

Conformations of Systems with Vicinal Lone Pairs

Basic problem: Compute geometries and heats of formation for isomers of the systems below. Determine the most stable conformation for each molecule, and the relative energies for higher energy conformations. Compute the HOMO for each conformation shown. What trends do you find relating the relative geometries of lone pairs to the most stable conformation? Look up whatever you can find about the known isomeric preferences. Do your results correspond to known literature preferences (either qualitatively or quantitatively)?

Method: PM3 and 6-31G* are reasonable levels of theory. Compare results for the semiempirical method to results for the ab initio method. Which one works better?

Literature: Use Beilstein Online, Chemical Abstracts, or the NIST Thermodynamic Database (available by request through P. M. Lahti) to get experimental heats of formation and literature references for them. Use any other references that will give information about presumed gas phase conformations for these systems.

