CONCEPT: CALCULATING CHAIR EQUILIBRIUM

We can use the difference in (ΔG^o) to calculate the percentage and/or ratio of chairs at any given temperature.

- First, use ΔG^o to solve for the equilibrium constant:

$$\Delta G^\circ = - R \bullet T \bullet \ln(K_e) \xrightarrow{\text{Solve for } K_e} K_e = e^{\left[\frac{(-\Delta G^\circ)}{(R \bullet T)}\right]}$$

where: ΔG° = Gibbs free energy (*in joules*)

R = Gas Constant 8.134 (*j/mol K*)

T = Temperature (*in kelvin*)

*Correction: Gas Constant = 8.314

- Then, use K_e to solve for the percentage of each conformer:

$$K_e = \frac{[\text{Products}]}{[\text{Reactants}]} = \frac{[\text{Equatorial}]}{[\text{Axial}]} = \frac{x}{1 - x} \xrightarrow{\text{Solve for } \mathbf{x}} \frac{K_e}{K_e + 1} \bullet 100$$

where: **x** = % of equatorial conformer

PRACTICE: Estimate the equilibrium composition of the chair conformers of the following cyclohexanes at room temp:

a) *cis*-1,3-diethylcyclohexane

b) *trans*-1-methyl-3-phenylcyclohexane