no longer update because there is no longer a form there to enforce the integrity of the table.

8.10.3 Editing the stoichiometry form

The stoichiometry form in ChemDoodle is a self-calculating table, meaning the form will automatically compute entries as you enter values and units into other entries.

8.10.3.1 Explicit vs. implicit entries

Entries that you input into the stoichiometry form are explicit entries, and are rendered as text that is both bold and italic. You may enter explicit entries into any blank cell in the form, and you may edit any explicit entry at anytime.

After you enter each explicit entry into the form, the form will self-calculate and update to display any other entries that are fully defined by explicit entries. For instance, if you define both the **Reacting Mass** and **Measured Mass** entries for a reactant, the **Excess Mass** entry for that reactant is automatically calculated and displayed. In this way, the form enforces integrity for the entries presented in the table. Entries that are calculated by the form based on explicit entries are called implicit entries. Implicit entries are rendered as plain, unstyled text and cannot be edited. To change an implicit entry, you will need to clear any explicit entries leading to the calculation of the implicit entry.

8.10.3.2 Default values

By default, all values are unknown and do not factor into any calculations. The only exceptions are entries corresponding to the percentage-based fields, which are assumed to be *100%*, unless defined.

8.10.3.3 Defining and changing values

You can only edit certain cells in the stoichiometry form, specifically the cells containing entries for values to be input into the calculations. You cannot edit titles. You cannot edit the Formula or Molecular Mass entries, as those are already defined by the reaction used to build the stoichiometry form.

To change a value in the stoichiometry form, perform the following steps:

1. Begin by selecting the **Text for Atoms and Captions** tool  in the **Drawing** toolbar.
2. Hover over the entry in the form you wish to input or change with the mouse so an amber highlight over the table cell appears as shown in Figure 8.21. Only the appropriate cells for editing will be hoverable.

Reactants				*Products*	
Formula	$C_9H_{12}O_3$	$C_8H_{14}O_2$		Formula	$C_{17}H_{26}O_5$
Molecular Mass	**168.19amu**	**142.20amu**		Molecular Mass	**310.38amu**
Coefficients	*1*	*1*		Coefficients	*1*
Equivalents				Equivalents	
Measured Mass				Measured Mass	
Purity (by mass)				Purity (by mass)	
Density				Output Mass	
Volume				Output Moles	
Molarity				%Completion	
Reacting Mass				Expected Mass	
Reacting Moles				Expected Moles	
Excess Mass				%Yield	

Figure 8.21: *Hovering an editable cell in a stoichiometry form with the Text for Atoms and Captions tool*

3. Click with the mouse and a customized popup to edit the entry will appear as shown in Figure 8.22. You will be able to edit values for blank and explicit entries, but values for implicit entries will be uneditable as they are defined by other entries in the form.

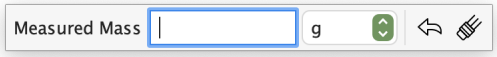


Figure 8.22: *Editing a stoichiometry form entry*

4. Edit your entry and confirm by clicking anywhere else in the document or by pressing the return or Enter key. If you wish to cancel your change, press the button in the popup or press the escape key.
5. Once confirmed, the form will self-calculate and update.

8.10.3.4 Clearing values

Only explicit values may be cleared. To clear a value in the stoichiometry form, perform the following steps:

1. Begin by selecting the **Text for Atoms and Captions** tool in the **Drawing** toolbar.
2. Hover over the entry in the form you wish to clear with the mouse so an amber highlight over the table cell appears as shown in Figure 8.21. Only cells containing explicit entries will be hoverable.
3. Click with the mouse and a customized popup to edit the entry will appear as shown in Figure 8.22.

4. Press the  button in the popup to clear the value. You may also enter a blank value and confirm, as this has the same effect.

5. Once cleared, the form will self-calculate and update, and dependent implicit entries will be removed from the form.

To more quickly clear explicit entries, you may also press the delete or backspace key while the cell containing the explicit entry is hovered.

8.10.3.5 Changing units

You can change units for both explicit and implicit entries. To change a unit in the stoichiometry form, perform the following steps:

1. Begin by selecting the **Text for Atoms and Captions** tool  in the **Drawing** toolbar.

2. Hover over the entry in the form you wish to change units for with the mouse so an amber highlight over the table cell appears as shown in Figure 8.21.

3. Click with the mouse and a customized popup to edit the entry will appear as shown in Figure 8.22.

4. On the right side of the popup will be a drop down selection containing unit options. Select the unit you desire. Confirm by clicking anywhere else in the document or by pressing the return/enter or escape key. If you wish to cancel your change, press the  button in the popup.

5. Once changed, the form will self-calculate and update.

Explicit entries with changed units will cause all implicit entries based on the explicit entry to update, but will not affect the units of those implicit entries. If you change units for an implicit entry, only that specific implicit entry will be affected.

Some entries may be unitless, and some may only have 1 unit option (*e.g.* the percentage-based fields can only be represented as percentages). In these cases, no edits to the unit are possible.

8.10.3.6 Flagged results

In all cases, the form will produce and present accurate results. However, there may be some suspicious entries caused by dubious user input, and in these cases the stoichiometry form will render such entries in the user defined error color of the application as shown in Figure 8.23.

Reactants				*Products*	
Formula	**$C_9H_{12}O_3$**	**$C_8H_{14}O_2$**		Formula	**$C_{17}H_{26}O_5$**
Molecular Mass	**168.19amu**	**142.20amu**		Molecular Mass	**310.38amu**
Coefficients	***1***	***1***		Coefficients	***1***
Equivalents	0.683	2.25		Equivalents	8.39
Measured Mass	***30.87g***	***86.11g***		Measured Mass	***700.38g***
Purity (by mass)				Purity (by mass)	
Density				Output Mass	700.38g
Volume				Output Moles	2.26mol
Molarity				%Completion	
Reacting Mass	***45.21g***	38.22g		Expected Mass	83.43g
Reacting Moles	0.269mol	0.269mol		Expected Moles	0.269mol
Excess Mass	-14.3g	47.89g		%Yield	839.46%

Figure 8.23: *Suspicious results are flagged in the stoichiometry form*

8.10.4 Examples

Several use cases for the stoichiometry form in ChemDoodle are presented in this section.

8.10.4.1 Determining the expected amount of product from measured reactant values

Question: For the following unbalanced reaction, we have 72.38g of Fe_2O_3 and unlimited carbon monoxide. How many grams of solid iron are produced if the reaction goes to completion?

$$Fe_2O_3(s) + CO(g) \longrightarrow Fe(s) + CO_2(g)$$

Answer: Draw the reaction in ChemDoodle and generate a stoichiometry form. The states of matter are irrelevant to our calculation.

Since we know we have a theoretical amount of Fe_2O_3, we simply input this value into the corresponding **Reacting Mass** entry (the default unit is already grams) and the stoichiometry form calculates the rest of the theoretical values as shown in Figure 8.24.

Reactants				*Products*		
Formula	**Fe_2O_3**	**CO**		Formula	**Fe**	**CO_2**
Molecular Mass	**159.69amu**	**28.01amu**		Molecular Mass	**55.84amu**	**44.01amu**
Coefficients	***1***	***3***		Coefficients	***2***	***3***
Equivalents				Equivalents		
Measured Mass				Measured Mass		
Purity (by mass)				Purity (by mass)		
Density				Output Mass		
Volume				Output Moles		
Molarity				%Completion		
Reacting Mass	***72.38g***	38.09g		Expected Mass	50.62g	59.84g
Reacting Moles	0.453mol	1.36mol		Expected Moles	0.907mol	1.36mol
Excess Mass				%Yield		

Figure 8.24: *Stoichiometry example: calculating expected mass of product*

The answer we are looking for is the calculated entry of **Expected Mass** for Fe, which is 50.62g.

8.10.4.2 Determining the required amount of reactant to produce a specific amount of product

Question: For the following drawn reaction (Figure 8.25), we want to produce 6.5 moles of 2-chloropropane. How many grams of 2-propanol and hydrochloric acid are required if the reaction goes to completion?

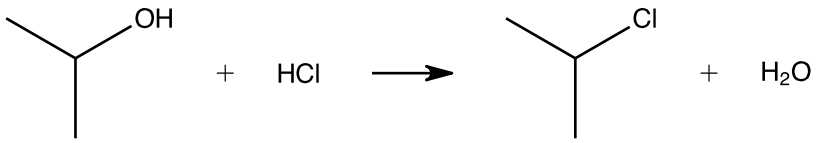


Figure 8.25: *Reaction to produce 2-chloropropane*

Answer: Draw the reaction in ChemDoodle and generate a stoichiometry form.

We want to theoretically produce 6.5 moles of 2-chloropropane. Simply input this value into the corresponding **Expected Moles** entry (the default unit is already moles) and the stoichiometry form calculates the rest of the theoretical values as shown in Figure 8.26.

Reactants				*Products*		
Formula	**C_3H_8O**	**ClH**		Formula	**C_3H_7Cl**	**H_2O**
Molecular Mass	**60.10amu**	**36.46amu**		Molecular Mass	**78.54amu**	**18.02amu**
Coefficients	***1***	***1***		Coefficients	***1***	***1***
Equivalents				Equivalents		
Measured Mass				Measured Mass		
Purity (by mass)				Purity (by mass)		
Density				Output Mass		
Volume				Output Moles		
Molarity				%Completion		
Reacting Mass	390.62g	236.99g		Expected Mass	510.51g	117.10g
Reacting Moles	6.50mol	6.50mol		Expected Moles	***6.5mol***	6.50mol
Excess Mass				%Yield		

Figure 8.26: *Stoichiometry example: calculating required mass of reactants*

The answers we are looking for are the calculated entries of **Reacting Mass** for each reactant, which are 390.62g of 2-propanol and 236.99g of hydrochloric acid.

8.10.4.3 Calculating the percent yield of an experiment

Question: The following organic reaction (Figure 8.27) has a known 90% completion rate. For an experiment, we mixed two solutions together, one of the ketone and one of the aldehyde and let them react to completion. The ketone solution has a known density of .12g/mL and 20 mL was used. The aldehyde solution has a known density of .47g/mL and 20mL was used. The resulting product was purified and crystallized out of solution, where the observed mass was 4.06g. What is the percentage yield of this experiment?

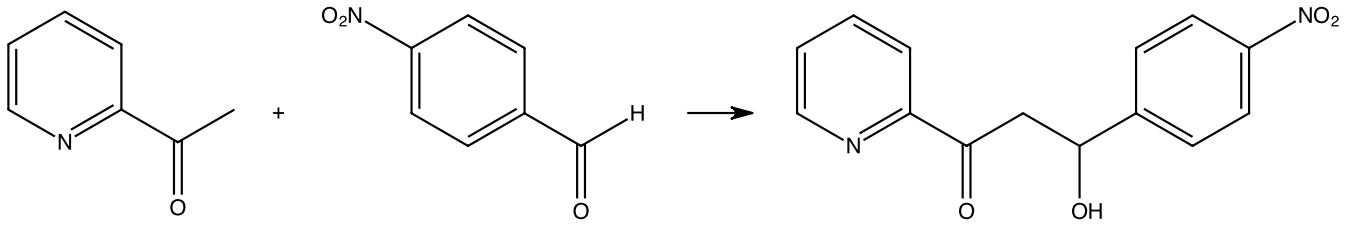


Figure 8.27: *Determining the percentage yield of a reaction*

Answer: Draw the reaction in ChemDoodle and generate a stoichiometry form.

We know that the theoretical percent completion of the reaction is 90%. So we input 90% into the **%Completion** field for the products. Next, we input the entries for the measured reactants, in this case both are solutions with a known density and volume, so we input the corresponding values and units into the **Density** and **Volume** fields. At this point, the table will have updated to give us expected entries for the product, but we are not done yet. We also know that 4.06g of pure product was recovered, so we input 4.06g into the **Measured Mass** entry for the product, completing the table with all of our known values as shown in Figure 8.28.

Reactants				*Products*	
Formula	**C_7H_7NO**	**$C_7H_5NO_3$**		Formula	**$C_{14}H_{12}N_2O_4$**
Molecular Mass	**121.14amu**	**151.12amu**		Molecular Mass	**272.26amu**
Coefficients	***1***	***1***		Coefficients	***1***
Equivalents	1.00	3.14		Equivalents	0.836
Measured Mass	2.40g	9.40g		Measured Mass	***4.06g***
Purity (by mass)				Purity (by mass)	
Density	***.12g/mL***	***.47g/mL***		Output Mass	4.06g
Volume	***20mL***	***20mL***		Output Moles	0.0149mol
Molarity	0.991mol/L	3.11mol/L		%Completion	***90%***
Reacting Mass	2.40g	2.99g		Expected Mass	4.85g
Reacting Moles	0.0198mol	0.0198mol		Expected Moles	0.0178mol
Excess Mass	0.00g	6.41g		%Yield	83.63%

Figure 8.28: *Stoichiometry example: calculating required mass of reactants*

The answer we are looking for is the **%Yield** entry for the product, which is calculated at 83.63%.

8.10.4.4 Determining the limiting reagent for a reaction

Question: For the following unbalanced reaction, we have 50mg each of ammonia and oxygen. Which reactant is the limiting reactant?

$$NH_3(g) + O_2(g) \longrightarrow N_2(g) + H_2O(g)$$

Answer: Draw the reaction in ChemDoodle and generate a stoichiometry form. The states of matter are irrelevant to our calculation.

We have two measured reactant masses, so we input these values into the **Measured Mass** entries for each reactant and the stoichiometry form calculates the rest of the theoretical values as shown in Figure 8.29. Don't forget to also set the units for the entries to milligrams as specified in the question.

Reactants				*Products*		
Formula	**NH_3**	**O_2**		Formula	**N_2**	**H_2O**
Molecular Mass	**17.03amu**	**32.00amu**		Molecular Mass	**28.01amu**	**18.02amu**
Coefficients	***4***	***3***		Coefficients	***2***	***6***
Equivalents	1.41	1.00		Equivalents		
Measured Mass	***50mg***	***50mg***		Measured Mass		
Purity (by mass)				Purity (by mass)		
Density				Output Mass		
Volume				Output Moles		
Molarity				%Completion		
Reacting Mass	0.0355g	0.0500g		Expected Mass	0.0292g	0.0563g
Reacting Moles	2.08E-3mol	1.56E-3mol		Expected Moles	1.04E-3mol	3.13E-3mol
Excess Mass	0.0145g	0.00g		%Yield		

Figure 8.29: *Stoichiometry example: determining the limiting reagent using experimental fields*

The theoretical amount of reactants used will be automatically determined by the stoichiometry form, and the **Excess Mass** entries will tell us how much of each reactant is leftover. If the value of the **Excess Mass** entry for a reactant is 0, then that reactant is the limiting reagent; in our case, oxygen is the limiting reagent. Keep in mind more than one reactant can have an **Excess Mass** entry with a value of 0, in which case there are technically multiple limiting reagents.

You may wonder why we put these values into the **Measured Mass** field rather than the **Reacting Mass** field. The **Reacting Mass** field is theoretical and therefore inputting only one entry defines the rest of the theoretical values. We can input 50mg into the **Reacting Mass** entry for ammonia, and the resulting table is shown in Figure 8.30. Notice the **Reacting Mass** entry for oxygen is calculated at 70.46mg (the unit for the **Reacting Mass** entry for oxygen was changed to mg for comparison). So theoretically, 70.46mg of oxygen is required to react with 50mg of ammonia to completion. This is more than the allotted 50mg provided, so oxygen is therefore the limiting reagent. Using the **Measured Mass** fields just makes things easier to comprehend as we can input both.

Reactants				*Products*		
Formula	**NH_3**	**O_2**		Formula	**N_2**	**H_2O**
Molecular Mass	**17.03amu**	**32.00amu**		Molecular Mass	**28.01amu**	**18.02amu**
Coefficients	***4***	***3***		Coefficients	***2***	***6***
Equivalents				Equivalents		
Measured Mass				Measured Mass		
Purity (by mass)				Purity (by mass)		
Density				Output Mass		
Volume				Output Moles		
Molarity				%Completion		
Reacting Mass	***50mg***	70.46mg		Expected Mass	0.0411g	0.0793g
Reacting Moles	2.94E-3mol	2.20E-3mol		Expected Moles	1.47E-3mol	4.40E-3mol
Excess Mass				%Yield		

Figure 8.30: *Stoichiometry example: determining the limiting reagent using theoretical fields*

8.10.4.5 Calculating partial stoichiometry using coefficients

Question: Consider a very complex reaction, consisting of many reactants, reagents and products, or a complex multistep reaction. It will be very time consuming to draw the reaction in its entirety and evaluate the stoichiometry of each step individually. Instead, we want to focus on a small number of input reactants and output products for a quick stoichiometric analysis. This is possible using ChemDoodle, as coefficients in stoichiometry tables can be defined, even if a reaction cannot be balanced.

The following multistep reaction describes the production of acetaminophen from phenol (Figure 8.31). There are several steps and reagents involved, however, we want to know the maximum amount of acetaminophen possible to be produced from 500g of phenol. How do we calculate that?

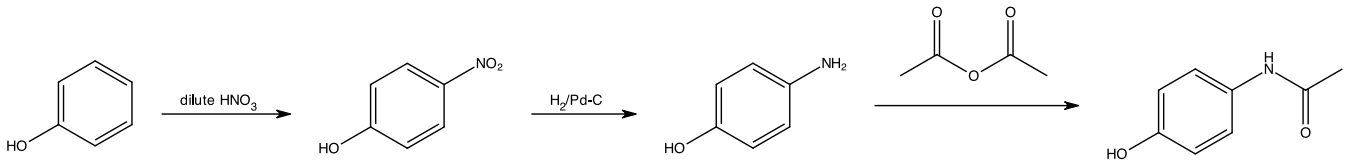


Figure 8.31: *The multistep synthesis of acetaminophen*

Answer: Draw a reaction in ChemDoodle with phenol as the reactant and acetaminophen as the product as shown in Figure 8.32.

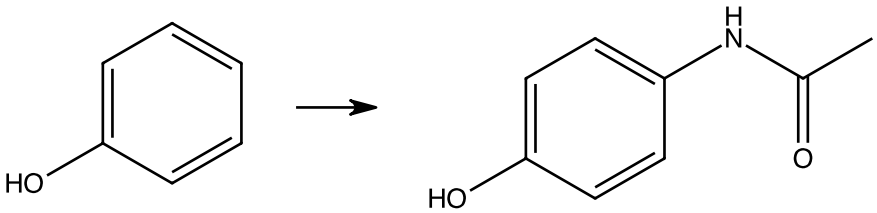


Figure 8.32: *A partially drawn reaction*

When you generate a stoichiometry form in ChemDoodle, a warning message will appear to notify you that the reaction cannot be balanced as shown in Figure 8.33.

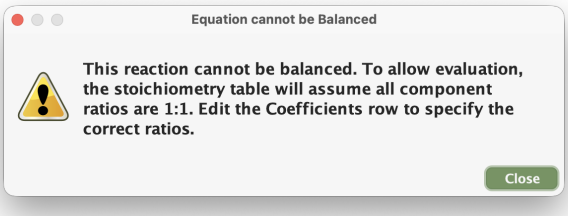


Figure 8.33: *Stoichiometry warning for an unbalancable reaction*

Select the **Close** button, and a stoichiometry form will be generated anyway. You will notice the entries in the **Coefficients** fields are automatically defined, by default, to 1 for each reactant and product. This specifies a 1:1 ratio for the stoichiometry between phenol and acetaminophen. This is correct, but if it is not correct for your case, you will need to change the coefficients values accordingly, and non-integer values may be used.

The rest is fairly simple, we start with 500g of phenol, so we input this value into the **Reacting Mass** entry for phenol. The table then updates as shown in Figure 8.34.

Reactants			*Products*	
Formula	C_6H_6O		Formula	$C_8H_9NO_2$
Molecular Mass	**94.11amu**		Molecular Mass	**151.16amu**
Coefficients	***1***		Coefficients	***1***
Equivalents			Equivalents	
Measured Mass			Measured Mass	
Purity (by mass)			Purity (by mass)	
Density			Output Mass	
Volume			Output Moles	
Molarity			%Completion	
Reacting Mass	***500g***		Expected Mass	803.11g
Reacting Moles	5.31mol		Expected Moles	5.31mol
Excess Mass			%Yield	

Figure 8.34: *Stoichiometry example: partial stoichiometry*

The answer we are looking for is the **Expected Mass** entry for acetaminophen, which is calculated at 803.11g. So in the best case scenario, where all steps in the multistep reaction go to 100% completion, we should expect to produce 803.11g of acetaminophen from 500g of phenol.

CHAPTER 9

Spectra

Contents

9.1 Overview **211**

9.2 Inserting spectra **211**
9.2.1 Spectra types 211
9.2.2 JCAMP NTUPLES 212
9.2.3 Uninterpretable spectra 213

9.3 Saving spectra **214**

9.4 Simulating spectra **214**
9.4.1 Nuclear Magnetic Resonance (NMR) simulations 214
9.4.1.1 Shift prediction 214
9.4.1.2 Splitting 215
9.4.1.3 Roof effects 215
9.4.1.4 Solvent peaks 215
9.4.1.5 ^{1}H rapid exchange 215
9.4.1.6 ^{1}H anisotropic effects 215
9.4.1.7 ^{1}H diastereotopic pairs 215
9.4.1.8 ^{13}C quaternary carbon intensity reductions 215
9.4.1.9 Limitations 215
9.4.2 Mass spectrometry (MS) simulations 215
9.4.2.1 Mass parent peak simulations 216
9.4.2.2 Fragmentation 216

9.5 Editing spectra **217**
9.5.1 Moving spectra 217
9.5.2 Resizing spectra 217
9.5.3 Removing spectra 218
9.5.4 Expanding the perspective 218
9.5.5 Editing the perspective 218
9.5.6 Changing the title 219
9.5.7 Changing the axes 219
9.5.8 Showing grids 219
9.5.9 Showing integration lines 220

9.1 Overview

ChemDoodle understands several spectroscopy and spectrometry techniques. These spectra can be loaded and edited to create graphics. This section introduces the new user to spectra within ChemDoodle. It covers the following topics:

- What types of spectra are supported.
- How to load spectra.
- How to save spectra.
- How to simulate spectra.
- How to edit spectra.

9.2 Inserting spectra

Spectra can be read in from the *JCAMP-DX* format which is the standard defined by *IUPAC*. The currently supported *JCAMP* formats are for nuclear magnetic resonance spectroscopy (NMR), infrared spectroscopy (IR), mass spectrometry (MS) and chemical structures.

To insert spectra from *JCAMP* files, execute the following steps:

1. Select the File > Open... menu item.
2. In the file chooser that appears, change the format filter on the bottom to **UPAC JCAMP-DX {jdx, dx}]**.
3. Find the *JCAMP* file on your computer and select it with the file chooser.
4. Press the **Open** button at the bottom-right of the file chooser to load the spectrum.

The spectrum will be loaded and displayed in the center of a new document.

9.2.1 Spectra types

Both continuous and discontinuous spectra are supported. An example of NMR input is shown in Figure 9.1. An example of IR input is shown in Figure 9.2. An example of MS input is shown in Figure 9.3.

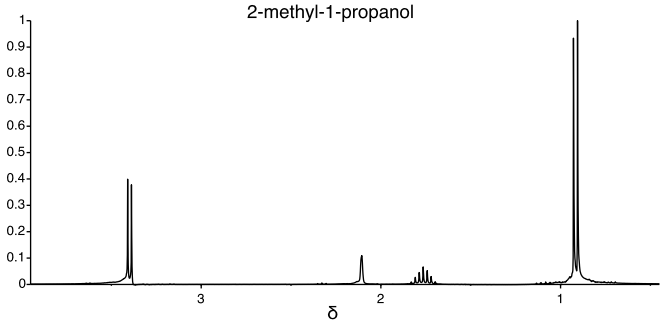


Figure 9.1: *An NMR Spectrum Loaded from a JCAMP File*

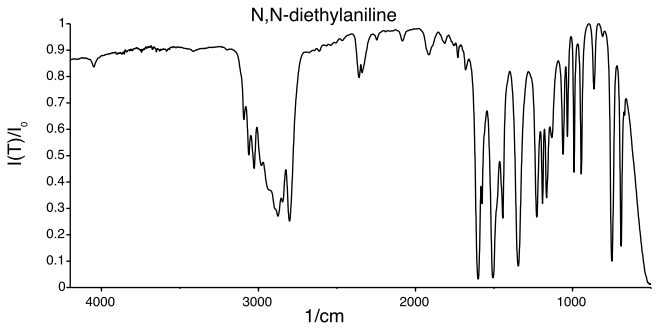


Figure 9.2: *An IR Spectrum Loaded from a JCAMP File*

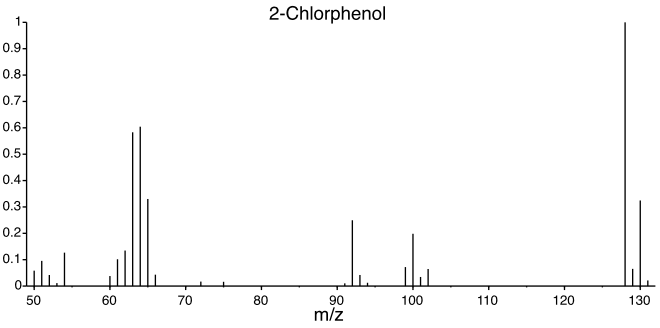


Figure 9.3: *An MS Spectrum Loaded from a JCAMP File*

9.2.2 JCAMP NTUPLES

ChemDoodle can understand multiple spectra from a single JCAMP file when described by the *NTUPLES* specification. Multiple spectra will be placed in a vertical column in the document on load. Typically, an *NTUPLES* file will contain both a real and imaginary spectrum for an NMR run as shown in Figure 9.4.

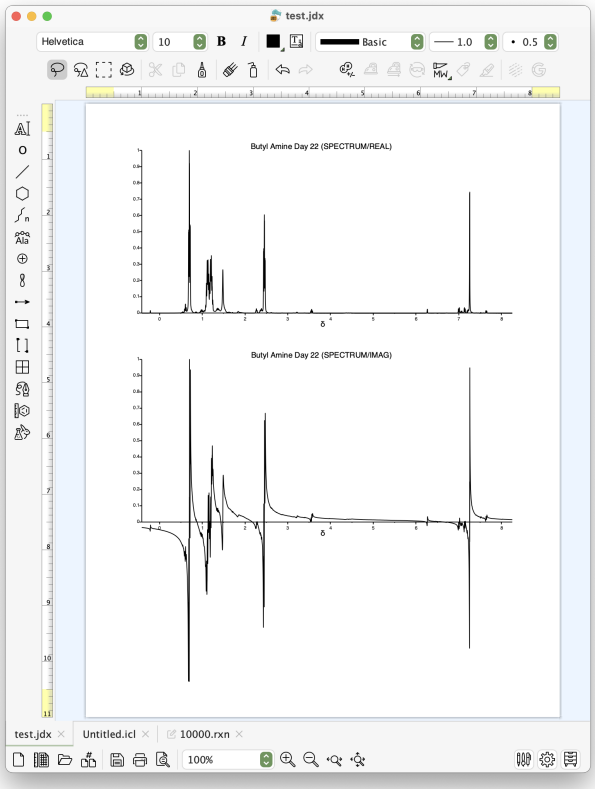


Figure 9.4: *Sample NTUPLES input from a JCAMP File*

9.2.3 Uninterpretable spectra

Some producers make non-conforming or custom JCAMP files. Therefore, ChemDoodle may not be able to understand a JCAMP file. If ChemDoodle was not able to interpret any spectra from the JCAMP file, you will see the message shown in Figure 9.5. Please send us the JCAMP file if you encounter this problem so that we may make it work for you.

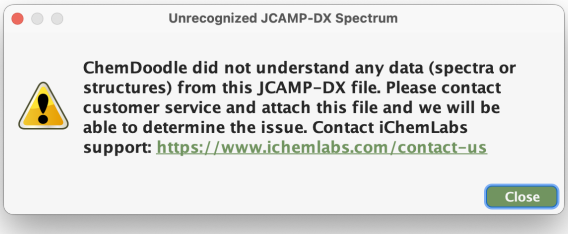


Figure 9.5: *ChemDoodle could not obtain any data from the JCAMP file.*

9.3 Saving spectra

ChemDoodle can output spectra in the following formats:

1. ChemDoodle Documents {*.icl*, *.icxml*}
2. IUPAC JCAMP-DX {*.jdx*, *.dx*}

To save your spectrum as a file, select the Save or Save As... menu items from the File menu. Save will automatically save the spectrum to the file it is associated with, while Save As... will allow you to save that file to a new location or overwrite another file. If there is no file associated with the current document, the Save function is identical to the Save As... function.

When saving a new file or using the Save As... function, a file chooser will appear. First, select the output format. For spectra, you will need to choose an output type from the previous list. Then select the location to save the file to and type a preferred file name or accept the default name. You do not need to type in an extension.



Be very careful when overwriting spectra to formats other than the *ChemDoodle Document*. ChemDoodle only reads and writes the information that is relevant to the display of its graphics, and other data will be lost. If you are saving third party spectra files for any reason, always save them as a new file.

9.4 Simulating spectra

ChemDoodle can simulate spectra for various techniques. Currently the following techniques are implemented:

- ^{1}H Nuclear Magnetic Resonance Spectroscopy
- ^{13}C Nuclear Magnetic Resonance Spectroscopy
- Mass Spectrum Parent Peak

To simulate spectra, execute the following steps:

1. Select the chemical structure you would like to simulate a spectrum for using the selection tools.
2. Expand the Spectrum > Generate submenu to view available techniques.
3. Click on the technique you would like to use.

The generated spectrum will then appear in the current document. Very intensive simulations may take a few seconds to complete.

9.4.1 Nuclear Magnetic Resonance (NMR) simulations

ChemDoodle can simulate ^{1}H and ^{13}C nuclear magnetic resonance spectroscopy. The **NMR Simulation** widget provides many customization options for the simulation and will present data on the output. This widget is covered in detail in the WIDGETS chapter.

The algorithms to simulate NMR spectra are continuously developed and improved. Important aspects of these algorithms are described in the rest of this section.

9.4.1.1 Shift prediction

ChemDoodle estimates chemical shifts for all hydrogen or carbon atoms for which incremental constants are available. The algorithm is an empirical approach and begins by identifying key functional groups in a structure. The identified functional

groups are used to determine base values for the estimated shifts of the nuclei.

After determining a base shift, a breadth-first algorithm is employed to look at the chemical environment surrounding each nucleus. Based on the functional groups around it, incremental constants are added to the base shift to calculate the estimated shift. Other contributions may be included such as ring strain and other algorithms.

9.4.1.2 Splitting

Splitting is determined by a table of typical j-constant magnitudes and the spin of the interacting nuclei. Splitting is calculated for all spins. Splitting magnitudes are determined from Pascal's triangle.

9.4.1.3 Roof effects

The magnitude for roof effects is determined by the resolution of the spectrum, set by the **Pulse Frequency** parameter, and the relative adjacency of the interacting peaks. The simulated roof effects will show a leaning of the split peak towards the peak that is splitting it. Peaks split by multiple peaks will lean towards all of them.

9.4.1.4 Solvent peaks

Solvent peaks are simulated using the same algorithms. Splitting from deuterium occurs. The magnitude ratio for solvent to solute peaks is determined by the **Dilution** parameter.

9.4.1.5 ^{1}H rapid exchange

If the temperature is above 273K, rapid exchange will occur for hydrogen bonded protons. These peaks will merge into a single broadened peak with a shift calculated at their weighted average. The shift will then be moved downfield relative to the magnitude of the temperature.

9.4.1.6 ^{1}H anisotropic effects

If the solvent or solute contains aromatic or antiaromatic rings, then ^{1}H nuclei will be appropriately shielded or deshielded based on the solvent/solute ratio and the types of rings involved.

9.4.1.7 ^{1}H diastereotopic pairs

If a methylene is adjacent to a stereocenter, then the two methylene protons will be separated into individual peaks. The peaks will be separated by 0.3 ppm centered around the predicted shift for the methylene group. The choice of nucleus to be shifted upfield or downfield is random.

9.4.1.8 ^{13}C quaternary carbon intensity reductions

To simulate a lack of Overhauser effects, quaternary carbons have their peak intensities reduced by 33 percent.

9.4.1.9 Limitations

ChemDoodle can only predict shifts for nuclei where environments are well described in its database. Functional groups that are not described well will have poorly calculated shifts and may result in values around 0 ppm, which should be ignored.

Since incremental constants do not take into account structure topography, 3D conformations will be poorly analyzed. It is essential that you fully scrutinize all NMR simulation results from ChemDoodle.

To learn more about the algorithms implemented in ChemDoodle and their accuracy, obtain the references listed under the *Algorithms* > *Spectroscopy* > *Nuclear Magnetic Resonance* section of ChemDoodle's reference list. The reference list can be viewed by selecting the Help » References menu item.

9.4.2 Mass spectrometry (MS) simulations

9.4.2.1 Mass parent peak simulations

The **Elemental Analysis** widget provides more elemental analysis calculations for your structures along with controls for the resolution of mass parent peak simulations. This widget is covered in detail in the WIDGETS chapter.

9.4.2.2 Fragmentation

ChemDoodle contains a powerful tool for fragmenting molecules. By using this tool, you can quickly break molecules apart and see the resulting masses. This facilitates the analysis of mass spectrometry peaks. The **Mass Fragmentation** tool 

can be found in the **Fragmentation Tools** group button in the **Content** toolbar.

To fragment a molecule or group of molecules, execute the following steps:

1. Select the **Mass Fragmentation** tool 

, which can be found in the **Fragmentation Tools** group button in the **Content** toolbar.

2. Press the mouse down and drag through all of the bonds to be broken, defining how the molecule is to be fragmented. A green line will follow the mouse path as shown in Figure 9.6.

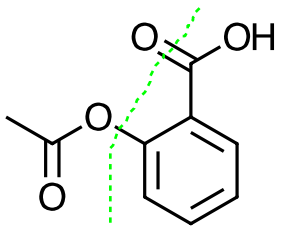


Figure 9.6: *Fragmenting an aspirin molecule*

3. Release the mouse to complete the function. Electrons will be added appropriately to account for the split bonds. Molecular mass calculations will be shown next to each fragment as displayed in Figure 9.7.

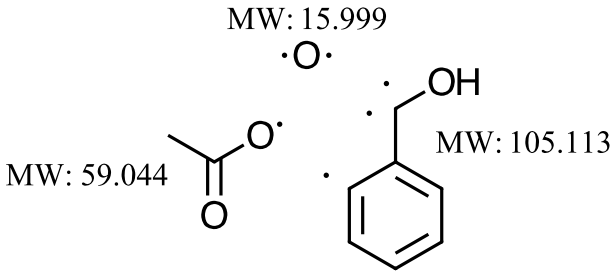


Figure 9.7: *The results of fragmenting an aspirin molecule*

When using the **Molecular Weight** fragmentation tool, monoisotopic masses will be calculated for the fragments generated. If you prefer to calculate molecular masses instead, in the **Settings** window under the **Tools** tab, select **Molecular Mass** for the **Mass Fragmentation Calculator** setting in the **Fragmentation** section.

9.5 Editing spectra

Spectra are shapes that can be edited like other shapes in ChemDoodle and are defined by an anchor box that controls its dimensions. When hovered, controls for the anchor box will appear as shown in Figure 9.8.

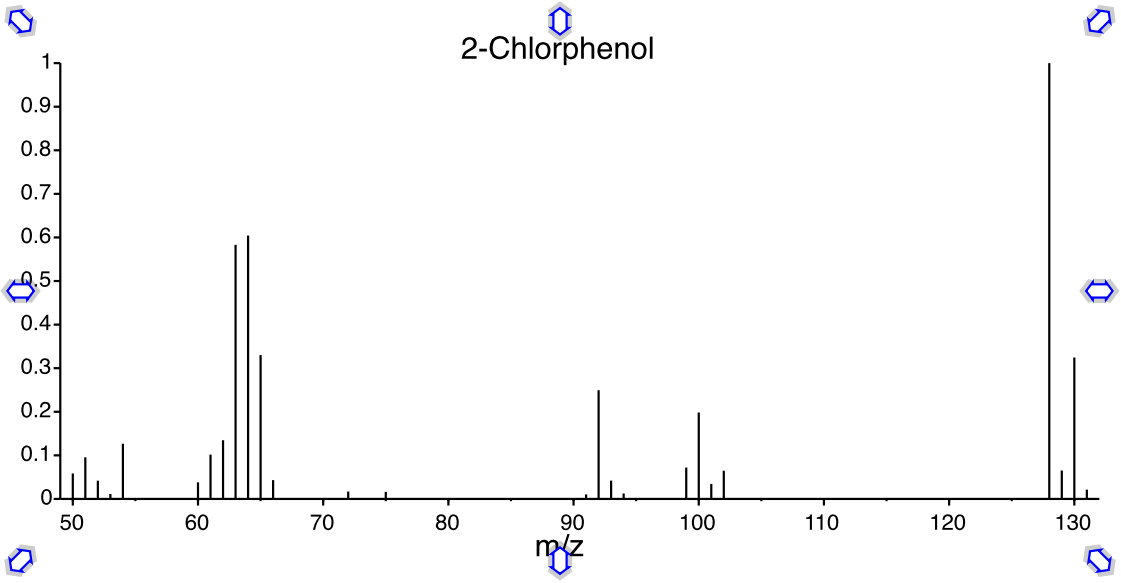


Figure 9.8: *Hovering Over a Spectrum to Display its Anchor Points*

9.5.1 Moving spectra

To move spectra, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the spectrum so an open hand mouse cursor appears and the spectrum anchor points are drawn as shown in Figure 9.8.
2. Press the mouse down and drag to move the spectrum.
3. Release the mouse to finish the move action.

9.5.2 Resizing spectra

To resize spectra, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the spectrum so an open hand mouse cursor appears and the spectrum anchor points are drawn as shown in Figure 9.8.
2. Move the mouse pointer over one of the anchor points so that anchor point is filled with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.

4. Drag the anchor point to resize the rectangle.
5. Release the mouse to finish the resize action.

9.5.3 Removing spectra

Spectra can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the spectrum until an open hand mouse cursor appears and the spectrum anchor points are drawn as shown in Figure 9.8. Then press either the backspace or delete key.
- Use the **Eraser** tool to hover the mouse pointer over the spectrum so the spectrum anchor points are drawn. Then click with the mouse.
- Select the spectrum using any of the selection tools. Then press either the delete or backspace key.

9.5.4 Expanding the perspective

Expanding the spectrum will fit the entire range and domain of the plot to the display rectangle. Execute the following steps.

1. Use the selection tools to select any number of spectra.
2. Click on the Spectrum ⟩ Expand Perspective menu item.

All selected spectra will have their perspectives expanded.

9.5.5 Editing the perspective

Editing the perspective will allow you to modify how the plot fits in the viewing rectangle and will also allow you to edit the axes and title. These functions are presented in the **Spectrum Edit** window as shown in Figure 9.9. You access the **Spectrum Edit** window by highlighting the spectrum you want to edit with a selection tool, right-clicking, and then choosing the Edit Perspective... menu item.

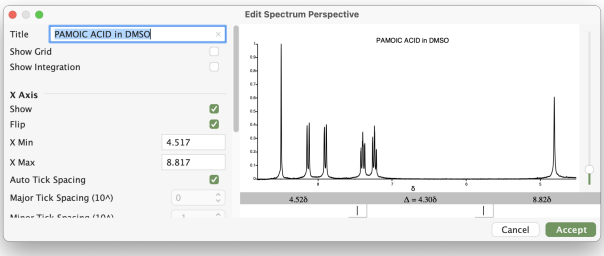


Figure 9.9: *The Spectrum Edit Window*

To specifically define the start and end parameters of the plot domain, change the **X Min** and **X Max** number fields in the **X Axis** section. To roughly change the plot domain, click and drag the sliders presented directly under the spectrum. The sliders display, from left to right, the minimum domain cutoff, the magnitude of the domain, and the maximum domain cutoff. You can also change the plot domain by clicking and dragging on the main spectrum panel. Click on the placement where you would like the domain to begin, then drag to where you would like the domain to end and release the mouse. A dotted grey line will display while dragging to mark the new domain. Holding the shift key while dragging on the spectrum will translate the domain of the spectrum.

To specifically define the plot range scale, change the **Y Max** number field in the **Y Axis** section. To roughly change the range scale, click and drag the vertical slider directly to the right of the spectrum. You can also change the range scale by using the mouse scroll gesture on the main spectrum panel. Scroll up to increase the range scale and scroll down to decrease the range scale.

To expand the perspective, double-click on the main spectrum panel.

9.5.6 Changing the title

To change the title of the spectrum, in the **Spectrum Edit** window shown in Figure 9.9, click on the **Title** text field located to the left and type in the desired title.

9.5.7 Changing the axes

There are several options for editing the axes.

X-axis options are presented in the **X Axis** section of the **Spectrum Edit** window shown in Figure 9.9. You can choose to show or hide the *x*-axis by clicking the **Show** check box. You can choose whether or not to flip the domain by clicking the **Flip** check box. You can select the **Auto Tick Spacing** check box to have the spectrum ticks automatically allocated appropriately for you. Alternatively, you can adjust the increments for the major and minor tick spacings using the **Major Tick Spacing** and **Minor Tick Spacing** drop-down selections. The values in the drop-down selections are exponents for base 10. You can change the title of the *x*-axis by clicking on the **Unit** text field and typing the desired title.

Y-axis options are presented in the **Y Axis** section of the **Spectrum Edit** window shown in Figure 9.9. You can choose to show or hide it by clicking the **Show** check box. The **Baseline Bump** check box will positively offset the plot by a small value. You can adjust how many major ticks appear on the *y*-axis using the **Tick Divisions** drop-down selection. You can change the title of the *y*-axis by clicking on the **Unit** text field and typing the desired title.

9.5.8 Showing grids

Grids can be displayed by executing the following steps:

1. Hover the spectrum to display the grid.
2. Right-click on the spectrum and select the Format Spectrum... menu item.
3. Scroll down to the **Grid** section and select the **Show Grid** checkbox.

The color and thickness of the grid lines can also be set in this format window. A grid appears as shown in Figure 9.10.

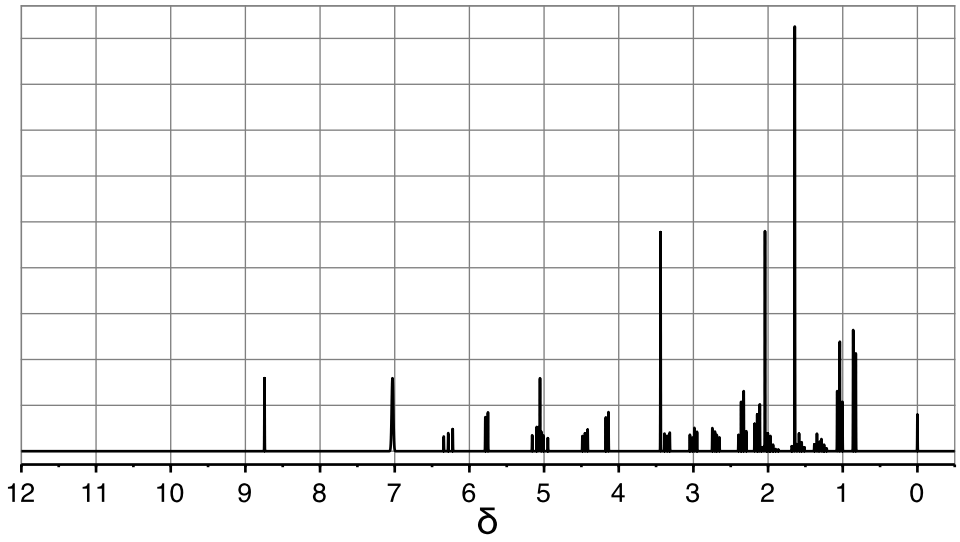


Figure 9.10: *A Grid Displayed Over a Spectrum*

9.5.9 Showing integration lines

Integration lines can be displayed by executing the following steps:

1. Hover the spectrum to display the integration line.
2. Right-click on the spectrum and select the Format Spectrum... menu item.
3. Scroll down to the **Integration Line** section and select the **Show for NMR Spectra** checkbox.

The color and thickness of the integration line can also be set in this format window. While intended for NMR spectra, integration lines can be added to any plot if desired. An integration line appears as shown in Figure 9.11.

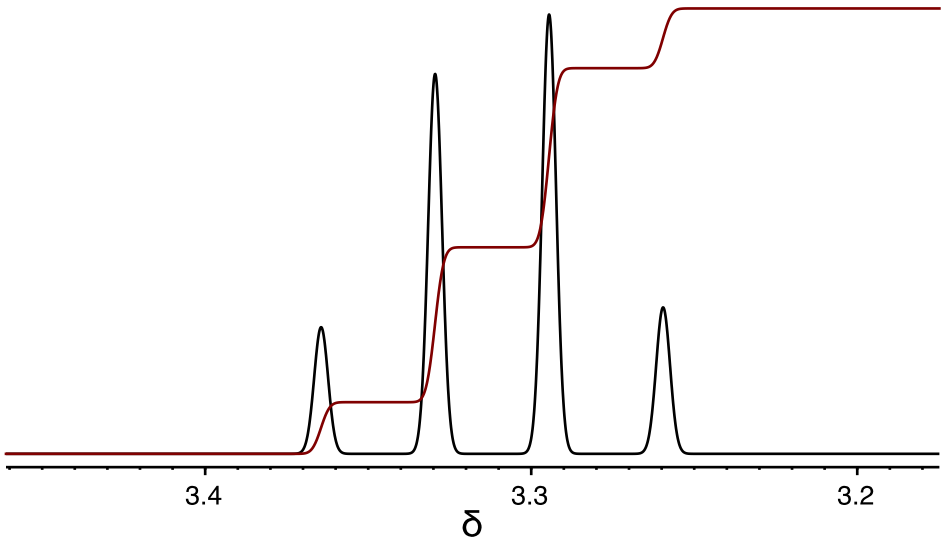


Figure 9.11: *An Integration Line Calculated Over an NMR Multiplet*

CHAPTER 10

Shapes

Contents

10.1 Overview **225**

10.2 Shape types **225**
10.2.1 Manual shapes 225
10.2.1.1 Anchors 225
10.2.1.2 Control anchors 226
10.2.1.3 Corner/edge anchors 226
10.2.1.4 Moving 226
10.2.1.5 Resizing 226
10.2.1.6 Removing 227
10.2.1.7 Edit shapes while drawing shapes 227
10.2.2 Automatic shapes 227
10.2.2.1 Moving 227
10.2.2.2 Resizing 227
10.2.2.3 Removing 227

10.3 Lines **228**
10.3.1 Drawing lines at fixed angles 228
10.3.2 Drawing lines at non-fixed angles 228
10.3.3 Forcing lines to be drawn vertically and horizontally 228

10.4 Arcs **228**
10.4.1 Drawing arcs at fixed angles 229
10.4.2 Drawing arcs at non-fixed angles 229
10.4.3 Forcing arcs to be drawn vertically and horizontally 229
10.4.4 Changing arc angles 229
10.4.5 Flipping an arc's orientation 230
10.4.6 Changing arc lengths 230

10.5 Rectangles **230**
10.5.1 Drawing rectangles 230
10.5.2 Drawing squares 231
10.5.3 Converting between rounded & non-rounded rectangles 231

10.6 Ovals **231**
10.6.1 Drawing ovals 231
10.6.2 Drawing circles 232

10.7 Brackets **232**
10.7.1 Drawing brackets 232
10.7.2 Drawing brackets with equal width and height 232
10.7.3 Editing bracket lip protrusion 232

10.8 Custom shapes **233**
10.8.1 Drawing with the pen tool 234
10.8.2 Drawing with the polyline tool 234
10.8.3 Modifying pen paths and polylines 234
10.8.4 Drawing with the Bézier tool 235
10.8.5 Modifying Bézier curves 235
10.8.6 Deleting Bézier control points 236
10.8.7 Adding arrowheads to custom shapes 236
10.8.8 Closing and opening custom shapes 236

10.9 Rulers . . . **237**
10.9.1 Drawing rulers at fixed angles . . . 237
10.9.2 Drawing rulers at non-fixed angles . . . 237
10.9.3 Forcing rulers to be drawn vertically and horizontally . . . 237
10.9.4 Automatically measuring object width and height . . . 237
10.9.5 Automatically measuring object diagonal . . . 237
10.9.6 Showing and hiding major and minor ticks . . . 238
10.9.7 Changing the measurement unit . . . 238

10.10 Tables . . . **238**
10.10.1 Creating tables . . . 239
10.10.1.1 Drawing tables . . . 239
10.10.1.2 Defining a table by rows and columns . . . 239
10.10.1.3 Drawing square tables . . . 240
10.10.2 Editing tables . . . 240
10.10.2.1 Adding a row . . . 240
10.10.2.2 Resizing a row . . . 241
10.10.2.3 Removing a row . . . 241
10.10.2.4 Adding a column . . . 241
10.10.2.5 Resizing a column . . . 241
10.10.2.6 Removing a column . . . 241
10.10.2.7 Fitting a table to its contents . . . 242
10.10.3 Editing cells . . . 242
10.10.3.1 Adding content . . . 243
10.10.3.2 Editing content . . . 243
10.10.3.3 Setting or editing a cell label . . . 243
10.10.3.4 Clearing content . . . 244
10.10.3.5 Styling . . . 244
10.10.3.6 Defining a rowspan . . . 244
10.10.3.7 Defining a colspan . . . 245
10.10.3.8 Alignment . . . 245
10.10.3.9 Padding . . . 245

10.11 Labels . . . **246**
10.11.1 Adding text with the text tool . . . 246
10.11.2 Token and line spacing . . . 247
10.11.3 Controlling fonts . . . 247
10.11.4 Creating equally spaced labels . . . 247
10.11.5 Copying formatted text from labels . . . 247
10.11.6 Moving labels . . . 247
10.11.7 Editing label text . . . 248
10.11.8 Auto-updating labels . . . 248
10.11.8.1 Adding updating labels . . . 248
10.11.8.2 Editing updating labels . . . 249
10.11.8.3 Reattaching moved updating labels . . . 249
10.11.8.4 Updating label options . . . 249

10.12 Atom mappings . . . **250**
10.12.1 Adding atom mappings . . . 250
10.12.2 Editing atom mapping rendering styles . . . 251
10.12.3 Working with atom mappings . . . 251

10.13 Electron pushers . . . **251**
10.13.1 Adding electron pushers . . . 252
10.13.2 Flipping electron pushers . . . 252

10.13.3 Special cases . . . 252
10.13.3.1 Bond to atom shortcuts . . . 252
10.13.4 Editing electron pusher styles . . . 253
10.13.5 Converting to Bézier arrows . . . 253

10.14 Highlights . . . **254**
10.14.1 Adding highlights . . . 254
10.14.2 Customizing highlights . . . 254
10.14.3 Color in rings . . . 255
10.14.4 Merging highlights . . . 255

10.15 Repeat unit brackets . . . **256**
10.15.1 Adding repeat units . . . 256
10.15.2 Defining the repeat unit display value . . . 257
10.15.3 Flipping repeat units . . . 257
10.15.4 Editing repeat units styles . . . 257
10.15.5 Repeat unit bracket types . . . 258
10.15.6 Enclosing shortest paths . . . 258
10.15.7 Working with repeat units . . . 259

10.1 Overview

In addition to chemical structures, ChemDoodle provides tools for drawing shapes for advanced figures.

In this chapter the new user is introduced to shapes within ChemDoodle. Topics covered include:

- The different types of shapes.
- How to draw shapes.
- Adding text to figures.
- How to move shapes.
- How to resize shapes.
- How to remove shapes.
- What the anchor decorations mean.

10.2 Shape types

There are two categories of shapes in ChemDoodle: *manual* and *automatic*. *Manual* shapes are controlled by anchors and their shapes and sizes are fully defined by the user. *Automatic* shapes are set to other objects and their layout is automatically controlled by those other objects.

Then there is one last unique shape, the LABELS, which is controlled by a single control point, and its bounds is based on the text that defines it.

10.2.1 Manual shapes

ChemDoodle allows the user to create the following *manual* shapes:

- LINES
- ARCS
- RECTANGLES
- OVALS
- BRACKETS
- CUSTOM SHAPES
- RULERS
- TABLES

There a few more. Orbitals are covered in the DRAWING CHEMICAL STRUCTURES chapter. Arrows are covered in the REACTIONS chapter. Spectra are covered in the SPECTRA chapter. Vector art is covered in the iChemLabs ART chapter.

10.2.1.1 Anchors

Anchors are points that define a given shape. Anchors are only present on *manual* shapes. By moving anchors, you modify how the shape appears. There are two types of anchors, control anchors and corner/edge anchors.

10.2.1.2 Control anchors

Control anchors represent points that can be moved anywhere and have no relationship to other anchors. Shapes that are controlled by these achors include lines, custom shapes or orbitals. They appear as compass shapes as shown in Figure 10.1.



Figure 10.1: *Control Anchors*

10.2.1.3 Corner/edge anchors

Corner edge anchors define corners and edges of shapes. Moving these anchors will change the shape in relationship to the other anchors. For instance, if you move a left-right pointing anchor, you will not affect the vertical positioning of the other anchors. These anchors are present for box shaped objects, like rectangles and ovals. They appear as double sided arrows as shown in Figure 10.2.

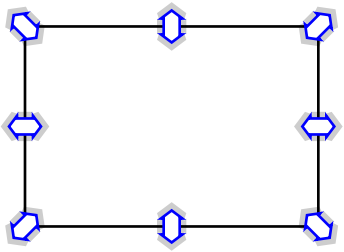


Figure 10.2: *Corner/Edge Anchors*

10.2.1.4 Moving

To move *manual* shapes, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the shape so an open hand mouse cursor appears and the anchor points are shown for the shape.
2. Press the mouse down without selecting any of the anchors and drag to move the shape.
3. Release the mouse to finish the move action.

10.2.1.5 Resizing

To resize *manual* shapes, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the shape so an open hand mouse cursor appears and the anchor points are shown for the shape.
2. Move the mouse pointer over one of the anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.

4. Drag the anchor point to resize the shape.
5. Release the mouse to finish the resize action.

10.2.1.6 Removing

Manual shapes can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the shape so an open hand mouse cursor appears and the shape anchor points are shown for the shape. Then press the backspace or delete key.
- Use the eraser tool  to hover the mouse pointer over the shape so the shape anchor points are drawn. Then click with the mouse.

10.2.1.7 Edit shapes while drawing shapes

For convenience and quick editing when drawing shapes, you can use the same tool to edit shapes, without having to switch to a selection tool. By default, you can edit any shape type that is the **Same** type as the one you are currently drawing (you may edit other rectangles when drawing rectangles). There is a setting in the **Settings** window, in the **Controls** tab named **Edit Shapes while Drawing Shapes**. You may change this setting to expand the range to editing **All** shapes or restrict it to editing **None**. The **None** choice is optimal if you have a very congested figure and want more control over precisely drawing shapes.

10.2.2 Automatic shapes

ChemDoodle allows the user to create the following *automatic* shapes:

- ATOM MAPPINGS
- ELECTRON PUSHERS
- HIGHLIGHTS
- REPEAT UNIT BRACKETS

10.2.2.1 Moving

Automatic shapes are defined by the objects they are set to, and cannot be moved.

10.2.2.2 Resizing

Automatic shapes are defined by the objects they are set to, and cannot be resized.

10.2.2.3 Removing

Automatic shapes can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the shape so the shape is outlined by an amber color. Then press the backspace or delete key.
- Use the eraser tool  to hover the mouse pointer over the shape so the shape is outlined by an amber color. Then click with the mouse.
- Delete any of the objects that define the *automatic* shape, and the shape will also be removed.

10.3 Lines

Lines are the most basic shape and are defined by two anchors placed at their endpoints as shown in Figure 10.3. There is also a third anchor at the midpoint for controlling the arc angle. This anchor point is discussed in the next section (Arcs). Lines are *manual* shapes.

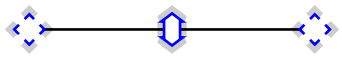


Figure 10.3: *Line Shape and Anchors*

10.3.1 Drawing lines at fixed angles

To draw a line at fixed angles, execute the following steps:

1. Select a line tool from the **Shapes** palette in the **Drawing** toolbar.
2. Press and hold the mouse down on the current document to set the start point of the line.
3. Drag the mouse to preview the placement of the end of the line.
4. Release the mouse to set the line.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

By default, lines will be oriented at fixed angles every 15° starting at 0°.

10.3.2 Drawing lines at non-fixed angles

To place lines at non-fixed angles, hold down the alt key while dragging the mouse when defining the line.

10.3.3 Forcing lines to be drawn vertically and horizontally

To place lines oriented vertically or horizontally, hold down the shift key while dragging the mouse when defining the line. The line preview will then automatically orient vertically or horizontally depending on the angle from the start point to the current mouse cursor position.

10.4 Arcs

Arcs are segments of a circle and are defined by two anchors placed at their endpoints as shown in Figure 10.4. There is a third anchor at the middle of the arc for controlling the arc angle. And finally there are two anchors flanking the end points for controlling the arc length.

The only difference between the line shape in the previous section and an arc shape is the angle, and either shape can be converted into the other by changing this value. Only 90°, 120°, 180° and 270° arc drawing tools are directly available in the **Shapes** palette, but an arc of any angle can be drawn in ChemDoodle. Arcs are *manual* shapes.

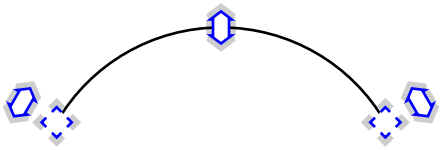


Figure 10.4: *Arc Shape and Anchors*

10.4.1 Drawing arcs at fixed angles

Here, the angle we are referring to is the reference from one end point to the other, not the arc angle. To draw an arc at fixed angles, execute the following steps:

1. Select an arc tool by expanding the **Shapes** palette in the **Drawing** toolbar.
2. Press and hold the mouse down on the current document to set the start point of the arc.
3. Drag the mouse to preview the placement of the end of the arc.
4. Release the mouse to set the arc.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

By default, arcs will be oriented at fixed angles every 15° starting at 0°.

While placing the arc, if the z key is clicked, the arc will toggle to the opposite side.

10.4.2 Drawing arcs at non-fixed angles

Here, the angle we are referring to is the reference from one end point to the other, not the arc angle. To place arcs at non-fixed angles, break from the fixed orientation angles by holding down the alt key while dragging the mouse when defining the arc.

10.4.3 Forcing arcs to be drawn vertically and horizontally

To place arcs oriented vertically or horizontally, hold down the shift key while dragging the mouse when defining the arc. The arc preview will then automatically orient vertically or horizontally depending on the angle from the start point to the current mouse cursor position.

10.4.4 Changing arc angles

Arc angles can be changed using the midpoint anchor. Choose a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the arc so an open hand mouse cursor appears and the arc anchor points are drawn as shown in Figure 10.4.
2. Move the mouse pointer over the middle anchor point so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to change the arc angle.
5. Release the mouse to set the new arc angle.

While changing the angle of arcs, the arc angle will be displayed below the mouse cursor.

10.4.5 Flipping an arc's orientation

To flip an arc's orientation, so that the curve faces the opposite direction. use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the arc so an open hand mouse cursor appears and the arc anchor points are drawn as shown in Figure 10.4.
2. Right-click on the hovered arc.
3. Select the Flip Arc menu item to flip the arc's orientation.

You can also click and drag the midpoint to the other side of the arc to perform this task.

If you are viewing the preview of the arc while drawing it, you can click the z key to quickly flip it in the other direction.

10.4.6 Changing arc lengths

Arc lengths can be changed using the anchors flanking the endpoints. Choose a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the arc so an open hand mouse cursor appears and the arc anchor points are drawn as shown in Figure 10.4.
2. Move the mouse pointer over either flanking anchor point so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to change the arc length.
5. Release the mouse to set the new arc length.

While changing the length of arcs, the resulting arc angle will be displayed below the mouse cursor.

10.5 Rectangles

Rectangles can be drawn in several styles and are defined by an anchor box set that controls its dimensions as shown in Figure 10.5. Rectangles are *manual* shapes.

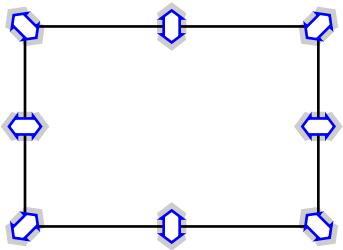


Figure 10.5: *Rectangle Shape and Anchors*

10.5.1 Drawing rectangles

To draw a rectangle, execute the following steps:

1. Select a rectangle tool from the **Shapes** palette in the **Drawing** toolbar.

2. Press the mouse down on the current document to set one corner of the rectangle.
3. Drag the mouse to preview the placement of the opposite corner along the diagonal of the rectangle.
4. Release the mouse to set the rectangle.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

10.5.2 Drawing squares

To draw squares, hold down the shift key while dragging the mouse when defining the rectangle to force the width and height to be equal.

10.5.3 Converting between rounded & non-rounded rectangles

To change a rectangle into a rounded rectangle or vice versa, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the rectangle so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in Figure 10.5.
2. Right-click on the hovered rectangle and select the Format Rectangle... menu item.
3. Scroll to the **Rectangle** section and use the **Rounded** on/off choice to set the rectangle to be rounded or not.

10.6 Ovals

Ovals can be drawn in several styles and are defined by an anchor box set that controls its dimensions as shown in Figure 10.6. Ovals are *manual* shapes.

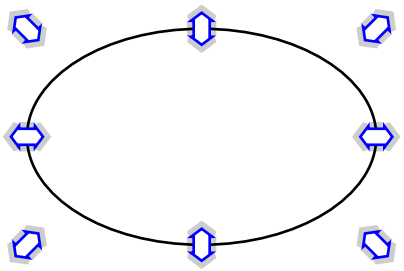


Figure 10.6: *Oval Shape and Anchors*

10.6.1 Drawing ovals

To draw an oval, execute the following steps:

1. Select an oval tool from the **Shapes** palette in the **Drawing** toolbar.
2. Press and hold the mouse on the current document to set one corner of the circumscribing rectangle.
3. Drag the mouse to preview the placement of the opposite corner along the diagonal of the circumscribing rectangle.
4. Release the mouse to set the oval.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

10.6.2 Drawing circles

To draw circles, hold down the shift key while dragging the mouse when defining the oval to force the major and minor axes lengths to be equal.

10.7 Brackets

Brackets can be drawn in several styles and are defined by an anchor box set that controls its dimensions as shown in Figure 10.7. Brackets are *manual* shapes.

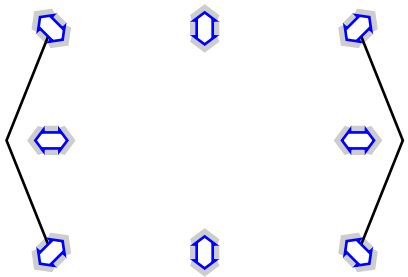


Figure 10.7: *Bracket Shape and Anchors*

There are currently 4 bracket styles:

- **Square Brackets** - [ ]
- **Parentheses** - ( )
- **Curly Brackets** - { }
- **Chevrons** - < >

10.7.1 Drawing brackets

To draw a set of brackets, execute the following steps:

1. Select a bracket tool by expanding the **Brackets** palette in the **Drawing** toolbar.
2. Press and hold the mouse down on the current document to set one corner of the bracket.
3. Drag the mouse to preview the placement of the opposite corner along the diagonal of the bracket.
4. Release the mouse to set the bracket.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

10.7.2 Drawing brackets with equal width and height

To draw square brackets, hold down the shift key while dragging the mouse when defining the bracket to force the width and height of the bracket content to be equal.

10.7.3 Editing bracket lip protrusion

To change the widths of the current bracket rendering style, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the brackets so an open hand mouse cursor appears and the bracket anchor points are drawn as shown in Figure 10.7.
2. Right-click on the hovered bracket and select the Format Bracket... menu item.
3. Scroll to the **Bracket** section and use the **Wideness** number slider to define how protruded bracket lips are rendered.

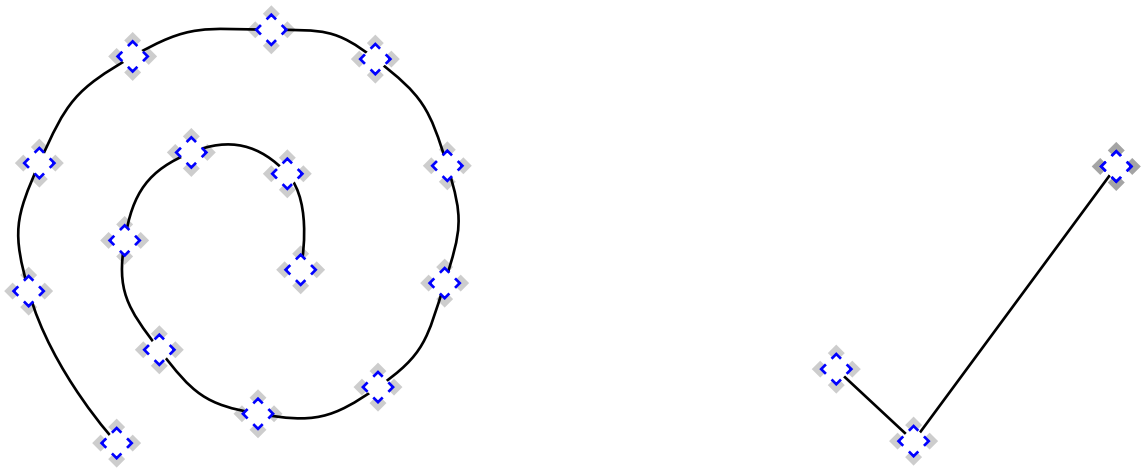
10.8 Custom shapes

In addition to the standard defined shapes previously discussed, ChemDoodle allows you to create custom shapes. All custom shapes are *manual* shapes. Currently there are three types of custom shapes:

Table 10.1: Available Custom Shapes

Icon	Tool	Action
	**Pen**	Allows you to draw any shape by clicking and dragging an outline.
	**Bézier Curve**	Allows you to draw a Bézier curve by defining its control points.
	**Polyline**	Allows you do draw any polygon shape that can be convex or concave.

Both pen paths and polylines can be open or closed and are defined by their control points, which the shape will pass through as shown in Figure 10.8.



(a) *Pen Shape and Anchors* (b) *Polyline Shape and Anchors*

Figure 10.8: *Pen and Polyline Control Points*

Bézier curves can be open or closed and are defined by a more complex set of control points as shown in Figure 10.9.

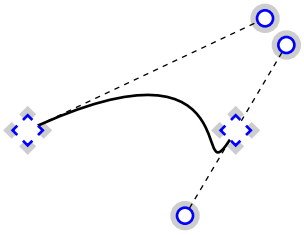


Figure 10.9: *Bézier Control Points*

10.8.1 Drawing with the pen tool

To draw a custom shape with the **Pen** tool, execute the following steps:

1. Select the **Pen** tool  from the **Pen** palette in the **Drawing** toolbar.
2. Press the mouse down on the current document to begin drawing.
3. Drag the mouse in an outline of the shape you would like.
4. Release the mouse to set the shape.

ChemDoodle will automatically simplify your path for you and generate a cubic interpolation.

10.8.2 Drawing with the polyline tool

To draw a custom shape with the **Polyline** tool, execute the following steps:

1. Select a **Polyline** tool  from the **Pen** palette in the **Drawing** toolbar.
2. Press the mouse down on the current document and release to set the first point.
3. Move the mouse to the location you prefer the next point to be placed.
4. Click to place the next point. Points will automatically connect to previous points.
5. Repeat steps 3 and 4 until finished.
6. Click on the first point drawn or double-click the last point to complete the shape and set it.

10.8.3 Modifying pen paths and polylines

You can move the control points that define pen paths and polylines. To do so, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the custom shape so an open hand mouse cursor appears and the control points are drawn as shown in Figure 10.8.
2. Move the mouse pointer over one of the control points that you desire to be moved so that control point is filled with an amber color.
3. Press the mouse down so the control point is filled with a blue color.

4. Drag the control point to move it.
5. Release the mouse to finish.

10.8.4 Drawing with the Bézier tool

Bézier curves are defined by a set of control point triplets, an intersect point and two tangent points. The curve passes through the intersect point, while the line between the tangent points describes the tangent line to the curve at the intersect point. To draw a Bézier curve, execute the following steps:

1. Select the **Bézier Curve** tool  from the **Pen** palette in the **Drawing** toolbar.
2. Press the mouse down on the current document to set the first intersect point.
3. Drag your mouse to set the tangent point that defines the tangent line to the curve at the first intersect point. The further from the intersect point you make this tangent point, the tighter the curve will hug the tangent line.
4. Release the mouse to set the tangent point.
5. Move the mouse to the location you prefer for the next intersect point the curve will pass through.
6. Press the mouse down to place the next intersect point. A segment will automatically be drawn between the intersect points.
7. Drag your mouse to set the tangent point that defines the tangent of the curve at the second intersect point. The further from the second intersect point you make this new tangent point, the tighter the curve will hug the latest tangent line.
8. Repeat steps 5 through 7 until finished.
9. Press the escape key to complete the shape and set it.

All intersect points you place will have two tangent points associated with them mirrored across the intersect point. The only exception is the first intersect point, which will only have a single tangent point, as there is no segment leading to it.

10.8.5 Modifying Bézier curves

You can move the control points defining Bézier curves in one of two ways. The first way is by following the same instructions as in the MODIFYING PEN PATHS AND POLYLINES section. However, you will only be able to move the intersect points this way. The second is by using the **Bézier Curve** tool which will allow you to move all control points. Execute the following steps:

1. Select the **Bézier Curve** tool  from the **Pen** palette in the **Drawing** toolbar.
2. Move the mouse pointer over the Bézier curve that you desire to be modified so its control points are rendered.
3. Click on the Bézier curve so that all of its control points are rendered as shown in Figure 10.9.
4. Hover over any of the control points so an amber color fills the one you wish to move.
5. Press the mouse down and drag the point to the new desired location.
6. Release the mouse to finish moving the control point.
7. Press the escape key to finish editing the shape and set it.

By default, when you move one tangent point to an intersect point, the opposite tangent point will also move such that it remains exactly opposite the tangent point you are editing. This way, the Bézier curve will remain continuous in the first and second derivative, leading to a smooth shape. If you wish to detach the paired tangent points from each other, hold down any combination of the shift and alt keys while moving a tangent point. By holding down the shift key, you will break the length dependency between the two tangent points and one may be further from the intersect point than the other, but the angle between them will remain 180°. By holding down the alt key, you will break the angle dependency between the two tangent

points and the angle between the two tangent points will no longer be preserved to 180°, however the distances between the intersect and both tangent points will remain equal. If you hold down both the shift + alt keys, then the opposite tangent point will remain in place as you move a tangent point.

10.8.6 Deleting Bézier control points

Only the intersect points (that have the curve pass through them) may be deleted. Deleting one of these intersect points will also remove the corresponding paired tangent points. To delete a Bézier intersect point, execute the following steps:

1. Select the **Bézier Curve** tool from the **Pen** palette in the **Drawing** toolbar.
2. Move the mouse pointer over the Bézier curve that you desire to be modified so that its control points are rendered.
3. Click on the Bézier curve so that all of its control points are rendered as shown in Figure 10.9.
4. Hover over the intersect point that you wish to remove so that it is filled with an amber color.
5. Press the backspace or delete key to delete the intersect point.
6. Press the escape key to finish editing the shape and set it.

10.8.7 Adding arrowheads to custom shapes

To add arrows to custom shapes, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Then right-click on the custom shape after it is hovered, select the appropriate Format Custom Shape... menu item, and define the arrow sections to your preference. Arrowheads are covered in detail in the REACTIONS chapter.

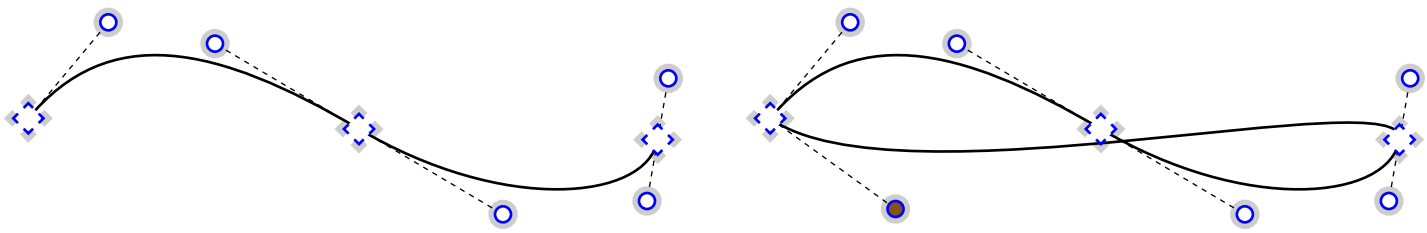
10.8.8 Closing and opening custom shapes

To close or open a custom shape, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the custom shape so an open hand mouse cursor appears and the control anchor points are drawn as shown in Figure 10.8.
2. Right-click on the hovered custom shape and select the Format Custom Shape... menu item.
3. Scroll to the **Path** or **Bézier Curve** section and use the **Close** on/off choice to specify whether the custom shape path is closed or not.

If closed, the custom shape can be filled with any desired color.

One more note about closed Bézier curves. Once closed, the first tangent point for the first intersect point will appear to allow you to define how the final Bézier segment will close the custom shape as shown in Figure 10.10. In Figure 10.10b, the now visible and editable first tangent point is highlighted.



(a) *An open Bézier curve does not show the first tangent point* (b) *An closed Bézier curve does show the first tangent point*

Figure 10.10: *Closed vs. open Bézier curves*

10.9 Rulers

Rulers measure distances in 2 dimensions, and are defined by two anchors placed at their endpoints as shown in Figure 10.11. Rulers are *manual* shapes.



Figure 10.11: *Ruler Shape and Anchors*

10.9.1 Drawing rulers at fixed angles

To draw a ruler at fixed angles, execute the following steps:

1. Select the **Ruler** tool in the **Drawing** toolbar.
2. Press the mouse down on the current document to set the start point of the ruler.
3. Drag the mouse to preview the placement of the end of the ruler.
4. Release the mouse to set the ruler.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

By default, rulers will be oriented at fixed angles every 15° starting at 0°.

10.9.2 Drawing rulers at non-fixed angles

To place rulers at non-fixed angles, hold down the alt key while dragging the mouse when defining the ruler to break from the fixed chain orientation angles.

10.9.3 Forcing rulers to be drawn vertically and horizontally

To place rulers oriented vertically or horizontally, hold down the shift key while dragging the mouse when defining the ruler. The ruler preview will then automatically orient vertically or horizontally depending on angle from the start point to the current mouse cursor position.

10.9.4 Automatically measuring object width and height

To measure the width and height of selected objects, execute the following procedure:

1. Select the content to be measured using the selection tools.
2. Select the Content › Measure › Width and Height menu item.

Two rulers will be placed to measure the width and height of the selected content.

10.9.5 Automatically measuring object diagonal

To measure the diagonal of selected objects, execute the following procedure:

1. Select the content to be measured using the selection tools.

2. Select the Content ⟩ Measure ⟩ Diagonal menu item.

A single ruler will be placed across the diagonal of the selected content.

10.9.6 Showing and hiding major and minor ticks

To show and hide ruler major and minor ticks, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the ruler so an open hand mouse cursor appears and the anchor points are drawn as shown in Figure 10.11.
2. Right-click on the hovered ruler and select the Format Ruler... menu item.
3. Scroll to the **Ruler** section and use the **Show Major Ticks** and **Show Minor Ticks** on/off choices to set whether major and minor ticks are visible or not.

10.9.7 Changing the measurement unit

To change the ruler's measurement unit, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the ruler so an open hand mouse cursor appears and the anchor points are drawn as shown in Figure 10.11.
2. Right-click on the hovered ruler and select the Format Ruler... menu item.
3. Scroll to the **Ruler** section and use the **Unit** drop-down selection to select the unit to be displayed.

You can also hide the measurement completely by deselecting the **Show Measurement** option in this **Ruler Settings** window.



If you use the Ångström unit with a ruler, the conversion is based on the **Ångströms/Bond Length** style defined in the **Styles** window under the **Pages** tab in the **Dimensions** section. The reference bond length is defined the by **Bond Length** style defined in the **Styles** window under the **Bonds** tab in the **Settings** section. This is useful if you have built 3D coordinates rendered in ChemDoodle as the original Ångström coordinates will be multiplied by the **Bond Length** style to achieve the pixel coordinates for the 2D chemical structure drawing. Always be mindful of what your input coordinates are for 3D structures!

10.10 Tables

Tables are very powerful shapes for creating organized groupings of content in grid patterns. You can control the table grid and its formatting as well as the content that appears within each table cell and cell formatting. Tables can be drawn in several styles and are defined and controlled by an anchor box set as shown in Figure 10.12. Tables are *manual* shapes. While the large number of anchors may at first seem overwhelming, each anchor performs a specific function for the table and provides instant feedback for edits you may want to perform.

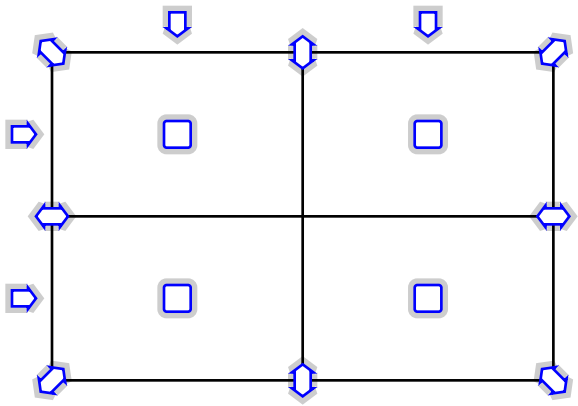


Figure 10.12: *Table Shape and Anchors*

10.10.1 Creating tables

Tables can be added in one of two ways, by using a form to define the number of rows and columns, or by using the mouse to draw the outline of the table.

10.10.1.1 Drawing tables

To draw a table, execute the following steps:

1. Select the table tool  from the **Drawing** toolbar.
2. Press the mouse down on the current document to set one corner of the table.
3. Drag the mouse to preview the placement of the opposite corner along the diagonal of the table.
4. Release the mouse to set the table. By default a 2x2 table will be produced.

10.10.1.2 Defining a table by rows and columns

To define a table by a specific number of rows and columns, execute the following steps:

1. Select the table tool  from the **Drawing** toolbar.
2. Click the mouse down in the current document where you would like to have the center of the table defined.
3. A window will appear to define the number of rows and columns as shown in Figure 10.13. Use the number fields to define positive integer values to each input. Press the **Accept** button when done. Press the **Cancel** button if you do not want to create the table.

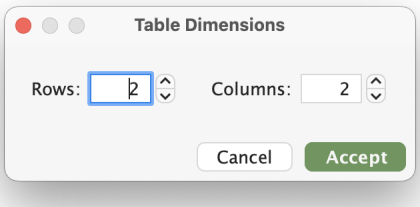


Figure 10.13: *Defining a table by the number of rows and columns*

4. The defined table will now appear in the current document where you originally clicked the mouse.

Any newly created tables will now be initialized with the number of rows and columns from the last defined table.

10.10.1.3 Drawing square tables

To draw square tables, hold down the shift key while dragging the mouse when defining the table to force the width and height to be equal.

10.10.2 Editing tables

You can edit tables after they have been created. This includes moving, resizing and removing them as discussed in the MANUAL SHAPES section at the beginning of this chapter.

Tables are more complex than other shapes, and have more functions than other shapes. For instance, you can add and remove columns and rows, or fit them to the content inside of the table. This section will cover table editing features.

10.10.2.1 Adding a row

To add a row to an existing table, highlight a row next to the position where you would like the new row to go by hovering over the corresponding row anchor to the left of the row as shown in Figure 10.14. With the row now highlighted, right-click and select the Insert Row Before or the Insert Row After menu item depending on where you would like to place the new row. The currently highlighted row will then be split in half, with a blank row placed according to the menu item chosen.

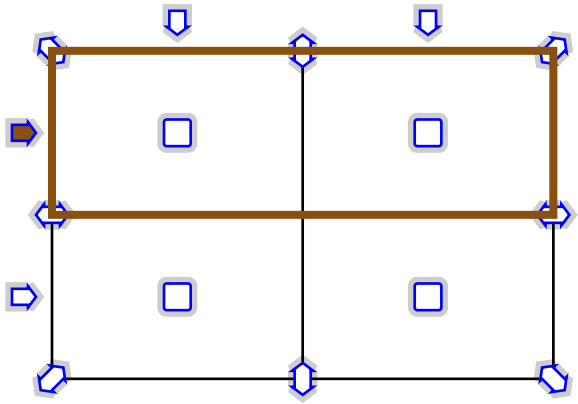


Figure 10.14: *Highlighting a Table Row*

10.10.2.2 Resizing a row

To resize a row, using a selection tool, hover the mouse directly over a row separator so the cursor changes to the table adjust cursor. Press the mouse down and drag to move the separator to the desired position and release the mouse to set the new separator position.

A separator cannot be moved beyond the bounds of the two rows it separates and a minimum of 2% of the total table height is reserved for each row. If the separator separates two rows where the sum of both heights adds up to less than 5% of the total table height, then the separator will be automatically centered and cannot be moved.

10.10.2.3 Removing a row

To remove a row from an existing table, highlight the row you wish to remove by hovering over the corresponding row anchor to the left of the row as shown in Figure 10.14. With the row now highlighted, right-click and select the Delete menu item and the row will be removed.

10.10.2.4 Adding a column

To add a column to an existing table, highlight a column next to the position where you would like the new column to go by hovering over the corresponding column anchor to the top of the column as shown in Figure 10.15. With the column now highlighted, right-click and select the Insert Column Before or the Insert Column After menu item depending on where you would like to place the new column. The currently highlighted column will then be split in half, with a blank column placed according to the menu item chosen.

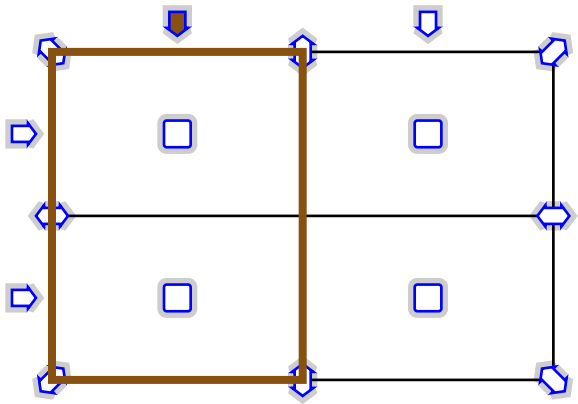


Figure 10.15: *Highlighting a Table Column*

10.10.2.5 Resizing a column

To resize a column, using a selection tool, hover the mouse directly over a column separator so the cursor changes to the table adjust cursor. Press the mouse down and drag to move the separator to the desired position and release the mouse to set the new separator position.

A separator cannot be moved beyond the bounds of the two columns it separates and a minimum of 2% of the total table width is reserved for each column. If the separator separates two columns where the sum of both widths adds up to less than 5% of the total table width, then the separator will be automatically centered and cannot be moved.

10.10.2.6 Removing a column

To remove a column from an existing table, highlight the column you wish to remove by hovering over the corresponding column anchor to the top of the column as shown in Figure 10.15. With the column now highlighted, right-click and select the Delete menu item and the column will be removed.

10.10.2.7 Fitting a table to its contents

ChemDoodle will automatically fit tables to contained content for you. To do so, simply hover the table using a selection tool, right-click and select the Fit Table to Contents menu item.

An example of table fitting is shown in Figure 10.16.

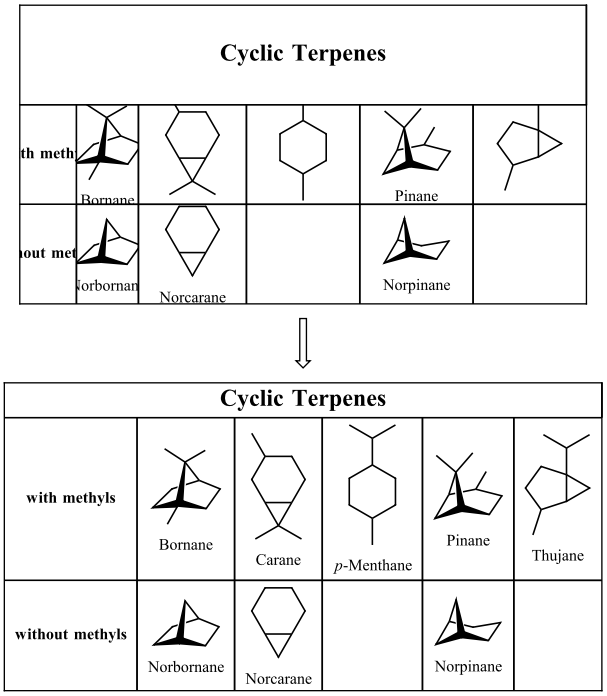


Figure 10.16: *Here is a complex table with a title row, row titles and different sized molecules with IUPAC names. The bottom table was fit to its contents.*

10.10.3 Editing cells

Each cell of the table may contain unique content and has an individual set of styles. To interact with a table cell, the cell needs to be highlighted. This is achieved by hovering over the cell anchor point as shown in Figure 10.17. Any functions pertaining to cells will then affect the highlighted cell.

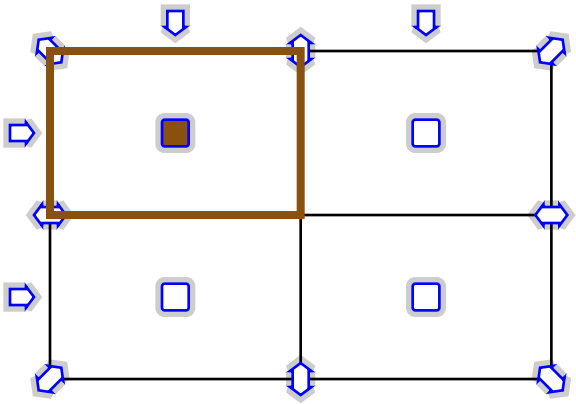


Figure 10.17: *Highlighting a Table Cell*

10.10.3.1 Adding content

Adding content to cells is done by pasting. Draw the figure that you wish to be displayed in a table cell. Copy it with a selection tool and hover the table cell it should be placed in as shown in Figure 10.17. Then right-click and select the Paste menu item to set the content to the table cell. You may also use the ctrl+V keyboard shortcut to achieve the same result.

Adding content to cells may also be done via dropping a selection when using a selection tool. First select the content you wish to be placed in a table cell, then drag the selection and move the mouse pointer over the table cell so the table cell is hovered and release the mouse. The content from the document will be removed and will appear in the table cell. If you wish to keep a copy of the content in the document, then duplicate the content during the lasso drag action as described in the DUPLICATING CONTENT section.

Any structures or shapes from ChemDoodle can be placed in a table cell. If content is already present in the cell when contents are deposited, the previous content will be replaced.

Cell content will not be rendered outside of the cell bounds, so if the cell dimensions become smaller than the content defined within, the content will be cut off.

10.10.3.2 Editing content

Once content has been placed in a table cell, it is protected and no longer editable directly. To edit content from a cell, you will need to copy the content from the cell, paste in a document to edit, and then re-paste the edited content back into the cell. To do so, perform the following steps:

1. Hover the table cell to be edited an as shown in Figure 10.17.
2. Right-click and select the Copy or Cut menu item to copy the content from the table cell. You may also use the ctrl+C or ctrl+X keyboard shortcuts.
3. Somewhere else in the document, or in a different document, paste the copied content from the table cell. You may also use the ctrl+V keyboard shortcut.
4. Edit the pasted content.
5. When editing is complete, select the altered content with a selection tool. Right-click and select the Copy menu item.
6. Hover the table cell it should be placed in as shown in Figure 10.17.
7. Right-click and select the Paste menu item to replace the previous content in the table cell.

10.10.3.3 Setting or editing a cell label

Cell labels can be added or edited without the need to first create the label in the document and paste into the cell. To set a label to a cell, that cell will need to be blank. And to edit a label within a cell, the only contents of that cell must be a single label shape (not a lone atom label). If either of those two conditions is met, then that table cell will be highlighted when hovered and using the **Text for Atoms and Captions** tool [A] in the **Drawing** toolbar. The hovered cell will be highlighted with an amber outline as shown in Figure 10.18. The mouse cursor will also change to the text edit cursor.

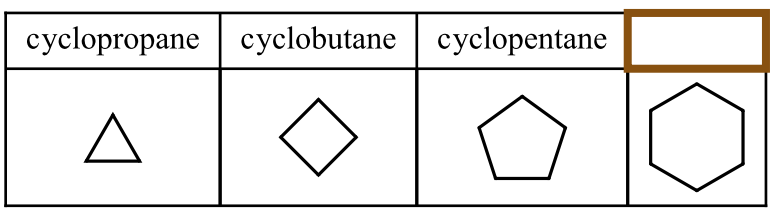


Figure 10.18: *Hovering over a table cell with the text tool to set a label*

When the desired table cell is highlighted, click the mouse to edit that cell's label. Editing this label will work identically to editing an individual label shape in the document. When done, click anywhere else in the document or press the return or Enter key to close and set the label (You may also press the excape key to disregard your current changes.). If there was a label originally present in the cell, and the newly set label is blank, the original label will be removed. If the cell was originally blank, and the newly set label is blank, then nothing will happen.

10.10.3.4 Clearing content

To clear a table cell of its content, so it becomes blank, hover the table cell to be cleared an as shown in Figure 10.17. Then right-click and select the Delete menu item. You may also press the backspace or delete key to achieve the same result.

10.10.3.5 Styling

Table cells can be individually styled. To do so, hover the table cell to be edited an as shown in Figure 10.17. Then right-click and select the Format Table Cell... menu item. A window will appear to allow you to define table cell styles as shown in Figure 10.19. You may also press the comma , key while the table cell is highlighted to show the styles window.

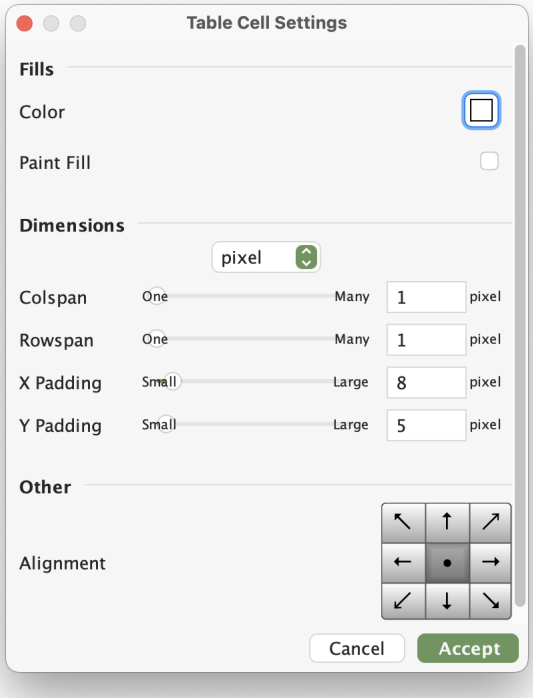


Figure 10.19: *Styling a Table Cell*

Using the components in this window, you can control how the table cell is rendered.

You may also define styles for an entire row or column of table cells at the same time. To do so, hover the table row or column anchor corresponding to the row or column to be edited as shown in Figures 10.14/10.15. Then right-click and select the Format Table Row/Column... menu item (or press the comma , key). You will be able to edit the table cell styles for the entire row/column. Certain styles only applicable to a single table cell, such as **Colspan** and **Rowspan** will not be present when editing the styles of a group of table cells at once.

10.10.3.6 Defining a rowspan

To define a rowspan to a table cell, which will cause it to absorb the space of the number of cells below it, perform the following steps:

1. Hover the table cell to be edited an as shown in Figure 10.17.
2. Right-click and select the Format Table Cell... menu item.
3. Scroll down to the **Dimensions** section.
4. Adjust the **Rowspan** style to the desired value. You can watch the table update in real time.
5. When satisfied, press the **Accept** button.

10.10.3.7 Defining a colspan

To define a colspan to a table cell, which will cause it to absorb the space of the number of cells to its right, perform the following steps:

1. Hover the table cell to be edited an as shown in Figure 10.17.
2. Right-click and select the Format Table Cell... menu item.
3. Scroll down to the **Dimensions** section.
4. Adjust the **Colspan** style to the desired value. You can watch the table update in real time.
5. When satisfied, press the **Accept** button.

10.10.3.8 Alignment

To define the alignment of a table cell, which will determine how content is placed within the bounds of the cell, perform the following steps:

1. Hover the table cell to be edited an as shown in Figure 10.17.
2. Right-click and select the Format Table Cell... menu item.
3. Scroll down to the **Other** section.
4. Select the arrow corresponding to the direction of the alignment for the **Alignment** style. The center dot represents both a vertical and horizontal center alignment You can watch the table update in real time.
5. When satisfied, press the **Accept** button.

Alignment will affect what is visible when content does not fit completely inside the table cell.

10.10.3.9 Padding

To define the horizontal or vertical padding of a table cell, which will determine how much space is placed between the content in the cell and the borders of the cell, perform the following steps:

1. Hover the table cell to be edited an as shown in Figure 10.17.
2. Right-click and select the Format Table Cell... menu item.
3. Scroll down to the **Dimensions** section.
4. Adjust the **X Padding** and **Y Padding** styles to the desired value. You can watch the table update in real time.
5. When satisfied, press the **Accept** button.

Note that padding styles will not affect content that is centered, as centered content location is not determined by distances from any border of the cell.

10.11 Labels

Labels render formatted text in your figures. They can be added anywhere, and any text can be specified. Labels are controlled by a single point defining its position; its bounds will automatically be determined by the text it renders. A hovered label will show an amber rectangle around the bounds as seen in Figure 10.20.

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Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Figure 10.20: *A Hovered Label*

10.11.1 Adding text with the text tool

To add text to your document, execute the following steps:

1. Select the **Text for Atoms and Captions** tool  in the **Drawing** toolbar.
2. Click the mouse on the current document where you would like the text to be placed. This point defines the text anchor and will be used to layout the text glyphs. Vertically, this point represents the middle of the first line. Horizontally, this point represents the left/center/right justification point.
3. A text area will appear with a formatting toolbar above it as shown in Figure 10.21. Use the keyboard to type your text or paste in the desired text. Use the Shift+Enter or Ctrl+Enter keys (shift+return or control+return on macOS) to start a new line.

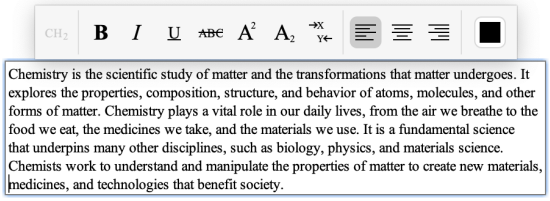


Figure 10.21: *Editing a label*

4. Using the formatting toolbar that appears above the text area, select text and format it as desired.
5. Click outside of the text area in the document, or press the return or Enter key to set the label. You may also press the excape key to cancel the creation of the label.



The **Text for Atoms and Captions** tool [AI] is the same tool that you will use to set atom text. If you click on an atom, you will be editing atom text, if you click on a label or any other part of the document, you will be creating/editing label text.

10.11.2 Token and line spacing

You have control over the token and line spacing used to render text. In the **Styles** window under the **Pages** tab, you will find the **Text** section. Here you will find the following options:

1. **Main Font**
2. **Horizontal Spacing**
3. **Vertical Spacing**
4. **Subscript Reduction**
5. **Subscript Shift**
6. **Superscript Reduction**
7. **Superscript Shift**

These options affect all text across the entire document and are covered in the STYLES chapter.

10.11.3 Controlling fonts

The main font used in the document is for structures and other text. Labels have their own separate font definition, called a caption font. The caption font can be set in the **Styles** window under the **Shapes** tab, in the **Labels** section. Here you can set a custom default font to labels that will be different from atom labels. When you create a non-chemical label using the **Text for Atoms and Captions** tool [AI], the caption font will be used. You can also simply set it to the main font, if you wish all fonts to be the same.

You can also use the font tools in the **Formatting** toolbar to edit the fonts of all selected objects, including labels.

10.11.4 Creating equally spaced labels

When adding labels, sometimes it is convenient to create an evenly spaced row of text. You can do this by pressing the [tab] key while editing a labels. A new label will then open for edit at the same height using a standard length between the positions of the labels.

10.11.5 Copying formatted text from labels

To copy formatted text in a label to the system clipboard, hover the label with a selection tool so that it is bordered in an amber color as shown in Figure 10.20 and right-click. Select the [Copy Text] menu item to copy the displayed text and its formatting to the system clipboard. You can define which formatted text data types are included in the **Settings** window under the **Clipboard** tab. This is covered in detail in the SHARING INFORMATION chapter.

10.11.6 Moving labels

To move labels, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the label so an open hand mouse cursor appears and it is bordered in an amber color as shown in Figure 10.20.

2. Press the mouse down and drag to move the shape.
3. Release the mouse to finish the move action.

10.11.7 Editing label text

To edit a label that has already been defined, execute the following steps:

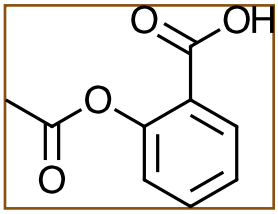
1. Select the **Text for Atoms and Captions** tool [A] in the **Drawing** toolbar.
2. Hover the mouse pointer over the label you wish to edit so an text mouse cursor appears and the label is bordered in an amber color as shown in Figure 10.20.
3. Press the mouse down to open the text area for edit.
4. Click outside of the text area in the document, or press the [return] or [Enter] key to set your changes. You may also press the [excape] key to disregard your current changes.

You can also double click on a hovered label when using a selection tool to open the text area for edit.

10.11.8 Auto-updating labels

Updating labels can be attached to structures and will update dynamically to display a certain descriptor for the associated molecule as the molecule is edited. Updating labels are very convenient for figures that change often or for dynamically generating IUPAC names or molecular formulas, for instance. Updating labels can be edited just like regular labels.

Updating labels automatically move to be located at the bottom center of the associated structure. If you hover over the label, it will highlight both itself and the associated structure, as shown in Figure 10.22.



o-Acetoxybenzoic acid

$C_9H_8O_4$

Figure 10.22: *Two updating labels associated with aspirin showing its IUPAC name and molecular formula*

You can assign multiple updating labels to the same structure. The labels will simply stack below the structure in the order that they were added.

10.11.8.1 Adding updating labels

Updating labels can only be created by ChemDoodle using a form. To attach an updating label to a molecule, execute the following steps:

1. Select the molecule(s) you would like to add an updating label to.
2. Select the [Structure] [Attach Updating Label] menu item, or press the **Attach Updating Label** [🏷] button in the **Chemistry** toolbar.

3. In the popup that appears as show in Figure 10.23, select the types of labels you would like to attach to the selected molecule(s) among the options.

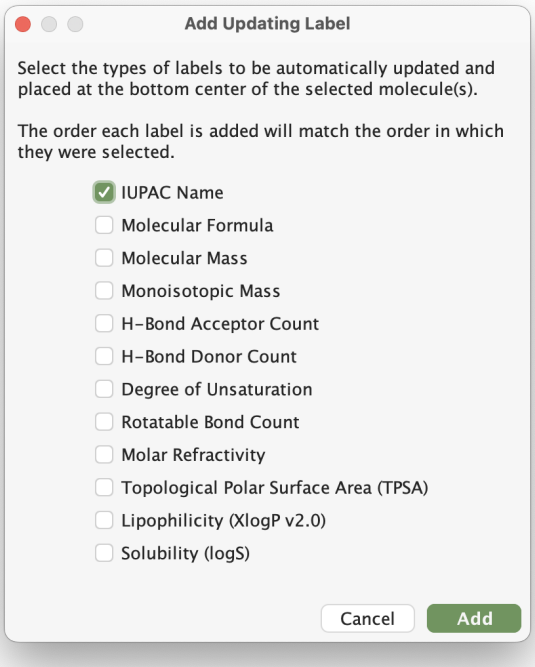


Figure 10.23: *The interface for adding updating labels*

4. Press the **Add** button to add the updating labels.

10.11.8.2 Editing updating labels

You can move an updating label by hovering the label with a selection tool and then clicking and dragging. Note once you move the label, it will no longer automatically adjust itself to be placed at the bottom center of the associated molecule. It will, however, continue to update its content dynamically.

You can also edit updating labels just as you would regular labels. But once you edit the content, it will break from the associated molecule and become a standard label graphic.

10.11.8.3 Reattaching moved updating labels

If you have moved an updating label, and would like to restore its automatic positioning below the molecule it describes, perform the following steps:

1. Hover the updating label you would like to reattach so it is outlined by an amber rectangle, as shown in Figure 10.20. You should also see the associated molecule bordered by an amber rectangle. If you do not, this means the link to the structure has been broken and it cannot be reattached. Instead, create a new updating label.

2. Right-click on the label and select the Reattach Updating Label menu item.

10.11.8.4 Updating label options

When displaying calculations in updating labels, you can control the decimal resolution of the calculation (for fractional output) by changing the **Resolution** slider in the **Calculations** section of the **Descriptors** tab of the **Settings** window. You

can suppress the unit designation at the end of the calculation output by deselecting the **Include Unit** checkbox in the same section.

10.12 Atom mappings

An atom mapping is a direct association between two atoms. Typically, they are used to show the atom-to-atom mapping between reactants and products in a reaction, but may serve other purposes. You define atom mappings by designating a starting atom and an ending atom. A mapping designation number will be display near those atoms to designate the specific mapping, as shown in Figure 10.24. The numbers are automatically generated, incremented starting at 1, based on the order they exist within the document. Atom mappings are *automatic* shapes.

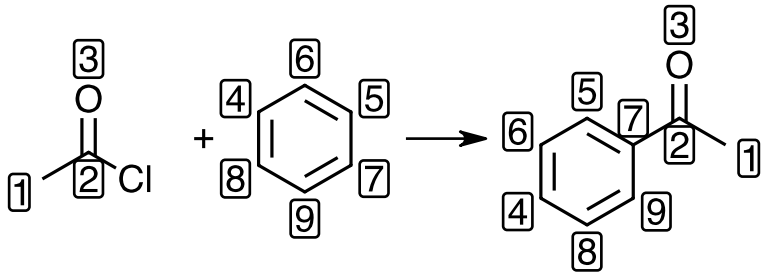


Figure 10.24: *An atom mapping for the acylation of benzene*

When hovered, atom mapping designations will be outlined with an amber color as shown in Figure 10.25.

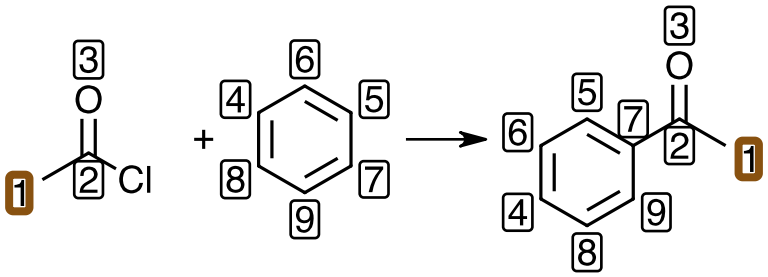


Figure 10.25: *A hovered atom mapping*

10.12.1 Adding atom mappings

To add an atom mapping, execute the following steps:

1. Draw your chemical structures and reactions with atoms the mappings will be applied to.
2. Select the **Atom Mapping** button in the **Arrows** palette in the **Drawing** toolbar.
3. Hover over the first atom in the mapping.
4. Press and hold the mouse down, drag to the second atom in the mapping, and release the mouse to apply the atom mapping.

10.12.2 Editing atom mapping rendering styles

To edit the rendering styles for atom mapping designations, execute the following steps:

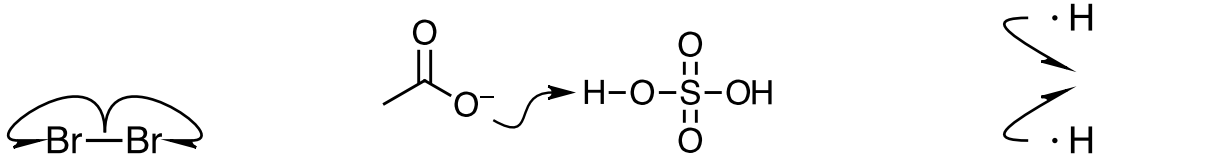
1. For convenience, select the **Lasso only Shapes** button  . Make sure no other content is selected.
2. Hover the atom mapping you wish to edit so an amber outline surrounds it as shown in Figure 10.25.
3. Right-click and select the Format Atom Mapping... menu item.
4. Set the styles as desired to determine how the atom mapping should be rendered.
5. Press the **Accept** button to finish editing the atom mapping.

10.12.3 Working with atom mappings

Atom mappings serve a much more important role in ChemDoodle than just a convenient way to graphically show atom correspondence. Atom mappings may be used to define characteristics of reactions and will be output to various chemistry file formats that support reaction data. Please see the ATOM-TO-ATOM MAPPINGS section of the REACTIONS chapter for further instruction.

10.13 Electron pushers

Electron pushers show electron movement between atoms and bonds in molecules. You define electron pushers by designating a starting atom or bond and an ending atom or bond. Electron pushers will automatically render a Bézier arrow between those two objects. There are three types of electron pushers, shown in Figure 10.26. Electron pushers are *automatic* shapes.



(a) *Single electron pushing arrows* (b) *An electron pair pushing arrow* (c) *A bond forming pushing arrow*

Figure 10.26: *Three different types of electron pushing arrows*

When hovered, electron pushers will be outlined with an amber color as shown in Figure 10.27.

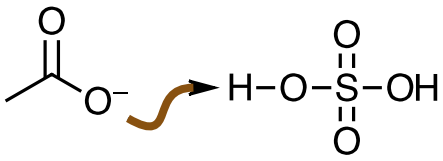


Figure 10.27: *A hovered electron pusher*

If a radical or electron pair attribute is present on an atom that an appropriate pusher starts from, the start of the arrow shaft will automatically originate from the attribute location as shown in Figure 10.25.

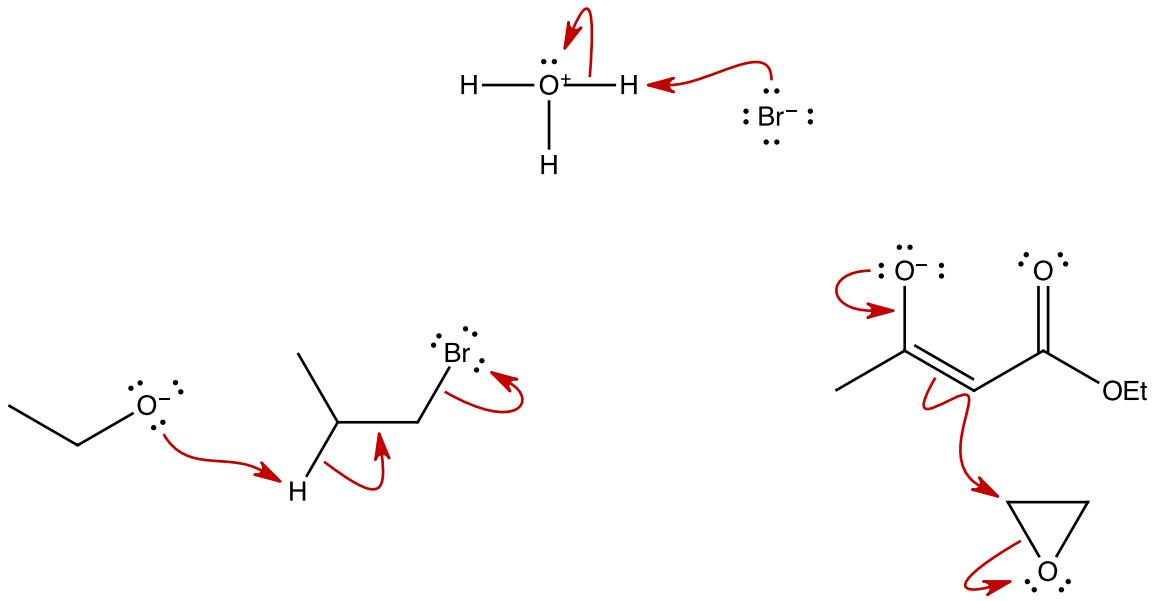


Figure 10.28: *Electron pusher shapes will automatically start from radical and electron pair attributes, when applicable.*

10.13.1 Adding electron pushers

To add electron pushers, execute the following steps:

1. Draw your chemical structures with atoms and bonds that the electron pushers will be added to.
2. Select the **Single Electron Pusher**  , **Electron Pair Pusher**  , or **Bond Forming Pusher**  button in the **Arrows** palette in the **Drawing** toolbar.
3. Hover over the atom or bond where the electrons will be pushed from.
4. Press and hold the mouse down, drag to the atom or bond the electrons are moving to, and release the mouse to set the electron pushing arrow. Of course, for bond forming electron pushers, electrons will come from both the start and ending objects.

10.13.2 Flipping electron pushers

You may reverse the direction of an electron pusher by simply clicking on a hovered pusher shape (as shown in Figure 10.27) while using the **Single Electron Pusher** tool or the **Electron Pair Pusher** tool.

10.13.3 Special cases

The following special cases for electron pushing arrows are handled.

10.13.3.1 Bond to atom shortcuts

In many cases, an electron pair pusher from a bond to an independent atom will be drawn as shorthand for two electron pair pushers, one going from the bond to one of the atoms in that bond and then a second electron pair pusher going from that bond's atom to the independent atom. For these cases, ChemDoodle will show a humped arrow first directing towards the side of the bond to be used to connect to the independent atom. To toggle to the other side of the bond, simply hover the electron pair pusher as shown in Figure 10.27 using the **Electron Pair Pusher** tool and click.

Figure 10.29 shows the result of toggling such a pusher to the other side of the bond.

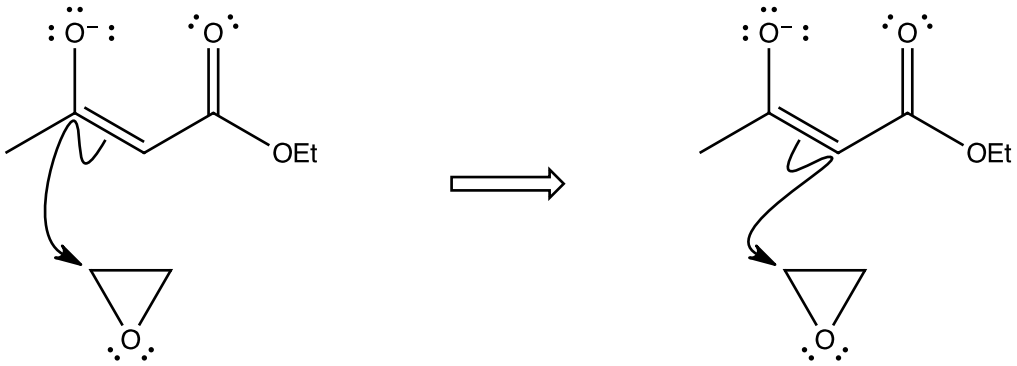


Figure 10.29: *Toggling a bond-to-atom electron pair pusher to the opposite side of the bond*

10.13.4 Editing electron pusher styles

To edit electron pusher styles, execute the following steps:

1. For convenience, select the **Lasso only Shapes** button  . Make sure no other content is selected.
2. Hover the electron pusher you wish to edit so an amber outline surrounds it as shown in Figure 10.27.
3. Right-click and select the Format Electron Pusher... menu item.
4. Set the styles as desired to determine how the electron pusher should be rendered.
5. Press the **Accept** button to finish editing the electron pusher.

10.13.5 Converting to Bézier arrows

Electron pusher graphics are automatically determined based on the objects they are assigned to. You can convert electron pushers into custom Bézier curves, which are manual shapes and can be fully controlled. To convert electron pushers into Bézier curve custom shapes, execute the following steps:

1. For convenience, select the **Lasso only Shapes** button  . Make sure no other content is selected.
2. Hover the electron pusher you wish to edit so an amber outline surrounds it as shown in Figure 10.27.
3. Right-click and select the Convert to Bézier Shape menu item.

The manual Bézier shape will replace the automatic electron pusher shape, and you can use the selection and Bézier tools to edit.

10.14 Highlights

Highlights emphasize a section of a structure by creating an outlining shape behind certain atoms and bonds. A molecule with highlights included is shown in Figure 10.30. Highlights are *automatic* shapes.

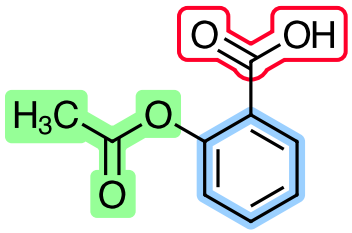


Figure 10.30: *A molecule with highlight shapes*

When hovered, highlights will be outlined with an amber color as shown in Figure 10.31.

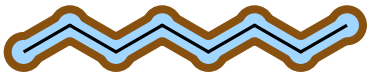


Figure 10.31: *A hovered highlight*

10.14.1 Adding highlights

To add highlights, execute the following steps:

1. Draw your structure that the highlights will be added to.
2. Using a selection tool, select the atoms and bonds in that structure the highlight will encompass.
3. Select the **Structure Highlighter** button  in the **Chemistry** toolbar.
4. The highlight will be placed and the styles for the highlight will appear in a window.
5. Set the styles as desired to determine how the highlight should be rendered.
6. Press the **Accept** button to finish creating the highlight.

10.14.2 Customizing highlights

To customize highlights, execute the following steps:

1. For convenience, select the **Lasso only Shapes** button  . Make sure no other content is selected.
2. Hover the highlight you wish to edit so an amber outline surrounds it as shown in Figure 10.31.
3. Right-click and select the Format Highlight... menu item.
4. Set the styles as desired to determine how the highlight should be rendered.
5. Press the **Accept** button to finish customizing the highlight.

10.14.3 Color in rings

You may also use highlights to color or fill in rings.



Filling in rings is off by default, but may be enabled by default in the **Styles** window under the **Shapes** tab in the **Highlights** section.

To color in rings, perform the following steps:

1. For convenience, select the **Lasso only Shapes** button  . Make sure no other content is selected.
2. Hover the highlight you wish to edit so an amber outline surrounds it as shown in Figure 10.31.
3. Right-click and select the Format Highlight... menu item.
4. In the **Highlight** section, enable the **Fill in Rings** style.
5. Press the **Accept** button to finish customizing the highlight.

Rings that are part of the highlight will then be colored in with the defined **Fill** color for the highlight object. A ring is determined to be part of the highlight if all of the atoms in the ring are highlighted. Use multiple highlights for different color rings in the same structure as shown in Figure 10.32, where we also disabled the **Draw Border** and **Paint Fill** styles so only the colored rings were shown.

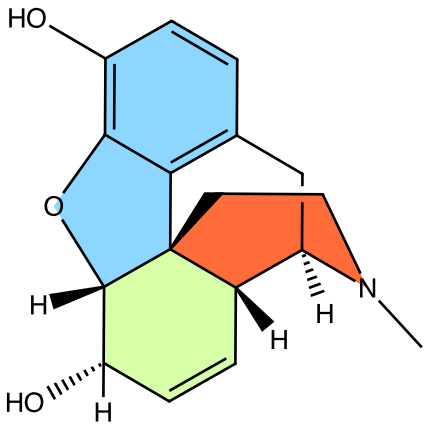


Figure 10.32: *Colored in rings using highlights*

10.14.4 Merging highlights

Highlights may sometimes overlap, and need to be visibly merged. Depending on how many highlights are merging, be sure to use an appropriate alpha value (which sets transparency) when choosing fill colors for the overlapping highlights.

10.15 Repeat unit brackets

Repeat units are rendered in ChemDoodle with a special bracket shape defined between two bonds. The brackets will automatically update to fit the appropriate content between those two bonds. Repeat unit brackets will also place and render text for any display value you define. A structure with repeat unit brackets present is shown in Figure 10.33. Repeat unit brackets are *automatic* shapes.

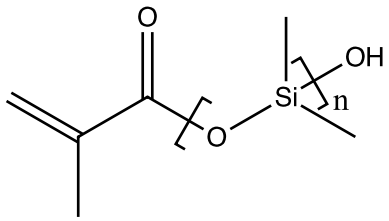


Figure 10.33: *A structure containing a repeat unit*

When hovered (over the end bracket shapes or the display text), repeat unit brackets will be outlined with an amber color as shown in Figure 10.34.

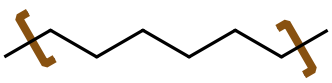


Figure 10.34: *A hovered repeat unit*

10.15.1 Adding repeat units

To add repeat unit brackets, execute the following steps:

1. Draw your structure the repeat unit brackets will be added to.
2. Select the **Repeat Unit** button [ ]n in the **Brackets** palette in the **Drawing** toolbar.
3. Hover over one of the two bonds you would like to define the brackets to.
4. Press and hold the mouse down, drag to the second of the two bonds you would like to define the brackets to and release the mouse to set the brackets.
5. A text field will appear as shown in Figure 10.35. Enter any value you desire to be displayed along with the brackets.

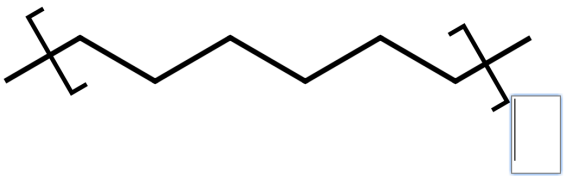


Figure 10.35: *A text field appears to edit the repeat unit display value*

6. When you are finished defining the display value, press the escape key or click elsewhere in the document to close the text field and finish the creation of the repeat unit brackets.

10.15.2 Defining the repeat unit display value

When you first create a repeat unit, you will automatically be presented with an empty text field to define the associated display value as described in the previous section. You may change this display value at any time. To do so, make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Select the **Repeat Unit** button $[]_n$ in the **Brackets** palette in the **Drawing** toolbar.
2. Hover the mouse pointer over the repeat unit brackets so the brackets are outlined in an amber color as shown in Figure 10.34.
3. Click the mouse while the repeat unit is hovered and a text field will appear to edit the display value as shown in Figure 10.35.
4. When you are finished editing the display value, press the escape key or click elsewhere in the document to close the text field and commit your edits.

Alternatively, while repeat unit brackets are hovered with any tool, you may press the space key or double click with the mouse to edit the repeat unit display value.

10.15.3 Flipping repeat units

Flipping repeat units is only possible in a ring, as there are two possible directions for a repeat unit to be defined in a ring. To flip a repeat unit in a ring, make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the repeat unit brackets so the brackets are outlined in an amber color as shown in Figure 10.34.
2. Right-click on the hovered repeat unit and select the Flip Repeat Unit menu item.

Figure 10.36 shows the result of flipping a repeat unit.

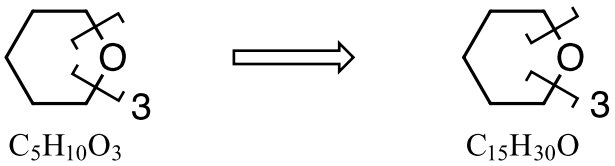


Figure 10.36: *Flipping a repeat unit in a ring*

10.15.4 Editing repeat units styles

To change the heights, widths or bond buffers of the current bracket rendering style for the repeat unit, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Execute the following steps:

1. Hover the mouse pointer over the repeat unit brackets so the brackets are outlined in an amber color as shown in Figure 10.34.
2. Right-click on the hovered repeat unit and select the Format Repeat Unit... menu item.
3. Scroll to the **Repeat Unit** section and edit the **Height**, **Lip Width** and **Bond Buffer** sliders as desired.

Please note, when the repeat unit is improperly defined, there may be no contents, in which case the brackets may not orient in the way you desire and some settings may have no effect. For instance, if you set a repeat unit between two bonds in separate chemical structures as shown in Figure 10.37, there will be no contents and the **Bond Buffer** style will have no effect. The bracket ends will still attempt to orient towards each other.

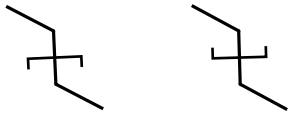


Figure 10.37: *Some styles will have no effect if the repeat unit is invalid*

Instead, use *manual* bracket objects, which are described in the BRACKETS section. For more information on invalid bracket definitions, please see the REPEAT UNITS section of the CHEMINFORMATICS chapter.

10.15.5 Repeat unit bracket types

You may change the style of bracket used for rendering. There are currently 4 bracket styles:

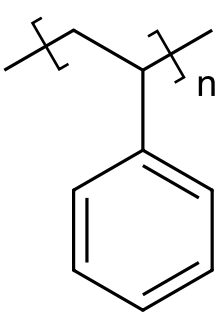
- **Square Brackets** - [ ]
- **Parentheses** - ( )
- **Curly Brackets** - { }
- **Chevrons** - < >

To change the repeat unit bracket style, execute the following steps:

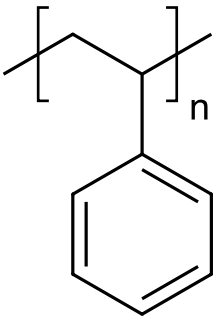
1. Hover the mouse pointer over the repeat unit brackets so the brackets are outlined in an amber color as shown in Figure 10.34.
2. Right-click on the hovered repeat unit and select the Format Repeat Unit... menu item.
3. Scroll to the **Repeat Unit** section and edit the **Style** style to the desired type.

10.15.6 Enclosing shortest paths

All of the repeat unit brackets shown so far have been aligned with the bonds they are attached to. This is the default rendering for repeat unit brackets in ChemDoodle and conveys the meaning of the repeat unit in the most clear and versatile way, given any random structure layout. Some users may prefer aligned brackets in their figures. If you wish for more aligned brackets, you may enable the **Enclose Shortest Path** style. This will render brackets for the rectangular bounds of the shortest path between the two assigned bonds, and still pass through those two bonds. Enable enclosing shortest paths with the **Enclose Shortest Path** style for the repeat unit. Figure 10.38 shows the results.



(a) *Repeat unit brackets aligned by bond*



(b) *Repeat unit brackets enclosing shotest path*

Figure 10.38: *Different methods for rendering repeat unit brackets*

ChemDoodle will properly render the appropriate dimensions for the shortest path, and therefore the **Height** and **Bond Buffer** styles will have no effect when the **Enclose Shortest Path** style is enabled. Please be aware, rendering repeat unit brackets while enclosing shortest paths will not be appropriate for all situations, such as in rings, or where the shortest path between the two assigned bonds is not regularly linear, or when other bonds may intersect with the brackets, reducing the clarity of the figure.

10.15.7 Working with repeat units

Repeat units serve a much more important role in ChemDoodle than just a convenient way to render a bracket. Repeat units are a chemically interpreted part of the molecule they are assigned to and can be used to actually define repeating substructures in molecules. Please see the REPEAT UNITS section of the CHEMINFORMATICS chapter for further instruction.

CHAPTER 11

iChemLabs Art

Contents

11.1 Overview **262**

11.2 What is iChemLabs art? **262**
11.2.1 iChemLabs art vs. vector graphics 263
11.2.2 Restrictions on using iChemLabs art 263

11.3 Categories of iChemLabs art **264**
11.3.1 Laboratory Glassware 264
11.3.1.1 Editing glassware styles 265
11.3.1.2 Removing solution (liquid) from templates 265
11.3.1.3 Tubing 266
11.3.2 BioArt 267
11.3.3 Flipping art 268
11.3.4 Z-ordering 268

11.4 Importing your own art **269**

11.1 Overview

The graphics artists at iChemLabs have created a large number of publication quality scientific images for use in your figures and projects through ChemDoodle. We call these images iChemLabs art. There are two main categories of iChemLabs art in ChemDoodle: glassware, which are greyscale by default and BioArt, which are full color. All iChemLabs art are vector graphics, which mean that these images are resolutionless and fully scalable, so you can be sure figures created with them are always of the highest quality. Using iChemLabs art allows you to create very advanced scientific figures to cover a wide range of materials.

This section introduces the new user to using the iChemLabs art resources provided within ChemDoodle. It covers the following topics:

- What is iChemLabs art?
- The types of iChemLabs art available in ChemDoodle.
- How to put together glassware diagrams.
- How to edit glassware.
- How to draw tubing for glassware.
- How to remove liquid from glassware.
- How to put together BioArt diagrams.
- How to import your own art.
- Restrictions on the use of the iChemLabs art from ChemDoodle.

11.2 What is iChemLabs art?

The predrawn art in ChemDoodle has been hand drawn by graphics artists at iChemLabs. These are images that are not only very well drawn, but are also what we call vector graphics, or resolutionless images. This means that they can be scaled to any size and they will still be rendered cleanly, without the blurriness that plagues bitmap graphics. You can see a range of iChemLabs art in Figure 11.1.

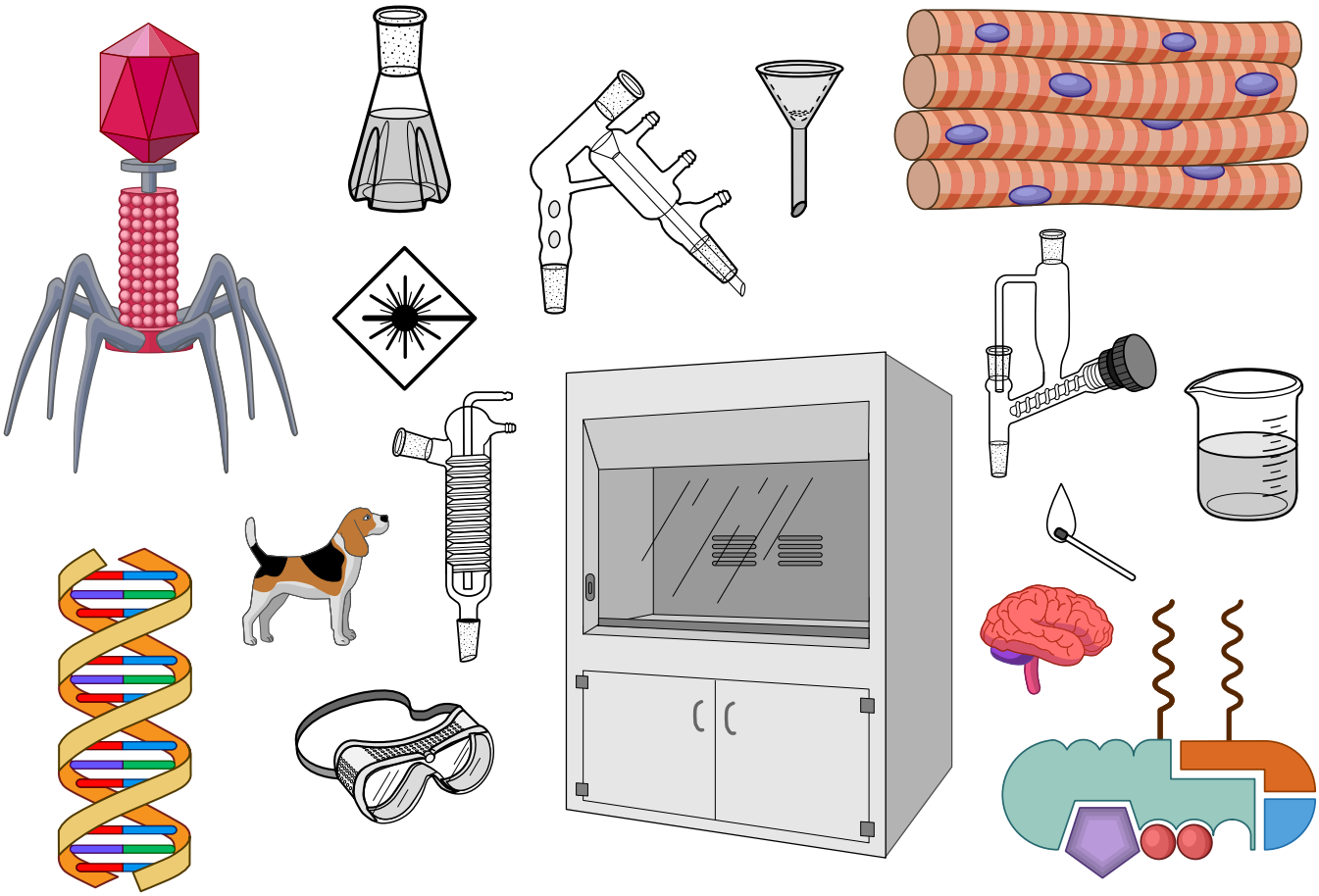


Figure 11.1: *Sample iChemLabs Art*

iChemLabs art can be used in conjunction will the other graphics tools in ChemDoodle to produce very advanced and descriptive figures.

11.2.1 iChemLabs art vs. vector graphics

Vector graphics are covered in detail in the SHARING INFORMATION chapter. All of the predrawn iChemLabs art provided in ChemDoodle are vector graphics. We are simply calling all of the hand drawn vector graphics from iChemLabs and provided in ChemDoodle as iChemLabs art. So vector graphics are protocols for defining resolutionless images, and iChemLabs art is the set of predrawn vector graphics provided by iChemLabs in ChemDoodle.

11.2.2 Restrictions on using iChemLabs art

While copyright for the output from this software belongs to the author of said content (the licensee of this software), iChemLabs owns the copyright on all of the individual iChemLabs art images provided in ChemDoodle. We certainly want you to be able to use these images to create your figures and work, but please note that the copyrights on the individual images are owned by iChemLabs. As such, using ChemDoodle to output the glassware graphics or the BioArt graphics for the sole purpose of publishing, selling, or distributing them individually or as a set is forbidden.

11.3 Categories of iChemLabs art

There are two main categories of vector art provided in ChemDoodle: glassware and BioArt.

11.3.1 Laboratory Glassware

Figures for glassware setups can be created by using the glassware clipart library within ChemDoodle. ChemDoodle contains hundreds of different glassware clipart and other laboratory clipart that can be put together to create very complex laboratory setups. The clipart is organized into a window for easy selection, shown in Figure 11.2. This is accessed by clicking on the **iChemLabs Art** button  in the **Drawing** toolbar.



Figure 11.2: *The Glassware Clipart Window*

The right side contains tabs for selecting the category of clipart to view. While moving your mouse over the clipart, a grey highlight will appear with a description of the clipart. An amber highlight means that the clipart is selected.

To build glassware setups, execute the following steps:

1. Click on the **iChemLabs Art** button  in the **Drawing** toolbar.
2. In the window that appears, select the tab category on the right and then select the glassware piece you would like to place into your figure.
3. Press the mouse down on the current document and drag to place it where you prefer the piece to be placed. Hold down the shift key to flip the template horizontally while placing.
4. Release the mouse to set the glassware piece.
5. Repeat steps 2-4 until your figure is complete.

11.3.1.1 Editing glassware styles

All glassware clipart is governed by the same styles that other shapes are. So you can change the stroke thickness and the colors of the various components in the clipart as shown in Figure 11.3. Note that only liquid filling in the glassware have colors that can be modified.

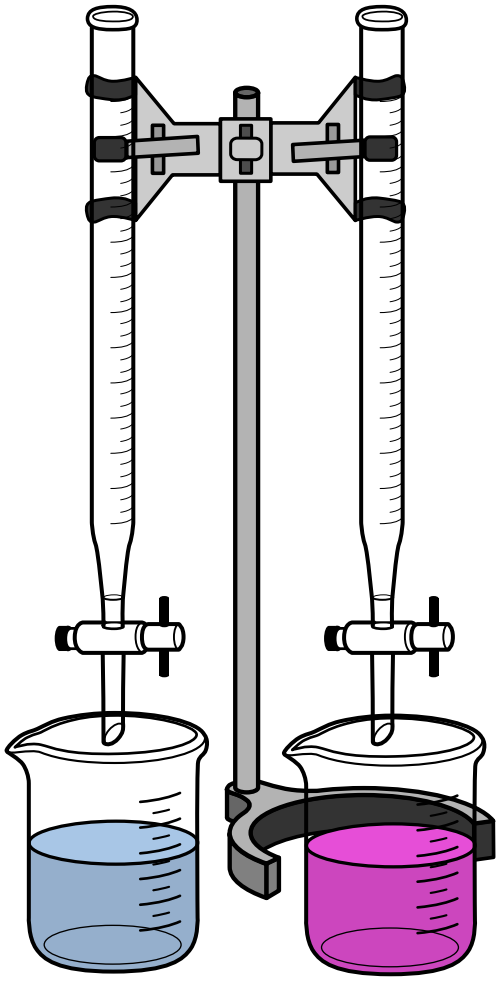


Figure 11.3: *A Glassware Setup with Altered Colors*

11.3.1.2 Removing solution (liquid) from templates

Many glassware clipart contain solution. You may desire to have this solution removed for your figures. To do so, execute the following steps:

1. In your document (not in the glassware window), hover over the glassware clipart with the solution you would like removed using a selection tool with nothing selected.
2. Right-click on the glassware clipart and select the **Format Clipart…** menu item, or press the comma [,] key.
3. Scroll down to the **Clipart** section and deselect the **Fill with Solution** on/off choice.

The solution will then be removed from the glassware clipart as shown in Figure 11.4.

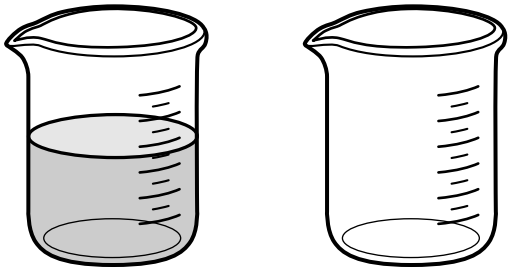


Figure 11.4: *A Beaker with and without Solution*

11.3.1.3 Tubing

You may wish to connect pieces of glassware via tubing. A good technique for doing this is by using the **Bezier Curve** tool to draw the path of the tubing, and then increasing the stroke width of the path to the desired thickness.

One method for doing so is as follows:

1. Select the **Bezier Curve** tool in the **Drawing** toolbar.
2. Press the mouse down in the middle of the outlet in the glassware figure where the first tubing connection will be made.
3. Drag the mouse out in the direction that the first outlet faces. The longer you drag out the control point, the longer the curve will be straight at that point.
4. Press the mouse down in the middle of the outlet in the glassware figure where the second tubing connection will be made.
5. Drag the mouse out in the direction that the second outlet faces. The longer you drag out the control point, the longer the curve will be straight at that point.
6. Edit the bezier curve if necessary, or press the escape key to finish drawing the curve.
7. Hover the curve using a selection tool and right-click, selecting the Format Bezier Curve... menu item.
8. In the **Strokes** section of the settings window that appears, change the **Thickness** setting to 10 pixels.
9. Select the **Accept** button to close the settings window.

Your completed figure will then contain a nice smooth curve connecting the outlets that represents tubing as shown in Figure 11.5.

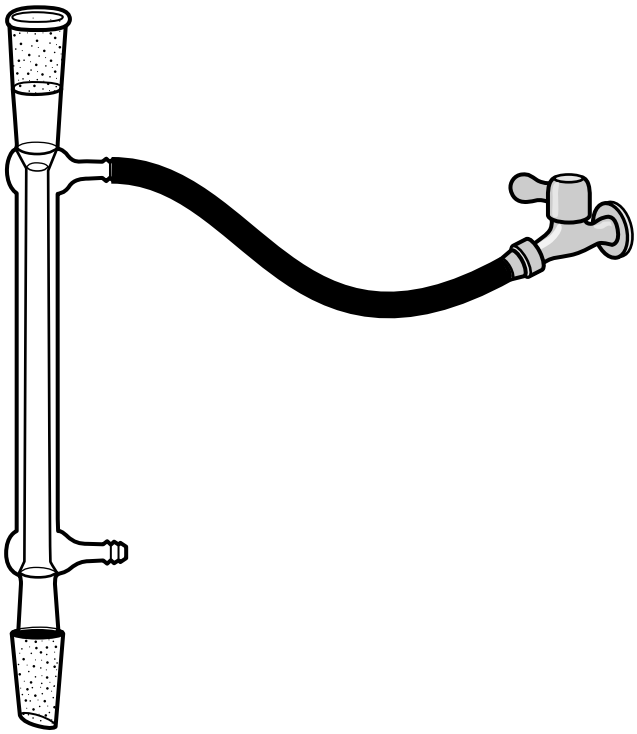


Figure 11.5: *Glassware Figure with Tubing*

11.3.2 BioArt

In addition to laboratory clipart, ChemDoodle includes BioArt for creating biological diagrams. The BioArt is organized into a window for easy selection along with the Laboratory Glassware, as shown in Figure 11.6. This is accessed by clicking on the **iChemLabs Art** button  in the **Drawing** toolbar.

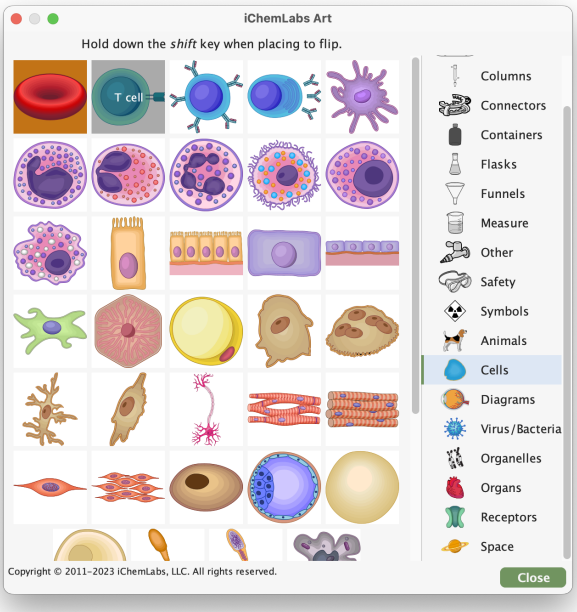


Figure 11.6: *The BioArt Window*

The right side contains tabs for selecting the category of clipart to view. While moving your mouse over the clipart, a grey highlight will appear with a description of the clipart. An amber highlight means that the clipart is selected.

To build biological diagrams, execute the following steps:

1. Click on the **iChemLabs Art** button  in the **Drawing** toolbar.
2. In the window that appears, select the tab category on the right and then select the BioArt piece you would like to place into your figure.
3. Press the mouse down on the current document and drag to place it where you prefer the piece to be placed. Hold down the shift key to flip the template horizontally while placing.
4. Release the mouse to set the BioArt image.
5. Repeat steps 2-4 until your figure is complete.

11.3.3 Flipping art

To flip iChemLabs art graphics, just hold down the shift key while placing them. The preview will then show you the flipped graphic.

You can also manually specify whether iChemLabs art is flipped or not by right-clicking on the graphic (in the document, not the art windows) with nothing selected, selecting the Format Clipart... menu item and then changing the **Flip** on/off choice in the **Clipart** section.

11.3.4 Z-ordering

To achieve the desired front-to-back order for iChemLabs art, care must be taken when placing them in a figure. The last piece added will be rendered on top.

Each piece of iChemLabs art is a complete image, and it is not possible to show one piece in between the front and back of another piece in ChemDoodle. However, because they are vector graphics, you may export your figure to be post-edited in

vector editing software (such as Adobe Illustrator) to achieve this effect.

11.4 Importing your own art

Inserting images is covered in detail in the SHARING INFORMATION chapter. So you can easily incorporate other art or your own art into your figures. It is recommended that you import vector graphics for the best quality figures. ChemDoodle can import both the Adobe Portable Document Format {.pdf} and Web Scalable Vector Graphics {.svg, .svgz} as vector graphics. Be sure to respect the copyrights on all images that you use.

CHAPTER 12

Content Management Tools

Contents

12.1 Overview **273**

12.2 Selecting content **273**
12.2.1 Selecting individual objects 274
12.2.2 Selecting groups of objects 274
12.2.3 Select all 274
12.2.4 Adding/removing individual objects from a selection 274
12.2.5 Adding/removing groups of objects from a selection 274
12.2.6 Selecting whole molecules 274
12.2.7 Selecting chemical objects by SMARTS 275
12.2.7.1 Extensions 275
12.2.8 Navigating through single shapes 276
12.2.9 Selecting only shapes 276
12.2.10 Select the inverse of the current selection 276
12.2.11 Deselecting objects 276
12.2.12 Reselecting objects 276

12.3 Transforming content **277**
12.3.1 Translating 277
12.3.1.1 Arbitrarily 277
12.3.1.2 Horizontally or vertically 277
12.3.2 Rotating 277
12.3.2.1 Arbitrarily 277
12.3.2.2 By 30 degree increments 277
12.3.2.3 By 90 degree increments 277
12.3.2.4 By a specifically defined angle 278
12.3.2.5 Rotating in 3D 278
12.3.2.6 Moving the rotation anchor 278
12.3.3 Rotating labels 279
12.3.3.1 Rotating selected atom labels 279
12.3.3.2 Rotating individual labels 279
12.3.3.3 Reset the rotation of atom labels 279
12.3.4 Scaling 279
12.3.4.1 Arbitrarily 279
12.3.4.2 Locking the aspect ratio 279
12.3.4.3 Precisely 279
12.3.4.4 Scaling by bond 280

12.4 Organizing content **281**
12.4.1 Aligning 281
12.4.2 Aligning parts of molecules 281
12.4.3 Aligning by bond 281
12.4.4 Centering 281
12.4.5 Centering parts of molecules 281
12.4.6 Distributing 281
12.4.7 Distributing parts of molecules 282
12.4.8 Flipping 282
12.4.9 Flipping a bond 282
12.4.10 Torsioning a bond 282
12.4.11 Placing in grid 282
12.4.12 Stacking 283

12.5 Z-orders **283**
12.5.1 Changing the z-order of bonds 283
12.5.1.1 Using the context menu 283
12.5.1.2 Re-adding the bond 284
12.5.1.3 3D coordinates 284
12.5.1.4 Automatically layering bonds by wedges 284
12.5.2 Changing the z-order of shapes 285
12.5.2.1 In relation to other shapes 285
12.5.2.2 In front of or behind atoms and bonds 285

12.6 Framing content **286**

12.7 Grouping content **286**
12.7.1 Grouping 286
12.7.2 Ungrouping 286

12.8 Duplicating content **287**
12.8.1 Copy and paste 287
12.8.2 Cut and paste 287
12.8.3 While transforming 287

12.9 Removing content **288**
12.9.1 Removing individual objects 288
12.9.2 Removing groups of objects 288
12.9.3 Clearing the document 288

12.10 Drawing aids **288**
12.10.1 Atom aids 288
12.10.2 Bond aids 288
12.10.3 Ring aids 288
12.10.4 Molecule aids 289
12.10.5 Background aids 289

12.11 Fonts **289**

12.12 Colors **289**
12.12.1 Quick colors button 289
12.12.2 Color detection 290
12.12.3 Advanced colors button 290
12.12.4 RGB/HSB color chooser 292
12.12.5 Pinwheel color chooser 293
12.12.6 Recent colors chooser 294
12.12.7 Responsive color controls 295
12.12.8 Custom element color set 295

12.1 Overview

In this chapter the new user is introduced to content management tools within ChemDoodle. It covers the following topics:

- Selecting content
- Duplicating content
- Editing content
- Organizing content
- Grouping content
- Removing content
- How to enable drawing aids
- Using the color choosers
- Defining a custom element color set

12.2 Selecting content

Content can be selected by using any of the selection tools. There are three types of selection tools provided in ChemDoodle:

Lasso		Define an arbitrary boundary that follows the mouse and selects any objects contained within.
Lasso Only Shapes		Define an arbitrary boundary that follows the mouse and selects only shape objects contained within.
Rectangular Marquee		Define a rectangle that selects any objects contained within.

Selected content will be highlighted in amber and will be surrounded by an animated (called a "crawling ants" effect) blue outline as shown in Figure 12.1.

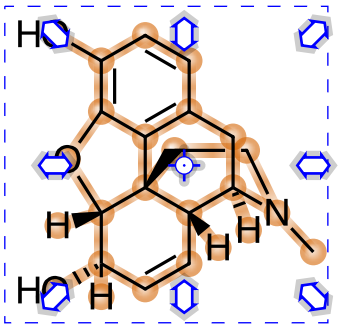


Figure 12.1: *Selected Content*

The crawling ants animation can be turned off in the **Settings** window under the **Appearance** tab.

12.2.1 Selecting individual objects

To select an individual object, first choose a selection tool and make sure no content is currently selected. Then hover the object to be selected and click. The single object will then be selected.

12.2.2 Selecting groups of objects

To select groups of objects, execute the following steps:

1. Choose a selection tool.
2. Click and drag to draw an outline with a lasso or to draw a rectangle with the rectangular marquee to surround all of the objects you would like to select.
3. Release the mouse to select the contained objects.



It may be difficult to see the full bounds for some shapes, such as with iChemLabs art that doesn't fully fill its rectangle bounds. If you have trouble selecting a shape, make sure to discover where its bounds are and draw the selection bounds around all anchors.

12.2.3 Select all

To select all content in the scene, use the Content » Select » All menu item. For quick use, the keyboard shortcut for this function is ctrl + A.

12.2.4 Adding/removing individual objects from a selection

If a selection has already been made, you can add or remove an individual object from the selection. While still using the selection tool, hold down the alt key and hover the object to be added or removed and click the mouse. If that object was previously selected, it will be removed from the selection, otherwise it will be added to the selection.

12.2.5 Adding/removing groups of objects from a selection

If a selection has already been made, you can add or remove groups of objects from the selection. While still using the selection tool, hold down the shift key and click and drag to draw an outline with a lasso or to draw a rectangle with the rectangular marquee to surround all of the objects you would like to select or deselect. Then release the mouse. Any objects contained within the new boundary will be removed from the selection if they were previously selected, otherwise they will be added to the selection.

12.2.6 Selecting whole molecules

Instead of tracing an entire molecule with the selection tools to select it, which may become difficult in complex scenes, the following techniques will allow you to precisely select individual molecules:

- Using a selection tool, double click on a constituent atom or bond. The entire molecule will become selected. This behavior may be changed to edit the styles of the atom or bond instead by changing the **Double Click on Atom/Bond** setting to **Edit Object Styles** in the **Settings** window under the **Controls** tab.
- Using a selection tool, hold down the alt + shift keys and then click on an atom or bond within the molecule you wish to select. This will result in the whole molecule being selected. If part of that molecule is already selected, that part will be removed from the selection.

- Alternatively, press the tab key to navigate through molecules, selecting one at a time, starting at the last drawn molecule and then navigating through them chronologically. If you hold down the alt key while pressing tab, you will navigate through the molecules in reverse chronological order.

12.2.7 Selecting chemical objects by SMARTS

SMARTS is single line, text-based query system for matching chemical objects. Sometimes it is convenient to select content in scenes by *SMARTS* queries. To do so, execute the following steps:

1. Select the Content » Select » SMARTS... in the application menu toolbar.
2. A window will appear prompting you for the *SMARTS* query. Input your query here and press the **Accept** button.

Any content that matches the *SMARTS* string will then be selected. *SMARTS* stands for *SM*iles *AR*bitrary *T*arget *S*pecification and is defined by Daylight: http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html

12.2.7.1 Extensions

In addition to the Daylight *SMARTS* specification, ChemDoodle supports the following atomic and bond-query extensions:

Table 12.1: Extended SMARTS Atomic Primitives

Symbol	Symbol name	Atomic property requirements	Default
`#G`⟨n⟩	periodic group	(identity) element belonging to historical main group ⟨n⟩, where 1 and 2 correspond to IUPAC groups 1 and 2, and 3–8 correspond to IUPAC groups 13–18; transition metals are not included	group 1 (alkali metals, including hydrogen)
`#M`	metal	(identity) matches any metal element	(no default)
`#N`	electronegative class	(identity) matches N, O, F, Cl, or Br	(no default)
`#X`	heteroatom	(identity) any element other than hydrogen or carbon	(no default)
`d`⟨n⟩	Non-hydrogen degree	Exactly ⟨n⟩ directly bonded non-hydrogen atoms; multiple bonds count once	exactly one
`i`⟨n⟩	π-bonding degree	Exactly ⟨n⟩ π bond participations: *i.e.* `i2` matches an alkyne carbon or central allene carbon	at least one
`k`⟨n⟩	size of SSSR ring	Atom lies in an SSSR ring of size ⟨n⟩; unlike Daylight `r`, this can match any participating SSSR ring size rather than only the smallest	any ring atom
`Z`⟨n⟩	aliphatic heteroatom degree	Exactly ⟨n⟩ directly bonded nonaromatic heteroatoms, where a heteroatom is any atom other than carbon or hydrogen	at least one
`z`⟨n⟩	heteroatom degree	Exactly ⟨n⟩ directly bonded heteroatoms, where a heteroatom is any atom other than carbon or hydrogen	at least one
`^`⟨n⟩	hybridization	(caret symbol) perceived atomic hybridization ⟨n⟩, where 0 = s, 1 = sp, 2 = sp^2, 3 = sp^3, 4 = sp^3d, and 5 = sp^3d^2	0 (s)
`'`⟨n⟩	radical count	(apostrophe symbol) exactly ⟨n⟩ assigned radical electrons	exactly one (" is 2, etc)
`|`⟨n⟩	lone-pair count	(pipe symbol) exactly ⟨n⟩ assigned lone electron pairs	exactly one (|| is 2, etc)

Table 12.2: Extended SMARTS Bond Primitives

Symbol	Description
$	quadruple bond



We based the inclusion of these extensions on what has already been adopted in the industry by other toolkits. Our intention is to maximize functionality, but remain consistent. This may not mean that all of the extensions present in another package are available, some may be redundant already with the extensions provided or offer no meaningful benefit over the official *SMARTS* specification. But the extensions we have implemented should be easily adaptable, or even familiar, to the query you are trying to execute.

The #M, apostrophe, and pipe atom-environment primitives are ChemDoodle-specific additions. Where another dialect assigns different semantics to the same symbol, the behavior documented in this section is authoritative for ChemDoodle.

12.2.8 Navigating through single shapes

Instead of selecting a shape object with a selection tool, you can press the tab + shift key to navigate through shapes, selecting one at a time, starting at the last drawn shape and then navigating through them chronologically. If you hold down both shift+alt while pressing tab, you will navigate through the shapes in reverse chronological order.

12.2.9 Selecting only shapes

When figures are highly congested, it may be difficult to select shapes from surrounding structures. In this case, use the **Lasso Only Shapes** tool  which will only recognize shapes. The behavior of the **Lasso Only Shapes** tool is identical to that of the **Lasso** tool, except that it only recognizes shapes.

12.2.10 Select the inverse of the current selection

To select the inverse of the current selection on a page, select the Content › Select › Inverse menu item. The keyboard shortcut to use this function is shift+ctrl+I.

12.2.11 Deselecting objects

To deselect the current selection, execute one of the following actions:

- Move the mouse cursor away from the selection so that the lasso cursor icon appears. Then click the mouse.
- When the mouse cursor is within the current selection boundary, double-click the mouse.
- Press the space key to deselect the current selection and return to the structure drawing mode.
- Use the Content › Deselect menu item.

12.2.12 Reselecting objects

If you lost the current selection, you can reselect it by selecting the Content › Reselect menu item. The keyboard shortcut to use this function is ctrl+shift+D.

12.3 Transforming content

The selection area is context sensitive and you can click and drag on the various features of the selection to perform different actions.

12.3.1 Translating

Selected content can be translated, or in other words, moved around the document.

12.3.1.1 Arbitrarily

To translate content arbitrarily, or move it on the page, execute the following steps:

1. Select the content to be translated.
2. Hover the mouse cursor over the selection so that an open hand cursor appears.
3. Press the mouse down so the mouse cursor turns into a closed hand cursor.
4. Drag the mouse to translate the content.
5. Release the mouse to finish the translation.

During the translation, the change in x position and change and y position will be displayed below the mouse cursor. You can disable this feedback in the **Settings** window under the **Appearance** tab.

12.3.1.2 Horizontally or vertically

Pressing down the shift key after beginning a translate action on a selection will lock the content horizontally or vertically to the original position of the content.

12.3.2 Rotating

Selected content can be rotated.

12.3.2.1 Arbitrarily

To rotate content any arbitrary angle, execute the following steps:

1. Select the content to be rotated.
2. Hover the mouse just outside the edge of the selection border so that the rotation cursor appears.
3. Press the mouse down and drag it to rotate the content.
4. Release the mouse to finish the rotation.

During the rotation, the rotation angle will be displayed below the mouse cursor. You can disable this feedback in the **Settings** window under the **Appearance** tab.

12.3.2.2 By 30 degree increments

Pressing down the shift key after beginning a rotate action on a selection will lock the content to 30° angles from the original orientation.

12.3.2.3 By 90 degree increments

To rotate content by 90°or 180°, execute the following steps:

1. Select the content to be rotated.
2. Expand the Content › Rotate submenu and press the 90 °CW, 90 °CCW or 180 ° menu items.

12.3.2.4 By a specifically defined angle

To rotate content by a specifically defined angle, execute the following steps:

1. Select the content to be rotated.
2. Expand the Content › Rotate submenu and press the Arbitrary... menu item.
3. Enter a degree value in the number field that appears and select clockwise or counterclockwise as the direction of rotation.
4. Press the **Rotate** button to complete the rotation with the settings you provided.

12.3.2.5 Rotating in 3D

Even though ChemDoodle generates graphics for structures in two dimensions, the underlying structures are defined in three dimensions.

ChemDoodle will read in 3D coordinates from all chemical files and provides functions for rotating structures in 3D.



While ChemDoodle has some 3D editing features, it is not a molecular modeler and is not the appropriate tool for building 3D coordinates for structures. You can use ChemDoodle 3D to build chemical 3D coordinates:
https://www.chemdoodle.com/3d

To rotate structures in 3D execute the following steps:

1. Select the molecules to be rotated in 3D using a selection tool.
2. Press the **Rotate in 3D** button  in the **Content** toolbar.
3. Hover the mouse over the selection so that the 3D rotation cursor appears.
4. Press the mouse down and drag it to rotate the content.
5. Release the mouse to finish the rotation.

By default, mouse movements while rotating structures in 3D will rotate the structure around the x- and y-axes based on horizontal and vertical movement respectively. You can also set the 3D rotations to be defined by a quaternion trackball in the **Settings** window under the **Controls** tab if that is more comfortable for you.

12.3.2.6 Moving the rotation anchor

By default, content is rotated about its center; both for 2D and 3D rotations. Rotation about an alternative point can be achieved by moving the rotation anchor which, by default, is located at the center of the selection. This is useful, for instance, for rotating structures about an atom.

To move the rotation anchor, execute the following steps:

1. Move the mouse over the rotation anchor so that the anchor fills with an amber color and the mouse cursor changes to a resize cursor.
2. Press the mouse down and drag the rotation anchor to the desired position.
3. Release the mouse to set the new rotation anchor position.

Henceforth, all rotations will proceed around the new rotation anchor position.

When moving the rotation anchor, it will automatically lock onto atoms within the selection as you get close to them, aiding you in setting the rotation anchor over atom positions.

12.3.3 Rotating labels

Atom and caption labels can be rotated from the horizontal axis.

12.3.3.1 Rotating selected atom labels

By default, labels are not rotated when selected structures are rotated. To change this behavior, in the **Settings** window, in the **Controls** tab, enable the **Rotate Atom Text with Structures** option. When you rotate structures, atom labels will now rotate as well.

12.3.3.2 Rotating individual labels

Individual atom labels and captions can be rotated. To rotate an individual caption or atom label, execute the following steps:

1. Select the individual caption or atom label, ensuring that no other content is selected.
2. Hover the mouse just outside the edge of the selection border so that the rotation cursor appears.
3. Press the mouse down and drag it to rotate the label.
4. Release the mouse to finish the rotation.

12.3.3.3 Reset the rotation of atom labels

To reset a rotated atom label back to its original alignment, hover that atom label with a selection tool, right-click and select the Reset Label Rotation menu item.

12.3.4 Scaling

Selected content can be scaled.

12.3.4.1 Arbitrarily

To scale content arbitrarily, execute the following steps:

1. Select the content to be scaled.
2. Hover the mouse over one of the anchor points in the selection so that the mouse resize cursor appears.
3. Press the mouse down and drag the anchor to scale the content.
4. Release the mouse to finish the scale action.

The x scale factor and y scale factor will be displayed below the mouse cursor during scaling. You can disable this feedback in the **Settings** window under the **Appearance** tab.

12.3.4.2 Locking the aspect ratio

To preserve the width-to-height ratio while scaling content along the diagonals, just hold down the shift key while performing the above steps.

12.3.4.3 Precisely

To precisely scale content, execute the following steps:

1. Select the content to be scaled.
2. Press the Content » Scale... menu item.
3. Select whether to scale the content by dimension or bond length and then specify the remaining settings.
4. Press the **Scale** button to scale the content to the settings you provided.

12.3.4.4 Scaling by bond

To scale an individual bond, and take into account the rest of the molecule, execute the following steps:

1. Hover the bond to be scaled.
2. Right-click on the bond and select the Scale Bond... menu item. The **Scale Bond** interface will appear as shown in Figure 12.2.

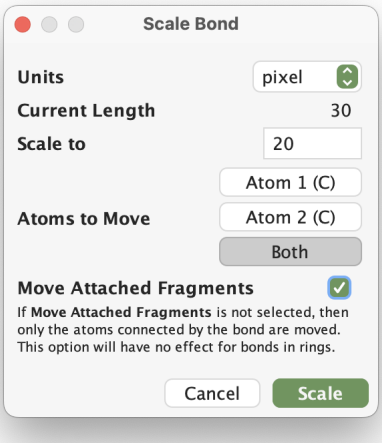


Figure 12.2: *Scaling a individual bond*

3. The current length will be displayed in the **Current Length** line. Set the new length in the **Scale to** line. You can change the units using the **Units** drop down on the top.
4. Select how you would like the bond to be adjusted in the **Atoms to Move** section. **Atom 1** means that the atom at the start of the bond will be moved to achieve the new length. **Atom 2** means that the atom at the end of the bond will be moved to achieve the new length. **Both** means that both atoms of the bond will be moved equally to achieve the new length. The labels of the atoms will be displayed in the choice to help show you which atom is which.
5. Select the **Move Attached Fragments** check box if you wish to also move the fragments in the molecule attached to the atoms that are being moved.
6. Press the **Scale** button to scale the bond as defined.



If you select **Move Attached Fragments**, it must be true that the two fragments on the opposite sides of the bond are separated and only connected by the bond being scaled. If they are not, they cannot be moved independently, such as if the bond being scaled is in a ring. So in these cases, selecting the **Move Attached Fragments** check box will have no effect.

12.4 Organizing content

ChemDoodle provides several tools for laying out content in the document.

12.4.1 Aligning

To align content relative to each other, execute the following steps:

1. Select the content to be aligned.
2. Expand the Content » Align submenu and press the Left Edges, Centers Horizontally, Right Edges, Top Edges, Centers Vertically or Bottom Edges menu items. A small icon for the menu items will help you decide which alignment you need.

12.4.2 Aligning parts of molecules

It is possible to align substructures and individual atoms with other objects. Simply use a selection tool to only select the parts of the molecule you wish to align and follow the instructions in the previous section.

12.4.3 Aligning by bond

To align an entire molecule by a given bond, execute the following steps:

1. Hover the bond to align the molecule by.
2. Press the ↑, ↓, ←, or → arrow keys to align the bond from its first to second constituent atom in the selected direction. This will rotate the entire molecule with the bond.

12.4.4 Centering

To center all content on the page, select the Content » Center » All on Page menu item.

To center selected content on the page, execute the following steps:

1. Select the content to be centered.
2. Expand the Content » Center submenu and press the Selection on Page, Selection Horizontally or Selection Vertically menu items.

12.4.5 Centering parts of molecules

It is possible to center substructures and individual atoms with other objects. Simply use a selection tool to only select the parts of the molecule you wish to center and follow the instructions in the previous section.

12.4.6 Distributing

To distribute content across the document, execute the following steps:

1. Select the content to be distributed.
2. Expand the Content » Distribute submenu and press the Horizontally on Page or Vertically on Page menu items.

To distribute content across the document using a buffer spacing that you provide, execute the following steps:

1. Select the content to be distributed.

2. Expand the Content › Distribute submenu and press the Horizontally by Buffer Space... or Vertically by Buffer Space... menu items.
3. Input a buffer space value into the number field that appears.
4. Click the **Accept** button to perform the distribution.

12.4.7 Distributing parts of molecules

It is possible to distribute substructures and individual atoms along with other objects. Simply use a selection tool to only select the parts of the molecule you wish to distribute and follow the instructions in the previous section.

12.4.8 Flipping

To flip content horizontally or vertically, execute the following steps:

1. Select the content to be flipped.
2. Expand the Content › Flip submenu and press the Horizontally or Vertically menu item.

There is one option in the **Settings** window under the **Tools** tab that will modify how the flipping functions work:

- **Flip Retains Stereochemistry** - By default, when flipping content horizontally or vertically, stereocenters will *not* have bond types adjusted and the flip functions will invert chiral stereocenters. Enable this option to preserve stereochemical configurations when using the content flip functions.

12.4.9 Flipping a bond

You may wish to flip non-symmetrical bonds when you need them to face the other direction, such as when working with wedge bonds. There are a few quick ways to do so:

- Hover the bond and press the F key to flip it.
- Hover the bond, right-click and select the Flip Bond Orientation menu item.
- Use the bond tool of that bond type and click on the bond after hovering it. ChemDoodle will detect the bond is being set to its current bond type and will instead flip the bond.

12.4.10 Torsioning a bond

There may be cases where you would like to flip the structure on one side of a bond, through the axis of the bond, independent of the other side. For instance, if you want to change a *cis* double bond to its *trans* counterpart. To do so, hover the bond, right-click and select the Torsion Bond menu item.

12.4.11 Placing in grid

To place all content in a grid that covers the document, execute the following steps:

1. Select the Content › Grid All on Page... menu item.
2. In the prompt that appears, select whether you want to specify the grid dimensions by columns or by rows by choosing the corresponding selection from the drop-down menu.
3. Input the dimension of the grid in the number field. The other dimension will be calculated automatically based on the number of objects being placed in the grid.
4. Select the **Grid** button.

12.4.12 Stacking

Stacking will place all content on the page starting from the top-left of the document to the bottom- right, such that their visual bounds are separated by a small buffer and that all objects are within the page margins (if possible). To stack all content on the page, press the Content > Stack All on Page menu item.

If content is ever placed outside of the page bounds, red strips will appear at the sides of the page that the content extends from as shown in Figure 12.3. Click on the red strip to stack all of the content that extends from that side of the page back onto the page.



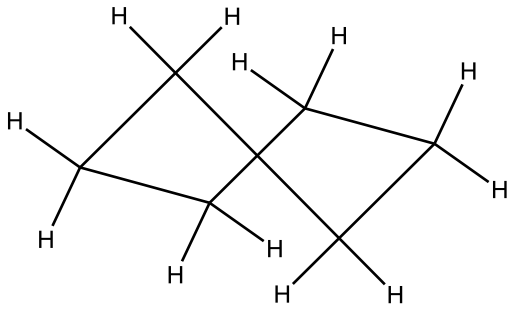
Figure 12.3: *When content is off-page, a red strip will appear. When clicking, the off-page content from that side will be stacked.*

12.5 Z-ORDERS

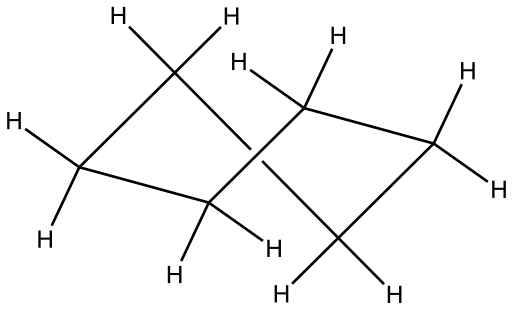
The *z*-order is the order that objects are rendered in. The higher the *z*-order, the later the object is rendered in the document. Those rendered last are rendered on top of the objects rendered before it.

12.5.1 Changing the z-order of bonds

It is often difficult to represent depth in 2D. When bonds intersect, the viewer may be confused as to which bond is on top of the other. Even worse, the overlap may mistakenly portray the existence of an extra atom at the intersection. ChemDoodle will retract a bond rendering from an intersection to aid in visualization as shown in Figure 12.4.



(a) *The two center bonds intersect, creating ambiguity*



(b) *The bond with the lower z-order is retracted at the intersection, generating a clearer image*

Figure 12.4: *Intersecting Bonds*

By default, bond overlaps are retracted. If you wish to disable or modify bond overlap retractions, the behavior is controlled by the **Clear Bond Overlaps** and **Overlap Clear Width** styles for bonds. Please see the STYLES chapter for further instruction.

The *z*-order for bonds is determined by the order the bonds were added to the document, if *z*-coordinates are not present. Therefore, bonds drawn earlier will be rendered below bonds drawn after. For structures with 3D coordinates, the bond with the most positive *z*-coordinates will be rendered on top. The following sections provide instructions to modify the *z*-order of bonds.

12.5.1.1 Using the context menu

If you desire to change the rendering such that a bond drawn below another is instead drawn on top, you may do so in ChemDoodle. To modify the *z*-order of a bond, execute the following steps:

1. Hover the bond to change its z-order.
2. Right-click on the bond.
3. Expand the Arrange submenu.
4. Select the Send Forward, Send Backward, Send to Bottom or Send to Top menu item depending on your preference.

Depending on the current z-order of the bond, some of the options in the Arrange submenu may be disabled. For instance, if the hovered bond has no intersections with other bonds, then the Send Forward and Send Backward menu items will be disabled.

12.5.1.2 Re-adding the bond

Bonds will be rendered in chronological order such that the last bond drawn will be rendered on top. To quickly change the z-order of bonds while drawing the structure, execute the following steps:

1. Delete the bond that is to be rendered on top. You may quickly do this by hovering over the bond and pressing the delete or backspace key.
2. Redraw the bond.

12.5.1.3 3D coordinates

For structures with 3D coordinates, the bond with the most positive z-coordinates will be rendered on top. To change the z-order of bonds when z-coordinates are present, execute the following steps:

1. Select the structure with the z-orders to be changed.
2. Select the **Rotate in 3D** tool  in the **Content** toolbar.
3. Click and drag the mouse to rotate the structure in 3D so the desired bond is placed on top.
4. Release the mouse to stop the rotation and set the new coordinates.



If z-coordinates are present in the structure, using the context menu or re-adding the bond will be ineffective at changing which bond is rendered on top as the z-order will be explicitly defined by the coordinates of the atoms. If you wish to manually control the overlaps within a 3D structure rendering, first flatten the structure using the Content » Flatten menu item to set all z-coordinates to 0.

12.5.1.4 Automatically layering bonds by wedges

In perspective structures with wedges, bond overlaps are often inevitable. ChemDoodle can help you quickly layer the bonds in structures containing wedges to show appropriate overlaps within the perspective structure without altering the x and y-coordinates of the atoms. This function is performed by assigning a small z-coordinate value to each atom based on the wedges within the structure. Therefore, molecule output formats that support z-coordinates will retain such overlap ordering when opened in another application that properly respects z-coordinates.

Perform the following steps to use this function:

1. Select the perspective structure with the bonds to be layered. At least one wedge bond must be defined for the function to have any effect.
2. Execute the Structure » Auto-layer Bonds by Wedges menu item.

Figure 12.5 shows some examples of the function.

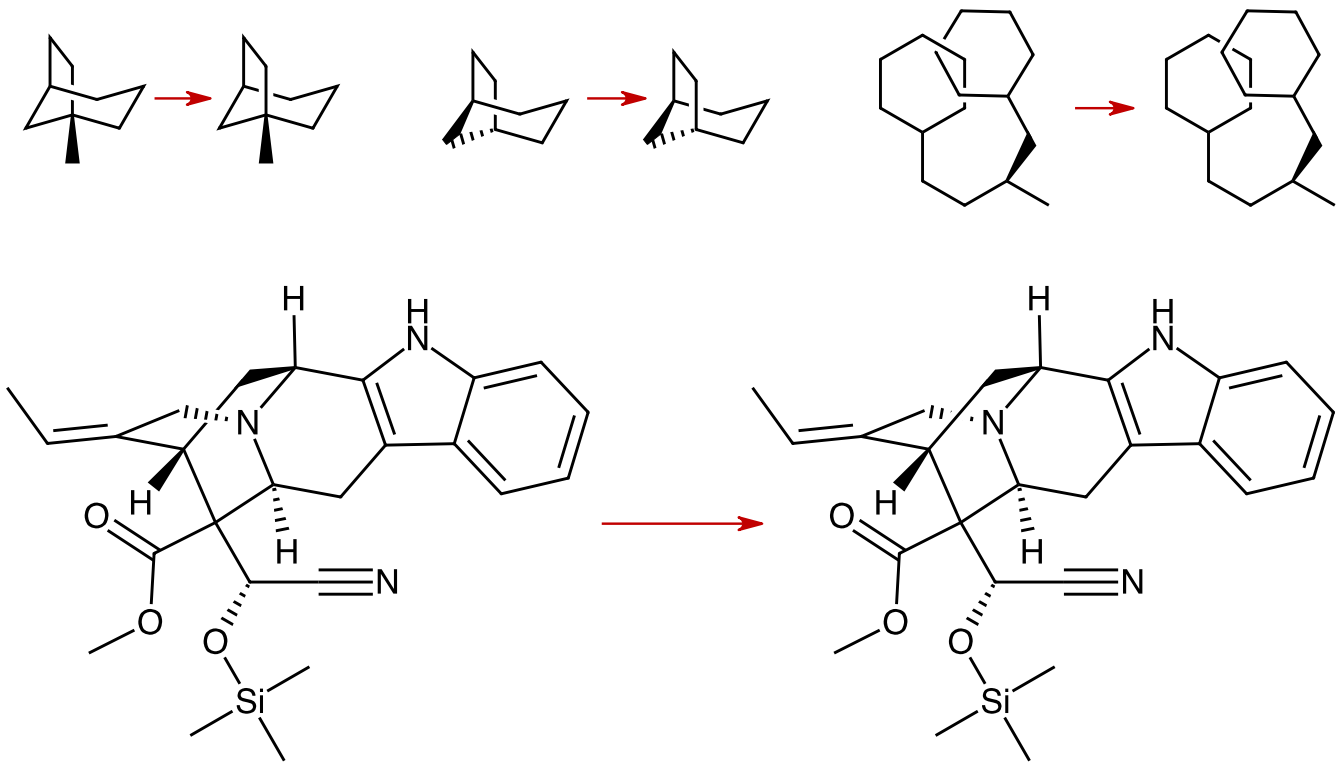


Figure 12.5: *ChemDoodle can automatically layer your bonds for you by inferring z-order from wedges.*

12.5.2 Changing the z-order of shapes

Shapes, by default, will always render behind atoms and bonds and will be *z*-ordered chronologically. Occasionally, you may want to change how shapes are *z*-ordered with respect to each other and with respect to atoms and bonds.

12.5.2.1 In relation to other shapes

To modify the *z*-order of a shape in relation to other shapes, execute the following steps:

1. Hover the shape to change its *z*-order.
2. Right-click on the shape.
3. Expand the Arrange submenu.
4. Select the Send Forward, Send Backward, Send to Bottom or Send to Top menu item depending on your preference.

Depending on the current *z*-order of the shape, some of the options in the Arrange submenu may be disabled. For instance, if only the hovered shape exists in the document, then all of the menu items in the Arrange submenu will be disabled.

12.5.2.2 In front of or behind atoms and bonds

Shapes, by default, will always render behind atoms and bonds. An exception to this rule are orbital shapes, which are rendered in front of atoms and bonds by default.

To make a shape render on top or atoms and bonds, or to reverse this action and render the shape below atoms and bonds, perform the following steps:

1. Hover the shape to change its *z*-order with respect to atoms and bonds.
2. Right-click on the shape.

3. Expand the Arrange submenu.
4. At the bottom of the submenu, either the **Place in Front of Structures** or **Place in Back of Structures** menu item will be present, depending on the current *z*-order of the shape with respect to atoms and bonds. Execute this menu item to switch to the other side.

12.6 Framing content

Content can be automatically framed with various different shapes. To frame objects, execute the following steps:

1. Select the objects to be framed using the selection tools.
2. Expand the Content > Add Frame submenu.
3. Select the type of frame to use.

The selected content will then be framed.

12.7 Grouping content

Content in ChemDoodle can be grouped. Once grouped, you will no longer be able to edit the member objects individually. Any transformations performed on the group will affect all member objects. Groups can be transformed as a whole just like other shapes.

Grouping can be nested, so groups can be grouped into further groups. Ungrouping is not recursive, so ungrouping a group containing groups will leave those contained groups intact.

12.7.1 Grouping

To group content, execute the following steps:

1. Select the content to be grouped.
2. Press the Content > Group menu item.

12.7.2 Ungrouping

To ungroup content, execute the following steps:

1. Select the groups to be ungrouped.
2. Press the Content > Ungroup menu item.

12.8 Duplicating content

Content in ChemDoodle can be duplicated in the current document or between separate documents through copy and paste actions. To have ChemDoodle objects copied and pasted correctly in the document, keep **ChemDoodle Collage** enabled in the **Settings** window under the **Clipboard** tab.

12.8.1 Copy and paste

To duplicate content, execute the following steps:

1. Select the content to be duplicated.
2. Press the Edit > Copy menu item. The keyboard shortcut to use this function is ctrl + C. You can also use the **Copy** button in the **Content** toolbar.
3. Press the Edit > Paste menu item. The keyboard shortcut to use this function is ctrl + V. You can also use the **Paste** button in the **Content** toolbar.

12.8.2 Cut and paste

To duplicate content and remove the original, execute the following steps:

1. Select the content to be duplicated.
2. Press the Edit > Cut menu item. The keyboard shortcut to use this function is ctrl + X. You can also use the **Cut** button in the **Content** toolbar.
3. Press the Edit > Paste menu item. The keyboard shortcut to use this function is ctrl + V. You can also use the **Paste** button in the **Content** toolbar.

12.8.3 While transforming

You can quickly duplicate selected content as you are transforming it. Just perform the following steps:

1. Select the content to be duplicated.
2. While holding down the Ctrl key on Windows and Linux or the command key on macOS, press the selection tool down and perform your transform action (translate, rotate or scale).
3. The selected content will be duplicated and the current transform action will affect the duplicated content.
4. Release the mouse to complete the transform action on the duplicated content.

You may also press the Ctrl key on Windows and Linux or the command key on macOS at any time during a transform action to immediately create a duplicate at that moment. This way, you can quickly create complex layouts of duplicates.



If you press and hold the shift key down after duplicating content while performing a transform action, you will restrict the transform action on the duplicated content as described in the TRANSFORMING CONTENT section.

12.9 Removing content

12.9.1 Removing individual objects

Individual objects can be removed by using the **Eraser** tool  in the **Content** toolbar to hover the object and then clicking to remove it. Additionally, at any time, when an object is hovered, press the backspace or delete key to remove it.

12.9.2 Removing groups of objects

Groups of objects can be removed in a number of ways. You can do the following:

- Use a selection tool to select the content to be removed. Then press the backspace or delete key.
- First select the content to be removed. Then use the **Eraser** tool  in the **Content** toolbar to click on the current document.
- Select the **Eraser** tool, then press the mouse down and drag over all of the content to be removed. Selected content will be highlighted. Then release the mouse to remove all highlighted objects. Dragging over content that has already been highlighted will unhighlight it.

12.9.3 Clearing the document

Clear the entire document by executing the Edit > Clear menu item or by pressing the **Clear** button  in the **Content** toolbar.

12.10 Drawing aids

Drawing guides are helpful when precision is important. There are several categories of drawing guides, and each has its own use. Guides can be enabled and disabled in the View > Drawing Aids submenu.

12.10.1 Atom aids

Two types of aids can be drawn for atoms:

- **Orthogonal** - Will show a horizontal and vertical line through the center of each atom to help with alignment.
- **Circular** - Will show a circle around each atom with radius equal to the current standard bond length to help with distances.

12.10.2 Bond aids

A single type of aid can be drawn for bonds:

- **Parallel** - Will draw a line through each bond, parallel to its direction to help with extrapolation.

12.10.3 Ring aids

Rings can be colored in with a different color corresponding to the size of the ring to help with perception.

12.10.4 Molecule aids

Two types of aids can be drawn for molecules:

- **Bounds** - Will show a rectangle representing the bounds of each molecule to help with placement.
- **Orthogonal** - Will show a horizontal and vertical line through the center of each molecule to help with alignment.

12.10.5 Background aids

Three types of aids can be drawn on the background:

- **Crosshair** - Will render a crosshair and grid to help with partitioning and aligning objects. The crosshair may be moved by clicking and dragging on the center target using a selection tool. If you double click on the center target, the target will be reset to the center of the document. Each page in a multi-page document will present its own crosshair which may be moved independently of the others. To reset all crosshairs in a multi-page document, disable the **Crosshair** aid and then reenable it. By default, the crosshair will be segmented in inches, but you may instead switch to **Metric (cm)** mode in the **Settings** window in the **Appearance** tab in the **Other Settings** section with the **Ruler Mode** setting.
- **Grid** - Will render a grid at an interval that you specify to help with aligning objects. Both metric and US lengths are available.
- **Margins** - Will render the bounds for the margins.

12.11 Fonts

To change the fonts of atom labels and text-based shapes, execute the following steps:

1. Select the atoms and shapes whose fonts you would like to change.
2. Choose the font family, font size and font style from the **Formatting** toolbar to change the fonts.

Caption fonts for label shapes can be set independently of fonts used for the rest of the document, including molecular structures. You can set the **Caption Font** in the **Styles** window under the **Shapes** tab in the **Labels** section.

12.12 Colors

There are two features in the **Formatting** toolbar for changing the colors of content, the **Quick Colors** button and the **Advanced Colors** button.

12.12.1 Quick colors button

The **Advanced Colors** button, although powerful, is not a quick way to change colors. To quickly change colors, use the **Quick Colors** button. Select the content for which you would like the colors changed and press the **Quick Colors** button. All of the content will be changed to that color regardless of the content type.

If you click and hover (or drag) over the **Quick Colors** button, a palette will appear to select a new color. Drag the mouse pointer over one of the preset colors to select it and immediately change the selected content to that color.

You can also add custom colors to the last three rows of the **Quick Colors** palette. Release your mouse over the circled plus icon (⊕) and release to show a color chooser. Choose the desired color and press **OK** to add it to the palette and change the currently selected content to that color.

The **Quick Colors** palette is shown in Figure 12.6.

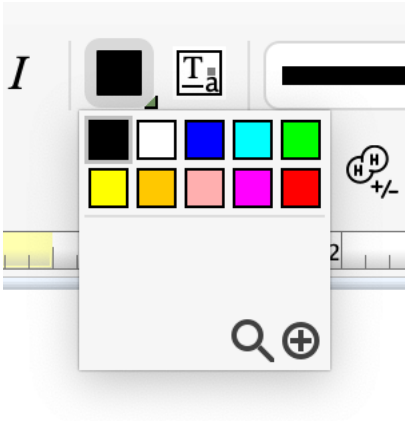


Figure 12.6: *The Quick Colors Palette*

12.12.2 Color detection

When working with content that uses nonstandard colors, you may wish to detect what those colors are. To do this, expand the **Quick Colors** button and release the mouse over the **Detect Color** (🔍) button. Then hover over the color in the document you wish to detect and press the mouse down when that color is centered in the cursor. That color will be added to the **Quick Colors** button for further use.

12.12.3 Advanced colors button

The **Advanced Colors** button in ChemDoodle is a bit more complex of a function. When you click on this button, you will see a window appear, shown in Figure 12.7.

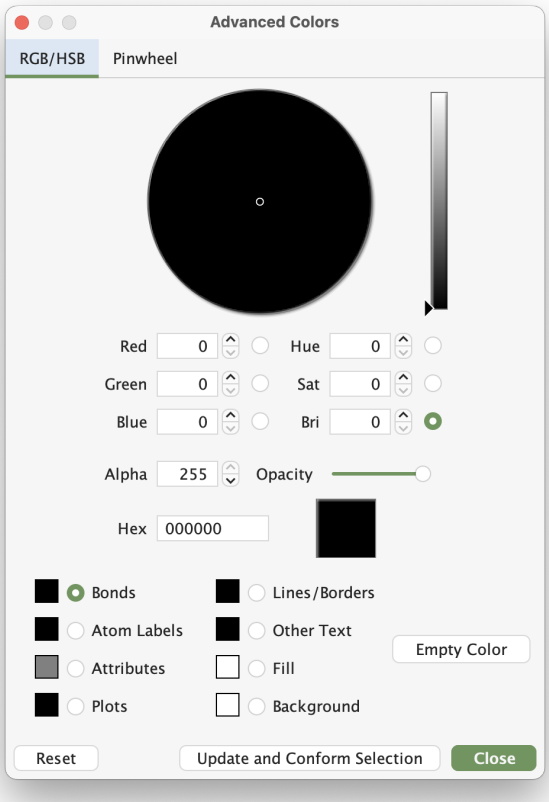


Figure 12.7: *Advanced Colors Window*

On the top of this window will be color pickers, and the bottom will contain a list of object groups. This window can remain open while you are creating figures. You may define a color to each of these groups to quickly control the style sheet colors for your figures.

There are eight colors defined by the **Color** button:

1. Bonds
2. Atom Labels
3. Attributes
4. Plots
5. Lines/Borders
6. Other Text
7. Fill
8. Background

To change the color for a specific group of objects, select the radio button for the group you wish to define. Then use the color pickers at the top to decide your color (including alpha channel transparency). The color next to the radio button will automatically update as you pick your color. If you wish for a certain group color to be empty and to not be rendered, then click the **Empty Color** button to the right of the color groups.



Note an empty color is different from a color with an alpha value of 0 (fully transparent). If you export your figure to SVG format, for instance, the object rendered with a 0 alpha color will still be present in the SVG (although you should not see it), while an object with an empty color will be excluded.

Once you have decided upon the colors for the different groups, press the **Update and Conform Selection** button to apply your color choices and modify any selected objects in your document, if there is a selection. To reset the group colors to their original colors, press the **Reset** button. You will still need to press the **Update and Conform Selection** button to apply the reset colors for the groups. If you do not wish to commit any further changes, and you want to close the window, press the **Close** button.

The **Advanced Colors** button displays the currently defined style sheet colors for the groups as a quick reference. A breakdown of the **Advanced Colors** button icon is shown in Figure 12.8.



Figure 12.8: *Advanced Colors Icon*

- The background color is represented by the color behind the rectangle border.
- Lines/Borders have their colors represented by the rectangle border.
- Fill color is represented by the fill inside the rectangle border.
- Bond color is represented by the line leading to the “a” character.
- Atom text color is represented by the “a” character.
- Attribute color is represented by the small square above the “a” character.
- Other text color is represented by the “T” character.

12.12.4 RGB/HSB color chooser

The RGB/HSB color chooser is shown in Figure 12.9.

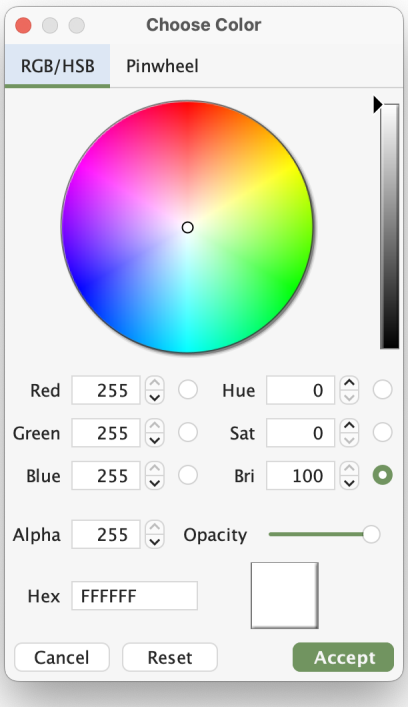


Figure 12.9: *The HSB/RGB Color Chooser*

The color selected can be seen in the preview square at the bottom right, with the hex value shown to the left.

To select a color, just move the mouse pointer over the color panel and press the mouse down and drag until the color you would like to use is selected.

If the pinwheel appears all black, you will need to increase the **Brightness** setting by moving the **Brightness** slider up (located to the right of the color wheel).

The chosen colors and the values in the text fields will mirror each other, and editing the color by the color panel will change the text values and changing the text values will edit the defined color.

The left text fields of **Red**, **Green** and **Blue** refer to the red, green and blue components of the RGB color model. The right text fields of **Hue**, **Sat** and **Bri** refer to the hue, saturation and brightness components of the HSB color model. To edit a single component of these models, select the radio button next to the component to be controlled individually. The min value for these fields is 0 and the max value is 255. The color panel will change to reflect this mode and the slider will show the range of the selected value.

You can also set the **Alpha** value here, which is directly related to the opacity of the color. A value of 0 means the color is completely transparent, and a value of 255 means that the color is completely opaque. You can also use the **Opacity** slider.

12.12.5 Pinwheel color chooser

The pinwheel color chooser is shown in Figure 12.10.

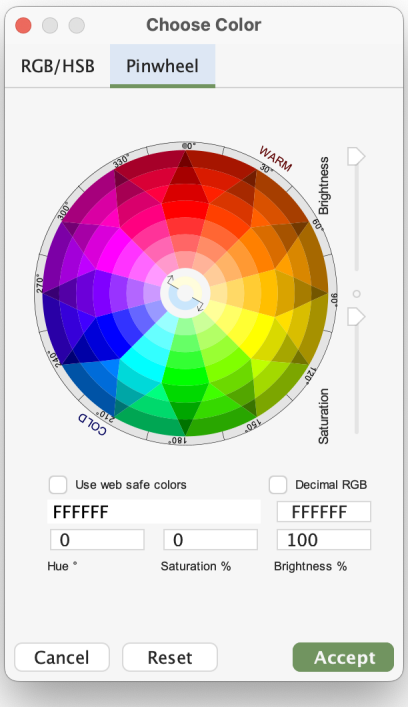


Figure 12.10: *The Pinwheel Color Chooser*

The color selected can be seen in the preview bar at the bottom, with the hex value shown by default. You can also view the RGB value by enabling the **Decimal RGB** checkbox.

To select a color, just move the mouse pointer over the pinwheel until the color you would like to select is hovered, then click the mouse. You can also use the mouse wheel to scroll through colors.

If the pinwheel appears all black, you will need to increase the **Brightness** setting by moving the **Brightness** slider up. If the pinwheel appears all white, you will need to decrease the **Saturation** setting by moving the **Saturation** slider down.

The chosen colors and the values in the text fields will mirror each other, and editing the color by the pinwheel wheel will change the text values and changing the text values will edit the defined color.

12.12.6 Recent colors chooser

The recent colors chooser is shown in Figure 12.11.

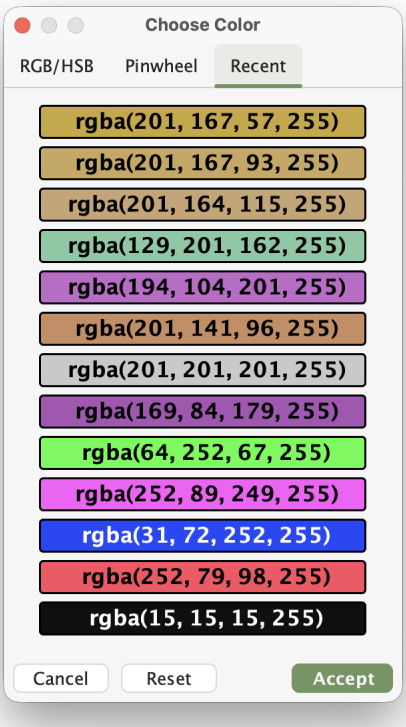


Figure 12.11: *The Recent Colors Chooser*

This chooser simply lists the last 13 selected colors in a column, with the most recent at the top. Each color is represented by a button filled in with the color and labelled by the *RGBA* values for that color. Simply click on a color button to select it.

12.12.7 Responsive color controls

Color choosers will update the graphics in real time. So keep an eye on your figure as you use color choosers for immediate feedback and precise color choice.

12.12.8 Custom element color set

If you wish to use a different color set from the built-in sets provided by ChemDoodle, you can do so with the custom element color set.

To edit the custom element color set, perform the following steps:

1. Open the **Styles** window and select the **Atoms** tab.
2. In the **Elements** section, click the **Custom Color Set** button  .
3. The **Custom Color Set** window will appear as shown in Figure 12.12.

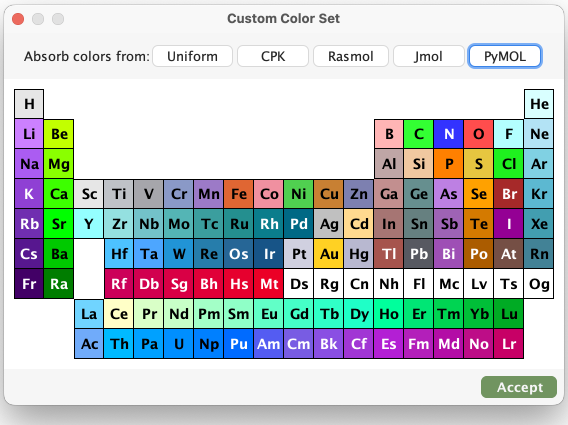


Figure 12.12: *Defining a custom color set for elements*

4. Start from the default colors or choose any of the buttons on the top of the window to choose a different starting set.
5. To change an element's color, click on that element and use the color chooser that appears.
6. Press the **Accept** button when you are finished.

You can now use your custom color set just like the built-in color sets by choosing **Custom** for the **Element Coloring** style.

CHAPTER 13

Styles

Contents

13.1 Overview **300**

13.2 Document styles **300**
13.2.1 Style sheets 300
13.2.2 Saving style sheets 301
13.2.3 Setting the default document style sheet 301
13.2.4 Restore the original default document style sheet 302

13.3 Editing styles **302**
13.3.1 For single objects 302
13.3.2 For a group of objects 302
13.3.3 Conforming a group of objects to the current style sheet 302
13.3.4 Conforming the entire document to a different style sheet 303

13.4 Individual styles **303**
13.4.1 Style types 303
13.4.2 Pages 304
13.4.2.1 Colors 304
13.4.2.2 Text 304
13.4.2.3 Dimensions 305
13.4.2.4 Margins 305
13.4.3 Atoms 305
13.4.3.1 Colors 305
13.4.3.2 Labels 305
13.4.3.3 Hydrogens 306
13.4.3.4 Carbons 306
13.4.3.5 Elements 306
13.4.4 Attributes 307
13.4.4.1 Colors 307
13.4.4.2 Logistics 307
13.4.4.3 Text 307
13.4.4.4 Charges 307
13.4.4.5 Electrons 307
13.4.4.6 Stereochemistry 307
13.4.5 Bonds 307
13.4.5.1 Colors 307
13.4.5.2 Settings 308
13.4.5.3 Stroke 308
13.4.5.4 Merges 308
13.4.5.5 Conjugation 309
13.4.5.6 Options 309
13.4.6 Rings 310
13.4.6.1 Fused 310
13.4.6.2 Aromatics 310
13.4.7 Reactions 310
13.4.7.1 Layout 310
13.4.7.2 Arrowheads 310
13.4.8 Shapes 311
13.4.8.1 Colors 311
13.4.8.2 Settings 311
13.4.8.3 Strokes 311

13.4.8.4 Fills . . . 311
13.4.8.5 Shadows . . . 311
13.4.8.6 Brackets . . . 311
13.4.8.7 Repeat Unit Brackets . . . 311
13.4.8.8 Highlights . . . 312
13.4.8.9 Labels . . . 312
13.4.8.10 Orbitals . . . 312
13.4.8.11 Paths . . . 312
13.4.8.12 Pushers . . . 312
13.4.8.13 Rectangles . . . 312
13.4.8.14 Rulers . . . 313
13.4.9 Spectra . . . 313
13.4.9.1 Colors . . . 313
13.4.9.2 Plot Strokes . . . 313
13.4.9.3 Grids . . . 313
13.4.9.4 Integration Lines . . . 313

13.5 Bond stroke styles . . . **314**

13.6 Advanced document rendering . . . **315**
13.6.1 Anti-aliasing . . . 315
13.6.2 Font fractional metrics . . . 315
13.6.3 Dithering . . . 316
13.6.4 Rendering algorithm . . . 316
13.6.5 Alpha interpolation algorithm . . . 316
13.6.6 Color rendering algorithm . . . 317
13.6.7 Stroke control . . . 317
13.6.8 Image scaling . . . 318

13.1 Overview

All graphics in ChemDoodle are fully customizable. Styles for the graphics can be defined for the entire document, and may be saved and applied to another file.

This section introduces the new user to ChemDoodle document styles and style sheets. It covers the following topics:

- How to customize the graphics of your figures.
- What are styles and style sheets?
- How to create, share and install custom *ChemDoodle Style Sheet* files.
- Which graphic styles can be customized.

13.2 Document styles

Document styles are the variables that determine how graphics are rendered in the document. They can define the entire document, a group of objects or an individual object.

Document styles are separate from application settings and are found in the **Styles** window as shown in Figure 13.1. The **Styles** window may be accessed using the Content ▸ Edit Styles... menu item or by pressing the **Edit Styles** button  at the bottom-right of the main interface.

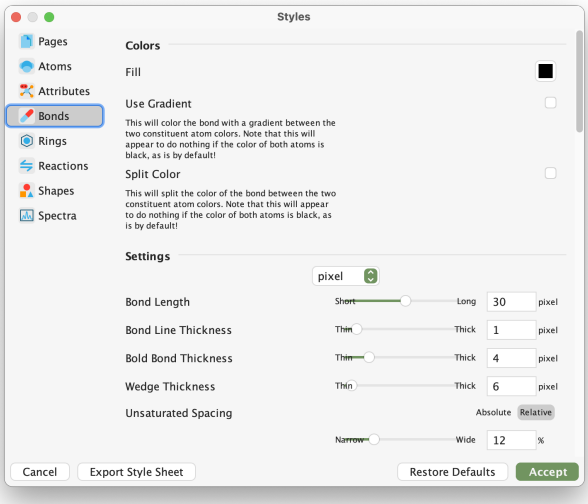


Figure 13.1: *Styles Window*

13.2.1 Style sheets

The entire set of styles defined to a document is called a style sheet. When a style sheet from ChemDoodle is saved to a file, it is called a *ChemDoodle Style Sheet* file. Style sheets can be chosen when creating formatted documents. The creation of formatted documents is discussed in ChemDoodle BASICS.

Style sheets are useful when creating new graphics from previously defined options or for sharing a standardized style among many users.

13.2.2 Saving style sheets

To save your currently selected styles as a style sheet, execute the following steps:

1. Open the **Styles** window and customize the document styles to your preference.
2. Press the **Export Style Sheet** button on the bottom left of the **Styles** window. Outside of the **Styles** window, you may also select the Edit ⟩ Export Style Sheet... menu item.
3. A new window will appear as shown in Figure 13.2. Type in the name of the *ChemDoodle Style Sheet* file.
4. Choose three fonts to cascade through. This is important because different operating systems have different font sets and you may have selected a font not accessible on another operating system. *Serif* and *SansSerif* will always be defined on all operating systems, so select one of those fonts as the third option for a guaranteed font.
5. Press the **Export** button to save the *ChemDoodle Style Sheet* file.

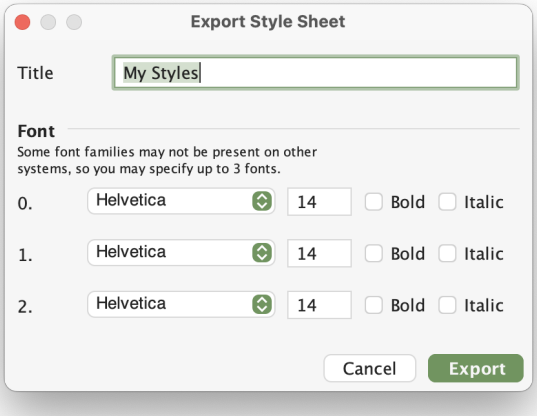


Figure 13.2: *Choose options for exporting a style sheet*

All *ChemDoodle Style Sheet* files are saved to the `styleSheets` folder in the `ChemDoodleSettings` folder located in your operating system's standard `Documents` folder. Any functions for using *ChemDoodle Style Sheet* files or for conforming documents will now list the new style sheet file.

If you want to use *ChemDoodle Style Sheet* files provided by other users of ChemDoodle, just copy their file into the `styleSheets` folder in the `ChemDoodleSettings` folder located in your operating system's standard `Documents` folder. If you have ChemDoodle open while copying the file, close and restart it. The copied style sheets will then be accessible in ChemDoodle.

13.2.3 Setting the default document style sheet

When you globally change the styles for a document, ChemDoodle will ask you if you would like the changed styles to become the new default style sheet. There are two cases when this happens:

1. After opening the **Styles** window and changing styles.
2. After conforming a document using the Edit ⟩ Conform Document... menu item.

Just click **Yes** to set the changed styles as the default document style sheet. Now when a new document is opened, the current default style sheet will be used to define the graphics. Alternatively, you may answer **No** to the question, and later, if you decide to indeed use the current styles as the default style sheet, then select the Edit ⟩ Remember Style Sheet... menu item.

13.2.4 Restore the original default document style sheet

To restore the original default document style sheet, open the **Styles** window and click the **Restore Defaults** button at the bottom of the window, located next to the **Accept** button. Then close the window and select **Yes** when asked to set the current styles as the new default style sheet.

13.3 Editing styles

You can easily edit styles in ChemDoodle for single objects, selections of objects or the entire document.

13.3.1 For single objects

To edit the styles of a single object, execute the following steps:

1. Switch to a selection tool and make sure the current selection is empty.
2. Hover the mouse pointer over the object for which the styles are to be changed.
3. Right-click on the object and select the Format Object... menu item or double-click on the object. You can also press the comma , key.
4. Change the styles in the window that appears. You will see the graphics update in real-time in the document.
5. Click the **Accept** button in the object's **Styles** window to set the changes.

You can also press the **Cancel** button to cancel all changes.

Alternatively, you may access the individual Object Styles window by double-clicking on a hovered object using a selection tool. Note, the default behavior for double-clicking on atoms and bonds will select the entire molecule. This behavior may be changed to open the styles window for the atom or bond instead by changing the **Double Click on Atom/Bond** setting to **Edit Object Styles** in the **Settings** window under the **Controls** tab.

13.3.2 For a group of objects

To edit the styles for a group of objects, execute the following steps:

1. Switch to a selection tool.
2. Select all of the content for which the styles are to be changed.
3. Open the **Styles** window via the Content > Edit Styles... menu item or by selecting the **Edit Styles**  button at the bottom-right of the interface.
4. Change all the styles in the **Styles** window to your preference. You will see the graphics update for selected content in real-time in the document.
5. Click the **Accept** button in the **Styles** window to set the changes.

You can also press the **Cancel** button to cancel all changes or press the **Restore Defaults** button to return all specifications to the defaults.

A quick way to edit the styles of all objects in the document is to quickly select all of the content by using the Content > Select > All menu item or by pressing the menu accelerator ctrl + A.

13.3.3 Conforming a group of objects to the current style sheet

To conform a group of objects to the current style sheet, perform the following steps:

1. Switch to a selection tool.
2. Select all of the content for which the styles are to be changed.
3. Press the Content › Conform to Current Styles menu item or select the **Conform Selection to Current Style Sheet** button in the **Content** toolbar.

All content will conform to the styles defined in the document's style sheet. This function will also change fonts and scale structures to match the defined bond length.

13.3.4 Conforming the entire document to a different style sheet

To conform the entire document to a different style sheet, perform the following steps:

1. Press the Edit › Conform Document... menu item.
2. In the window that appears, choose the style sheet you prefer from the drop-down selection.
3. You will be asked if you would like to conform atom text by changing fonts; choose **Yes** or **No**.
4. If the bond length has changed, you will be asked if you would like the structures to be scaled to match the new values; choose **Yes** or **No**.

The entire document will now conform to the chosen style sheet.

13.4 Individual styles

13.4.1 Style types

All styles provided in ChemDoodle are listed in the **Styles** window as shown in Figure 13.1.

Each style is controlled by a interface consisting of a title to the left and a component to the right. These components include:

- **On/Off Choices** ☑ - Click the check box to choose whether the style is enabled or not. For example, the following check box will enable or disable the **Clear Bond Overlaps** style.



Figure 13.3: *On/Off Choice*

- **Single Option Choices** ◎ - Choose one of the options from the group to exclusively define it as the value to use for the style. For example one option can be chosen from the following group set to determine the value for the **Covalent Style** style.



Figure 13.4: *Single Option Choice*

- **Drop Down Choices** ☰ - If there are many choices to choose from, a drop down will be displayed instead of a **Single Option Choice**. Choose one of the options from the group to exclusively define it as the value to use for the style. For example one option can be chosen from the following group set to determine the value for the **Ruler Unit** style.

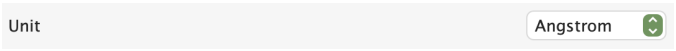


Figure 13.5: *Drop Down Choice*

- **Number Sliders** - Define a number value by clicking and dragging the slider or by explicitly typing the value in the text field. Some number components will be associated with a dimension drop down selection to easily set values in other units, such as centimeters instead of pixels. For example, slide the slider or type a value into the text box of the following number component to define the value for the **Bond Line Thickness** style.



Figure 13.6: *Number Slider*

- **Color Buttons** - Click on color buttons and use the color selection window that appears to select a new color. For example, click on the color button and choose a color to set the value for the **Fill Color** style. For more instruction on using the color choosers, please see the COLORS section.

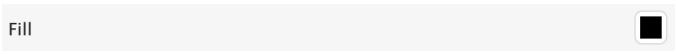


Figure 13.7: *Color Button*

- **Complete Fonts** - A complete font is a streamlined interface that allows you to set a font family, size and style in a single line. The interface consists of a drop down to select an available font family, a integer field to input the font size and two checkboxes to set the font to be **Bold** or **Italic**. For example, set the desired values for the **Caption Font** style.



Figure 13.8: *Complete Font*

All objects created in the document after changing the styles in the **Styles** window will conform to the newly defined styles. The exception to this is pasted content, which will retain its original styling (if any); you can use the Edit ⟩ Paste and Match Style menu item to override this behavior. All styles are listed in the following sections.

13.4.2 Pages

The **Page** tab contains all the styles related to page formatting.

13.4.2.1 Colors

Background A color button for the background color of the document.

13.4.2.2 Text

Main Font This is the main font used in the document for structures and other text. The caption font for non-chemical labels can be set independently in the **Shapes** panel chosen on the left of the **Styles** pane.

Query Font This is the font used to render query atoms and bonds. Font style is not editable as it is important to the meaning of the query label.

Horizontal Spacing A number slider to set the horizontal whitespace between each label token.

Vertical Spacing A number slider to set the vertical whitespace between each label token.

Subscript Reduction A number slider to set the size of subscript font relative to the label font.

Subscript Shift A number slider to set the magnitude of the offset from the label font baseline for drawing subscripts.

Superscript Reduction A number slider to set the size of superscript font relative to the label font.

Superscript Shift A number slider to set the magnitude of the offset from the label font ascent to draw superscripts from.

13.4.2.3 Dimensions

Page Size Customize the page layout by page size, page orientation, height and width. The width setting has a drop down menu that has multiple units available including centimeters, inches, millimeters, and pixels.

Ångströms/Bond Length A number slider for setting the ratio between Ångströms and the Bond Length specification in pixels. This specification is useful when finding covalent bonds and when reading in files with Ångström coordinates.

13.4.2.4 Margins

Margins The options listed are top, bottom, right and left and each refers to the margin size of the respective direction. A drop down menu is available with different units including centimeters, inches, millimeters, and pixels.

13.4.3 Atoms


The **Atoms** tab contains all the styles related to atom rendering and representations.

13.4.3.1 Colors

Text A color button for the text color of atom labels.

13.4.3.2 Labels

Buffer Type A single option choice that changes the shape of the label buffer. The default setting will shape the buffer as a convex hull around the label. The other choice will set the buffer as a rectangle around the label.

Buffer Space A number slider to set the amount of whitespace between atom text and the bonds connected to that atom.

Vertical Alignment A number slider to control the baseline for rendering text relative to the center of the atom.

Subtoken Alignment Multicharacter tokens attached to bonds will be centered by either the entire token center, or by the edge character center. For instance, if your terminal label consists of a single "Ala" token, disabling this style will center the label around the center of the entire "Ala" string (close to the "l" character), regardless of orientation. If subtoken alignment is applied, the rendering will center the label around the starting "A" or ending "a" depending on whether the label is oriented to the left or the right.

You may choose to **Never** apply subtoken alignment, **Always** apply it to every atom label, apply it to **Only Terminal** atom labels or apply an **Optimized** algorithm. When in **Optimized** mode, ChemDoodle will strive to produce the best possible layout for the specific situation of each atom label.

Token Stacking A single option choice to set whether atom labels will stack all tokens, stack only the second token or will never stack tokens.

Stack Lone/Terminal ☑ An on/off choice to set whether lone and terminal atoms will stack their label tokens.

Minimize Line Spacing ☑ This is enabled by default and collapse line spacing to reduce whitespace in atom labels. Deselect this to force uniform line spacing between the baselines of each line.

13.4.3.3 Hydrogens

Show Implicit Hydrogen ☑ Checking this box will display hydrogens not explicitly drawn in the document.

Implicit Hydrogen Coloring By default, implicit hydrogens automatically shown on hetereoatom labels will be colored based on the heteroatom's color (**Inherit from Heteroatom**). You may instead change this setting to **Explicit Hydrogen Coloring** to use the color that would be assigned to an explicit hydrogen instead.

13.4.3.4 Carbons

Display Carbon Labels A single option choice to set if carbon labels display always, only on lone and hidden carbons, only on hidden carbons, or never show.

Hidden Carbon Angle An angle number slider for setting the hidden carbon angle. The hidden carbon angle is the deviation from 180° between bonds on a carbon atom that only has two bonds attached to it.

Show Terminal Labels ☑ An on/off choice to set whether terminal carbon labels are displayed or not.

Show Attributed Labels ☑ An on/off choice to set whether attributed carbon labels are displayed or not.

13.4.3.5 Elements

Use Circles ☑ An on/off choice for controlling if element labels are rendered as text or as circles.

Coloring A single option choice for determining whether user chosen colors, *CPK* colors, *Jmol* colors, *PyMOL* or *Rasmol* colors are used for element labels.

Custom Color Set Use this button to open the **Custom Color Set Window** (see CUSTOM ELEMENT COLOR SET) to manually define a color set to use to render element types.

Radius Convention A single option choice to control if circles are rendered with a constant radius, the atomic radius of their element, the covalent radius of their element or the van der Waals radius of their element.

Constant Radius A number slider to set the constant radius with which to render element atom circles. This number may be set to 0, in which case the circle and border will not be rendered at all.

Border Width A number slider to set the width of the circle outlines when atoms are rendered as circles.

13.4.4 Attributes


The **Attributes** tab contains all the styles related to attribute objects.

13.4.4.1 Colors

Fill/Text A color button for the text color of attribute labels and graphics.

13.4.4.2 Logistics

Optimal Distance A number slider to control the maximum distance an attribute can be translated away from the object it defines.

13.4.4.3 Text

Font Size Reduction A number slider to control the font size reduction of attribute text from its defined font. This is so attribute text is smaller than the text of the object with which is associated.

13.4.4.4 Charges

Surround with a Circle ☑ An on/off choice to set whether charges are rendered with a circle around them.

Circle Line Width A number slider that determines the width of the charge circle in pixels.

13.4.4.5 Electrons

Diameter A number slider to set the diameter of rendered electrons.

Separation A number slider to set the separation distance between electrons or electrons and charges in paired attributes such as electron pairs and radical cation symbols.

13.4.4.6 Stereochemistry

Parenthesis and Italics ☑ An on/off choice to define whether stereochemical configuration descriptors will be italicized and surrounded with parenthesis.

13.4.5 Bonds


The **Bonds** tab contains all the styles related to bond rendering and representations.

13.4.5.1 Colors

Fill A color button for the bond line color.

Use Gradient ☑ An on/off choice for rendering bonds with a gradient between the constituent atom colors.

Split Color ☑ An on/off choice for rendering bonds that will split the bond color between the constituent atom colors.

13.4.5.2 Settings

Bond Length A number slider to define the length of bond lines. The bond length of selected structures will not update in real time while editing this style, but ChemDoodle will ask if you want to scale your structures after you commit your changes.

Bond Line Thickness A number slider to define the width of bonds.

Bold Bond Thickness A number slider to define the width of bold bonds.

Wedge Thickness A number slider to define the width of the wide end of wedge bonds.

Unsaturated Spacing A number slider to define the spacing between bond lines in higher order bonds.

Clip Angle A number slider to define the angle at which secondary bond lines are cropped.

Hash Width A number slider to define the width of hashes in bonds rendered with a hash.

Hash Spacing ☑ A number slider to define the width of the spacing between hashes in bonds rendered with a hash.

Hash Offset A number slider to define the translation from the origin of hashes in bonds rendered with a hash.

Dot Size A number slider to determine the size of dots in zero-order ionic bonds.

Arrow Length A number slider to define the arrowhead length of dative bonds.

Arrow Angle An angle number slider to define the arrowhead angle of dative bonds.

Wavy Length A number slider to define the amplitude of wavy bonds.

Zigzag Length A number slider to define the amplitude of zigzag bonds.

13.4.5.3 Stroke

Style A drop down selection to set the default bond stroke style.

Texture A number slider for setting the magnitude of texture in stroke styles. For instance, a higher number will cause *Bristle* strokes to look more bristled.

Bond Ends A single option choice to set how bond ends are rendered; with no cap, a round cap or a square cap.

13.4.5.4 Merges

Join Bond Connections ☑ When enabled, ChemDoodle will merge bonds together where they connect for the most aesthetic graphics.

Miter Joint Limit This number slider determines how far out a joint of two bonds should protrude from the connection.

Cut Bold/Wedge Ends ☑ When the wide end of a wedge, or either end of a bold bond merges to 2 or more other bonds, the end will be cut to match the shape of the other bonds, instead of being rendered flat.

Wedge Merging ◎ Choose the way that wedges are merged, either **Radial** or **Parallel**. **Radial** merging preserves the wedge thickness by altering the merge angle, while **Parallel** preserves the wedge angle while ignoring wedge thickness.

13.4.5.5 Conjugation

Render Curves ☑ For chains of resonance bonds, render a dash curve line across all bonds in the chain instead of individual dashed line segments.

Curve Sharpness ⊣⊢ This style defines the depth of the conjugated curves. The higher the value, the more kinked the curve will appear.

13.4.5.6 Options

If Terminal (but not simple chain) ☑ If enabled, terminal double bonds will be symmetrical unless they are in a simple chain.

Between Two Shown Labels ☑ If enabled, double bonds between two shown atom labels will be symmetrical.

In Cumulenes (including allenes) ☑ If enabled, double bonds in cumulenes will be symmetrical.

In a Chain ☑ If enabled, double bonds in chains will be symmetrical.

In a Ring ☑ If enabled, double bonds in rings will be symmetrical.

Anchor cis Interior ☑ An on-off choice that forces the second unsymmetrical line to face the interior of cis configuration.

Heteroatom Retraction ☑ An on/off choice that defines whether asymmetric double bonds will retract the second line from an atom or not based on whether that atom is a heteroatom.

Terminal Retraction ☑ An on/off choice that defines whether terminal double bonds will retract the second line from a terminal atom or not.

Autocenter Hashes ☑ An on/off choice which automatically centers hashes for aesthetic appeal and may use whitespace buffers at bond ends. When enabled, the *Hash Offset* setting has no effect.

Even Hashes ☑ An on/off choice to determine if the **Hash Width** and **Hash Offset** specifications only affect **Bold Dashed** and **Recessed** bonds.

Clear Bond Overlaps ☑ An on/off choice to determine if an overlapped bond will erase the section of overlap.

Overlap Clear Width ⊣⊢ A number slider that defines how much of the bond that is rendered behind is to be removed.

Dative Style ◎ A single option choice to set if dative bonds are rendered as **Polar Covalent** bonds with a slash in the stroke, or as **Coordinate Covalent** bonds.

Indent Arrow Bond ☑ An on/off choice to set if dative bond arrowheads are indented.

Use Lewis Dot Style ☑ An on/off choice to draw bonds as if they are part of a Lewis dot structure.

13.4.6 Rings


The **Rings** tab contains all the styles related to ring representations.

13.4.6.1 Fused

Favor Aromatics ☑ An on/off choice to force double bonds in fused systems to face aromatic rings over non-aromatic rings.

Double Bond Orientation ◎ A single option choice to determine if double bonds in fused ring systems will face larger rings or smaller rings.

13.4.6.2 Aromatics

Display Electron Count ☑ When enabled, the number of electrons participating in the delocalized ring will be drawn in the center of the ring.

Use Circles for Aromatics ◎ A single option choice to render aromatics with a circle instead of in Kekulé form. **Never** will never show aromatic circles, always displaying the second bond line. **Always** will always show the aromatic circle. **Resonance Bond Rings Only** will not alter Kekulé structures, but any rings that are defined by **All Resonance Bonds** will display an aromatic circle.

Circle Radius ⊣ A number slider to define the diameter of the aromatic circle relative to the dimensions of the ring.

13.4.7 Reactions


The **Reactions** tab contains all the styles related to reaction representations.

13.4.7.1 Layout

Double Line Spacing ⊣ A number slider to define the spacing between the lines in equilibrium arrows.

Automatically Place Pluses ☑ An on/off choice to set whether reactions automatically place pluses between constituent reactants and products.

Text Buffer ⊣ A number slider to define the buffer between the text set as the reaction conditions and the ends of the associated arrow when the text is centered. This value times two will determine the default length that arrows without associated text are cleaned to when cleaning reactions.

Constituent Buffer ⊣ A number slider to define the spacing between reaction constituents when cleaning reactions.

13.4.7.2 Arrowheads

Length ⊣ A number slider to define the arrowhead length of arrow shapes.

Angle ⊣ An angle number slider to define the arrowhead angle of arrow shapes.

Sculpting ◎ This style determines the shape of the arrow head. Sharp will lead to pointed ends and are better for larger or scaled up rendering. Smooth uses rounded ends and will lead to much better graphics at standard scales and for equilibrium arrows (as sharp ends will protrude past the line length).

13.4.8 Shapes



The **Shapes** tab contains all the styles related to shapes representations.

13.4.8.1 Colors

Borders and Lines A color button for the lines and borders of shapes.

Fill A color button for the fill color of shapes.

Text A color button for the text color of shapes.

13.4.8.2 Settings

Shapes Add A single option choice to set whether shapes are drawn in front of atoms or behind atoms.

13.4.8.3 Strokes

Draw Borders An on/off choice that will render borders around shapes.

Thickness A number slider to define the width of solid strokes in shapes.

Hash Width A number slider to define the width of hashes in shapes rendered with a hash.

Hash Spacing A number slider to define the width of the spacing between hashes in shapes rendered with a hash.

Hash Offset A number slider to define the translation from the origin of hashes in shapes rendered with a hash.

13.4.8.4 Fills

Paint Fill An on/off choice that determines whether shapes are filled with the current **Fill** color.

13.4.8.5 Shadows

Translation A number slider to define the distance from the shape the shadow should be rendered.

Angle An angle number slider to define the angle in relation to the shape to place the shadow.

Opacity A number slider to define the transparency of shadows.

Color A color button for the shadow color.

13.4.8.6 Brackets

Wideness A number slider to define the width of bracket lips relative to the standard size.

13.4.8.7 Repeat Unit Brackets

Height This number slider determines the height of dynamic brackets.

Lip Width This number slider determines the lip width of dynamic brackets.

Bond Buffer This number slider determines how far into the bond the dynamic brackets are rendered at.

Style Choose between square brackets [], parenthesis () and chevrons {} for the display of the repeat unit.

Enclose Shortest Path ☑ If enabled, brackets will be rendered vertically and will be sized to enclose all of the atoms within the shortest path between the connected bonds.

13.4.8.8 Highlights

Atom Label Buffer This number slider determines how much space to extend past atom labels.

Atom Diameter This number slider determines how much space to extend past atoms without labels.

Bond Width This number slider determines how much space to extend past bonds.

Fill in Rings ☑ An on/off choice that determines whether rings are filled with the current **Fill** color. A ring is determined to be part of the highlight if all of the atoms in the ring are highlighted.

13.4.8.9 Labels

Caption Font Abc This font is the default font for captions, which can be controlled separately from the main font for chemical structures.

13.4.8.10 Orbitals

Length Multiplier A number slider to define the default extent of orbitals in bond lengths. So if the length multiplier is one, then all orbitals placed will have a length of one bond length.

Stroke Shaded Lobes ☑ An on/off choice to set whether shaded lobes in orbitals will also be outlined.

13.4.8.11 Paths

Close ☑ An on/off choice to set if paths are closed by default.

13.4.8.12 Pushers

Distance Extent Control the distance that Pusher shapes will protrude from their bounds objects.

Nucleophile Hint When a two electron pusher originates from a bond and ends at an independent atom, the following convention will be used to render the arrow and designate the nucleophile from the atom to create the incipient bond: **Undetermined**, **Hump**, **Metaline** or **Cambridge Swoop**.

13.4.8.13 Rectangles

Rounded Arc Width A number slider to define the width of the corner arcs in rounded rectangles.

Rounded Arc Height A number slider to define the height of the corner arcs in rounded rectangles.

13.4.8.14 Rulers

Show Major Tick Marks ☑ An on/off choice to set if major ticks are shown in rulers.

Show Minor Tick Marks ☑ An on/off choice to set if minor ticks are shown in rulers.

Show Measurement ☑ An on/off choice to set if the value of the distance measured is shown in rulers.

Unit ☰ A drop-down selection to set the default units of ruler objects.

13.4.9 Spectra

 The **Spectra** tab contains all the styles related to spectra representations.

13.4.9.1 Colors

Plots A color button for the spectrum plots.

Grids A color button for the spectrum grids.

Integration Limits A color button for the spectrum integration lines.

13.4.9.2 Plot Strokes

Thickness A number slider to define the width of solid strokes in spectrum plots.

Hash ☑ An on/off choice to render spectrum plots with a hashed stroke.

Hash Width A number slider to define the width of hashes in spectrum plots rendered with a hash.

Hash Spacing A number slider to define the width of the spacing between hashes in spectrum plots rendered with a hash.

Hash Offset A number slider to define the translation from the origin of hashes in spectrum plots rendered with a hash.

13.4.9.3 Grids

Show ☑ An on/off switch to set whether spectrum grids are shown by default.

Thickness A number slider to define the line thickness of spectrum grids.

13.4.9.4 Integration Lines

Show for NMR Spectra ☑ An on/off switch to set whether spectrum integration lines are shown by default.

Thickness A number slider to define the line thickness of spectrum integration lines.

13.5 Bond stroke styles

ChemDoodle provides several bond stroke styles to style your structures for presentations, posters and more casual media. To change bond stroke styles, select the bonds to be changed with a selection tool and use the **Strokes** drop down components in the **Formatting** toolbar.

The default bond line stroke thickness is 1.2 pixels on macOS and 1.0 pixels on Windows and Linux. This is not sufficient to see some stroke styles and the value will need to be increased. Other stroke styles, such as the **Brush** style, will not display well for really short bonds and structures rendered with those styles should be expanded.

The following bond stroke styles are currently provided:

- **Basic** - 
- **Bristle** - 
- **Brush** - 
- **Charcoal** - 
- **Scribble** - 
- **Slant** - 
- **Wobble** - 

13.6 Advanced document rendering

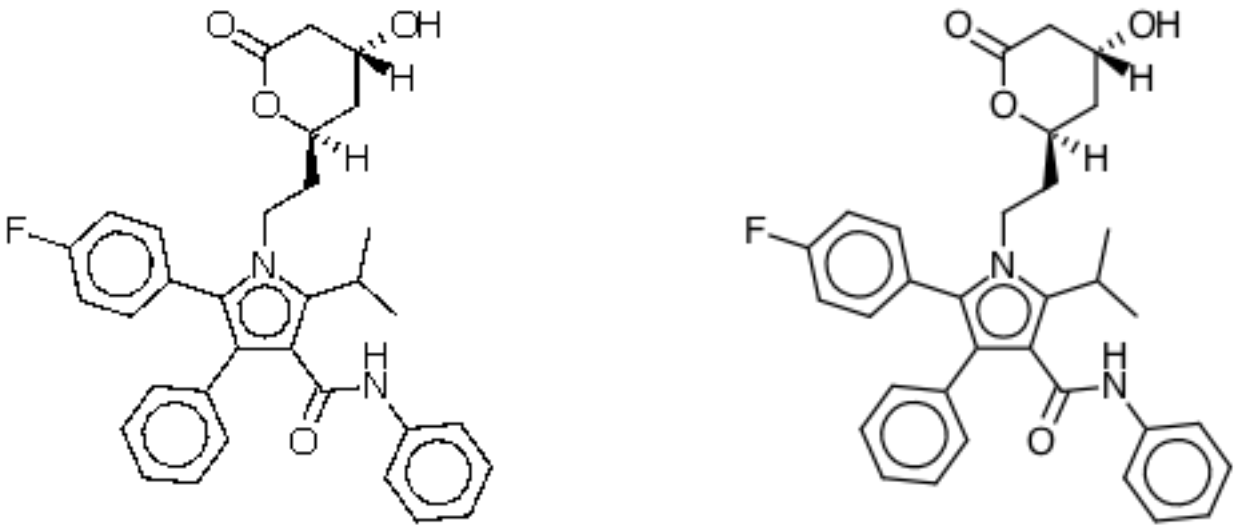
The graphics defined by ChemDoodle are always exact and based on very precise coordinates. However, the screen that you use to display ChemDoodle and bitmap images that are output will need to define the graphics in a much less precise resolution. Algorithms have been developed to minimize the perception of this loss of resolution and ChemDoodle provides full access to control how the graphics are rendered. In contrast, note that scalable vector graphics are exact and based on precise coordinates and are therefore resolution-less. The following settings will only affect the display of graphics on your computer monitor and the output of bitmap graphics; scalable vector graphics will not be affected.

To access these options, select the **Rendering** tab in the **Settings** window.

13.6.1 Anti-aliasing

Anti-aliasing controls whether or not the geometry rendering methods will attempt to reduce aliasing artifacts along the edges of shapes. Anti-aliasing is enabled by default.

A typical anti-aliasing algorithm works by blending the existing colors of the pixels along the boundary of a shape with the requested fill paint according to the estimated partial pixel coverage of the shape. This function reduces the appearance of jagged edges. Figure 13.9a is a structure rendered without anti-aliasing enabled, while Figure 13.9b is a structure rendered with anti-aliasing enabled.



(a) *Anti-aliasing Disabled* (b) *Anti-aliasing Enabled*

Figure 13.9: *Anti-aliasing*

13.6.2 Font fractional metrics

Font fractional metrics controls whether the positioning of individual character glyphs takes into account the sub-pixel accuracy of the scaled character advances of the font or whether such advance vectors are rounded to an integer number of whole device pixels. This hint only recommends how much accuracy should be used to position the glyphs and does not specify or recommend whether or not the actual rasterization or pixel bounds of the glyph should be modified to match. Font fractional metrics are disabled by default to produce better graphics for bitmap images and for the computer screen. In ChemDoodle, this property does not affect printing. Since printing is usually with a high resolution device, ChemDoodle will always enable font fractional metrics for printer rendering.

Rendering text to a low resolution device like a screen will necessarily involve a number of rounding operations as the high quality and very precise definition of the shape and metrics of the character glyphs must be matched to discrete device pixels. Ideally the positioning of glyphs during text layout would be calculated by scaling the design metrics in the font according

to the point size, but then the scaled advance width will not necessarily be an integer number of pixels. If the glyphs are positioned with sub-pixel accuracy according to these scaled design metrics then the rasterization would ideally need to be adjusted for each possible sub-pixel origin.

Unfortunately, scaling each glyph customized to its exact sub-pixel origin during text layout would be prohibitively expensive, so a simplified system based on integer device positions is typically used to lay out the text. The rasterization of the glyph and the scaled advance width are both adjusted together to yield text that looks good at device resolution and has consistent integer pixel distances between glyphs so that the glyphs are uniformly and consistently spaced and readable.

This process of rounding advance widths for rasterized glyphs to integer distances means that the character density and the overall length of a string of text will be different from the theoretical design measurements due to the accumulation of a series of small differences in the adjusted widths of each glyph. The specific differences will vary from glyph to glyph, some being wider and some being narrower than their theoretical design measurements. Thus the overall difference in character density and length will vary with a number of factors including the font, the specific device resolution being targeted, and the glyphs chosen to represent the string being rendered. As a result, rendering the same string at multiple device resolutions can yield widely varying metrics for whole strings.

When font fractional metrics are enabled, the true font design metrics are scaled by the point size and used for layout with sub-pixel accuracy. The average density of glyphs and total length of a long string of characters will therefore more closely match the theoretical design of the font, but readability may be affected since the distance separating individual pairs of characters may not always be consistent depending on how the sub-pixel accumulation of the glyph origins meshes with the device pixel grid. Enabling this hint may be desirable when text layout is being performed that must be consistent across a wide variety of output resolutions. Specifically, this hint may be desirable in situations where the layout of text is being previewed on a low resolution device like a screen for output that will eventually be rendered on a high resolution printer or typesetting device.

When disabled, the scaled design metrics are rounded or adjusted to integer distances for layout. The distances between any specific pair of glyphs will be more uniform on the device, but the density and total length of long strings may no longer match the theoretical intentions of the font designer. Disabling this hint will typically produce more readable results on low resolution devices like computer monitors.



Disabling **Font Fractional Metrics** can lead to more readable text on the computer screen, but will cause adverse effects in the text layout. If you see text overlapping and becoming inconsistent at different scales, make sure this option is re-enabled.

13.6.3 Dithering

Dithering controls how closely to approximate a color when storing to a destination with limited color resolution. Dithering is enabled by default.

Some rendering destinations may support a limited number of color choices which may not be able to accurately represent the full spectrum of colors that can result during rendering operations. For such a destination, dithering controls whether rendering is done with a flat solid fill of a single pixel value which is the closest supported color to what was requested, or whether shapes will be filled with a pattern of colors which combine to better approximate that color.

13.6.4 Rendering algorithm

This setting provides a high level recommendation as to whether to bias algorithm choices more for speed or quality when evaluating tradeoffs. This hint could be consulted for any rendering or image manipulation operation, but decisions will usually honor other, more specific settings in preference to this setting. The rendering algorithm is set to **Quality** by default.

13.6.5 Alpha interpolation algorithm

The alpha interpolation setting is a general setting that provides a high level recommendation as to whether to bias alpha blending algorithm choices more for speed or quality when evaluating tradeoffs. The alpha interpolation algorithm is set to

Quality by default.

This setting controls the choice of alpha blending calculations that sacrifice some precision to use fast lookup tables or lower precision SIMD instructions. This hint could also control whether or not the color and alpha values are converted into a linear color space during the calculations for a more linear visual effect at the expense of additional per-pixel calculations.

13.6.6 Color rendering algorithm

The color rendering algorithm controls the accuracy of approximation and conversion when storing colors into a destination image or surface. The color rendering algorithm is set to **Quality** by default.

When a rendering or image manipulation operation produces a color value that must be stored to a destination, it must first convert that color into a form suitable for storing to the destination image or surface. Minimally, the color components must be converted to bit representations and correctly ordered or an index into a color lookup table must be chosen before the data can be stored to the destination memory. Without this minimal conversion, the data in the destination would likely represent random, incorrect or possibly even unsupported values. Algorithms to quickly convert the results of rendering operations into the color format of most common destinations are well known and fairly optimal to execute.

Simply performing the most basic color format conversion to store colors to a destination can potentially ignore a difference in the calibration of the color space of the source and destination or ignore other factors such as the linearity of the gamma correction. Unless the source and destination color space are identical, to correctly perform a rendering operation with the most care taken for the accuracy of the colors being represented, the source colors should be converted to a device independent color space and the results then converted back to the destination color space. Furthermore, if calculations such as the blending of multiple source colors are to be performed during the rendering operation, greater visual clarity can be achieved if the intermediate device independent color space is chosen to have a linear relationship between the values being calculated and the perception of the human eye to the response curves of the output device.

13.6.7 Stroke control

Stroke control defines whether a rendering implementation should or is allowed to modify the geometry of rendered shapes for various purposes. Stroke control is set to **Best Compromise** by default.

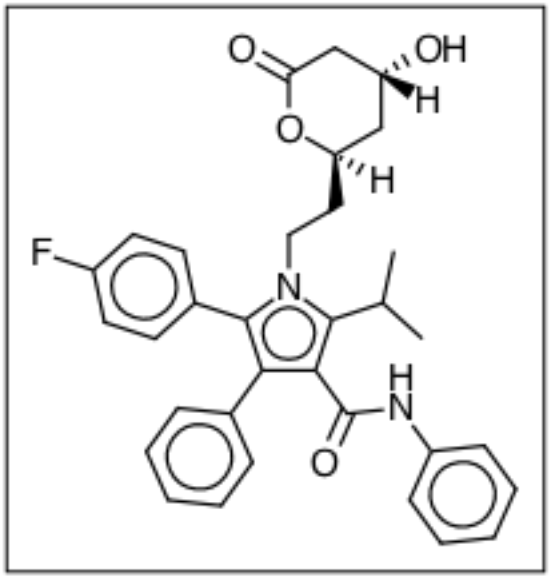
Some implementations may be able to use an optimized platform rendering library which may be faster than traditional software rendering algorithms on a given platform, but which may also not support floating point coordinates. Some implementations may also have sophisticated algorithms which perturb the coordinates of a path so that wide lines appear more uniform in width and spacing.

If an implementation performs any type of modification or "normalization" of a path, it should never move the coordinates by more than half a pixel in any direction.

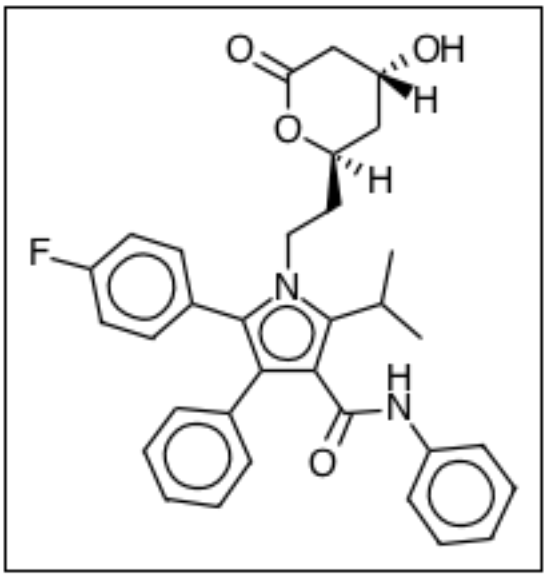
When stroke control is set to **Normalize**, geometry will be altered to improve uniformity or spacing of lines and overall aesthetics. The compromise is that geometry will be offset to fit to the pixel resolution of the rendering device. A consequence is that lines that are parallel may not appear exactly parallel, such as in double bonds.

When stroke control is set to **Pure**, geometry will be left unmodified and rendered with sub-pixel accuracy. There will be noticeable lightness and bolding in straight lines that are vertical or horizontal.

Figure 13.10a shows a rectangle and structure displayed with stroke control set to *Pure*, while Figure 13.10b shows the same objects with stroke control set to **Normalize**.



(a) *A structure and rectangle rendered with stroke control set to Pure. Note the bolding and blurring of the horizontal and vertical lines.*



(b) *A structure and rectangle rendered with stroke control set to Normalize. Note that parallel lines are not preserved and circles are not accurate.*

Figure 13.10: *Stroke Control*

For even better graphics, a third option called **Best Compromise** is provided. This option will use pure stroke control for all chemical structures. All other shapes will first be analyzed for vertical and horizontal lines, and any found will be rendered with normalized stroke control while the rest of the graphics will be rendered with pure stroke control.

13.6.8 Image scaling

Image scaling controls how image pixels are filtered or resampled during an image rendering operation. This will have noticeable effects on images that are not rendered in their natural scale. The image scaling algorithm is set to **Bicubic** by default.

Implicitly images are defined to provide color samples at integer coordinate locations. When images are rendered upright with no scaling onto a destination, the choice of which image pixels map to which device pixels is obvious and the samples at the integer coordinate locations in the image are transferred to the pixels at the corresponding integer locations on the device pixel grid one for one. When images are rendered in a scaled, rotated, or otherwise transformed coordinate system, then the mapping of device pixel coordinates back to the image can raise the question of what color sample to use for the continuous coordinates that lie between the integer locations of the provided image samples. Interpolation algorithms define functions which provide a color sample for any continuous coordinate in an image based on the color samples at the surrounding integer coordinates.

Bicubic is better than **Bilinear** which is better than **Nearest-Neighbor** at producing reasonable graphics of stretched or shrunken bitmap images. The better the algorithm used, the longer the runtime.

CHAPTER 14

Cheminformatics

Contents

14.1 Overview **323**

14.2 References **323**

14.3 Atom properties **324**
14.3.1 Formal charges 324
14.3.2 Lone pairs 324

14.4 Chemical labels **325**
14.4.1 Interpretation 325
14.4.1.1 Abbreviations 325
14.4.1.2 Bond types 326
14.4.1.3 Charges 326
14.4.1.4 Hydrogens 327
14.4.1.5 Fragments 328
14.4.1.6 Formulas 328
14.4.1.7 Linear notations 329
14.4.1.8 Multiplicity 329
14.4.1.9 Repetition 329
14.4.2 Interface functions 330
14.4.2.1 Expanding labels to structures 330
14.4.2.2 Collapsing structures to labels 330

14.5 Chemical suppliers **331**
14.5.1 ChemExper 331
14.5.2 SciFinder-n 331

14.6 Chemical warnings **331**
14.6.1 Warning rendering 331
14.6.1.1 Hiding warning rendering 332
14.6.2 Disabling warnings 332
14.6.2.1 Globally 332
14.6.2.2 For a single object 333
14.6.3 Warning types 333
14.6.3.1 Atoms 333
14.6.3.2 Bonds 334
14.6.3.3 Atom mappings 335
14.6.3.4 Repeat units 335

14.7 Coordinate generation **335**
14.7.1 2D 335
14.7.1.1 Optimizing structures in 2D 335
14.7.2 3D 336
14.7.2.1 Build 3D model 336
14.7.2.2 Universal force field minimization 336
14.7.2.3 Distance geometry embedding 337
14.7.2.4 Flattening atomic coordinates 337

14.8 Covalent bond deduction **337**
14.8.1 Bonding variables 338
14.8.2 Bond order algorithm 338

14.9 Descriptors **339**

14.9.1 Constitutional . . . 339
14.9.2 Topological . . . 340
14.9.3 Physicochemical . . . 341
14.9.4 ADME . . . 341

14.10 Elemental data . . . 342
14.10.1 Viewing the data . . . 342
14.10.2 Interactive periodic table . . . 342
14.10.3 Isotopic data in calculations . . . 344
14.10.3.1 Defining extraterrestrial isotopes . . . 345
14.10.3.2 Elemental analysis . . . 345
14.10.3.3 Isotopic distributions . . . 345
14.10.3.4 Molecular mass calculations . . . 346

14.11 Functional groups . . . 346

14.12 Graph reduction . . . 348
14.12.1 Reduce 0° (lone) . . . 348
14.12.2 Reduce 1° (terminals) . . . 348
14.12.3 Repeatedly reduce 1° . . . 348
14.12.4 Reduce 1° + 0° . . . 348
14.12.5 Reduce 2° (chains) . . . 348
14.12.6 Reduce 2° + 1° + 0° . . . 348

14.13 Hydrogens . . . 348
14.13.1 Implicit hydrogens . . . 348
14.13.1.1 Overriding implicit hydrogen counts . . . 348
14.13.1.2 Hiding implicit hydrogens . . . 349
14.13.1.3 Valence Model . . . 349
14.13.2 Building explicit hydrogens . . . 349
14.13.2.1 Adding hydrogens as atoms . . . 349
14.13.2.2 Removing hydrogens . . . 350
14.13.2.3 Adding hydrogens as text . . . 350
14.13.2.4 Defining when hydrogens are added to carbons . . . 350

14.14 Literature and Patent Searching . . . 351
14.14.1 Google Patents . . . 351
14.14.2 SciFinder-n . . . 351

14.15 Repeat units . . . 351
14.15.1 Repeat values . . . 351
14.15.2 End bond types . . . 352
14.15.3 Embedded repeat units . . . 353
14.15.4 Repeat units in rings . . . 354
14.15.5 Drawing repeat units . . . 355
14.15.6 Expanding repeat units . . . 355

14.16 Resonance systems . . . 357
14.16.1 Representation . . . 357
14.16.2 Aromaticity . . . 357
14.16.2.1 Displaying electron counts . . . 357
14.16.2.2 Circle representations for aromatics . . . 358
14.16.2.3 Forcing aromaticity . . . 358
14.16.2.4 Ambiguously aromatic resonance rings . . . 358
14.16.3 Conjugated chains . . . 359
14.16.4 Kekulé structures . . . 359

14.16.4.1 Kekulizing a single bond frame . . . 360
14.16.4.2 Kekulizing a substructure of resonance bonds . . . 360
14.16.4.3 Delocalizing a Kekulé structure . . . 360

14.17 Ring perception . . . **361**
14.17.1 Supported ring sets . . . 361
14.17.2 Exploding ring sets . . . 362
14.17.3 Performance considerations . . . 362

14.18 Text descriptions . . . **362**
14.18.1 Support . . . 363

14.19 Valence . . . **363**

14.1 Overview

The previous chapters of this guide have discussed how to use ChemDoodle to draw and create images of chemistry. This chapter will go in depth into how ChemDoodle understands and handles that chemistry, not just how it is displayed.

ChemDoodle is powered by an advanced cheminformatics engine that understands chemistry and aids you in handling chemical information. These functions are typically handled behind the scenes in ChemDoodle, so you may not even realize they are being done at all. For example, ChemDoodle perceives rings for all the structures you draw so that double bonds face the inside of rings, and ChemDoodle can understand the stereochemistry of your wedge drawings and warn you when things appear incorrect.

All of the publications that were consulted in the development of the algorithms in ChemDoodle are referenced in the Help 〉 References menu item. It is recommended you go through this list for a deeper understanding of the methods in this software.

This section introduces the new user to the cheminformatics system within ChemDoodle. It covers the following topics:

- How does ChemDoodle understand chemistry?
- The database of elemental data provided in and used by ChemDoodle.
- The cheminformatics algorithms implemented in ChemDoodle.
- How to use and take full advantage of these functions to perform various advanced tasks.
- How to edit your structures in a more advanced way than described in DRAWING CHEMICAL STRUCTURES.
- How to interpret the warning system in ChemDoodle.

14.2 References

All algorithms performed by ChemDoodle and data within ChemDoodle's databases are based on published resources and are referenced from the source it originated from so you may assess its quality. The entire set of references can be viewed at any time by selecting the Help 〉 References menu item as shown in Figure 14.1. Other references used by the iChemLabs development team are also displayed in this list, including filetype specifications and graphics recommendations.

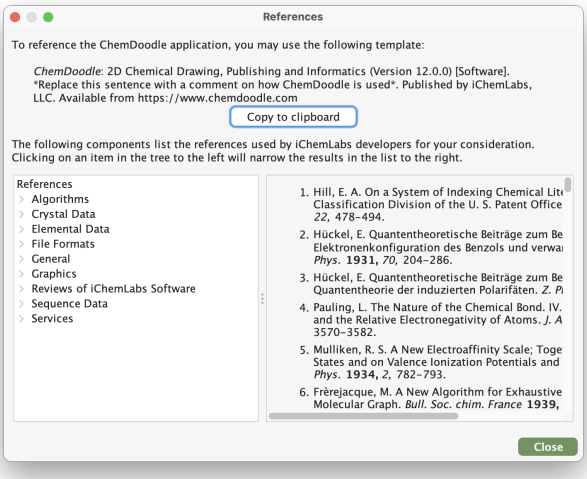


Figure 14.1: *ChemDoodle's References List*

If at any time you are skeptical about the output from ChemDoodle or believe we have done something wrong, please do not hesitate to report it to us. The APPENDIX: TECHNICAL SUPPORT shows how to quickly open a support ticket in ChemDoodle.

14.3 Atom properties

ChemDoodle can automatically determine certain atom properties from the existing molecular structure. Currently, the following properties can be determined:

- Formal charges
- Lone pairs

14.3.1 Formal charges

Although formal charges can be placed on atoms manually, ChemDoodle can also calculate and assign them when the remainder of the molecular structure is complete and correct. All bonds, implicit hydrogen counts, unpaired radical electrons, and lone pairs must be defined.

To calculate and assign formal charges, execute the following steps:

1. Select the atoms whose formal charges you want to calculate.
2. Choose the Structure » Atom Properties » Place Formal Charges menu item.

ChemDoodle will replace the existing formal charge on each selected atom when the calculated value is different. If no formal charges are changed, ChemDoodle will display a warning stating that no changes were made.

14.3.2 Lone pairs

Although lone pairs can be placed on atoms manually, ChemDoodle can also calculate and place the appropriate number of lone pairs when the remainder of the molecular structure is complete and correct. All bonds, implicit hydrogen counts, unpaired radical electrons, and formal charges must be defined.

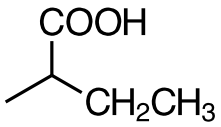
To calculate and place lone pairs, execute the following steps:

1. Select the atoms whose lone pairs you want to calculate.
2. Choose the Structure » Atom Properties » Place Lone Pairs menu item.

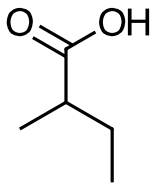
ChemDoodle will adjust the number of lone pairs on each selected atom, adding or removing lone pairs as needed. If no lone pairs are added or removed, ChemDoodle will display a warning stating that no changes were made.

14.4 Chemical labels

Atom labels can be much more than just an element symbol. They may contain hydrogens, formulas, charges, abbreviations and more and any combination. ChemDoodle includes an expert system for working with advanced chemical labels. This section describes how chemical labels are interpretted and the interface functions available to work with them.



(a) *Condensed Chemical Labels*



(b) *Expanded All-atom Model for the Same Structure*

Figure 14.2: *Condensed vs. Expanded Chemical Structures*

14.4.1 Interpretation

Labels that are interpretted chemically will be automatically parsed, rendered and understood by ChemDoodle in a chemical sense. Only atom labels defined with chemical interpretation enabled will be interpretted chemically. Do this by enabling the **Interpret Chemically** button CH_2 when defining your atom label using the **Text for Atoms and Captions** tool A in the **Drawing** toolbar.

14.4.1.1 Abbreviations

Abbreviations can be used to define fragments in atom labels. For instance, the "Ph" abbreviation defines a phenyl group. All supported abbreviations are listed in the **Symbols** widget in the **Abbreviations** section. When expanded, abbreviations will be replaced by the all atom model they define as shown below in the figure on the right.

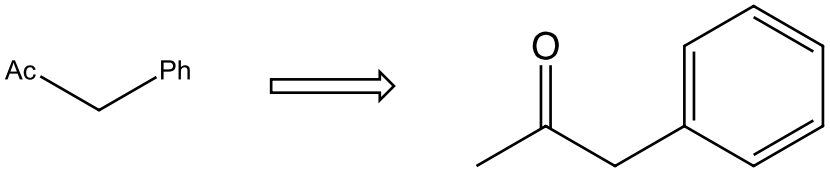


Figure 14.3: *Abbreviations in chemical labels*

ChemDoodle can only expand abbreviations that represent discrete molecules, monovalent or divalent fragments. ChemDoodle will attempt to interpret abbreviations properly based on their valency. For instance, the "CO2" abbreviation with a valency of zero is a carbon dioxide molecule while that same label with a valency of two denotes an ester group.

Adding custom abbreviations Custom abbreviations can be added by executing the following steps:

1. Select the Structure › Abbreviations › Add New… menu item.
2. Type the abbreviation label to be used in atom labels in the **Abbreviation Label** text field.
3. Type the full name of the abbreviation in the **Full Description/Name** text field.
4. Provide the SMILES string for the full atom model of the abbreviation in the **SMILES for Abbreviation** text field. If the valency of the abbreviation is greater than zero, then the attachment atom is the first atom defined by the SMILES string. If the abbreviation is divalent, then the last atom defined in the SMILES string will be used as the second attachment atom.

5. Select the valency of the abbreviation using the **Valency** drop down selection.

6. Press the **Add** button to add the new abbreviation.

ChemDoodle will update to recognize the added abbreviation and when used, that abbreviation will be expanded to the SMILES string defined.

14.4.1.2 Bond types

If no bonds are placed between components in the label, then single bonds are used to connect them.

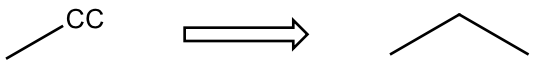


Figure 14.4: *Single bond order in a chemical label*

The "=" (equals) character will specify a double bond connection.

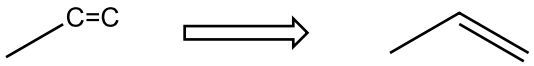


Figure 14.5: *Double bond order in a chemical label*

The "#" (pound) character will specify a triple bond connection.

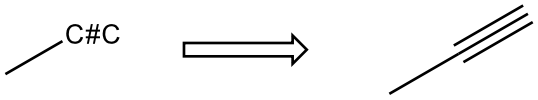


Figure 14.6: *Triple bond order in a chemical label*

Finally, The "$" (dollar) character will specify a quadruple bond connection.

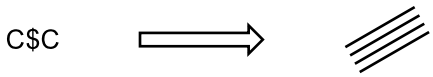
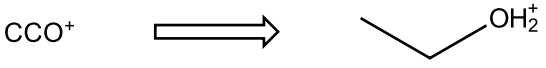


Figure 14.7: *Quadruple bond order in a chemical label*

14.4.1.3 Charges

When a positive or negative symbol is written manually in an atom label, ChemDoodle will interpret that symbol as a positive or negative charge associated with the previous atom. Positive symbols include both plus (+) and circled plus symbols (⊕). Negative symbols include minus (-), en dash (–), emdash (—) and circled minus (⊖) symbols.



(a) *A negative charge in a chemical label*



(b) *A positive charge in a chemical label*

Figure 14.8: *Charge symbols in chemical labels*

If the charge symbol follows a hydrogen, and unless the hydrogen is lone, the charge will be applied to the atom the hydrogen is attached to.

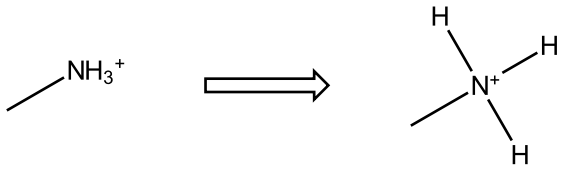


Figure 14.9: *A charge symbol in a chemical label following hydrogen is applied to the atom the hydrogen is attached to.*

If the charge symbol cannot be clearly associated with a previous atom, then it will be applied to the next atom defined.

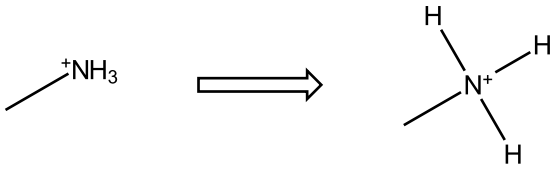


Figure 14.10: *A charge symbol in a chemical label applied to the next element*

A positive integer or "0" stated after a charge symbol will change the magnitude of the charge. Recognized charge values will appear superscripted in labels, with the magnitude displayed before the charge symbol, unless the magnitude of the value is 1, for which only the symbol implies.

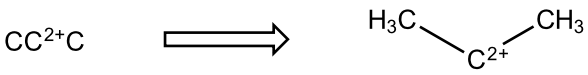


Figure 14.11: *A charge symbol followed by the number 2 (input as "+2") is understood and rendered as a "2+" charge.*

You may also repeat the plus or minus symbol multiple times or combine them.

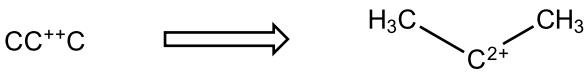


Figure 14.12: *Multiple charge symbols (in this case "++") is understood as a +2 charge.*

14.4.1.4 Hydrogens

Hydrogens can be presented explicitly as chemical text in an atom label. The handling of hydrogens in ChemDoodle is covered extensively in the HYDROGENS section.

When expanded, explicit hydrogens in labels are converted into implicit hydrogens. So the label "NH2" will become an "N" label when expanded with an implicit hydrogen count of 2. The label "CH5" will become an "C" label when expanded with an implicit hydrogen count of 5.

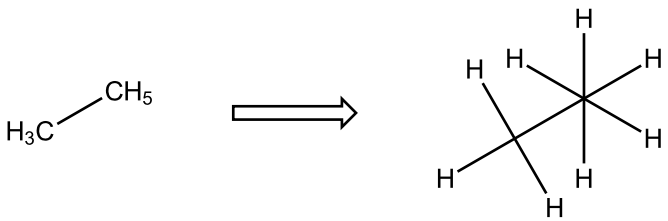


Figure 14.13: *Hydrogen counts explicitly defined in chemical labels will be enforced*

14.4.1.5 Fragments

A fragment may be defined with a breaking character. Acceptable breaking characters include space ( ), period (.) and bullet (•) characters.

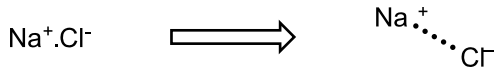


Figure 14.14: *A period character (.) is used to denote fragmentation*

You may also use any combination of breaking characters to define a fragmentation.



Figure 14.15: *A space ( ) and bullet (•) character pair is used to denote fragmentation*

ChemDoodle will also try to understand when fragmentation is not explicitly defined, but implied, when resolving connections between charged atoms.

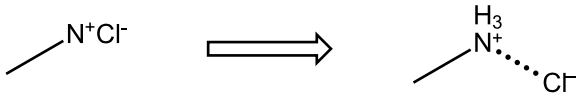


Figure 14.16: *ChemDoodle understands the connection between the nitrogen and chlorine atoms is an implied fragmentation*

14.4.1.6 Formulas

Sometimes you may wish to enter a chemical formula directly into an atom label, for instance, to calculate the molecular mass of an isomer without drawing its complete structure. When a formula is entered, ChemDoodle will associate the atom with the elemental composition of the molecular formula and construct an appropriate chemical representation as best it can, as shown in Figure **??**. Calculations based solely on elemental composition, such as molecular mass, will therefore be correct. However, ChemDoodle cannot determine which specific isomer you intend, so calculations that depend on structure may not produce the expected results. For accurate structural results, draw the all-atom structure or use a non-formula label.

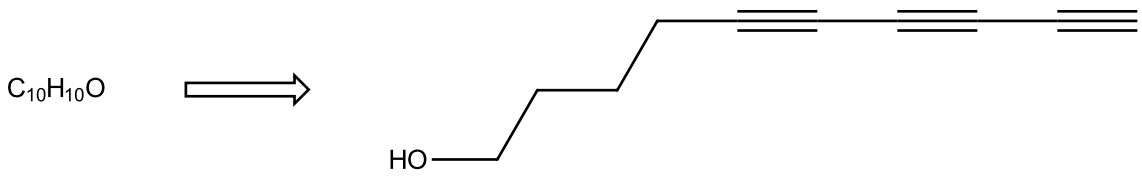


Figure 14.17: *ChemDoodle expands a molecular formula to an isomer all-atom model.*

ChemDoodle recognizes and validates molecular formulas using the following rules:

- There are no spaces in the string.
- Only valid elemental labels, numbers and the plus (+) and minus (-) characters are present in the string.
- Each element is only expressed once in the string.
- The maximum value for an element multiplicity is 1000. This is to avoid performance issues.
- The charge must be defined at the end of the string.

Molecular vs. radical formulas If a chemically interpretted atom label is input with a formula, it may be interpretted by ChemDoodle as either a molecular formula or a radical formula.

In order for a chemically interpretted atom label to be recognized as a radical formula, the atom must have a bond attached to it. Radical formulas must start with a carbon label and the second token must be a number. So "C3F7" will be recognized as a perfluoropropyl radical. ChemDoodle will also interpret labels terminating with a radical formula, such as "OC2H5". Keep in mind radical formulas can be ambiguous, and ChemDoodle will only be able to match the elemental composition of the formula; ChemDoodle will not be able to know which isomer you prefer.

Hydrogens in formulas ChemDoodle will handle hydrogen counts from formulas. This is done by intelligently saturating the structure to remove hydrogens, matching the input value. This way, when you enter a formula, an appropriate molecular data structure is defined for processing. For instance, if you input "C6H6", not only will ChemDoodle recognize this as a molecule containing exactly six carbons and six hydrogens, but if you calculate the *degree of unsaturation* of this label, ChemDoodle will produce the value 4. Make sure to input the correct number of hydrogens in your formulas, as that is exactly the number of hydrogens (both implicit and explicit) that will be present in the resolved structure. To illustrate this, if you input the lone label "C2H5", the output structure will contain a methyl group connected through a single bond to another carbon atom with only 2 implicit hydrogens defined.

The only exception to this rule is when handling radical formulas, or an atom label that contains a formula that is connected by a bond to another atom. In these cases, one valence spot on the attachment atom is reserved for the bond connection, replacing a potential hydrogen spot.

Charges in formulas ChemDoodle will handle charges in formulas. The charge will be assigned to the heaviest atom in the formula. No attempt is made to provide any particular valid structure, just to satisfy the formula input. When defining charges in formula labels, be sure to put the magnitude of the charge after the charge symbol and not before. So a chromate ion should be defined as "CrO4-2", not "CrO42-". The later denotes 42 oxygens to ChemDoodle.

14.4.1.7 Linear notations

Stringing elements together will place them in a chain, so "CCCC" or "CH2CH2CH2CH3" denotes a *n*-butyl group.

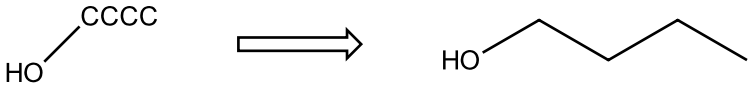


Figure 14.18: *Linear notation in chemical labels*

14.4.1.8 Multiplicity

Using parentheses (not at the start of the label) will denote multiple attachments, so the label "C(CH3)3" will denote a *t*-butyl group.

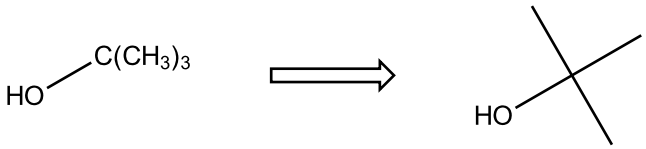


Figure 14.19: *Multiplicity in chemical labels*

14.4.1.9 Repetition

Using parentheses to begin a label will denote a repeating chain, so "(CH2)4" will represent four-carbon methylene chain.



Figure 14.20: *Repetition in chemical labels*

If this label is attached to two bonds, the two bonds will be placed on opposite ends.



Figure 14.21: *Two bonds connected to a chemical label of a repeating unit will be attached at both ends of the expanded structure.*

14.4.2 Interface functions

Use the following interface functions to quickly convert between all-atom models and more concise chemical labels.

14.4.2.1 Expanding labels to structures

To automatically expand labels, execute the following steps:

1. Select the atoms with labels to be expanded using any of the selection tools.
2. Select the Structure » Expand Labels menu item.

14.4.2.2 Collapsing structures to labels

The reverse of expanding labels can also be done, this is called label collapsing. This can be done automatically by ChemDoodle or manually.

Automatically ChemDoodle can automatically collapse your drawn structures to labels, including custom abbreviations that you have defined. This can help you quickly condense drawn structures. To do so, executing the following steps:

1. Select the structure you would like to collapse using a selection tool.
2. Select the Structure » Auto-Collapse to Labels menu item.

Manually You can replace a certain fragment in your structure with a custom label that can later be expanded to the original fragment. To do so, executing the following steps:

1. Select the part of the structure you would like to collapse using a selection tool.
2. Select the Structure » Collapse to Labels menu item.
3. An atom label text field will appear, type the desired label and format the label if required.
4. Click anywhere else in the document or press the escape key to close the text field and set the condensed label.

Using the Structure » Expand Labels menu item on this collapsed label will then expand it back to its original structure. Keep in mind that this label only represents this single collapsed fragment, and other typed labels with the same text will not represent the same fragment.

14.5 Chemical suppliers

Two partner services are available through ChemDoodle:

- **ChemExper** - No account needed.
- **SciFinder-n** - Account login required. (*ChemDoodle 2D only for now!*)

14.5.1 ChemExper

To search for chemical suppliers for the structures you draw using ChemExper, execute the following steps:

1. Draw the structure for which you would like to search.
2. Select the structure with a selection tool.
3. Expand the File › Interfaces › ChemExper menu item.
4. Select the Substructure Match or Exact Match menu item depending on whether you want to search for a substructure or exact match for the selected structure.
5. The ChemExper database will appear in your default browser with a listing of matches. Select the match to view the chemical suppliers.

The ChemExper database provides the supplier information and you must abide by their terms of use and any copyrights or disclaimers presented when using their service.

14.5.2 SciFinder-n

To search for chemical suppliers for the structures you draw using SciFinder-n, please refer to APPENDIX: THIRD PARTY APPLICATIONS.

14.6 Chemical warnings

ChemDoodle will check your structures and provide warnings for questionable objects, which are rendered as red flags over the corresponding objects in the structure. Chemical warnings are only flags displayed by the software, and will never appear in any image output or printouts. However, they should act as "red flags" and bring your attention to issues in drawn chemical data, as there may be incompatibility with cheminformatics functions. For instance, if you have an unknown label on a chemical structure, you will not be able to calculate a molecular mass for the structure.

14.6.1 Warning rendering

A warning is rendered on a chemically interpreted object (atom, bond, repeat unit, etc.) as a transparent red rectangle with a number on the top right as shown in Figure 14.22. The number corresponds to an associated note that describes the warning. If multiple warnings are assigned to an atom, all of the numbers will be listed in the red rectangle, separated by commas.

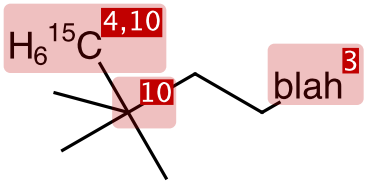


Figure 14.22: *Chemical warnings as rendered on atoms*

The warning descriptions will always be rendered at the top left of the document as shown in Figure 14.23. You can disable the rendering of warning descriptions by deselecting the **Display Warning Descriptions** checkbox in the **Settings** window under the **Warnings** tab.

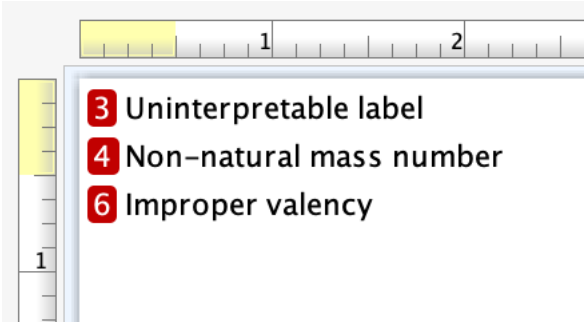


Figure 14.23: *Explanations for chemical warnings*

14.6.1.1 Hiding warning rendering

Chemical warnings will never appear in any image output or printouts.

If the rendering of warnings bothers you and clutters the document while drawing, they can be immediately suppressed by selecting the View > Hide Warnings menu item.

14.6.2 Disabling warnings

You may choose to disable warnings for a single object, or globally for all content in ChemDoodle.

14.6.2.1 Globally

Chemical warnings can be enabled/disabled individually in the **Settings** window under the **Warnings** tab as shown in Figure 14.24. This tab also contains an option to enable/disable the display of chemical warning explanations at the top-left of the document in which the warnings are present.

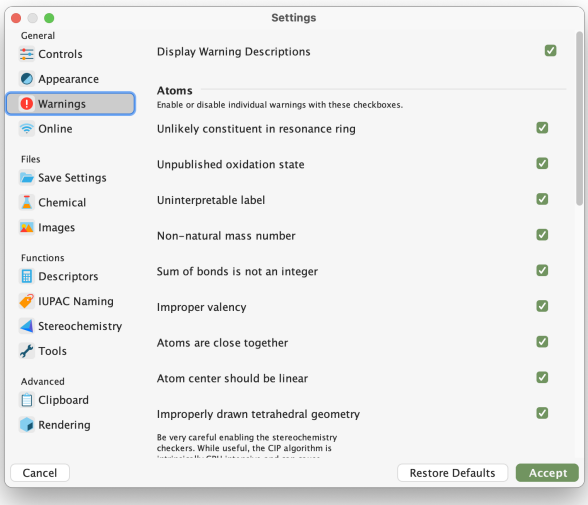


Figure 14.24: *Chemical Warnings*

14.6.2.2 For a single object

To disable warnings for a single chemically interpreted object, execute the following steps:

1. Hover the chemically interpreted object with the warning shown to be disabled.
2. Right-click on the hovered object and select the Disable Warnings menu item.

To enable warnings for a chemically interpreted object where warnings are currently disabled, simply right-click on the object after hovering it and select the Check for Warnings menu item. If no warnings are found, a confirmation message will display to notify you, as shown in Figure 14.25.

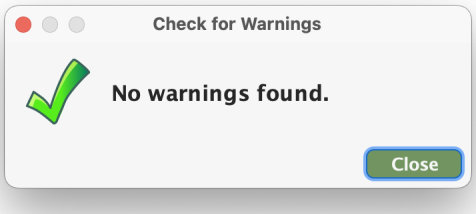


Figure 14.25: *No chemical warnings found*

14.6.3 Warning types

Warnings can be associated with any chemically interpreted objects.

14.6.3.1 Atoms

The following atom warnings are currently checked:

- **Unlikely constituent in a resonance ring** - The atom is not a resonance system contributor as drawn. For instance, it may not be sp^2 hybridized.

- **Unpublished oxidation state** - The oxidation state of this atom is not found in ChemDoodle's database of published oxidation states for the element.
- **Uninterpretable label** - ChemDoodle does not understand or interpret the text present in the atom label as chemically relevant.
- **Non-natural mass number** - This mass number is not found in ChemDoodle's database of published isotopes for the element.
- **Sum of bonds is not an integer** - The coordination number of this atom is not a whole number.
- **Improper valency** - It is unlikely that this element can have the current coordination number. Or the atom label is an abbreviation and the valency is overextended.
- **Atoms are close together** - This pair of atoms has very similar coordinates and will be perceived as a single atom in graphical output.
- **Atom center should be linear** - The geometry of the atom should be linear, but there is too much of a bend in the drawing.
- ***Improperly drawn tetrahedral geometry** - This center has exactly four unique attachments, but given how the bonds have been laid out or selected as wedge bonds, no configuration can be assigned.
- ***Not a stereocenter** - Wedge bonds are provided on a center that is not a stereocenter. ChemDoodle will be able to differentiate these cases from perspective structures.
- ***Stereocenter needs wedge bonds defined** - This warning will appear on centers that are detected as being a possible stereocenter, but no wedge bonds are provided.
- ***Both wedge and wavy bonds defined** - This warning will appear on potential stereocenters when both wedge and wavy bonds are attached, which makes no sense.



Be very careful enabling the stereochemistry checkers (marked with asterisks). While useful, the CIP algorithm is intrinsically CPU intensive and can cause ChemDoodle to run slowly. For this reason, they are disabled by default.

14.6.3.2 Bonds

The following bond warnings are currently checked:

- **Ambiguous double type is discouraged** - While some cheminformatics systems may use the ambiguous (crossed) double bond, IUPAC recommendations discourage any use of ambiguous double bonds.
- ***Trans configuration unlikely in small ring** - This double bond is drawn in a *trans* configuration, which is unlikely in a small ring. Instead, draw it with a *cis* configuration.
- ***Improperly drawn rectangle geometry** - Each side of the double bond has one or two unique attachments, but given how the attached bonds have been laid out around the double bond, no configuration can be assigned.
- ***Not an atropisomer** - Wedge bonds are provided on a bond center that is not a stereocenter. Wedges only make sense for bond centers in an atropisomer. ChemDoodle will be able to differentiate these cases from perspective structures.
- ***Atropisomer needs wedge bonds defined** - This warning will appear on atropisomer center bonds that are detected as being a possible atropisomer, but no wedge bonds are provided.
- ***Wavy bond should not connect stereocenters** - IUPAC recommendations forbid wavy bonds (defining unknown configuration) between two stereocenters, as the resulting figure would be ambiguous.
- ***No stereocenter connected to wavy type** - When a wavy bond is connected to a potential stereocenter, it specifies the configuration of that stereocenter as undefined. This warning will appear for wavy bonds not connected to any

potential stereocenter. Lone wavy bonds (which are sometimes used as bond breakers), will not be flagged.

14.6.3.3 Atom mappings

The following atom mapping warnings are currently checked:

- **Mapping between atoms within same structure** - This mapping correlates two atoms within the same structure, which may or may not be intended.
- **Overlapping atom maps** - Two or more atom mappings contain the same atom, which is unlikely to be intended.
- **Mapping is on one side of a reaction** - Both atoms in the mapping are on the same side of the reaction (*i.e.* both are reactant atoms or both are product atoms).

14.6.3.4 Repeat units

The following repeat unit warnings are currently checked:

- **End bond orders do not match** - Repeat units define a substructure that repeats linearly in the chemical structure. As such, it must be that each of the two brackets in a repeat unit reside on bonds sharing identical bond orders. If not, the repeat unit is invalid and will not be able to be expanded.
- **Disconnected brackets** - A repeat unit defines a substructure of a chemical structure, which is not possible if the two brackets reside on bonds in different chemical structures.
- **Units exactly overlap** - There are two repeat units that define the exact same substructure of a chemical structure. The multiples are likely a mistake.
- **Units partially intersect** - The contents of two repeat units partially intersect, which is an invalid state for either of the two repeat units, and neither will be able to be expanded.
- **A ring split exists within the unit** - If a repeat unit exists within a ring system, both brackets must be on bonds participating in exactly 1 ring each and both bonds must be part of the same exact ring. Otherwise, the repeat unit is ambiguous and will not be able to be expanded because repeat units define a linear repetition.
- **Repeat multiplicity must be a positive integer or 0** - Repeat units can only be expanded in positive whole numbers. A value of zero cuts the substructure from the chemical structure.

14.7 Coordinate generation

ChemDoodle can generate 2D and 3D coordinates for structures.

14.7.1 2D

The goal of 2D coordinate generation is to produce a graphic of a chemical structure that is aesthetically pleasing on a page and follows certain layout rules that are standard amongst chemists communicating chemical structures. 2D coordinate generation does not consider physics when choosing positions. The z-coordinate will be ignored and set to a 0 value in ChemDoodle.

14.7.1.1 Optimizing structures in 2D

If your structures do not have acceptable or aesthetic coordinates, ChemDoodle can clean them. To clean your structures, execute the following steps:

1. Select the structures to be cleaned.
2. Select the Structure » Clean » Beautify Structure Drawing menu item or press the **Optimize Structures in 2D** button  in the **Chemistry** toolbar.

ChemDoodle employs the published Clark algorithm for cleaning structures. This method is a statistical approach. Therefore, repeated applications of the function may produce different results. If you are not happy with the first result of the function, try it again, something you like better may be generated.

There are two options in the **Settings** window under the **Tools** tab that will modify how 2D cleaning works:

- **Clean Retains Stereochemistry** - By default, this option is enabled and will make sure that stereocenters after the clean have the same configuration as before the clean.
- **Chain Angle** - This option allows you to define the chain angle used. 120° is selected by default and is preferred for skeletal figures, while 180° is useful for drawing Lewis Dot Structures and other educational figures.

14.7.2 3D

The goal of 3D coordinate generation is to produce a physical model of the molecule that is consistent with observed measurements of real molecules. These are typically ab initio based approaches and can sometimes take a long time to run, if a molecule is very large or complex.



Keep in mind that methods that rely on properly mapping the chemistry of the atoms, like 3D coordinate generation, rely on the structure being a valid chemical model. If you do not have a valid chemical model (using sextuple bonds between oxygens or having an uninterpretable label), then the results will not be available.

After 3D coordinates have been produced for your structure, you can rotate the structure in 3D using the **Rotate in 3D** tool  in the **Content** toolbar.

14.7.2.1 Build 3D model

This is a very fast and high-quality template-based approach to generating 3D coordinates. Stereochemistry is retained. Hydrogens will be added appropriately.

This function uses the NIH Cactus service, and will require an internet connection. To use this method, execute the following steps:

1. Ensure you have a valid internet connection.
2. Select the structures to generate 3D coordinates for.
3. Select the Structure › Clean › Build 3D Model (NIH Cactus) menu item.

The structures will update to use their new 3D coordinates.



The NIH Cactus service may be down for any number of reasons. You can verify by trying to get to the NIH Cactus website (https://cactus.nci.nih.gov). If this is the case, please try again later and it will likely be back up.

14.7.2.2 Universal force field minimization

Force fields are the typically method for producing 3D coordinates. This is an ab initio approach that sets a force field to your structure and minimizes that force field to produce the smallest potential energy, hopefully resulting in an ideal conformation. Force field approaches attempt to find a local minimum in the potential energy landscape, but are not guaranteed to find the absolute minimum. Hydrogens will be added appropriately.

ChemDoodle has built in support for force fields and minimization. To use this method, execute the following steps:

1. Select the structures to generate 3D coordinates for.
2. Select the Structure » Clean » Universal Force Field Minimization menu item.

The structures will update to use their new 3D coordinates. For larger and more complex structures, please give this method some extra time.



For advanced force field functions and tools for building molecules in 3D, see the ChemDoodle 3D product: https://www.chemdoodle.com/3d

14.7.2.3 Distance geometry embedding

Distance geometry embedding sets 3D coordinates for a structure based on a regression of its bond distance matrix. This function works best on highly embedded structures such as fullerenes, carbon nanotubes and cage-like ring systems such as adamantane or norbornane. To use this method, execute the following steps:

1. Select the structures to generate 3D coordinates for by distance geometry embedding.
2. Select the Structure » Clean » Distance Geometry Embedding (3D) menu item.

The structures will update to use their new 3D coordinates.

14.7.2.4 Flattening atomic coordinates

In cases where your structures or imported chemical data contains 3D coordinates and you do not want them to have z-coordinates, you can set all the z-coordinates to zero by selecting those structures and choosing the Content » Flatten menu item.

14.8 Covalent bond deduction

Commonly, molecule data files do not include any bond information. Files including *PDB*, *XYZ* and output from quantum mechanics programs do not officially store bond data. Instead of having to draw bonds by hand, ChemDoodle contains tools for deducing covalent bonds based on just the atom elements and 3D coordinates alone. ChemDoodle can even assign bond orders to those bonds based on several algorithms.

To deduce covalent bonds, execute the following steps:

1. Select the atoms that you would like covalent bonds deduced between.
2. Select the Structure » Deduce Covalent Bonds... menu item.
3. A window will appear as shown in Figure 14.26.

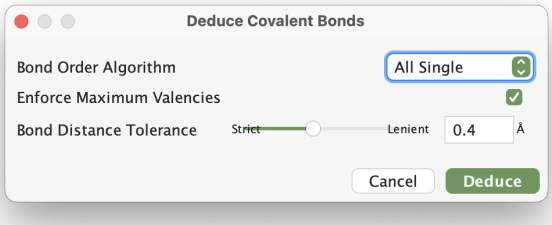


Figure 14.26: *Deduce Covalent Bonds Window*

4. Define the settings as appropriate and press the **Deduce** button.

The deduced bonds will be added to the selected atoms. If no bonds are found, a warning message will appear and you may modify the settings, if necessary, to try again. Bonds and the orders already defined to the selected atoms will not be modified by this function.

14.8.1 Bonding variables

The initial step in deducing covalent bonds involves analyzing the distances between the atoms and determining which distances are candidates for a bond. This determination uses published atomic covalent radii. Covalent radii are a best fit from a large number of experimentally observed covalent radii. For more flexibility, a **Bond Distance Tolerance** option is provided. By default, the value is .4 Ångströms. Increase this value to discover bonds at longer distances, and decrease this value to make the bond deduction more strict.

The bond deduction algorithm will enforce maximum valencies by default. So if 5 different bonds containing the same carbon atom are all of an acceptable distance, then the least likely of the bonds will be discarded. Maximum valencies are more difficult to evaluate for metal centers. To disable this behavior and allow as many bonds as possible, deselect the **Enforce Maximum Valencies** check box.

14.8.2 Bond order algorithm



While many algorithms for bond order deduction employ advanced techniques to reduce runtime, the runtime for this part of the function will scale exponentially and may take a very long time to complete if there are a large number of bonds to analyze. If you do not care about bond orders and simply want to generate the topology quickly, select the **All Single** option.

ChemDoodle has the ability to assign bond orders to the deduced bonds. Several algorithms are available:

- **All Single** - No further bond order evaluation is made, all deduced bonds will be single bonds.
- **Antechamber** - The Antechamber algorithm for the AMBER system is employed to deduce bond orders.
- **Auto-UFF** - The Auto-UFF algorithm deduces bond orders based on UFF atom types, as described by Artemova *et al.*

14.9 Descriptors

ChemDoodle calculates a large number of molecular descriptors. The descriptors are currently categorized into four types: constitutional, topological, physicochemical and ADME.



All of these descriptors are based on published methods, and they are all empirical methods. While our implementations are accurate to the methods provided for the results in the publications, that does not mean that they will correspond accurately at all to experimental results. Be sure to review the references in ChemDoodle thoroughly before using these calculations.

When using either the Structure » Descriptors menu items or displaying calculations in updating labels, you can control the decimal resolution of the calculation (for fractional output) by changing the **Resolution** slider in the **Calculations** section of the **Descriptors** panel of the **Settings** window. You can suppress the unit designation at the end of the calculation output by deselecting the **Include Unit** checkbox in the same section.

14.9.1 Constitutional

Constitutional descriptors are based on the makeup of the molecule, such as atom counts and molecular formula. The following constitutional descriptors are provided:

- **Atom Count** - The number of atoms in a molecule.
- **Bond Count** - The number of bonds in a molecule.
- **Degree of Unsaturation** - The sum of all bond orders less one for each, plus the number of rings.
- **Element Counts** - The number of each element that is present in a molecule.
- **Cyclomatic Number** - The fundamental ring count. Also known as the cyclomatic number or the SSSR count.
- **Euler Facet Ring Count** - The count of all Euler facets in a molecule. This is defined as all of the sides of the 3D shape that is created by expanding the 2D structure on a 3D sphere.
- **Exhaustive Ring Count** - The total number of graph cycles present in the molecule.
- **Hydrogen Bond Acceptor Count** - Counts the number of atoms with lone pairs capable of hydrogen bonding.
- **Hydrogen Bond Donor Count** - Counts all nitrogens, oxygens and fluorines that have hydrogens attached.
- **Nominal Mass** - Calculates the mass of a molecular ion or molecule calculated using the isotope mass of the most abundant constituent element isotope of each element rounded to the nearest integer value and multiplied by the number of atoms of each element.
- **Rotatable Bond Count** - Counts all saturated bonds. Exceptions are single bonds connected to hydrogens or terminal atoms, single bonds of amides, thioamides, sulphonamides and those connecting two hindered aromatic rings (having at least three ortho substituents).
- **Total Electron Count** - Counts all electrons in a molecule taking into account charges.
- **Lightest Isotopic Mass** - Calculates the lightest isotopic mass by summing the lightest isotope for each atom given its element.
- **McGowan Characteristic Volume** - Calculates the vdW volume using McGowan's method.
- **Molecular Mass** - Calculates the molecular mass from atomic masses based on the IUPAC technical reports.
- **Monoisotopic Mass** - Calculates the monoisotopic mass from isotopic masses based on the IUPAC technical reports.

- **Volume as a Sum of Atomic and Bond Contributions** - Calculates the VABC vdW volume.
- **Empirical Formula** - Generates the empirical formula for the molecule. The empirical formula is just the molecular formula, where all element multiplicities have been divided by the greatest common denominator.
- **Molecular Formula** - Generates the molecular formula for the molecule in the form of $C_xH_y\ldots$ where … denotes all other elements and their counts in alphabetical order. This is based on the Hill system, so if no carbon atoms are present, the hydrogen count will be in alphabetical order with the rest of the elements.

14.9.2 Topological

Topological descriptors are solely based on the connectivity between atoms in a molecule, such as a bond distance matrix. The following topological descriptors are provided:

- **Centric Index** - Calculates the Centric index for the molecule (Bonchev *et al.*).
- **Diameter** - Calculates the longest topological distance in a molecule.
- **Hosoya Index** - Calculates the Hosoya index for the molecule.
- **Molecular Topological Index** - Calculates the Molecular Topological index for the molecule (Schultz *et al.*).
- **Platt Index** - Calculates the Platt index for the molecule.
- **Ring Complexity** - Calculates the Ring Complexity for the molecule.
- **Szeged Index** - Calculates the Szeged index for the molecule.
- **Wiener Index** - Calculates the Wiener index for the molecule.
- **Zagreb Indexes** - First and second order calculations are supported. (Z_1, Z_2)
- **Balaban Index** - Calculates the Balaban index for the molecule.
- **Bertz Complexity Index** - Calculates the Bertz Complexity index for the molecule.
- **Branching Index** - Calculates the Branching index for the molecule. The Branching index is equivalent to ${}^1\chi$.
- **Chi Molecular Connectivity Indexes** - Indexes from zeroth to third order are supported. Both simple and valence models are calculated. (${}^0\chi$, ${}^1\chi$, ${}^2\chi$, ${}^3\chi$, ${}^0\chi_v$, ${}^1\chi_v$, ${}^2\chi_v$, ${}^3\chi_v$)
- **Fraction Molecular Framework** - Calculates the Fraction Molecular Framework (fMF) ratio for the molecule.
- **Harary Index** - Calculates the Harary index for the molecule.
- **Kappa Shape Indexes** - Indexes from the first to third order are supported. Both simple and alpha models are calculated. (${}^1\kappa$, ${}^2\kappa$, ${}^3\kappa$, ${}^1\kappa_\alpha$, ${}^2\kappa_\alpha$, ${}^3\kappa_\alpha$)
- **Superpendentic Index** - Calculates the Superpendentic index for the molecule.
- **Adjacency Matrix** - Generates a matrix *M* of size $A \times A$, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals one if there is a bond connecting atoms *i* and *j*, and equals zero otherwise.
- **Bond Distance Matrix** - Generates a matrix *M* of size $A \times A$, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals the shortest bond distance between atoms *i* and *j*.
- **Bond Electron Matrix** - Generates a matrix *M* of size $A \times A$, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals the number of electrons shared between atoms *i* and *j*.
- **Detour Matrix** - Generates a matrix *M* of size $B \times A$, where , where B is the number of bonds in the molecule and A is the number of atoms in the molecule. $M(B_i, A_j)$ equals one if bond *i* contains atom *j*, and zero otherwise.
- **Incidence Matrix** - Generates a matrix *M* of size $A \times A$, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals the longest bond distance between atoms *i* and *j*.

- **Laplacian Matrix** - Generates a matrix M of size $A \times A$, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals one if there is a bond connecting atoms i and j and equals zero otherwise. $M(i, i)$ equals the number of bonds connected to atom A_i.

14.9.3 Physicochemical

Physicochemical descriptors describe the physical or chemical properties of a molecule. These are estimations of their real physical values. The following physicochemical descriptors are provided:

- **Average Molecular Polarizability** - Estimates the average molecular polarizability. Both the average hybrid components (Miller) and average hybrid polarizabilities (Kang) methods are implemented.
- **Critical Pressure** - Estimates the critical pressure (P_c) of a substance based on Joback's method.
- **Critical Temperature** - Estimates the critical temperature (T_c) of a substance based on Joback's method.
- **Critical Volume** - Estimates the critical volume (V_c) of a substance based on Joback's method.
- **Enthalpy of Formation** - Estimates the enthalpy of formation ($\Delta H^0_{f,298}$) of a substance (ideal gas at 298K) based on Joback's method.
- **Enthalpy of Fusion** - Estimates the enthalpy of fusion (ΔH_f) of a substance based on Joback's method.
- **Enthalpy of Vaporization** - Estimates the enthalpy of vaporization (ΔH_{vb}) of a substance (at T_b) based on Joback's method.
- **Gibbs Energy of Formation** - Estimates Gibbs energy of formation ($\Delta G^0_{f,298}$) of a substance (ideal gas, unit fugacity, at 298K) based on Joback's method.
- **Heat Capacity** - Estimates the heat capacity (C^0_p) of a substance (ideal gas) based on Joback's method.
- **Lipophilicity ($\log P$)** - Estimates the octanol/water partition coefficient ($\log P$) of a substance. The NC+NHET, AlogP98, and XlogP v2.0 (Wang) algorithms are implemented.
- **Liquid Viscosity** - Estimates the liquid viscosity (η_L) of a substance (at 298K) based on Joback's method.
- **Molar Refractivity** - Estimates the molar refractivity of a substance. Both the CMR3 and AMR algorithms are implemented.
- **Normal Boiling Point** - Estimates the normal boiling point (T_b) of a substance based on Joback's method.
- **Normal Freezing Point** - Estimates the normal freezing point (T_f) of a substance based on Joback's method.
- **pKa** - Estimates the acid dissociation constant on a logarithmic scale, where $\mathrm{p}K_\mathrm{a} = -\log_{10}(K_\mathrm{a})$, using the SMARTS $\mathrm{p}K_\mathrm{a}$ method.
- **Solubility ($\log S$)** - Estimates the solubility ($\log P$) of a substance using the Hou method.
- **Topological Polar Surface Area** - Estimates the topological polar surface area (TPSA) of a molecule with the algorithm developed by Ertl *et al.*

14.9.4 ADME

Descriptors that rank bioactivity of drugs (ADME is an acronym for *absorption*, *distribution*, *metabolism*, and *excretion*):

- **Bioavailability Score** - Calculates the bioavailability score (Martin).
- **Egan Violations Count** - Calculates the number of violations to Egan's rules.
- **Lipinski's Rule of 5 Violations Count** - Counts the number of violations to Lipinski's rule of 5.
- **Veber Violations Count** - Calculates the number of violations to Veber's rules.

14.10 Elemental data

The built-in elemental database allows ChemDoodle to perform many tasks, from filling the dynamic periodic table to deducing covalent bonds to calculating a molecular mass. The data itself can be viewed by opening various data tables in ChemDoodle or by using the dynamic periodic table.

14.10.1 Viewing the data

The data tables are found in the View menu. Currently ChemDoodle provides three data tables:

- **Elemental Data** - Displays all data in the elemental database not contained in other tables.
- **Ionization Energies** - Displays ionization energies for the elements.
- **Isotopes** - Displays isotopes, their masses, natural abundances and half-lives.

Each table is interactive, and you can click on a column header to reorder the content by that column. By clicking again you can reverse the order of that column. By pressing down on the header and dragging, you can reorder the columns to more easily correlate different columns.

14.10.2 Interactive periodic table

ChemDoodle contains an interactive periodic table of elements for reference, printing and demonstrations. It is viewable by selecting the View » Interactive Periodic Table menu item. The window that opens is shown in Figure 14.27.

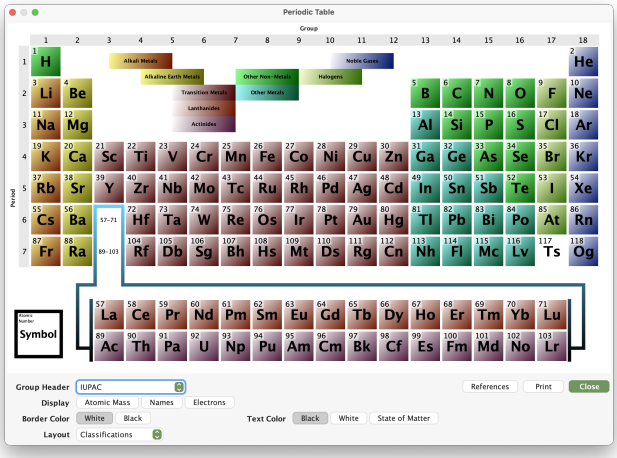


Figure 14.27: *The Interactive Periodic Table*

You may hover over elements and click on them for additional information. There may also be classifications listed in the top region. Hovering over a classification will desaturate all other classifications. This is shown in Figure 14.28 when the mouse pointer hovers over the **Other Non-Metals** classification.

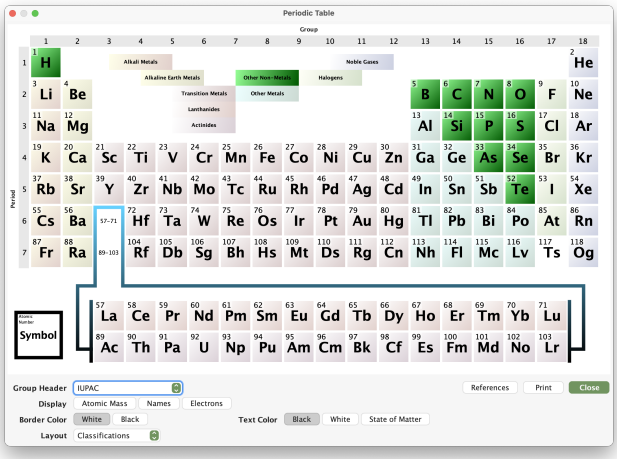


Figure 14.28: *Focusing on a classification*

The table is customizable and you can choose from several format options, including the **Display** of atomic mass, names and electron configurations in addition to the element symbol. The block in the bottom-left corner of the periodic table will display the current format of each element box as shown in Figure 14.29.

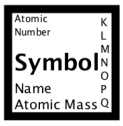


Figure 14.29: *Element Format*

You may define which designation is used for the **Group Header**:

- **IUPAC**
- **Mendeleev (I-VIII)**
- **CAS (US, A-B-A)**
- **old IUPAC (Europe, A-B)**

You can also customize graphical options, such as the element **Border Color** and **Text Color**.

In addition to the traditional **Classifications** display, you can also choose to display these other features of the elements:

- **CPK Colors** - Displays each element with its CPK (Corey, Pauling, Koltun) color.
- **Rasmol Colors** - Displays each element with its Rasmol color.
- **Jmol Colors** - Displays each element with its Jmol color.
- **PyMOL Colors** - Displays each element with its PyMOL color.
- **State of Matter** - Each element is colored based on its state of matter at the set temperature. Solids are black, liquids are blue and gases are red. Unknown states are grey. A temperature slider will appear in the controls to set the temperature which is displayed on the top right of the table.
- **Years of Discovery** - Each element is colored if discovered before the set year of discovery. A year slider will appear in the controls to set the year of discovery which is displayed on the top right of the table.

Each display format shows off interesting properties and makes for great in-class demonstrations, such as the **State of Matter** display shown in Figure 14.30.

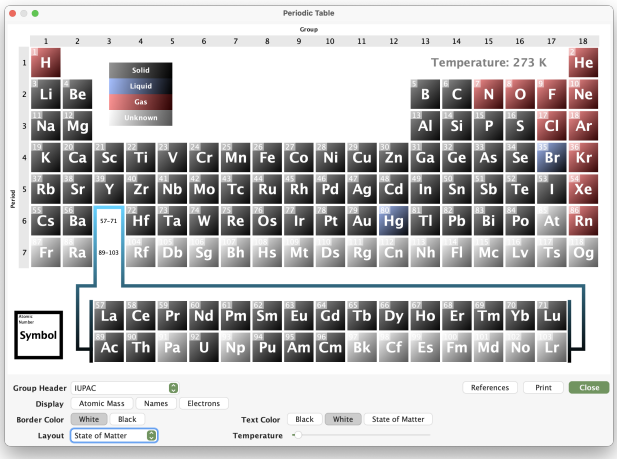


Figure 14.30: *States of Matter Display*

If you click on any of the elements in the periodic table, additional information about that element will be displayed as shown in Figure 14.31.

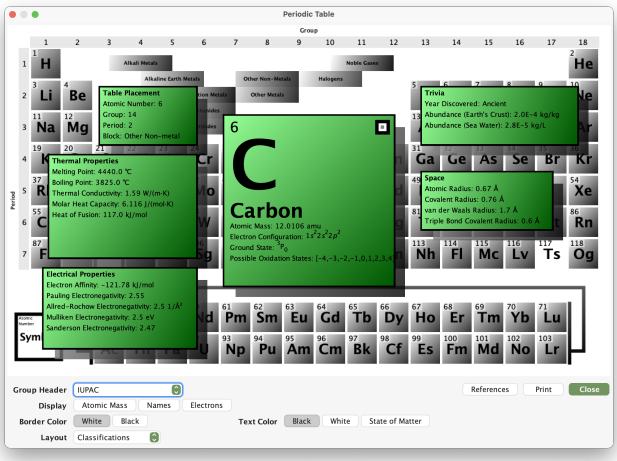


Figure 14.31: *Additional information for carbon*

To print the periodic table, click the **Print** button at the bottom-right of the window. The **References** button will display ChemDoodle's references and the **Close** button will close the **Periodic Table** window.

14.10.3 Isotopic data in calculations

The elemental database used by ChemDoodle is derived from the sources listed in the program references, see the REFERENCES section. Isotopic data is notably important as any elemental analysis calculation is dependent on the experimentally measured masses, given we cannot calculate an isotopic mass directly from the number of protons, neutrons and electrons present in the atom. The isotopic data in ChemDoodle includes both isotopes with natural abundance on planet Earth and those that are not naturally found on planet Earth. Therefore, molecular mass and elemental analysis calculations can be performed on molecules containing a wide range of isotopes. Keep in mind, if an isotope with no mass data is defined in a molecule,

ChemDoodle will be unable to perform elemental analysis calculations for that molecule. The follow sub-sections describe the various functions in ChemDoodle where this is important.

14.10.3.1 Defining extraterrestrial isotopes

In the ISOTOPES section, we show how to specify isotope values on atoms. Isotopes with no natural abundance on Earth (including tritium, ^{3}H) will be excluded from the default list that appears. To set a mass value to an isotope with no natural abundance on Earth, use the Mass Number ⟩ Other... menu item after right-clicking on the specific atom you wish to define the isotope value to.

14.10.3.2 Elemental analysis

The Elemental Analysis widget is described in the ELEMENTAL ANALYSIS WIDGET section. If an isotope with no mass data is included in the focused molecular structure, the only possible output will be the molecular formula. The Elemental Analysis widget will show a warning message in the Elemental Analysis section stating which isotope(s) there is no data for as shown in Figure 14.32.

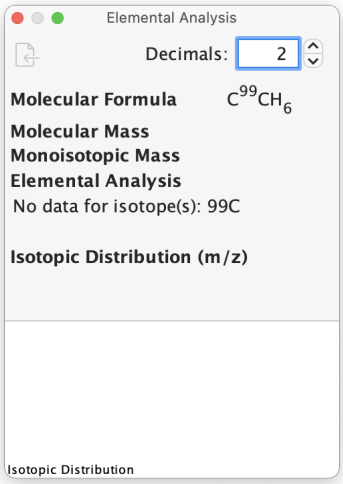


Figure 14.32: *How the Elemental Analysis widget handles an isotope with no mass data*

14.10.3.3 Isotopic distributions

Isotopic distributions are covered in MASS SPECTROMETRY (MS) SIMULATIONS section. If a mass parent peak is generated for a chemical structure including an isotope with no mass data, the following error stating which isotope(s) there is no data for will appear as shown in Figure 14.33.

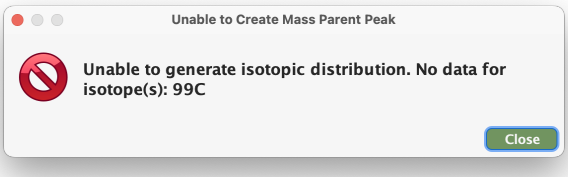


Figure 14.33: *Generating a mass parent peak for a chemical structure including an isotope with no mass data will show this error*

14.10.3.4 Molecular mass calculations

Any mass (molecular, monoisotopic, etc.) calculations on chemical structures containing an isotope with no mass data will output "NaN", to signify the input is not valid. Any further calculations using the "NaN" value will fail.

14.11 Functional groups

ChemDoodle may be used to automatically highlight the functional groups present in drawn structures. To do so, perform the following steps:

1. Select the molecule(s) where the functional groups should be automatically highlighted.
2. Choose the Structure » Highlight Functional Groups… menu item.
3. A window will appear as shown in Figure 14.34. Using the **Algorithm** dropdown, select the algorithm you wish to use to highlight functional groups. You may select the **Analyze Structures Individually** checkbox if you wish to process each selected structure separately.

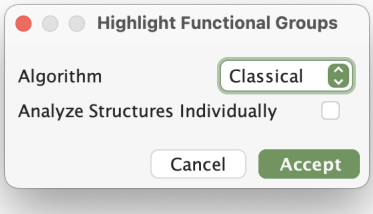
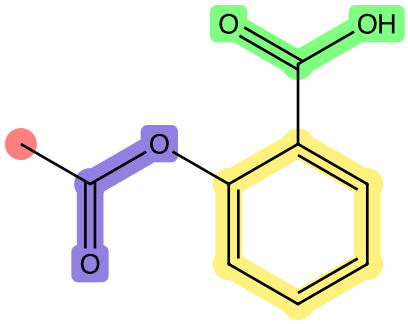


Figure 14.34: *Options for the Highlight Functional Groups function.*

4. Press the **Accept** button to execute the function.

Each functional group of a specific type will be highlighted in the same color. A table will also appear below the selected structure(s) listing the included functional groups and the corresponding highlight color as shown in Figure 14.35.



Color	*Functional Group*
	Alkane
	Aromatic
	Carboxylic Acid
	Ester

Figure 14.35: *Functional groups for the structure of aspirin are automatically highlighted.*

There are currently two types of algorithms available for functional group highlighting:

1. **Classical** - Based on classical definitions of functional groups. The produced table will also list the names of the functional groups highlighted.

2. **Ertl** - Based on the Ertl algorithm for functional group perception. This algorithm does not name functional groups, it instead attempts to perceive and generalize any functional groups present in a structure, regardless of their novelty. The produced table will also list the number of occurances of each functional group in the selected structures.

If the **Analyze Structures Individually** checkbox is selected when this function is executed, each individual structure in the selection will be highlighted separately and have its own associated table produced.



This function is meant to be performed on all-atom structures only. If there are any condensed labels included in the analyzed structure, such as “CH2CH3”, “COOH” or “Ph”, those labels will be classified as **Unknown** or ignored. You may quickly expand condensed labels for a structure by selecting the structure and executing the Structure 〉 Expand Labels menu item.

14.12 Graph reduction

To reduce molecule graphs, execute the following steps:

1. Select the structure with the graph you would like to be reduced.
2. Expand the Structure ⟩ Graph Reduction submenu and select the preferred reduction method.

14.12.1 Reduce 0° (lone)

Will remove all selected atoms that have no bonds attached.

14.12.2 Reduce 1° (terminals)

Will remove all selected atoms that have only one bond attached to them. This process will stop after the first iteration.

14.12.3 Repeatedly reduce 1°

Will remove all selected atoms that have only one bond attached to them. This process will continue until it has pruned all terminal chains from the selection.

14.12.4 Reduce 1° + 0°

Will remove all selected lone and terminal atoms.

14.12.5 Reduce 2° (chains)

Will remove all chains from a molecule, leaving single bonds connecting any remaining 3° atoms.

14.12.6 Reduce 2° + 1° + 0°

Will remove all lone, terminal and chain atoms, leaving a simplified core that represents the embedded ring structure of a graph.

14.13 Hydrogens

Hydrogens do not need to be drawn on structures as they are implicitly declared. At any time, hydrogens can be added to a structure as text in atom labels or as atoms with bonds attached. ChemDoodle employs an advanced system for handling hydrogens, whether implicit or explicit. You can also manually control how many implicit hydrogens are assigned to an atom and even hide implicit hydrogens from rendering.

14.13.1 Implicit hydrogens

Implicit hydrogens are important in completing the understand of chemical diagrams. When drawing structures, most chemists will understand how many hydrogens should be on an atom, and drawing them explicitly will crowd the figure, so they are implied. However, there may be times when you will need to control this behavior.

14.13.1.1 Overriding implicit hydrogen counts

You may manually define the number of implict hydrogens assigned to an atom. This is convenient for structures that you need to modify the valence for but do not wish to drawn explicit hydrogen atoms, such as metal complexes. To manually change the implicit hydrogen count on an atom, executing the following steps:

1. Hover the atom with implicit hydrogens to set.
2. Right-click on the atom.
3. Expand the Implicit Hydrogens submenu.
4. Select the menu item corresponding to the number of implicit hydrogens you wish to set to the atom.

You can reset the implicit hydrogen count by right-clicking on the hovered atom and selecting the Implicit Hydrogens > Auto menu item.

14.13.1.2 Hiding implicit hydrogens

By default, implicit hydrogens are automatically rendered on any element labels and appropriate abbreviations that are visible. To disable the auto-rendering of implicit hydrogens, uncheck the **Show Implicit Hydrogens** style in the **Hydrogens** section of the **Atoms** tab of the **Styles** window.

You can also disable the auto-rendering of implicit hydrogens for a specific atom by executing the following steps:

1. Hover the atom with implicit hydrogens to remove.
2. Right-click on the atom.
3. Select the Hide Implicit Hydrogens menu item.

This will stop the auto-rendering of implicit hydrogens on that atom. To restore the implicit hydrogen auto-rendering, follow the same steps as above, but choose the Show Implicit Hydrogens menu item.

Keep in mind, that even though the rendering of the implicit hydrogens has been disabled, the implicit hydrogen count will still be the same value internally for that atom, even if it is not rendered. To modify the implicit hydrogen count, please see the OVERRIDING IMPLICIT HYDROGEN COUNTS section.

14.13.1.3 Valence Model

ChemDoodle implements the MDL valence model, as defined in the *Chemical Representation* document from MDL/Symyx/Accelrys/BIOVIA, which instructs the default calculation of implicit hydrogen counts.

There are two versions of the MDL valence model, **Modern** and **Legacy**. The legacy MDL valence model defines valency for many non-organic elements, leading to covalent models where implicit hydrogens are placed on those elements. The only metal atom to have a valency for implicit hydrogens in the modern MDL valence model is aluminum with a charge of -1 (valence of 4).

By default, ChemDoodle uses the modern MDL valence model, but you may switch to the legacy model if you choose by changing the **MDL Valence Model** option in the **Settings** window in the **Tools** tab, in the **Hydrogens** section. Reasons to use the legacy model include remaining consistent with legacy MDL CT files (*.mol*, *.rxn*, etc.) and allowing a neutral pentavalent nitrogen center to support legacy drawings of pyridine-*N*-oxide compounds.

14.13.2 Building explicit hydrogens

ChemDoodle provides features for building hydrogens on structures both as explicit atoms and as text in labels.

14.13.2.1 Adding hydrogens as atoms

To add hydrogens to a structure as atoms as shown in Figure 14.36, execute the following steps:

1. Select the structure to add hydrogens to.
2. Select the Structure > Add/Remove Hydrogens > From Selection menu item. You can also use the **Add/Remove Hydrogens** button  in the **Chemistry** toolbar.

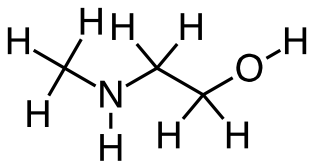


Figure 14.36: *Hydrogens Added as Atoms*

14.13.2.2 Removing hydrogens

To remove hydrogens from a structure, execute the following steps:

1. Select the structure to remove hydrogens from.
2. Select the Structure » Add/Remove Hydrogens » From Selection menu item. You can also use the **Add/Remove Hydrogens** button  in the **Chemistry** toolbar.

When using the remove hydrogens functions, explicit hydrogen atoms will be retained for the following cases:

1. Hydrogens with an explicitly defined mass number, including a value of 1.
2. Hydrogens with an explicitly defined charge value.
3. Lone hydrogen atoms.
4. Hydrogens connected to more than one atom.
5. Hydrogens connected by a bond order that is not equal to 1
6. Hydrogens in all atom-models of molecular hydrogen.
7. Hydrogens connected to a stereocenter by a wedge bond.

14.13.2.3 Adding hydrogens as text

To add hydrogens as text into atom labels as shown in Figure 14.37, change the **Add as** setting in the **Hydrogens (Add/Remove)** section in the **Settings** window, under the **Tools** tab, to **Text**. After doing so hydrogens will be explicitly added as text when using the **Add/Remove Hydrogens** functions.

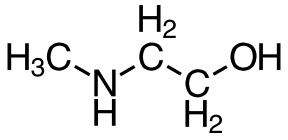


Figure 14.37: *Hydrogens Added as Text*

14.13.2.4 Defining when hydrogens are added to carbons

You can modify how explicit hydrogens are added to carbon atoms: whether they are always added, only added to lone isolated carbons, only added to hidden carbons (such as those between two bonds forming a 180° angle), or never added to carbons. These options are available in the **Styles** window, under the **Atoms** tab, in the **Carbons** section.

14.14 Literature and Patent Searching

Two partner services are available through ChemDoodle:

- **Google Patents** - No account needed.
- **SciFinder-n** - Account login required.

14.14.1 Google Patents

To search for relevant patents and non-patent literature for the structures you draw using Google Patents, please refer to APPENDIX: THIRD PARTY APPLICATIONS.

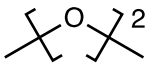
14.14.2 SciFinder-n

To search literature for the structures you draw using SciFinder-n, please refer to APPENDIX: THIRD PARTY APPLICATIONS.

14.15 Repeat units

Repeat units are used to define linearly repeating substructures in molecules. A repeat unit consists of a pair of square brackets denoting the substructure to be repeated and a repeat value defining how many times the substructure is repeated. Most conveniently, when properly defined in chemical structures in ChemDoodle, repeat units are automatically recognized, evaluated and expanded so you can quickly draw complex structures and perform cheminformatics tasks such as calculating molecular masses and formulas.

To demonstrate, Figure 14.38 shows the molecular formula generated in ChemDoodle for a dimethyl peroxide structure, where the two oxygens in the peroxide are defined by a single oxygen within a repeat unit of value 2. You can see the molecular formula of $C_2H_6O_2$ is correct.



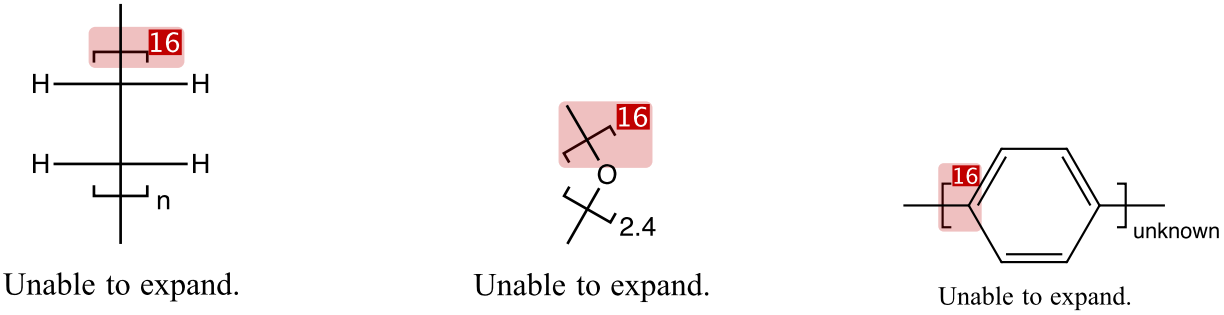
$C_2H_6O_2$

Figure 14.38: *Repeat units are automatically interpreted*

See the REPEAT UNIT BRACKETS section of the SHAPES chapter for instructions to create and edit repeat units in ChemDoodle.

14.15.1 Repeat values

As a graphics application, ChemDoodle will allow you to create any graphic you desire, and you can associate any value with a repeat unit. However, only a positive integer or zero is appropriate, and any other value will be flagged as invalid. Repeat units show chemical warnings just like atoms and bonds in ChemDoodle. See the CHEMICAL WARNINGS section for more information. Figure 14.39 shows several repeat unit values that cannot be expanded as they are not positive integers or zero.



(a) *Repeat value is a variable* (b) *Repeat value is a fraction* (c) *Repeat value is not a number*

Figure 14.39: *Examples of invalid repeat unit values*

For invalid cases, no expansion by the system is possible, as expected, and any output will either be an error or will have ignored the invalid repeat unit(s). In Figure 14.39, ChemDoodle states it is unable to expand these structures and no molecular formula is displayed.

So it is important to always use a positive integer when defining repeat units if you want the associated structure to be handled properly by the cheminformatics engine. You may also use a value of zero (0), which essentially cuts the substructure out of the molecule. For instance, Figure 14.40 shows the molecular formula for our dimethyl peroxide structure becomes C_2H_6 when we change the repeat unit value to 0. The oxygen is simply cut out of the structure entirely, and when the two ends are connected together, we are left with ethane.

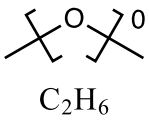


Figure 14.40: *Repeat values of 0 cut out the contained substructure*

14.15.2 End bond types

A repeat unit is only valid if the bond order is the same for both bonds assigned to the brackets in the repeat unit. Up until this section, all examples have shown repeat units where both ends are single bonds, which will not impose any issues. Repeat units can exist between two different types of single bonds, as long as they are both single bonds. For instance, Figure 14.41 shows a stereocenter where a protruding bond starts a repeat unit. This is valid as long as the closing bond in the repeat unit is also a single bond, which it is in this case.

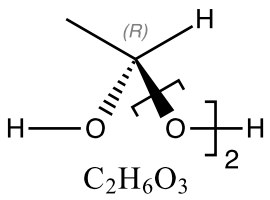


Figure 14.41: *A stereo bond can start a repeat unit as long as the closing bond is a single bond*

We can also use bond orders other than 1, Figure 14.42 shows a valid repeat unit where both ends are double bonds.

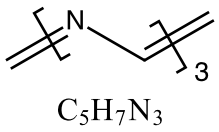


Figure 14.42: *Repeat unit on a substructure where both ends are double bonds*

Figure 14.43 shows an invalid repeat unit where one end is a single bond and the other end is a triple bond. There is no logical way to expand this repeat unit.

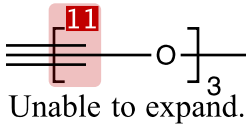


Figure 14.43: *Repeat unit bond ends must have the same bond order*

14.15.3 Embedded repeat units

Embedded repeat units are valid in ChemDoodle as long as there are no partial intersections. To demonstrate, Figure 14.44 shows how to represent a trimer of nylon 6/6 drawn with 3 repeat units. The two methylene repeat units are both embedded in the outer repeat unit.

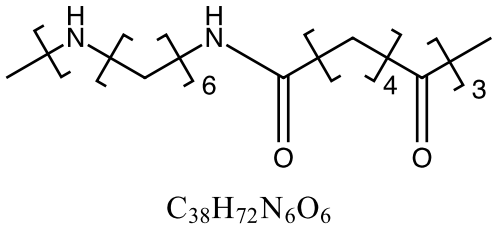


Figure 14.44: *A trimer of nylon 6/6 drawn with 3 repeat units, 2 of which are embedded in the third*

It is also convenient to note the inner repeat units in nylon 6/6 are simple enough to be described with chemical labels instead (CHEMICAL LABELS), if you choose, as shown in Figure 14.45.

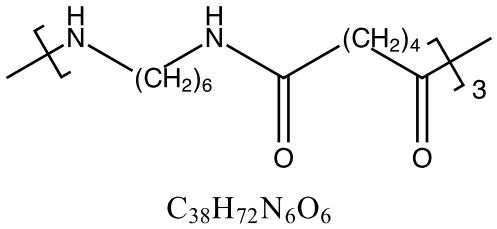


Figure 14.45: *You may mix condensed labels with repeat units*

It is not acceptable for two repeat units to partially intersect, as shown in Figure 14.46. Such repeat units will be flagged as invalid.

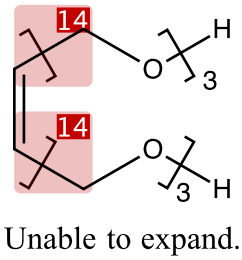


Figure 14.46: *Partially intersecting repeat units are invalid*

Two exactly overlaping repeat units are also not acceptable and will also be flagged as invalid, as shown in Figure 14.47. Instead, delete one of the repeat units, and add the repeat value of the repeat unit being deleted to the one being retained.



Figure 14.47: *Exactly overlapping repeat units are invalid*

However, it is acceptable for the embedded repeat unit to share only one bond with the repeat unit it is embedded in as shown in Figure 14.48.

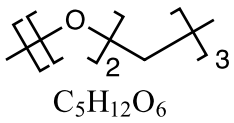


Figure 14.48: *An embedded repeat unit that shares one bond with the outer repeat unit is valid*

14.15.4 Repeat units in rings

Repeat units are allowed in rings, as long as their definition is unambiguous. In the simplest case, you have only a single ring as shown in Figure 14.49. There are two directions a repeat unit can be defined in a ring. To flip a repeat unit to contain the other side of the ring, hover the repeat unit with a selection tool, right-click and select the Flip Repeat Unit menu item.

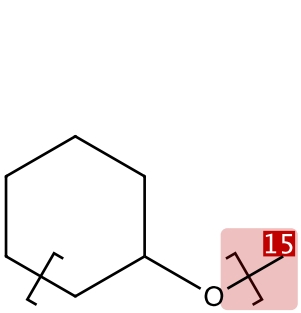


(a) *The oxygen is the only atom in the repeat unit*

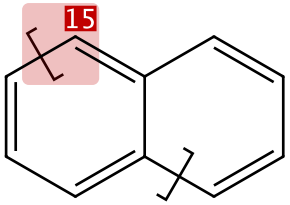
(b) *Only the carbons compose the repeat unit*

Figure 14.49: *There are two directions for a repeat unit in a ring*

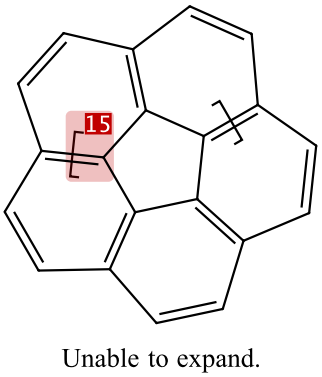
This case is unambiguous. However, you can introduce ambiguity if you define a repeat unit where a path can connect both sides of a bracket without using the bond the bracket is associated with (a ring split to an outer atom exists within the bracket contents). These cases mostly occur in fused ring systems. These ambiguous repeat units will not be able to be expanded and are invalid. Figure 14.50 shows some ambiguous repeat units where a ring split occurs.



(a) *One side is in a chain, while the other is in a ring*



(b) *An ambiguous repeat unit within naphthalene*



(c) *An ambiguous repeat unit at the center of corannulene*

Figure 14.50: *Examples of ambiguous repeat units*

As a rule of thumb, to define a valid repeat unit in a ring, both ends of the repeat unit must be on bonds that exist in 1 and only 1 ring each, and both of those bonds must be in the same exact ring. Figure 14.51 demonstrates a valid repeat unit in a fused ring system.

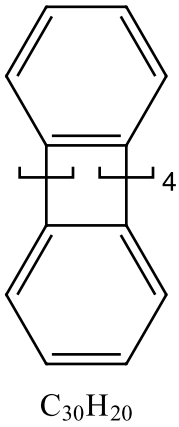


Figure 14.51: *Repeat units are possible in fused ring systems*

14.15.5 Drawing repeat units

The drawing and editing of repeat units is covered in the REPEAT UNIT BRACKETS section of the SHAPES chapter.

14.15.6 Expanding repeat units

ChemDoodle can expand a repeat unit into an all-atom model. To do so, perform the following steps:

1. Hover the mouse pointer over the brackets of the repeat unit you wish to expand so the brackets are outlined in an amber color.

2. Right-click on the hovered repeat unit and select the Expand Repeat Unit menu item.

On successful expansion, you will see the all-atom model and the repeat unit will be removed from the structure. For chains, the coordinates of the repeating substructure will be propogated linearly as shown in Figure 14.52.

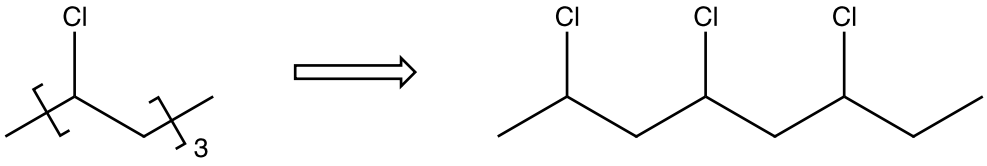


Figure 14.52: *Expanding a repeat unit*

When expanding ring based repeat units, there is no good place to insert the repeated substructure, so the complete structure will be cleaned after the expansion as shown in Figure 14.53.

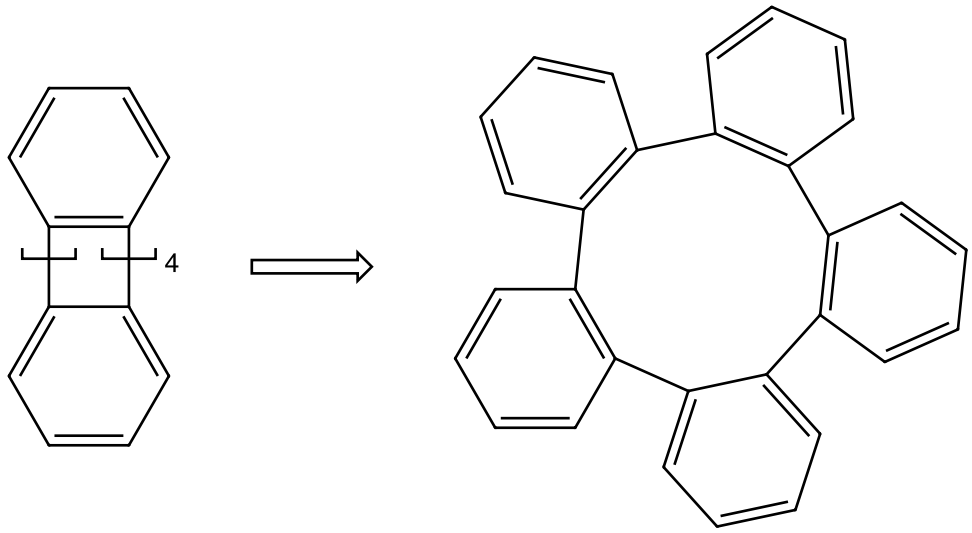


Figure 14.53: *Expanding a ring based repeat unit*

If the repeat unit is invalid, you will see the following error message and the repeat unit will not be expanded.



Figure 14.54: *Invalid repeat units cannot be expanded*

You will also see an error message if you attempt to expand a repeat unit containing another repeat unit. Make sure to expand any inner repeat units before expanding outer repeat units.

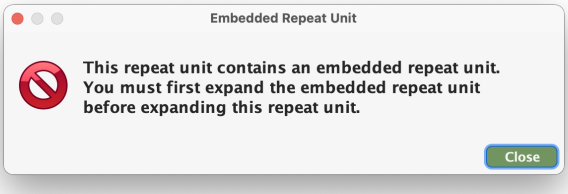


Figure 14.55: *Inner repeat units must be expanded before outer repeat units*

14.16 Resonance systems

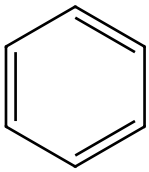
Resonance systems are expertly modeled in ChemDoodle. The most important resonance systems are aromatics. Many tools are provided for specifying resonance and converting to other models.

14.16.1 Representation

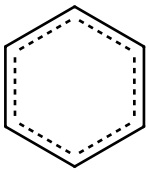
Resonance systems can be rendered in several different ways in ChemDoodle:

- **Kekulé** - All bonds are explicitly typed. Multiple Kekulé structures exist for the same molecule.
- **Delocalized** - All or most bonds are defined as resonance bonds.
- **Aromatic Circles** - This representation is reserved only for aromatic rings, and a circle replaces all bond order information.

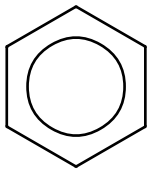
The different ways of representing benzene are seen in Figures 14.56.



(a) *Kekulé Model*



(b) *Delocalized Model*



(c) *Aromatic Circle*

Figure 14.56: *Aromatic Representations*

ChemDoodle will recognize all three of these models as aromatic benzene.

14.16.2 Aromaticity

Aromaticity is detected based on the Hückel model. Electron contributions are calculated based on an extended *SMILES Aromaticity Model*, and therefore any appropriately hybridized heteroatoms can be constituents in an aromatic ring. All rings are assumed to be planar.

14.16.2.1 Displaying electron counts

ChemDoodle calculates the number of electrons present in resonance rings, to evaluate the ring for aromaticity based on the Hückel model. You can view the results of this calculation for aromatic and anti-aromatic rings by enabling the **Display Electron Count** style in the **Styles** window in the **Rings** tab. The electron count for aromatic rings will be displayed in the center of the ring as shown in Figure 14.57. Anti-aromatic rings will show a negative symbol in front of the count to

denote an anti-aromatic ring. Using this feature, you can see which rings ChemDoodle considers as aromatic, anti-aromatic or non-aromatic.

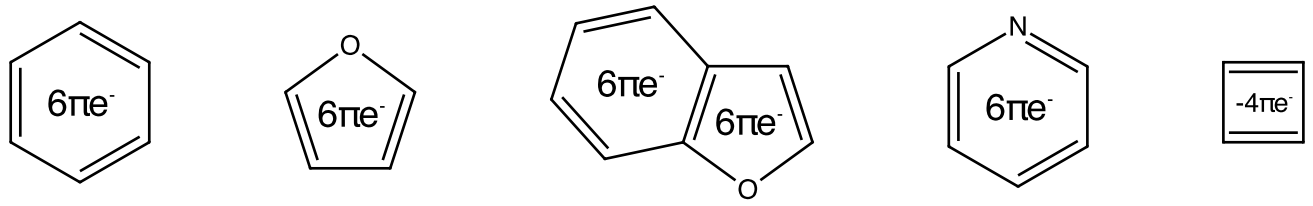


Figure 14.57: *Showing aromatic and anti-aromatic electron counts*

14.16.2.2 Circle representations for aromatics

To toggle between viewing aromatics with circles or not, execute the following steps:

1. Open the **Styles** window.
2. Select the **Rings** tab.
3. Select the preferred setting for the **Use Circles for Aromatics** style under the **Aromatics** section based on your preference.

The **Always** option will render circles for all aromatics. The **Resonance Bond Rings Only** option will render circles only for rings completely defined by resonance bonds. The **Never** option will never render aromatic circles. Use this style for full control over the aromatic ring representations in your figures.

14.16.2.3 Forcing aromaticity

In rare cases, ChemDoodle may determine a ring to have no aromatic character when it should be aromatic for some purpose. To force a ring to be recognized as aromatic, change all of the ring bonds to *resonance* bonds.

You should also use all *resonance* bonds to define an aromatic ring that you want to be represented by an aromatic circle in mixed structures, such as when displaying a Kekulé benzene next to a benzene represented by an aromatic circle.

14.16.2.4 Ambiguously aromatic resonance rings

In simple aromatic resonance rings, there is no question what the explicit bond types or implicit hydrogen counts should be. For instance, in benzene, we know that the double bonds should alternate and each carbon is assigned a single implicit hydrogen. However, this quickly becomes difficult to assess when fused ring systems with heteroatoms are involved. Imidazole is a good example. Nitrogen can have either 0 or 1 implicit hydrogens in aromatic rings as shown in the Kekulé representation in Figure 14.58. But when this ring is fully defined using delocalized resonance bonds, it is no longer clear where the double bonds or implicit hydrogens should go.

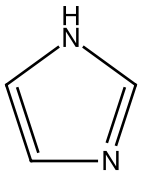


Figure 14.58: *A Kekulé model of imidazole, it is clear where implicit hydrogens should go as we have double bonds defined*

ChemDoodle attempts to resolve this issue by making intelligent choices and distribute implicit hydrogens appropriately to maintain aromaticity in a delocalized ring. Therefore, you will see the implicit hydrogen assigned correctly in a delocalized model of imidazole as shown in Figure 14.59. ChemDoodle will even adapt the model if you manually define an implicit hydrogen on the other nitrogen.

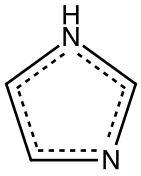


Figure 14.59: *A delocalized imidazole ring, ChemDoodle can intelligently resolve these systems*



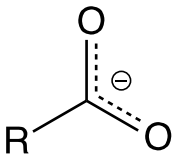
Resonance systems should be avoided when describing aromatic rings because they are ambiguous, even if there may be multiple Kekulé structures for the same molecule. Resolving aromatic resonance systems in ChemDoodle is also computationally expensive, so it is best to avoid them for many reasons.

14.16.3 Conjugated chains

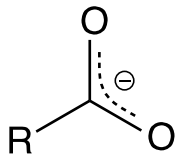
Conjugated chains are defined by making chains of resonance bonds. Sometimes, you may want to render the dashed lines not as separate segments, but as a continuous curve. You may do so in ChemDoodle using two global styles in the style sheet. These styles are located in the **Bond** styles, under the **Conjugation** section.

- **Render Curves**
- **Curve Sharpness**

Enabling the **Render Curves** style will instruct ChemDoodle to automatically find and render chains of conjugated resonance bonds as curves as shown in Figure 14.60.



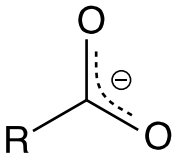
(a) *Conjugated curves disabled, dashed segments join at angles*



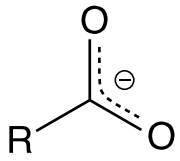
(b) *Conjugated curves enabled*

Figure 14.60: *Rendering conjugated chain resonance lines as a curve*

The **Curve Sharpness** style defines the depth of the curve. The higher the value, the more kinked the curve will appear. Figure 14.61 shows two values of the **Curve Sharpness** style and the results.



(a) *A curve sharpness value of 0.25*



(b) *A curve sharpness value of 0.338*

Figure 14.61: *Conjugated Curve Sharpness*

14.16.4 Kekulé structures

ChemDoodle contains a function for assigning double bonds to a structure so that pi electron delocalization is maximized. Both frames of single bonds and substructures consisting of only resonance bonds may be considered.

14.16.4.1 Kekulizing a single bond frame

To easily draw Kekulé structures, you may begin by just drawing a single bond frame. This way, ChemDoodle can optimally assign double bonds to the structure. If there are other bond types present, ChemDoodle will not Kekulize the structure. However, the Structure » Saturate function will change all bond types to single bonds.

To Kekulize a structure of only single bonds, execute the following steps:

1. Select the structure containing only single bonds to be Kekulized.
2. Select the Structure » Kekulize menu item.

For example, corannulene is generated from a Kekulization of a single bond frame in Figure 14.62.

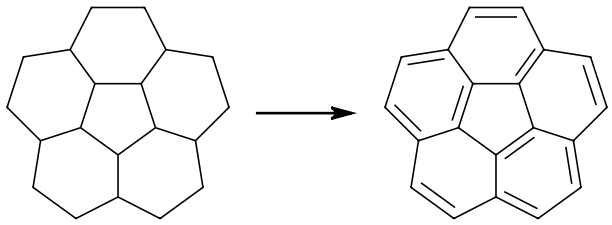


Figure 14.62: *Kekulizing a Single Bond Frame to Generate Corannulene*

14.16.4.2 Kekulizing a substructure of resonance bonds

In some cases, structures may be read into ChemDoodle with resonance bonds. This is very common for *SMILES* strings. It may be necessary to present a Kekulé structure instead of the resonance model. When Kekulizing a structure with resonance bonds, only the resonance bonds will be affected.

To Kekulize a substructure of resonance bonds, execute the following steps:

1. Select the structure containing the substructure of resonance bonds to be Kekulized.
2. Select the Structure » Kekulize menu item.

For example, the aromatic rings in Viagra are Kekulized in Figure 14.63.

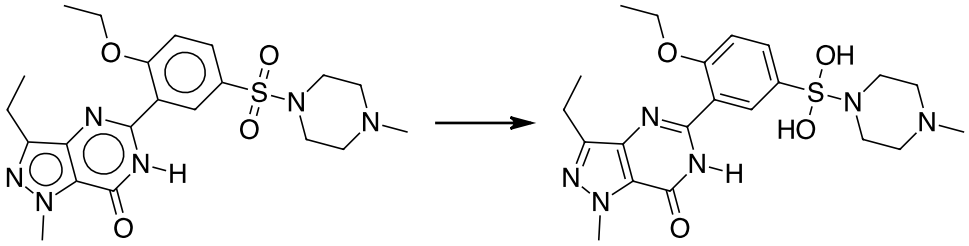


Figure 14.63: *Kekulizing the Aromatic Rings in the Resonance Model for Viagra*

14.16.4.3 Delocalizing a Kekulé structure

You can also delocalize a Kekulé structure. Do this by selecting the content to delocalize and select the Structure » Delocalize menu item. Any aromatic rings will be converted into a delocalized model.

14.17 Ring perception

Rings are cycles of atoms and are important, because ChemDoodle uses them to define graphics such as which direction double bonds face and for algorithms such as aromaticity detection. There are several published algorithms to define rings in structures producing different ring sets.

In the vast majority of the cheminformatics algorithms that ChemDoodle executes, the *Smallest Set of Smallest Rings* set is the ring set that is used.

14.17.1 Supported ring sets

Currently, ChemDoodle recognizes the following sets:

- **Smallest Set of Smallest Rings** - The smallest set of smallest rings (SSSR) is the standard for defining ring sets in flat 2D structures.
- **Euler Facet Rings** - The Euler facet ring set is better than the SSSR at defining essential rings in 2D depictions of 3D structures. It is defined by all the rings that make up the faces of a 3D object when the 2D chemical graph is placed on a 3D sphere.
- **Hanser (All) Rings** - Every last graph cycle in selected structures.

You can see the differences in these sets for cubane in Figure 14.64 and Figure 14.65.



(a) *The SSSR set for cubane, 5 rings*

(b) *The Euler facet ring set for cubane, 6 rings*

Figure 14.64: *Different ring sets for cubane*

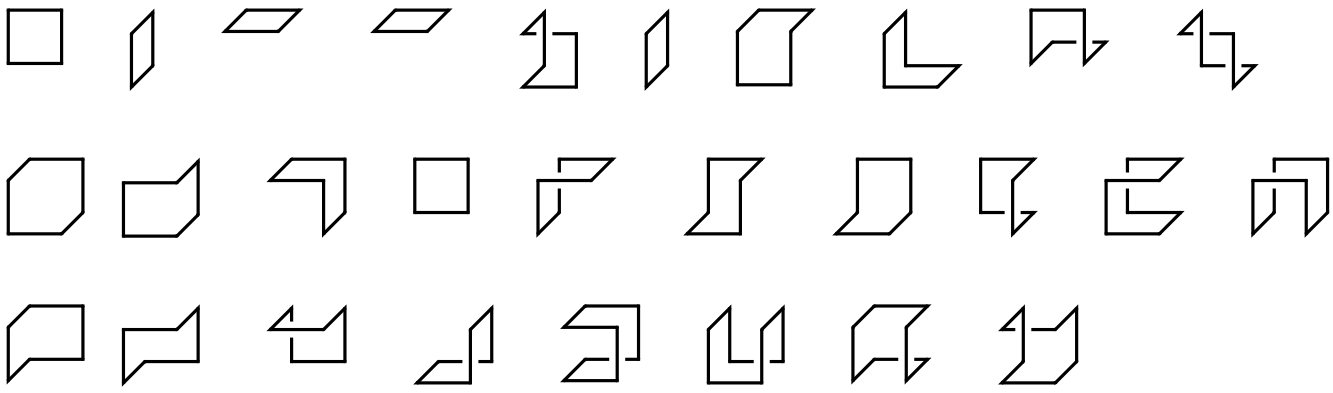


Figure 14.65: *All of the graph cycles in cubane, 28 in total, this is also the Hanser ring set*

14.17.2 Exploding ring sets

Ring sets can be exploded from the structure. In other words, they will be laid out around the structure to show the rings and where they are contained. To explode ring sets, execute the following steps:

1. Select the structures with the rings to be exploded.
2. Expand the Structure » Rings submenu and select the desired set to explode.

In very complex structures, the exploded ring diagram will be highly overlapped. Just stack the rings (in the Content menu) to view them all clearly.

14.17.3 Performance considerations

The default SSSR algorithm employed by ChemDoodle is the **RP-Path** algorithm, which is very fast, but requires a significant amount of memory to perform. Large structures may cause issues as they will quickly overrun the available memory for the application. Therefore, the **Euler Facet** algorithm is used to generate the SSSR for structures with more than 1000 constituent atoms, with a ring cutoff size of 13. So very large structures will still be handled quickly by ChemDoodle, but only rings of sizes 13 and smaller will be found.

14.18 Text descriptions

ChemDoodle will generate text descriptions of your drawn figures. To do so, first select the content you wish to describe and then execute the Structure » Generate Text Description menu item. The description will appear in the text area of a new window as shown in Figure 14.66.

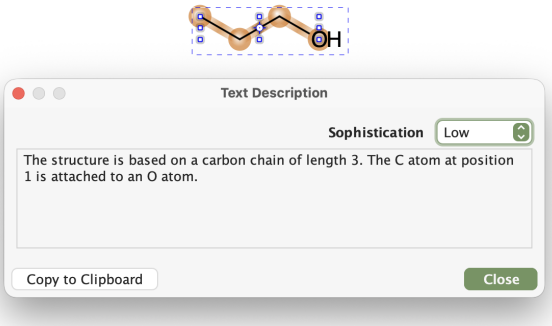


Figure 14.66: *A generated text description for 1-propanol with low sophistication*

On the bottom of the window that appears, you will see two buttons. The **Copy to Clipboard** button will copy the contents of the text area to the system clipboard (you may also copy and paste selections in the text area using standard keyboard shortcuts). The **Close** button will close the **Text Description** window.

There are 3 **Sophistication** levels:

1. **Low** - The text description will describe the content using as little chemistry terms as possible.
2. **Medium** - The text description will break down the content, but still use some chemistry terminology.
3. **High** - This text will be an advanced and concise description of the content.

14.18.1 Support

The algorithm attempts to create an accurate, thorough, instantaneous, consistent, canonical text description of chemical figures based on IUPAC naming rules. No LLM or AI use.

These current features of chemical figures are currently considered:

- individual molecules
- multiple molecules
- language to describe reactions

Please contact support if you encounter any issues or have any recommendations.

14.19 Valence

Valence for elements is important, as it determines how many implcit hydrogens are to be displayed, or if any warnings or errors should appear for drawn chemical structures. ChemDoodle implements the MDL Valence model. For more information on controlling implicit hydrogen counts, please see the HYDROGENS section.

CHAPTER 15

IUPAC Naming

Contents

15.1 Overview **366**

15.2 IUPAC naming scope **366**
15.2.1 Types of names 367
15.2.1.1 Traditional IUPAC names 367
15.2.1.2 Preferred IUPAC names (PINs) 367
15.2.1.3 Other IUPAC names 367
15.2.1.4 CAS nomenclature 367
15.2.2 Systematic nomenclature systems 368
15.2.3 Elements 368
15.2.4 Bond types 368
15.2.4.1 Covalent 368
15.2.4.2 Zero order 369
15.2.4.3 Resonance 369
15.2.4.4 Dative 370
15.2.5 Ligands 372
15.2.6 Radicals 374
15.2.7 Ions 374
15.2.8 Isotopes 375
15.2.9 Stereochemistry 375
15.2.10 Unsupported names 375
15.2.11 References 376

15.3 Converting between names and structures **377**
15.3.1 Name to structure 377
15.3.1.1 Window with instructions 377
15.3.1.2 Pasting from the system clipboard 378
15.3.2 Structure to name 378
15.3.2.1 Multiple structures in a single name 378

15.4 Automatically updating IUPAC labels **379**
15.4.0.1 Multiple structures in a single name 380

15.5 Copying IUPAC names with formatting **381**
15.5.1 Unicode IUPAC name output 381

15.6 IUPAC locants **382**

15.7 IUPAC naming options **383**
15.7.1 Base Nucleus 383
15.7.2 Functional Groups 384
15.7.3 Rings and Ring Blocks 385
15.7.4 Benzenes 388
15.7.5 Templates 388
15.7.6 Isotopes 389
15.7.7 Ions 389
15.7.8 Radicals 389
15.7.9 Stereochemistry 390
15.7.10 Complexes 390
15.7.11 Metals 391
15.7.12 Hydrogens 391
15.7.13 Locants 392
15.7.14 Punctuation 392

15.1 Overview

IUPAC stands for the International Union of Pure and Applied Chemistry. Their goal is stated on their website: https://iupac.org/who-we-are/

> A neutral and objective scientific organization, IUPAC was established in 1919 by academic and industrial chemists who shared a common goal – to unite a fragmented, global chemistry community for the advancement of the chemical sciences via collaboration and the free exchange of scientific information. Throughout its long history IUPAC has fulfilled that goal through the creation of a common language and the standardization of processes and procedures.

IUPAC naming is an incredibly important part of chemistry. While much communication involves pictures and structural drawings, we still need a way to quickly communicate chemistry through text and language. This is where IUPAC naming comes into play. IUPAC defined standards for language communication of chemistry and related fields in their well-known "Color Books". That being said, the IUPAC naming rules are very extensive and very complex, and users need quick and accurate methods for working with IUPAC names without having to spend years learning the rules. iChemLabs develops and distributes software that interprets those rules and can read and write IUPAC names for chemical structures. ChemDoodle provides access to these features.

This section introduces the new user to the IUPAC naming features within ChemDoodle. It covers the following topics:

- What is IUPAC naming?
- The scope of IUPAC naming within ChemDoodle.
- Generating IUPAC names from a chemical structure.
- Converting IUPAC names into a chemical structure.
- Copying IUPAC names with formatting into other software.
- Using updating labels to display IUPAC names in real time as you draw molecules.
- An overview of all of the options available to you in ChemDoodle to customize IUPAC names.

15.2 IUPAC naming scope

IUPAC naming is governed by an incredibly complex and extensive set of rules. iChemLabs develops software to handle these rules. Our IUPAC naming work is a continuous development project, and we are always adding in support for new groups of molecules and updating to the latest rules and standards.

For ChemDoodle, the focus is on organic and simple inorganic molecules. Our main references are the IUPAC Blue and Red books along with the associated corrections and revisions.

Additionally, the history of IUPAC naming literature spans many decades and changes to the rules have occured since they were first published. This leads to rules that are no longer used or have become internally inconsistent. One of the goals of ChemDoodle is to give the user complete control over how their chemistry is described and we have used the entire history of IUPAC publications to guide the implementation of our algorithms. ChemDoodle does not enforce a single IUPAC naming paradigm on users. As such, many options are exposed to allow you to control how ChemDoodle generates IUPAC names (on the other hand, IUPAC names can be parsed and converted into chemical structures irrespective of rules as long as they are correctly written). This is covered in the IUPAC NAMING OPTIONS section later in this chapter.

And of course, even with IUPAC's careful consideration of their extensive rules, there are still some disagreements on the interpretation of those rules and there can be possibly multiple correct names for a single structure. In these situations, ChemDoodle will prefer clear names that exclude redundant information and produce the shortest text length.

15.2.1 Types of names

IUPAC names consist of traditional names and Preferred IUPAC Names (PINs). You may have also heard of systematic or trivial IUPAC names. This section describes in more detail what these are. While knowledge of different types of IUPAC names is not necessary for parsing, as any valid IUPAC name will be appropriately handled, it is important for output, as you will need to understand the features in ChemDoodle to derive the specific format of the name you desire.

15.2.1.1 Traditional IUPAC names

A traditional IUPAC name is any valid IUPAC name defined by any part of the IUPAC naming specification, present or past. Traditional IUPAC names consist of both systematic and trivial names. Systematic IUPAC names are fully defined by rules. Names that can be algorithmically derived, such as "methane", "ethane", "propane", "butane", etc. are systematic names. Alternatively, trivial names are common names that cannot be derived by any algorithm, but were historically used to reference a specific compound and have been codified by the IUPAC specification. Examples of trivial names are "benzene", "alanine", and "acetylene". Both systematic and trivial names are valid IUPAC names, and may be used depending on the situation. For control over how ChemDoodle derives traditional IUPAC names, modify the options in the **Settings** window, under the **IUPAC Naming** tab, as descibed in the IUPAC NAMING OPTIONS section.

It should be noted that systematic naming may lead to many different names for the same structure, for instance "1-chloropropane" and "3-chloropropane" both describe the same exact structure. IUPAC naming declares various rules to exclude certain naming choices, and "3-chloropropane" is not acceptable. ChemDoodle takes care of these rules for you when generating names, but any recognizable name, including "3-chloropropane", or even "chloroethylmethane", can be parsed by ChemDoodle into the structure without error.

15.2.1.2 Preferred IUPAC names (PINs)

IUPAC names are not canonical. Which means multiple correct names exist for any given structure. For instance, "*o*-xylene" and "1,2-dimethylbenzene" are both valid and acceptable IUPAC names that describe the same exact chemical structure. Now, the average chemist may be happy communicating either of these names, but even more may be derived, especially as the molecular structure becomes more complex. To further improve the utility of IUPAC naming, the 2013 Blue book introduced a "Preferred IUPAC Name", also known as a PIN. When describing a chemical structure, only one specific name is the correct PIN. All other names are still valid traditional IUPAC names.

Understandably, generating PINs is an incredibly massive and difficult task, and the rules can change over time. In ChemDoodle, the goal is to generate accurate PINs, but such output is not guaranteed. Therefore, ChemDoodle produces what we refer to as an "Attempted PIN", in which the algorithm outputs a name as close as possible to the true PIN. The Attempted PIN may not be accurate and would therefore require some correction to be the actual PIN. Of course, we are continuously working hard on our IUPAC naming algorithms to ensure our Attempted PINs are as accurate as possible and consistent progress will be made as time goes on.

Because only one PIN is acceptable for any given structure, there are no options to modify PIN output in ChemDoodle.

15.2.1.3 Other IUPAC names

There are many options in ChemDoodle available to you to control the IUPAC name output for your structures. To define how ChemDoodle derives traditional IUPAC names, modify the options in the **Settings** window, under the **IUPAC Naming** tab, as descibed in the IUPAC NAMING OPTIONS section.

If you are a student, you are likely looking for the simple systematic name for the structure you are drawing. For such output, in the IUPAC naming settings, deselect the **Use Non-systematic Names** option under the **Templates** title.

15.2.1.4 CAS nomenclature

It is important to note that CAS nomenclature, which is used in SciFinder, is not IUPAC naming, but rather a dialect of it: https://www.iupac.org/publications/ci/2012/3404/nn.html

> A system of nomenclature which is independent of IUPAC, but which is widely used by chemists, is due to the Chemical Abstracts Service (CAS) of the American Chemical Society. This has been developed to produce names for CAS use in both running text and indexes.

15.2.2 Systematic nomenclature systems

IUPAC naming attempts to describe chemical structures as human-communicable language. However, there are different classes of chemical structures and the method for describing an organic molecule with only covalent bonds is not ideal for describing a periodic salt with ionic bonds. Therefore, there are several systems available for describing chemical structures as language:

- Substitutive
- Radicofunctional
- Additive
- Subtractive
- Conjunctive
- Replacement
- Stoichiometric

It is important to understand how these different systems are used by ChemDoodle. When dealing with organic molecules, ChemDoodle will attempt to name the structure substitutively by investigating carbon base chains. If no base chain inclusive of carbon is found, but a parent hydride made up of heteroatoms is present, ChemDoodle will continue to name the structure substitutively with the employment of replacement nomenclature to describe the parent hydrides.

Radicofunctional names are used occassionally. Radicofunctional names should not be confused with functional replacement nomenclature. Functional replacement nomenclature is a procedure for deriving names of complex functional groups from more basic ones, which ChemDoodle will do as necessary.

In simple to moderately complex cases, where a central atom (typically metal or overvalenced) can be isolated, ChemDoodle will employ additive nomenclature. Currently, only a single additive center is allowed for a single discrete structure.

And by using the **Force Stoichiometric Naming** option, ChemDoodle will output stoichiometric names, which only convey element types, their ratios to each other, and whether parts are cationic or anionic, but not the topology of the structure.

Subtractive and conjunctive nomenclature will be rarely used by ChemDoodle, if at all. Please reference the IUPAC specifications for more information.

15.2.3 Elements

The entire periodic table of elements may be used in structures.

15.2.4 Bond types

Many bond types are available in ChemDoodle, but not all are relevant to IUPAC naming. For instance, the hextuple and half order bonds are not applicable to IUPAC naming, at least not at the time of writing this section. The following bond types are acceptable in drawn structures to be converted into IUPAC names.

15.2.4.1 Covalent

Single, double and triple bonds are all acceptable. Any bond types with bond orders of 1, 2 or 3 will be handled as basic bonds of those orders. Figure 15.1 shows some examples.

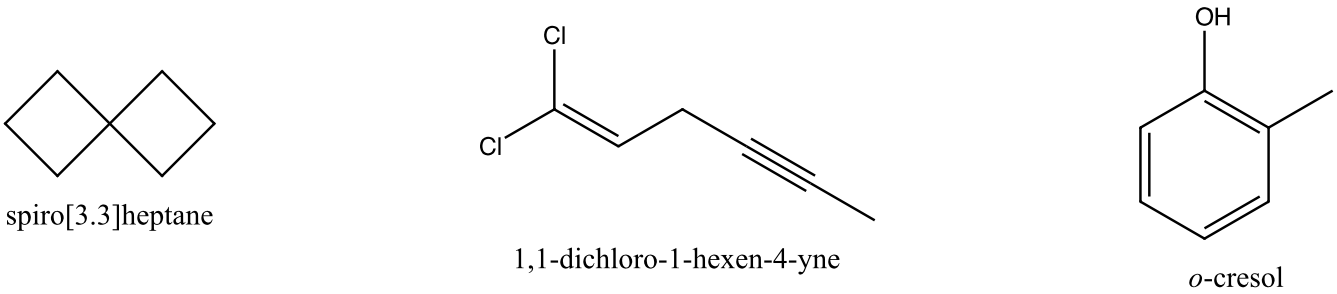


Figure 15.1: *IUPAC naming of various structures with covalent bond types*

Stereochemistry may be defined or excluded by using stereochemical bonds, such as wedges or the ambiguous double bond. Figure 15.2 shows some examples.

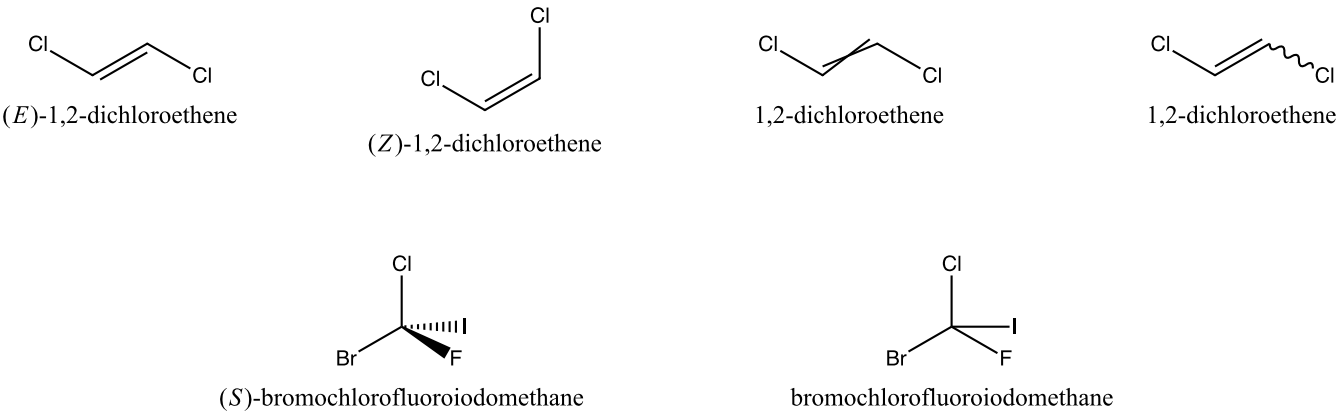


Figure 15.2: *IUPAC naming of stereocenters*

15.2.4.2 Zero order

Zero order bonds specify to ChemDoodle the structure should be split up into separate structures by cutting the zero order bonds before naming. This is helpful when drawing ionic compounds and mixtures, but is most useful for drawing fully connected structures when using auto-updating labels. Figure 15.3 shows some examples.

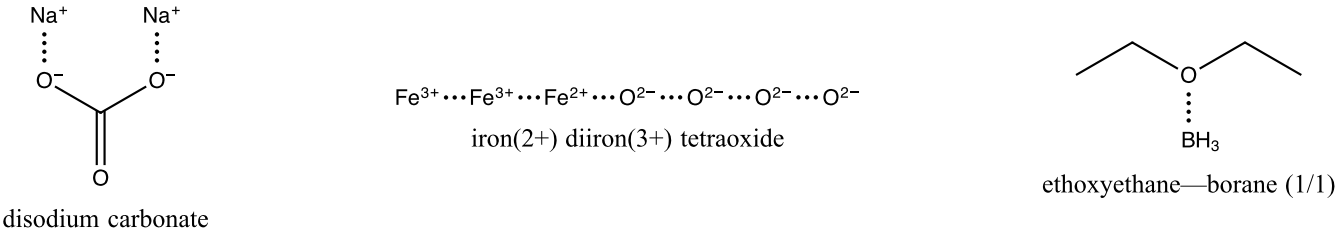


Figure 15.3: *IUPAC naming of various structures with zero order bonds*

15.2.4.3 Resonance

Resonance bonds are acceptable when defining fully delocalized ring blocks, such as benzene or naphthalene. Figure 15.4 shows some examples.

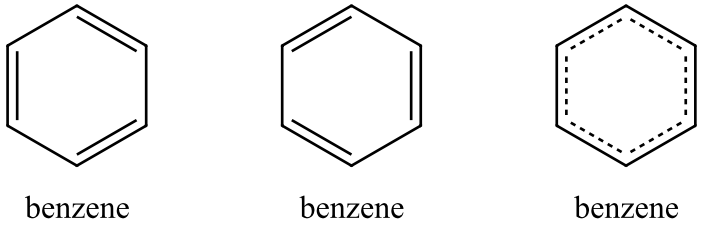
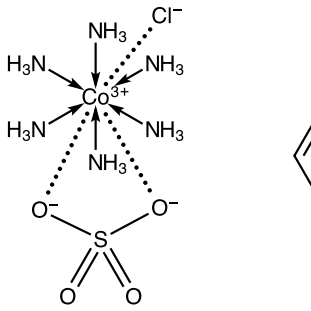


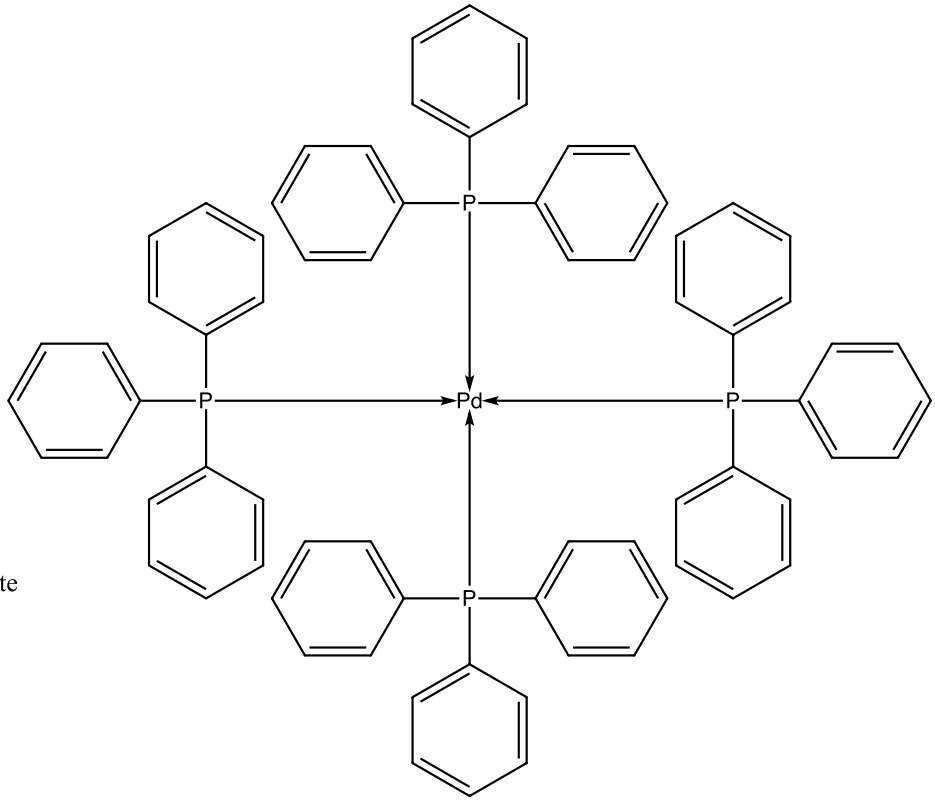
Figure 15.4: *IUPAC naming will work on both Kekulé and delocalized structures*

15.2.4.4 Dative

Dative bonds are used to designate a ligand is attached to a complex center by the contribution of an electron pair or pairs. While ChemDoodle will make intelligent decisions for whether or not to name a center via additive nomenclature, the presence of dative bonds will force the center to be named additively (if possible, otherwise the function will fail with a warning). Figure 15.5 shows some examples.



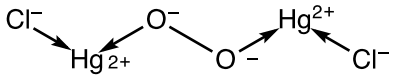
hexaamminecobalt(3+) chloride sulfate



tetrakis(triphenylphosphanyl)palladium

Figure 15.5: *IUPAC naming of various structures with dative bonds*

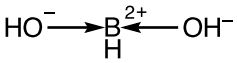
Only one additive center is currently allowed per structure. If more than one additive center is defined with dative bonds, the following output in Figure 15.6 will be presented.



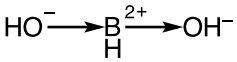
Only a single center (forced by dative bonds) is allowed for additive nomenclature.

Figure 15.6: *Only a single additive center may be defined per structure*

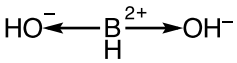
Care should be taken when drawing dative bonds, as they are directional. The arrow should point towards the dative center, or the atom that is receiving the electrons in the dative bond. Typically the dative bond should point from the anion or neutral component with a lone electron pair to the cation. Figure 15.7 shows the output message with dative bonds pointed incorrectly. See the LIGANDS section for more information.



Hydridodihydroxidoboron



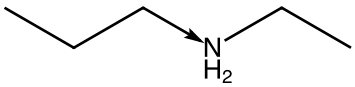
Only a single center (forced by dative bonds) is allowed for additive nomenclature.



Only a single center (forced by dative bonds) is allowed for additive nomenclature.

Figure 15.7: *The directionality of dative bonds is important*

On a final note, in some situations, a dative bond does not make sense and ChemDoodle will not be able to name your structure, as in Figure 15.8.



Unable to name this molecule via additive nomenclature, therefore dative bonds are not allowed.

Figure 15.8: *A dative bond in this context does not make any sense and this structure cannot be named*

15.2.5 Ligands



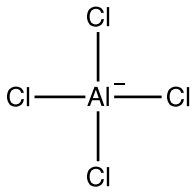
This section is for advanced users, and the discussion in this section may seem overly complex. IUPAC naming is not a simple or even straightforward specification and therefore such complexity is ultimately desired for full control. If you do not care about the nomenclature systems used and the choices made by ChemDoodle, the default options will produce the most desired output in the majority of cases.

When naming molecules, ChemDoodle will almost always name the structure using substitutive nomenclature. In some cases, where additive naming will lead to a better name, ChemDoodle will instead name the center additively and the substituents will be named as ligands. A couple examples are shown in Figure 15.9.



Figure 15.9: *ChemDoodle may automatically employ additive nomenclature, depending on the structure*

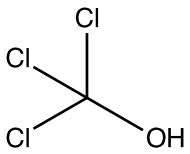
The name “Hydridosodium” is much preferred to “Sodamethane” and the name “Chloridoiron” is much preferred to “Chloroferramethanediylium”. Yet, other cases may not be as simple to decide. For example, in Figure 15.10, both the substitutive name and the additive name are equally acceptable. Because this structure is relatively simple, ChemDoodle produces the additive name by default. If instead you want the substitutive name, disable the **Allow Additive Nomenclature** option as described in the IUPAC NAMING OPTIONS section below.



Substitutive: Tetrachloroalumanuide
Additive: Tetrachloridoaluminate(1-)

Figure 15.10: *Both the additive and substitutive name may be equally desirable*

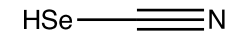
There may also be cases where you want ChemDoodle to be more agressive in producing additive names, such as when carbon is the central atom as shown in Figure 15.11. ChemDoodle will always choose to name these structures substitutively, but by enabling the **Expand Additive Scope** option, ChemDoodle will be more likely to name a structure additively and does so in this case.



Substitutive: Trichloromethanol
Additive: Trichloridohydroxidocarbon

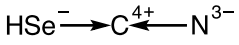
Figure 15.11: *You may expand the additive scope so ChemDoodle will more likely name structures via additive nomenclature*

Now up to this point, we have been describing ligands using covalent bonds and employing options to increase and decrease the additive scope. ChemDoodle has to detect such a center makes sense to be named additively, and then name the substituents as ligands, properly allocating charges. For more explicit control, you may instead draw ligands using dative bonds and explicit charges to force additive nomenclature. There is no multiple dative bond, for multiido ligands you would draw the appropriate multiple charges on the anionic ligand. Figure 15.12 shows some examples. ChemDoodle will always name centers drawn with dative bonds additively, but only a single additive center is allowed per structure. Additive centers may be explicitly defined with a mix of dative and covalent bonds, as shown in Figure 15.12c. Please see the Dative bond type section above for more instructions.



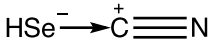
Selenocyanic acid

(a) *Covalent bonds*



Nitridoselanidocarbon

(b) *Dative bonds*

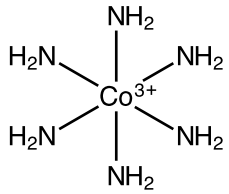


Nitridoselanidocarbon

(c) *A mix of covalent and dative bonds*

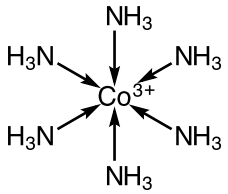
Figure 15.12: *Dative bonds and explicit charges may be used to manually define additive centers*

Dative bonds are the only way to communicate to ChemDoodle you wish to have neutral ligands named additively. Figure 15.13 demonstrates why this is the case. Notice in Figure 15.13a the nitrogen substituents are defined as amido ligands because breaking the covalent bond assigns a negative charge to the nitrogen atom, and therefore only 2 implicit hydrogens make sense (NH_2^-). Figure 15.13c shows using zero order bonds will instruct ChemDoodle to split the structure and name the individual molecules separately.



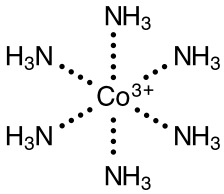
Hexaamidocobalt(3+)

(a) *Single bonds*



Hexaamminecobalt(3+)

(b) *Dative bonds*

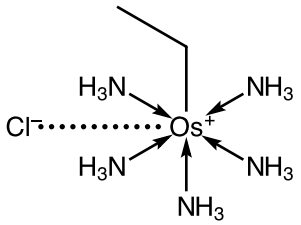


Cobalt(3+)—ammonia (1/6)

(c) *Zero bonds*

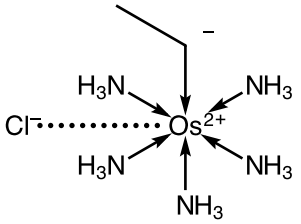
Figure 15.13: *Bond type choice is very important for neutral ligands*

One exception is when it is preferable to name an alkyl substituent substitutively on an additive center. An alkyl substituent may be connected to a metal center by a purely covalent bond where splitting would create a radical. In these cases, ChemDoodle will name the substituent substitutively. If you wish to instead name the substituent as an anionic ligand, draw the alkyl group as an anion with a dative bond to the additive center. Figure 15.14 exemplifies this concept.



Pentaammineethylosmium chloride

(a) *Neutral "ethyl" substituent*



Pentaammineethanidoosmium chloride

(b) *Anionic "ethanido" ligand*

Figure 15.14: *Alkyl groups will be named as neutral substituents in additive centers when single covalent bonds are used*

15.2.6 Radicals

Radicals are named. Multiple radicals may be present in the same structure and on the same atom. Several options modify how ChemDoodle will name radicals. Figure 15.15 shows some examples.

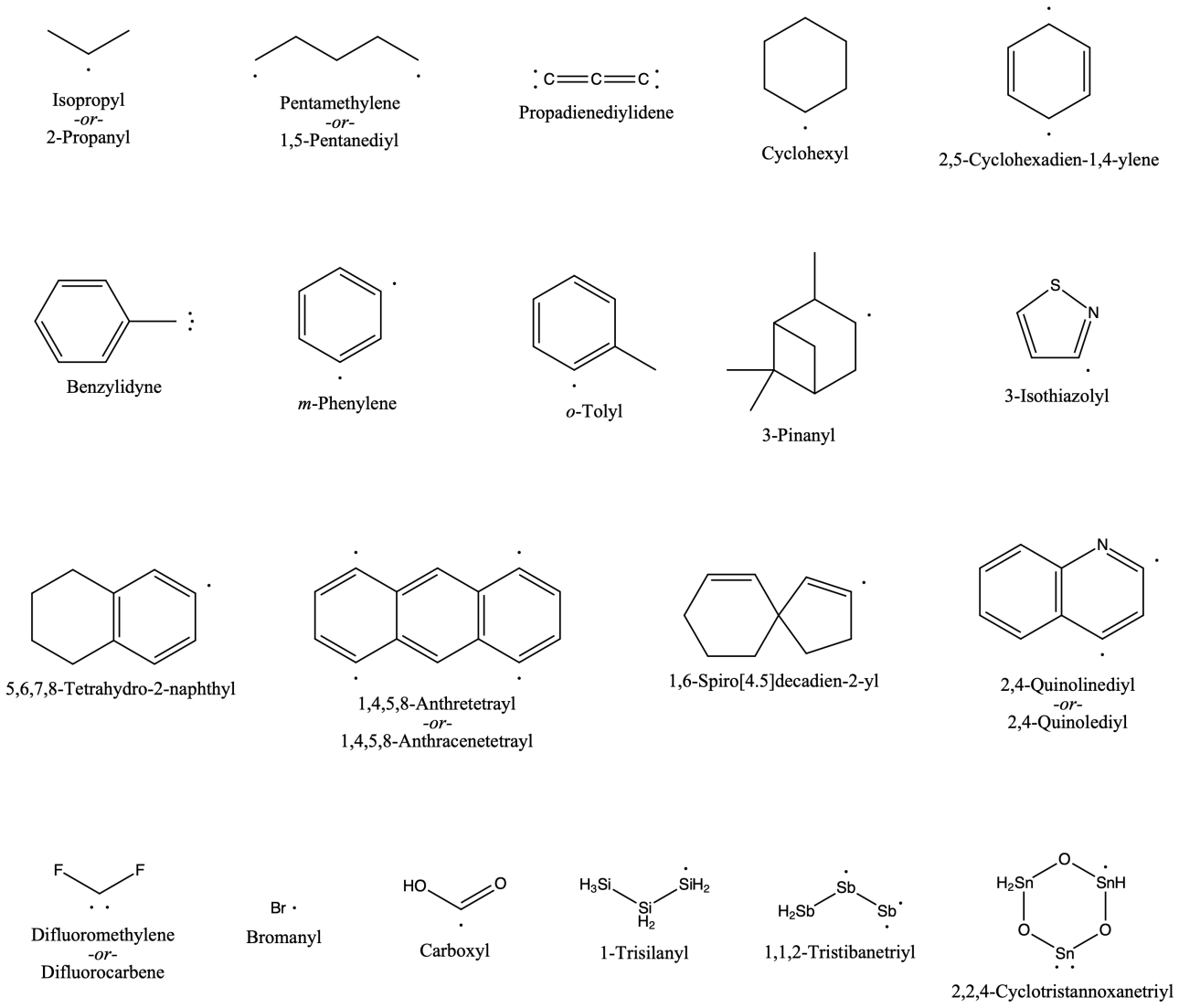


Figure 15.15: *IUPAC naming of various radicals by ChemDoodle*

15.2.7 Ions

Both positive and negative ions are named. Multiple ionic centers may be present in the same structure. Several options modify how ChemDoodle will name ions. Figure 15.16 shows some examples.

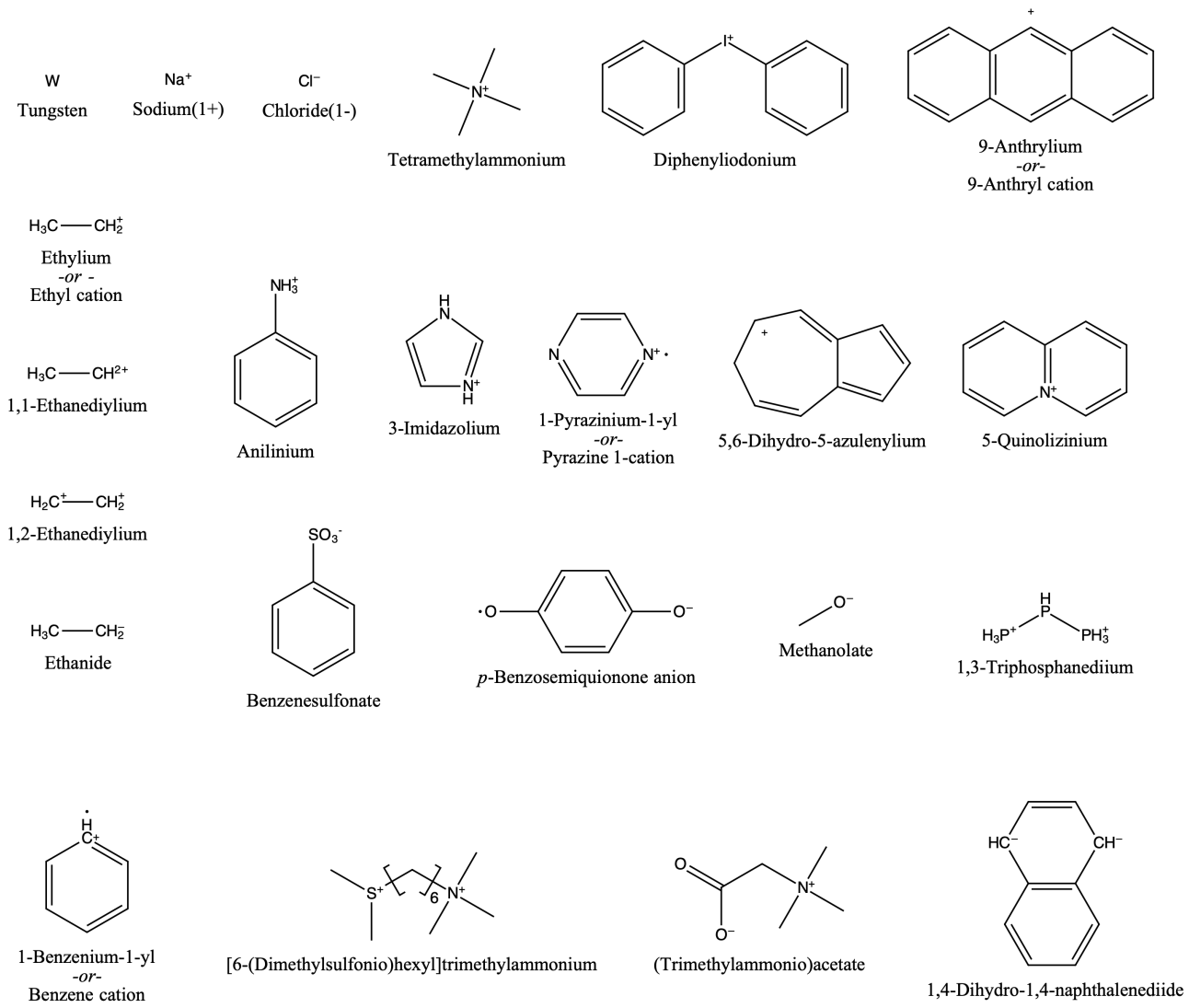


Figure 15.16: *IUPAC naming of various ionic structures by ChemDoodle*

15.2.8 Isotopes

Support for both modern and Boughton principle rules is provided by ChemDoodle for naming isotopic structures.

15.2.9 Stereochemistry

The scope of the stereochemistry understood by ChemDoodle is supported. The proper CIP labels will be included in output IUPAC names. For more information on the stereochemistry engine in ChemDoodle, please see the STEREOCHEMISTRY chapter.

15.2.10 Unsupported names

The vast majority of IUPAC names and structures the average chemist works with can be handled with ease, however, given the entire scope of what IUPAC naming defines, you will likely draw a structure that ChemDoodle cannot generate a name for or a name that ChemDoodle cannot parse.

If you try to parse a name that ChemDoodle cannot handle, a message will be presented as the contents of the text areas as shown in Figure 15.17.

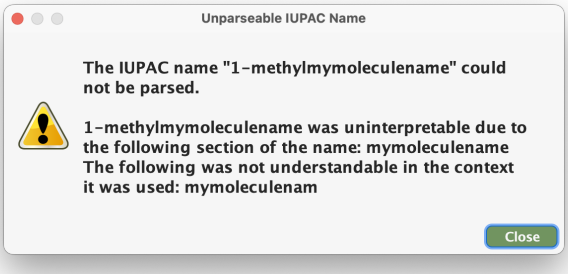


Figure 15.17: *A warning is displayed describing why a name cannot be parsed*

If you see this message, please double check that you have correctly written your IUPAC name and have it properly formatted to be parsed. If it is certainly correct, please contact iChemLabs as described in APPENDIX: TECHNICAL SUPPORT, so that we can improve our support for your use.

If ChemDoodle fails to generate a name for a structure you have drawn, a message similar to the following will appear as shown in Figure 15.18. If you are using an updating label to display your IUPAC names, the explanation will be presented as the contents of the label.

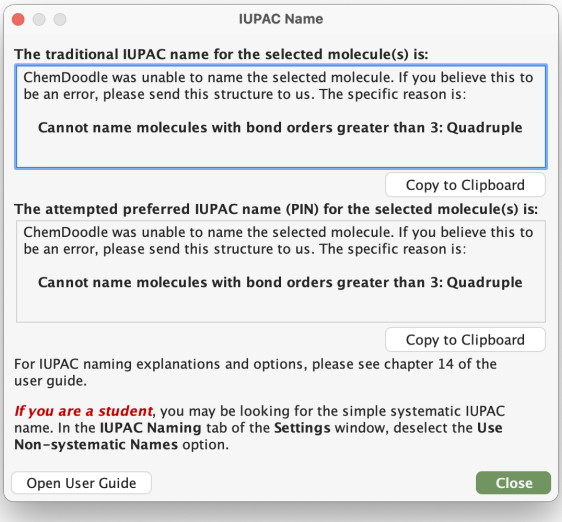


Figure 15.18: *A warning is displayed describing why a name cannot be generated*

If you see this message, please contact iChemLabs as described in APPENDIX: TECHNICAL SUPPORT, so that we can improve our support for your use.

15.2.11 References

References used in the development of our IUPAC naming algorithms can be found by selecting the Help > References menu and expanding the **Nomenclature** subfolder in the **Algorithms** folder in the references tree.

15.3 Converting between names and structures

ChemDoodle can generate IUPAC names for drawn structures as well as parse IUPAC names into chemical structures.

15.3.1 Name to structure

To parse an IUPAC name and generate a chemical structure or structures, choose one of the following methods.



If you are looking to generate a structure from a common name or synonym (such as “aspirin” or “cefuroxime” or “c60 fullerene”), not an IUPAC name, then use the MOLGRABBER WIDGET instead.

15.3.1.1 Window with instructions

You may view instructions and edit the name you are parsing using the application menu. This is helpful if you are trying to parse an IUPAC name with complex formatting.

1. Select the Structure ⟩ Parse IUPAC Name… menu item.
2. A window will appear with a text area as shown in Figure 15.19. Enter (or paste) the IUPAC name in this text area. Instructions are provided in this window for inputting more complex names including greek letters and superscripts.

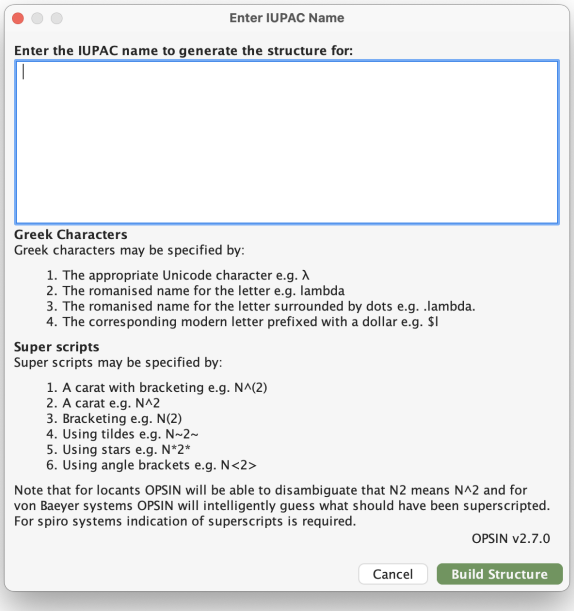


Figure 15.19: *The Enter IUPAC Name window*

3. Press the **Build Structure** button to parse the IUPAC name and place the associated structure(s) in your current document. The placed structure(s) will be automatically selected.
4. If you see a warning message, your name could not be parsed. Please double check the accuracy of the name and try again.

15.3.1.2 Pasting from the system clipboard

If you have an IUPAC named copied to the system clipboard, you may simply paste parsed structures by right-clicking anywhere in the document and selecting the Paste Text as Chemical ⟩ IUPAC Name menu item.

15.3.2 Structure to name

To generate an IUPAC name from a chemical structure, execute the following steps:

1. Make sure the structure you would like to generate the name for is in your current document.
2. Select the structure you would like to produce an IUPAC name for.
3. Select the Structure ⟩ Structure to IUPAC Name menu item.
4. Both the Traditional IUPAC name and Attempted PIN (with formatting) will be displayed in the popup that appears as show in Figure 15.20. You can copy directly from the text area, but be careful of formatting. Use the **Copy to Clipboard** button below each IUPAC name to copy the text with formatting to the system clipboard.
5. When you are done, press the **Close** button to dismiss the window.

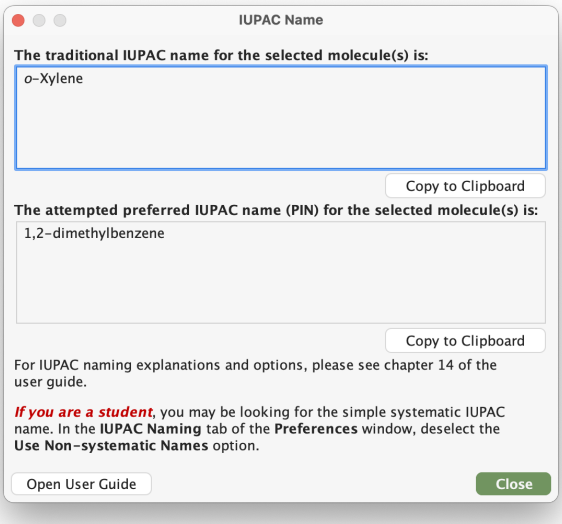


Figure 15.20: *The Traditional IUPAC name and the Attempted PIN will be shown in a window*

15.3.2.1 Multiple structures in a single name

To generate a single name from multiple separate structures, select all of the structures using a selection tool before following the procedure above. The compound name will be displayed in the text area as shown in Figure 15.21.

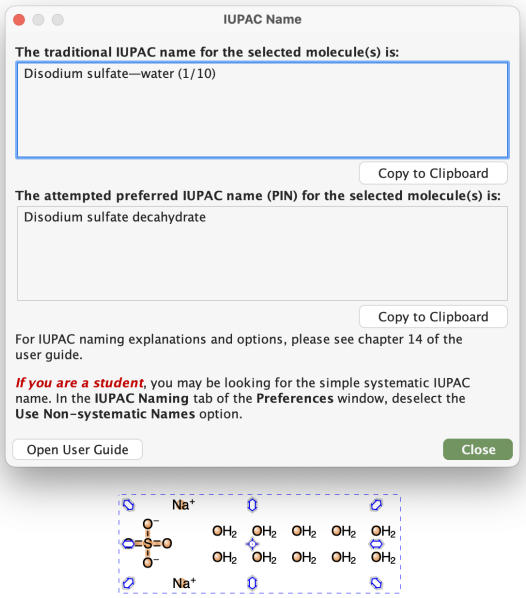


Figure 15.21: *Generating a name from multiple components, such as this ionic compound*

15.4 Automatically updating IUPAC labels

At times, it may be more convenient to have an IUPAC name associated with a molecule, and have that name automatically update while drawing. This is possible using auto-updating labels, which are covered in detail in the SHAPES chapter. To attach an auto-updating label to a molecule to display the IUPAC name, execute the following steps:

1. Select the molecule you would like to name.
2. Select the Structure » Attach Updating Label menu item, or press the **Attach Updating Label** button in the **Chemistry** toolbar.
3. In the popup that appears as show in Figure 15.22, make sure **IUPAC Name** is selected among the options.

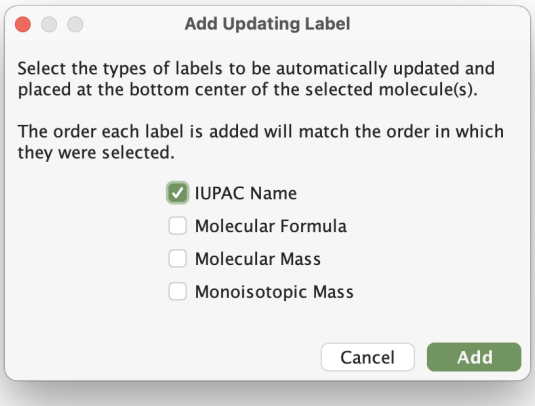
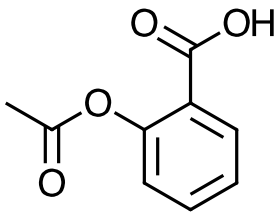


Figure 15.22: *The interface for adding an IUPAC updating label*

4. Press the **Add** button to add the updating label.



o-Acetoxybenzoic acid

Figure 15.23: *An updating label displaying an IUPAC name*

As you edit or move your molecule, the updating label will update accordingly. To copy the IUPAC name from an updating label to the system clipboard with formatting, right click on the label with a selection tool and select the Copy Text menu item.

By default, the Attempted PIN will be displayed in the updating label. If you wish to display a traditional IUPAC name, with full control via the options in ChemDoodle, open the **Settings** window. In the **IUPAC Naming** tab, change the **Auto-updating labels display** option to **Traditional**.

15.4.0.1 Multiple structures in a single name

To generate a single name from multiple separate structures, connect all of the structures using zero order bonds before following the procedure above. It does not matter how the zero order bonds connect the structures, as zero order bonds do not affect calculations for atom properties, but linking counterions leads to nicer images. The compound name will be displayed below the connected compound structure as shown in Figure 15.24.

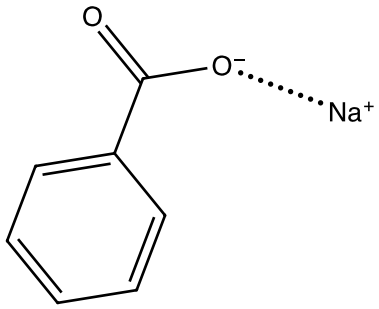


Figure 15.24: *An auto-updating label to show the IUPAC name for multiple components connected with zero order bonds*

15.5 Copying IUPAC names with formatting

Copying text is simple enough, and IUPAC names are text. However, some IUPAC names contain formatting, such as italicized letters (for stereochemical designations) and superscripts (for von Baeyer systems). Additionally, IUPAC names can include text outside of the normal ASCII range, such as greek symbols. Such formatting and symbols will not be copyable as plain text. ChemDoodle can place formatted text on the system clipboard as *RTF* or *HTML* for pasting into compatible applications, such as your text editor or web page. Not all applications will be able to handle formatted text. Controls over the text types ChemDoodle places on the system clipboard are found in the **Settings** window in the **Clipboard** panel. These controls are covered in detail in the SHARING INFORMATION chapter.

To copy formatted text to the system clipboard when using the Structure › Structure to IUPAC Name function, select the **Copy to Clipboard** button in the popup that displays the name, as described in the STRUCTURE TO NAME section.

To copy formatted text to the system clipboard from an updating label, right click on the label with a selection tool and select the Copy Text menu item, as described in the AUTOMATICALLY UPDATING IUPAC LABELS section.

15.5.1 Unicode IUPAC name output

Because some platforms do not support markup language for formatted text like *RTF* or *HTML*, ChemDoodle will output a unicode converted string as plain text. Superscript and subscript characters are replaced by equivalent character glyphs in the unicode range. All other formatting, such as italics, will be lost. This is useful to generate readable names in plain text, as long as the font used for rendering supports those character glyphs. But be aware many of these glyphs are typically deprecated and not intended as a replacement for proper markup language handling, leading to poorly aligned and spaced characters. Please also keep in mind that name-to-structure software and functions may not be able to recognize some of the character glyphs used. Unicode IUPAC name output is simply a means to create a more readable string for humans without formatting markup.

To demonstrate, here is a properly formatted IUPAC name using markup language:

9-[(*E*)-2-Chloroethenyl](3-$^{2}H_{1}$)tetracyclo[8.8.0.0^{2,7}.0^{13,18}]octadecane

And here is the same name output as plain text making use of equivalent character glyphs in the unicode range (rendered as an image, as LaTeX doesn't support all of these unicode characters):

9-[(E)-2-Chloroethenyl](3-²H₁)tetracyclo[8.8.0.0²·⁷.0¹³·¹⁸]octadecane

Figure 15.25: *A formatted IUPAC name converted into unicode plain text*

ChemDoodle will convert formatted IUPAC names to UTF-8 when using the **Copy to Clipboard** button in the Structure › Structure to IUPAC Name popup, and when outputting to certain file formats, such as FAIR data headers in *SDF* files.

15.6 IUPAC LOCANTS

IUPAC locants are the indexes, or number prefixes, you see before modifications to the names of chains. So for instance, in 2-propanol, 2 is a locant that defines the alcohol on the second carbon of the propane chain. Because ChemDoodle needs to calculate these locants to properly produce IUPAC names, a feature is provided to show this locant numbering, which may be useful for a number of applications. To show IUPAC locants, perform the following steps:

1. Select the View » Unique IDs » On Atoms » IUPAC Locants menu item.
2. Draw the structure you wish to view IUPAC locants for.

Any structures you draw will now present IUPAC locants in real time. Figure 15.26 shows how this will look.

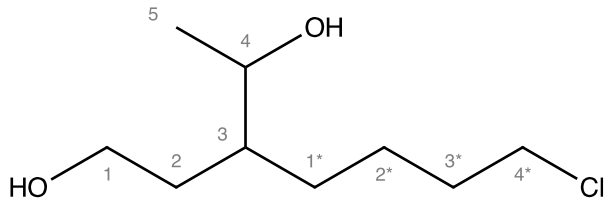


Figure 15.26: *Showing IUPAC locants can help clarify main chains*

This feature can be especially useful for complex structures. Separate chains will be differentiated by the number of asterisks following the locant, spreading out from the base chain system as shown in Figure 15.27.

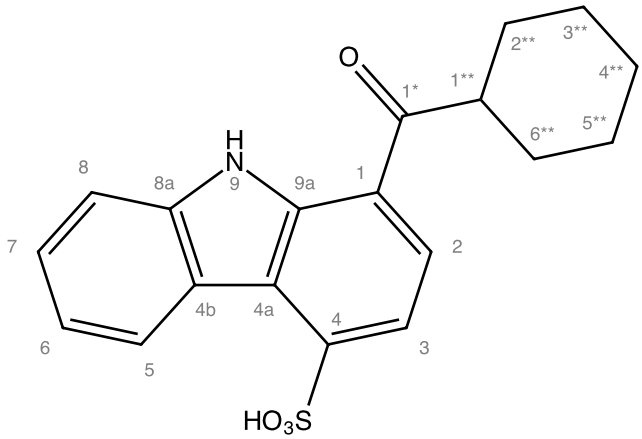


Figure 15.27: *Complex IUPAC names with specifically numbered base systems are elucidated*

To disable showing IUPAC locants on structures, simply select the View » Unique IDs » On Atoms » IUPAC Locants menu item again.

15.7 IUPAC NAMING OPTIONS

There are many options you can define to control how ChemDoodle generates IUPAC names. These options are organized in the **Settings** window, in the **IUPAC Naming** tab as shown in Figure 15.28.

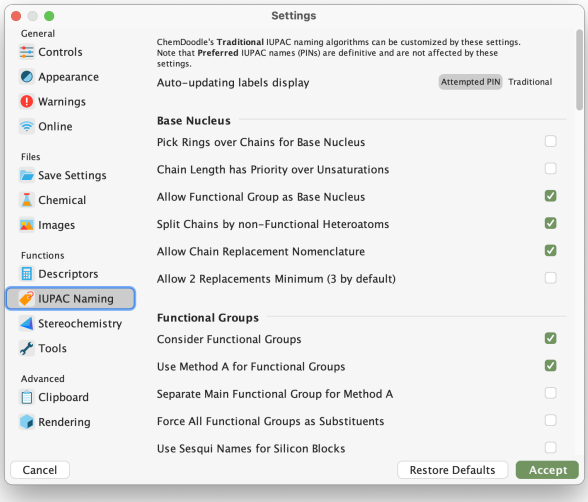


Figure 15.28: *IUPAC naming options in the Settings window*

Controlling these options can be very useful for certain purposes. For instance, if you are teaching a class about systematic IUPAC names and you don't want trivial IUPAC names to be shown for simple molecules, you can deselect the **Use Non-systematic Names** option.



While these options will affect the generation of names from structures, they will not affect the parsing of names into structures. This makes sense as an IUPAC name only refers to a single structure, while one structure can have several names. So when a name is generated, you have control over the output. When parsing an IUPAC name, as long as that name is legitimate, the corresponding structure will be created.

The options are categorized below by type. Each option is described with its default value and example output is demonstrated for when the option is on or off.

15.7.1 BASE NUCLEUS

Base Nucleus Priority Chosen when Unclear

Default:	**chains**
rings:	2-Butyrylpyridine
chains:	1-(2-Pyridyl)-1-butanone

Chain (length/unsaturations) Priority based on

Default:	**unsaturations**
chain length:	3-Methylenepentane
unsaturations:	2-Ethyl-1-butene

Chain (heteroatoms/suffixes) Priority based on

Default:	**suffixes**
heteroatoms:	5-oxa-2,8-dithia-11-silatetradecan-14-oic acid
suffixes:	10-oxa-7,13-dithia-4-silatetradecan-1-oic acid

Allow Functional Group as Base Nucleus

Default:	**on**
on:	Ethylamine
off:	Ethanamine

Split Chains by non-Functional Heteroatoms

Default:	**on**
on:	Tetraethylplumbane
off:	3,3-Diethyl-3-plumbapentane

Allow Chain Replacement Nomenclature

Default:	**on**
on:	3-Oxa-2,4-disila-1-hexanethiol
off:	(3-Ethyldisiloxanyl)methanethiol

Minimum Number of Heteroatoms for Replacement Nomenclature

Default:	**3**
2:	3,6-Dioxa-1,8-octanediol
3:	2-[2-(2-Hydroxyethoxy)ethoxy]ethanol

15.7.2 Functional Groups

Consider Functional Groups

Default:	**on**
on:	Methylhydrazine
off:	Methyldiazane

Functional Group Suffix Method

Default:	**(a) merge**
(a) merge:	Hexanoic acid
(b) append:	Pentanecarboxylic acid

Separate Main Functional Group to Apply Suffix Method (a)

Default:	**off**
on:	3-Formylhexanedial
off:	1,2,4-Butanetricarbaldehyde

Force All Functional Groups as Substituents

Default:	**off**
on:	1-Oxo-1,2-dihydronaphthalene
off:	2*H*-Naphthalen-1-one

Use Sesqui Names for Silicon Blocks

Default:	**off**
on:	Tetracyclo[5.5.1.1^{3,11}.1^{5,9}]hexasilasesquioxane
off:	Tetracyclo[5.5.1.1^{3,11}.1^{5,9}]hexasiloxane

Sulfur Described as

Default:	**thio**
sulfanyl:	tris(methylsulfanyl)germane
thio:	tris(methylthio)germane

Olate as Oxide when Appropriate

Default:	**off**
on:	Methoxide
off:	Methanolate

15.7.3 Rings and Ring Blocks

Merge Ring Assemblies

Default:	**on**
on:	Biphenyl
off:	Phenylbenzene

Ring Assembly Naming

Default:	**radical**
full:	2,2´-Binaphthalene
radical:	2,2´-Binaphthyl

Merge Subspiros

Default:	**on**
on:	Trispiro{cyclopentane-1,1'-perhydropentalene-5',2''-spiro[4.4]nonane-3',2'''-spiro[4.4]nonane}
off:	Pentaspiro[cyclopentane-1,1'-cyclopentane-3',1''-perhydropentalene-5'',1'''-cyclopentane-3''',1''''-cyclopentane-3'',1''''-cyclopentane]

Allow Contracted Polycycle Radical Names

Default:	**on**
on:	2-Naphthyl
off:	2-Naphthylenyl

Collapse Nitro-Ketone Ring Names

Default:	**off**
on:	1*H*-Pyrid-2-one
off:	1*H*-Pyridin-2-one

Monocyclic Naming

Default:	**(i) Hantzsch/Widman**
(i) Hantzsch/Widman:	1*H*-Silole
(ii) replacement:	Pentazacyclopentane
(iii) chain cyclization:	Cyclopentaazane

Hantzsch/Widman Rule Set

Default:	**1982**
1979:	Phosphorin
1982:	Phosphinin

Force ending 'e' in Hantzsch/Widman Names

Default:	**off**
on:	Phosphinine
off:	Phosphinin

Use Polyacene Names

Default:	**on**
on:	Nonacene
off:	Nonacyclo[20.16.0.0^{3,20}.0^{5,18}.0^{7,16}.0^{9,14}.0^{24,37}.0^{26,35}.0^{28,33}]octatriaconta-1,3,5,7,9(14),10,12,15,17,19,21,23,25,27,29,31,33,35,37-nonadecaene

Use Polyaphene Names

Default:	**on**
on:	Octaphene
off:	Octacyclo[16.16.0.0^{2,15}.0^{4,13}.0^{6,11}.0^{20,33}.0^{22,31}.0^{24,29}]tetratriaconta-1(18),2,4(13),5,7,9,11,14,16,19,21,23,25,27,29,31,33-heptadecaene

Use Polyalene Names

Default:	**on**
on:	Nonalene
off:	Bicyclo[7.7.0]hexadeca-1,3,5,7,9,11,13,15-octaene

Use Polyphenylene Names

Default:	**on**
on:	Pentaphenylene
off:	Hexacyclo[24.4.0.0^{2,7}.0^{8,13}.0^{14,19}.0^{20,25}]triaconta-1(30),2,4,6,8,10,12,14,16,18,20,22,24,26,28-pentadecaene

Use Polynaphthylene Names

Default:	**on**
on:	Tetranaphthylene
off:	Nonacyclo[30.8.0.0^{2,11}.0^{4,9}.0^{12,21}.0^{14,19}.0^{22,31}.0^{24,29}.0^{34,39}]tetraconta-1(40),2,4(9),5,7,10,12,14(19),15,17,20,22,24(29),25,27,30,32,34(39),35,37-icosaene

Use Polyhelicene Names

Default:	**on**
on:	Hexahelicene
off:	Hexacyclo[12.12.0.0^{2,11}.0^{3,8}.0^{17,26}.0^{20,25}]hexacosa-1,3(8),4,6,9,11,13,15,17(26),18,20(25),21,23-tridecaene

Use Annulene Names

Default:	**on**
on:	[10]Annulene
off:	1,3,5,7,9-Cyclodecapentaene

Use Benzo Fusing

Default:	**on**
on:	1-Benzophosphinin
off:	1-Phosphanaphthalene

Use Special Ring Systems

Default:	**on**
on:	Tetrahydroselenophene
off:	Selenacyclopentane

15.7.4 Benzenes

Use Ortho/Meta/Para

Default:	**on**
on:	*p*-Diethylbenzene
off:	1,4-Diethylbenzene

Use Benzene Exceptions

Default:	**on**
on:	3,4-Xylenol
off:	3,4-Dimethylphenol

15.7.5 Templates

Use Template Overrides

Default:	**on**
on:	Cubane
off:	Pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane

Use Non-systematic Names

Default:	**on**
on:	Isopentane
off:	2-Methylbutane

Non-systematic Dictionary

Default:	**Traditional**
Traditional:	Vinylbenzene
PIN:	ethenylbenzene

15.7.6 Isotopes

Isotopes are Specifically Labeled

Default:	**off**
on:	[^{14}C]Methane
off:	(^{14}C)Methane

Suffix Isotope Placement

Default:	**attached to suffix**
attached to suffix:	2-Cyclohexen-1-($^{2}H_2$)amine
prepended to chain:	(*N*,*N*-$^{2}H_2$)-2-Cyclohexen-1-amine

Use Boughton Principles

Default:	**off**
on:	2-(Chloro-^{35}*Cl*)-3-(methyl-d_3)pentane-*1-d*
off:	2-(^{35}Cl)Chloro-3-[($^{2}H_3$)methyl](1-$^{2}H_1$)pentane

15.7.7 Ions

Explicit Ion Naming

Default:	**off**
on:	Phenyl cation
off:	Phenylium

Ion Designation

Default:	**charge**
charge:	Tetraoxoarsenate(3-)
oxidation state:	Tetraoxoarsenate(V)

15.7.8 Radicals

Rules from section

Default:	**A**
A:	Hexamethylene
D:	1,6-Hexanediyl

Contract Radical Chain Names

Default:	**on**
on:	Bicyclo[3.2.1]oct-2-yl
off:	Bicyclo[3.2.1]octan-2-yl

Name Carbenes Where Possible

Default:	**on**
on:	Dicyanocarbene
off:	Dicyanomethylene

Radical Suffix Placement

Default:	**before ions**
after ions:	1-Ethid-1-yl
before ions:	1-Ethyl-1-ide

15.7.9 Stereochemistry

Include Double Bond Stereochemistry

Default:	**on**
on:	(*E*)-2-Butene
off:	2-Butene

Exo Stereodescriptors Placement

Default:	**pull to parent chain**
pull to parent chain:	(1*E*)-1-(butan-2-ylidene)-1*H*-indene
on substituent:	[(2*E*)-butan-2-ylidene]-1*H*-indene

Include Stereodescriptor for Bond in Ring <8

Default:	**never**
if larger ring present:	(2*Z*,6*Z*)-spiro[4.7]dodeca-2,6-diene
never:	(6*Z*)-spiro[4.7]dodeca-2,6-diene

15.7.10 Complexes

Allow Additive Nomenclature

Default:	**on**
on:	Trichloridostannate(1-)
off:	Trichlorostannanide

Expand Additive Scope

Default:	**off**
on:	Tetrahydridoaluminate(1-)
off:	Alumanuide

Additive Ruleset

Default:	**1979**
1979:	Tetrachloroaluminate(1-)
2005:	Tetrachloridoaluminate(1-)

Automatically Split Structure

Default:	**on**
on:	Sodium benzoate
off:	(Sodamethyloxycarbonyl)benzene

Force Stoichiometric Nomenclature

Default:	**off**
on:	Phosphorus trichloride oxide
off:	Phosphoric trichloride

Name Hydrates

Default:	**on**
on:	Ammonium magnesium phosphate hexahydrate
off:	Ammonium magnesium phosphate—water(1/6)

15.7.11 Metals

Use Abandoned Metal Substituent Names

Default:	**off**
on:	1-Sodiopropane
off:	1-Sodamethylpropane

15.7.12 Hydrogens

Detach Hydro Prefixes

Default:	**off**
on:	1,2,3,4-Tetrahydro-4-oxo-1-naphthoic acid
off:	4-Oxo-1,2,3,4-tetrahydro-1-naphthoic acid

Exclude Indicated Hydrogen on Defined Cycles

Default:	**on**
on:	Pyrrole
off:	1*H*-Pyrrole

Define Added Indicated Hydrogens

Default:	**-one suffixes only**
never:	1,4-Dihydro-4-pyridylidene
-one suffixes only:	2(3*H*)-Pyrazinone
always:	4(1*H*)-Pyridylidene

15.7.13 Locants

Locants Are Implied

Default:	**when obvious**
never:	1-Bromo-1-chloro-1-fluoromethane
PIN rules:	(2*Z*)-2-Butene
when obvious:	Bromochlorofluoromethane

Place First Suffix Locant Before

Default:	**base chain name**
base chain name:	1-Butene
suffix:	But-1-ene

von Baeyer Replacement Locant Separators

Default:	**commas (,)**
periods (.):	3.6.8-Trioxabicyclo[3.2.2]nonane
commas (,):	3,6,8-Trioxabicyclo[3.2.2]nonane

15.7.14 Punctuation

Capitalize First Character

Default:	**on**
on:	Methane
off:	methane

Only use Parenthesis

Default:	**off**
on:	2-(2-(1-(2-Aminoethoxy)ethoxy)ethoxy)propiononitrile
off:	2-{2-[1-(2-Aminoethoxy)ethoxy]ethoxy}propiononitrile

Encapsulation Rules

Default:	**Traditional**
Traditional:	cyclopropylphenylmethanol
PIN:	cyclopropyl(phenyl)methanol

Append Warnings

Default:	**off**
on:	2,2,2-Trimethylpropane (Unusual valences)
off:	2,2,2-Trimethylpropane

Use "per" Nomenclature

Default:	**on**
on:	Perchloromethane
off:	Tetrachloromethane

Use "bis" Nomenclature

Default:	**on**
on:	Bis(2-napthyl)methane
off:	Di-2-naphthylmethane

CHAPTER 16

Stereochemistry

Contents

16.1 Overview **396**

16.2 Geometry **396**
16.2.1 Evaluation 396
16.2.1.1 IUPAC 397
16.2.1.2 MDL/BIOVIA 397
16.2.2 Standard geometries 398
16.2.2.1 Tetrahedral 398
16.2.2.2 Rectangular 398
16.2.3 Projections 398
16.2.3.1 Enabling and disabling projection analysis 399
16.2.3.2 Fischer 399
16.2.3.3 Haworth 399
16.2.3.4 Chair 400
16.2.4 Input and Output 401
16.2.4.1 0D/1D 402
16.2.4.2 2D 402
16.2.4.3 3D 402

16.3 Configuration **403**
16.3.1 Cahn-Ingold-Prelog (CIP) descriptors 403
16.3.1.1 Tetrahedral centers 404
16.3.1.2 Alkenes and other isolated double bonds 405
16.3.1.3 Odd-numbered cumulenes 405
16.3.1.4 Allenes and even-numbered cumulenes 405
16.3.1.5 Atropisomers 406
16.3.1.6 Limitations 406
16.3.2 Alkene cis/trans descriptors 407
16.3.3 Unspecified stereochemical configurations 407

16.4 Software functions **407**
16.4.1 Resolving stereochemical configurations 407
16.4.2 Removing stereochemical configurations 407
16.4.2.1 In bulk 407
16.4.2.2 Individually using a mouse tool 408
16.4.3 Forcing stereochemical configurations 408

16.5 Enhanced stereochemistry **410**
16.5.1 Defining enhanced stereochemistry 410
16.5.2 Grouping 411
16.5.3 Removing an enhanced stereochemistry designation 414
16.5.4 File format support 414

16.1 Overview

Stereochemistry is a very important part of chemistry for functional reasons, and it is very important the structures and images created in ChemDoodle properly depict stereochemistry. ChemDoodle provides a best-in-class system for processing geometric features in conjunction with an accurate and current Cahn-Ingold-Prelog (CIP) algorithm for assigning configuration descriptors to stereochemical features.

This section introduces the new user to the stereochemistry engine within ChemDoodle. It covers the following topics:

- What is a stereochemical feature?
- How does ChemDoodle understand stereochemistry?
- What is the difference between a geometry and a stereochemical feature?
- The different types of stereochemical projections ChemDoodle supports.
- The extent and support for CIP descriptors.
- Software functions for working with stereochemistry.
- Enhanced stereochemistry, and how stereochemical queries can be output to different file formats.

16.2 Geometry

Stereochemistry is a three-dimensional consideration where two or more configurations of substituents around a feature are chemically unique. The first expectation of a user will be to assign a configuration descriptor for a stereochemical feature (for instance *cis/trans* or *R/S*). But before any stereochemical analysis is possible, the geometrical features of the molecule need to be discovered and defined. ChemDoodle can then evaluate the geometrical features and assign stereochemical configurations. In three dimensions, this analysis is trivial as the coordinates themselves (if properly defined) explicitly define the geometries of the structure. In two dimensions, this process is much more complex. For instance, a tetrahedral geometry is defined using wedge bonds in conjunction with two dimensional coordinates.

It is important for our software to recognize geometrical features in molecules regardless of the dimensions they are described in. It does this by storing geometry information for features in the molecule irrespective of the coordinates or drawing standards used to define them on input so they may be unambiguously represented, modified and output.

It should be noted that a geometry may apply to a molecular feature that is not a stereochemical feature. For instance, methane forms a tetrahedral geometry, even though all four hydrogens are chemically identical. As such, the geometry system in ChemDoodle evaluates drawings before stereochemical features are considered. In this way, ChemDoodle can evaluate your drawings based on geometric rules alone, such as flagging the use of 4 protruding wedge bonds to a methane carbon, in addition to flagging features for stereochemical issues.

16.2.1 Evaluation

ChemDoodle will scan molecular structures to (a) categorize a feature as a certain geometry based on the number of substituents attached and (b) evaluate whether the substituents are correctly placed or drawn around the feature.

If a feature does not match any defined geometry, it is no longer considered. If a feature does match a defined geometry, and the substituents are not correctly described around the feature, ChemDoodle will display a warning message, excluding this feature from further processing. Please see the CHEMICAL WARNINGS section in the CHEMINFORMATICS chapter for more information on the warning system in ChemDoodle.

Converting a 2D drawing into 3D geometric features is not a simple task. There are two main specifications for facilitating this conversion, IUPAC and MDL/BIOVIA, and both are implemented in ChemDoodle.

16.2.1.1 IUPAC

The IUPAC specification is written by Brecher. This is a very thorough and complex ruleset for properly conveying 3D geometric features in a 2D chemical drawing. It is recommended that all users make themselves familiar with this specification. ChemDoodle uses the IUPAC specification for interpretation of geometric features by default, and will always modify or output 2D figures to satisfy IUPAC rules, if possible, when using the features of the software.

Brecher, J. Graphical Representation of Stereochemical configuration. *Pure Appl. Chem.* **2006**, *78*, 1897-1970.

16.2.1.2 MDL/BIOVIA

The MDL/BIOVIA specification, on the other hand, attempts to be concise and aims to always interpret geometric features in a 2D drawing, regardless of how they are drawn. A 3D model of the structure is envisioned for the perspective the 2D structure conveys, leading to the definition of the geometries. We consider this approach to take the opposite stance of the IUPAC specification interpretations in almost every way, even though the majority of 2D drawings will have the exact same geometries defined by both algorithms.

CHEMICAL REPRESENTATION; Dassault Systèmes: San Diego, CA, 2018.

The MDL/BIOVIA specification is useful if you have input that does not conform to IUPAC rules, and you do not want to adjust it. For instance, consider the structure shown in Figure 16.1. The geometric center on the bridge is not correctly represented via IUPAC rules and ChemDoodle displays a warning (Figure 16.1a) because a tetrahedral center may have at most 2 wedges connected to it. IUPAC prefers assignment of wedges to bridge bonds, so changing the assignment to the other ring bonds or the hydrogen bonds is less than ideal. In fact, the best option would be to redraw the structure making the unsubstituted bottom half of the ring the bridge instead of the substituted sections. This is not always possible or reasonable to do. Alternatively, this drawing is completely acceptable in the MDL/BIOVIA specification, and all stereochemical features are resolved (Figure 16.1b).



(a) *The bridge stereocenter is not compliant with IUPAC rules* (b) *The MDL/BIOVIA specification accepts this drawing*

Figure 16.1: *The same structure evaluated for stereochemical features using both IUPAC and MDL/BIOVIA specifications*

To have ChemDoodle interpret 2D drawings of geometries using MDL/BIOVIA rules, in the **Settings** window, under the **Stereochemistry** tab, set the **2D Stereo Interpretation** choice to **MDL/BIOVIA**. ChemDoodle will only modify or output 2D figures to satisfy IUPAC rules, and not MDL/BIOVIA, when using the features of the software.

Please note, while the MDL/BIOVIA rules handle more geometry drawing possibilities, the scope comes at a cost. MDL/BIOVIA definitions are often arbitrary as stated, especially in ambiguous cases, and will not always match what you intended to convey. Additionally, projection analysis is only compatible with IUPAC rules, please see the PROJECTIONS section below for more information.

16.2.2 Standard geometries

The following sections describe the standard stereochemical geometries supported by ChemDoodle.

16.2.2.1 Tetrahedral

Tetrahedral geometries describe any atomic center where four explicit substituents align most closely with the vertices of a tetrahedron. This is opposed to a square planar arrangement, where the four attachments most closely match a flat square or rectangle. Additionally, one and only one explicit substituent may be replaced by a single implicit hydrogen or a single pair of electrons.

Figure 16.3 shows a couple examples of incorrectly drawn tetrahedral geometries.

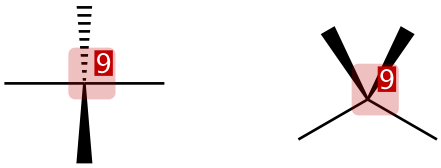


Figure 16.2: *Examples of incorrectly drawn tetrahedral geometries*

16.2.2.2 Rectangular

A rectangular geometry represents any feature where one or two substituents on one side have a coupled spatial relationship with one or two substituents on the other side.

Rectangular geometries are used in ChemDoodle to represent alkenes, allenes, both odd and even-numbered cumulenes, and atropisomers. Related functional groups are also included, such as imines.

Figure 16.3 shows a couple examples of incorrectly drawn rectangular geometries.



Figure 16.3: *Examples of incorrectly drawn rectangular geometries*

16.2.3 Projections

Stereochemical projections are standardized ways of depicting chemical structures while representing stereochemistry, recognized between chemists. Perspective bonds, like wedges, may or may not be included, but the important concept is the shared understanding of how these images should be interpreted. Separate substructures in a single connected structure can be represented by different projection types, including standard wedge diagrams, given each system is clearly separated. ChemDoodle will automatically recognize the following stereochemical projections in drawn chemical structures, as well as evaluate the stereochemical features defined.

1. Fischer
2. Haworth

3. Chair

The following sections describe these stereochemical projections, and how ChemDoodle will recognize and interpret them. For more information, please refer to the IUPAC rules:

> Brecher, J. Graphical Representation of Stereochemical configuration. *Pure Appl. Chem.* **2006**, *78*, 1897-1970.

16.2.3.1 Enabling and disabling projection analysis

Projections are supported and allowed under IUPAC rules for geometry interpretation, but are not allowed under MDL/BIOVIA rules. Please see the EVALUATION section above for more information.

By default, and if the **2D Stereo Interpretation** setting is set to **IUPAC**, projections are automatically recognized. However, the system is designed to be flexible and allow drawings of structures close to matching projection rules. Therefore, you may wish to disable the evaluation of projections. To do so, deselect the **Allow Projections** option in ChemDoodle's **Settings** window, under the **Stereochemistry** tab.

16.2.3.2 Fischer

A Fischer projection is mainly used to depict the tetrahedral stereochemistry of carbohydrate chains and derivatives. Fischer projections may be used to represent non-carbohydrate structures, but this may lead to ambiguity and is not recommended. An example of a Fischer projection is shown in Figure 16.4.

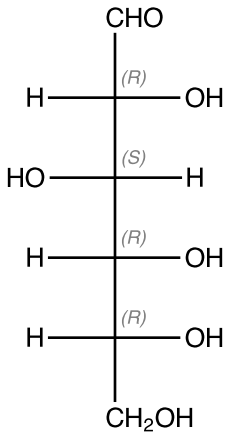


Figure 16.4: *An example of a Fischer projection evaluated in ChemDoodle*

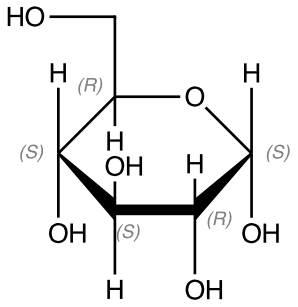
Fischer projections are always drawn vertically, and never horizontally or at an angle.

ChemDoodle will interpret any drawn carbon center as a Fischer projection if there are exactly four single bonds, one pointing in each of the four cardinal directions. One implicit hydrogen is allowed if there are bonds pointing north and south. The east and west bonds must end in terminal atoms.

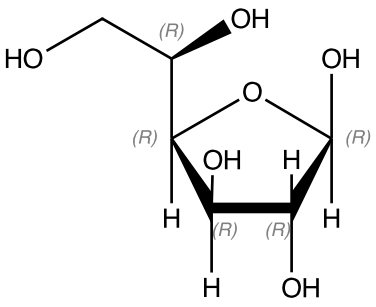
In Fischer projections, each tetrahedral center is evaluated with the east and west connections protruding out of the plane from the center, while the north and south bonds recede into the plane.

16.2.3.3 Haworth

Haworth projections are typically used to depict the tetrahedral stereochemistry of cyclic sugars and similar molecules. A couple examples of Haworth projections are shown in Figure 16.5.



(a) *A Haworth projection of a 6-membered ring*



(b) *A Haworth projection of a 5-membered ring*

Figure 16.5: *Example Haworth projections evaluated in ChemDoodle*

For ChemDoodle to recognize and interpret a drawn structure as a Haworth projection, the molecule can only include one single ring consisting of only five or six atoms. All of the ring bonds must be plain single bonds. If any of the ring bonds are drawn vertically, the structure will not be recognized as a Haworth projection.

The projection may also be represented in perspective style. So there may be two protruding wedges pointing into a bold bond. The bold bond needs to be horizontal and situated at the bottom of the ring.

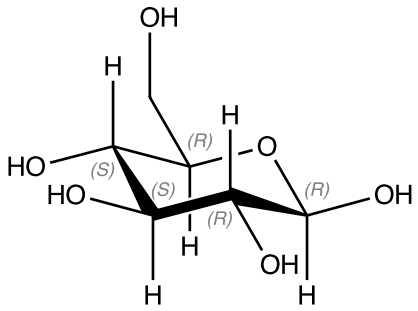
In Haworth projections, ChemDoodle will interpret ring carbons as tetrahedral centers if the atom has two plain non-ring bonds pointing directly upward and downward, exactly aligned with the *y*-axis. Removing one substituent to represent a single implicit hydrogen is allowed. The tetrahedron is evaluated with the ring rotated into the *xz*-plane (the bold or bottom horizontal bond is facing forward) and the two non-ring bonds bent away from the center of the ring, keeping their upward and downward relationship.



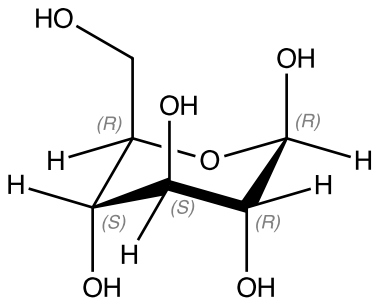
If a single center in a Haworth projection is drawn incorrectly, the entire structure will be disregarded as a Haworth projection with warnings shown. The most common reason is substituents not aligned with the *y*-axis.

16.2.3.4 Chair

A chair projection is meant to portray the 3D geometry of a six-membered ring in a low energy chair conformation. There are two variations of this shape, as the chair can invert through conformations to the other side. This projection is easy to recognize as the bonds of the ring are drawn in a zigzag pattern, like a lightning bolt. A chair projection and its inversion are shown in Figure 16.6.



(a) *A chair projection*



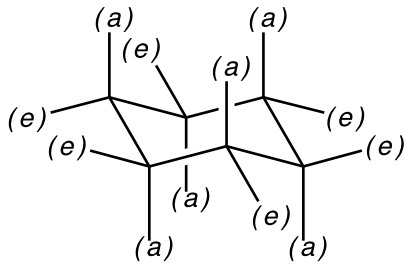
(b) *A conformational inversion of the other projection*

Figure 16.6: *A chair projection and its inversion evaluated in ChemDoodle*

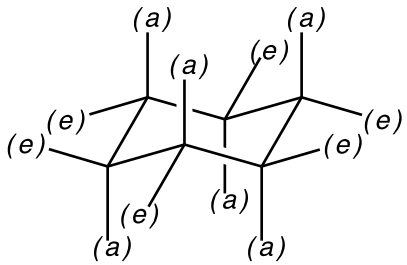
All of the ring bonds must be plain single bonds. When evaluating the projection, ChemDoodle will rotate the drawn molecular structure to best match the drawn chair ring to one of the horizontal layouts as pictured above. The rotation direction requiring

the smaller angle will be preferred. The projection may also be represented in perspective style. So there may be two protruding wedges pointing into a bold bond. In this case, ChemDoodle will always rotate the molecule so that the bold bond is rotated to the bottom.

Each tetrahedral atom of the ring has an axial substituent and an equitorial substituent. The axial substituents are parallel to the axis of the ring, and are drawn pointing vertically up or down when the ring is horizontal, whichever direction points away from the ring. Equitorial substituents are drawn parallel to the pair of opposite ring bonds of distance two from the atom. Figure 16.7 shows the correct directions for the axial (*a*) and equitorial (*e*) substituents for both chair conformations. For ChemDoodle to interpret the projection correctly, drawn substituent bonds must match these directions as closely as possible after rotation to the horizontal position.



(a) *Substituent directions for the chair projection…*



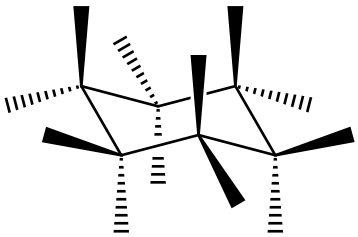
(b) *… and for the inversion*

Figure 16.7: *Axial (a) and equitorial (e) substituents*

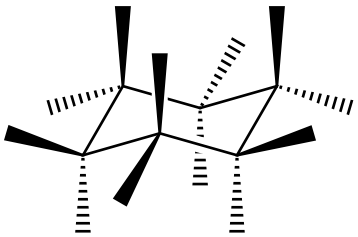


Wavy bonds should not be used as ring bonds in perspective drawings of chairs. If you want to mark a stereocenter in a chair projection as undefined, use a wavy bond for either the axial or equatorial substituent bond.

The bonds pointing off of the ring do not need to be wedges, but if they are, the wedges should match the implied wedge direction from the perspective of the drawing. Figure 16.8 shows the correct wedges.



(a) *Correct wedge types for projection substituents…*



(b) *… and for the inversion*

Figure 16.8: *Wedge types for chair projection substituents*

16.2.4 Input and Output

The geometry system unambiguously defines the configuration of geometrical features in a molecular structure. Regardless, the software first has to input the geometrical features from various sources to handle the information, and then output the geometrical features for further processing and communication. Geometrical features may be present in different formats, for instance, encoded in a SMILES string, drawn using wedges or from coordinates in a 3D molecular format. The following subsections describe how the geometry of molecular features is input and output by ChemDoodle.

16.2.4.1 0D/1D

When no coordinates are provided, geometrical configurations are assumed to be undefined unless coming from a format where specific configurations are defined. ChemDoodle fully supports the input and output of tetrahedral, alkene (and related functional groups), allene and cumulene stereochemical configuration information from *SMILES* and *InChI* strings.



Always be aware of the capabilities of the file format, in addition to the features in ChemDoodle. At the time of writing this warning, *InChI* does not support stereochemical configurations for cumulenes of length 4 or more, and neither *InChI* nor *SMILES* support stereochemical configurations for atropisomers.

On input, ChemDoodle will produce coordinates for the atoms as an 2D drawing. Stereochemical features that depend on specific 2D coordinate layouts are enforced, such as a *cis* or *trans* layout of substituents on double bonds. After coordinates are generated, wedges are applied to the appropriate bonds to correctly represent the remaining stereochemical configurations.

SMILES defines more types of stereochemical features than what ChemDoodle supports. These stereochemical configurations are correctly read in by ChemDoodle, but are disregarded. If you are using the **Line Notation Pad** widget, an appropriate warning will be displayed for the disregarded stereochemical configurations.

16.2.4.2 2D

In two dimensions, stereochemical features are defined by both two dimensional coordinates and perspective bond types, the protruding and recessed wedges. Some stereochemical features, such as alkenes, only require two dimensional coordinates, while others like tetrahedral and allene features require both two dimensional coordinates and wedge bonds.

In addition to evaluating wedge-based tetrahedral drawings, ChemDoodle will also recognize tetrahedral geometries in 2D drawn projections, such as Fischer, Haworth and chair projections. Please see the PROJECTIONS section for more information.

2D drawings will come from both chemical sketch files and user drawn content. ChemDoodle will interpret 2D drawings based on one of two rulesets controlled by the user. These rulesets are described in the EVALUATION section above.

ChemDoodle can modify drawn structures to match a certain configuration. For double bonds and odd numbered cumulenes, ChemDoodle will torsion the bond, if necessary. For wedge based stereochemical features, ChemDoodle will apply or change wedges to correctly represent the internally defined geometry by IUPAC rules, when applicable. The only exception is if a geometry is being forced on a single stereochemical feature where there are no good choices for assigning wedges (for instance, all connections are to previously defined stereochemical features and any assignment would invalidate the other stereochemical features). In these cases, an appropriate warning message will appear stating the software is unable to complete the action and you should modify the structure manually.



Conveniently, ChemDoodle will automatically preserve stereochemical configurations when using the 2D clean function. However, when editing graphics and flipping content horizontally or vertically, stereocenters will *not* have bond types adjusted and the flip functions will invert chiral stereocenters. Both of these behaviors are controlled by settings in the **Settings** window under the **Tools** tab. The **Cleaning** > **Clean Retains Stereochemistry** setting controls whether stereochemical configurations are preserved when using the 2D clean function while the **Flipping** > **Flip Retains Stereochemistry** setting controls whether stereochemical configurations are preserved when using the content flip functions.

16.2.4.3 3D

In three dimensions, all stereochemical features are explicitly defined by the three dimensional coordinates of the atoms. ChemDoodle does not input nor output stereochemical features from three dimensional coordinates. ChemDoodle inputs *z*-coordinates when present, but will only analyze stereochemistry from a 2D perspective. ChemDoodle will output *z*-coordinates only as explicitly set in the document. Instead, use ChemDoodle 3D.

16.3 Configuration

In the GEOMETRY section above, we described how you may define and how ChemDoodle will be able to recognize the features in a 2D drawing that should be considered for stereochemical significance. In this section, we discuss the various configuration descriptors ChemDoodle can assign to those geometrical features.

Configuration descriptors are very important for the communication of chemical information. While basic cases are trivial to resolve, complexity can increase quickly, especially in organic molecules and such analysis is best left to a software program like ChemDoodle. The functions in ChemDoodle allow you to check your work to ensure the figure you have drawn is accurate.

16.3.1 Cahn-Ingold-Prelog (CIP) descriptors

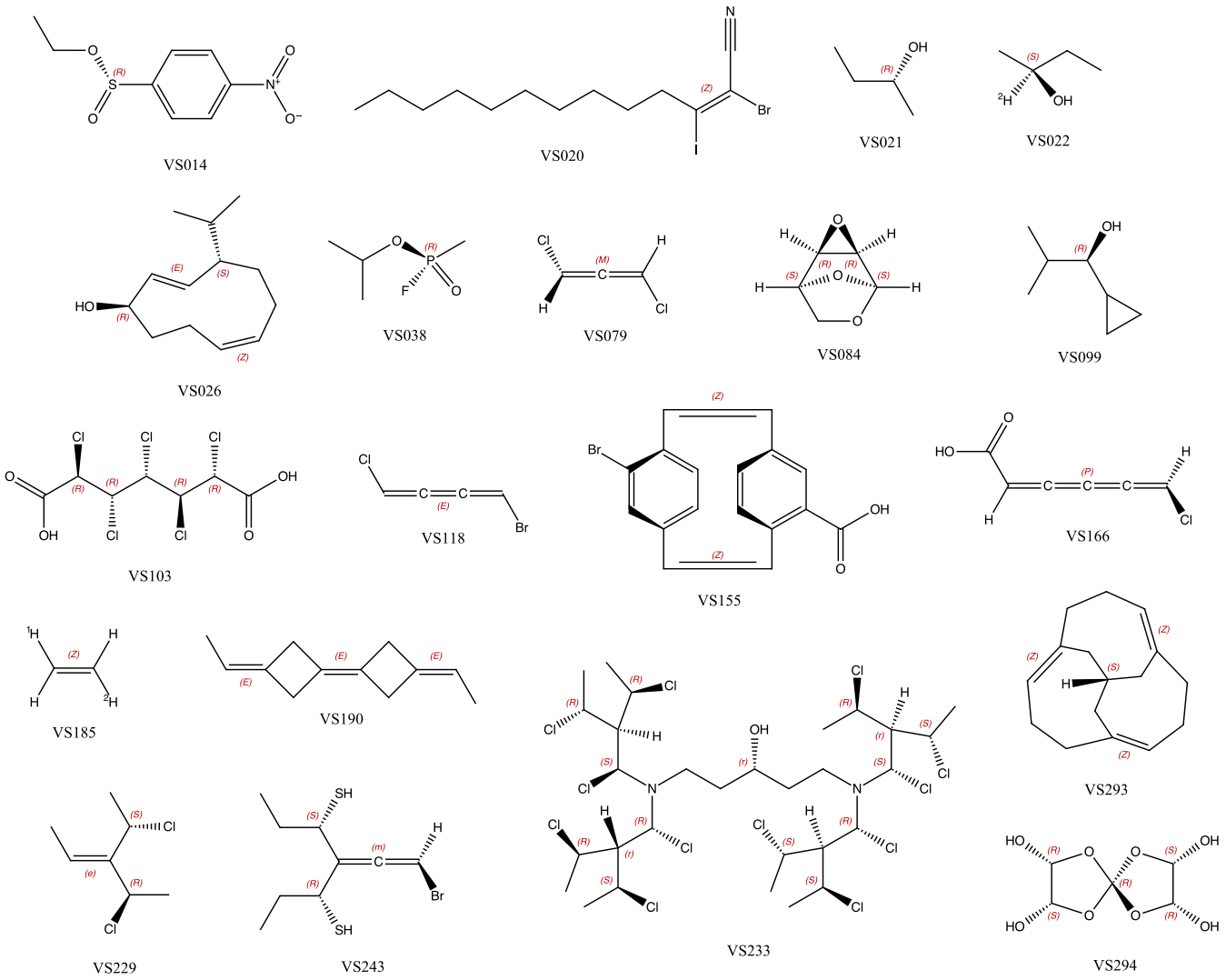


Figure 16.9: *ChemDoodle expertly assigns CIP descriptors, as validated by the Hanson validation suite*

The CIP rules have long been the standard for describing configurations of stereochemical features in a molecule. While flawed, they have seen many revisions over the decades and were clarified by the work of Paulina Mata. These rules were adopted by IUPAC for naming standards and fully described in the Blue books. The most recent CIP rules from IUPAC were then algoritihmically analyzed and standarized by Hanson *et al.* to remove any ambiguities and describe a completely consistent system for CIP assignments.

Hanson, R. M.; Musacchio, S.; Mayfield, J. W.; Vainio, M. J.; Yerin, A.; Redkin, D. Algorithmic Analysis of Cahn-Ingold-Prelog Rules of Stereochemistry: Proposals for Revised Rules and a Guide for Machine Implementation. *J. Chem. Inf. Model.* **2018**, *58*, 1755-1765.

ChemDoodle implements all 6 current CIP rules as well as auxilliary desciptors and mancude ring support. The CIP algorithm in ChemDoodle is validated against the test suite provided by Hanson *et. al.* and is 100% accurate in all 300 test cases provided. A sample of the variety and scope of the Hanson validation suite is shown in Figure 16.9, along with the CIP descriptors assigned by ChemDoodle.

Additionally, NextMove Software released a test suite for stress testing CIP systems, and the results for ChemDoodle are fully accurate and recorded in Figure 16.10.

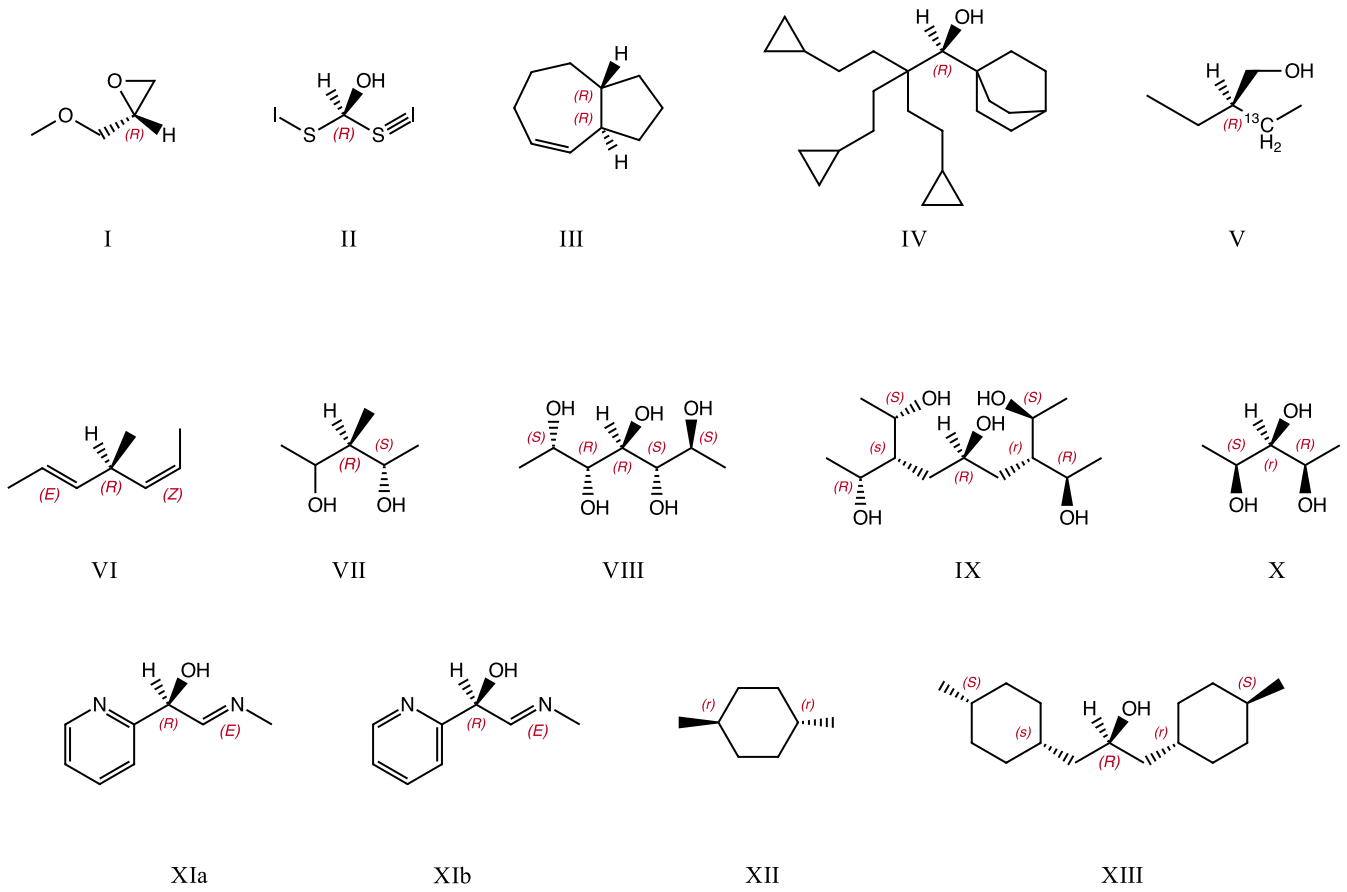


Figure 16.10: *Thorough CIP rule handling*



CIP rules have evolved over the decades, and a correct configuration descriptor from the past may no longer be correct today. As such, you may notice new analysis of a stereochemical feature yields a different configuration. ChemDoodle will match the rules of the latest work from Hanson *et al.*

16.3.1.1 Tetrahedral centers

CIP rules are used to resolve *rectus* (R) and *sinestra* (S) configurations for tetrahedral chiral centers. Pseudo-asymmetric tetrahedral centers are also resolved with lower case *rectus* (r) and *sinestra* (s) identifiers.

Forcing a configuration will interchange the protruding and recessed bonds, if necessary and possible. If only single bonds are present, then the appropriate wedge bonds will be placed when a configuration is forced, if possible.

16.3.1.2 Alkenes and other isolated double bonds

CIP rules are used to resolve *entgegen* (E) or *zusammen* (Z) configurations around double bonds. Any equivalent functional group where the substituents on both sides of the double bond are fixed with respect to each other are included, *e.g.* imines. Pseudo-asymmetric double bonds are also resolved with lower case *entgegen* (e) and *zusammen* (z) identifiers. Some publications and software may designate pseudo-asymmetric double bonds with (seqcis) or (seqtrans) descriptors, but ChemDoodle uses the little (e) and (z) descriptors for brevity.

IUPAC recommendations (*IUPAC Blue Book 2013 P-93.5.1.4.1*) state "In three- to seven-membered monocycles, cyclic double bonds have a 'cis' configuration; the stereodescriptor, 'Z' or 'cis', denoting the configuration of the cyclic double bonds (double bonds that are included in the ring) is permanently omitted. From eight-membered monocycles members onward, cyclic double bonds can be either 'cis' or 'trans'; the stereodescriptors 'Z' and 'E', must be used in preferred IUPAC names, to specify such arrangements; the stereodescriptors 'cis' and 'trans' may be used in general nomenclature." Therefore, ChemDoodle will not produce by default stereochemical configurations for double bonds in any ring with a size of 7 or smaller. To override this recommendation, enable the **Consider Small Ring Double Bonds** option in the **Settings** window in the **Stereochemistry** tab.

Forcing double bond stereochemistry will flip both substituents on one atom's side of the double bond through the double bond axis, if necessary and possible. Double bonds in rings may not have their stereochemical configuration forced to the opposite configuration.

16.3.1.3 Odd-numbered cumulenes

Stereochemical configurations for odd-numbered cumulenes (3 or more consecutive double bonds) are resolved by ChemDoodle. The center bond will be assigned to the correct *entgegen* (E) or *zusammen* (Z) configuration as shown in Figure 16.11. Pseudo-asymmetric odd-numbered cumulenes are also resolved with lower case *entgegen* (e) and *zusammen* (z) identifiers.

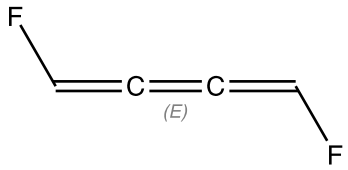


Figure 16.11: *An odd numbered cumulene system with an (E) configuration*

16.3.1.4 Allenes and even-numbered cumulenes

Stereochemical configurations for allenes (2 consecutive double bonds) and even-numbered cumulenes (4 or more consecutive double bonds) are resolved by ChemDoodle.

The center atom will be assigned to the correct *minus* (M) or *plus* (P) configuration to define helicity for the cumulene axis as shown in Figure 16.12. Pseudo-asymmetric allenes and even-numbered cumulenes are also resolved with lower case *minus* (m) or *plus* (p) identifiers. You may have CIP equivalent substituents present on both sides of system as long as each of the pairs of substituents on the same side of the system are CIP unique.

Under IUPAC rules, wedges will need to be correctly drawn on one side and only one side of the cumulene system, however, under MDL/BIOVIA rules, both sides may have wedges, but one side should have more wedges than the other for proper interpretation.

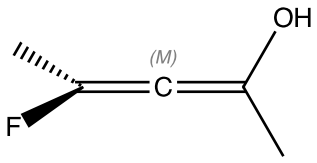


Figure 16.12: *An allene stereocenter with a (M) configuration*

IUPAC recommendations (*IUPAC Blue Book 2013 P-93.4.2.2*) state "Stereodescriptors 'M' and 'P' are preferred to 'R_a' and 'S_a' in preferred IUPAC names." The 'M' and 'P' stereodescriptors define helicity, while 'R_a' and 'S_a' describe axial chirality. For a chirality axis, 'M' corresponds to 'R_a' and 'P' to 'S_a'. You may instruct ChemDoodle to use the descriptors you prefer by defining the **Chirality Axis Descriptors** choice in the **Settings** window in the **Stereochemistry** tab.

16.3.1.5 Atropisomers

Stereochemical configurations for atropisomers are resolved by ChemDoodle. An atropisomer is defined by hindered rotation around a single sigma bond caused by bulky subsituents, typically in the *ortho* positions of aryl rings. The sigma bond will be assigned to the correct *minus* (M) or *plus* (P) configuration to define helicity for the sigma bond axis as shown in Figure 16.13.

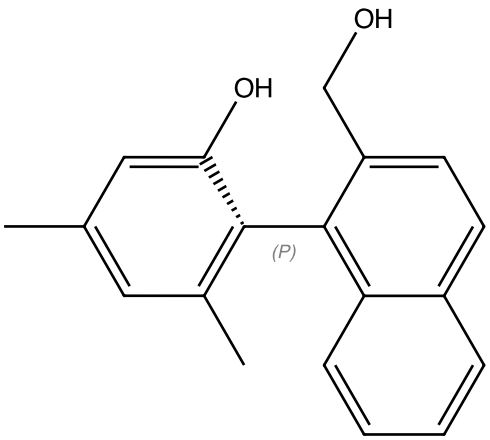


Figure 16.13: *An atropisomer with a (P) configuration*

Currently, ChemDoodle will recognize atropisomerism for a single sigma bond connecting two aromatic rings with at least 3 substitutions or embedded ring atoms in *ortho* positions. Only one bond from an aromatic ring directly connected to the sigma bond needs to be defined as a wedge bond to be recognized.

16.3.1.6 Limitations

Resolving CIP stereochemical configurations is a very computationally expensive graph theoretical algorithm as a thorough CIP hierarchical digraph must be generated for every potential feature. You may notice slowdown in ChemDoodle when analyzing very complex structures, especially with embedded ring systems. Some cases may cause your computer to lock up. One of the ways we reduce this runtime and avoid any freeze is by enforcing a maximum size on the CIP digraph generated for any stereochemical feature at 10000 nodes. If a stereochemical feature exceeds this threshold, then the CIP algorithm will not proceed for the feature and it will not be assigned a CIP descriptor even though it may be defined by a CIP descriptor. This will also affect pseudo-asymmetric stereochemical features in the same structure, as their assignments may be dependent on the configuration of the skipped feature. Figure 16.14 is an example of a structure where the threshold is met and stereochemical features are not assigned a CIP descriptor.

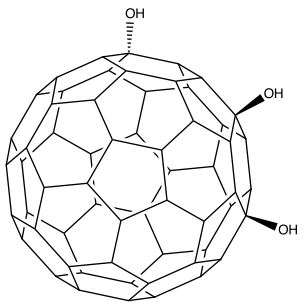


Figure 16.14: *The CIP configurations for this structure would take a very long time to resolve and may likely lockup your computer, so they are skipped*

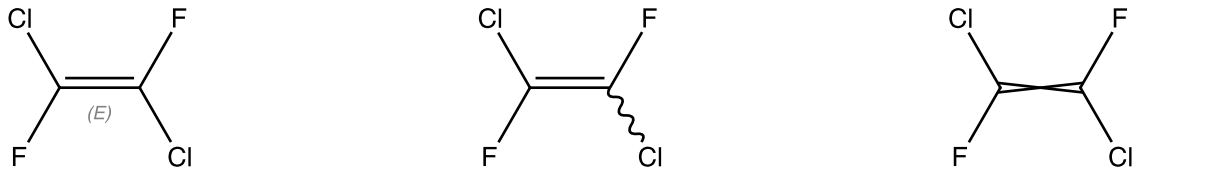
16.3.2 Alkene cis/trans descriptors

The less systematic cis/trans conventions can also be used to define olefin enantiomers, in addition to the CIP E/Z system. However, the CIP E/Z system will work for any double bond presented, while the cis/trans conventions will not return results in ambiguous cases.

16.3.3 Unspecified stereochemical configurations

In some cases, a drawn structure unintentionally conveys a specific stereochemical configuration, when you wish to portray the stereochemical feature as undefined. For instance, if you draw 1,2-dichloro-1,2-difluoroethene, no matter how you draw it, the configuration will be explicitly E, Z or incorrectly drawn.

IUPAC recommendations state a wavy bond should be placed from the stereochemical feature to a single substituent to explictly mark a stereochemical feature as being undefined. MDL recommendations use an ambiguous double bond for undefined alkene stereochemical configurations. ChemDoodle will not recognize geometric features as stereochemical features if either a wavy bond to a substituent or an ambiguous double bond type is used, as the following Figure 16.15 demonstrates. Note using a wavy bond to a substituent is more versatile as it can be applied to stereochemical features that do not contain a double bond.



(a) *Correct drawing always defined* (b) *Using a wavy bond* (c) *Using an ambiguous double bond*

Figure 16.15: *Using a wavy or ambiguous double bond will mark a stereochemical feature as undefined*

16.4 Software functions

16.4.1 Resolving stereochemical configurations

To resolve stereochemistry for structures, execute the following steps:

1. Select the structures or parts of structures with stereochemical features to be resolved with the selection tools.
2. Expand the Structure ⟩ Stereochemistry submenu.
3. Choose the appropriate Assign menu item to resolve stereochemical features of that type.

Note meso centers cannot be resolved until all other stereochemical configurations the meso center configuration is dependent on are resolved first (or at the same time).

You may also access these functions through the right-click menu.

16.4.2 Removing stereochemical configurations

Stereochemical configuration assignments shown as attributes on stereochemical features in your drawings may be quickly removed.

16.4.2.1 In bulk

To remove all of the attributes representing stereochemical configurations in a selection at once, perform the following steps:

1. Select all of the atoms and bonds that are attributed with stereochemical configurations using a selection tool.

2. Use the Structure » Stereochemistry » Remove Assignments menu item.

16.4.2.2 Individually using a mouse tool

To remove a single attribute representing a stereochemical configuration that is displaying in the document, perform the following steps:

1. Hover the attribute that represents the sterechemical configuration and delete it by pressing the backspace or delete key. You can also use the **Eraser** tool  .

16.4.3 Forcing stereochemical configurations

In addition to resolving stereochemical features, ChemDoodle can potentially force a feature into a particular configuration by changing the 2D drawing. To force a stereochemical configuration on an atom or bond, perform the following steps:

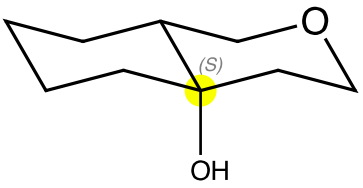
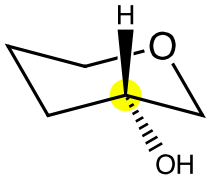
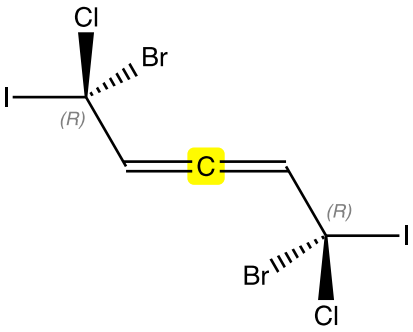
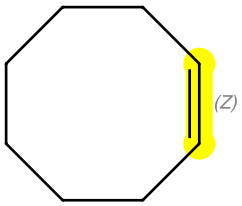
1. Hover the atom or bond on which the configuration will be forced.
2. Right-click on the hovered object.
3. If that object is a stereochemical feature of the molecule, then the Stereochemistry submenu will be present. Expand this submenu.
4. Choose the appropriate Force menu item to force the configuration.

Along with bond and wedge based stereochemical configurations, projection centers may be forced using these functions. These functions will only work on correctly drawn projections and will switch the two substituent locations to invert the drawn configuration, if necessary. For more information on projections, please see the PROJECTIONS section above.

Meso centers cannot be forced until any other stereochemical configurations the meso center configuration is dependent on are resolved first. ChemDoodle will not be able to force stereochemical configurations on incorrectly drawn geometric features, so please refer to the IUPAC recommendations when drawing geometric features.

Stereochemical configurations also cannot be forced when there are no good choices for modifying coordinates or assigning wedges. In these cases, an appropriate warning message will appear stating the software is unable to complete the action. Table 16.1 collects examples for when the force stereo function will not succeed. You should modify the structure manually in these cases.

Table 16.1: Situations where stereochemical configurations cannot be forced

Example (feature highlighted in yellow)	**Stereo Force Error**
	A projection center is constrained by external rings (when forcing to the opposite configuration), and ChemDoodle will not modify ring bond locations when forcing stereochemical configurations.
	A projection center is incorrectly drawn, and neither configuration can be assigned.
	The stereochemical configuration cannot be made explicit, as it would assign or be in conflict with an adjacent stereocenter.
	ChemDoodle will not modify ring bonds when forcing alkene (and odd-numbered cumulene chain) configurations in rings to the opposite configuration.

16.5 Enhanced stereochemistry

When you draw a stereochemical configuration for a chiral center in ChemDoodle, it is recognized by the software exactly as drawn, being one of two enantiomers (Figure 16.16). In certain cases, you may wish to define a current chiral center as one configuration *or* the other (Figure 16.17), or as a mixture of both (*and*, Figure 16.18). This can be defined using the enhanced stereochemistry features in ChemDoodle. You may then output this information into several file formats for use by compatible registration and search engines, for instance.

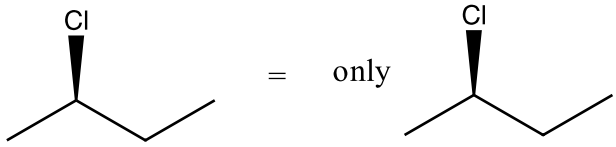


Figure 16.16: *Absolute enhanced stereochemistry is defined by default, designating only a single enantiomer*

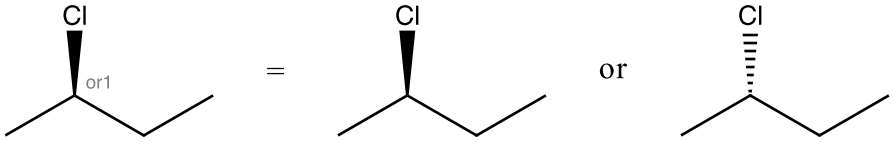


Figure 16.17: *"Or" enhanced stereochemistry defines the current enantiomer or the opposite configuration*

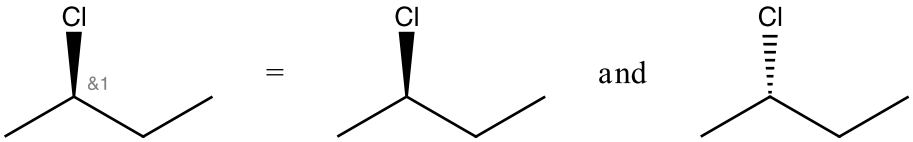


Figure 16.18: *"And" enhanced stereochemistry defines the current enantiomer and the opposite configuration*

Just a note, a racemic mixture is a 1:1 mixture of both enantiomers. While the *and* enhanced stereochemistry designation may be used with a racemic mixture, the actual ratio is not defined using this tool.

16.5.1 Defining enhanced stereochemistry

By default, all chiral centers in ChemDoodle are designated as *absolute* configurations. Therefore, if you draw a *rectus* center, that center may only be interpreted as *rectus*, and if you draw a *sinestra* center, that center may only be interpreted as *sinestra*. No additional steps are required.



Other software may force you to define an *absolute* designation and then show an **abs** tag on the center. This originates from an "undefined" enhanced stereochemistry state, which is not really useful and may be ambiguous in cheminformatics engines. In ChemDoodle, there is no "undefined" state and all centers are designated *absolute* by default. Therefore no **abs** tag is shown in ChemDoodle as it is implied.

To define a chiral center as representing either the *rectus* or *sinestra* configuration (**or** tag), or as representing both the *rectus* and *sinestra* configurations (**&** tag), perform the following steps:

1. Hover the atom (chiral center), where you would like to specify an enhanced stereochemistry designation.
2. Right-click on the atom.

3. If that object is a chiral center of the molecule, then the Enhanced Stereochemistry submenu will be present. Expand this submenu.

4. By default, the Absolute designation will already have been applied. You may choose the Or and And designations instead.

If a chiral center is defined with an enhanced stereochemistry designation other than *absolute*, stereochemistry assignment functions will disregard the center. For instance, you will not be able to assign a CIP configuration to a center flagged with an *or* or *and* enhanced stereochemistry.

16.5.2 Grouping

You may have noticed the numbers following the *and* and *or* tags. These are groupings. And when you group enhanced stereochemistry designations over several chiral centers, you are defining relative stereochemistry. Because *absolute* enhanced stereochemistry designations define only a single configuration, they are always independent of other centers and therefore have no associated grouping.

Take for example, Figure 16.19. The two chiral centers in this molecule are both designated as *or*. Therefore, we have either *rectus-rectus* or *rectus-sinestra* or *sinestra-rectus* or *sinestra-sinestra*. However, if we place both chiral centers in the same enhanced stereochemistry group as shown in Figure 16.20, the definition becomes *rectus-rectus* or *sinestra-sinestra*.

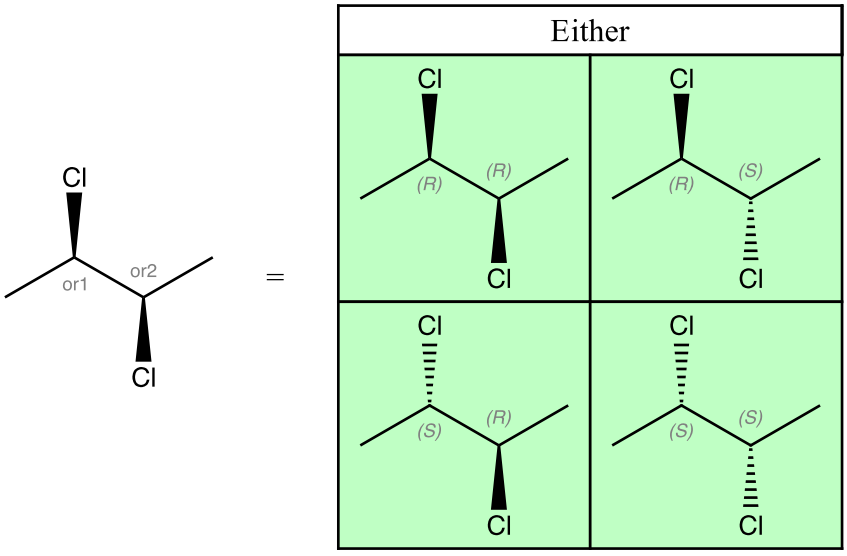


Figure 16.19: *Enhanced stereochemistry, using "or" operators on two separate chiral centers in two separate groups, representing all 4 stereoisomers*

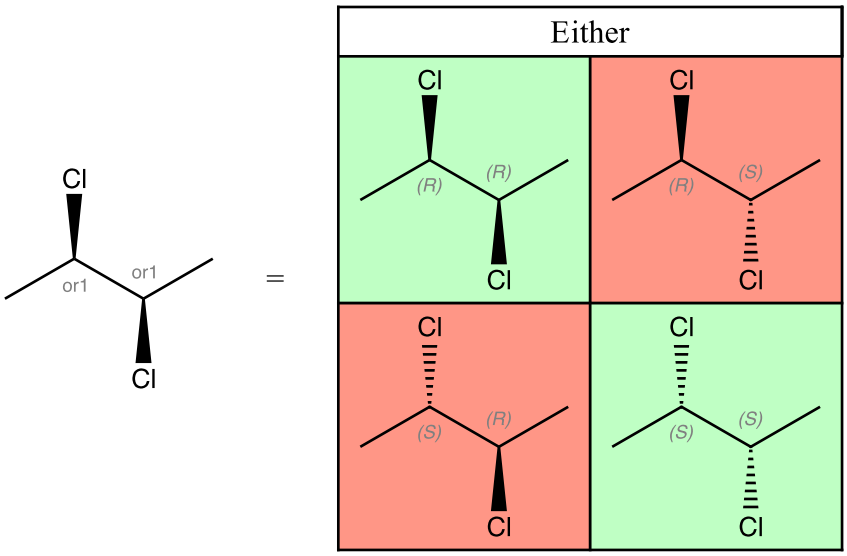


Figure 16.20: *Enhanced stereochemistry, using "or" operators on two separate chiral centers in the same group, representing only a pair of diastereomers*

Similarly in Figure 16.21, the two chiral centers in this molecule are both designated as *and*. Therefore, we have a mixture of *rectus-rectus* and *rectus-sinestra* and *sinestra-rectus* and *sinestra-sinestra*. When we place both chiral centers in the same enhanced stereochemistry group as shown in Figure 16.22, the definition becomes *rectus-rectus* and *sinestra-sinestra*.

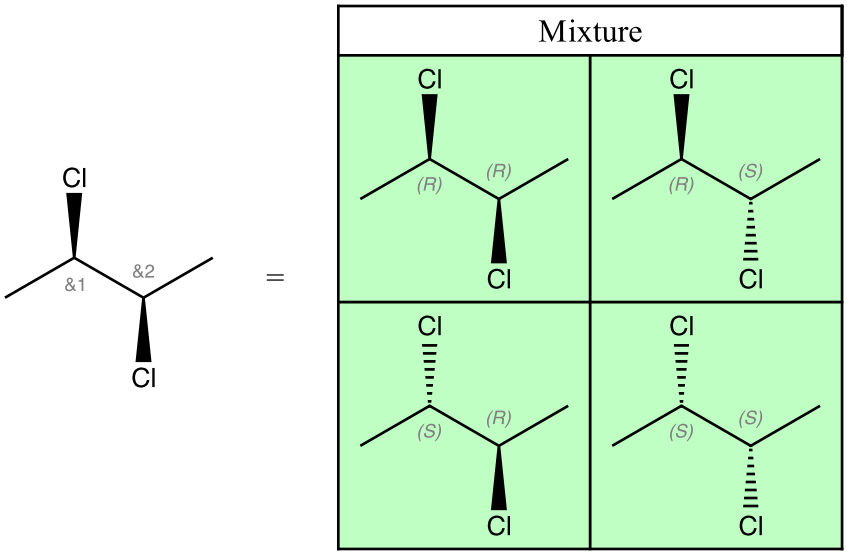


Figure 16.21: *Enhanced stereochemistry, using "and" operators on two separate chiral centers in two separate groups, representing all 4 stereoisomers*

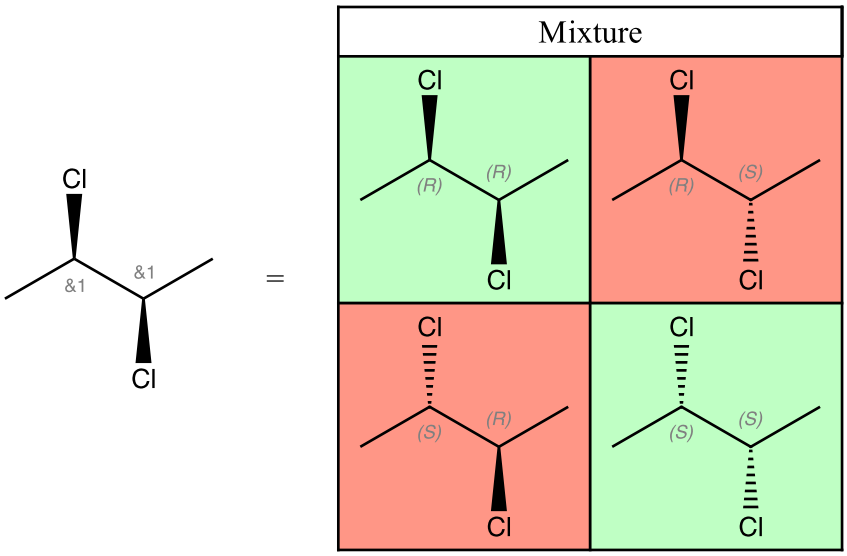


Figure 16.22: *Enhanced stereochemistry, using "and" operators on two separate chiral centers in the same group, representing only a pair of diastereomers*

The *and* and *or* groups are independent of each other, so they should be permuted with their operator, where the *and* operator takes precedence.

To define an absolute stereochemistry designation to a chiral center using a desired grouping number, perform the following steps:

1. Hover the atom (chiral center), where you would like to specify an enhanced stereochemistry designation.
2. Right-click on the atom.
3. If that object is a chiral center of the molecule, then the Enhanced Stereochemistry submenu will be present. Expand this submenu.
4. Choose the Or x... or And x... menu item.
5. A window will appear prompting you to enter the desired grouping number as shown in Figure 16.23. Enter a positive integer greater than 0.

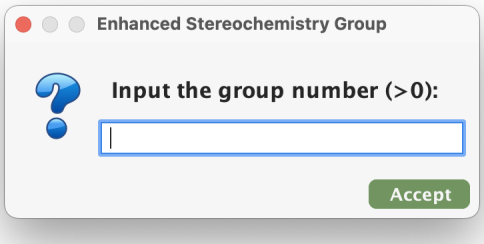


Figure 16.23: *Prompt for enhanced stereochemistry grouping number*

6. Press the **Accept** button to set the new enhanced stereochemistry designation and group number to the chiral center.

When using the regular enhanced stereochemistry menu items, ChemDoodle will automatically choose a grouping number that is 1 greater than the maximum grouping number present in the current document for that operator.

16.5.3 Removing an enhanced stereochemistry designation

To remove an enhanced stereochemistry designation, perform the following steps.

1. Hover the atom with the enhanced stereochemistry designation you would like to remove.
2. Right-click on the atom.
3. Select the Enhanced Stereochemistry 〉 Absolute menu item.

You may also simply hover the enhanced stereochemistry attribute tag directly with a selection tool and then press the backspace or delete key.

16.5.4 File format support

In ChemDoodle, the enhanced stereochemistry designations are not useful beyond a quick graphical explanation. Other systems may do more with the enhanced stereochemical designations, such as chemistry search engines. To communicate the information to those systems, ChemDoodle outputs enhanced stereochemistry designations into the following compatible formats:

- CambridgeSoft ChemDraw Exchange (*.cdx*)
- CambridgeSoft ChemDraw XML (*.cdxml*)
- ChemAxon Marvin Document (*.mrv*)
- iChemLabs ChemDoodle Document (*.icl, .icxml*)
- iChemLabs ChemDoodle JSON (*.js*)
- MDL MOLFiles (*.mol*, *.mdl*)*
- MDL RDFiles (*.rdf*, *.rd*)*
- MDL RXNFiles (*.rxn*)*
- MDL SDFiles (*.sdf*, *.sd*)*
- MMI SketchEl Molecule (*.el*)*

All of these formats completely support enhanced stereochemistry designations of *absolute*, *or* and *and*, as well as grouping. Note the MDL connection table formats (marked with asterisks), only support enhanced stereochemistry using the V3000 extended connection tables. By default, ChemDoodle outputs V2000 MDL connection tables for maximum compatibility. To have ChemDoodle instead output V3000 extended connection tables, in the **Settings** window, under the **Chemical Files** tab, under the **MDL Connection Table Files** subsection, enable the **Output V3000 Extended Connection Table** option.

The V2000 MDL connection tables do support a *chiral* flag for each individual structure. ChemDoodle will set this flag to true on molecular output where one or more chiral centers is present and all have an enhanced stereochemistry designation of *absolute*. Of course, this limitation of the V2000 connection table does not allow full recovery of the enhanced stereochemistry information. When inputting V2000 connection tables without a *chiral* flag set, ChemDoodle will automatically define the enhanced stereochemical designations of chiral centers as *absolute*, *or* and *and* in the default groupset 1. The choice of *absolute*, *or* and *and* will be determined by the **No Chiral Flag, Input Centers as** option in the **Settings** window, under the **Chemical Files** tab, under the **MDL Connection Table Files** subsection.

One final note about MDL connection table files. ChemDoodle will only set the *chiral* flag and output enhanced stereochemistry information if the molecule contains a chiral center and that center is resolved. Otherwise, ChemDoodle would need to run computationally intensive CIP algorithms on every molecule output to an MDL file. So, to make sure your enhanced stereochemistry information is output correctly, before saving your MDL file, select the molecule(s) and execute the Structure 〉 Stereochemistry 〉 Assign All(CIP) menu item.

CHAPTER 17

Sharing Information

Contents

17.1 Overview **419**

17.2 The system clipboard **419**
17.2.1 MIME types 419
17.2.2 Clipboard settings 420
17.2.3 Non-chemical text 420
17.2.4 Images 420
17.2.4.1 Scalable vector graphics 421
17.2.4.2 Embedded chemical data 421
17.2.5 Chemical data 421
17.2.6 Non-MIME types 422

17.3 Copying data to other applications **422**
17.3.1 Using the copy function 422
17.3.2 Using the copy as function 422
17.3.3 Copying formatted text 422

17.4 Pasting data from other applications **423**
17.4.1 Where content is pasted 423
17.4.2 Paste and match style 423
17.4.3 Paste special… 423
17.4.4 Pasting text as chemical data 424

17.5 File Input/Output **424**
17.5.1 Hiding file types when saving 424
17.5.2 File output settings 425

17.6 Chemical format compatibility **426**
17.6.1 Native file format 426
17.6.2 Adherence to third party specifications 426
17.6.3 Use caution saving third party formats 427
17.6.4 Testing third party file type output 427
17.6.5 Supported chemical file types 427
17.6.6 Chemistry file annotations 428
17.6.7 Chemistry file conversion tool 429
17.6.8 Chemistry file options 430
17.6.8.1 Input partial charges 431
17.6.8.2 Center output in molecular formats 431
17.6.8.3 Warn about object compatibility 432
17.6.9 iChemLabs ChemDoodle Document 432
17.6.9.1 Embed images 432
17.6.10 ChemDraw files 432
17.6.10.1 Combine multiple pages on input 432
17.6.10.2 Breakup groups on input 432
17.6.10.3 Discard lone invisible atoms 432
17.6.11 ChemAxon Marvin Document 432
17.6.11.1 Lone Pair Input 432
17.6.12 Chemical Markup Language 432
17.6.12.1 Output dimension 433
17.6.12.2 Store data in arrays 433
17.6.12.3 Store reaction molecules 433
17.6.13 Daylight SMILES 433

17.6.13.1 Allow extensions . . . 433
17.6.13.2 Kekulize input . . . 433
17.6.13.3 Infer ambiguous double bonds on input . . . 433
17.6.13.4 Asterisk (*) as query on input . . . 433
17.6.13.5 Output aromaticity . . . 433
17.6.13.6 Output all explicit hydrogens . . . 433
17.6.13.7 Output stereochemistry . . . 434
17.6.13.8 Output implied double bond stereo . . . 434
17.6.14 Gaussian CUBE . . . 434
17.6.14.1 Output unit . . . 434
17.6.15 Gaussian input . . . 434
17.6.15.1 Output atom ID type . . . 434
17.6.15.2 Output z-matrix . . . 434
17.6.15.3 Use variables in output (z-matrix only) . . . 434
17.6.16 IUPAC InChI . . . 434
17.6.16.1 Include auxiliary information . . . 434
17.6.16.2 Include InChI key . . . 434
17.6.17 IUPAC JCAMP-DX . . . 434
17.6.17.1 Convert Hz to PPM . . . 434
17.6.18 ISIS Sketch files . . . 435
17.6.18.1 Binary output format . . . 435
17.6.19 MDL connection table files . . . 435
17.6.19.1 Input data records as tables . . . 435
17.6.19.2 Output FAIR data headers . . . 435
17.6.19.3 Output eCTD data headers . . . 435
17.6.19.4 No chiral flag, input centers as . . . 435
17.6.19.5 Bond length conversion . . . 435
17.6.19.6 Output v3000 extended connection table . . . 435
17.6.19.7 Output hydrogen counts . . . 435
17.6.19.8 Output atom stereo parity . . . 435
17.6.20 RCSB macromolecular formats . . . 436
17.6.20.1 Read CONECT records . . . 436
17.6.20.2 Output higher bond orders (unofficial) . . . 436
17.6.20.3 Deduce covalent bonds if none found . . . 436
17.6.21 XYZ . . . 436
17.6.21.1 Atom identifier . . . 436

17.7 Round-trip editing . . . 436
17.7.1 Support . . . 436
17.7.2 Windows . . . 437
17.7.2.1 Setup . . . 437
17.7.2.2 Clipboard Settings . . . 437
17.7.2.3 Procedure . . . 437
17.7.2.4 Troubleshooting . . . 438
17.7.3 macOS . . . 438
17.7.3.1 Setup . . . 438
17.7.3.2 Clipboard Settings . . . 438
17.7.3.3 Procedure . . . 439
17.7.3.4 Workaround for iWork Applications . . . 439
17.7.3.5 Troubleshooting . . . 439
17.7.4 Linux . . . 440
17.7.5 LibreOffice . . . 440
17.7.5.1 Compatibility . . . 440
17.7.5.2 Setup . . . 440

17.7.5.3 Clipboard Settings . . . 441
17.7.5.4 Procedure . . . 441
17.7.5.5 Troubleshooting . . . 443
17.7.5.6 Questions and Answers (Q&A) . . . 445

17.8 Chemical data recovery . . . **445**
17.8.1 Level 0: Reading chemical files . . . 446
17.8.2 Level 1: Pasting directly from other chemical applications . . . 446
17.8.3 Level 2: Pasting embedded data from other (non-chemical) applications . . . 446
17.8.4 Level 3: Recovering data from Microsoft Office files . . . 447
17.8.5 Summary . . . 449

17.9 Image format compatibility . . . **449**
17.9.1 Supported input formats . . . 449
17.9.2 Supported output formats . . . 449
17.9.3 Importing chemical content from images . . . 450
17.9.4 Exporting the document to an image . . . 450
17.9.5 Exporting only certain objects to an image . . . 450
17.9.6 Image sizing . . . 450
17.9.6.1 Previewing the image size . . . 452
17.9.7 Image output options . . . 452
17.9.7.1 Automatically Size . . . 453
17.9.7.2 Force Output Size . . . 453
17.9.7.3 Scale Contents to Fit . . . 453
17.9.7.4 Border Buffer . . . 453
17.9.7.5 Scale (bitmap only) . . . 453
17.9.7.6 Resolution (bitmap only) . . . 454
17.9.7.7 Transparency (bitmap only) . . . 454
17.9.7.8 Color Space (bitmap only) . . . 454
17.9.7.9 Compression Quality (bitmap only) . . . 454
17.9.7.10 Text as Shapes (vector only) . . . 454
17.9.8 Encapsulated Postscript . . . 454
17.9.8.1 Preserve chemnum Tags . . . 454
17.9.8.2 chemnum Tag . . . 454
17.9.9 CompuServ graphics interchange format options . . . 454
17.9.9.1 Semi-transparent pixel merge . . . 454
17.9.10 Web scalable vector graphics options . . . 455
17.9.10.1 Use CSS output . . . 455

17.10 Inserting images . . . **455**

17.11 Chemical image recovery . . . **456**
17.11.1 Input . . . 457
17.11.2 Support . . . 457
17.11.2.1 Atoms . . . 457
17.11.2.2 Bonds . . . 457
17.11.2.3 Rings . . . 457
17.11.2.4 Attributes . . . 457
17.11.2.5 Shapes . . . 457
17.11.3 Performance . . . 458
17.11.3.1 Optical character recognition . . . 458

17.12 Printing . . . **459**
17.12.1 Page setup . . . 459
17.12.2 Flipping the page orientation . . . 459
17.12.3 Print preview . . . 459
17.12.4 Printing a document . . . 459

17.1 Overview

ChemDoodle has advanced functions for interacting with other applications on your computer. This is essential for importing graphics into word processors or for transferring chemical data into other scientific applications.

This section introduces the new user to ChemDoodle's system clipboard capabilities. It covers the following topics:

- Introducing the system clipboard.
- How to copy data and graphics from ChemDoodle into other applications.
- How to copy data and graphics from other applications into ChemDoodle.
- What types of data can be transferred?
- What is a *MIME* type?
- What text formats are supported?
- What image formats are supported?
- What chemical formats are supported?
- How to annotate chemical files.
- How to save images.
- How to insert images.
- How to convert between chemical file types.
- How to take advantage of roundtrip editing.

17.2 The system clipboard

The system clipboard is a construct of the operating system that contains data for sharing between applications. Only one application can place data on the system clipboard at a time. Other applications can then see that data and load it. This construct forms the basis for copy and paste functionality. ChemDoodle will place a wide range of chemical, text and graphic data on the system clipboard as well as associate that data with the correct *MIME* types for other applications to use.

17.2.1 MIME types

A *MIME* type is an identifier to define the data it is associated with. For example, a structure can be represented in *MDL MOLFile* format. The *MDL MOLFile* format is a plain text format and can be associated with the *MIME* type, "text/plain". However, this is a very generic description and other applications will only recognize it as plain text, rather than as a chemical structure. Therefore a different *MIME* type is associated with this data, "chemical/x-mdl-molfile", to define it as a structure in the *MDL MOLFile* format. In this manner, other applications will recognize this data as a chemical.

ChemDoodle follows the MIME standards put forth by the Chemical MIME Project (https://www.ch.ic.ac.uk/chemime/). This should be regarded as the standard; however, many chemical software developers do not follow these rules, thereby causing issues when transferring data between chemical applications.

Additionally, since many items can be present on the system clipboard at once, applications may paste a certain data type by default that may not be the data you want to paste. For instance, Microsoft Word can paste both text data types and image data types. If both are present on the system clipboard, Microsoft Word will automatically select the text data type when pasting, even if you wanted the image to be pasted. There can even be different image types, confusing the situation further.

Therefore, ChemDoodle allows you to define which data is placed on the system clipboard and how the data is to be used when working with other applications.

17.2.2 Clipboard settings

ChemDoodle can transfer data to almost any application that has been created. But it is impossible for ChemDoodle to determine which data should be transferred. Therefore, you need to set the appropriate copy settings to make sure any ambiguities are resolved with the application you are pasting to. Copy settings can be set in the **Settings** window under the **Clipboard** tab as shown in Figure 17.1. These settings will allow you to explicitly control what data ChemDoodle will transfer to other applications.

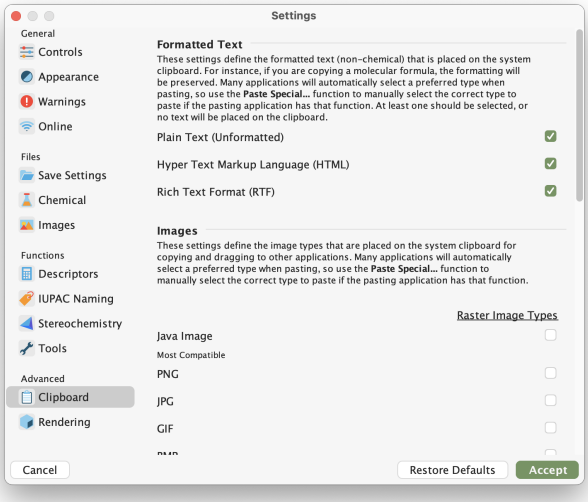


Figure 17.1: *Copy Settings*

To work with other applications, first decide what type of data you would like to transfer and what types of data the other application accepts. Then set the appropriate copy settings to continue. By default, ChemDoodle is set up for the optimal communication of graphics into common word processors.

17.2.3 Non-chemical text

Text may be copied from ChemDoodle that isn't a chemical, for instance a calculated thermodynamic property or a formatted IUPAC name. ChemDoodle supports the following text types for communicating with the system clipboard:

- **Plain Text (Unformatted)** - Only the text is present; there is no formatting.
- **Hyper Text Markup Language (HTML)** - The formatted text is presented in HTML format. This is great for working with web editors and most word processing tools.
- **Rich Text Format (RTF)** - The formatted text is presented in RTF format. This is a very common formatted text protocol that most applications can receive.

At least one should be selected, or no text will be placed on the clipboard when you copy text from ChemDoodle.

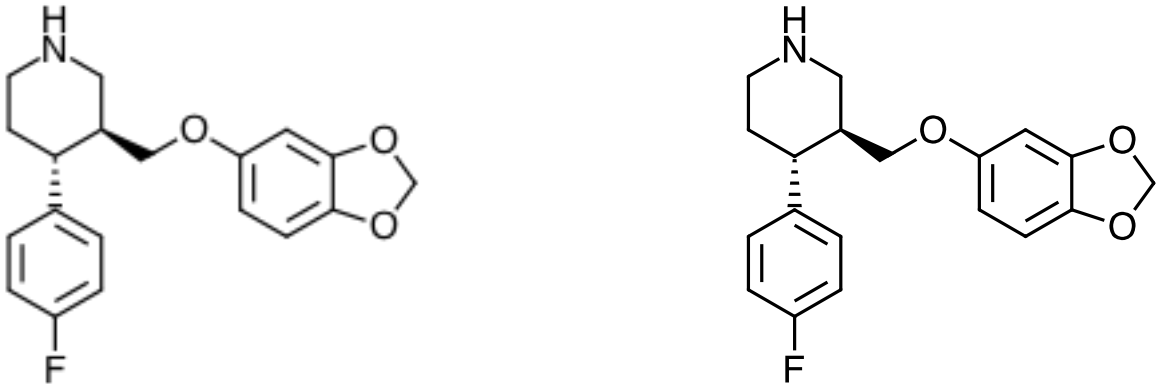
17.2.4 Images

There are two main classes of images:

- **Raster Image Types** - Raster image types are compatible with almost any program that can handle images, but they are not scalable in resolution. These are all disabled by default as many applications will paste a raster image instead of a vector image if both are present on the system clipboard.
- **Vector Image Types** - Vector images are much more versatile and will remain crisp and clear regardless of resizing or transformation. Vector image types are not universally accepted by applications.

17.2.4.1 Scalable vector graphics

There are two types of images, raster and vector. Raster images are traditional images and define a rectangle of pixels and their colors, while vector images define drawing instructions for rendering it. When resizing, the raster will become blurry, pixelated and lose its quality while the vector image will remain crisp and clear. Figure 17.2a shows a raster image of a structure, while Figure 17.2b shows a vector image of the same structure. Both were created by ChemDoodle. Try zooming in on both images using your PDF reader and you can see the difference in quality for yourself.



(a) *A Raster Image* (b) *A Vector Image*

Figure 17.2: *Raster Image vs. Vector Image*

Raster images will suffer from this issue with any change of resolution, including printing to a printer. Because of this, we recommend you insert vector images into your documents. The only downside to using vector graphics is that some programs may not support them. ChemDoodle compatibility with third party applications is discussed in APPENDIX: THIRD PARTY APPLICATIONS.

If you must use a raster image, then ChemDoodle provides high resolution options (such as scaling and DPI control) for some raster formats as discussed in the IMAGE OUTPUT OPTIONS section later in this chapter.

17.2.4.2 Embedded chemical data

Some programs communicate chemical data embedded in images. It is possible to embed chemical data in both raster and vector image types. See the IMAGE FORMAT COMPATIBILITY section for more information.

17.2.5 Chemical data

There are two main types of chemical data that may be transferred:

- **Text Types** - Some common chemical formats are listed here to be pasted as plain text into other applications. Contains a line or lines of text that will be interpretable by other applications as plain text. All text data will be interpreted as plain text by other applications and any chemical significance will be lost unless the receiving application intends to receive the chemical data as text and will create the chemical from it. Only one text data type will be placed on the system clipboard at a time.
- **Chemical Types** - Chemical types include chemical structure information and may include styling and other features. Only other chemical aware programs will see these.

17.2.6 Non-MIME types

There are some non-*MIME* type based chemical clipboard protocols that are also available for working with a number of programs. ChemDoodle includes the *MDLCT* and *MDLSK* clipboard formats for communicating chemical data on Windows. These formats are listed in the **Chemical Types** section.

17.3 Copying data to other applications

17.3.1 Using the copy function

To copy data from ChemDoodle into other applications, execute the following steps:

1. Determine which data you would like to transfer and the types of data that the other application can accept and configure the copy settings in the **Settings** window under the **Clipboard** tab accordingly.
2. Select the objects in the current document that you would like to copy using the content selection tools.
3. Click on the Edit ⟩ Copy menu item or press its menu accelerator keyboard shortcut which is ctrl + C. You can also press the **Copy** button  in the **Content** toolbar.
4. Use the **Paste** function present in the other application to paste the content. If the other application has a **Paste Special...** function, you may use that to specify which data type to paste if multiple are present.

17.3.2 Using the copy as function

The **Copy As** functions are preset shortcuts for placing specific chemical data on the system clipboard without changing the data types to be copied in the **Clipboard** tab of the **Settings** window.

Select the content in the document to be copied and then select one of the menu items in the Edit ⟩ Copy As submenu. The most popular data types are supported. These functions will place both text and chemical data on the system clipboard for maximum compatibility with third party applications. This function will not place image data on the system clipboard.

17.3.3 Copying formatted text

Most text that is copied is unformatted text, but there will be many times when you would like to preserve the formatting of text between applications, such as when copying a molecular formula or IUPAC name. You can copy formatted text from most objects in ChemDoodle that present formatted text. This includes objects like auto-updating labels and atom labels. Just right-click on the object with a selection tool while nothing is selected and choose the Copy Text menu item. You can then paste that formatted text into another application that supports formatted text.

Certain widgets, such as the **Properties** widget will also place formatted text on the system clipboard.

17.4 Pasting data from other applications

To paste data from other applications into ChemDoodle, execute the following steps:

1. Use the copy function present in the other application.
2. Click on the Edit ⟩ Paste menu item or press its menu accelerator keyboard shortcut which is ctrl + V to paste the highest priority data to the current document. You can also press the **Paste** button in the **Content** toolbar.

17.4.1 Where content is pasted

The pasted content will be located according to the following rules:

1. If your mouse pointer is hovering over the document, the center of the pasted content will be located at the mouse pointer.
2. If the mouse pointer is not hovering over the document, and the lasso is active, then the pasted content will appear to the bottom-right of the lassoed content. If the mouse pointer is not hovering over the document and the lasso is inactive, then the pasted content will appear at the top left of the current viewed page of the document.

17.4.2 Paste and match style

When styled chemical structure data is pasted from another source, including ChemDoodle content pasted between currently edited documents, that content will retain its original styling. Instead of selecting the Content ⟩ Conform to Current Styles menu item after pasting, you can save some time and directly paste and conform the settings by choosing the Edit ⟩ Paste and Match Style menu item.

17.4.3 Paste special...

Since an application can place different data types on the system clipboard, the data that ChemDoodle chooses to paste by default may not always be the desired type. In general, ChemDoodle pastes chemical data in preference to images, and images in preference to text. If you would like to paste a data type that is not chosen by default by ChemDoodle, click on the Edit ⟩ Paste Special... menu item. A window will appear listing all ChemDoodle compatible data and options for loading it as shown in Figure 17.3. Just select the list item you would like to paste and press the **Paste** button.

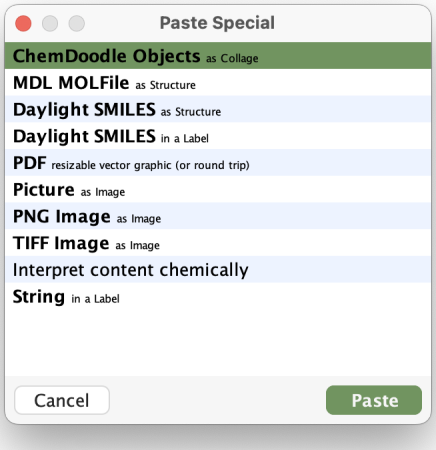


Figure 17.3: *Paste Special Window*

17.4.4 Pasting text as chemical data

Sometimes it may be necessary to handle text data from the system clipboard. For instance, a chemical application may paste the *MOLFile* format in plain text, or you may be copying a *SMILES* string from a web browser. ChemDoodle provides the **Paste Text as Chemical** function to conveniently handle this situation. To paste text content from another application as chemical data, execute the following steps:

1. Use the copy function present in the other application to place the text on the system clipboard.
2. Expand the Edit > Paste Text as Chemical submenu.
3. Depending on the type of data being represented by the text (which you will know), select the appropriate menu item in the submenu to paste.

Using this method, any of the line notations that ChemDoodle understands can be pasted as chemical data. Additionally, there is an XYZ-Like Data menu item for pasting text as chemical data in an XYZ-like format. This option will automatically scan the text to extract atom labels and positions. The final menu item in this submenu is Guess Chemical Format. This will detect the chemical format of the text data on the system clipboard and paste the chemical data accordingly, which is perfect for ASCII or XML data types, such as *MOLFiles* or *CML*. This function will alert you if no chemical format could be associated with the text data.

17.5 File Input/Output

ChemDoodle inputs and output the following categories of file data, discussed in detail later in the chapter:

1. **Chemistry files** - see the CHEMICAL FORMAT COMPATIBILITY section
2. **Images** - see the IMAGE FORMAT COMPATIBILITY section

17.5.1 Hiding file types when saving

You can choose to hide certain file types from the **Save As** file choosers. Use this feature to reduce the number of formats shown when saving if you only use a few types and want to save time from scrolling or if you find the file types you do not commonly use to be distracting. You set what types are excluded by pressing the **Format Excludes List** button in the **Save Settings** tab of the **Settings** window. The **File Chooser Format Exclusions** window will appear to hide selected chemical and image file types as shown in Figure 17.4.

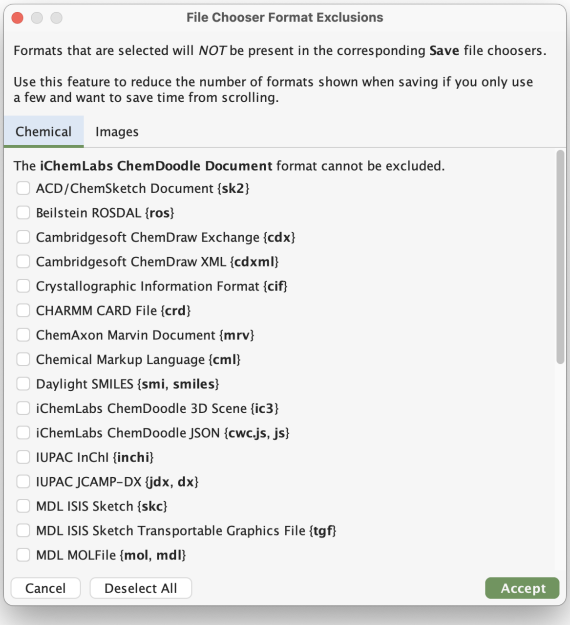


Figure 17.4: *Excluding file types from the Save As file choosers*

Formats that are selected will *NOT* be present in the corresponding **Save As** file choosers. The main ChemDoodle format cannot be excluded. If all image types are excluded, the *PNG* type will be default.

17.5.2 File output settings

You may define the default file output settings in the **Settings** window under the **Files** tabs. These are the default settings that will be used when outputting files. You will also be given the opportunity to manually define settings to be used when saving each individual file. Such settings will be displayed after you choose a location to save your file, and only relevant settings for that file type will be presented, as shown in Figure 17.5. This way, you have full control over the output of files from ChemDoodle.

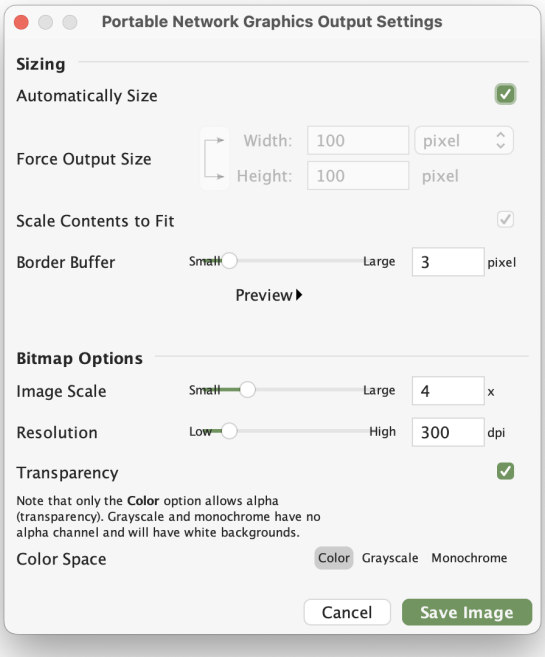


Figure 17.5: *When saving a file, an individualized output settings window will be presented, in this case for PNG image output*

You may specify in the **Settings** window whether the individualized output settings window is displayed for each category of file data. In the **Save Settings** tab, under the **Output Options** section, select or deselect the checkbox for the specific category of file data you wish to change. If selected, each time you save a file for that category of file data, the individual settings window for that file type will be displayed. If not selected, each time you save a file for that category of file data, the default settings will be used.

17.6 Chemical format compatibility

ChemDoodle supports one of the largest chemical format libraries in the industry and can interpret various chemical formats for input to and output from other chemical applications. ChemDoodle can currently read and write 36 different chemical file types.

17.6.1 Native file format

The *ChemDoodle Document* is the native format of the ChemDoodle application, and no data loss should occur when saving your work to this format.

17.6.2 Adherence to third party specifications

File formats implemented in ChemDoodle strictly follow their published specifications. ChemDoodle does not take liberties with their rules or inject ChemDoodle-only content into them. All file format objects and properties are mapped as closely as possible to objects and properties in ChemDoodle. Specification references can be found by selecting the Help » References menu item.

ChemDoodle will try to interpret all third party files as best as possible, so if you do find a file that doesn't read well, please send it to us so we can improve our compatibility.

17.6.3 Use caution saving third party formats

ChemDoodle does its best to preserve the data it reads in from third party formats, however it may not be perfect as those formats may have been intended for systems that are very different from ChemDoodle. For instance, one program may define a charge by placing a text box near an atom, while ChemDoodle defines a charge by associating a charge attribute with that atom. When read, ChemDoodle may decide to convert that text box to a charge attribute, thereby changing the data that is in the file.

When saving as third party files, ChemDoodle will display a warning as a reminder before allowing you to continue. These warnings can be disabled in the **Settings** window under the **Chemical Files** tab.

That being said, it is very important that you carefully consider whether to allow ChemDoodle to save over third party data files as ChemDoodle may not retain all essential information that the other program requires.

Instead, we recommend that you first save a copy of that file to edit, instead of saving over files created by other applications.

17.6.4 Testing third party file type output

If you are unsure about whether your document will be saved in its entirety to a third party format, save a test file in ChemDoodle, close the document you just saved, and then reopen the file in ChemDoodle. If some content is missing or any object properties have changed in some way, then the format you are trying to save to does not support those objects and/or properties or ChemDoodle does not yet support the input/output of those objects and/or properties for that format.

17.6.5 Supported chemical file types

1. ACD/ChemSketch Document (*.sk2*)
2. Beilstein ROSDAL (*.ros*)
3. CambridgeSoft ChemDraw Exchange (*.cdx*)
4. CambridgeSoft ChemDraw XML (*.cdxml*)
5. Crystallographic Information Format (*.cif*)
6. CHARMM CARD File (*.crd*)
7. ChemAxon Marvin Document (*.mrv*)
8. Chemical Markup Language (*.cml*)
9. Daylight SMILES (*.smi*, *.smiles*)
10. Gaussian Cube (*.cub*, *.cube*)
11. Gaussian Input (*.gjf*, *.gau*, *.gzmat*, *.com*)
12. HyperChem HIN (*.hin*)
13. iChemLabs ChemDoodle Document (*.icl, .icxml*)
14. iChemLabs ChemDoodle 3D Scene (*.ic3*)
15. iChemLabs ChemDoodle JSON (*.cwc.js*)
16. IUPAC InChI (*.inchi*)
17. IUPAC JCAMP-DX (*.jdx*, *.dx*)
18. MDL ISIS Sketch File (*.skc*)
19. MDL ISIS Sketch Transportable Graphics File (*.tgf*)

20. MDL MOLFiles (*.mol*, *.mdl*)
21. MDL RDFiles (*.rdf*, *.rd*)
22. MDL RXNFiles (*.rxn*)
23. MDL SDFiles (*.sdf*, *.sd*)
24. MMI SketchEl Molecule (*.el*)
25. Molinspiration JME String (*.jme*)
26. ORCA Input File (*.orcainp*, *.inp*)
27. RCSB BinaryCIF (*.bcif*)
28. RCSB Macromolecular Crystallographic Information File (*.cif*, *.mcif*, *.mmcif*)
29. RCSB Protein Data Bank Files (*.pdb*, *.ent*)
30. RCSB Protein Data Bank Markup Language (*.xml*, *.pdbml*)
31. Schrödinger MacroModel (*.mmd*, *.mmod*)
32. Schrödinger Maestro (*.mae*)
33. Standard Molecular Data (*.smd*)
34. Tripos Mol2 (*.mol2*, *.ml2*, *.sy2*)
35. Tripos Sybyl Line Notation (*.sln*)
36. XYZ Files (*.xyz*)

17.6.6 Chemistry file annotations

Annotations can be read and written to files where possible. Each document has its own set of annotations. To view previously defined annotations, edit them or create your own, select the File ⟩ Annotations... menu item. Then edit the fields shown in Figure 17.6.

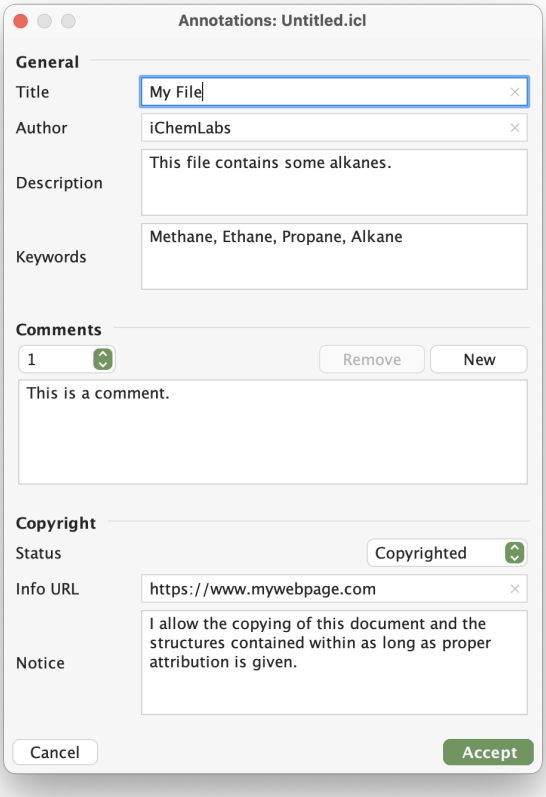


Figure 17.6: *File Annotations Window*

All data associated with a file through annotations will be stored in *ChemDoodle Documents* and *ChemDoodle 3D Scenes*. Other users opening your annotated *ChemDoodle Document* or *ChemDoodle 3D Scene* files will be able to easily access the annotations. Other file types may be able to store annotations as well, either partially or completely.

17.6.7 Chemistry file conversion tool

ChemDoodle contains robust functionality for easily and quickly converting files between different formats. This tool is accessed by clicking the File » Convert... menu item and is shown in Figure 17.7. Unlike other chemical conversion utilities, ChemDoodle converts all document objects and properties in addition to just atoms and bonds; this including shapes, fonts, colors, annotations, styles, etc (when possible).

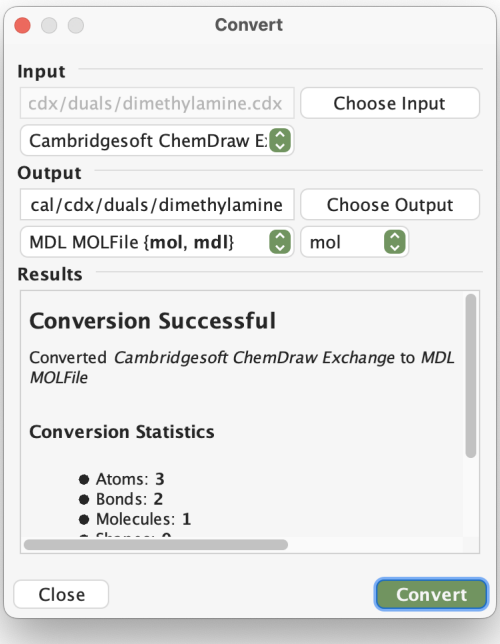


Figure 17.7: *Chemical File Conversion Utility*

Perform the following steps to convert a file:

1. Choose a recognized input file with the file chooser that appears after clicking the **Choose Input** button. Use the file format filter at the bottom of the file chooser to select different file formats.
2. Choose the location to store the output by clicking the **Choose Output** button or by manually typing in the path to the file. You can change the name of the output file this way.
3. Choose an output format and extension from the drop-down selection below the output location.
4. Click the **Convert** button.

When complete, ChemDoodle will display statistics about the conversion or any issues encountered.

17.6.8 Chemistry file options

There are several options you can define that will affect the input and output of chemistry files in ChemDoodle. You can define defaults for these options in the **Settings** window, under the **Chemical** tab as shown in Figure 17.8.

Additionally, relevant output options will appear when you are saving your file, if showing such options is enabled as described in FILE OUTPUT SETTINGS.

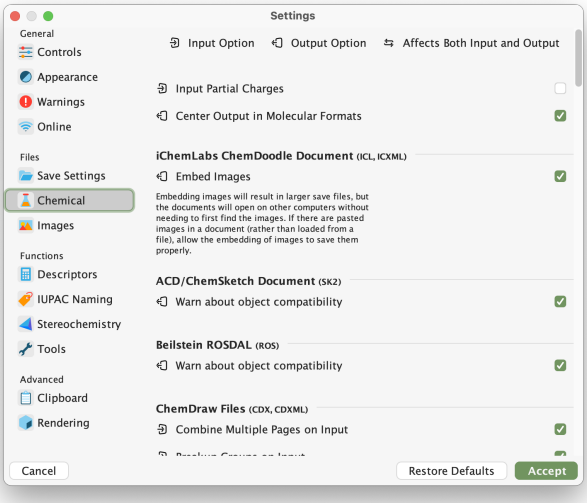


Figure 17.8: *Chemistry Format Options*

The multitude of formats and options may be confusing. To help clarify the option types, we use the following icons to describe whether an option affects input, output or both. These icons are used both here in the following sections, as well as in the application settings panel.

Table 17.1: File Option Types

Cursor	Meaning	Function
	Input	This option is strictly an input option, and will modify how ChemDoodle opens and loads files of the associated format.
	Output	This option is strictly an output option, and will modify how ChemDoodle saves and exports files of the associated format.
	Both	This option affects both input and output of the associated chemistry file format.

The following general options are available:

17.6.8.1 Input partial charges

Some chemistry formats may have specific attributes to describe partial charges, as opposed to or in addition to full formal charges. This data may be useful when performing certain functions or calculations, but will be graphically shown in the application. To include partial charges when inputting a chemistry file, enable this option.

17.6.8.2 Center output in molecular formats

When outputting molecular data to molecule files, enabling this option will center the atom coordinates around the origin. This option will not affect formats where the coordinates are important in relation to the origin, such as in chemistry publishing formats.

17.6.8.3 Warn about object compatibility

If this option is enabled, ChemDoodle will show a warning when saving the file that data may be lost on output. Please see the USE CAUTION SAVING THIRD PARTY FORMATS section for more information. All formats, except the native format of the application, will have this option. The *ChemDoodle Document* is the native format of the application, and no data loss should occur when saving your work to this format.

17.6.9 iChemLabs ChemDoodle Document

In addition to the general options, *ICL* files have their own options.

17.6.9.1 Embed images

Images may be embedded in *ChemDoodle Documents* or defined locally via a file path. Embedding images will result in larger save files, but the documents will open on other computers without needing to first find the images. If there are pasted images in a document (rather than loaded from a file), allow the embedding of images to save them properly.

17.6.10 ChemDraw files

In addition to the general options, ChemDraw files have their own options.

17.6.10.1 Combine multiple pages on input

ChemDraw files, like *ChemDoodle Documents*, may consist of several pages. However, ChemDraw files exclude the page margins, and when opening content from ChemDraw that crosses between pages in ChemDoodle, you will see such content stretched across the page margins. Select this option to merge ChemDraw file pages into one large canvas on input to avoid this issue.

17.6.10.2 Breakup groups on input

Keep this options selected to break up grouped objects on input.

17.6.10.3 Discard lone invisible atoms

ChemDraw files may contain empty lone atom labels that are not visible. Enabling this option removes these labels on input.

17.6.11 ChemAxon Marvin Document

In addition to the general options, MRV files have their own options.

17.6.11.1 Lone Pair Input

Lone pair counts may be defined to atoms in *MRV* files. On input, choose whether this information creates lone pair attributes to the atoms. The option values are **Ignore** (never create lone pair attributes), **Mechanism Atoms Only** (only add lone pair attributes for atoms that are members of mechanism pushing arrows) or **All** (always create lone pair attributes and match the value from the *MRV* file). **Mechanism Atoms Only** is the default.

17.6.12 Chemical Markup Language

In addition to the general options, *CML* files have their own options.

17.6.12.1 Output dimension

Define the output dimension as **2D** or **3D**.

17.6.12.2 Store data in arrays

Select this option to output objects as data arrays instead of individual elements.

17.6.12.3 Store reaction molecules

By default, molecules in reactions are only stored in a *reaction* element (**in Reaction**). If you prefer to store molecule data in separate *molecule* elements and have reactions reference these molecules by *id*, change this setting to **as Separate Molecules**.

17.6.13 Daylight SMILES

In addition to the general options, *Daylight SMILES* output have their own options.

17.6.13.1 Allow extensions

ChemDoodle implements the original Daylight SMILES specification. Parts of the OpenSMILES specification are also viewed as canon and are implemented as native *SMILES* support in ChemDoodle (for instance '$' denotes a quadruple bond).

If this option is enabled, unofficial SMILES extensions will be allowed, as described here.

- **Radicals** - Radicals may be defined in atom environments using the apostrophe "'" symbol. You may use multiples of the symbol, or the symbol followed by a number to denote radical multiplicity.
- **Lone Pairs** - Lone pairs may be defined in atom environments using the pipe "|" symbol. You may use multiples of the symbol, or the symbol followed by a number to denote lone pair multiplicity.

17.6.13.2 Kekulize input

If enabled, delocalized input will be kekulized.

17.6.13.3 Infer ambiguous double bonds on input

If enabled, ambiguous double bonds will be used for input double bonds with no explicit stereochemistry defined.

17.6.13.4 Asterisk (*) as query on input

If enabled, and an input atom is defined by the asterisk wildcard, it will be replaced by a query "any" atom.

17.6.13.5 Output aromaticity

If enabled, the aromaticity model will be output in the SMILES string, using lowercase letters.

17.6.13.6 Output all explicit hydrogens

If enabled, all explicitly drawn hydrogen atoms will be output in the SMILES string as explicit atoms.

17.6.13.7 Output stereochemistry

If enabled, any properly defined stereocenters compatible with the SMILES protocol, will be output in the SMILES string.

17.6.13.8 Output implied double bond stereo

In structures where multiple cis/trans systems exist, one of the slash characters may be implied by another substituent in the SMILES string. This implied slash character is then excluded. Enable this option to force implied slash characters.

17.6.14 Gaussian CUBE

In addition to the general options, *CUBE* files have their own options.

17.6.14.1 Output unit

Define whether the output dimension for the CUBE file is in **Bohr** or **Ångström**.

17.6.15 Gaussian input

In addition to the general options, *Gaussian Input* files have their own options.

17.6.15.1 Output atom ID type

Define what value is used for the atom ID, either **Atomic Number**, **Element Symbol** or a **Unique ID**.

17.6.15.2 Output z-matrix

If enabled, output will be defined by a z-matrix, instead of Cartesian coordinates.

17.6.15.3 Use variables in output (z-matrix only)

If enabled, and when outputting to a z-matrix, variables will be used to condense the data into a smaller file.

17.6.16 IUPAC InChI

In addition to the general options, *InChI* output have their own options.

17.6.16.1 Include auxiliary information

If enabled, InChI auxiliary information will be appended to the output InChI string on a new line.

17.6.16.2 Include InChI key

If enabled, the InChI key will be appended to the output InChI string on a new line.

17.6.17 IUPAC JCAMP-DX

In addition to the general options, *JCAMP* files have their own options.

17.6.17.1 Convert Hz to PPM

If enabled, input data in Hz will be converted to PPM based on the defined resolution.

17.6.18 ISIS Sketch files

In addition to the general options, *ISIS Sketch* files have their own options.

17.6.18.1 Binary output format

(SKC only) Define the endianness of the output SKC file. Choosing **Current System** will use little endian on Windows and Linux and big endian on macOS.

17.6.19 MDL connection table files

In addition to the general options, *MDL CT* files have their own options.

17.6.19.1 Input data records as tables

(SDF only) If enabled, the data records will be rendered in a table along side each connection table entry, either **Horizontally** or **Vertically**. Please note this feature is read-only, and custom data records outside of the file annotations will not be written to SD files.

17.6.19.2 Output FAIR data headers

(SDF only) If enabled, automatically generated FAIR data headers will be output in the SDF file.

17.6.19.3 Output eCTD data headers

(SDF only) If enabled, automatically generated eCTD data headers will be output in the SDF file.

17.6.19.4 No chiral flag, input centers as

If no chiral flag is defined in the input CT file, chiral centers should be input using either **And** or **Or** enhanced stereochemistry logic. Define the desired behavior using this option.

17.6.19.5 Bond length conversion

When normalizing the bond lengths in two-dimensional CT file output, choose whether the **Standard Bond Length** (20px) or **Current Bond Length** is used.

17.6.19.6 Output v3000 extended connection table

If enabled, CT files will be output using the V3000 extended connection table format. Otherwise the more compatible V2000 connection table format will be used.

17.6.19.7 Output hydrogen counts

If enabled, hydrogen counts will be explicitly output in the atom block.

17.6.19.8 Output atom stereo parity

If enabled, for properly defined chiral stereocenters, the stereo parity as defined by MDL will be output in the atom block. This feature is deprecated by MDL in CT files.

17.6.20 RCSB macromolecular formats

In addition to the general options, *RCSB* files have their own options.

17.6.20.1 Read CONECT records

(PDB only) If enabled, bonds will be defined only by the CONECT records in PDB files.

17.6.20.2 Output higher bond orders (unofficial)

(PDB only) PDB files cannot output bond order information. An unofficial method of using the PDB protocol to output higher bond orders is used by many software packages. Enabling this option will use this unofficial method to output higher bond orders.

17.6.20.3 Deduce covalent bonds if none found

If enabled and no bonds are explicitly defined in input data, ChemDoodle will automatically deduce those bonds based on internal bond deduction algorithms.

17.6.21 XYZ

In addition to the general options, *XYZ* files have their own options.

17.6.21.1 Atom identifier

Choose whether the atom **Symbol** or **Atomic Number** is used as the atom identifier in output.

17.7 Round-trip editing

Round-trip editing is a very advanced feature for allowing ChemDoodle content to transfer between applications by embedding it into images. In most cases, ChemDoodle will automatically perform this embedding for you. Through round-trip editing, you can copy ChemDoodle content into your word processor for instance, and then later copy that content back into ChemDoodle for re-editing.



Make sure you always save your drawings and figures in a *ChemDoodle Document* and never rely on a third party application to save your ChemDoodle data. The third party application may change how it works and you may lose your data!

17.7.1 Support

Round-trip editing requires that both ChemDoodle and the application you are inserting the ChemDoodle content into work together. Currently, ChemDoodle supports round-trip editing with LibreOffice on all operating systems and with any applications that understand Object Linking and Embedding (OLE) on Windows, or that preserve PDF comments on macOS. This covers a large number of applications that most scientists use and we are actively working to expand the range of applications with which ChemDoodle supports round-trip editing.



NOTE: It takes two applications to work together for round-trip editing. While ChemDoodle provides functionality for round-trip editing, the other application you want to round-trip with may not support round-trip editing. Other applications that do support round-trip editing may remove round-trip editing functionality at any time and without the consent of iChemLabs.

17.7.2 Windows

17.7.2.1 Setup

No additional setup is required for round-trip editing on Windows. The OLE server is automatically registered when ChemDoodle is installed.

17.7.2.2 Clipboard Settings

By default, in the **Settings** window, under the **Clipboard** tab, OLE is enabled. OLE is required to be enabled for round-trip editing to work on Windows.

17.7.2.3 Procedure

Round-trip editing is very simple on Windows. Just copy in ChemDoodle and paste into the receiving application. Some applications may not paste the OLE object by default. In this case, make sure to use a provided **Paste Special** function in the receiving application to choose the OLE object

There are two ways to edit the content after it has been pasted:

1. Copy the embedded object from the receiving application and paste back into ChemDoodle to recover the objects. Once you have finished editing, again copy in ChemDoodle and paste back into the receiving application to replace the original object.

2. As of version 6 of ChemDoodle, embedded objects may be edited through standard OLE embedded object activation. Double clicking the object inside the receiving application will start ChemDoodle if it is not already running, and load the content of the object for editing in a new tab. After you have made your changes, close the tab, and a dialog box asking if you would like to update the OLE object will appear. Select **Yes** to update the object in the receiving application.

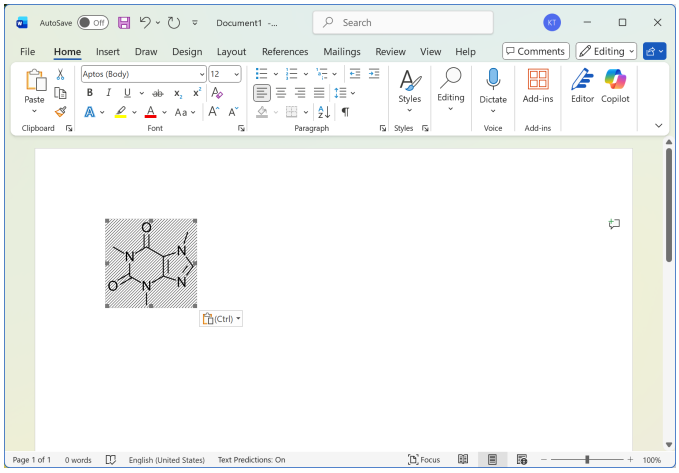


Figure 17.9: *An Activated ChemDoodle Embedded Object (Microsoft Word)*

Figure 17.9 shows an activated ChemDoodle embedded object within Microsoft® Word[1]. The hash marks on the object indicate

[1]Microsoft is a registered trademark of Microsoft Corporation

that it is open in ChemDoodle for editing, and disappear once the object is closed.

Not all Windows applications support OLE, and round-trip editing is not possible with those applications.

17.7.2.4 Troubleshooting

Since ChemDoodle is a Java application and Windows uses C, there are compatibility challenges when implementing OLE.

When pasting ChemDoodle OLE objects into other applications, everything should work fine. If you copy the OLE object back into ChemDoodle, you can recover and edit the original data, then paste it as a new OLE object to update the graphic.

However, problems may occur with OLE activation (the process of editing an OLE object in place, using double-click or the OLE object's right-click menu). iChemLabs has developed ChemDoodle's OLE functions, but OLE APIs are old and have limitations. The known issues are:

1. **Microsoft Word**: You can only edit an OLE object once using double-click or right-click. After editing, if you try to activate it again, the object will corrupt, and you will lose the ability to recover or edit it. To avoid this, after each edit, delete the OLE object and use Word's undo function to restore it, refreshing its state. This issue does not affect PowerPoint, Excel, or other Office apps. Copy-pasting the OLE object is safe—corruption only occurs when using double-click or right-click more than once.

2. **Activation issues**: If the OLE object doesn't activate, restart your computer to reset the OLE server. You can always copy-paste the object into ChemDoodle to recover the data and paste it back into the other application, even if activation doesn't work.

3. **Tampering with the executable**: The error in Figure 17.10 appears if our OLE server is tampered with in the installation folder. Make sure that the installation folder is not modified and important files are not removed.

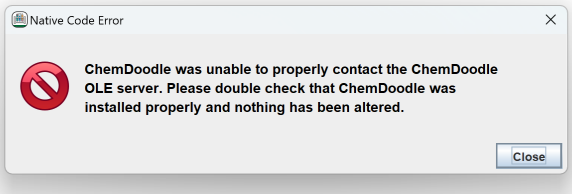


Figure 17.10: *OLE Server Installation Corruption*

.

In short, using copy-paste to manage OLE objects should avoid any issues. Relying on double-click or right-click will lead to the known problems described above.

17.7.3 macOS

17.7.3.1 Setup

No additional setup is required for round-trip editing on macOS.

17.7.3.2 Clipboard Settings

By default, in **Settings** window under the **Clipboard** tab, PDF is enabled. PDF is required to be enabled for round-trip editing to work on macOS.

17.7.3.3 Procedure

Round-trip editing is very simple on macOS. Just copy in ChemDoodle and paste into the receiving application. To edit the content, copy the image from the receiving application and paste back into ChemDoodle to recover the objects. Once you have finished editing, again copy in ChemDoodle and paste back into the receiving application to replace the original image.

Some applications may not paste the PDF by default. In this case, use a provided **Paste Special** function in the receiving application to choose the PDF.

Not all applications on macOS preserve PDF comments, and round-trip editing is not possible with those applications.

17.7.3.4 Workaround for iWork Applications

iWork applications (Pages, Keynote, Numbers) corrupt PDF comments, so round-trip editing will fail directly from them. There is a workaround to recover the original chemical data and facilitate round-trip editing. To perform this workaround, execute the following steps:

1. When working with a PDF figure pasted into iWork applications from ChemDoodle, click on the figure to select it.
2. In the **Inspector** panel on the right side of the iWork application, click on the **Image** tab on the top as shown in Figure 17.11.
3. In the **File Info** section, press the mouse down and drag the `pasted-image.pdf` file (drag the icon, not the name) onto your system desktop.
4. A `pasted-image.pdf` file will appear on your desktop where you released the drag action. Drag this PDF file onto the **Doodle Board** in ChemDoodle to recover the data.

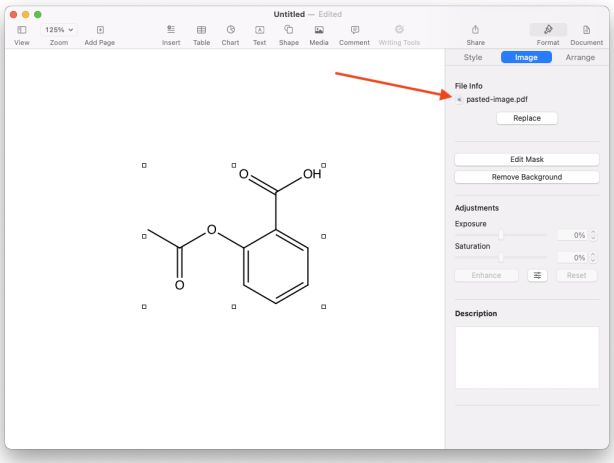


Figure 17.11: *Round-trip Editing: Workaround for iWork Applications*

17.7.3.5 Troubleshooting

You may encounter error messages with round-trip editing on macOS. We document the most common cases here.

The error in Figure 17.12 appears if the application you are performing round-trip editing with has failed to preserve the ChemDoodle data in the PDF. You will need to contact the producer of the other application to get this fixed.

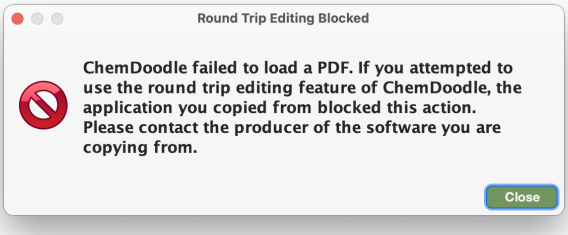


Figure 17.12: *PDF Round-trip Editing has been Blocked*

17.7.4 Linux

There is no system wide round-trip editing mechanism available on Linux platforms, and round-trip editing implementations are application specific on Linux.

ChemDoodle currently supports round trip editing with the following applications on Linux:

1. LibreOffice - please see the LIBREOFFICE section below.

17.7.5 LibreOffice

iChemLabs developed a plugin for LibreOffice to facilitate round-trip editing. This plugin is developed on the LibreOffice Universal Network Objects (UNO) API.

17.7.5.1 Compatibility

LibreOffice versions of 24.2 or more recent should function as described.

There are many flaws in the LibreOffice UNO system, used for round-trip editing functionality. We do our best to support and continue to improve this procedure, but your help is required to submit issues to the LibreOffice development teams and urge them to improve their software and APIs.

iChemLabs tests the **ChemDoodle UNO** plugin for LibreOffice on Windows, macOS and Linux. The Writer, Impress and Calc applications are used for testing.

Apache OpenOffice v4.1.12+ should be compatible, but we do not test OpenOffice and you may experience unexpected behavior.

17.7.5.2 Setup

Round-trip editing of ChemDoodle figures within LibreOffice is made possible after the user installs our **ChemDoodle UNO** plugin. The plugin is named `ChemDoodle.oxt` and can be found in the `resources` subfolder of the `ChemDoodle` installation folder.

To install the plugin, execute the following steps:

1. Launch LibreOffice.
2. Execute the Tools » Extensions... menu item in LibreOffice.
3. Click the **Add** button.
4. In the file chooser that appears, locate the `ChemDoodle.oxt` file in the `resources` folder of the `ChemDoodle` installation folder and select it. Confirm the installation in the next window by pressing the **OK** button.
5. You will be asked to restart LibreOffice for the plugin to take full affect. Do so.

If the plugin is successfully registered, it will appear in the **Extension** window as shown in Figure 17.13.

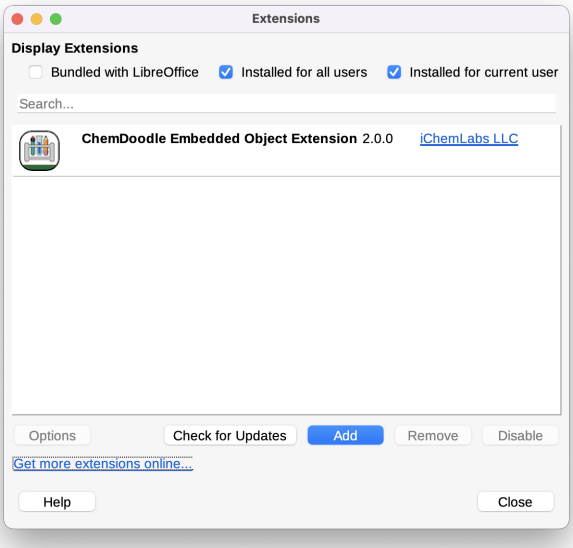


Figure 17.13: *The Extensions window in LibreOffice with the ChemDoodle plugin properly registered*

17.7.5.3 Clipboard Settings

In ChemDoodle's **Settings** window under the **Clipboard** tab, the appropriate data needs to be available on the system clipboard for the **ChemDoodle UNO** plugin to properly create the round-trip editable object. This data is different for each operating system:

- Windows - only **OLE Object** is required.
- macOS - only **Adobe PDF** is required.
- Linux - both **PNG (720dpi)** and **ChemDoodle Document** are required. Other raster image types should be disabled.

17.7.5.4 Procedure

To insert a round-trip editable ChemDoodle object into LibreOffice, execute the following steps:

1. Ensure the clipboard settings are correct as stated in the previous section.
2. In ChemDoodle select the content you wish to copy and use a copy function.
3. In the LibreOffice application you want to insert the object into, execute the Insert ⟩ OLE Object ⟩ OLE Object... submenu. (Figure 17.14)

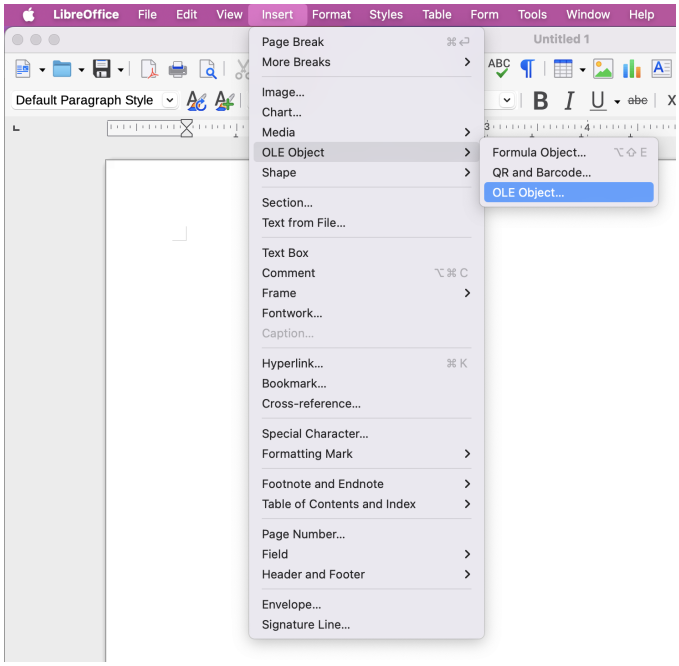


Figure 17.14: *The menu item used to insert OLE Objects in LibreOffice*

4. In the window that appears, select **ChemDoodle Embedded Object** and select the **OK** button. (Figure 17.15)

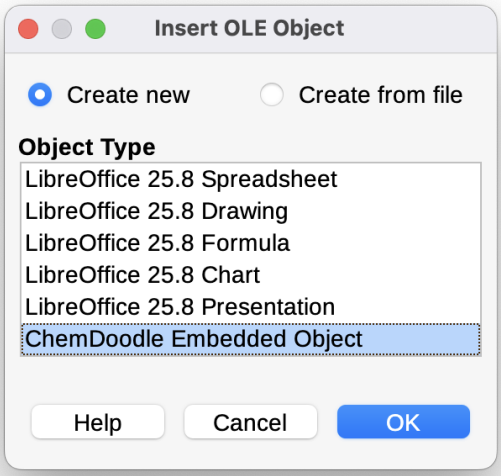


Figure 17.15: *Selecting ChemDoodle Embedded Object to insert in LibreOffice*

To edit the inserted ChemDoodle object, execute the following steps:

1. Select the inserted ChemDoodle object that you wish to edit, and double-click on it. The double-click action is required and is sufficient to place the corresponding ChemDoodle data on the system clipboard.

2. In ChemDoodle, use a paste function to paste the data.

3. Edit the pasted content in ChemDoodle as you desire.

4. Select the updated content in ChemDoodle and follow the procedure for inserting the ChemDoodle object into LibreOffice above to replace the previous object.

Double-click editing on Windows
LibreOffice on Windows has a second pipeline for round-trip editing of **ChemDoodle OLE** objects allowing for traditional in-place editing one would experience when double-clicking on a **ChemDoodle OLE** object in MS Office applications.

Instead of using the Insert menu, use the Edit > Paste Special > Paste Special... menu item as shown in Figure 17.16.

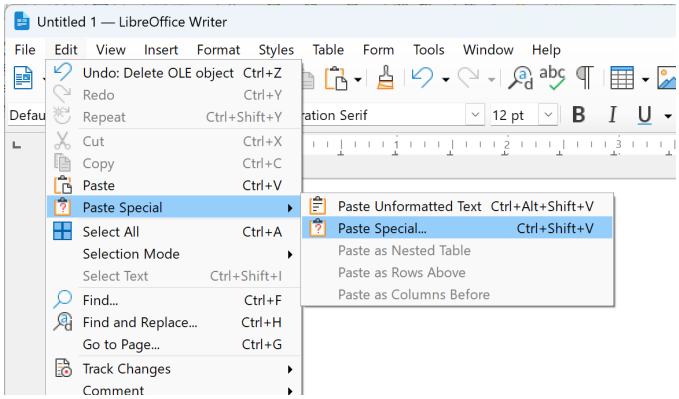


Figure 17.16: *Use the Paste Special menu item on Windows to paste a traditional Windows OLE object*

In the **Paste Special** window that appears, select **ChemDoodle OLE** as shown in Figure 17.17. The traditional Windows OLE object will then be pasted into the LibreOffice application.

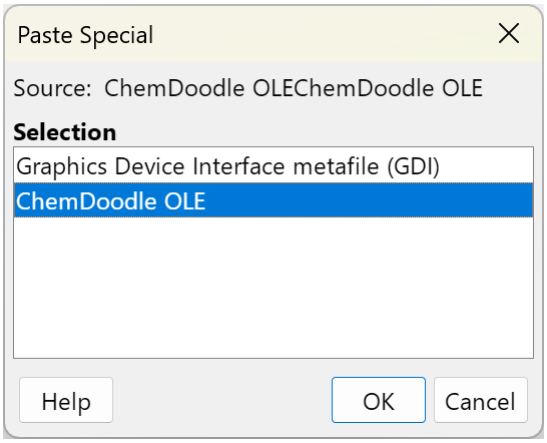


Figure 17.17: *Select "ChemDoodle OLE"*

When you double click on the **ChemDoodle OLE** object embedded through the Edit menu, double-clicking on the object will automatically activate (you will see a hashed overlay on the object) and load the associated data in ChemDoodle. When you are finished editing your figure, close the OLE document in ChemDoodle and it will automatically update in LibreOffice. Please note, while the aspect ratio of **ChemDoodle OLE** objects will automatically update when changes are committed in Writer, the aspect ratio will not change via this method in Impress or Calc.

17.7.5.5 Troubleshooting

Common error boxes may appear, troubleshoot them as follows.

The following warning means you should enable the correct metadata for the plugin to work properly in the **Clipboard** tab of the **Settings** window as discussed in the *Clipboard settings* section above.

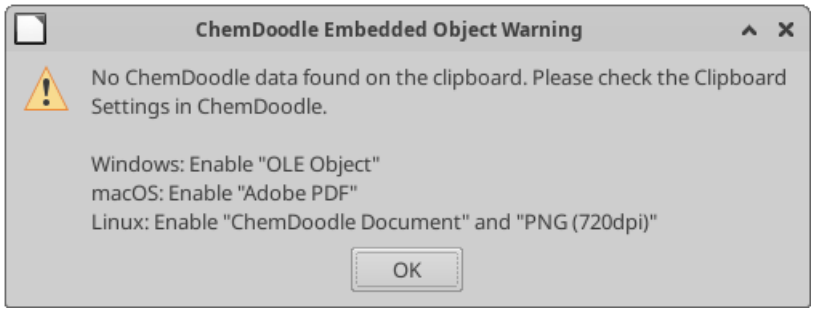


Figure 17.18: *Missing ChemDoodle Document and Image Data*

The following warning means you should enable the correct metadata for the plugin to work properly in the **Clipboard** tab of the **Settings** window as discussed in the *Clipboard settings* section above.

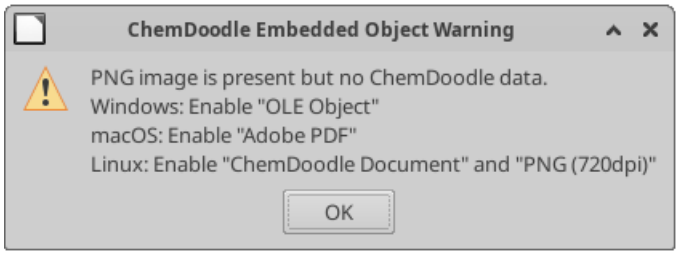


Figure 17.19: *Missing ChemDoodle Document*

On Linux, the following warning means that **PNG (720dpi)** needs to be enabled in the **Clipboard** tab of the **Settings** window.



Figure 17.20: *Missing Image Data*

This warning means something has gone wrong and the ChemDoodle data on the system clipboard has been corrupted. Please try again.

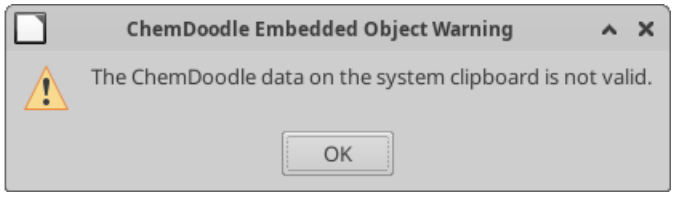


Figure 17.21: *Corrupted ChemDoodle Document*

17.7.5.6 Questions and Answers (Q&A)

Q: *On Linux, why is a bitmap image used instead of a vector graphic?*

A: LibreOffice does not support vector graphics through their Embedded Object insertion on Linux. We tried to use *ODG* files for scalable vector graphics, but this is not allowed. Please contact the appropriate Office development teams to urge them to add this functionality. For now, we use a 720 DPI image so print quality will still be excellent.

Q: *Why can't I just paste the object? Why do I need to go through the menu to insert it?*

A: Implementing direct pasting of the object exhibits many inconsistencies which make it unsuitable for regular use. This is something we are trying to work around. Please contact the appropriate Office development teams to urge them to improve this process.

Q: *Why can't I paste the object directly between Office applications?*

A: This is a limitation of LibreOffice.

Q: *Why do I have to double-click the object to round-trip it?*

A: This is what LibreOffice requires to execute the object.

17.8 Chemical data recovery

The handling of chemical data is extremely important, as without it, chemists would not be able to store or communicate chemistry information through computers. Over the past century, many file formats have been proposed to represent chemical information. Several formats have become essential and are implemented by the vast majority of chemical software. These formats include MDL connection table formats (*MOL*, *SDF*, etc.), Chemical Markup Language (*CML*), and *CDX*/*CDXML* formats. There are plenty of chemistry applications that "read" chemical files. However, most software that read chemical files understand little more than basic molecules and perhaps reactions, while there are a lot of objects and properties defined by the various formats for creating complex chemical data and figures. The goal of chemical file reading in ChemDoodle is to fully understand all objects and properties and to recover the graphics of the chemical figures drawn in other programs in a pixel-perfect manner.

Also prevalent in the professional chemistry community is an application process referred to as "round-trip editing" (fully supported by ChemDoodle and discussed in detail in the ROUND-TRIP EDITING section), which allows a user to create data in one program (such as ChemDoodle) and store the data in another program (such as Microsoft Office). This allows a chemist to easily manage chemical data, which is not an intrinsic data type in other programs like text or images are, without having to save and manage multiple files from different applications; for instance if a chemist includes a dozen reaction schemes in a word processor, then those reaction schemes can later be accessed and edited through the word processor's application and file.

Professional chemists have come to rely on the convenience of round-trip editing, but it is fraught with risk. On several occasions in the past decade or so, Microsoft Office has discontinued round-trip editing support on macOS, leading to many macOS users losing access to their chemical data. Therefore, as a practical consideration when working with niche data like chemical data, your computer and software will eventually change and there is a chance you will be locked out of accessing your data. Some software may become obsolete, the developer may change it, you may switch to a different operating system where software is no longer compatible, or you may no longer be able to afford the products you used in the past. In all of these cases, you will no longer have access to the original chemical data you created. Years of work and effort may be lost in this way.

ChemDoodle includes very thorough tools for recovering chemical data, whether through files, via interactions with other software, or through round-trip editing. In particular, ChemDoodle expertly handles chemical data and can recover embedded chemical data in other applications, regardless of the operating system you are using. This allows you to maintain control and access to your work. This process is very complex, and so we describe the different ways of recovering chemical data as levels. There are 4 different levels of chemical data recovery. ChemDoodle fully supports all 4 levels on Windows, macOS and Linux.

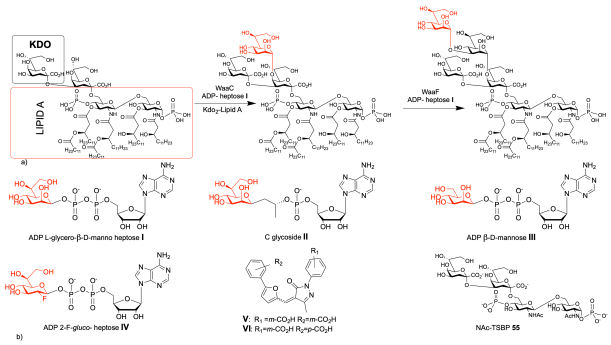
0. Reading chemical files
1. Pasting directly from other chemical applications

2. Pasting embedded data from other (non-chemical) applications
3. Recovering data from Microsoft Office files

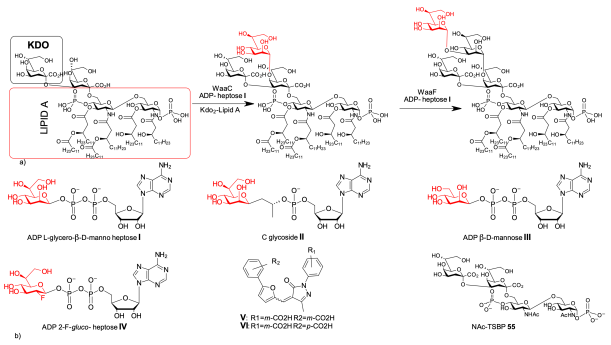
17.8.1 Level 0: Reading chemical files

The most basic function for recovering chemical data is to read chemical files. ChemDoodle understands over 30 widely used chemical file formats. As stated in the introduction to this section, the goal of chemical file interpretation in ChemDoodle is to fully and completely handle file contents and to recover the graphics in a pixel perfect manner.

Data and graphics support in ChemDoodle is an immense undertaking. Yet, the ChemDoodle application does this expertly. If you are not satisfied with the way ChemDoodle opens your chemical file, simply send it to us and tell us what you are not satisfied with, and our goal will be to improve it.



(a) *A complex ChemDraw figure, exported as an image from ChemDraw*



(b) *The same figure, imported into ChemDoodle as a CDX file, and exported as an image from ChemDoodle*

Figure 17.22: *ChemDoodle reads in chemical files in a pixel-perfect manner*

17.8.2 Level 1: Pasting directly from other chemical applications

While it may not seem sensible to need two separate chemistry applications or ever to need two different chemical drawing applications, the scope of each application is different, and there are functions ChemDoodle can perform that other chemical software cannot. For instance, you may want to use ChemDoodle to style bond strokes or generate 3D coordinates. You can copy from other chemistry applications and paste into ChemDoodle on both Windows and macOS. ChemDoodle is compatible with *ChemDoodle Collages*, *ChemDoodle JSON*, *MDLCT* and *MDLSK*, and *ChemDraw Interchange Format* clipboard data on Windows, and is compatible with *ChemDoodle Collages*, *ChemDoodle JSON* and *ChemDraw Interchange Format* clipboard data on macOS.

17.8.3 Level 2: Pasting embedded data from other (non-chemical) applications

Some chemical applications embed chemical metadata into figures pasted into 3rd party applications, in a process referred to as "round-trip editing". The technical procedure for recovering this data is different on Windows and macOS. However, on both operating systems, these figures can be copied from the 3rd party application and pasted into ChemDoodle to recover the original data for further editing without using or having access to the original chemical software that created the figure.

This process will be limited to the operating system the figure was created on. This is because Windows and macOS handle system metadata differently and most programs working on both operating systems (like Microsoft Office) do not convert the data for the other operating system.

As an example, if you have pasted a chemical figure into Microsoft Word on Windows, you will later be able to copy that chemical figure from Microsoft Word on Windows and paste into ChemDoodle for further editing. And if you have pasted a chemical figure into Microsoft Word on macOS, you will later be able to copy that chemical figure from Microsoft Word on

macOS and paste into ChemDoodle for further editing. This works for any application correctly storing the chemical metadata, including WordPad on Windows and Pages and Mail on macOS.

If you need to get around this operating system limitation for Microsoft Office, look at the next section, Level 3.

17.8.4 Level 3: Recovering data from Microsoft Office files

ChemDoodle provides a unique solution for searching and extracting chemical figures out of, specifically, Microsoft Office files, regardless of what application or operating system the embedding occurred with. Microsoft Word will be the most common filetype used to store embedded chemical data. This is especially useful if you are a macOS user collaborating with a chemist on Windows (and *vice versa*), or if you used to be a Windows user but switched to Linux, or if round-trip editing is broken by any part of the chain. To recover chemical data using this method in ChemDoodle, you do not need access to other chemistry software, Microsoft Office, or the original operating system the data was created on.

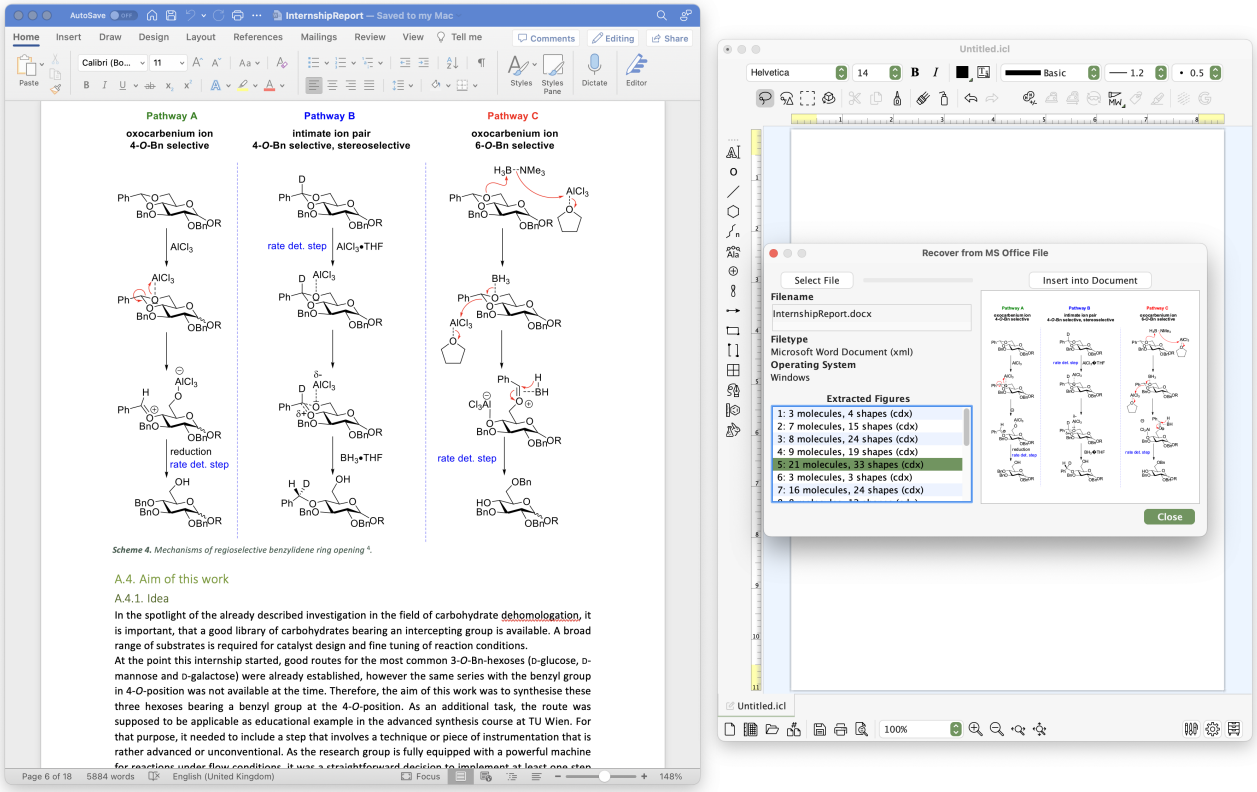


Figure 17.23: *In this image, ChemDoodle on macOS recovers complex chemical figures pasted from ChemDraw into Microsoft Word on Windows.*

Currently, the *XML* files from Word, Powerpoint and Excel can be handled, and ChemDoodle, BIOVIA Draw ®[2] (formerly known as ISIS/Sketch, Symyx Draw and Accelrys Draw), ChemSketch ™[3] and ChemDraw ®[4] embedded data can be recovered.

To recover chemical data from your Microsoft Office file, please follow these instructions:

1. In ChemDoodle, select the File > Recover from MS Office File... menu item. A window will appear as shown in Figure 17.24

[2]BIOVIA is a registered trademark of Dassault Systèmes
[3]ChemSketch is a trademark of ACD/Labs
[4]ChemDraw is a registered trademark of PerkinElmer, Inc.

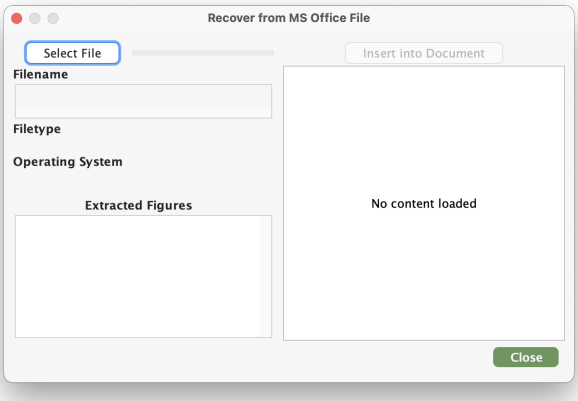


Figure 17.24: *Window to select a Microsoft Office file to recover chemical data from.*

2. Press the **Select File** button on the top left, and a file chooser will appear. Select the Microsoft Office document you wish to scan for chemical data and press the **Open** button.

3. ChemDoodle will scan the file for compatible chemical data. A progress bar will be animated while the scan is in progress, as the process may take a few seconds or longer. Once complete, the window will display which type of Microsoft Office file was detected and which operating system ChemDoodle believes the file was created on. Any recovered figures will be listed in the **Extracted Figures** list, denoted by the number of molecules and shapes contained in the figure as well as type of chemical data the figure was represented in surrounded by parentheses. This is shown in Figure 17.25.

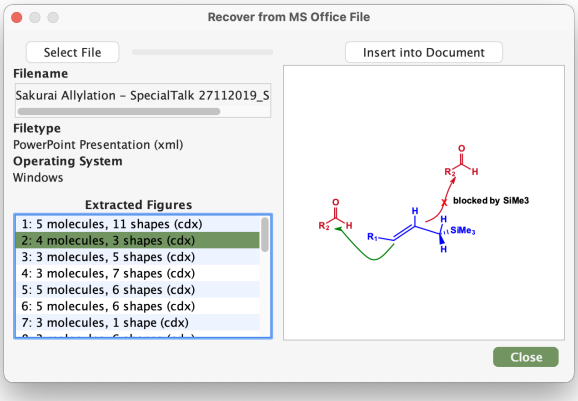


Figure 17.25: *Recovered chemical figures from a Microsoft Powerpoint file.*

4. The first extracted figure will automatically be selected and displayed in the preview on the right side of the window. Go through the **Extracted Figures** list and select the figure you wish to recover for further editing or any other purpose. You can zoom in on the preview by moving your mouse pointer over the preview panel.

5. Press the **Insert into Document** button to load the recovered figure into your current document.

You can then repaste your content back into the original Microsoft Office file to replace the original figure, but keep in mind the original data will be replaced by ChemDoodle embedded data, and programs other than ChemDoodle may not be able to edit the newly embedded data.

Now, you can share your Microsoft Office files including embedded chemical data with your colleagues on Windows, macOS or even Linux!

17.8.5 Summary

In summary, you can use ChemDoodle to recover chemical data created in ChemDoodle and other chemical programs. This means you will be able to recover data in files you thought were lost long ago, you can edit chemical figures from Microsoft Office files even if you do not have access to Microsoft Office, and you can finally collaborate with chemists in creating documents even if they use a different operating system. When you have ChemDoodle with you, you are in control of your chemical data.

17.9 Image format compatibility

ChemDoodle supports the input and output of a wide range of bitmap and vector images.

17.9.1 Supported input formats

ChemDoodle can read the following bitmap image formats:

- Joint Photographic Experts Group {.jpg, .jpeg, .jpe, .jfif, .jfi, .jif}
- Microsoft Bitmap {.bmp, .dib}
- Tagged Image File Format {.tiff, .tif}
- Wireless Bitmap {.wbmp}
- CompuServ Graphics Interchange Format {.gif}
- Portable Network Graphics {.png}
- UNIX Portable PixMap {.ppm, .pnm, .pbm, .pgm}
- Photoshop Document {.psd}

ChemDoodle can read the following vector image formats:

- Adobe Portable Document Format {.pdf}
- Web Scalable Vector Graphics {.svg, .svgz}

17.9.2 Supported output formats

ChemDoodle can write the following bitmap image formats:

- CompuServ Graphics Interchange Format {.gif}
- Joint Photographic Experts Group {.jpg, .jpeg, .jpe, .jfif, .jfi, .jif}
- Microsoft Bitmap {.bmp, .dib}
- Portable Network Graphics {.png}
- Tagged Image File Format {.tiff, .tif}
- UNIX Portable PixMap {.ppm, pnm, pbm, pgm}
- Wireless Bitmap {.wbmp}

ChemDoodle can write the following vector image formats:

- Adobe Portable Document Format {.pdf}
- Encapsulated Postscript {.eps, .epi, .epsi, .epsf}

- Macintosh Vector Pict {.pict}
- OpenDocument Graphics {.odg}
- Web Scalable Vector Graphics {.svg, .svgz}
- Windows Enhanced Metafile {.emf}

17.9.3 Importing chemical content from images

ChemDoodle will automatically embed chemical data in certain image formats. When these images are inserted into ChemDoodle, they will be checked for chemical information and that chemical information will be loaded if found.

ChemDoodle embeds chemical information into the following image formats:

- Adobe Portable Document Format {.pdf}
- Encapsulated Postscript {.eps}
- OpenDocument Graphics {.odg}
- Web Scalable Vector Graphics {.svg, .svgz}

17.9.4 Exporting the document to an image

To export all of the objects in the current document to an image, execute the following steps:

1. Select the File 〉 Save As Image... menu item.
2. A file chooser will appear. Select the location you would like to have the image saved in and type in a name for the file if you do not like the default name. You do not need to type in an extension as ChemDoodle will do this for you.
3. After you are satisfied with a location and name, select the image type of the image to be exported.
4. After selecting the file type to be used, press the **Save** button to export your document as an image.
5. If options are available, a window will be shown to allow you to set the options. Define the settings to your preference and then click the **Save Image** button.

17.9.5 Exporting only certain objects to an image

To export specific objects in the current document to an image, execute the following steps:

1. Use a selection tool to select the objects to be exported to an image.
2. Select the File 〉 Save Selection As Image... menu item.
3. A file chooser will appear. Select the location you would like to have the image saved in and type in a name for the file if you do not like the default name. You do not need to type in an extension as ChemDoodle will do this for you.
4. After you are satisfied with a location and name, select the image type of the image to be exported.
5. After selecting the file type to be used, press the **Save** button to export the selected objects to an image.
6. If options are available, a window will be shown to allow you to set the options. Define the settings to your preference and then click the **Save Image** button.

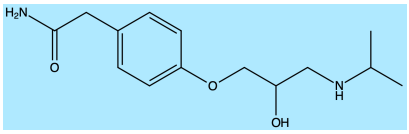
17.9.6 Image sizing

By default, images in ChemDoodle are automatically sized to fit the graphics content being output. So if you have a molecular structure that measures 100px by 50px in your document, then the output image size will be 100px by 50px. If you prefer to

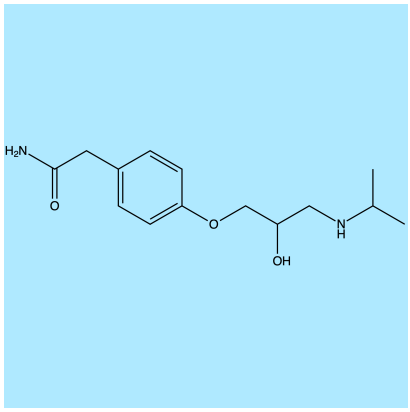
output your graphics to a predetermined image size, then deselect the **Automatically Size** setting, and the **Forced Output Size** setting will become editable so you may define a custom width and height. The **Image Border Buffer** setting adds to these dimensions. The **Image Scale** setting will multiply the image size and the border buffer.

When rendering content to an image of predetermined size, the graphic's dimensions may not be an ideal fit. For instance, if your molecule's dimensions are larger than the output image size, then parts of the molecule will be cutoff from the image. If your molecule's dimensions are smaller than the output image size, there will be a significant amount of empty space in the output image. If **Scale Contents to Fit** is enabled, then ChemDoodle will automatically scale the contents to best fit the custom output dimensions, preserving the aspect ratio of the graphics. In all cases, the contents of the image will be centered.

To illustrate these options, Figure 17.26 shows 3 images of the drug Tenormin. A blue background is used to easily describe the image bounds. In Figure 17.26a, ChemDoodle automatically measures the dimensions of the molecule (326x97). A border buffer of 3px is applied (332x103), and a 4x scale is applied for a final image dimension of 1328px by 412px. In Figure 17.26b, we instead wish to render the molecule in a square image. We define the image dimensions at 500px by 500px, and after a 3px border buffer and 4x scale, the final dimensions of the image are 2024px by 2024px. In this image, the molecule dimensions are the same as the first image at 326px by 97px, so to avoid empty space, ChemDoodle automatically scales the molecule to fit the available space, preserving the aspect ratio. In the final image, Figure 17.26c, the same custom dimensions are used leading to another image of 2024px by 2024px, but the contents are not scaled to fit, leading to empty space. Not scaling the contents may benefit you if you are trying to create a large number of images of the same size, where all of the structures have equivalent bond lengths.



(a) *Automatically sized image*



(b) *Custom sized image, scaled contents*



(c) *Custom sized image, unscaled contents*

Figure 17.26: *Image Sizing*

Be careful when creating images of a custom size with unscaled contents. If the contents do not fit within the bounds of the output image, they will be cut off as shown in Figure 17.27. The same molecule of Tenormin is rendered, but to a much smaller size of 100px by 100px. This is smaller than the molecule dimensions of 326px by 97px, so it is cut off.

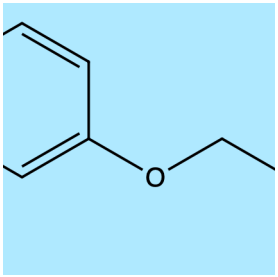


Figure 17.27: *Custom sized image with unscaled contents, leading to cutoff*

17.9.6.1 Previewing the image size

Since there are several options for defining the image size, it may not always be clear what the final calculated size of the output image is or how the graphics content will fit in the image. To clarify how these options alter the output image dimensions, a preview is provided in the image settings window as shown in Figure 17.28.

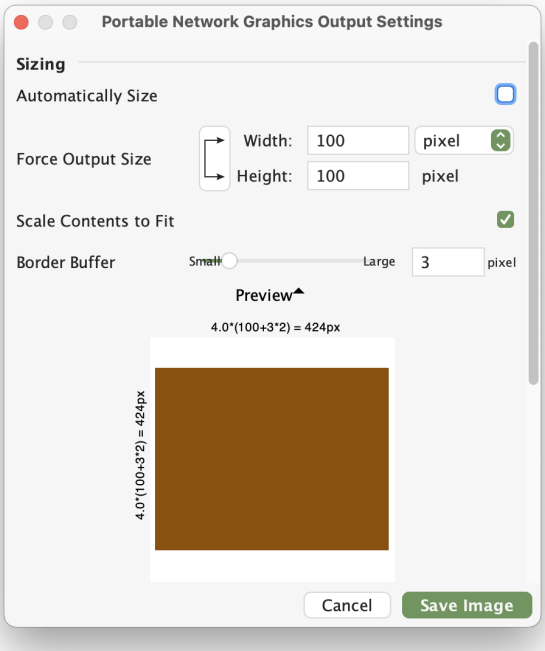


Figure 17.28: *Previewing the image size*

Click on the **Preview** toggle to show the image size preview. A depiction of the image dimensions will be shown, with calculations for the width and height of the image using the following formula:

$$scale * (dimension + border * 2)$$

The preview will update in real time as you change the output settings and you can see exactly what the dimensions are of the output image. Only bitmap images will show a scale parameter.

Additionally, the space the graphics content occupies will be rendered by a rectangle in the application defined highlight color. If any of the graphics content extend beyond the dimensions of the output image (this is only possible if you are using a custom image size and not scaling the content to fit), you will see a message warning you that content is cutoff.

17.9.7 Image output options

There are several options that you can define for output images. Some options are only available for bitmap or vector types, while other options are available for both. These options will appear when you are saving your image. However, you can define defaults for these options in the **Settings** window, under the **Images** tab as shown in Figure 17.29.

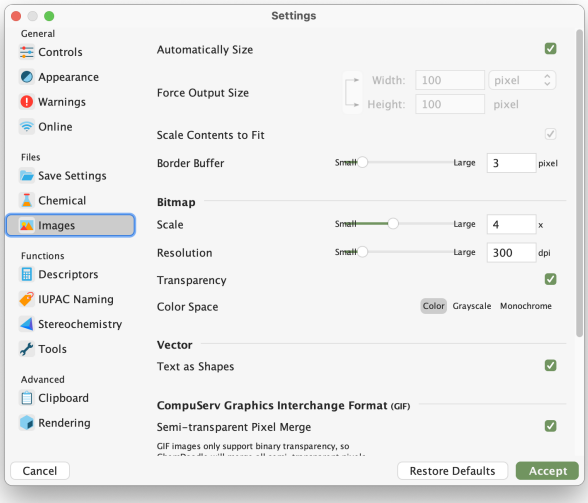


Figure 17.29: *Image Format Options*

The following options are available:

17.9.7.1 Automatically Size

By default, images in ChemDoodle are automatically sized to fit the graphics content being output. So if you have a molecular structure that measures 100px by 50px in your document, then the output image size will be 100px by 50px. The **Border Buffer** setting adds to these dimensions. The **Scale** setting will multiply the automatically determined image size and the border buffer.

17.9.7.2 Force Output Size

This setting is only relevant if the image output is not automatically sized. If you prefer to output your graphics to a predetermined image size, then deselect the **Automatically Size** setting, and the **Force Output Size** setting will become editable. Define the desired width and height of the output image. The **Border Buffer** setting adds to these dimensions. The **Scale** setting will multiply the defined image output size and the border buffer.

17.9.7.3 Scale Contents to Fit

This setting is only relevant if the image output is not automatically sized. When rendering content to an image of predetermined size, the graphic's dimensions may not be an ideal fit. For instance, if your molecule's dimensions are larger than the output image size, then parts of the molecule will be cutoff from the image. If your molecule's dimensions are smaller than the output image size, there will be a significant amount of empty space in the output image. If **Scale Contents to Fit** is enabled, then ChemDoodle will automatically scale the contents to best fit the custom output dimensions, preserving the aspect ratio of the graphics.

17.9.7.4 Border Buffer

You can control the image border buffer, or the amount of space surrounding the graphics in an image, by changing the **Border Buffer** setting. The default image border buffer is three (3) pixels. This setting is relevant for both bitmap and vector graphics.

17.9.7.5 Scale (bitmap only)

This setting will determine the scale of the output image. The larger the scale, the larger the output image. Vector graphics can be rescaled at any time, and therefore this setting is only available for bitmap images. You will need to scale bitmap images to a larger size if you want to use a higher resolution, but retain the same dimensions.

17.9.7.6 Resolution (bitmap only)

This setting will instruct printers and other renderers how to scale the image. The higher the DPI setting, then the crisper the image will look, but the smaller it will appear. By default, the DPI setting is 300 dpi. Currently, only the JPEG, PNG and TIFF output support this option. Vector graphics are resolution-less, and therefore this setting is only relevant for bitmap images.

17.9.7.7 Transparency (bitmap only)

If the bitmap image type supports transparency, this option will be available. This option is only relevant for bitmap images.

17.9.7.8 Color Space (bitmap only)

Define the color space of the image. **Color** will output the full color range, as possible, for the format. **Grayscale** will convert the colors to a grayscale (between white and black). **Monochrome** will use either and only solid white or solid black to represent each pixel. This option is only relevant for bitmap images.

17.9.7.9 Compression Quality (bitmap only)

For bitmap image formats that support compression, this setting will define the extent of the compression. A lower compression quality will result in a smaller image file size. A value of 100% defines no compression. Currently, only the JPEG format supports this output option. All other formats output without compression or with lossless compression.

17.9.7.10 Text as Shapes (vector only)

For vector graphics in ChemDoodle, the default behavior is to output text as shapes, so they are no longer recognized as text by other applications. This ensures that the graphics will remain consistent regardless of the fonts available or how the renderer draws those fonts. If you prefer to preserve the text characters for editing in other applications, then deselect this option. Note that the font you use for the text must be present on the system that you open the image in, or the font you used will be replaced with something similar, but not identical. This option is only relevant for vector images.

17.9.8 Encapsulated Postscript

In addition to the general options, *EPS* files have their own options.

17.9.8.1 Preserve chemnum Tags

The LaTeX package chemnum looks for label values of the form "<tag>n", where <tag> is typically "TMP" and n is a positive integer, for automatic replacement in output documents. If enabled, labels containing "<tag>n" (label shapes, not atom labels) will be preserved in EPS output as text, even if the **Render Text as Shapes** option is enabled.

Keep in mind, if the label including the chemnum tag contains characters outside of the standard EPS font ranges, those output characters may fail to render. In such cases, please split up your label into separate pieces, isolating the chemnum tag so that the rest of the label is rendered as shapes in the EPS file.

17.9.8.2 chemnum Tag

Define the tag used for the LaTeX package chemnum, this value is typically "TMP".

17.9.9 CompuServ graphics interchange format options

In addition to the general options, *GIF* files have their own options.

17.9.9.1 Semi-transparent pixel merge

GIF images only support binary transparency, so ChemDoodle will merge all semi-transparent pixels with white. Otherwise, all semi-transparent pixels will be dropped, unless you select a **Monochrome** color space or disable **Transparency**.



The *GIF* format only allows for binary transparency, which means that a pixel can either be on or off. When you output an image with partially transparent pixels on a transparent background, the software has to make a choice whether to show the partially transparent pixels as completely opaque or completely transparent. ChemDoodle chooses to make them completely transparent, while other software you are using may choose to make them completely opaque. Both options lead to a poor image output, which is why ChemDoodle provides the **Semi-transparent Pixel Merge** option. However, if you place this image on a background that is not white, you will see white artifacts around the border.

Turning transparency off will avoid this issue. However, if you do desire transparency in *GIF* images, we recommend outputting at 4x scale in monochrome for just black and white images.

17.9.10 Web scalable vector graphics options

In addition to the general options, *SVG* files have their own options.

17.9.10.1 Use CSS output

Web Scalable Vector Graphics {.svg, .svgz} files have a unique option. *Firefox* and *Opera* follow a different ruleset for CSS font size specifications, so make sure to uncheck this if you want SVG text to be displayed correctly in these browsers when text is not rendered as shapes.

17.10 Inserting images

For any of the image formats that ChemDoodle can read, you can import files of that format into your documents. To do so, execute the following steps:

1. Select the File ⟩ Insert Image... menu item.
2. In the file chooser that appears, navigate to and select the image you would like to insert.
3. Select the **Open** button to insert the image.

If you selected an image file type that is not understood by ChemDoodle, a message will appear to notify you of the issue.

In addition to inserting images via the **File** menu, you may also simply drag compatible images from your file system or from other applications on to the **Doodle Board**.



We recommend you always use vector graphics when importing images into your document as that will create the best looking figures.

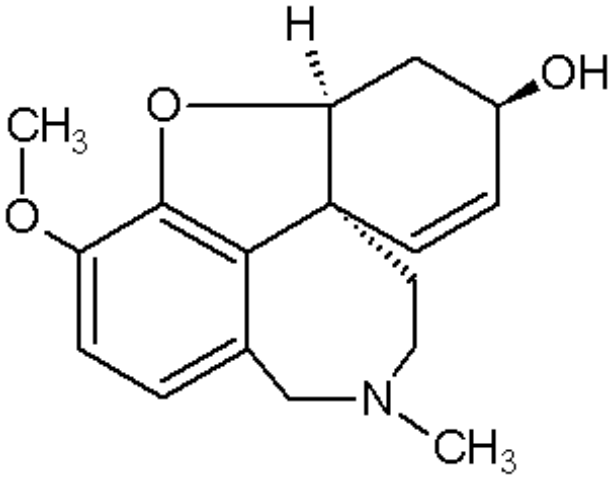
17.11 Chemical image recovery

ChemDoodle has the ability to recreate a chemical drawing from an image of a molecule, recovering the original chemical data. This is different from inserting the image from the previous section INSERTING IMAGES. Inserting an image provides you with just a graphic, while recovering the chemical drawing allows you to regain access to the chemical information to use or edit further. We call this function Chemical Image Recovery (CIR). Some may also refer to this function as Optical Structure Recognition (OSR).

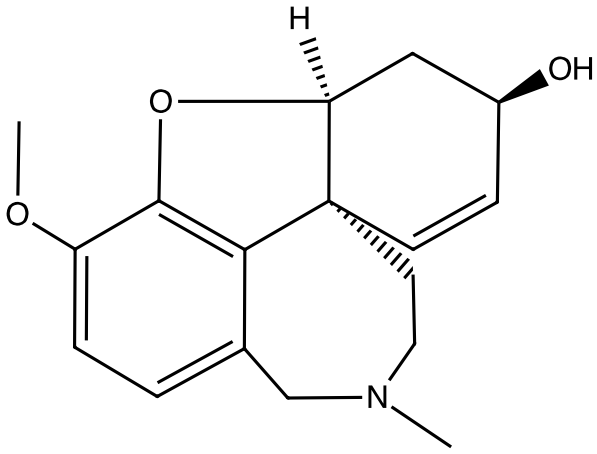
To use the CIR function in ChemDoodle, perform the following steps:

1. Select the File > Recover from Image... menu item.
2. Navigate to and select the image containing the desired chemical drawings to recover in the file chooser that appears.
3. Select the **Open** button to process the image. Any recovered chemical drawings will be placed into the current document, conformed to the current style sheet, and selected.

For example, an image of the molecule galanthamine in Figure 17.30a is processed using the CIR function in ChemDoodle, resulting in the recovered structure shown in Figure 17.30b.



(a) *An image of a molecule*



(b) *The recovered chemical drawing*

Figure 17.30: *Recovering a chemical drawing from an image. The recovered drawing may be further edited or used as input to a chemistry function.*

If no chemical drawings are recovered, you will be presented with the warning message in Figure 17.31.

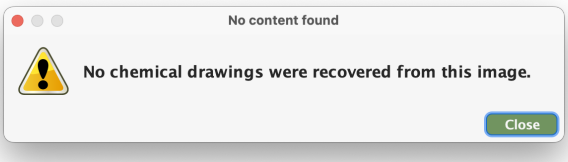


Figure 17.31: *No chemical drawings were recovered from the input image.*

17.11.1 Input

Any image file type recognized by ChemDoodle is valid input into the chemical image recovery function, including understood vector types like *PDF* and *SVG*. If a vector image type includes embedded data that ChemDoodle understands, that data will override the CIR procedure and be loaded instead.

17.11.2 Support

In this section, the chemical features of images the CIR algorithm perceives are described. Multiple structures within a single image will be properly handled, even if they have different styles.

17.11.2.1 Atoms

Atoms will be created at junctions between perceived bonds and where there is any chemically interpreted text. This may include lone labels, such as isolated elements or molecular formulae. Any complex labels ChemDoodle can understand, consisting of elements, numbers, abbreviations, formulae and more, will be properly handled. Text may be formatted including superscripts and subscripts.

17.11.2.2 Bonds

The following bond types are supported:

- **Single**
- **Double**
- **Triple**
- **Quadruple**
- **Quintuple**
- **Hextuple**
- **Recessed Wedge**
- **Protruding Wedge**
- **Bold Single**

Overlapping bonds are resolved, both where there is a break in the bond and those where the two bonds cross. Some features of perspective drawings are also handled, where protruding wedges and bold bonds are used to show some 3D view.

17.11.2.3 Rings

Rings are automatically created based on perceived atoms and bonds. Aromatic circles are also recognized and aromatic character is applied to the rings they are contained within.

17.11.2.4 Attributes

The following attributes are supported:

- **Charges** - both at the end of labels or placed around an atom
- **Radicals** - placed around an atom
- **Isotopes** - As defined in superscript before an element label

17.11.2.5 Shapes

The following shapes are supported:

- **Labels** - Arbitrary text that is not part of a chemical structure, or cannot be chemically interpreted, will be recreated as a label shape.

17.11.3 Performance

Chemical image recovery will work on computer generated skeletal images of chemical structures. Hand drawn images may not work well. Clearer images at a crisp resolution will have the best results. The messier or blurrier the image is, the more ChemDoodle will have to use intuition to resolve the chemical structure, similar to a human looking at an unclear image.

Chemical image recovery is performed by ChemDoodle through analyzing the features and shapes in an image to reconstruct the original chemical information. As such, ChemDoodle may interpret graphics differently than you may. Our goal is to have the chemical image recovery features perfectly match what you perceive in the image, but you should expect to perform some level of post-editing on some images.

We are continuously developing the CIR algorithms in ChemDoodle. Our goal is to eliminate 99% of the effort required in recovering chemical drawings from images, and ideally 100%, but this is not always possible. If you are not happy with the results, please send us the image so we may improve the algorithm.

17.11.3.1 Optical character recognition

Part of the process of recovering chemical structures is to recognize character glyphs from images. ChemDoodle does this by comparing potential glyphs to standard *serif* and *sans-serif* fonts on your computer. If your computer does not have common fonts like "Times" and "Arial", you may find the character matching of the CIR algorithm to be performing poorly. The training set used to match character glyphs is found in the `characterTraining` folder of the `ChemDoodleSettings` folder. You may add to this training set if there is a particular type of glyph shape present in your images that is not well represented by the standard *serif* or *sans-serif* font. To do so, perform the following steps:

1. Isolate what shape is not being recognized well and create an image (100 by 100 pixels) with a pure white background in your image editor of choice. Place the character shape in a black color on this white background, centered so it is not touching the edges.
2. Save this image as a *PNG*.
3. In the `ChemDoodleSettings/characterTraining` folder, locate the subfolder for the character glyph your new image represents. In that folder you will see several other glyph shapes for that character. Name your image as "g*[n]*.png", where *[n]* is replaced with the first number not used by the other images. iChemLabs may add more images as time goes on, so to be safe, you may start with a number greater than 10.
4. The next time you restart ChemDoodle, the new glyph will be used to match character shapes by the chemical image recovery algorithm.

Character support covers glyphs lowercase *a-z*, uppercase *A-Z*, the digits *0-9* and the symbols plus (*+*), dash (-) and apostrophe (*'*).

In the case you have mistakenly deleted or overwritten one or more of the default training set images, you can have ChemDoodle restore the original set by going into the application **Settings**, going to the **Tools** tab and clicking the **Update Character Training Set** button in the **Chemical Image Recovery** section. This function will override any changes you have made to the training set, but will not discard any newly added images (where names do not clash). For a complete reset, delete the entire `characterTraining` folder in the `ChemDoodleSettings` folder before using this function.

17.12 Printing

The document can be printed from ChemDoodle. In most cases, the procedure is identical to other applications you use on your operating system. You can define settings, preview, and print.

17.12.1 Page setup

By selecting the File › Page Setup... menu item, you will be able to set the printer settings. The window that appears will be identical to the window that appears in other applications on your operating system. Here, you can select the printer and set up the page orientation.

17.12.2 Flipping the page orientation

In some cases, you may wish to print your document in landscape mode. To do this, execute the following steps:

1. Select the File › Page Setup... menu item.
2. In the window that appears, find the appropriate setting for page orientation, and change it to landscape.
3. Press the confirm button in the window to save your settings and close it.
4. A dialog box will appear asking if you would like to swap the width and height of the current document in ChemDoodle. If this is appropriate for your document, select **Yes**, otherwise, select **No**.



The orientation of the printed document and its size are distinct. Printing in landscape mode simply means that the printer prints your content at a 90 degree angle. It does not alter your document in any way. So in some cases, you may want to flip the dimensions of your document and reorient your figures before printing in landscape mode.

This procedure gives you maximum control over your documents, by allowing you to control the dimensions of your document and separately to control the orientation in which your document is printed.

17.12.3 Print preview

To preview your document before you print, select the File › Print Preview menu item. You can also click on the **Print Preview** button  in the **Document** toolbar. Click the **Close** button on the bottom right when you are finished to close the preview. Only the content that should appear in the printed version will appear in the preview; no warnings, highlights or other interface decorations will be present.

17.12.4 Printing a document

To print a document, execute the following steps:

1. Select the File › Print... menu item. You can also click on the **Print** button  in the **Document** toolbar.
2. In the window that appears, confirm or change any available settings.
3. Press the **Print** button to print your document.

Appendices

Appendix A: THIRD PARTY APPLICATIONS 462

Appendix B: CHEMDOODLE WEB COMPONENTS 474

Appendix C: TECHNICAL SUPPORT 479

APPENDIX A

Third Party Applications

A.1 Overview

ChemDoodle works with many third party applications. The most common applications are listed in this section. It is not an comprehensive list. Discussed in this section are:

- Common applications that are used with ChemDoodle.
- Which types of data are transferred to common third party applications?
- Solutions to issues involved with the third party applications.
- Round-trip editing compatibility.

A.2 Apple iWork

A.2.1 Pages

Text, images and scalable vector graphics can be transferred. For scalable vector graphics, **PDF** must be selected in the copy settings. Round-trip editing is supported via the workaround detailed in the *Round-Trip Editing* section of SHARING INFORMATION.

A.2.2 Keynote

Vector graphics support is the same as Pages. Round-trip editing is supported directly.

A.2.3 Numbers

Vector graphics support is the same as Pages. Round-trip editing is not supported.

A.3 Adobe products

A.3.1 Photoshop

Images and scalable vector graphics can be transferred. For scalable vector graphics, **PDF** must be selected in the copy settings.

A.3.2 Illustrator

Scalable vector graphics can be transferred. First, save content as *PDF* and then open, insert or drag and drop the file into Illustrator. For direct pasting, make sure all vector graphics are disabled except for **Windows Enhanced Metafile** on Windows or **Macintosh Vector Pict** on macOS.

A.4 Browsers

Most browsers will support image and scalable vector graphic output from ChemDoodle for display in web pages. The best scalable vector graphic formats to use are *SVG* and *PDF*.

For information of ChemDoodle Web Components browser compatibility, visit the ChemDoodle Web Components website: https://web.chemdoodle.com/installation/browser-compatibility/.

A.5 CAS SciFinder-n

iChemLabs is partnered with the Chemical Abstracts Service (CAS). As such, our ChemDoodle is integrated with SciFinder-n. This integration allows you to draw and submit queries to SciFinder-n including a structure, any number of structures or a reaction. A SciFinder-n account is required to access SciFinder-n through ChemDoodle.

A.5.1 Submitting a Query

To submit a query to SciFinder-n, perform the following steps:

1. Draw your query in ChemDoodle. The query can be a single structure, multiple structures, or a single reaction.
2. Select your drawn query using a selection tool.
3. Press the **SciFinder-n** button  in the **Chemistry** toolbar. You may instead use the File » Interfaces » SciFinder-n menus.
4. A window will appear as shown in Figure A.1. If using the button and you have a reaction selected, the query will default to a **Reactions** query, otherwise it will default to a **Substances** query.

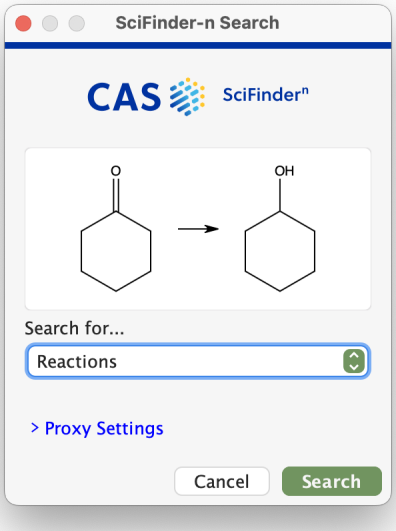


Figure A.1: *The SciFinder-n query window*

5. Your query will be previewed. You may choose a different search type using the drop down, and any search options will appear underneath the drop down, if available.

6. Once you have set up your search, press the **Search** button to execute. Your browser will open up with your search results.

A.5.2 Authentication

The first time you attempt to use SciFinder-n from ChemDoodle, you will be asked to authenticate your SciFinder-n account to give permission to ChemDoodle to submit queries on your behalf. So when you try to execute your first query search, your default browser will appear and ask you to log into SciFinder-n as shown in Figure A.2. Once successfully logged in, your search will appear in the browser.

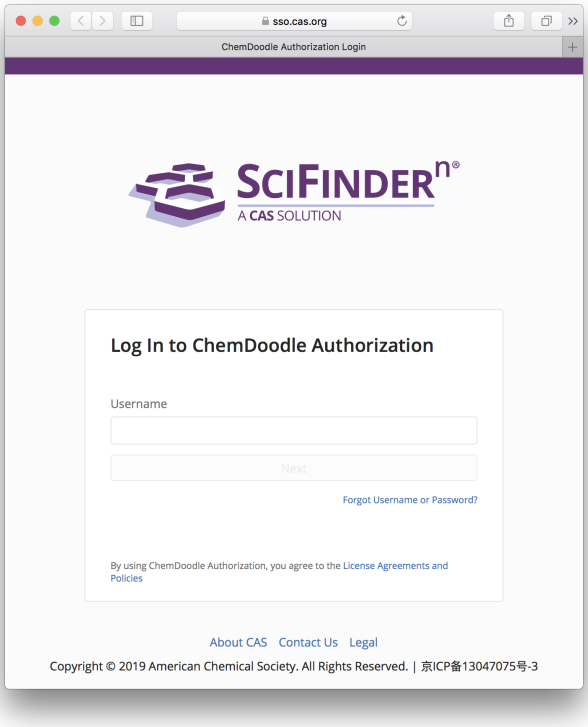


Figure A.2: *Logging into SciFinder-n*

A.5.3 Proxy settings

If your institution uses a proxy to access SciFinder-n services, you will need to specify the proxy URL in ChemDoodle. To do so, when the **SciFinder-n Window** is open, click on the **Proxy Settings** expandable label on the bottom left. A proxy URL input will be provided as shown in Figure A.3. Simply set the correct proxy URL in the **Proxy URL** field and press the **Save** button. If set to the correct value, your queries should then execute without issue.

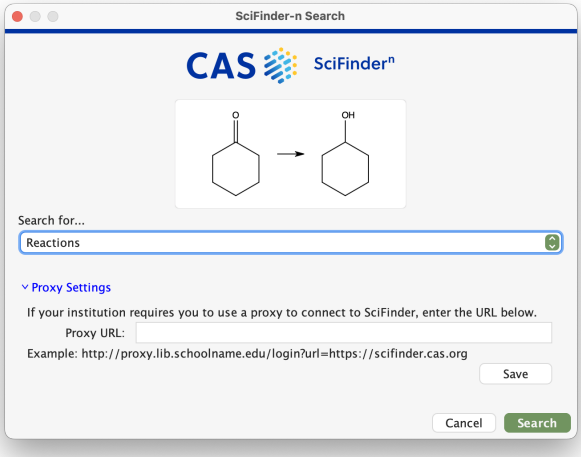


Figure A.3: *Setting up a proxy for SciFinder-n*

Once your proxy URL is saved, it will be remembered through restarts of the ChemDoodle application. To reset this value, open the **Settings** window and select the **Online** tab. Then press the **Purge 3rd Party Credentials** button.

A.6 CHEMNUM

The LaTeX chemnum package requires "<tag>n" tags to be preserved in *EPS* images, where <tag> is typically "TMP" and n is a positive integer. Based on the options you choose when outputting *EPS* images, ChemDoodle will detect "<tag>n" substrings in labels (label shapes, not atom labels) and will output such labels as complete text commands in *EPS* images for use with chemnum.

For more information, see the ENCAPSULATED POSTSCRIPT section and chapter 8 of the chemnum manual.

A.7 Google Patents

iChemLabs is partnered with the Google Patents team. As such, our ChemDoodle is integrated with Google Patents. This integration allows you to draw and submit queries to Google Patents.

A.7.1 Submitting a query

To submit a query to Google Patents, perform the following steps:

1. Draw your query in ChemDoodle. The query can be a single or multiple structures.
2. Select your drawn query using a selection tool.
3. Press the **Google Patents** button in the **Chemistry** toolbar. You may instead use the File » Interfaces » Google Patents menus.
4. A window will appear as shown in Figure A.4.

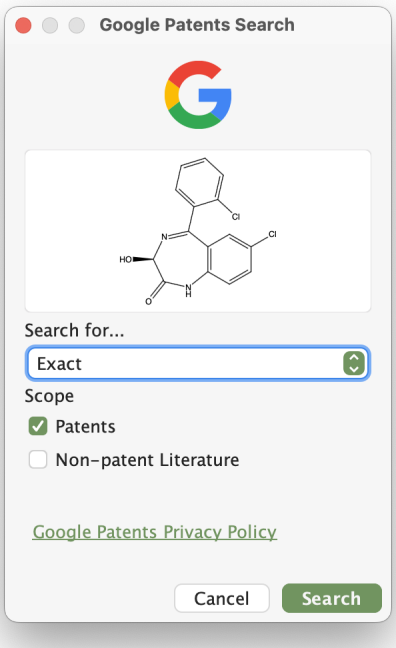


Figure A.4: *The Google Patents query window*

5. Your query will be previewed. You may choose a different search type using the drop down. You may then select a search scope, opting to search just Google Patents, non-patent literature (Google Scholar and Google Books), or both.

6. Once you have set up your search, press the **Search** button to execute. Your browser will open up with your search results.

A.8 GSRS

GSRS stands for Global Substance Registration System, which many government organizations use.

A.8.1 Submitting a query

To submit a query to GSRS, perform the following steps:

1. Draw your query in ChemDoodle. The query can be a single or multiple structures.

2. Select your drawn query using a selection tool.

3. Expand the File ⟩ Interfaces ⟩ GSRS submenu. Select the type of search you wish to perform.

4. A window will appear as shown in Figure A.5.

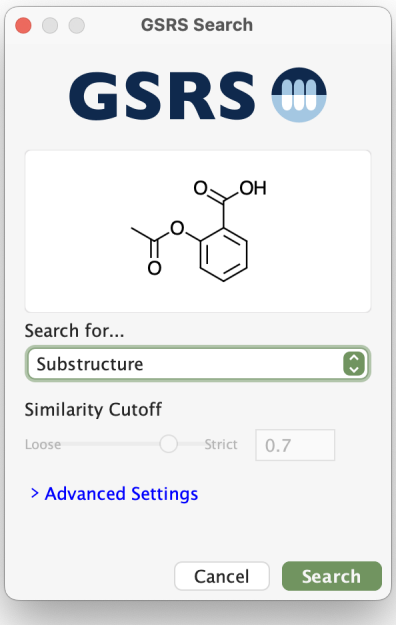


Figure A.5: *The GSRS query window*

5. Your query will be previewed. You may choose a different search type using the drop down. If you are performing a **Similarity** search, the **Similarity Cutoff** option will be enabled allowing you to control the looseness of the search.

6. Once you have set up your search, press the **Search** button to execute. Your browser will open up with your search results.

A.8.2 Advanced settings

The default GSRS instance ChemDoodle connects to will be the NIH: https://gsrs.ncats.nih.gov/ginas/app/beta

If your institution uses an internal GSRS database or you wish to switch to a different GSRS instance, you will need to specify the base URL in ChemDoodle. To do so, when the **GSRS Window** is open, click on the **Advanced Settings** expandable label on the bottom left. Additional settings will be available as shown in Figure A.6. Simply set the correct base URL in the **Base URL** field, and press the **Save** button. If setup correctly, your queries should then execute without issue.

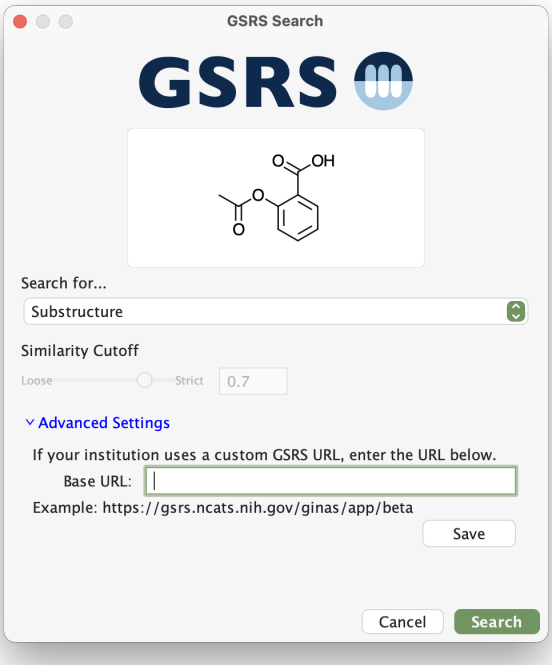


Figure A.6: *Advanced settings for the GSRS instance*

Once your advanced settings are saved, they will be remembered through restarts of the ChemDoodle application. To reset these settings, open the **Settings** window and select the **Online** tab. Then press the **Purge 3rd Party Credentials** button.

A.9 LabArchives

iChemLabs is partnered with LabArchives. As such, our ChemDoodle application is integrated with LabArchives. This integration allows you to post chemical data as an image and chemical file pair. A LabArchives account is required to access LabArchives through ChemDoodle.

A.9.1 Posting content

To post content to LabArchives, perform the following steps:

1. Draw your content in ChemDoodle.
2. Select your content using a selection tool.
3. Expand the File ⟩ Interfaces ⟩ LabArchives submenu. Select the **Post Selected Content** menu item.
4. A window will appear as shown in Figure A.7. An image preview for the post will be presented on the bottom. Enter your preferred values for the **Filename**, **Caption**, and **Keywords** fields.

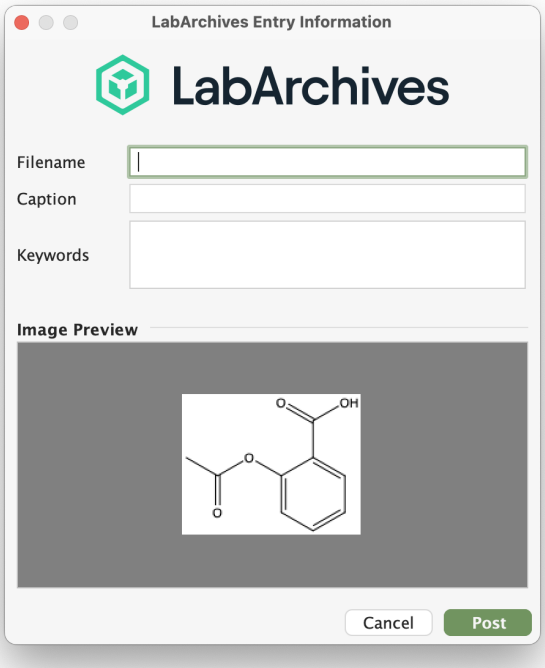


Figure A.7: *The LabArchives post window*

5. Once you are satisfied with the post content, press the **Post** button to complete your post. This post will appear in the inbox area of your LabArchives account for further action.

A.9.2 Authentication

The first time you attempt to use LabArchives from ChemDoodle, you will be asked to authenticate your LabArchives account to give permission to ChemDoodle to post content on your behalf. So when you try to execute your first post, an authentication window will appear as shown in Figure A.2. Once successfully authenticated, your post will proceed.

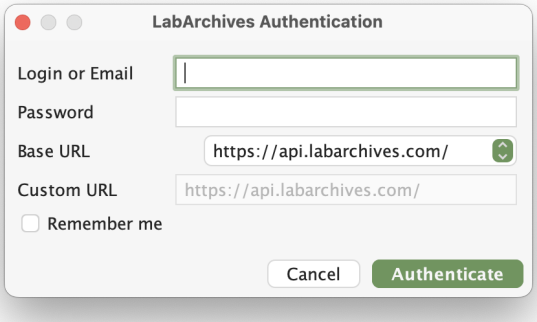


Figure A.8: *Authenticating your LabArchives account*

A.9.3 Base URL settings

If your institution uses a custom base URL to access LabArchives, you will need to specify the custom base URL in ChemDoodle during authentication by editing the **Base URL** and **Custom URL** fields. Press the **Authenticate** button to complete authentication. If set to the correct values, your post should then execute without issue.

A.9.4 Saving credentials

When authenticating, select the **Remember me** checkbox to store your authentication information with ChemDoodle for future use. The authentication information will be remembered through restarts of the ChemDoodle application. To reset this value, open the **Settings** window and select the **Online** tab. Then press the **Purge 3rd Party Credentials** button.

A.10 Microsoft Office

A.10.1 Word

On Windows and macOS, text, images and scalable vector graphics can be transferred.

For scalable vector graphics, if using Word on Windows, **Windows Enhanced Metafile** must be selected in the **Image Types** section of the **Clipboard** tab of the **Settings** window. For scalable vector graphics, if using Word 2004 on macOS, **Macintosh Vector PICT** must be selected in the **Image Types** section of the **Clipboard** tab of the **Settings** window; Word 2008 and all future versions on macOS require **PDF** to be selected in the copy settings. Make sure all bitmap image types are deselected.

Round trip editing is functional on Windows with Microsoft Office using ChemDoodle's OLE library.

Round trip editing is functional on macOS with Microsoft Office 2011 at update 14.0.1 or more recent and until version 16 where Microsoft has disabled round trip editing.

A.10.2 Powerpoint

Same as Word.

A.10.3 Excel

Same as Word.

A.11 OpenOffice

A.11.1 Writer

On all operating systems, text, images and scalable vector graphics can be transferred. For scalable vector graphics, if using Writer on Windows, **Windows Enhanced Metafile** must be selected in the **Image Types** section of the **Clipboard** tab of the **Settings** window. For scalable vector graphics, if using Writer on macOS, **Macintosh Vector PICT** must be selected in the **Image Types** section of the **Clipboard** tab of the **Settings** window. For scalable vector graphics, if using Writer on Linux, **OpenDocument Graphics** must be selected in the **Image Types** section of the **Clipboard** tab of the **Settings** window.

Round-trip editing is supported on Linux by using the *ChemDoodle UNO* plugin.

A.11.2 Calc

On all platforms, text, images and scalable vector graphics can be transferred.

For macOS, first save ChemDoodle content as **Macintosh Vector PICTs** and then insert or drag and drop the file into Calc.

Round-trip editing is supported on Linux by using *ChemDoodle UNO* plugin.

A.11.3 Impress

Same as Calc.

A.12 Other

ChemDoodle is compatible with any application that supports the data ChemDoodle places on the system clipboard. Because ChemDoodle expertly handles *Windows Enhanced Metafiles*, *Macintosh Vector PICT 2*, *PDF* and *OpenDocument Graphics*, scalable vector graphics can be directly pasted into all native applications on the different operating systems.

Round-trip editing will be supported with any application that supports OLE on Windows, or that will preserve PDF comments on macOS, or that can integrate with the *ChemDoodle UNO* plugin on Linux.

A.13 precisionFDA

precisionFDA is a secure, collaborative, high-performance computing platform that builds a community of experts around the analysis of biological datasets in order to advance precision medicine.

A.13.1 Submitting a UNIISearch query

To submit a UNIISearch query to precisionFDA, perform the following steps:

1. Draw your query in ChemDoodle. The query should be a single structure.
2. Select your drawn query using a selection tool. If multiple structures are selected, only the first molecule will be submitted.
3. Expand the File › Interfaces › precisionFDA submenu. Select the UNIISearch menu item.
4. Your browser will open up with your search results.

A.14 PubChem

ChemDoodle is integrated with PubChem. This integration allows you to draw and submit queries to PubChem.

A.14.1 Submitting a query

To submit a query to PubChem, perform the following steps:

1. Draw your query in ChemDoodle. The query can be a single or multiple structures.
2. Select your drawn query using a selection tool.
3. Press the **PubChem** button  in the **Chemistry** toolbar. You may instead use the File › Interfaces › PubChem menus.
4. A window will appear as shown in Figure A.9.

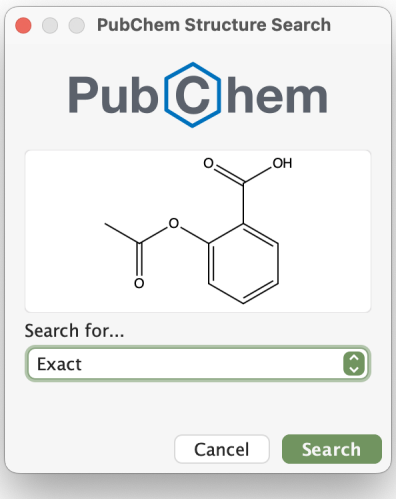


Figure A.9: *The PubChem query window*

5. Your query will be previewed. You may choose a different search type using the drop down. You may then select a search scope.

6. Once you have set up your search, press the **Search** button to execute. Your browser will open up with your search results.

APPENDIX B

ChemDoodle Web Components

B.1 Overview

In addition to creating graphics and chemical files, ChemDoodle can also create dynamic web components. This feature utilizes another iChemLabs technology, the ChemDoodle Web Components library. This appendix covers the following topics:

- Creating ChemDoodle Web Components in ChemDoodle.
- ChemDoodle rendering features that are available in the ChemDoodle Web Components library.
- Other functions for working with ChemDoodle Web Components.
- How generated components work for both desktop and mobile browsers.
- Restrictions on using ChemDoodle Web Components in your webpages.

B.2 Generating ChemDoodle web components

To generate a ChemDoodle Web Component, execute the following steps:

1. Select the File » Generate Web Component... menu item. Make sure to first have drawn or loaded any content you wish to be displayed in ChemDoodle.
2. If you had selected a *molecule* or *spectrum* before opening this window, then an appropriate viewer will be selected. Otherwise, choose the **Type** of component you would like to create.
3. If you did not previously select content for the component and you want to preload content or the **Type** of component chosen requires content, then click on the **Select** button and choose the content to be displayed in the component. You may also choose to include all compatible data from your current document using the **Select** button.
4. As is shown in Figure B.1, set the size of the component and the component name (a random name is generated for you to avoid name clashes).

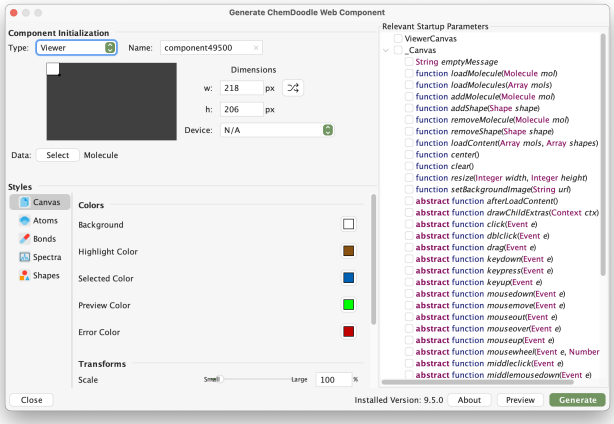


Figure B.1: *Generate ChemDoodle Web Component Window*

5. Define any styles for the component. It will inherit compatible styles from the current style sheet in ChemDoodle.
6. In the **Relevant Startup Parameters** tree, select any *Javascript* variables or functions you would like to define. Placeholders for them will be generated in the *Javascript* code.

7. Press the **Preview** button to preview your ChemDoodle Web Component in your main browser as shown with Apple Safari in Figure B.2.

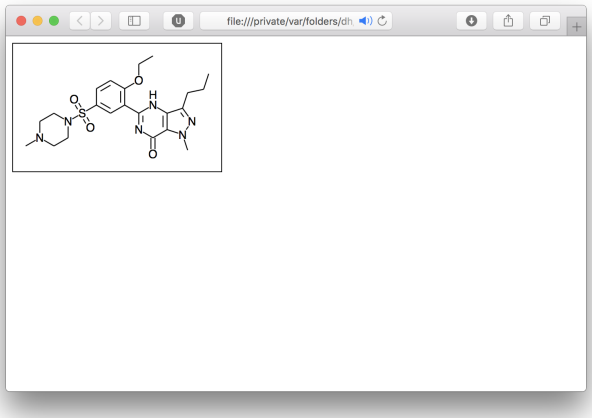


Figure B.2: *Previewing the Web Component (Apple Safari shown)*

8. Make any changes, if necessary.

9. Click the **Generate** button to generate the *Javascript* for the component.

Paste the generated *Javascript* directly in your webpage (in the *<body>* tag) in the location you prefer the component to appear. You must first install the ChemDoodle Web Components library for your webpage for these components to work. Installation instructions are provided on the official ChemDoodle Web Components website at https://web.chemdoodle.com/installation/download.

B.3 GENERATING CHEMDOODLE JSON DATA FILES FOR USE WITH CHEMDOODLE WEB COMPONENTS

If you are displaying several web components with the same molecule/spectrum or are doing advanced development, it may be more efficient to generate the data first in a *ChemDoodle JSON* data file to be loaded into your webpage. To do this, execute the following steps:

1. Draw all content to be used in your webpage in ChemDoodle.

2. Select the File ⟩ Save as... menu item.

3. In the file chooser that appears, select the location and the name of the file to be saved.

4. In the drop-down selection for the file type, choose *iChemLabs ChemDoodle JSON*.

5. Press the **Save** button.

All structures and spectra on the **Doodle Board** will be saved to the *ChemDoodle JSON* format in *Javascript*. To use this file, link it into the *HTML* page as a *Javascript* resource or copy and paste the source of the file into your *Javascript* code. Use the ChemDoodle Web Components' API to retrieve the chemical data from the JSON object. More information on the *ChemDoodle JSON* format can be found on the official ChemDoodle Web Components website at https://web.chemdoodle.com/docs/chemdoodle-json-format/.

B.4 Generating components for mobile devices

ChemDoodle Web Components will work in all browsers including those on mobile devices, notably iPhone OS (iPhone, iPod Touch, iPad) and Android devices. All rendering is supported on the mobile devices and touch events and gestures are recognized by the components.

There is no difference between generating components for desktop browsers versus for mobile browsers. The only consideration would be the size of the component. The ChemDoodle Web Component generator contains a drop down selection to the right of the dimension panel containing preset sizes for mobile devices. Use it to quickly set standard sizes if preferable.

B.5 Rendering compatibility

Even though ChemDoodle and the ChemDoodle Web Components library are in the same family of products, their feature sets are not identical. Many graphical features and styles provided in ChemDoodle may not yet be available in the ChemDoodle Web Components library.

Use the ChemDoodle Web Component window in ChemDoodle to help guide you through the available styles in the ChemDoodle Web Components library. Use the **Preview** button to ensure your graphics will be correctly represented to your satisfaction.

B.6 ChemDoodle web components version

The interface in ChemDoodle will always work with the latest version of the ChemDoodle Web Components when a ChemDoodle update is released. However, the ChemDoodle Web Components may have further updates after this release. In this case the latest version of the ChemDoodle Web Components may not work with the output from ChemDoodle, although incompatibilities should be minimal. You can see which version of the ChemDoodle Web Components is used by ChemDoodle on the bottom right of the ChemDoodle Web Components builder.

You can update the ChemDoodle Web Components in ChemDoodle manually by replacing the corresponding files in the `resources` folder in the `ChemDoodle` installation folder with the latest from the ChemDoodle Web Components website. Please note that while this will allow you to use the latest ChemDoodle Web Components with ChemDoodle, it will not add new features to ChemDoodle and it may require an update from iChemLabs before it works completely.

B.7 License

The ChemDoodle Web Components library is licensed under version 3 of the GNU GENERAL PUBLIC LICENSE: https://www.gnu.org/licenses/gpl-3.0.html

If you want to include ChemDoodle Web Components in your product or website, you must abide by this license, or contact iChemLabs for a commercial license.

B.7.1 Am I allowed to rebrand your components?

Not under the GPL license. Rebranding is identical to removing our copyright notice on the source code, which is also prohibited.

B.7.2 Attributions

Attributions on webpages for the use of ChemDoodle and ChemDoodle Web Components are greatly appreciated.

Several ChemDoodle Web Component badges are provided for this purpose at https://web.chemdoodle.com/installation/badges.

B.7.3 Further information

For further information regarding the ChemDoodle Web Components, including webpage installation instructions, the most recent version and updates, advanced programming and use of the API, examples and browser compatibility, visit the official ChemDoodle Web Components website at https://web.chemdoodle.com.

APPENDIX C

Technical Support

C.1 When to contact customer service

We certainly want your experience with iChemLabs software to be as enjoyable and hassle free as possible. While we do our best to debug and test ChemDoodle, a few bugs will always slip past us. We encourage you to report any bugs that you find and we will do our best to address them.

Before contacting us, please do the following:

- Check the system requirements for ChemDoodle on our website to ensure that your system is supported.
- Search this user guide to see if your issue is addressed here.
- Read the TROUBLESHOOTING section of this appendix and follow the possible resolution tactics outlined there.
- Double check that your problem is reproducible and outline the exact steps executed to cause it.
- Take screenshots of any relevant graphical issues or popup errors in their entirety.
- Make note of any steps you have taken in attempting to correct the problem.

C.2 How to contact customer service

After collecting all relevant information, click on the Help ⟩ Contact Customer Service menu item as shown in Figure C.1. We always respond to inquiries within one business day and frequently respond within an hour.

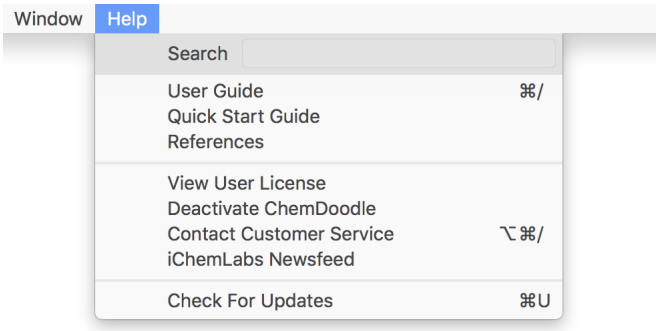


Figure C.1: *Contact Customer Service Menu Item*

This function will automatically pre-populate fields in our online customer support form at https://www.ichemlabs.com/contact-us. Fill in the remaining fields and send us your report. You may also attach supporting files.



The contact form only allows a single file to be attached and may not allow all types of files to be attached. If a file you are trying to upload is rejected, or you need to send us multiple files, please archive those file(s) into a *ZIP* archive and attach the *ZIP* instead.

C.3 Following ChemDoodle development

Our development process is an open process and you can learn more about what we are doing by visiting the iChemLabs homepage at https://www.ichemlabs.com. We regularly post stories about ChemDoodle development and compatibility checks with new operating systems. Subscribe to the iChemLabs newsfeed RSS or our social media accounts for immediate notifications.

The iChemLabs newsfeed RSS can also be viewed by selecting the Help > iChemLabs Newsfeed menu item.

C.4 Feature requests

We are happy to receive feature requests from users. You can submit a request using the customer service form as described in the previous section of this appendix.

Features that are not beyond the scope of ChemDoodle will be included in a future update. However, some features may take a long time to implement, so please be patient when requesting new features. If a feature is beyond the scope of ChemDoodle we will attempt to explain why in a response to the feature request.

The following steps describe how our feature request system works and how we prioritize the features that we work on.

1. All feature requests (from customers and non-customers) are considered and are reported to our development tracking system.
2. Feature requests are associated with a score based on the popularity of the request. Each feature begins with a score of 0. The score is then incremented by 1 for each unique customer that requests that feature (including the initial request if done by a customer). Non-customers that request features do not affect feature scores.
3. Once each month, we reevaluate the scores and plan our development around the features with the highest scores.
4. When a feature is implemented it is removed from our development tracking system.

Therefore, to get the features you want implemented in ChemDoodle as fast as possible, do the following two things:

- Let us know about the feature you would like to see implemented by contacting us using the method described in the previous section.
- Get as many unique ChemDoodle customers to request the same feature as possible.

C.5 Experimental Features

From time to time, iChemLabs may include experimental features in our builds, so that our customers can try them. These features are disabled by default. You may enable access to experimental features by editing the `config/application.config` file in the main installation `ChemDoodle` folder. Make sure you know what you are doing if you edit this file! Set the value for the "experimental_features" element to "true" to enable experimental features. Then restart the ChemDoodle application to see the experimental features.



The *experimental_features* option turns on features that are not yet tested or complete. These features may not work, or may cause data loss or other serious issues. By setting the *experimental_features* option to true, you agree to do so at your own risk.

C.6 Troubleshooting

C.6.1 Windows

Occasionally when you open ChemDoodle it will ask about connections, select “Keep Blocking". ChemDoodle creates a local socket to open files that are double-clicked, generating this warning. ChemDoodle never accesses the internet unless you allow it to.

Sometimes the JRE can corrupt and you may see weird behavior when using ChemDoodle. Restart your computer to resolve these issues.

C.6.2 macOS

If you have updated ChemDoodle and notice that the new filetype associations aren’t being recognized in Finder, restart your computer. The filetypes should now be recognized in Finder.

C.7 Performance improvements

C.7.1 Hardware

If you see poor responsiveness in ChemDoodle, access to system resources may need to be tweaked. Try the following solutions.

1. Upgrade to a more powerful CPU and/or GPU.
2. Increase the amount of memory accessible by the computer.

C.7.2 Software

Apart from hardware upgrades, a few base application features in ChemDoodle can be changed to improve performance.

1. Disable the application rendering decorations in the **Settings** window under the **Appearance** tab in the **Decorations** section.
2. Change the rendering parameters to the options that favor speed in the **Settings** window under the **Rendering** tab.

C.7.3 Memory Allocation

We specify a certain amount of memory to be allocated to the ChemDoodle application at startup. You may modify these values by editing the following application Java Virtual Machine (JVM) parameter files specific to each operating system:

- **Windows** - In the `ChemDoodle` installation folder, you will find a file named `ChemDoodle.vmoptions`.
- **macOS** - In the `ChemDoodle.app` application package, you will find a file at path `Contents/Java/ChemDoodle.cfg`. This file will contain a section titled **JVMOptions**.
- **Linux** - In the `ChemDoodle` installation folder, you will find a file named `ChemDoodle.ini`.

You may then change the JVM parameters as you see fit. This page from Oracle provides further instruction: https://docs.oracle.com/cd/E15523_01/web.1111/e13814/jvm_tuning.htm#PERFM161



You edit the ChemDoodle application files and JVM parameters at your own risk. iChemLabs does not warrant or support changes to these files.

C.8 Debug Log

In rare cases, an error may occur that iChemLabs cannot reproduce and we will need to see the debug log from the ChemDoodle application. Perform the following steps to create the log:

1. Make sure that ChemDoodle is currently closed.
2. In the user's documents folder, find the `ChemDoodleSettings` folder.
3. In the `ChemDoodleSettings` folder, add a subfolder named `log`.
4. Open ChemDoodle and take the necessary steps to reproduce the issue. Once that happens, close ChemDoodle. A log file should then be present in the `log` folder.
5. Compress the entire `log` folder and send it to iChemLabs. We will then be better equipped to solve the issue.

When the issue is resolved, be sure to delete the `log` folder, as logs will continue to be output there while it is present.



You may have changed the location of the `ChemDoodleSettings` folder by editing the `config/application.config` file in the main installation `ChemDoodle` folder. If you have done this, you will need to locate where the `ChemDoodleSettings` folder was placed to create the log.

Index

iChemLabs art, 262
    restrictions, 263
document
    styles, 300
document
    saving, 61
    tabs, 25
18-electron rule, 150
3D, 336
3d, 155
    rotating, 278

abbreviations, 325
    custom, 325
accessibility, 58
activation, 15
    vs installation, 7
ADME, 341
Adobe, 462
    Illustrator, 462
    Photoshop, 462
aligning, 281
alpha interpolation, 316
ambiguous double bonds, 407
anion, 132
anti-aliasing, 315
Apple
    iWork, 462
    Keynote, 462
    Numbers, 462
    Pages, 462
arcs, 228
aromatic circles, 358
aromaticity, 357, 358
    delocalization, 358
    electron counts, 357
aromatics
    ring circles, 157
arrowheads, 177, 236
arrows, 175, 236
    bezier, 180
    bold, 179
    connectors, 179
    electron pair, 179
    electron pushing, 181, 251
    equilibrium, 179
    palette, 47
    reaction, 179
    resonance, 179
    retrosynthetic, 179
    single electron, 179
asterisk, 132
atom mappings, 250
atoms, 109
    labels, 111, 113–116
    styles, 305
attributes, 129
    auto-placement, 129
    custom, 134
    styles, 307
autosaving, 61
axial chirality, 405

bezier
    arrows, 180
BioArt, 267
bold arrow, 179
bond
    z-order, 283
bond orders
    deduction, 338
bond types, 118
    IUPAC naming, 368
    labels, 326
bonds, 116
    palette, 43
    styles, 307
    zero order/ionic, 142
brackets, 232
    palette, 49
Browsers, 463
Bézier curves, 235

Cahn-Ingold-Prelog (CIP), 403
Calc, 470
calculations, 339
captions, 246
carbon
    atoms, 109
    labels, 112
carbon nanotubes, 161

CAS
    nomenclature, 367
    SciFinder, 463
cation, 132
centering, 281
chains, 120
    palette, 45
charges, 131
    dash length, 132
    formal, 324
    labels, 326
    partial, 431
ChemExper, 79, 81, 331
chemical files, 446
chemical formats, 426
chemical image recovery, 456
cheminformatics, 323
chemnum, 454, 465
ChemSpider, 79, 81
chevrons, 232
CIR, 456
cis/trans, 407
clipart, 262
clipboard, 419
color
    advanced colors button, 290
    detection, 290
    quick colors button, 289
color chooser
    pinwheel, 293
    recent colors, 294
    rgb/hsb, 292
color space, 454
compression quality, 454
CompuServ graphics interchange, 454
conjugation, 359
constitutional, 339
coordinate bonds, 143
coordinates, 335
    2D, 335
    3D, 336
copy, 287, 422
    formatted text, 381, 420, 422
copy as, 422
copy/paste, 286–287, 422–424
covalent bond deduction, 337
crown ethers, 123
curly braces, 232
cursors, 56
cut, 287

data
    elemental, 342
data recovery, 445
dative bonds, 143
delocalization, 360
delocalized, 357
descriptors, 339
deuterium, 113
dipole, 132
distance geometry embedding, 337
distributing, 281, 282
dithering, 316
document
    management, 59
    number of pages, 60
    resizing, 60
drawing
    cancelling, 109
drawing aids, 288
duplicating, 287
    while transforming, 287

electron, 132
    pair, 132
electron pair arrow, 179
electron pushing arrows, 181, 251
    flipping, 252
    special cases, 252
element
    custom color set, 295
elemental analysis
    undefined isotopes, 345
    widget, 74
elemental data, 342
elements
    IUPAC naming, 368
encapsulated postscript, 454
enhanced stereochemistry, 410
EPS
    image options, 454
equations
    balancing, 189
equilibrium arrow, 179
equivalents, 207
Euler facet rings, 361
Excel, 470
    chemical data recovery, 447

ferrocene, 150
File
    enabling individual filetype options, 425
    I/O, 424
    reducing file types on save, 424
file
    annotations, 428
    centering molecules on output, 431
    chemistry support, 427
    conversion, 429
    options, 430
    search widget, 91
file chooser, 63
    previews, 63
file type associations, 14

firewall, 16
flattening, 337
flipping, 282
folder
  installation, 13
  settings, 14
fonts
  caption, 247
  fractional metrics, 315
force field, 336
formats
  chemical, 426
  image, 449
  native, 426
forms
  stoichiometry, 194
formula
  molecular, 328
  radical, 328
fragmentation, 216
fragments
  labels, 328
framing, 286
functional groups, 346

geometric features, 396
GIF
  image options, 454
glassware, 50, 264
  solution, 265
  tubing, 266
Google
  Books, 465
  Patents, 465
  Scholar, 465
Google Patents, 351
graph reduction, 348
grayscale, 454
greek letters, 95, 133
grid, 282
grouping, 286
GSRS, 466

Hückel, 357
Hanser rings, 361
haptic bonding, 150
haptic bonds, 143
hapticity, 143
helicity, 405
high-DPI screens, 10
highlights, 254
history
  widget, 76
hovering, 108
hydrogens, 348
  explicit, 349
  implicit, 348
  labels, 327

icons
  file, 13
  mouse, 56
Illustrator, 462
image
  options, 452
  output, 449
  sizing, 450
image formats, 449
images
  insert, 455
  interpretation, 456
  raster, 420
  recovery, 456
  vector, 420
Impress, 471
incrementals, 133
infrared spectroscopy (IR), 211
installation, 7
  multiple users, 11
interface
  settings, 52
ionic bond, 142
ionization energies, 342
ions, 131
  IUPAC naming, 374
isotopes, 135, 342, 344
  calculations, 344
  IUPAC naming, 375
  natural abundance, 344
  with no natural abundance, 345
isotopic distribution, 216
  undefined isotopes, 345
  widget, 74
IUPAC naming, 366
  ionic compounds, 378, 380
  locants, 382
  name to structure, 377
  nomenclature systems, 368
  options, 383
  PINs, 367
  structure to name, 378
  Systematic, 367
  Traditional, 367
  Trivial, 367
iWork, 439, 462

JCAMP-DX, 211
  NTUPLES, 212

Kekulé, 357, 359
keyboard shortcuts, 106
  custom, 107
  drawing, 107
  tool, 107
Keynote, 439, 462

LabArchives, 468
label rotation, 279
labels, 246, 325
    auto-updating, 248
    collapsing, 330
    expansion, 330
landscape, 459
lewis dot structures, 160
LibreOffice plugin, 440
license
    restore, 18
    site, 15
    transfer, 17
    web components, 476
ligands
    IUPAC naming, 372
limiting reagent, 205
line notations
    widget, 77
lines, 228
locants
    IUPAC, 382
lone pairs, 324

macOS Gatekeeper, 11
macOS Notarization, 11
macromolecules, 161
mass calculations
    undefined isotopes, 346
mass fragmentation, 216
mass number, 135
mass spectrometry (MS), 211
    simulation, 215
MDLCT, 422
MDLSK, 422
menu
    chemdoodle, 26
    content, 31
    edit, 28
    file, 27
    help, 37
    main, 26
    purchase, 37
    reaction, 36
    spectrum, 36
    structure, 33
    view, 30
    window, 36
menu accelerators, 106
metal compounds
    bond types, 142
metallocenes, 143
Microsoft
    Excel, 470
    Powerpoint, 470
    Word, 470
Microsoft Office, 470
    chemical data recovery, 447
MIME types, 419
minimization, 336
molecular formula, 328
MolGrabber, 79
monochrome, 454
moving, 277
multi-center attachments, 143, 150
multiplets
    widget, 83

name to structure, 377
nanotubes, 161
new features, 4
Newman projections, 162
NIH Cactus, 336
nmr
    widget, 86
notation
    nuclear, 136
nuclear magnetic resonance (NMR), 211
    simulation, 214
    solvent, 215
nuclear notation, 136
Numbers, 439, 462

OLE server, 437
OpenOffice, 470
    Calc, 470
    Impress, 471
    Writer, 470
optical structure recognition, 456
optimization, 335
optimize zone, 117, 122, 125
orbitals, 137
    palette, 47
organizing, 281
OSR, 456
ovals, 231

Pages, 439, 462
palettes, 41
    arrows, 47
    bonds, 43
    brackets, 49
    chains, 45
    chemical attribute, 46
    elemental labels, 43
    macromolecular, 45
    orbitals, 47
    pens, 50
    rings, 44
    shapes, 48
    text input, 42
parenthesis, 232
paste, 287, 423
    match style, 423
    special, 423

text as chemical, 424
pasting
from other chemical applications, 446
pen, 234
performance, 481
periodic table, 342
perspective drawings, 156
photon, 179
Photoshop, 462
physicochemical, 341
polyline, 234
Powerpoint, 470
chemical data recovery, 447
precisionFDA, 471
Preferred IUPAC Names, 367
print
preview, 459
printing, 459
page setup, 459
prismanes, 161
processor
Apple Silicon, 8
properties
widget, 89
proxy, 16
pseudo-3d graphics, 158
PubChem, 79, 81, 471

queries
interface, 169
NOT operator, 169
structures, 166
uses, 171
variables, 167
query structures, 166
Quick Look, 64

racemic stereochemistry, 410
radical
anion, 132
cation, 132
radical formula, 328
radicals
IUPAC naming, 374
raster images, 420
reaction arrow, 179
reactions, 182
atom-to-atom mapping, 250
atom-to-atom mappings, 187
balancing, 189
builders, 184
cleaning, 186
conditions, 185
electron pushing, 183
equations, 189
mechanism result, 183
redox, 189
sprouting, 183
stoichiometry, 194
recovery
embedded chemical data, 446
rectangles, 230
references
IUPAC naming, 376
list, 323
referencing, 19
relative stereochemistry, 410
repeat units
drawing and editing, 256
resolution, 454
resonance, 357
resonance arrow, 179
restrictions
trial, 18
Retina screens, 10
retrosynthetic arrow, 179
rings, 121
arbitrary size, 123
crowns, 123
Euler facet rings, 361
exploding, 362
Hanser rings, 361
palette, 44
perception, 361
smallest set of smallest rings (SSSR), 361
styles, 310
roman numerals, 133
rotating, 277
3d, 278
round trip editing, 450
round-trip editing, 436, 445, 446
ruler, 50
rulers, 237
guides, 24

save
as image, 450
selection as image, 450
scalable vector graphics, 421
scale
rendering, 61
scaling, 279, 280
images, 318
SciFinder, 331, 351, 463
socket, 14
scrollbars, 24
selecting
atoms, 110
bonds, 118
selection, 273–276
lasso, 273
rectangular marquee, 273
sequences
amino acid, 163

Settings
controls, 53
settings
accessibility, 54
appearance, 54
button, 50
controls, 52
shapes, 225
anchors, 225
arcs, 228
atom mappings, 250
automatic, 227
brackets, 232, 256
Bézier curves, 235
custom, 233
electron pushers, 251
highlights, 254
lines, 228
manual, 225
editing, 226
ovals, 231
palette, 48
pen, 234
polyline, 234
rectangles, 230
repeat units, 256
styles, 311
tables, 238
z-order, 285
silent installation, 7
single electron arrow, 179
site license, 15
smallest set of smallest rings (SSSR), 361
SMARTS, 171, 275
socket, 14
solution, 265
spectra, 211
editing, 218
grid, 219
integration, 220
simulation, 214
styles, 313
stacking, 283
statistics
widget, 94
stereochemistry, 396
alkenes, 405
allene, 405
atropisomers, 406
chair projections, 400
cumulene, 405
enhanced, 410
Fischer projections, 399
forcing, 408
Haworth projections, 399
input/output, 401
IUPAC, 397
IUPAC naming, 375
MDL/BIOVIA, 397
preservation while editing, 282, 336, 402
projections, 398
removing, 407
tetrahedral, 404
unspecified, 407
stoichiometry, 194
coefficients, 207
form, 194
limiting reagent, 205
strokes, 314
structure to name, 378
style sheets, 300
loading, 301
saving, 301
styles, 300
document, 300
atoms, 305
attributes, 307
bonds, 307
button, 50
conforming, 302, 303
pages, 304
rings, 310
shapes, 311
spectra, 313
types, 303
suppliers, 331, 351
SVG
image options, 455
symbols, 132
mathematical, 95
templates, 97
widget, 95
system clipboard, 419
system requirements, 7

table, 49
tables, 238
adding content, 243
colspan, 245
rowspan, 244
stoichiometry, 194
tabs, 25
templates, 124
custom, 126
management, 126
perspective rings, 157
sets, 126
symbols, 97
tlc canvas, 99
text, 246, 420
formatting, 247, 381, 420
tlc plates
templates, 99
toolbar

chemistry, 40
content, 39
document, 41
drawing, 41
formatting, 39
toolbars, 39
topological, 340
torsioning, 282
Traditional IUPAC Names, 367
translating, 277
transparency, 454
tritium, 113
tubingn, 266

unicode, 95
universal force field (UFF), 336
updates, 16

valence, 363
vector graphics, 263, 420

warnings, 331
wavy bonds, 407
web components, 474–477
Web scalable vector graphics, 455
websites, 6
widgets, 50, 69–101
drawer, 70
elemental analysis, 74
expansion, 71
history, 76
line notation pad, 77
menu, 69
MolGrabber, 79
multiplet tool, 83
nmr simulation, 86
properties, 89
search, 91
statistics, 94
symbols, 95
Windows
admin privileges, 17
application signature, 10
registry, 14
SmartScreen, 10
Word, 470
chemical data recovery, 447
workspace, 51
Writer, 470

z-order, 283
zero order bond, 142