

Conformational Analysis of Substituted Cyclohexanes: 1,3-Diaxial Interactions



The equilibrium between **A** and **B** is described by the following equation:

$$K = e^{-\Delta G^\circ / RT}$$

where:

K = equilibrium constant

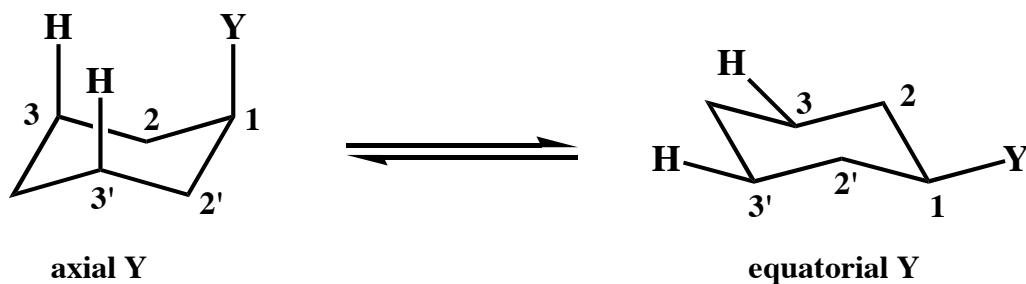
ΔG° = standard free-energy difference

R = 8.314 J/(mol K)

T = absolute temperature (Kelvin)

Calculated Equilibrium Values at T = 298 K

<u>energy difference (kJ/mol)</u>	<u>% more stable isomer</u>	<u>% less stable isomer</u>	<u>K</u>
0.000	50	50	1.00
0.497	55	45	1.22
1.00	60	40	1.50
1.53	65	35	1.86
2.10	70	30	2.33
2.72	75	25	3.00
3.43	80	20	4.00
4.30	85	15	5.67
5.44	90	10	9.00
7.30	95	5	19.0
11.4	99	1	99.0
17.1	99.9	0.1	999



substituent Y	<u>total strain due to two H-Y</u>	<u>strain due to one H-Y</u>
	<u>1,3-diaxial interactions (kJ/mol)</u>	<u>1,3-diaxial interaction (kJ/mol)</u>
-F	1.4	0.70
-Cl	2.4	1.2
-Br	2.4	1.2
-OH	4.4	2.2
-CH ₃	7.3	3.7
-CH ₂ CH ₃	7.5	3.8
-CH(CH ₃) ₂	9.2	4.6
-C(CH ₃) ₃	20.	10.
-Ph	12	6.0
-CO ₂ H	5.9	3.0
-CO ₂ CH ₃	5.2	2.6
-CH=CH ₂	7.0	3.5
-C≡CH	2.0	1.0
-C≡N	0.8	0.4