5 Electron Densities, Electrostatic Potentials, and Reactivity Indices

Exercise 1 Visualizing Different Bond Types.

Build a molecule of dihydrogen. Use the Text Tool and enter H2.
Minimize at the PM3 level and save as h2pm3.c3d.
Calculate the molecular electrostatic potential by clicking MOPAC / Compute Properties and choose Properties: Electrostatic Potential and Molecular Surfaces / Theory: PM3.
Save.
Click View / Molecular Electrostatic Potential and click Show Surfaces. Various surface types are available from the drop down menu.
Close and Save.

Build a molecule of hydrogen fluoride.
Minimize at the PM3 level and save as hfpm3.c3d.
Calculate the molecular electrostatic potential and save.
View. Do the colors make sense? _____

Compare/contrast the various surfaces for H_2 and HF. Are they what you expected?

Exercise 2 Charge Distribution in Aromatic Compounds.

Build a molecule of benzene using the Text Tool.
Minimize using PM3 and save as c6h6pm3.c3d.
Calculate the molecular electrostatic potential and molecular surfaces using PM3.
View.

Based on the electrostatic potential, draw a sketch of how you believe benzene molecules would stack together in the solid state.

Build a molecule of pyridine as in Exercise 1 of Session 2.
Minimize using PM3 and save as c5nh5pm3.c3d.
Calculate the molecular electrostatic potential and molecular surfaces using PM3.
View.

Describe the differences between the benzene and pyridine charge distribution. What causes this difference?

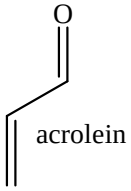
Exercise 3 Understanding Reactivity in a [4+2] Diels-Alder Reaction.

Build a molecule of furan.
Minimize at the PM3 level and save as c4h4opm3.c3d.
Calculate the molecular electrostatic potential and molecular surfaces using PM3.

furan

View the HOMO(N=13) molecular orbital by clicking View / Molecular Orbitals / Show Surface. Record the energy of the HOMO: _____ eV. Where are the largest lobes of the HOMO located?
_____
View the LUMO(N=14). Record the energy of the LUMO: _____ eV.
View the molecular electrostatic potential. On what atoms are the potentials centered?
_____
Save.
Redisplay the HOMO. Do not close.

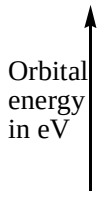
Open a New Model and build a molecule of acrolein.
Minimize at the PM3 level and save as c3h4opm3.c3d.
Calculate the molecular electrostatic potential and molecular surfaces using PM3.



acrolein

View the HOMO(N=11) molecular orbital and record the energy of the HOMO: _____ eV.
View the LUMO(N=12). Record the energy of the LUMO: _____ eV.
Where are the largest lobes of the LUMO located?
_____
View the molecular electrostatic potential. On what atoms are the potentials centered?
_____
Save.
Redisplay the LUMO. Do not close.

In the space below, plot the relative energies of the HOMO and LUMO of furan on the left, and the HOMO and LUMO of acrolein on the right. (Recall that more negative energies are more stable and are lower on the plot). What two orbitals will interact on these molecules?



Tile both windows (one with the furan, the other with the acrolein) onto the screen. View the HOMO of furan and the LUMO of acrolein in each window. Assuming that the blue lobe of the HOMO and the red lobe of the LUMO are both (+) in sign, make a sketch in the space below of how the two molecules will approach one another to react. You can separately rotate the images in each window to help with this. Recall that the largest lobe of the HOMO will overlap with the largest lobe of the LUMO.

Will the resulting product be the *endo* or *exo* isomer? _____ (*Endo* will have the =O pointing away from the furan oxygen, *exo* will have the =O pointing towards the furan oxygen). Is this the expected product? _____