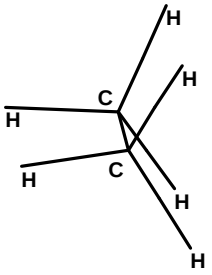
Chem 260 Laboratory B
(optional)

This lab demonstrates conformational analysis, i.e. finding the preferred conformations of "flexible" molecules.

VARIATION OF DIHEDRAL ANGLE IN ETHANE

1. Start HyperChem and draw ethane. Use model build but do not optimize the structure with Molecular Mechanics. Open a log file.
2. Select a H-C-C-H substructure and set the dihedral angle to 0º. Adjust the molecule's orientation so that you can readily view the conformation.



3. **Deselect** the structure and do a single point MM calculation.
4. Set the dihedral angle to values from 0–120º in steps of 15º, and for each conformation calculate the energy with Molecular Mechanics. Remember to deselect the H-C-C-H substructure before carrying out each calculation.
5. Plot the results (total energy versus dihedral angle) with Excel. Fit the data with the function: $E = A + B\cos(3\phi)$.
6. Now try optimizing the rest of the structure for each dihedral angle. Select H-C-C-H and name it with Select/Name Selection. Set its value as before but now use Setup/Restraints to set the force constant for your named selection to a very large value (100,000). This makes this part of the molecule rigid in comparison with the rest, when you then do structure optimization (remember to deselect first). You may need to repeat the optimization command if the convergence criterion is not met on the first set of calculations.

VARIATION OF DIHEDRAL ANGLE IN CHLOROETHANE

7. Change the molecule to Chloroethane, CH_3CH_2Cl and explore its conformations.