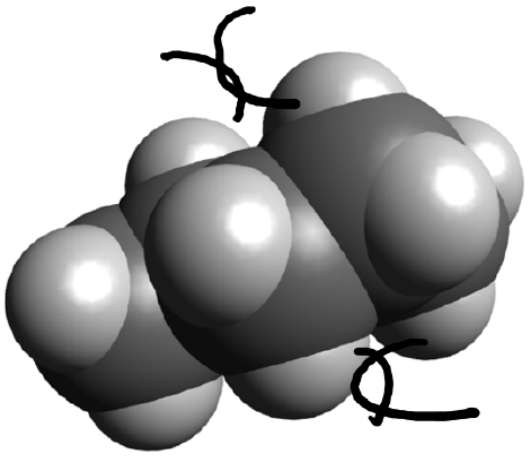
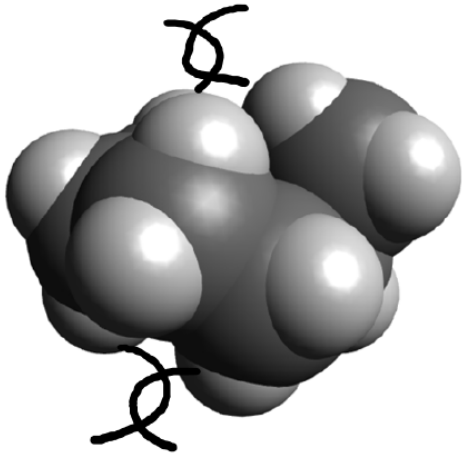
4.4: Exercise Questions

1. Open output file for both axial and equatorial conformations of methyl cyclohexane in Avogadro and view the molecule in space filling mode by clicking on Van Der Waals Spheres in the Display Types Window. Print a screen shot of both conformers and paste it below. Using a pen, indicate where the 1,3-diaxial interactions exist on the axial conformer.



Equatorial Conformer

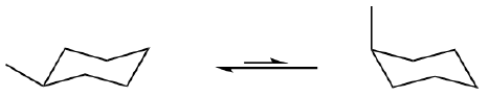


Axial Conformer

2. Please Complete the following table using the energy values you determined from your Orca output files. For the final conversion please note that 1 Hartree (E_H) = 627.5 kcal/mol.

Eq. Conformer Gibbs Free Energy (E_H)	Axial Conformer Gibbs Free Energy (E_H)	ΔG° (E_H) = Axial Energy – Equitorial Energy	A Value (Methyl Group), ΔG° converted to kcal/mol

3. Given the equilibrium from equatorial to axial conformers as written below, which side of the equilibrium is favored? Is the conformation change exergonic or endergonic?



Equitorial Conformer

Axial Conformer

4. Compare the A value that you obtained in question 3 to the literature A value. If there is a difference between the literature and calculated value, please propose a reason for the difference.
5. Using the equation that relates the change in free energy and the equilibrium (equation 1 shown above) constant, please calculate K_{eq} for the equilibrium as written in question 3.
6. What percentage of methyl cyclohexane is in the axial conformation and what percentage is in the equatorial conformation?