Molecular Modeling Lab
CHM 2210C

1. Construct a ball-and-stick model of butane. Draw and label Newman projections of both the CH_3/H eclipsed conformer and the staggered, anti conformer. Draw both along the C2 – C3 σ bond of butane. Depict the eclipsed and staggered positions clearly. (2 pts)

2. Construct a ball-and-stick model of 2,3-dimethylbutane. Review Figure 3.9 in McMurry. Draw a similar diagram of Energy versus Rotation along the C2 – C3 σ bond for 2,3-dimethylbutane. Include the Newman projections and energy values as well. Be sure to count your carbons carefully, there is a total of six. Keep either the front or back set of substituents in the same place, while you rotate the other side only. (3 pts)

3. Construct a model of *trans*-1,3-dichlorocyclopentane. Arrange the model so that one carbon atom is above the plane, and the other four carbons twist somewhat to relieve torsional strain from eclipsing. Draw this structure in 3D by showing the relative directions of all of the bonds. Write a short description of the overall shape. Also, explain whether or not a molecule could be systematically named 1,4-dichlorocyclopentane. (3 pts)

4. Construct a cyclohexane model and perform ring flips. Observe what happens to a pair of hydrogen atoms on the same carbon. Describe the change in their axial and equatorial positions. Does the new axial position point in the same direction as the old one? Draw both conformers and label the two hydrogen atoms on both molecules. (3 pts)

5. Construct a model of *cis*-1,2-dimethylcyclohexane and perform ring flips. Draw both conformers and label the axial and equatorial methyl groups. Calculate the total strains (gauche and 1,3-diaxial) for both conformers as well. (3 pts)

6. Repeat the procedure of problem 5 for *trans*-1,2-dimethylcyclohexane. (3 pts)

7. Construct a model of *tert*-butylcyclohexane and perform ring flips. Rotate (spin) the *tert*-butyl group on both conformers, and examine the interactions between the methyl groups and H atoms connected to the ring. Explain whether the axial or equatorial conformer is energetically preferred. Draw both conformers with labels for axial and equatorial positions. Calculate the total strains for both conformers as well.
(Note that the bond connecting the ring to the *tert*-butyl group
creates gauche interactions between the CH_3's and the ring C's.
Disregard these as they are identical in both conformers.)
(3 pts)