

CONFORMATIONAL ANALYSIS

"FREE" ROTATION

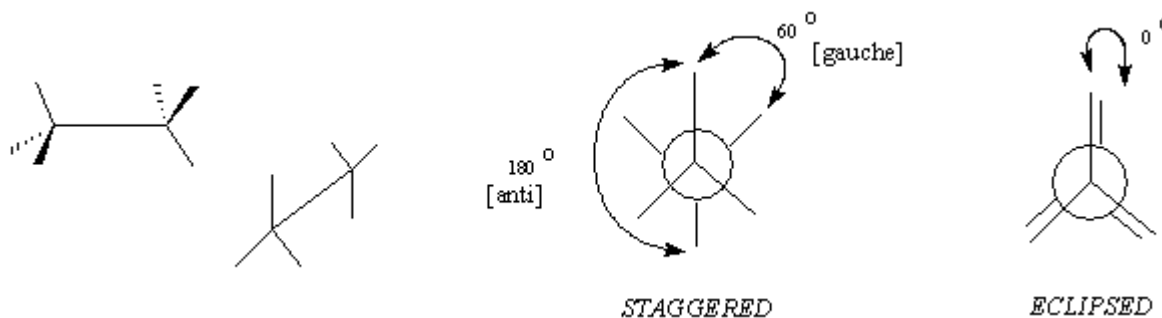
occurs around most non-cyclic single sigma bonds. This rotation may produce different spatial relationships between atoms bonded to the rotating carbons.

CONFORMATIONS

are the infinite number of non-identical momentary arrangements of the atoms in a molecule that result from rotation about one or more single bonds.

CONFORMERS

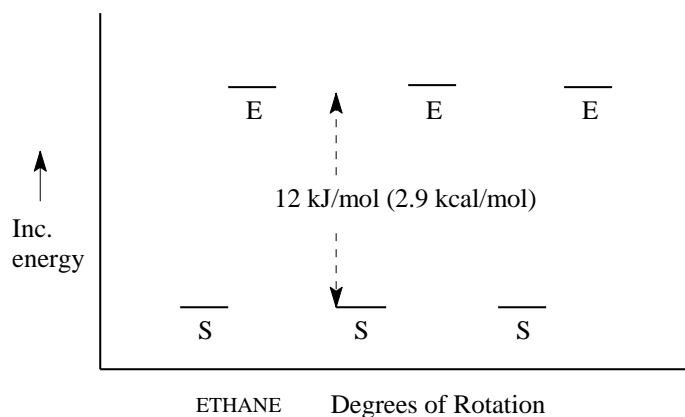
(conformational isomers; rotational isomers) are conformations of minimum energy and are therefore the most stable.



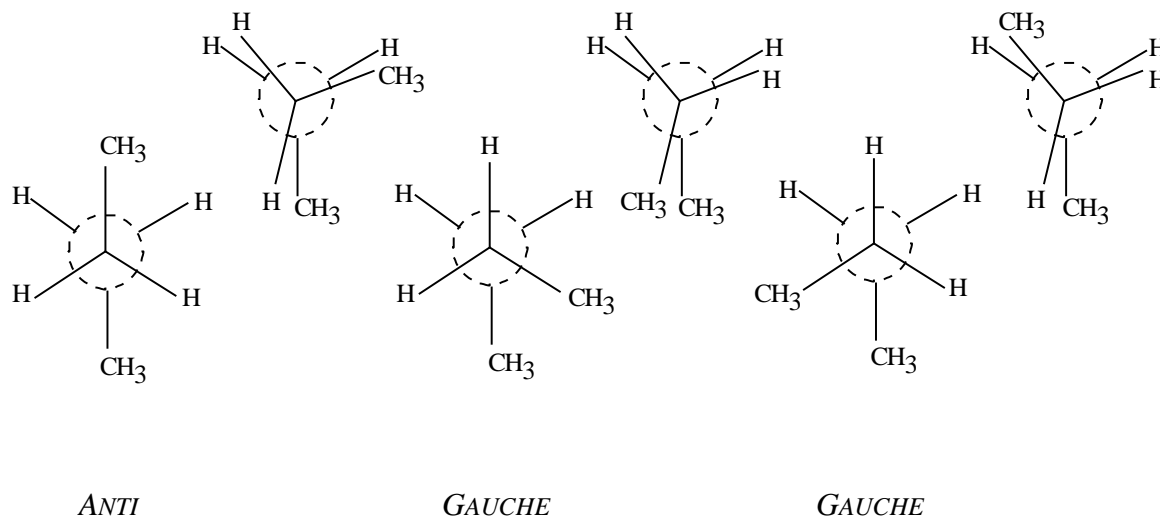
TORSIONAL STRAIN

is the force (energy barrier) that resists truly free rotation from one staggered conformation to another through an eclipsed conformation. The cause is not yet completely understood, although at one time it was thought to be the result of repulsion of the *electrons* in the *bonds* which are *eclipsed*.

The energy absorbed by the molecule to rotate through the eclipsed conformation raises the molecule to a higher energy level.



n-Butane CH₃-CH₂-CH₂-CH₃



STERIC STRAIN

(van der Waals strain or repulsion) occurs when *non-bonded atoms* interact repulsively by being too close to each other. It is important for atoms or groups other than H.

There is more steric strain in the 0° eclipsed conformation than in the other two eclipsed conformations (all three have torsional strain that is absent in the staggered conformations.) There is more steric strain in the *gauche* staggered conformations than in the *anti* staggered conformation.

