<u>Cyclohexane Conformations</u>

Let's use pcspartan to look at some cyclohexane structures. We will look at the equatorial and axial energy differences for methyl cyclohexane and isopropyl cyclohexane. We will also look at the energy difference for the two possible chair conformations of *cis* 1-isopropyl-3-methyl cyclohexane.

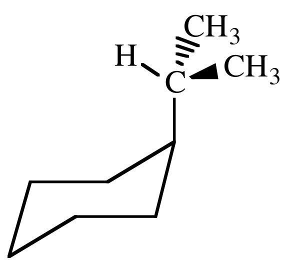
1. Log in and start pcspartan as before. Go to the "rings" menu on the right of the screen and choose cyclohexane. The ring will show up in the chair conformation.

2. To make methyl cyclohexane with the methyl group in the equatorial position, add a carbon (this will be a methyl group) to any of the six equatorial positions. Minimize the molecule as before, and record the energy in the table.

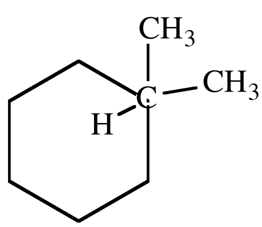
3. To make methyl cyclohexane with the methyl group in the axial position, make a new cyclohexane ring as before and add a carbon to any of the six axial positions. Minimize the molecule and record the energy in the table. The modeling program is not powerful enough to flip the ring and convert the methyl group to the equatorial position. Therefore, the minimized structure should still have the methyl group in the axial position.

4. Record the difference in energy between the equatorial and axial conformations. Compare this difference to the one provided by the textbook. Is it within 1-2 kJ/mole? This would be a reasonable value as our modeling program is not very advanced. If the program did more calculations, this lab would take a VERY LONG time to do!

5. Repeat steps 2-4 for isopropyl cyclohexane. When you put the isopropyl group in the axial position, pay attention to where the hydrogen (attached to the first "C" of the isopropyl group) is pointing. It should be pointing over the ring – as shown below. This will ensure that you get the correct minimized energy values. Again, compare the energy difference (between the axial and equatorial conformations) from pcspartan to the one from the textbook.



side view



top view (bond from the "C" to the ring is not shown)

6. Draw the two possible chair structures for *cis* 1-isopropyl-3-methyl cyclohexane and determine which is more stable (by using the values from Wade for monosubstituted rings). Label the more stable conformation as "**S**" and the less stable one as "**U**". Put each of these structures into pcspartan, minimize them, and record the energy values in the table shown. Calculate and record the energy difference between "**S**" and "**U**" as determined by pcspartan.

Molecule	Axial methyl cyclohexane	Equatorial methyl cyclohexane	Axial isopropyl cyclohexane	Equatorial isopropyl cyclohexane	**S**	**U**
Energy (kJ/mole)						
Energy Difference (ΔG)						

1. Draw the structures for **S** and **U** in the chair conformations. Show your calculations for deriving the energy difference between **S** and **U** by using the values for mono-substituted cyclohexane rings from the Wade textbook.

2. Now compare the energy differences from pcspartan with the energy differences from the Wade textbook. Do this for methyl cyclohexane, isopropyl cyclohexane, and for **S** and **U**. These ΔG values should agree (within 2 kJ/mole) for the monosubstituted rings, but not for **S** and **U**. Try to explain this difference (a picture can be worth a 1,000 words! – use your drawings from question 1 to help answer this question). Why is the energy difference between **S** and **U** so much larger than the calculation you did in question #1? Keep in mind that the values from Wade are for monosubstitued rings.