

An example from the Fall 1997 Hour Examination #1:

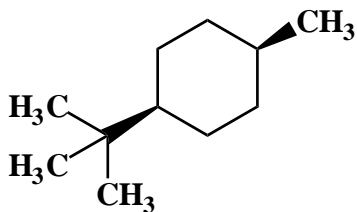
4. (20 points)

Draw the two possible chair conformations of *trans*-1,4-dimethylcyclohexane. Clearly denote all 1,3-diaxial interactions. Calculate the total strain energy for each conformation. Finally, circle the more stable conformation and estimate the ratio of the two conformations at 298 K.

An example from the Fall 1997 Final Examination:

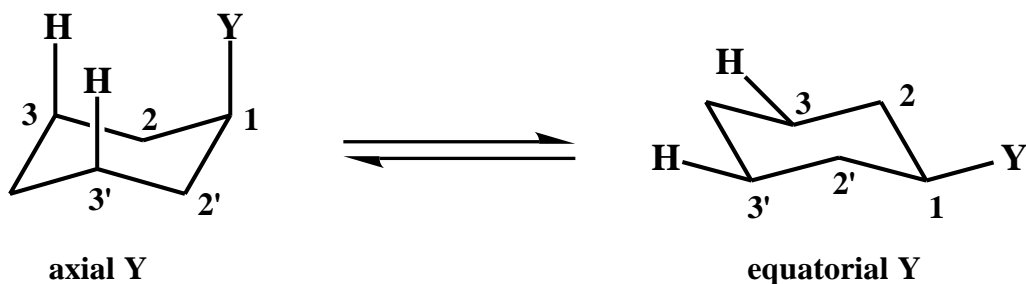
4. (25 points)

Draw the two possible chair conformations of the following 1,4-disubstituted cyclohexane. Show all 1,3-diaxial interactions for each chair. Circle the lowest energy conformation.



Calculated Equilibrium Values at T = 298 K

<u>energy difference (kcal/mol)</u>	<u>% more stable isomer</u>	<u>% less stable isomer</u>	<u>K</u>
0.000	50	50	1.00
0.119	55	45	1.22
0.240	60	40	1.50
0.367	65	35	1.86
0.502	70	30	2.33
0.651	75	25	3.00
0.821	80	20	4.00
1.028	85	15	5.67
1.302	90	10	9.00
1.745	95	5	19.0
2.723	99	1	99.0
4.092	99.9	0.1	999



<u>substituent Y</u>	<u>steric strain due to one H-Y</u>	<u>total steric strain due to two H-Y</u>
	<u>1,3-diaxial interaction (kcal/mol)</u>	<u>1,3-diaxial interactions (kcal/mol)</u>
-F	0.12	0.24
-Cl	0.25	0.50
-Br	0.25	0.50
-OH	0.50	1.0
-CH ₃	0.90	1.8
-CH ₂ CH ₃	0.95	1.9
-CH(CH ₃) ₂	1.1	2.2
-C(CH ₃) ₃	2.7	5.4
-C ₆ H ₅	1.5	3.0
-CO ₂ H	0.70	1.4
-C≡N	0.1	0.2