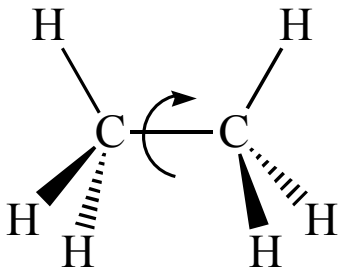
Conformers – Ethane

One important aspect of this bond's symmetry is that it is possible to rotate one end of the molecule with respect to the other leading to different molecular ***conformations***.



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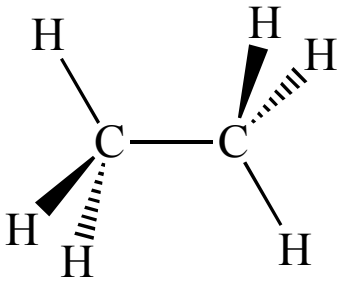
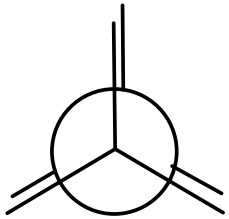
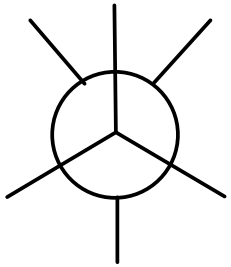
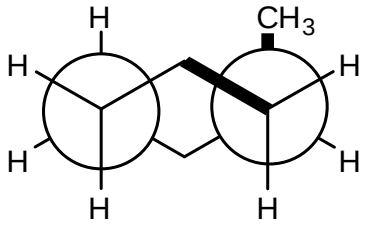


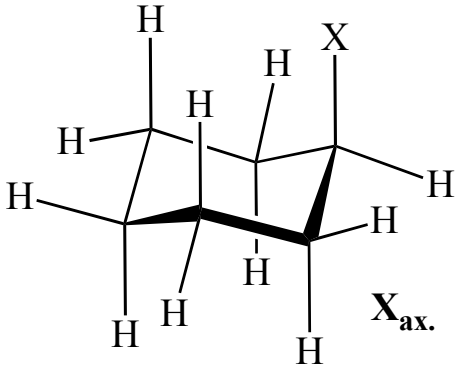
Staggered

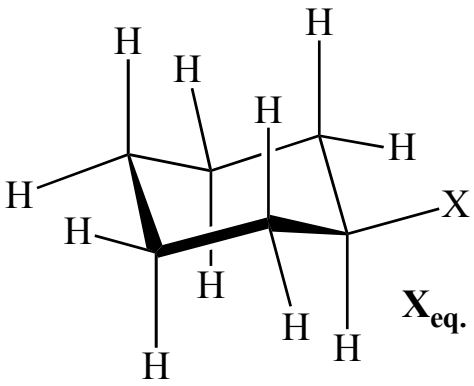


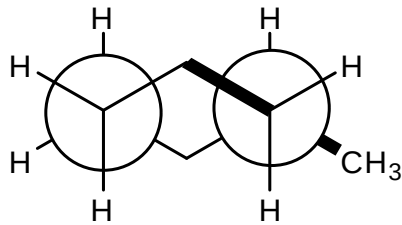


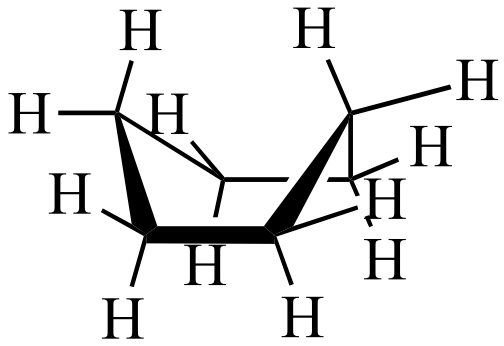
Newman Projections









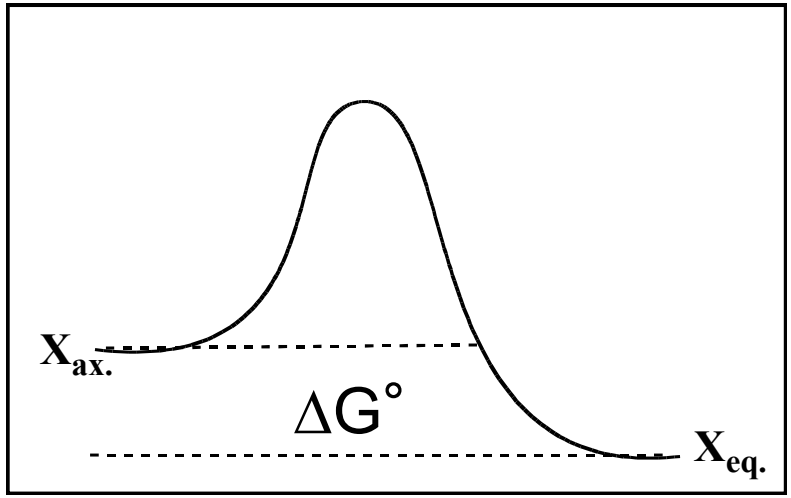


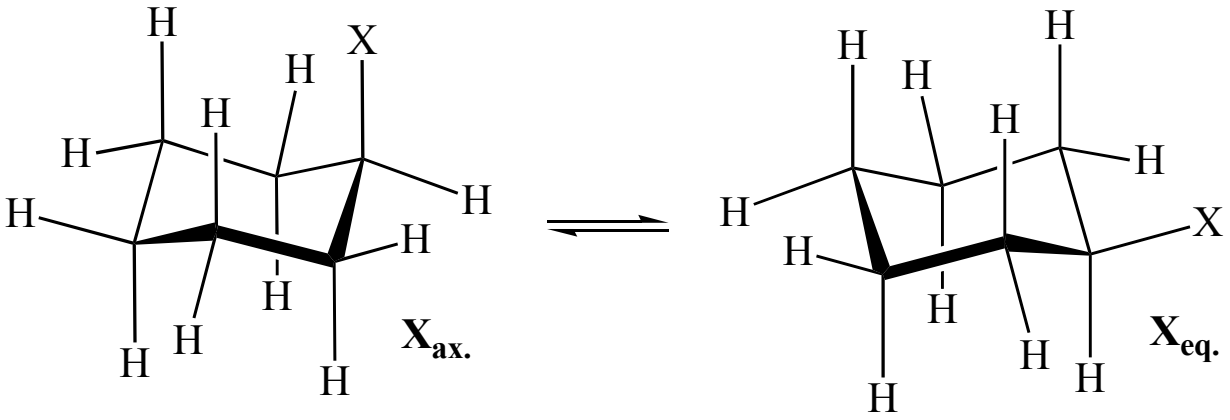
Flagpole interactions

$$K_{eq} = \frac{[X_{eq}]}{[X_{ax}]}$$

$$\Delta G^\circ = -RT\ln K_{eq}$$

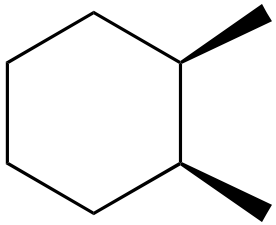
Define the "A value" as $-\Delta G^\circ$

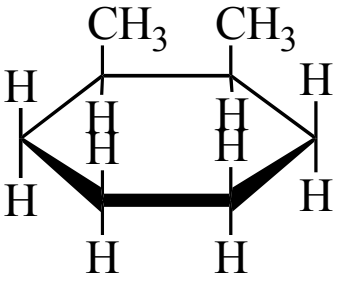


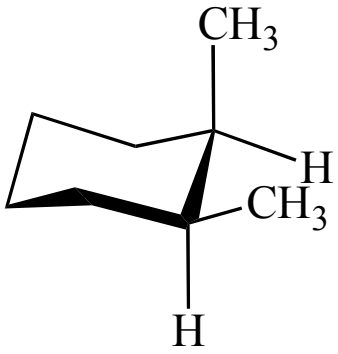


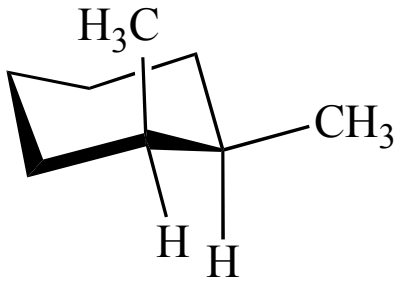
X	K_{eq}	$\Delta G°$ (kcal/mol)
H	1	0
CH_3	19	-1.74
CH_2CH_3	21	-1.79
$C(CH_3)_3$	3300	-4.8
—CH=CH_2	15	-1.6
—C≡CH	2.2	-0.46
F	1.7	-0.3
Cl	3	-0.6
Br	3	-0.6
I	2.3	-0.5

Conformers – Disubstituted Cyclohexanes

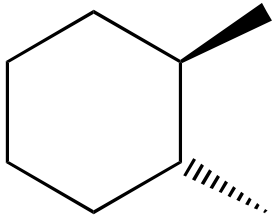


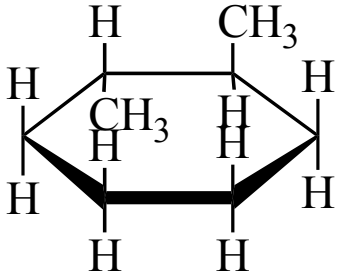


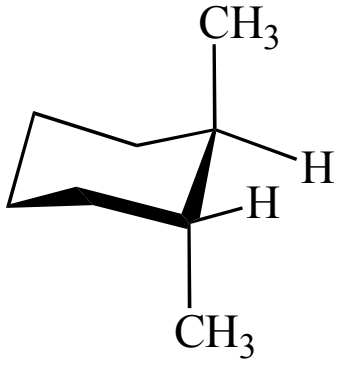


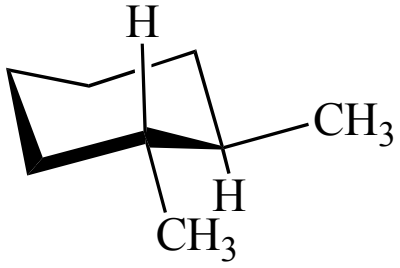


cis-1,2-dimethylcyclohexane



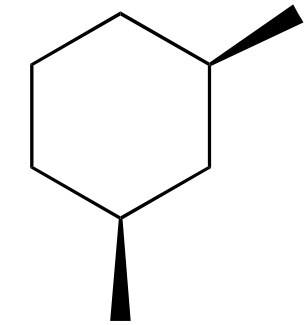


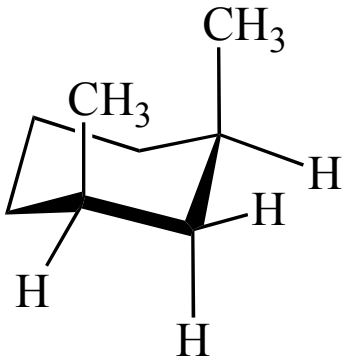


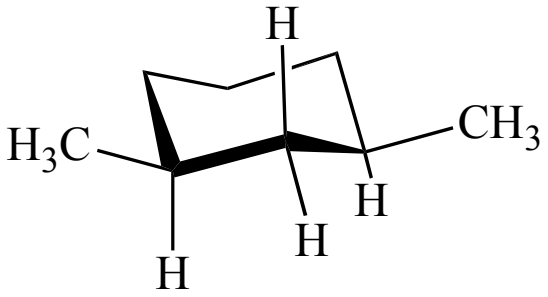


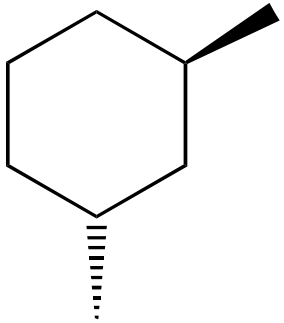
trans-1,2-dimethylcyclohexane

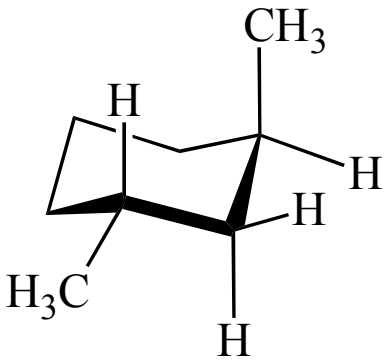
Conformers – Disubstituted Cyclohexanes

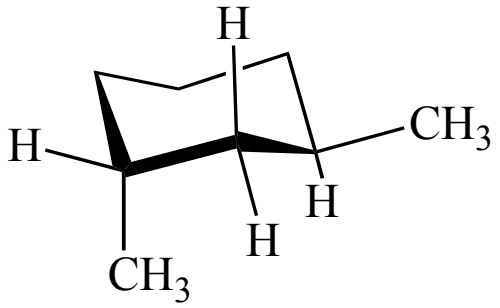




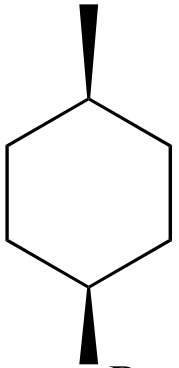




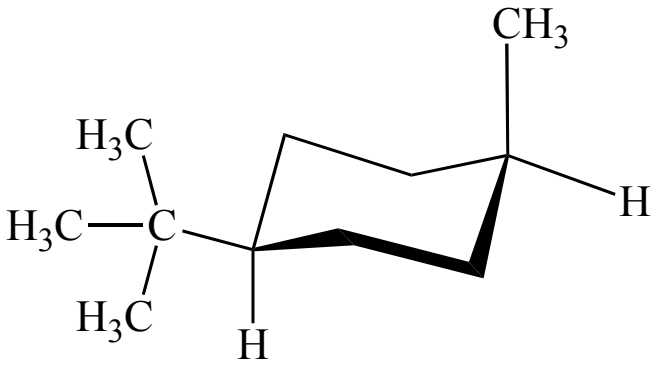


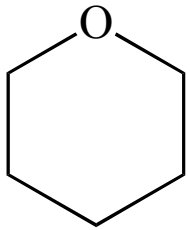


Conformers – Disubstituted Cyclohexanes

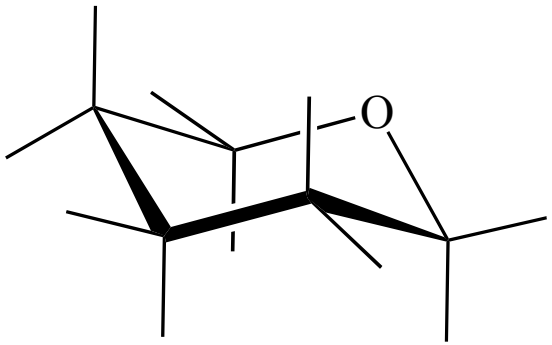


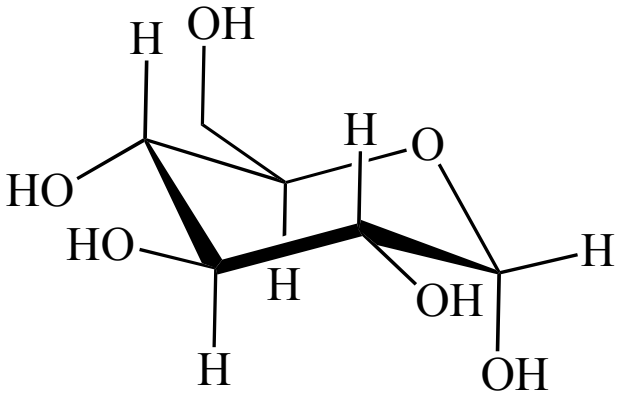
t-Bu





Tetrahydropyran





α-D-Glucose

Conformers – Cycloalkanes and Chirality

- Remember, ring flips are like bond rotations – they only change the conformation of the molecule. Therefore, you are allowed to do ring flips to determine if your molecule is chiral or not.

- Convince yourself that *cis*-1,2-dichlorocyclohexane is achiral.

- Convince yourself that *trans*-1,2-dichlorocyclohexane is chiral.

Conformers – Smaller Cycloalkanes

- Six-membered rings are prevalent in nature because they are relatively free from:
  - torsional strain: eclipsed bonds

  and
  - angle strain: bonds angles that deviate from those predicted by VSEPR theory

- Build cyclopentane, cyclobutane, and cyclopropane. Is there torsional strain? Angle strain? What do you think would be the most stable conformer for each of these rings? Use the amount of strain to rank these rings from most to least stable.