Conformations of n-butane

Structure 1 (nbutane1.mol)

The three important conformers of n-butane, anti, gauche and eclipsed. These conformations arise due to the rotation of central C-C bond. In the staggered conformation the two methyl groups are placed farthest from each other with a dihedral angle of 120 degrees. This is the most stable conformer with lower energy than gauche conformer.

Structure 2 (nbutane2.mol)

In the eclipsed conformation, the two methyl groups attached to center C-C bond are overlapping with each other. The dihedral angle is 0 degrees. This is the highest energy conformation for butane, due to steric repulsion between the two bulky methyl groups.

Structure 3 (nbutane3.mol)

The two methyl groups in this conformation are “gauche” to each other, hence it is referred to as “gauche” conformer. The two methyl groups are not as far apart and there is still significant steric repulsion between the two bulky methyl groups. The dihedral angle is 120 degrees.