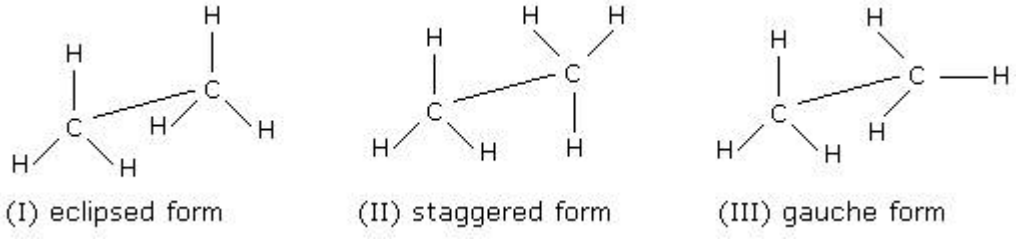
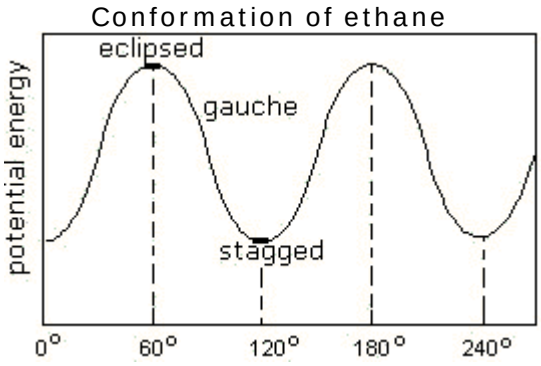
Study of Conformations

In a simple hydrocarbon like ethane, the free rotation of one carbon with respect to another gives rise to various arrangements of the atoms differing in relative positions of hydrogens attached to these carbon atoms. These momentary arrangements of atoms in space resulting due to free rotation around a single bond are called conformations or conformers or rotamers. Conformations of ethane are given below.



(This representation is referred to as the saw-horse formulae.)

In conformation (I) the hydrogen atoms of one carbon atom lie exactly parallel to the hydrogen atoms of the second carbon atom. This is called eclipsed conformation.
In conformation (II) the hydrogen atoms of one carbon atom are exactly in the middle position occupied by the hydrogen atoms of the other carbon atom. This arrangement is called staggered conformation.
Any other arrangement like (III) will be in-between these two extreme positions and thousands of such conformation are possible. Theoretically, ethane, therefore, should have infinite isomers but the energy differences between these conformations are so small that they are readily interconvertible at room temperature due to rotation around the single bond and hence cannot be isolated separately.



Potential energy diagram showing correlation of potential energy with rotation

A potential energy diagram of these structures suggests that the staggered conformation of ethane is about 12 kJ mol^{-1} lower in energy than the eclipsed conformation, making the former more stable. A number of factors are responsible for greater stability of the staggered conformation. They are as follows:

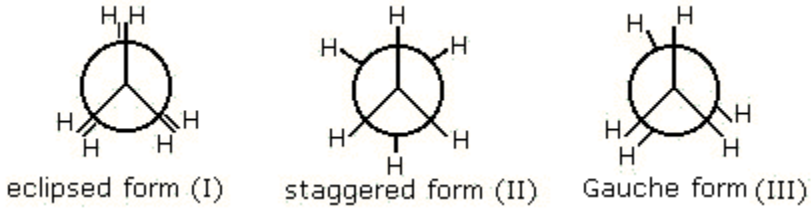
(a) In staggered conformation there is maximum separation of the bonded electron pair while in eclipsed conformation the electron pair repulsions are maximum. This is called torsional (Pitzer) strain.

(b) A small contribution of identical C-H dipole-dipole repulsion on adjacent carbon atoms makes the eclipsed form less stable.

(c) Any other conformation such as (III) must have the energy content and stability, between these two extremes.

Hence in a given sample of ethane, most molecules exist in staggered conformation and few in the (III) form and practically none in the eclipsed form at room temperature. However, the activation energy for conversion of staggered to eclipsed conformation being small, the rotation about the carbon-carbon bond increases with increase in temperature increasing the contribution of conformations like (III) and may be of the eclipsed form also.

These conformation cannot be separated from each other because of easy interconvertibility. Another way of representing these conformations is the Newman projection formula.



The important point of difference between configuration and conformation is that to change configuration, bonds must be broken while conformers are formed as a result of rotation around the same bond.

Examples

1. How many conformations are there for ethane?

Answer: Infinite

The answer to such questions can be either zero or infinite. For those molecules which will have conformation it will be infinite, since a slight rotation of the single bond (here C - C) gives another conformer.
For those molecules in which no conformation is possible, it will be zero.

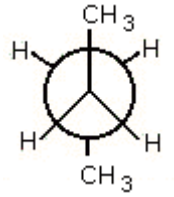
2. How many conformations are there for ethene?

Answer: Zero, as no conformations are possible.

3. Out of the various conformations of butane, which is most stable?

Answer: The most stable conformation is anti-conformer as there is least steric strain

because of bulky methyl groups anti to each other.



Anti-conformer