

Conformation of Cyclohexane

Cyclohexane exists in Folded form. All nuclear carbons do not lie in one plane.

1. Chair Conformation



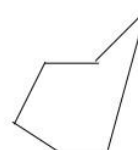
2. Boat Conformation



3. Twist Conformation or Skew Boat Conformation

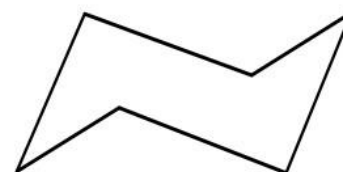


4. Half Chair Conformation



➤ Chair Conformation

- Shape : Like a Chair



- No. of Carbon atoms : 06

- All Carbon atoms : sp^3 hybridised

- Bond angle between any two bonds : $109^{\circ} 28'$

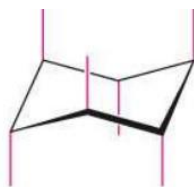
- No. of Hydrogen atoms : 12

- Two sets of Hydrogen atoms : 06 + 06

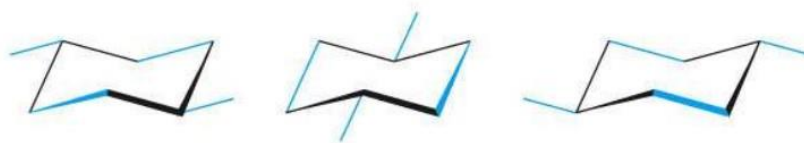
- a) Axial hydrogen atoms

- b) Equatorial hydrogen atoms

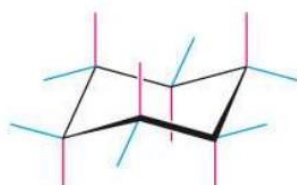
Axial bonds: The six axial bonds, one on each carbon, are parallel and alternate up-down.



Equatorial bonds: The six equatorial bonds, one on each carbon, come in three sets of two parallel lines. Each set is also parallel to two ring bonds. Equatorial bonds alternate between sides around the ring.



Completed cyclohexane

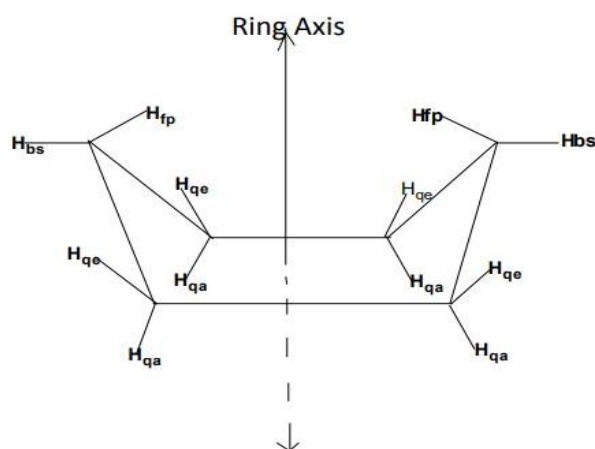


Boat Conformation of Cyclohexane

- Shape : Like a boat
- No. of Carbon atoms : 06
- All Carbon atoms : SP^3 hybridised
- Bond angle between any two bonds : $109^{\circ} 28'$
- No. of Hydrogen atoms : 12
- Four types of Hydrogen atoms : 2 + 2 + 4 + 4
 - a. Flag pole Hydrogen atoms : 2
 - b. Bow-sprit Hydrogen atoms : 2
 - c. Quasi axial Hydrogen atoms : 4
 - d. Quasi equatorial Hydrogen atoms : 4



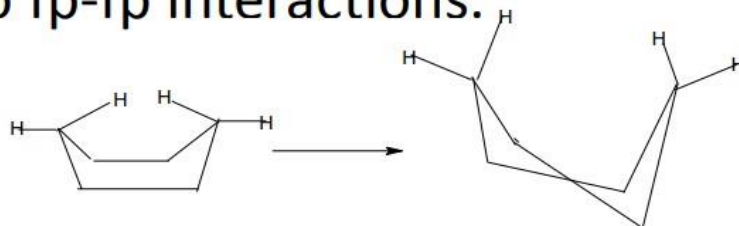
Types of Hydrogen atoms in Boat Conformation



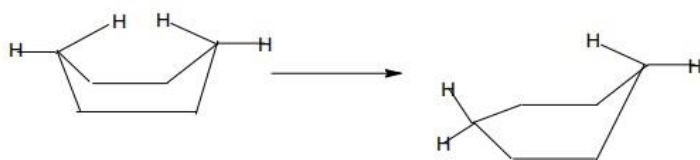
fp : Flag Pole, bs : Bow – sprit , qa : quasi axial, qe : quasi eqautorial

Twist Boat and Half Chair Conformations

- **Twist Boat** : Twisting of the boat results in release in steric strain due to fp-fp interactions.



- **Half Chair Conformation** : If C₁ or C₄ of chair conformation is brought in the average plane of the ring, the resulting conformation is known as Half chair conformation



Factors contribute to instability of conformations

1. Bond distortion strain
2. Charge repulsion strain
3. Bond opposition strain
4. Steric strain

- **Chair conformation:** Bond opposition and steric strain are minimum.

C-H bonds are perfectly staggered

∴ Bond opposition strain is minimum.

'H' atoms on adjacent carbon atoms have enough space for their accommodation.

∴ Steric strain is minimum.

Hence it is most stable.

- **Boat Conformation:** Suffers from two strains

Bond opposition strain: C-H bonds on the sides are eclipsed.

Fp – Fp interaction: Distance between two Fp Hs is 1.84 Å Distance required is 2.5 Å.

These two strains make boat conformation highly strained. Therefore boat conformation is less stable than chair conformation.

- **Twist or Skew boat Conformation:** Less torsional strain as compared to boat conformation. Flag pole H's are away from each other.

Therefore more stable boat but less stable than chair.

- **Half chair conformation:** Suffers from angle strain. It has more energy than chair conformation. Maximum energy content than any other conformation. Therefore it is least stable.

