Additional Reading Material

Conformational analysis of 1,2-Dichloroethane

Structures that can be interconverted by rotation about single bonds are conformers. The energy barrier for the rotation of C-C single bond in 1,2-dichloroethane molecule at room temperature in the gas phase is about 12.5 KJ/mol or 3.0 Kcal/mol. This is very similar to ethane, 12.1 KJ/mol or 2.9 Kcal/mol. The three most significant conformations for 1,2-dichloroethane are anti, gauche and eclipsed. These conformers are obtained when the C-C bond is rotated in 60 degree intervals.

In the anti conformation the two chlorine atoms appear to be facing in opposite directions. Here the dihedral angle is 180 degrees. The anti conformation is lower in energy than eclipsed by 12.1 KJ/mol. This is the value of the rotational barrier. In gaseous state at 22 degrees centigrade, 73% of 1,2-dichloroethane exists in anti form when compared to 67% for n-butane. The higher stability of anti (staggered) conformer, is because the two bulky chlorine atoms are furthest from each other. In the staggered conformation there may be some stabilizing interaction between the populated C-H σ bonding orbital on one carbon atom and the empty C-H σ* anti-bonding orbital on the neighbouring carbon. This stabilization is greatest when the two orbitals are parallel, this is present only in the anti conformation.

In the gauche conformation the two chlorine atoms are spaced apart with a dihedral angle of 60 degrees. It is more stable than the eclipsed conformation. This conformer exists in considerable quantities in the liquid state and in polar solvents. In polar solvents, the gauche conformer population increases due to decrease in the coulombic interaction of dipoles in the polar solvent. The gauche conformer with high dipole moment solvates in polar solvent, therefore its population increases. In liquid state both staggered and gauche conformers are almost equally populated.

In the eclipsed conformation, one chlorine atom in the front eclipses the rear second chlorine atom, the front and rear carbons are superimposing each other. The dihedral angle between two chlorine atoms is 0 degrees. The dihedral angle is also known as torsional angle. In this conformation, the atoms are very close to each other which results in the electrostatic repulsion between the electronic clouds of two bonded molecules. The dipole-dipole repulsions are strongest. It has the highest potential energy, hence it is the least stable conformation.