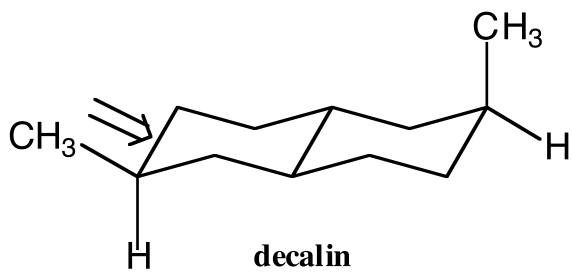
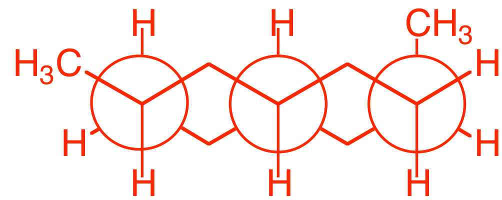
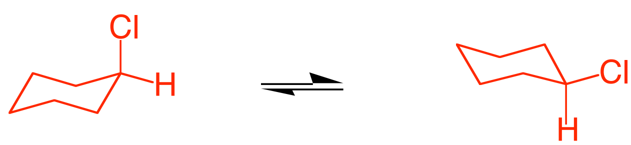
**1.** Draw a Newman projection for decalin looking down the indicated bond.




**decalin**




**2.** It's been calculated that the axial conformation of chlorocyclohexane is 0.52 kcal/mol *higher* in free energy than the equatorial conformation (therefore ΔG must be negative b/c $\Delta G_{rxn} = G_{products} - G_{reactants}$). If we cool a flask containing the compound to 10 °C, what will be the ratio of the two conformers at this temperature? Begin by drawing the two chair forms of chlorocyclohexane in the space provided below. Then show your calculations underneath that. **Hint:** recall the equation for free energy from gen. chem: $\Delta G° = -RT \ln K_{eq}$ where $T$ is in Kelvin and $R$ is the ideal gas constant (0.001987 kcal/K•mol).




**axial conformer** **equatorial conformer**

**Calculations**

$$\Delta G° = -RT \ln K_{eq}$$

$$-0.52 = (-0.001987 \text{ kcal/K•mol}) * (283.15 \text{ K}) \ln K_{eq}$$

$$1.08 = \ln K_{eq}$$

$$2.95 = K_{eq}$$

**For the above equilibrium...**

$$K_{eq} = \frac{[products]}{[reactants]} = \frac{[equatorial]}{[axial]}$$

**therefore...**

$$K_{eq} = 2.95 = \frac{[equatorial]}{[axial]}$$

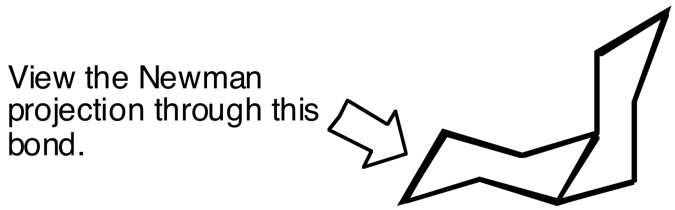
**If we express the relative amounts of equatorial to axial as a percentage, we can solve for the conformers...**

$$K_{eq} = 2.95 = \frac{x}{100 - x}$$

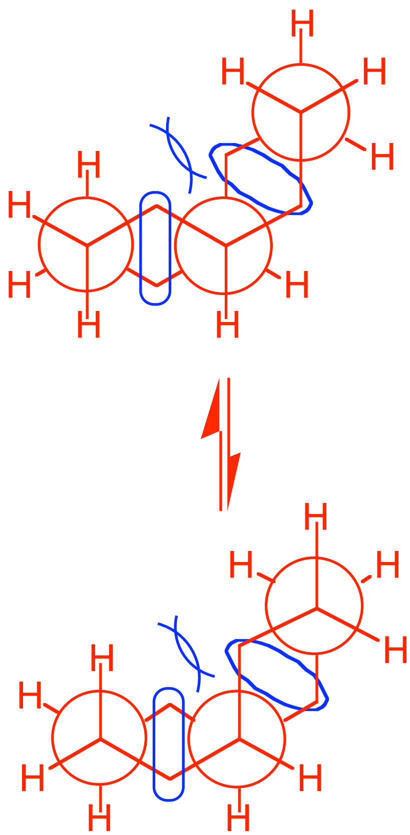
**Solving for x gives us a ratio of *74.7 equatorial* to *25.3 axial.***

****Notice how even a small energy difference (0.52 kcal/mol) can result in significant differences in stability****

**3.** Draw the two Newman projections for *cis*-decalin that represent the chair-to-chair interconversion of the molecule. One of the bonds you should look down has been indicated (remember that the Newman projection of any ring should include *all* parallel bonds). How many gauche interactions does each Newman projection possess (point them out if possible)? *Hint: use a model set to complete this assignment.*

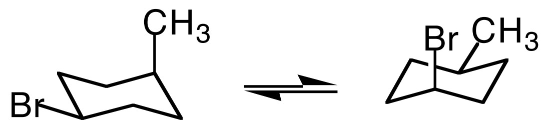



***cis*-decalin**




**Gauche relationships shown in blue.**

**4.** A-values are known to be additive. Using the table of A-values that was handed out in class, calculate the ratio of **a** to **b**. Based on your calculation, which conformer is more stable?




**<u>Calculations</u> (assuming room temp. = 25° C)**

**A Value = -0.38 + 1.70 = 1.32 = -ΔG°**

**$\Delta G° = -RT \ln K_{eq}$**

**$-1.32 = (-0.001987\ \text{kcal/K•mol}) * (298.15\ \text{K}) \ln K_{eq}$**

**$2.23 = \ln K_{eq}$**

**$9.30 = K_{eq}$**

**For the above equilibrium...**

$$K_{eq} = \frac{[products]}{[reac\tan ts]} = \frac{[equatorial]}{[axial]}$$

**therefore...**

$$K_{eq} = 9.30 = \frac{[equatorial]}{[axial]}$$

**If we express the relative amounts of equatorial to axial as a percentage, we can solve for the conformers...**

$$K_{eq} = 9.30 = \frac{x}{100 - x}$$

**Solving for x gives us a ratio of *90 equatorial* to *10 axial*.**