

## 5 Electron Densities, Electrostatic Potentials, and Reactivity Indices

### Exercise 1 Visualizing Different Bond Types.

Build a molecule of dihydrogen.

Minimize at the PM3 level and save as h2pm3.HIN.

Click Compute / Plot Molecular Graphs / Molecular Properties: Electrostatic Potential and Mapped Function Options: -1, 1. Click OK. The model may be resized by clicking the Magnify/shrink Tool (7<sup>th</sup> across) and dragging in the workspace.

Save.

Build a molecule of hydrogen fluoride.

Minimize at the PM3 level and save as hfpm3.HIN.

Calculate the molecular electrostatic potential and view. Do the colors make sense?

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Compare/contrast the various surfaces for H<sub>2</sub> and HF. Are they what you expected?

### Exercise 2 Charge Distribution in Aromatic Compounds.

Build a molecule of benzene.

Minimize using PM3 and save as c6h6pm3.HIN.

Calculate the molecular electrostatic potential and 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.

Minimize using PM3 and save as c5h5npm3.HIN.

Calculate the molecular electrostatic potential and view.

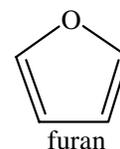
Describe the differences between the benzene and pyridine charge distribution. What causes this difference?

### 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.HIN.

Calculate the molecular electrostatic potential and molecular surfaces.



View the Number = 13 molecular orbital and record the energy of the HOMO: \_\_\_\_\_ eV. Where are the largest lobes of the HOMO located?

View the Number = 14 orbital. Record the energy of the LUMO: \_\_\_\_\_ eV.  
View the molecular electrostatic potential. On what atoms are the potentials centered?

Save. \_\_\_\_\_

Open a new worksheet and build a molecule of acrolein.

Minimize at the PM3 level and save as c3h4opm3.HIN.

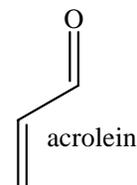
Calculate the molecular electrostatic potential and molecular orbitals.

View the Number = 11 molecular orbital and record the energy of the HOMO: \_\_\_\_\_ eV.

View the Number = 12. Record the energy of the LUMO: \_\_\_\_\_ eV. Where are the largest lobes of the LUMO located?

View the electrostatic potential. On what atoms are the potentials centered?

Save. \_\_\_\_\_



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?

Orbital  
energy  
in eV

Assuming that the purple lobe of the HOMO and the green 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. 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? \_\_\_\_\_