Quadrant I – Notes (Module 21)

Programme: Bachelor of Science (First year)
Subject : Chemistry
Paper code: CHC - 101
Paper Title: Inorganic and Organic Chemistry
Section : B
Unit : II : Stereochemistry
Module name : Conformation with respect to Ethane.
Name of the presenter: Mrs. Anuradha B. Kanolkar.

Structure of Ethane

Next in size after methane is **ethane**, C_2H_6 . If we connect the atoms of this molecule by covalent bonds, following the rule of one bond (one pair of electrons) for each hydrogen and four bonds (four pairs of electrons) for each carbon, we arrive at the structure



Ethane

Each carbon is bonded to three hydrogens and to the other carbon. Since each carbon atom is bonded to four other atoms, its bonding orbitals (sp³ orbitals) are directed toward the corners of a tetrahedron. As in the case of methane the carbon-hydrogen bonds result from overlap of these sp³ orbitals with the s orbitals of the hydrogens. The carbon-carbon bond arises from overlap of two sp³ orbitals.

The carbon-hydrogen and carbon-carbon bonds have the same general electron distribution, being cylindrically symmetrical about a line joining the atomic nuclei; because of this similarity in shape, the bonds are given the same name, o bonds (sigma bonds).

FREE ROTATION ABOUT THE CARBON- bond. Conformations. Torsional strain CARBON SINGLE BOND

In ethane, then, the bond angles and carbon-hydrogen bond lengths should be very much the same as in methane. that is, about 109.5° and about 1.10 A, respectively. Electron diffraction and spectroscopic studies have verified this structure in all respects, giving the following measurements for the molecule: bond angles, 109.5°: C-H length, 1.10 Ä: C-C length, 1.53 A. Similar studies have shown that, with only slight variations, these values are quite characteristic of carbon-hydrogen and carbon-carbon bonds and of carbon bond angles in alkanes.

Free rotation about the carbon-carbon single bond

This particular set of bond angles and bond lengths still does not limit us to a single arrangement of atoms for the ethane molecule, since the relationship between the hydrogens of one carbon and the hydrogens of the other carbon is not specified. If we examine models of ethane in which the hydrogens exactly oppose each other.

which the hydrogens are perfectly staggered, or an infinity of intermediate arrangements. Which of these is the actual structure of ethane? The answer is: all of them. We have seen that the o bond joining the carbon atoms is cylindrically symmetrical about a line joining the two carbon nuclei; overlap and hence bond strength.

should be the same for all these possible arrangements. If the various arrangements do not differ in energy, then the molecule is not restricted to any one of them, but can change freely from one to another. Since the change from one to another involves rotation about the carbon-carbon bond, we describe this freedom to change by saying that there is free rotation about the carbon-carbon single bond.

Different arrangements of atoms that can be converted into one another by rotation about single bonds are called **conformations.** Arrangement I is called the eclipsed conformation; arrangement II is called the staggered conformation. (The infinity of intermediate conformations are called skew conformations.) To represent such conformations, we shall often use two kinds of three dimensional formulas: andiron formulas.

FREE ROTATION ABOUT THE CARBON- CARBON SINGLE BOND

. Certain physical properties show that rotation is not quite free: there is an energy barrier of about 3 kcal/mol. The potential energy of the molecule is at a minimum for the staggered conformation, increases with rotation, and reaches a maximum at the eclipsed conformation Most ethane molecules, naturally, exist in the most stable, staggered conformation; or, put differently, any molecule spends most of its time in the most stable conformation.



How free are ethane molecules to rotate from one staggered arrangement to another? The 3-kcal barrier is not a very high one; even at room temperature the fraction of collisions with sufficient energy is large enough that a rapid interconversion between staggered arrangements occurs. For most practical purposes, we may still consider that the carbon-carbon single bond permits free rotation.

The nature of the rotational barrier in ethane is not understood or-what is not exactly the same thing--is not readily explained. It is too high to be due merely to van der Waals forces. Although thrown closer together in the eclipsed conformation than in the staggered conformation, the hydrogens on opposite carbons are not big enough for this to cause appreciable crowding. The barrier is considered to arise in some way from interaction among the electron clouds of the carbon-hydrogen bonds. Quantum mechanical calculations show that the barrier should exist, and so perhaps "lack of understanding" amounts to difficulty in paraphrasing the mathematics in physical terms. Like the bond orbitals in methane, the two sets of orbitals in ethane tend to be as far apart as possible-to be staggered. The energy required to rotate the ethane molecule about the carbon-carbon bond is called torsional energy. We speak of the relative instability of the eclipsed conformation-or any of the intermediate skew conformations-as being due to torsional strain.

As the hydrogens of ethane are replaced by other atoms or groups of atoms other factors affecting the relative stability of conformations appear: van der Waals forces. dipole-dipole interactions, hydrogen bonding. But the tendency for the bond.