

Alkanes

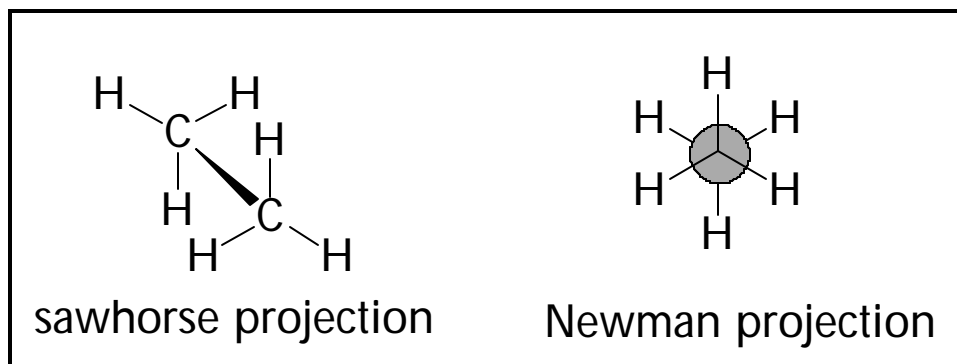
Carbons are sp^3 hybridized.

Bonds are s-bonds. C-C bonds $\sim 1.54\text{\AA}$;

C-H bonds $\sim 1.10\text{\AA}$.

Bond angles $\sim 109^\circ$.

Ethane —



Different arrangements of atoms in a molecule convertible into one another by rotation of groups of atoms about single bonds are called *conformations*. If the energy barrier to the rotation is nil or small, the rotation is said to be free or almost free.

The rotation of the methyl groups around the C-C bond in ethane is almost free; therefore, ethane can exist in an infinite number of conformations.

As one methyl group rotates relative to the other the energy of the molecule does change; the *staggered conformation* has the lowest energy and the *eclipsed conformation* has the highest energy.

See McMurry, 5th, Fig. 4.3, pg. 115

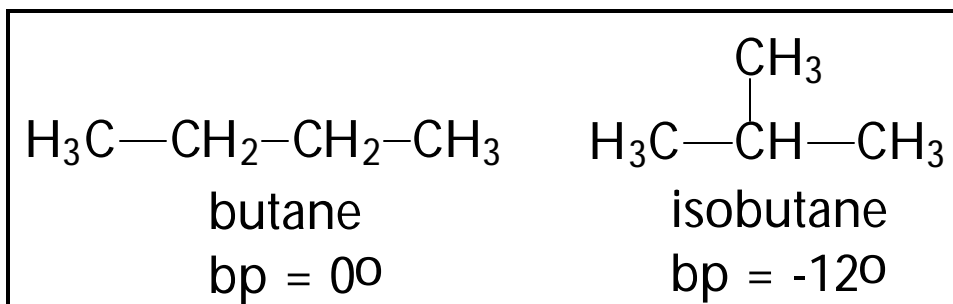
Eclipsed conformation has *torsional strain* --- probably due to repulsions between electrons in the C-H bonds on C-1 and on C-2.

Propane — C₃H₈

Rotational barrier ~ 14kJ/mole (3.3 kcal/mole): torsional strain.

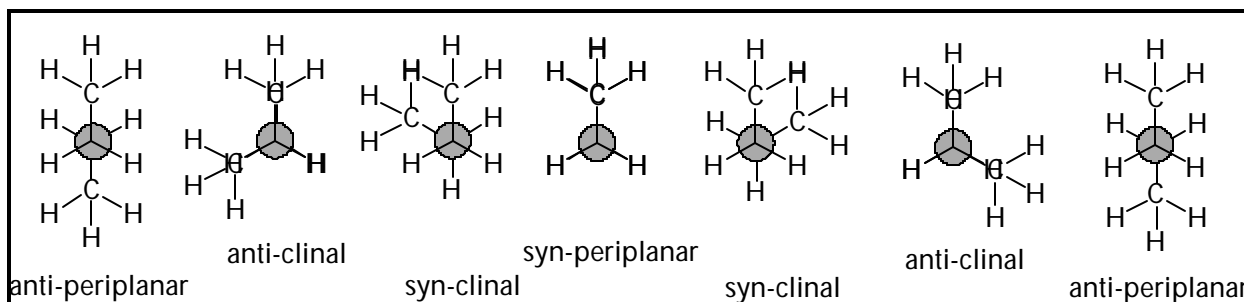
Butane — C₄H₁₀

Two structural isomers —



Let's examine *butane* by sighting down the C-2 to C-3 bond of the staggered conformation in which the methyl groups are 180° apart. Then we will rotate the rear ethyl group clockwise around the C-2 to C-3 bond until the methyl groups are again 180° apart. There will be an infinite number of conformations, but we will focus our attention on the staggered and eclipsed ones.

Sometimes the different conformations are named as follows:



See McMurry, 5th, Fig. 4.5, pg. 117.

Strain —

anti-periplanar: none

anti-clinal: torsional ~ propane

synclinal: steric

☞ methyl groups begin to approach each other

syn-periplanar: steric and torsional