

2.4 CONFORMATIONAL ISOMERISM

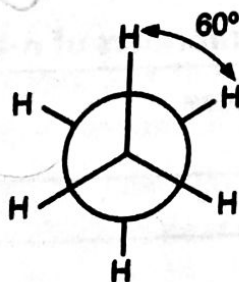
These are the isomers generated due to rotation around single bonds present in the molecule. They may be rapidly interconverted to each other again through further rotation around single bonds. There exists a rotational energy barrier that needs to be overcome to convert one conformer to another.

Some important examples of conformational isomerism include:

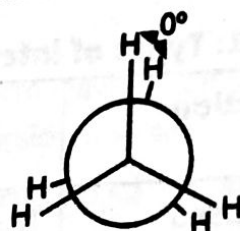
- (i) Open chain alkane conformations: Staggered, eclipsed and gauche conformers.
- (ii) Ring conformation: Chair and boat conformers.
- (iii) Atropisomerism: A molecule can become chiral due to restricted rotation about a bond.
- (iv) Folding of molecule.

2.4.1 Conformations of Ethane

Out of infinite conformations possible, most important conformers of ethane are:
(i) Staggered conformation and (ii) Eclipsed conformation.



(i) Staggered conformation



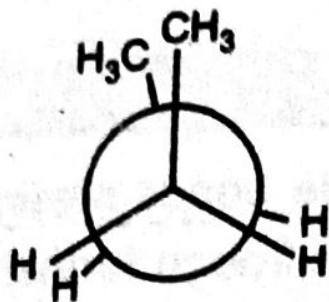
(ii) Eclipsed conformation

Since the angle between the C - H bonds of 1st and 2nd carbons is 60°, the staggered conformation is the most stable conformation of ethane. In eclipsed form, the angle is 0° between two C - H bonds leading to repulsion in their electron cloud which raises the energy and decreases the stability of the molecule. The eclipsed conformation of ethane is less stable than the staggered conformation by 3 kcal/mol.

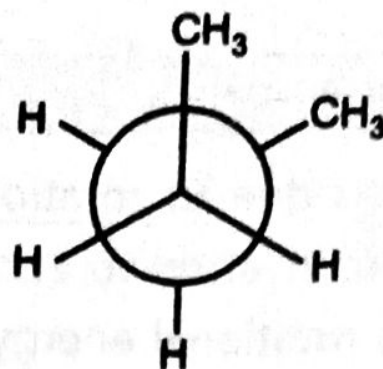
In eclipsed conformation, the bulky substituents of the molecule are brought closer leading to repulsion amongst them. This hindrance causes resistance to rotation (torsional strain i.e., force that opposes rotation due to the repulsion of bonding electrons.) It is not possible to isolate either of ethane conformations due to their rapid interconversion at room temperature.

2.4.2 Conformations of n-Butane

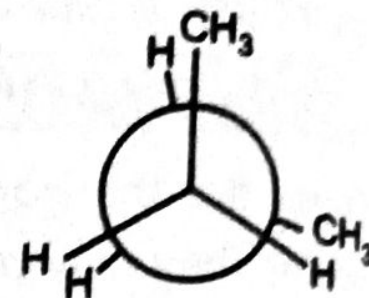
Various conformations of n-Butane include,



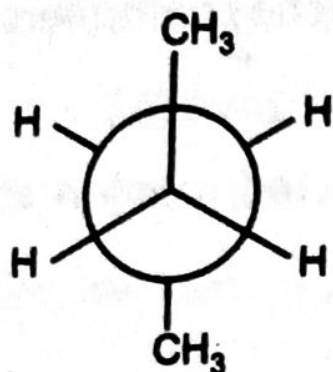
Syn (Eclipsed) (E_2)
Dihedral angle = 0° and 360°
Maximum energy



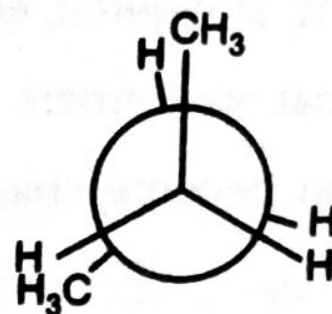
Gauche (Staggered)
Dihedral angle = 60°
Energy = 0.88 kcal/mol.



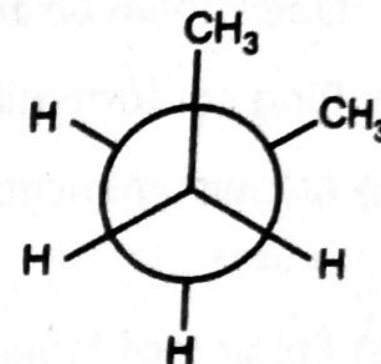
Eclipsed (E_1)
Dihedral angle = 120°
Lower energy



Anti (staggered)
Dihedral angle = 180°
Least energy



Eclipsed
Dihedral angle = 240°
Lower energy



Gauche (staggered)
Dihedral angle = 300°
Energy = 0.88 kcal/mol.

Dihedral angle: It is the angle created by two intersecting planes.

The gauche butane is less stable than antbutane by 3.8 kJ/mol, because of steric interference between H-atoms on the two methyl groups.

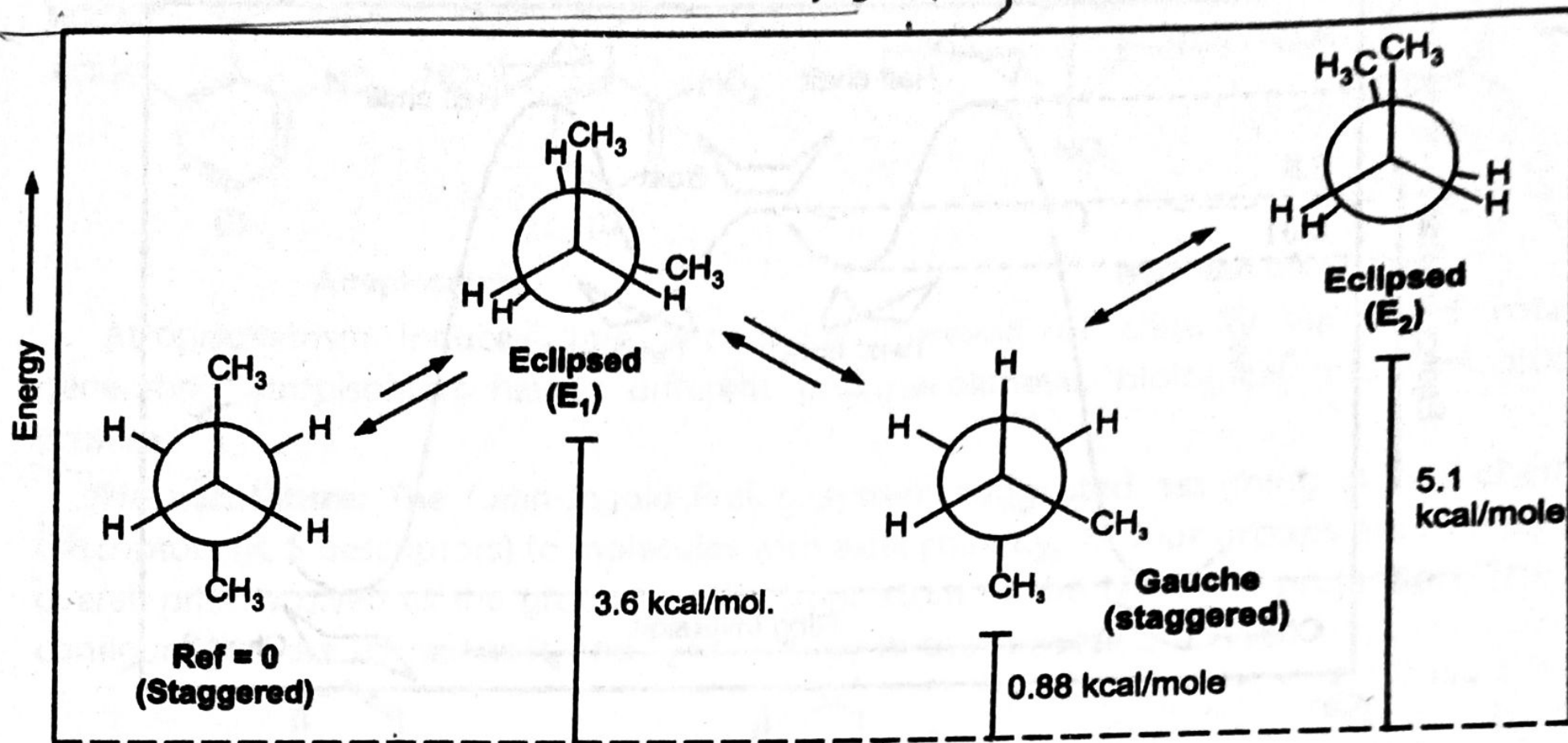


Fig. 2.1: n-Butane torsional energy profile