CONCEPT: THERMODYNAMICS OF CHAIR FLIPS

Sometimes we'll be asked to calculate the energy required (kJ/mol) to flip chairs into the axial position.

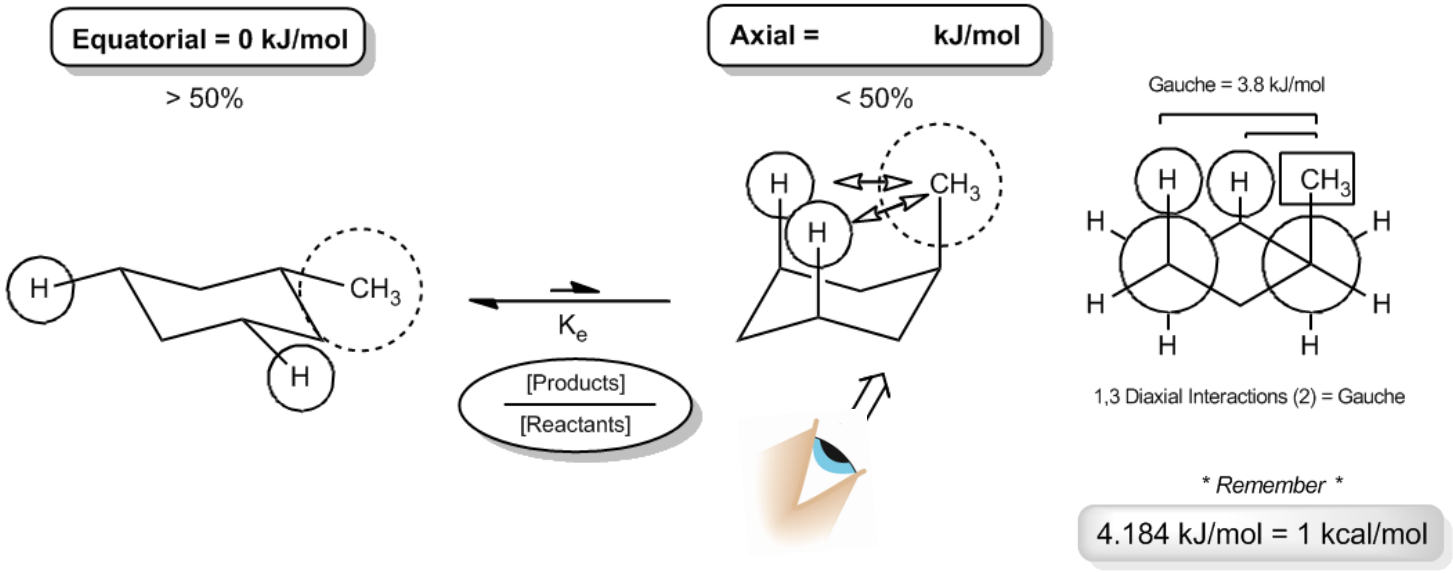
A-Values: 1,3-Diaxial Interactions for Common Substituents (ΔG°)

(Energy Difference Between Axial and Equatorial)

Group	kJ/mol
—H	0
—Me	7.6
—Et	8
—*t*-Bu	22.8

Group	kJ/mol
—F	1
—I	1.9
—Cl	2.2
—Br	2.4

Group	kJ/mol
—CN	0.8
—C≡C	1.7
—OH	4.2
—C_6H_5	12.6



PRACTICE: Calculate the difference in Gibbs free energy in (kJ/mol) ***and*** (kcal/mol) between the alternative chair conformations of the following disubstituted cyclohexanes:

a. *trans*-4-iodo-1-cyclohexanol

b. *cis*-2-ethyl-1-phenylcyclohexane