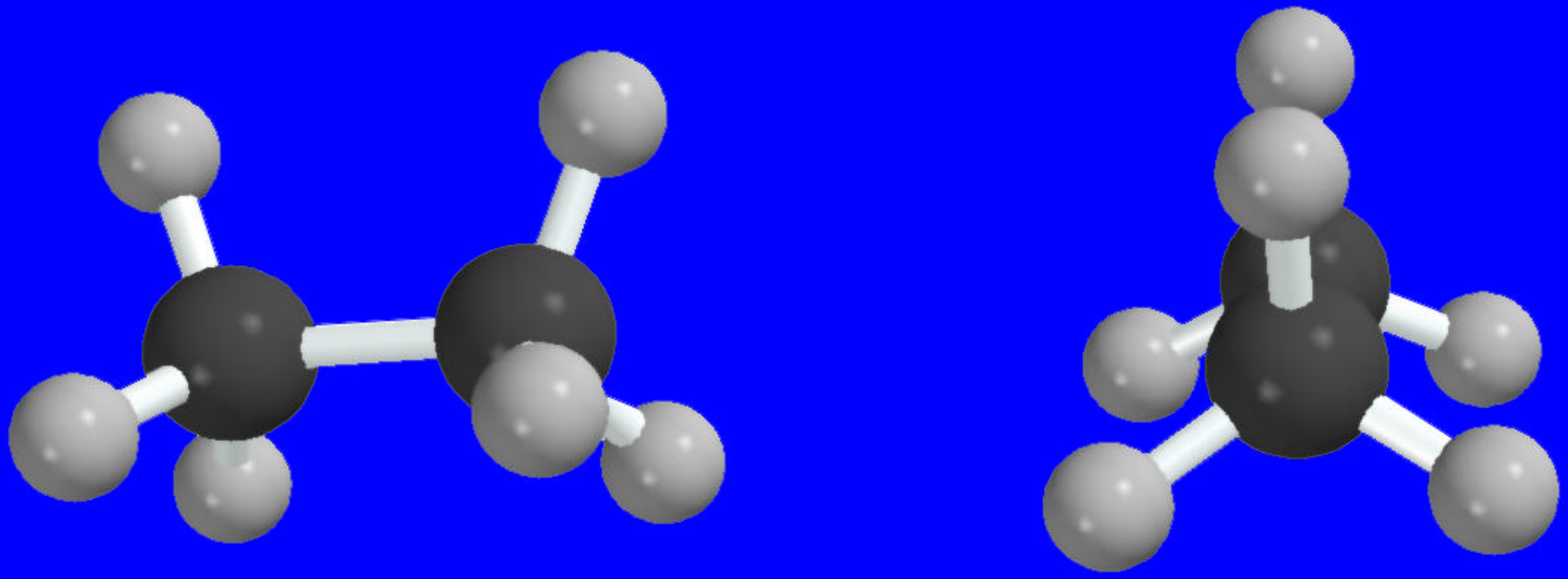
Chapter 3
Conformations of Alkanes and Cycloalkanes

3.1
Conformational Analysis of Ethane

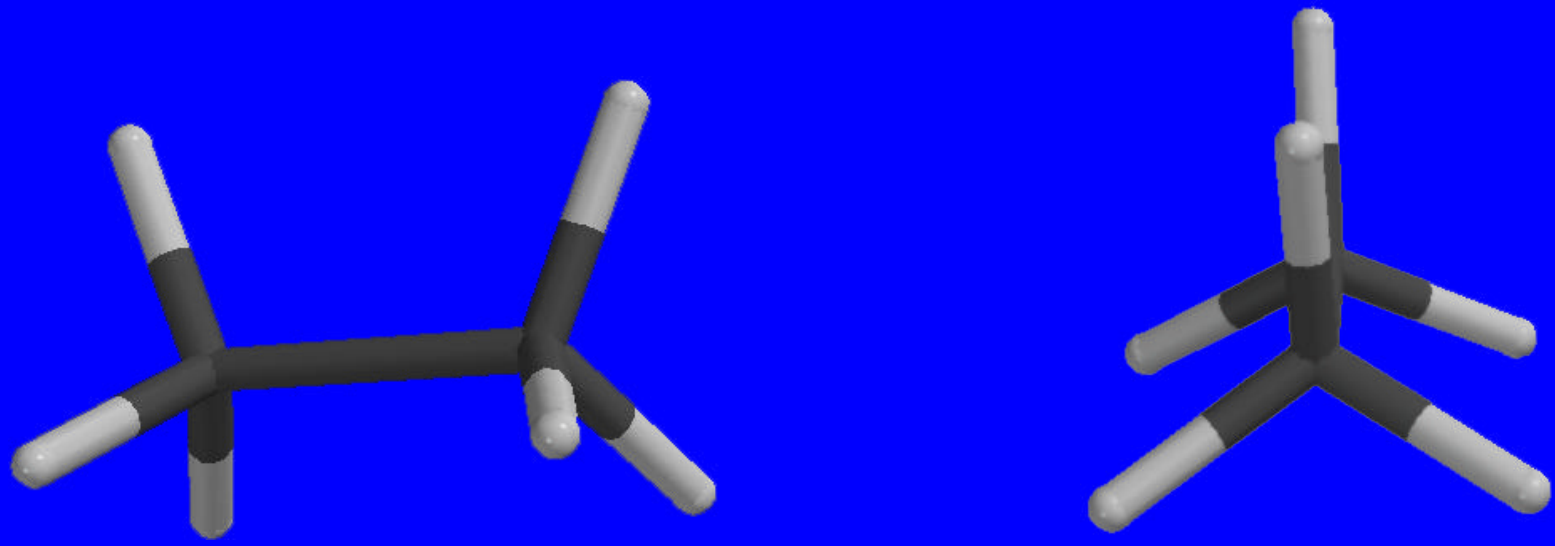
Conformations are different spatial arrangements of a molecule that are generated by rotation about single bonds.

Ethane



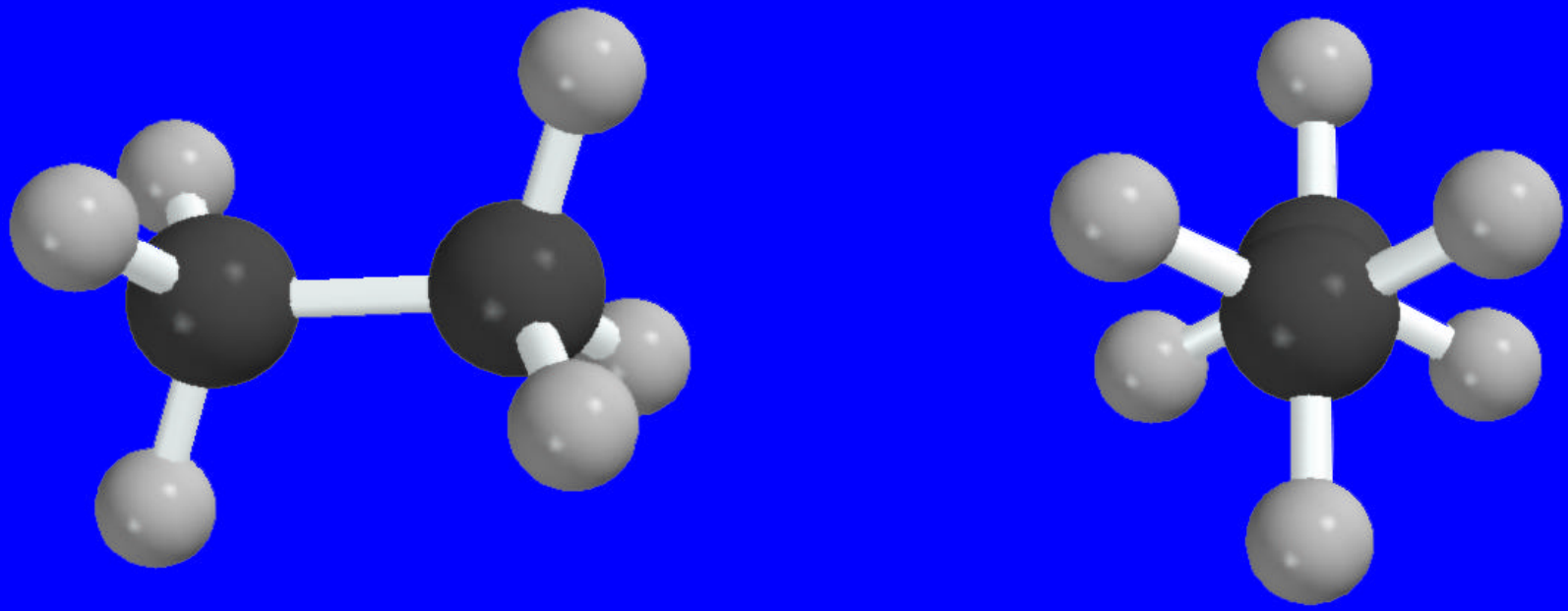
eclipsed conformation

Ethane



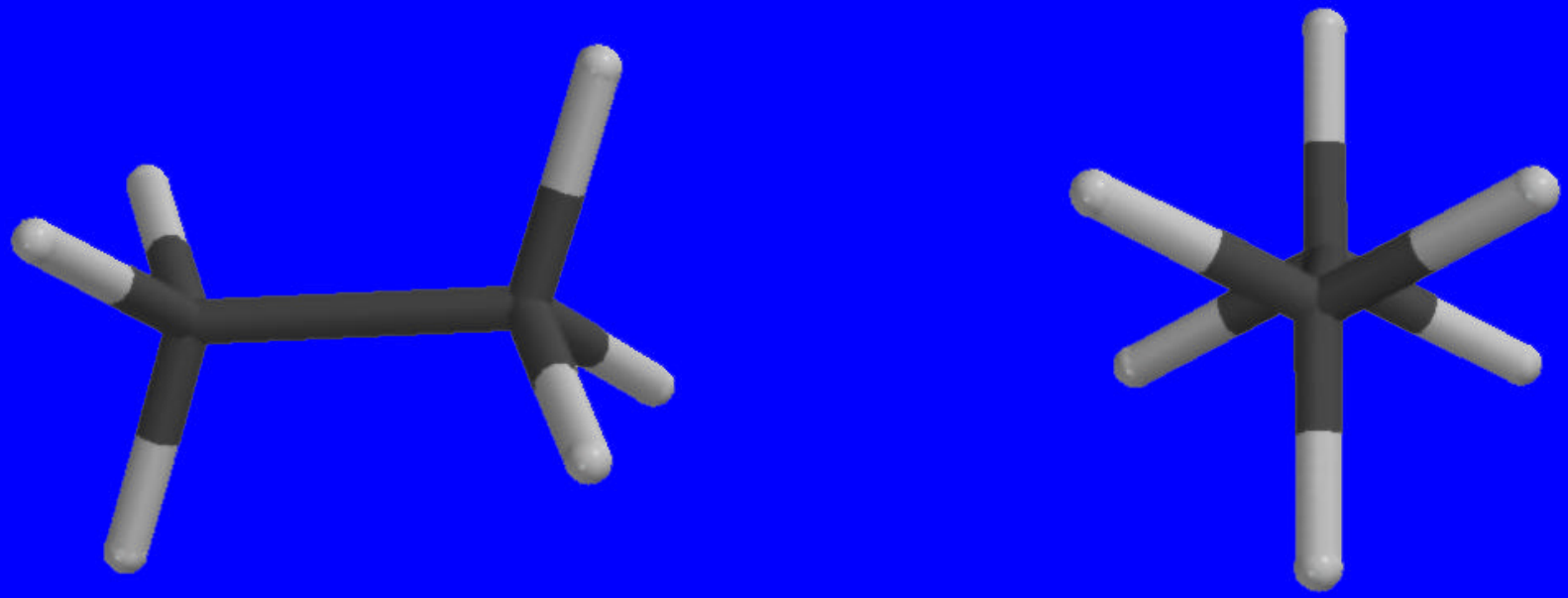
eclipsed conformation

Ethane



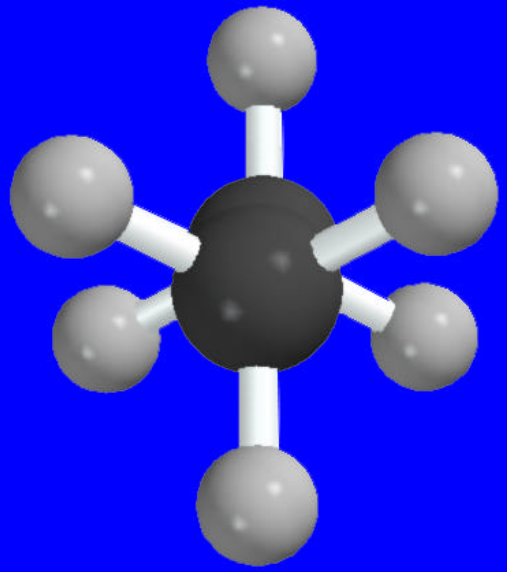
staggered
conformation

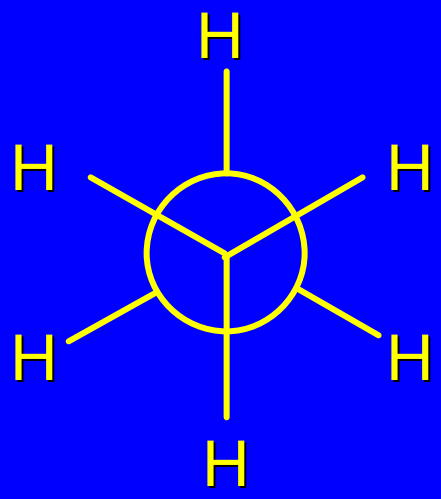
Ethane



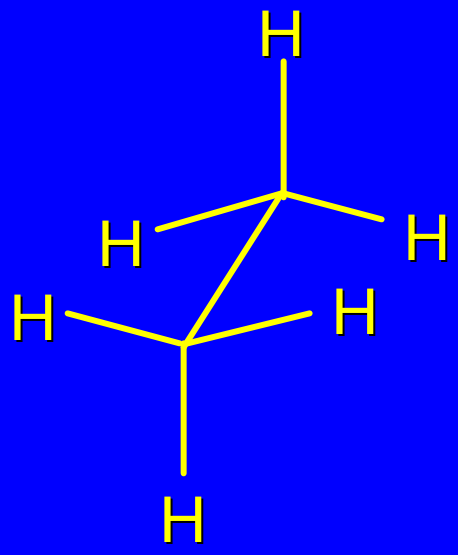
staggered
conformation

Projection Formulas of the Staggered Conformation of Ethane



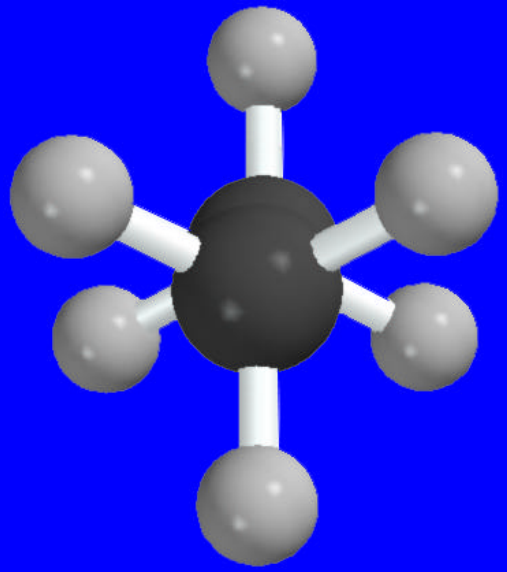


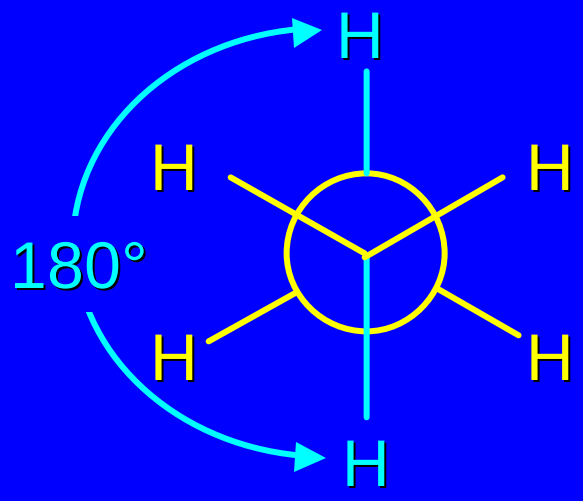
Newman

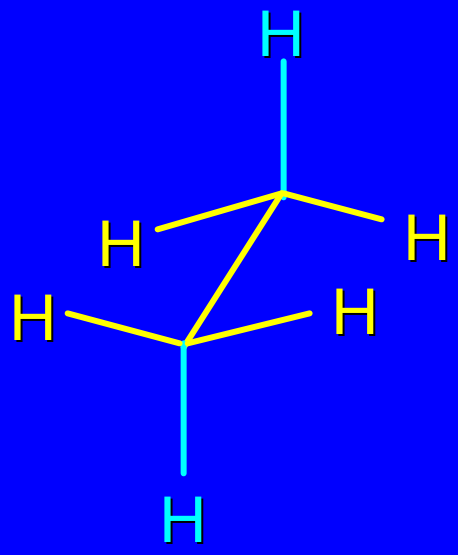


Sawhorse

Anti Relationships

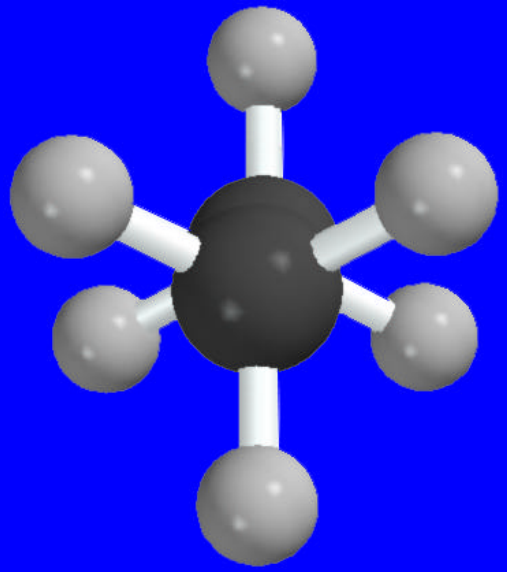


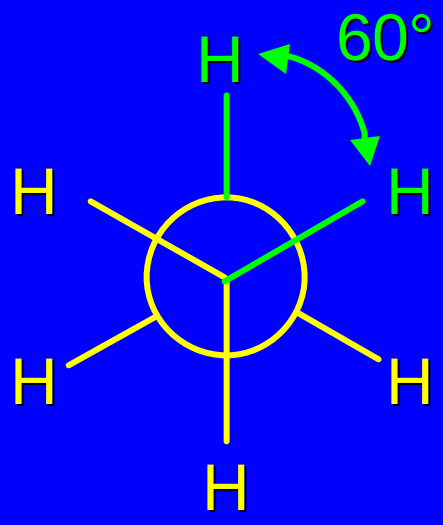


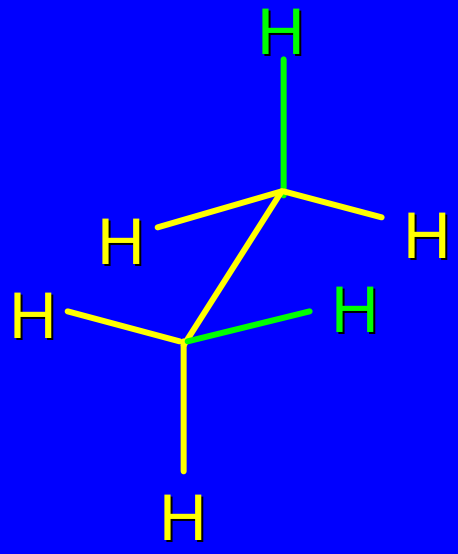


Two bonds are anti when the angle between them is 180°.

Gauche Relationships



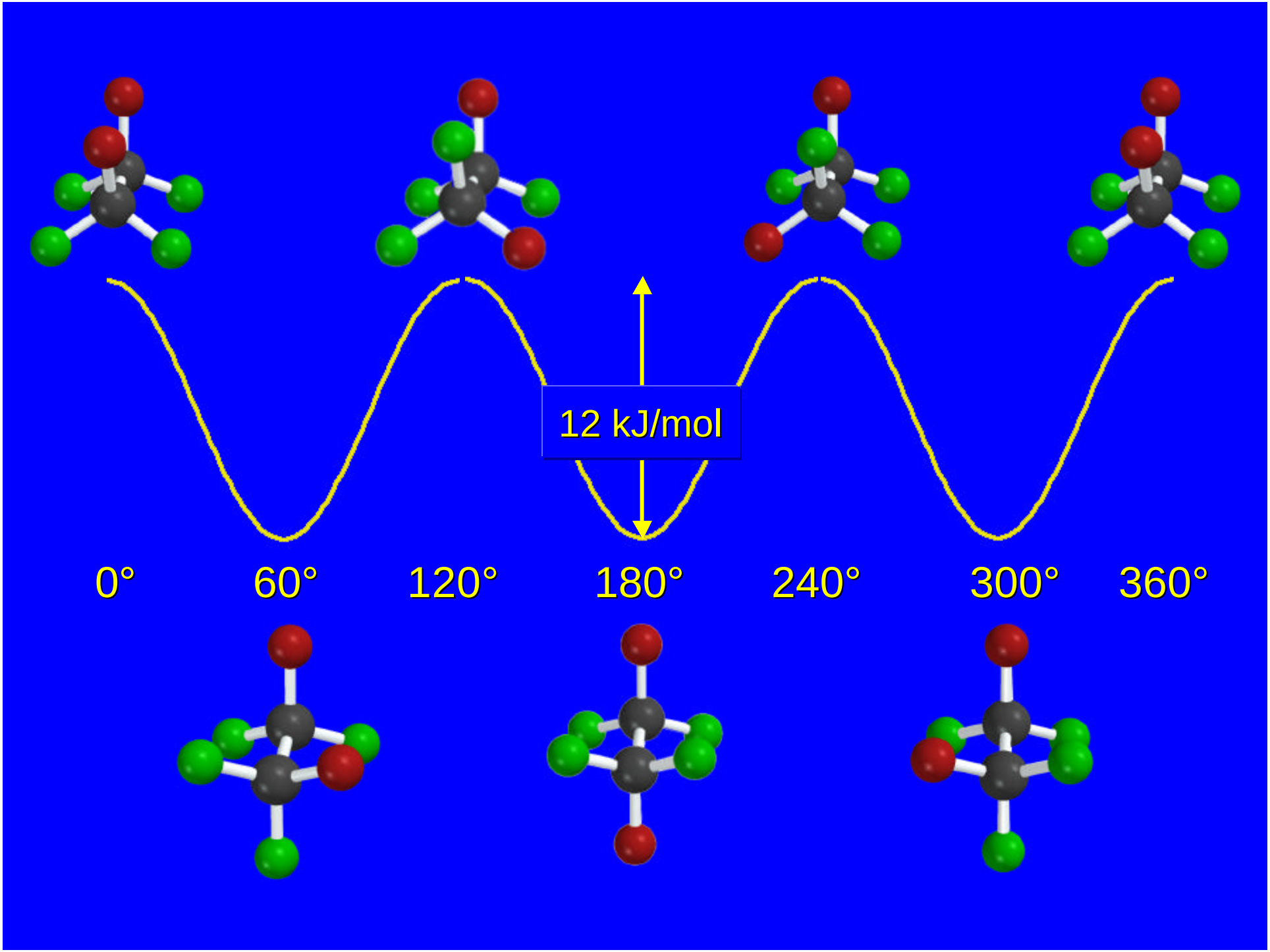




Two bonds are gauche when the angle between them is 180°.

An important point:

The terms anti and gauche apply only to bonds (or groups) on *adjacent* carbons, and only to *staggered* conformations.


12 kJ/mol
0°
60°
120°
180°
240°
300°
360°

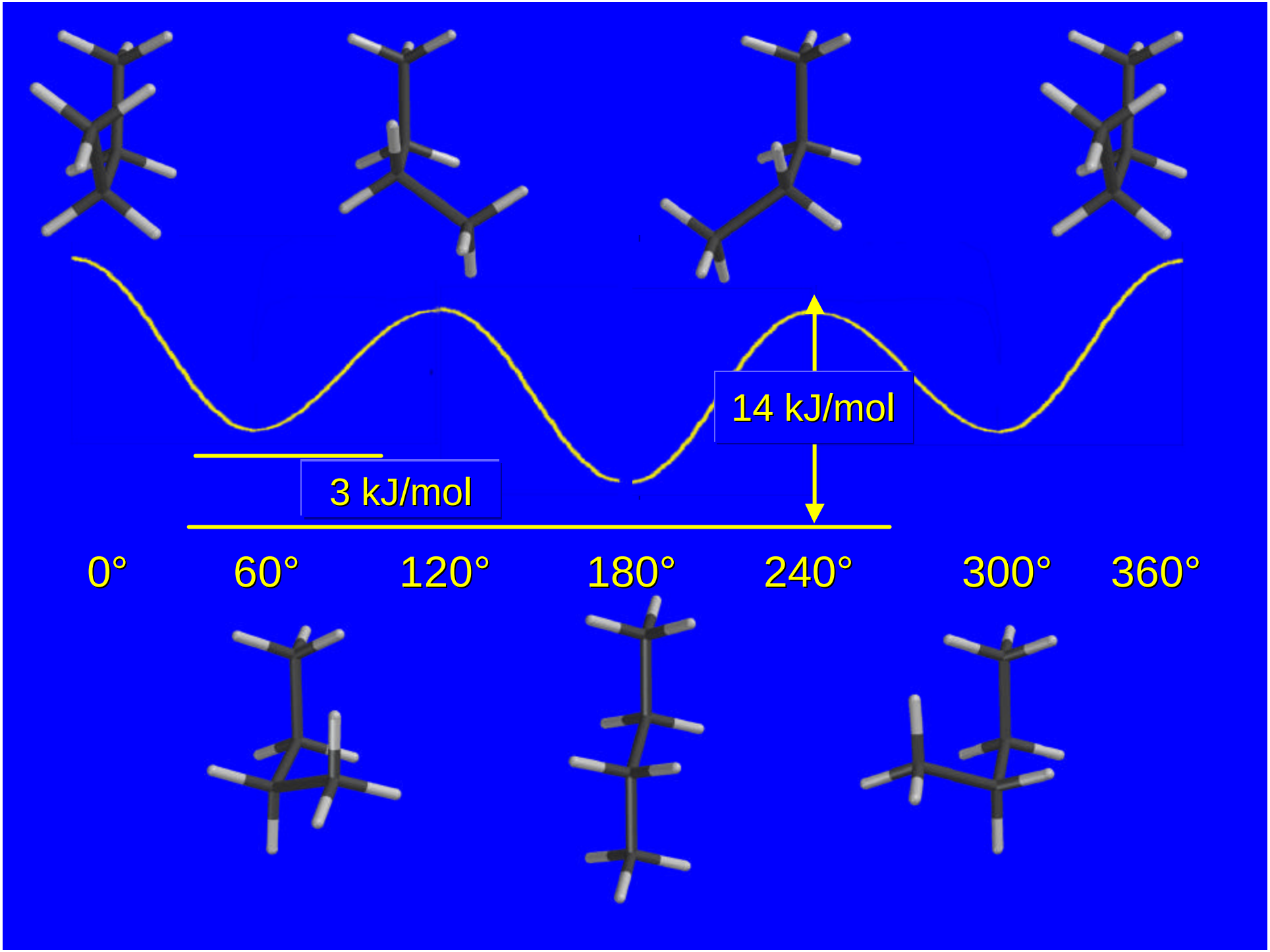
Torsional strain

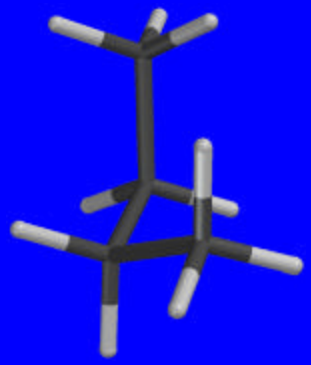
The eclipsed conformation of ethane is 12 kJ/mol less stable than the staggered.

The eclipsed conformation is destabilized by torsional strain.

Torsional strain is the destabilization that results from eclipsed bonds.

3.2
Conformational Analysis of Butane


14 kJ/mol
3 kJ/mol
0°
60°
120°
180°
240°
300°
360°



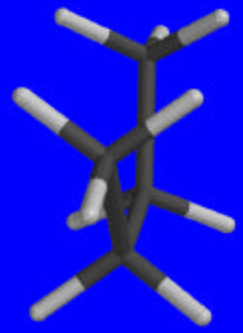
van der Waals strain

The gauche conformation of butane is 3 kJ/mol less stable than the anti.

The gauche conformation is destabilized by van der Waals strain (also called steric strain).

van der Waals strain is the destabilization that results from atoms being too close together.

van der Waals strain

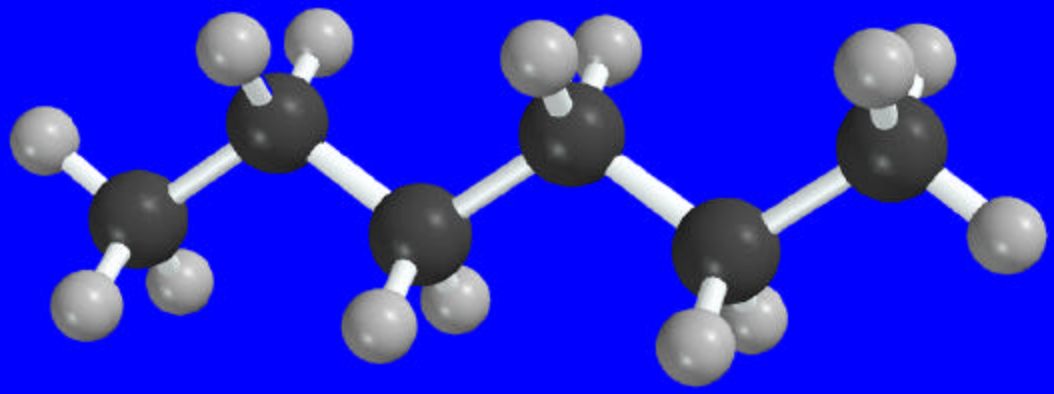


The conformation of butane in which the two methyl groups are eclipsed with each other is is the least stable of all the conformations.

It is destabilized by both torsional strain (eclipsed bonds) and van der Waals strain.

3.3
Conformational Analysis of Higher Alkanes

Unbranched alkanes



Hexane

The most stable conformation of unbranched alkanes has anti relationships between carbons.