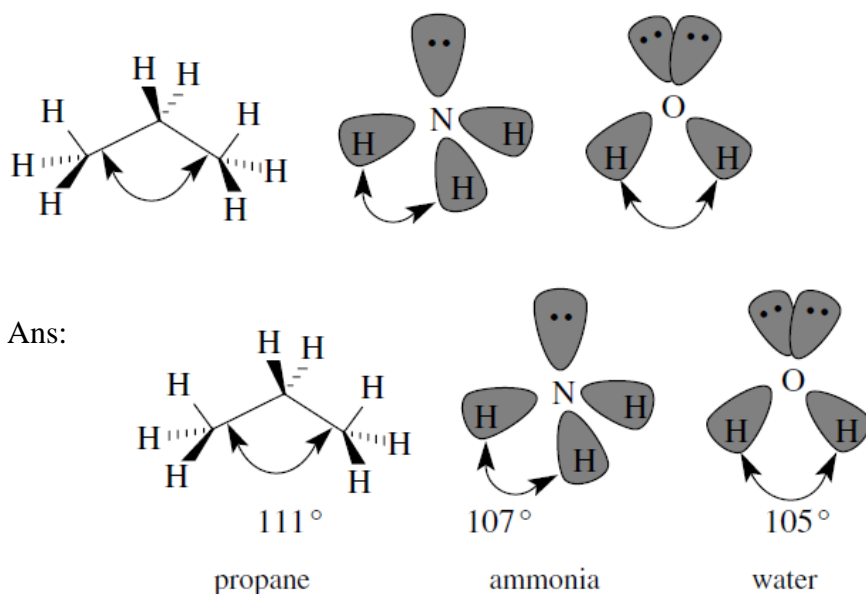


Topics covered in lecture 8 & 9 to be discussed in Tutorial 4

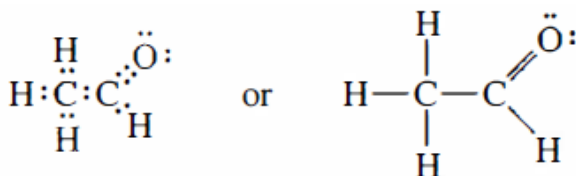
- Bonding & geometry of organic compounds
- Representation of organic molecules: Wedge-dash, Sawhorse, Newman projections
- Origin of various strains in organic molecules: Steric, torsional, angular strain
- Conformational analysis: ethane, propane, butane, Gauche effect, effect of H-bonding.
- Conformations of cyclic alkanes.
- Detailed conformational analysis of cyclohexane: Chair & boat conformations, drawing structures, axial, equatorial bonds, stability in mono and disubstituted cyclohexane and various interactions between substituents.

1. Assign the correct bond angle (as shown in the figure) for propane, ammonia and water from following values: 105° , 107° , 111° ,

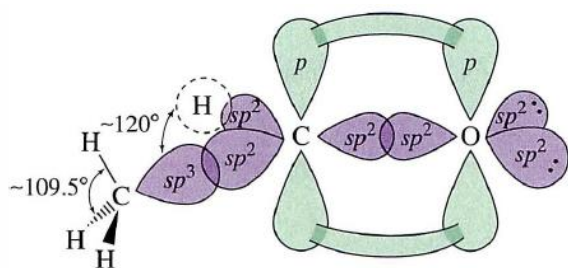


2. Predict hybridization, geometry and bond angles for the Carbon and Oxygen atoms in Acetaldehyde (CH_3CHO).

Ans. Lewis dot structure for acetaldehyde is



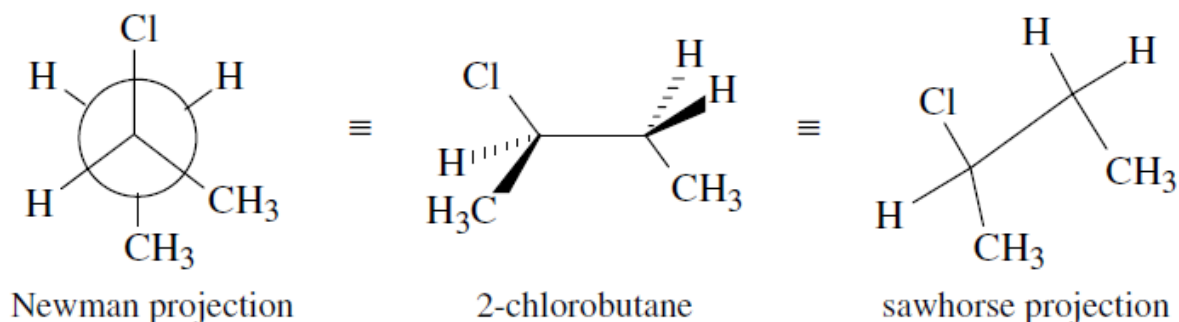
The CH_3 carbon in acetaldehyde is sp^3 hybridized, with tetrahedral bond angles of about 109° . The carbonyl ($\text{C}=\text{O}$) carbon is sp^2 hybridized, with bond



angles of about 120° . The oxygen atom is probably sp^2 hybridized.

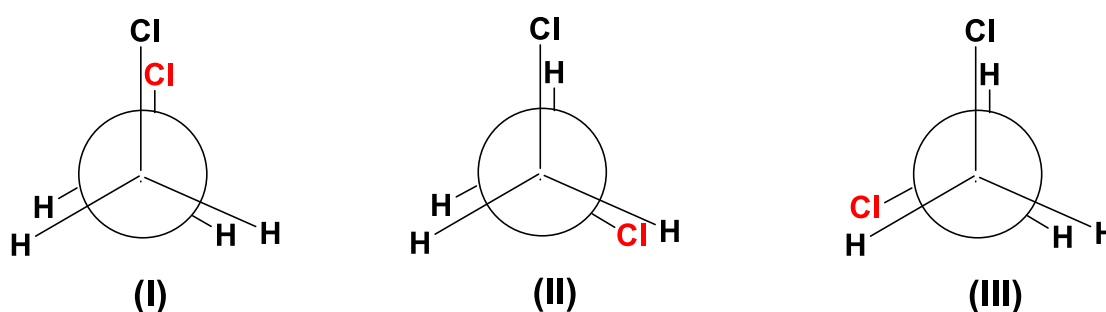
3. Draw the Sawhorse and Newman projections for 2-chlorobutane.

Ans:



4. (a) For 1,2-dichloroethane (a) draw Newman projections for all eclipsed conformations formed by rotation from 0° to 360° about the C-C bond.

Ans:

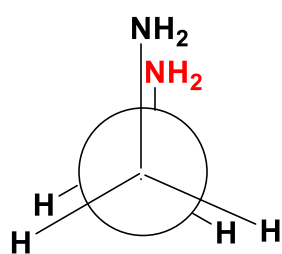


(b) Which eclipsed conformation(s) has the lowest energy? Which will have the highest energy?

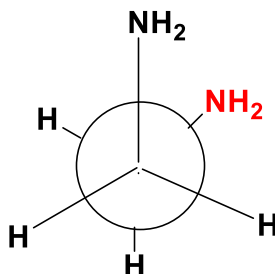
Ans: Conformation (I) will have highest energy (i.e. lowest stability) due higher torsional strain between C-Cl bonds due to stronger steric repulsion between two chloride along with dipole-dipole repulsion between them.

Conformation (II) and (III) will have lower in energy (they have same energy) as these conformations can avoid higher torsional strains as well as repulsive electronic interaction (dipole-dipole interaction) between chlorides.

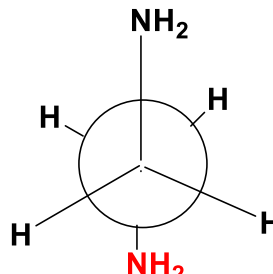
5. Draw the Newman projections for eclipsed, staggered and anti-conformations of ethylenediamine.



Eclipsed



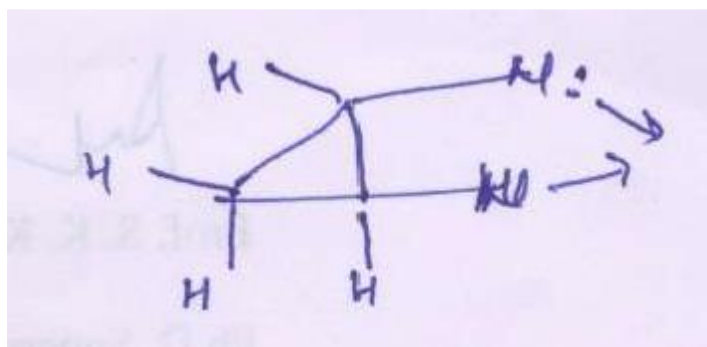
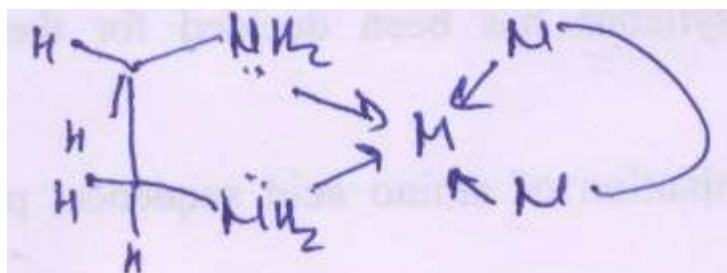
Staggered



Anti

(i) Which of these conformation will act as chelating ligand for metal ion?

Ans: Eclipsed conformation will act as chelating ligand as then only both the lone pair over N will be in same direction to form a chelated ring with metal.

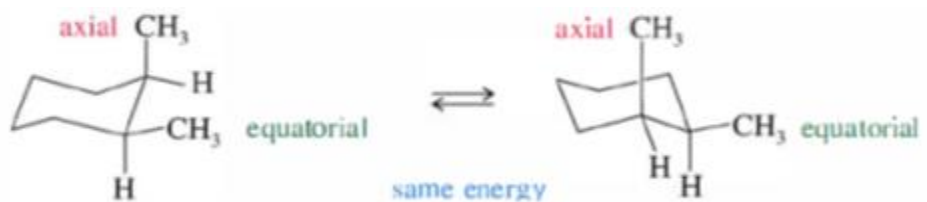


(ii) Comment on the dipole moments of these conformers.

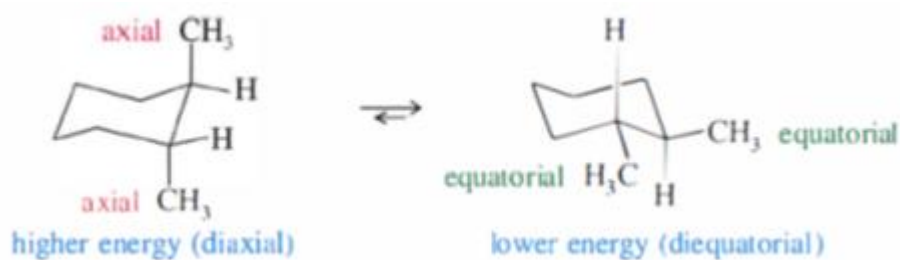
Eclipsed conformer will have highest dipole moment as both the dipole vectors are in same direction. Staggered conformation will have intermediate value (dihedral angle = 60°) between the dipole vectors. Anti-conformation will be having least value as vectors are opposing each other (dihedral angle = 180°), so resultant vector will be of least value.

6. Draw chair and boat conformations of *cis*-1,2-dimethylcyclohexane and *trans*-1,2-dimethyl cyclohexane. Predict which isomer is more stable.

Cis isomers:



Trans- isomers



The most stable isomer is *trans* di-equatorial isomer. This isomer is 7.6 kJ/mol (1.8 kcal/mol) lower in energy than either conformation of *cis*-isomers.

7. Name the following compounds

(a) *cis*-1,3-dimethylcyclohexane (b) *cis*-1,4-dimethylcyclohexane (c) *trans*-1,2-dimethylcyclohexane

