

# CONFORMATIONAL ANALYSIS OF n-Butane ①

## Conformation

Structures arising from rotation about single bonds (or flipping of rings) are called conformers.

When a C-C bond is rotated with its substituents, keeping one carbon static, an <sup>infinite</sup> number of spatial arrangements are obtained.

Each of these spatial arrangements are called as conformers.

## Conformational Analysis

The determination of the relative stabilities of the conformations of a compound and interpretation of their physical and chemical properties are referred to as conformational analysis.

The stability of a conformer depends on the following four main factors: They are

1. Torsional strain
2. Angle strain
3. Vander Waal's strain
4. Dipole-Dipole interaction

(1) Torsional Strain (2)  
<sup>conformation</sup>  
When a molecule is rotated to give an eclipsed <sup>conformation</sup>, the strain developed in a molecule is known as Torsional Strain. The strain is due to bond bond pair - bond pair repulsion. The greater the torsional strain, the lower is the stability of the conformation.

(ii) Angle Strain

Deviation from the normal angle will create a strain in the molecule which is known as Angle Strain. The greater the angle strain, the lower is the stability of the conformation.

(iii) Steric Strain (or) van der Waals Strain

If the distance between two substituents is less than the van der Waals radii, then a repulsive force is developed due to the repulsion between the electron clouds of the interacting substituents. This destabilizing interaction creates a strain in the molecule which is known as van der Waals strain. When the size of the non-bonded substituents are greater, greater will be the van der Waals



(3)

Strain and less is the stability of the conformation.

(1) Dipole-Dipole interaction

Non bonded substituents <sup>on each C atom</sup> of the C-C bond may undergo dipole-dipole interactions <sup>more</sup> which hydrogen bonding is the strongest. If the non bonded atoms have opposite partial charges/densities, then an attractive force develops between them and hence the stability of the conformation increases.

If the non bonded substituents <sup>have</sup> like charges, then a repulsive force is developed resulting in the destabilization of the conformation.

The potential energy of n-butane as a function of dihedral angle is given below:

n-Butane may exist in different conformations, such as eclipsed & staggered conformations which are represented by structures I to VI.

## Eclipsed conformations

(4)

The conformations I, III and V are eclipsed conformations. These conformations represent energy maxima in the potential energy diagram. Out of the three eclipsed conformations, conformations III and V have same potential energy, which is less than the conformation I at dihedral angle of  $0^\circ$  and  $360^\circ$ , conformations III and V have torsional strain and van der Waals strain.

## Staggered conformations

The conformations II, IV and VI are called as staggered conformations. These conformations have energy minima and are the stable conformations of n-butane.

However, not all the staggered conformations of butane are similar. The conformations II with a dihedral angle of  $60^\circ$  and conformation VI with a dihedral angle of  $300^\circ$  are called as Gauche conformations.

(b)

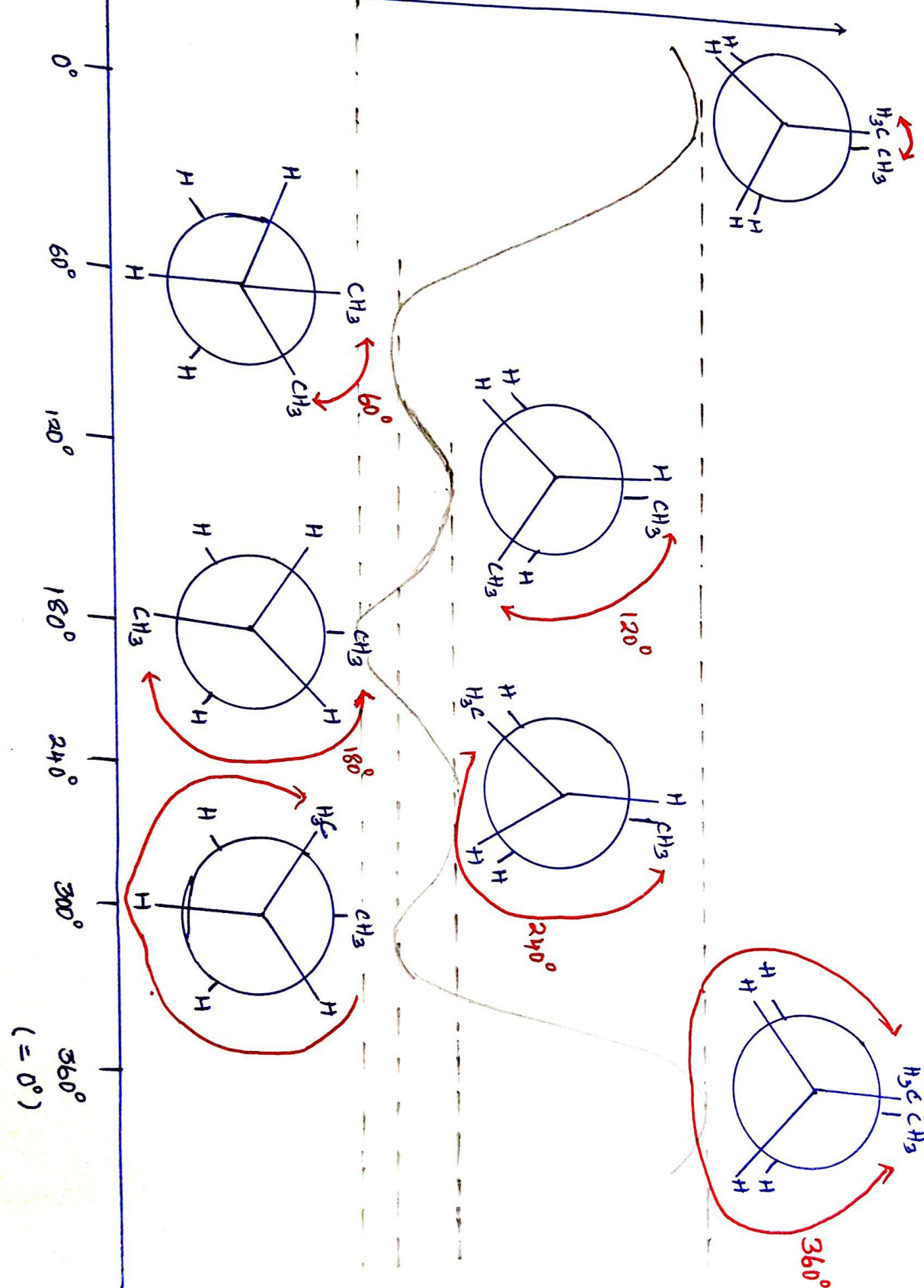
The conformation IV at a dihedral angle of  $180^\circ$  is called as anti conformation. (Anti - opposite in Greek). The anti conformation does not have torsional strain because the groups are staggered and the methyl groups are far apart. Anticonformation is more stable than the Gauche conformation.

The order of increasing stability of the conformation of n-butane is





Potential energy →



Dihedral angle →