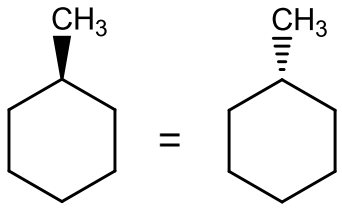
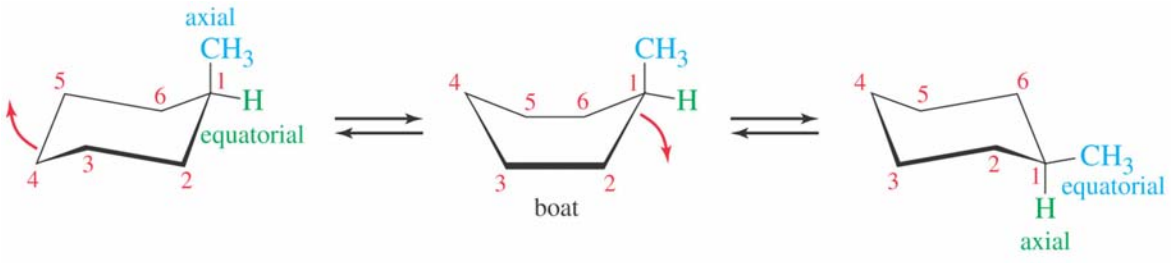
Substituted Cyclohexanes



methylcyclohexane



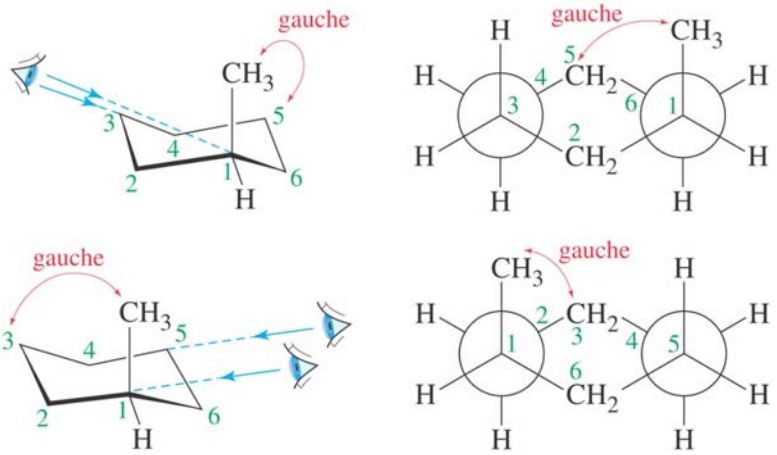
These two chair conformations are not identical.

Which is more stable?

Conformations of Methylcyclohexane

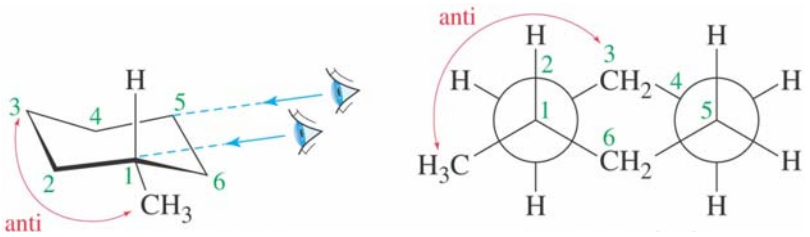
axial methyl

multiple gauche interactions between methyl and cyclohexane ring make this conformer **less** stable



equatorial methyl

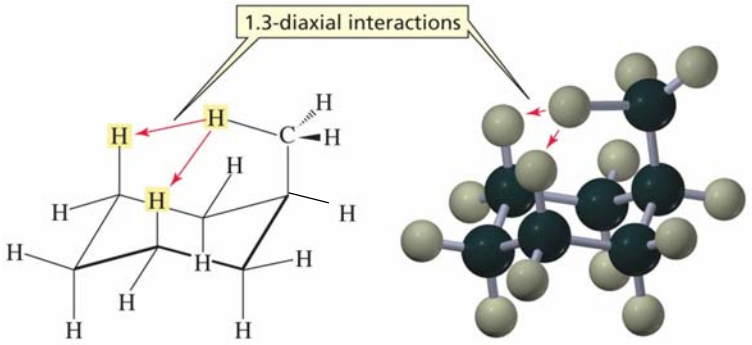
no adverse interactions; **more** stable



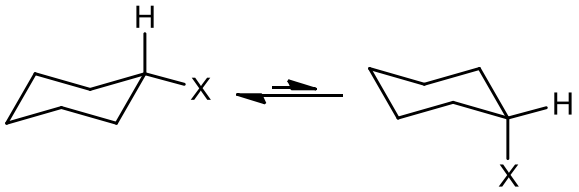
Substituted Cyclohexanes

Another effect: 1,3-diaxial interactions are *destabilizing*.

Conformer with <u>equatorial</u> substituent doesn't have this problem.



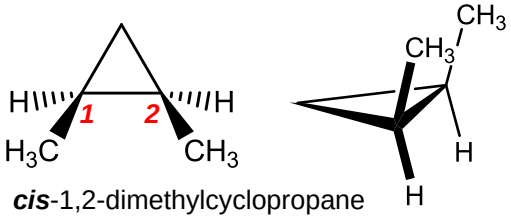
The larger the group, the bigger the preference.



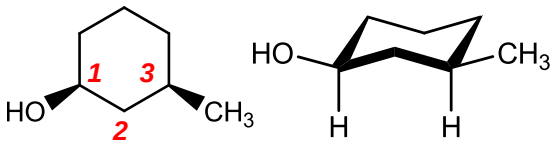
X	ΔG (kcal/mol)	[eq]/[ax]
-H	0	1
-F	0.2	1.5
-OH	1.0	5.4
$-CH_3$	1.8	18
$-C(CH_3)_3$	5.4	4800

Naming Disubstituted Cycloalkanes

***cis*-substituted:** Substituents on same side of ring.

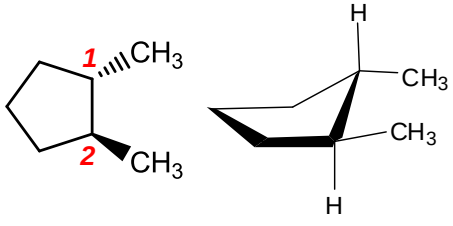


***cis*-1,2-dimethylcyclopropane**

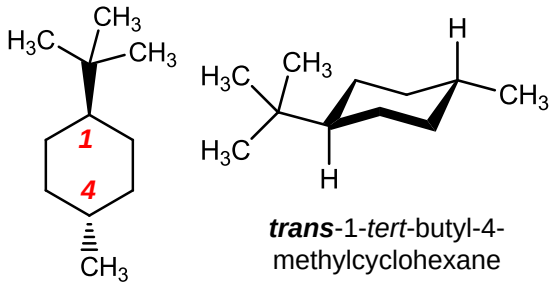


***cis*-1-hydroxy-3-methylcyclohexane**

***trans*-substituted:** Substituents on opposite side of ring.



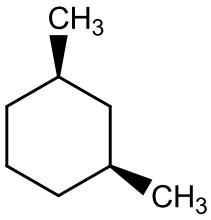
***trans*-1,2-dimethylcyclopentane**

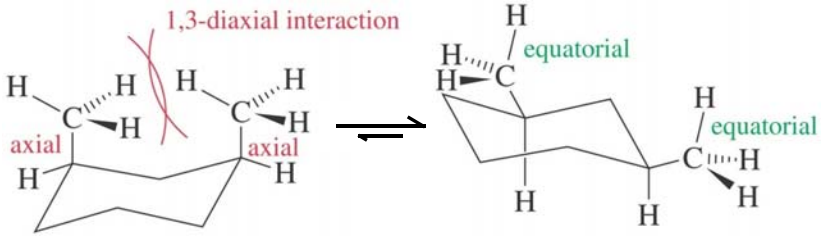


***trans*-1-*tert*-butyl-4-methylcyclohexane**

Multiply Substituted Cyclohexanes

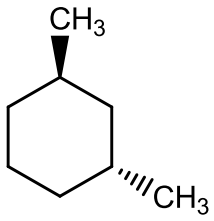
Chair conformations flip to minimize total 1,3-diaxial interactions.

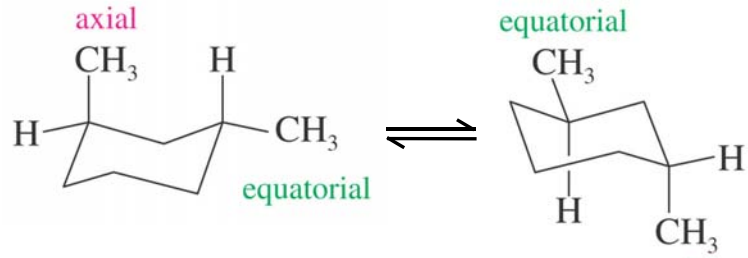




diaxial conformation:
very disfavored

diequatorial conformation:
favored





conformations identical