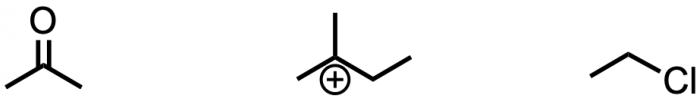
Name: _____
Class: _____

Nucleophiles & Electrophiles Worksheet

Warm-Up Questions:

Watch the Khan Academy videos on nucleophilicity and basicity.

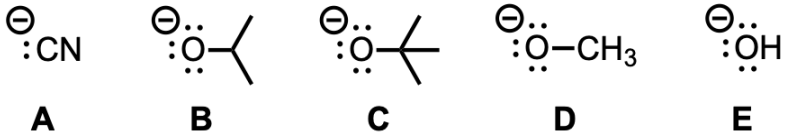
1) Identify the nucleophilic center of each molecule.



2) Identify the electrophilic center of each molecule.

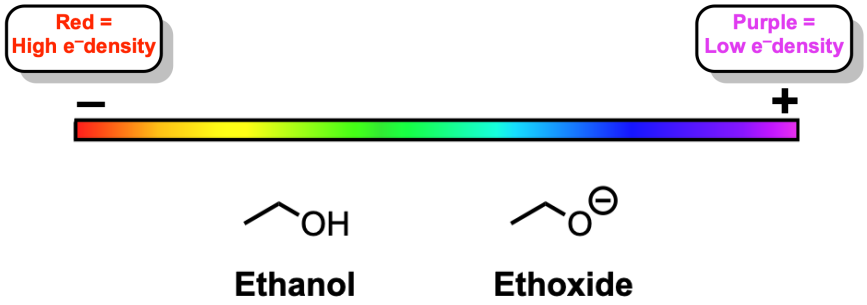
Example #1

Rank the following compounds in order of increasing nucleophilicity.



A **B** **C** **D** **E**

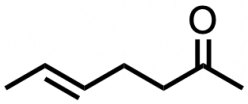
Computational Exercise #1:



Take a screenshot of the two electrostatic potential maps of ethanol and ethoxide. In a few sentences, analyze any differences you see between the two surfaces. Determine which regions of each nucleophile dictate its strength, or lack thereof, towards attack of an electrophile.

Example #2:

Predict where the nucleophilic and electrophilic centers are in the following molecule (E)-hept-5-en-2-one. Draw in any partial charges if applicable.

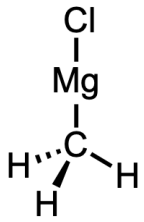


Computational Exercise #2:

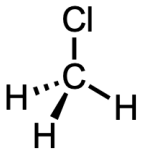
Take a screenshot of your electrostatic potential map. In a few sentences, analyze the nucleophilic and electrophilic regions of (*E*)-hept-5-en-2-one.

Individual Exercise:

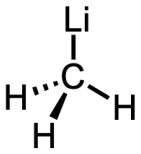
All three molecules below contain carbon atoms but some act as a nucleophile while some act as an electrophile.



A



B



C

For each of the molecules:

a) Build the molecules in Maestro using the 2D sketcher and minimize the structures.
b) Optimize their geometries using Jaguar. Take screenshots of your optimized structures with a ball-and-stick representation (from the Style toolbar).
    - Theory: B3LYP-D3, Basis set: 6-31gss
    - Use local host to run the jobs
c) Run single point calculations using Jaguar to generate electrostatic potential maps. Take screenshots of each ESP map.
    - Theory: B3LYP-D3, Basis set: 6-31gss
    - Use local host to run the jobs
d) Determine whether the carbon atoms are nucleophilic or electrophilic centers.

Screenshots of optimized geometries in ball-and-stick representations:

Screenshots of ESP maps:

Analysis: