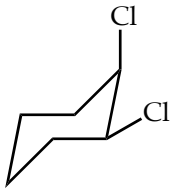
Cooperative Assignment 3

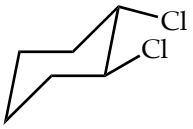
Chapter 4 - Conformations of Alkanes and Cycloalkanes

1. Use the tutorial on conducting dihedral angle coordinate scans, found here, to examine the conformation energy profiles of ethane and 1,2-dichloro ethane.

2. Structural drawings (molecular models, too) can be deceiving. For example, the chlorine atoms in 1,2-dichlorocyclohexane seem much closer to each other in a drawing of the trans stereoisomer than in the cis. Make models of each in WebMO and use the AM1 theory level to optimize the geometries. Measure the distance between the chlorines in both models. Report what you find.



cis-1,2-dichlorocyclohexane



trans-1,2-dichlorocyclohexane

3. Make a model of cyclohexanol with an equatorial hydroxyl group, optimize it's structure using AM1 theory. Do the same with a cyclohexanol model having an axial hydroxyl group. Which is the more stable conformation? What is the energy difference between them in kilocalories per mole?

4. What are the optimized energies of *cis*- and *trans*-4-methylcyclohexanol? How does the difference between these two compare with the difference between axial and equatorial cyclohexanol?

5. Predict whether 1,1,2,2-tetrafluoroethane has a dipole moment or not by drawing Newman projections of the various staggered conformations. Verify your answer by examining the anti and gauche conformations in WebMO. You can build the molecule and adjust the H-C-C-H dihedral angle to the appropriate value, similar to how you did in the dihedral angle scan in problem #1. Minimize the structures using AM1 theory level. Verify your dipole moments for each structure.

6. In WebMO build a model of 1,2-dichloro-1-fluoroethane. Conduct a dihedral angle coordinate scan by initially setting the Cl-C-C-Cl bond to 0^{o}. Scan from 0.01^{o} through 360^{o} using the AM1 theory level. Consult exercise #1 for more details about the calculation. At what dihedral angle is the minimum energy found? Explain why the angle is not exactly 180^{o}.