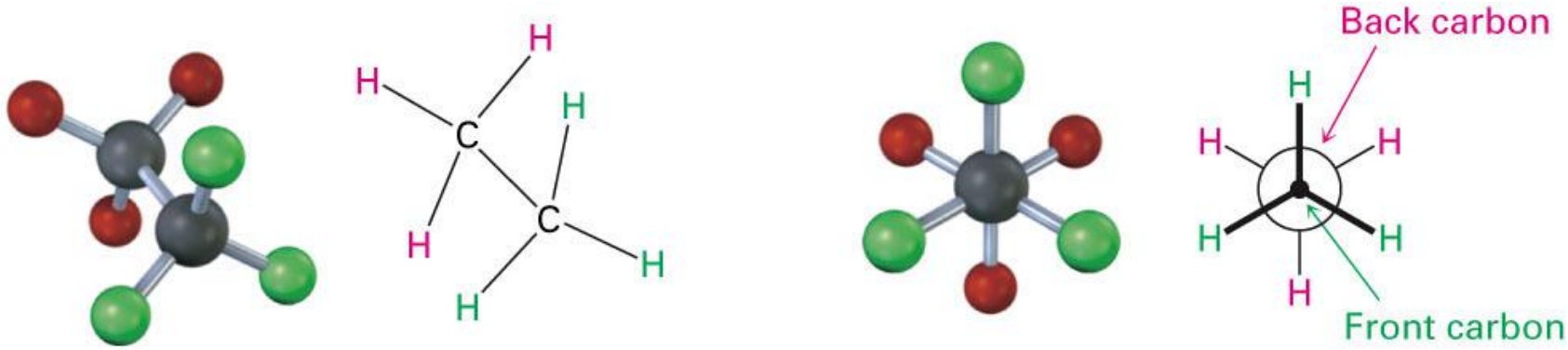
- **Conformation**- Different arrangement of atoms resulting from bond rotation

- Conformations can be represented in 2 ways:



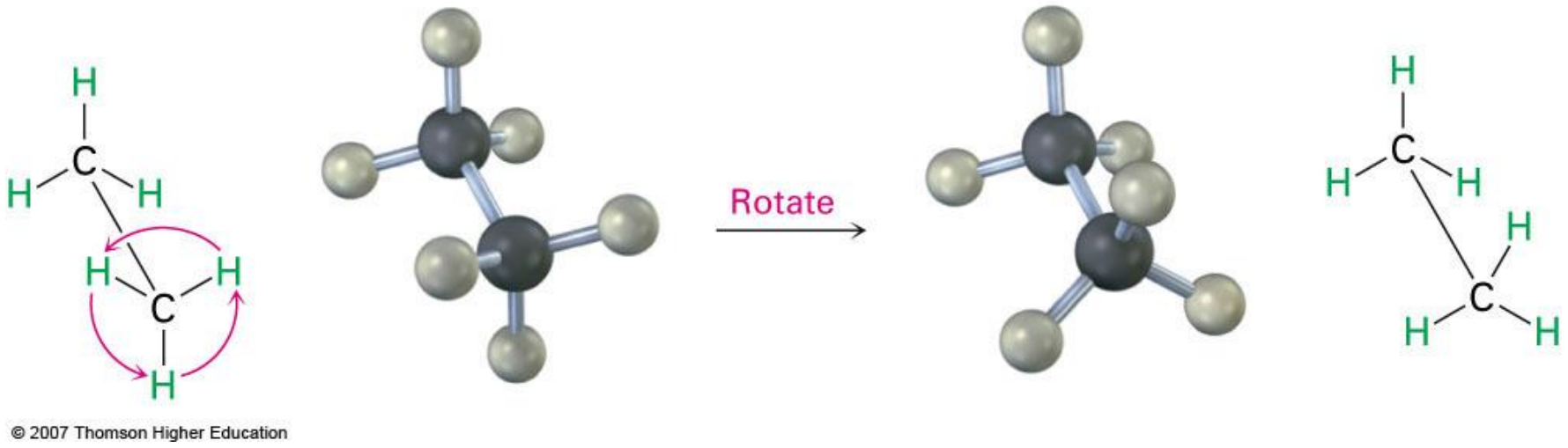
Sawhorse representation

Newman projection

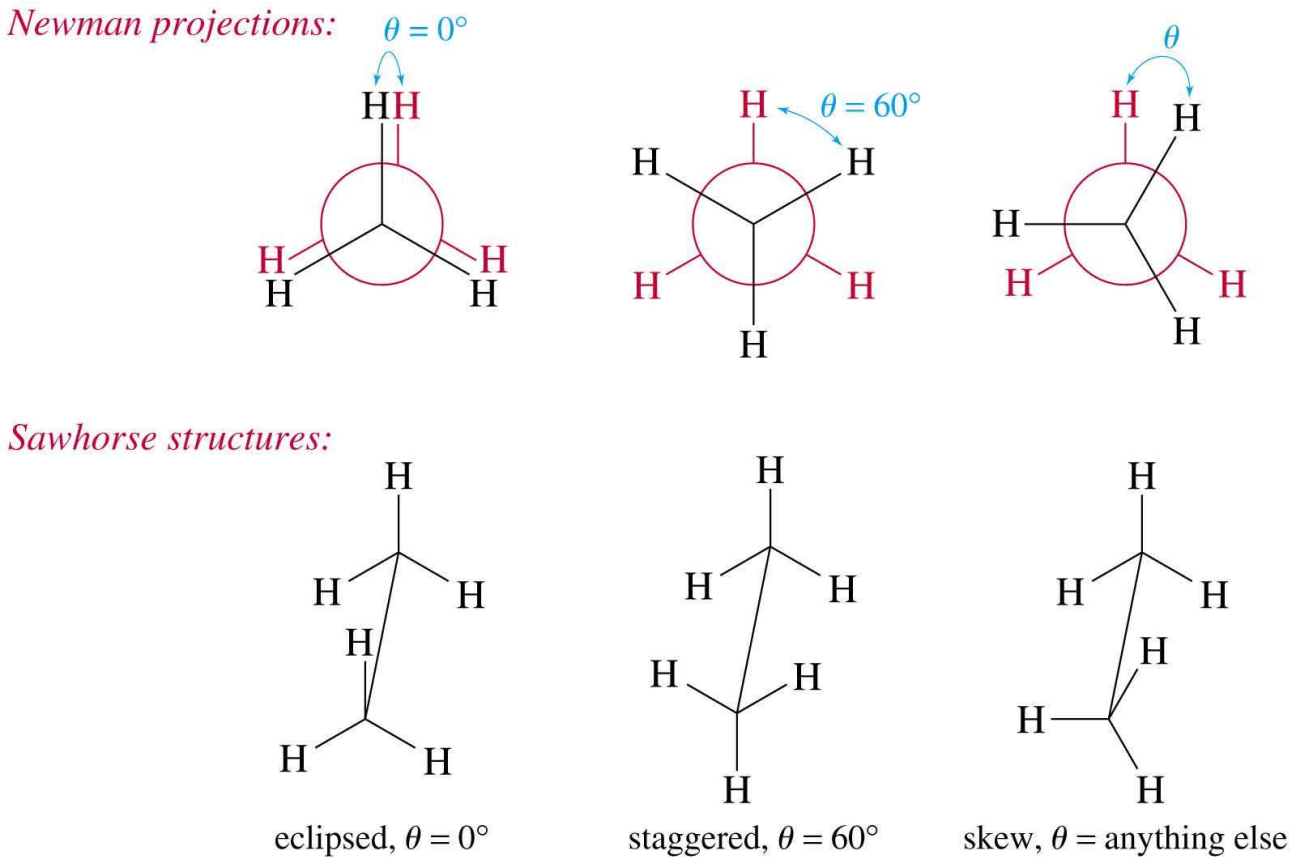
- We do not observe perfectly free rotation
- There is a barrier to rotation, and some conformers are more stable than others
- **Staggered**- most stable: all 6 C-H bonds are as far away as possible
- **Eclipsed**- least stable: all 6 C-H bonds are as close as possible to each other

- Stereochemistry concerned with the 3-D aspects of molecules

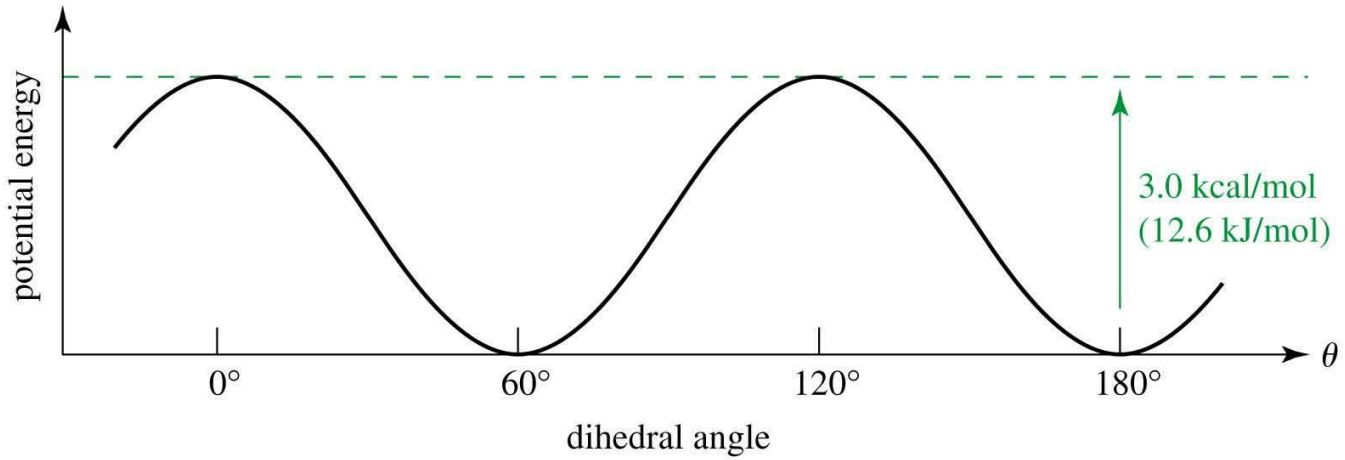
- Rotation is possible around C-C bonds in open-chain molecules (not cyclic)



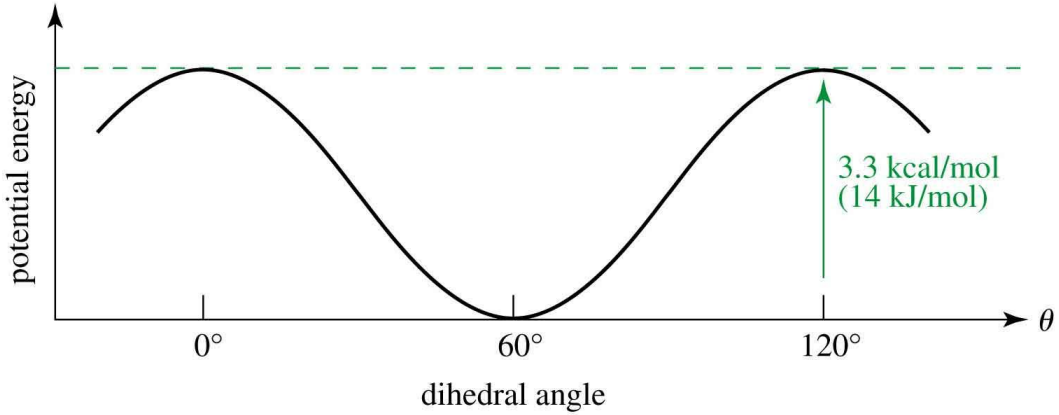
- Eclipsed conformer has highest energy
- Dihedral angle = 0 degrees



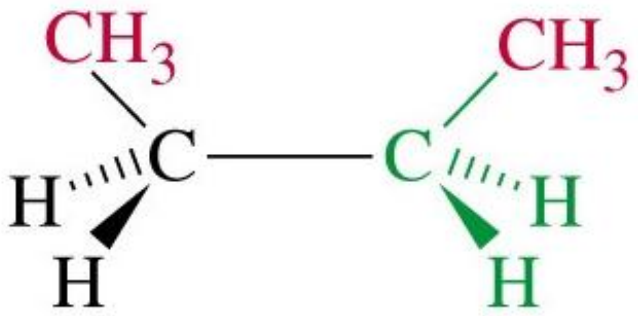
- Torsional strain: resistance to rotation.
- For ethane, only 3.0 kcal/mol

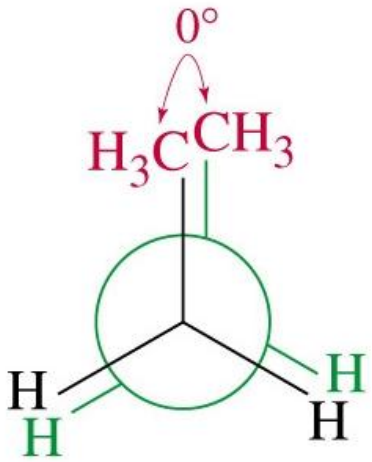


Note slight increase in torsional strain due to the more bulky methyl group.



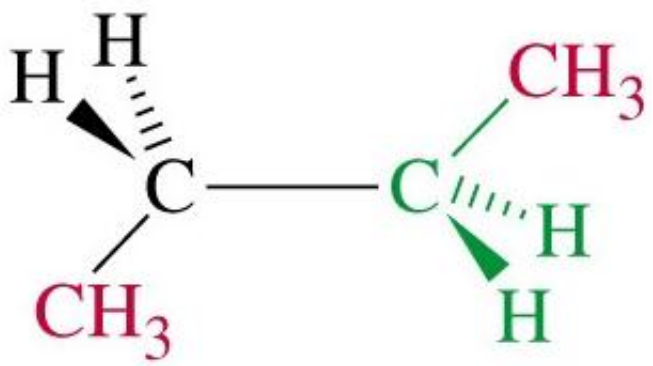
- Highest energy has methyl groups eclipsed.
- Steric hindrance
- Dihedral angle = 0 degrees



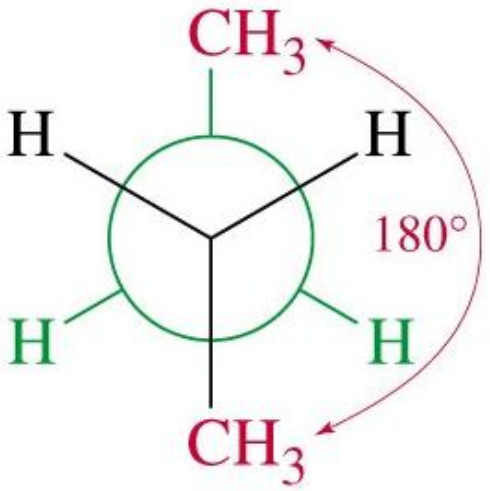


totally eclipsed

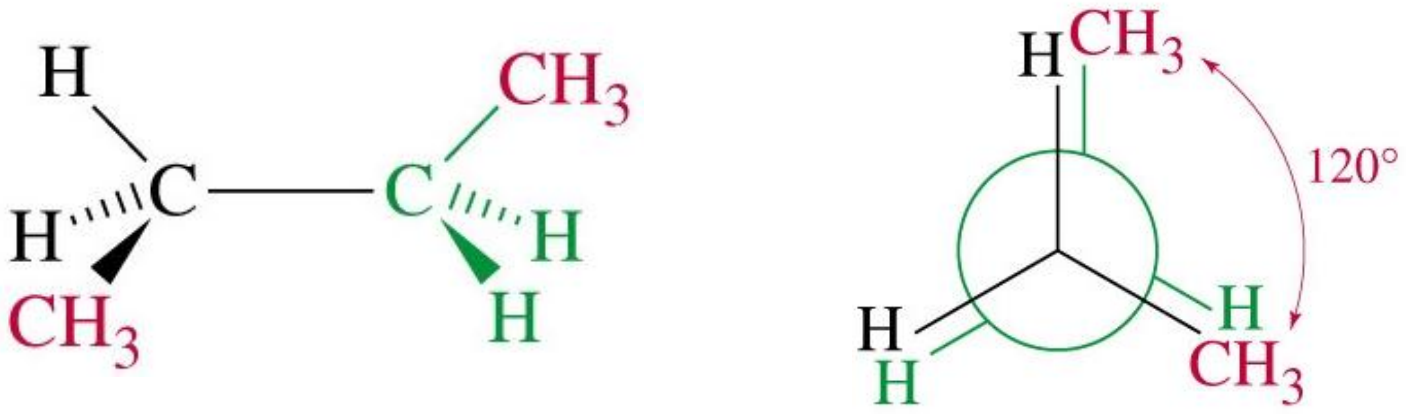
- Lowest energy has methyl groups anti.
- Dihedral angle = 180 degrees



anti

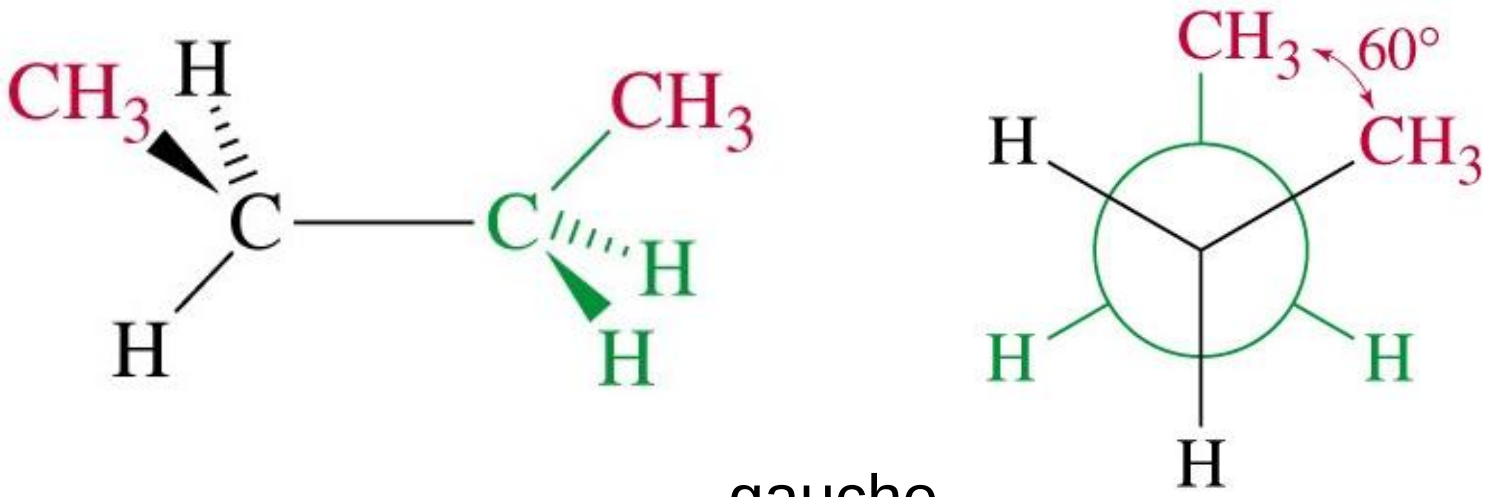


- Methyl groups eclipsed with hydrogens
- Higher energy than staggered conformer
- Dihedral angle = 120 degrees

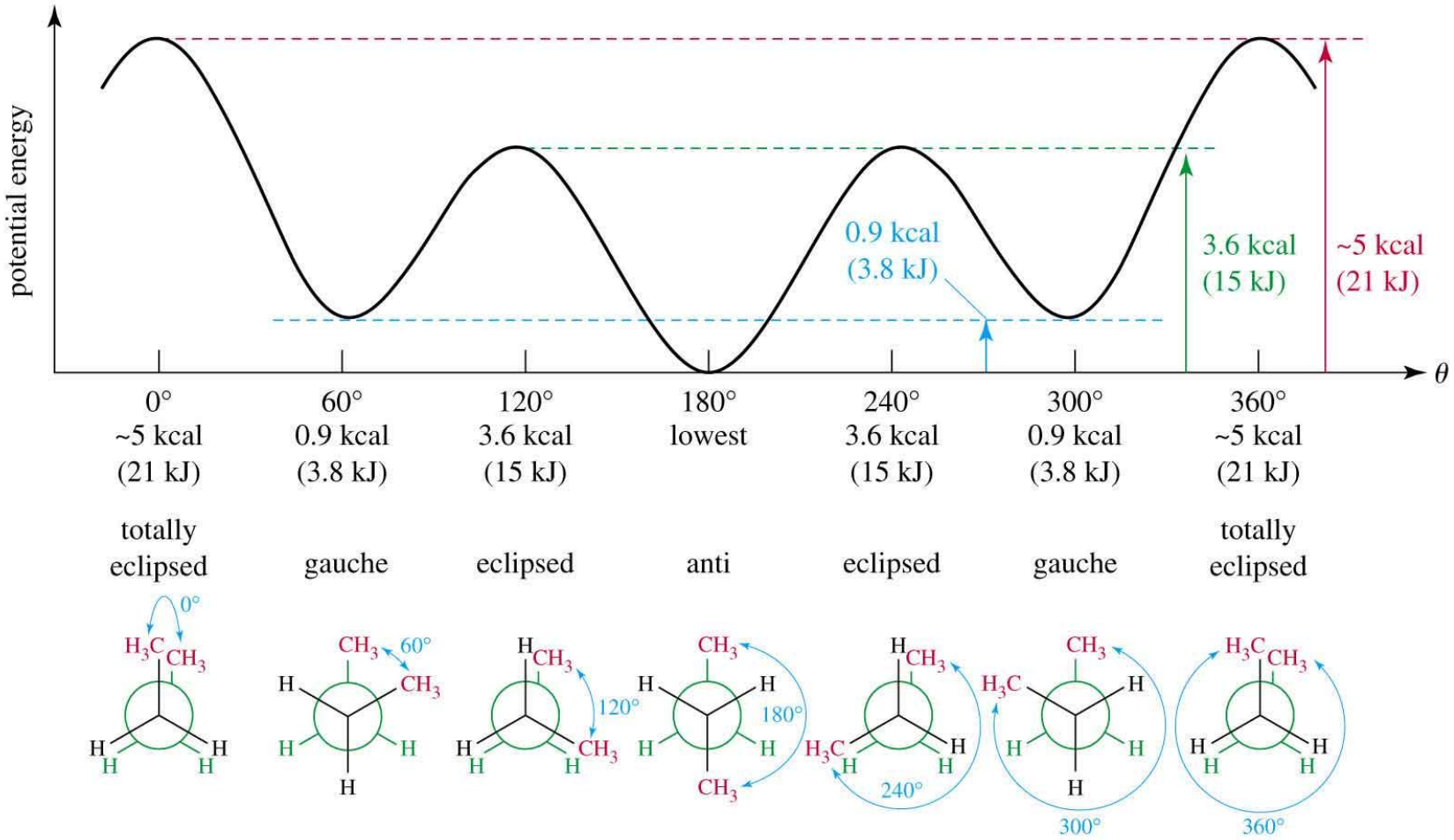


eclipsed

- Gauche, staggered conformer
- Methyls closer than in anti conformer
- Dihedral angle = 60 degrees

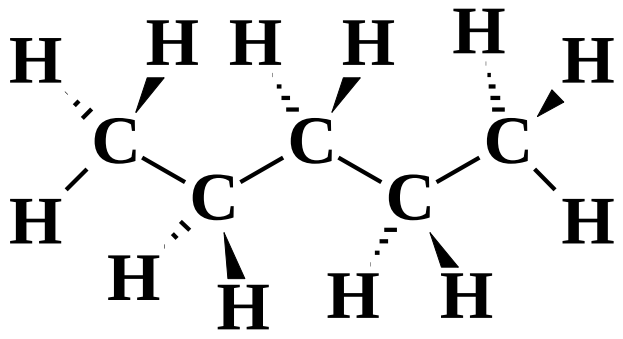


gauche


potential energy
0.9 kcal
(3.8 kJ)
3.6 kcal
(15 kJ)
~5 kcal
(21 kJ)
θ
0°
~5 kcal
(21 kJ)
totally
eclipsed
60°
0.9 kcal
(3.8 kJ)
gauche
120°
3.6 kcal
(15 kJ)
eclipsed
180°
lowest
anti
240°
3.6 kcal
(15 kJ)
eclipsed
300°
0.9 kcal
(3.8 kJ)
gauche
360°
~5 kcal
(21 kJ)
totally
eclipsed

- Anti conformation is lowest in energy.
- “Straight chain” actually is zigzag.

$$CH_3CH_2CH_2CH_2CH_3$$



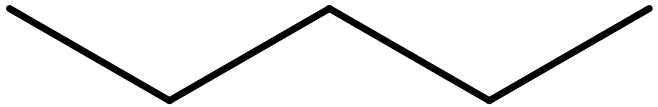


Table 3.5 | Energy Costs for Interactions in Alkane Conformers

Interaction	Cause	Energy cost (kJ/mol)	Energy cost (kcal/mol)
H⟷H eclipsed	Torsional strain	4.0	1.0
H⟷CH_3 eclipsed	Mostly torsional strain	6.0	1.4
CH_3⟷CH_3 eclipsed	Torsional and steric strain	11	2.6
CH_3⟷CH_3 gauche	Steric strain	3.8	0.9