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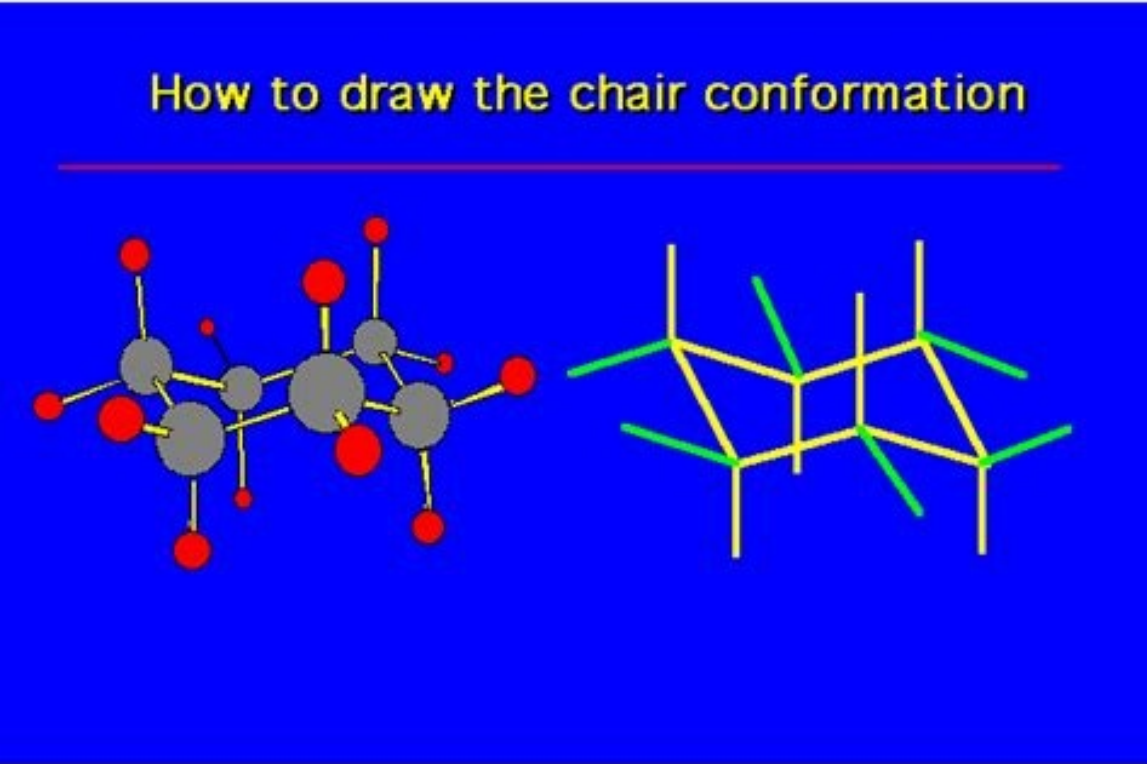
  
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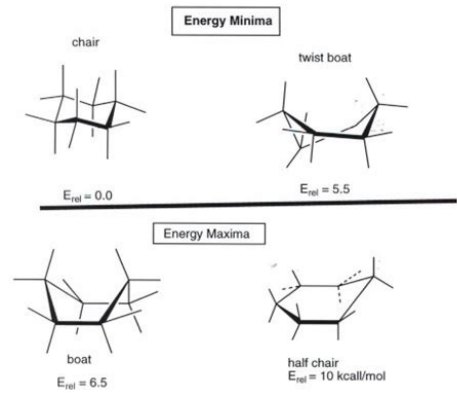
## Conformation of cyclohexane notes

**What is the chair conformation of cyclohexane. How to convert cyclohexane to chair conformation. Explain the conformation of cyclohexane. Conformation of cyclohexane stability order.**

Cyclohexane is a cycloalkane which is an alicyclic hydrocarbon. It is colorless with the molecular formula C6H6, consisting of a ring of six carbon atoms that is flammable and is considered to be a volatile liquid with a detergent-like odor, reminiscent of cleaning products.

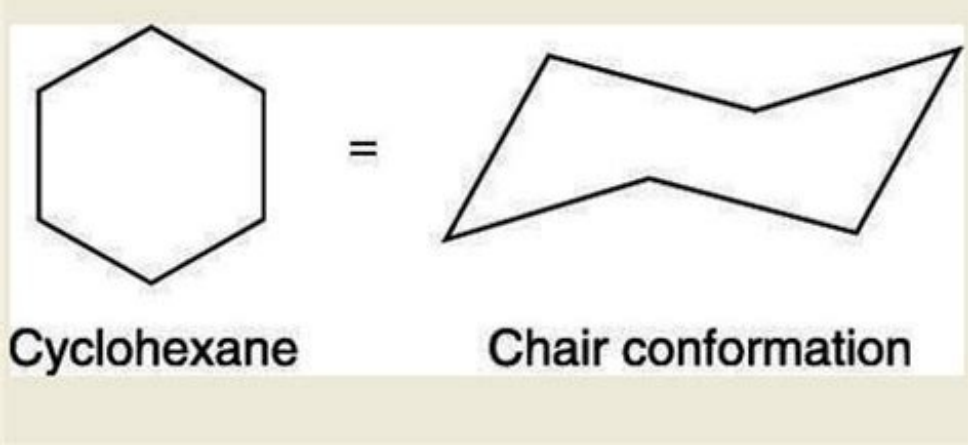


Cyclohexane has two non-planar puckered conformation and both are completely free from strain. These are called Chair Form and Boat Form because of their shape. There are so many examples of common cyclohexane conformations such as the chair form, boat form, twist boat form, and half chair conformations. The naming of the molecules is based on their own shape. Baeyer Strain Theory In 1885 Adolf Baeyer explained the relative stability of the first few cycloalkanes. He explained his theory on the fact that the normal angle between any pair of bonds of carbon atoms is 109°28'. In this theory, he has explained that any deviation of bond angles from the normal tetrahedral value would impose a condition of internal strain on the ring. And the Baeyer Strain theory is not valid for the Cyclohexane (Which is a cycloalkane). Sachse-Mohr Theory Sachse and Mohr proposed that seven rings can become free from strain if all the ring carbons are not forced into one plane, as meant by Baeyer. If a ring is assumed to have a 'puckered' or 'folded' condition, then the normal tetrahedral angles of 109°28' are retained and as a result, a strain within the ring is reduced. Cyclohexane exists as Chair Form and Boat Form because of its shape. Examination of the chair form of cyclohexane proves that the hydrogen atoms are divided into two categories. Six bonds of the hydrogen atom are found either straight up or down or almost perpendicular to the plane of the molecule. These are called Axial Hydrogen, and the other hydrogens which lie slightly above or slightly below the plane of the Cyclohexane ring, and these are known to us as Equatorial Hydrogen. The cyclohexane ring can assume many different shapes. A single cyclohexane molecule is in a continuous state of flexing or flipping into different shapes or conformations. Some of These Different Shapes are Given Below: Chair Form (more stable) Half Chair Form Twist Boat Boat Form (less stable) (Image will be Uploaded Soon) Half chair form has some angle strain and some torsional strain but the boat form has no significant angle strain and has the torsional strain. In this form hydrogen atoms are attached with the Van Der Waals forces. This interaction is known as flagpole interactions. Twist boat is twisted in nature and it has a consolation flagpole interaction. Also, it has less angle strain and less torsional strain. Mostly chair form has no angle strain and here in the chair form all C - C bonds are staggered. The conformations arise due to rotation around carbon-carbon bonds, but the chair form and the boat form are the two extreme cases. Energy Levels of the Cyclohexane Conformers are: Half Chair Form (Ring Strain=108 kcal/mol) Boat Form (Ring Strain=7.0 kcal/mol) Twist Boat (Ring Strain=5.5 kcal/mol) Chair Form (Ring Strain=0 kcal/mol) Stability of Cyclohexane Conformers is: Half Chair < Boat Form < Twist Boat Form < Chair Form. Mechanism of cyclohexane ring flip is like (Image will be Uploaded Soon) Conformation of the carbon atoms of the chair made up of cyclohexane roughly lie in one plane, and an axis can be drawn perpendicular to this plane. Each carbon atom of cyclohexane is bonded to two hydrogens. The bond to one of these hydrogen lies in the rough plane of the ring; this hydrogen is called Equatorial Hydrogen. The bond to the other hydrogen atom is parallel to the axis; this hydrogen atom is called Axial Hydrogen. Each of the six carbon atoms of cyclohexane has one equatorial and one axial hydrogen atom, we have to remember that there are six equatorial hydrogens and six axial hydrogens. In the flipping and re-flipping between conformations, the axial evolves into equatorial, while equatorial becomes axial. A methyl group is bulkier than a hydrogen atom. When the methyl group in methylcyclohexane is in the axial position, the methyl group and the m hydrogen of the ring repel each other. These interactions are called Axial-Axial Interactions. When the methyl group is in the equatorial position, the repulsions are minimum. The bulkier the group, the greater is the energy difference between equatorial and axial conformations. In other words, a cyclohexane ring with a bulky substituent (eg:- t-Butyl group) is more likely to have that group in the equatorial position. Chair conformation of cyclohexane Cyclohexane is the most stable cycloalkane. It is strain-free, meaning neither angle strains nor torsional strains apply, and it shows the same stability as chain alkanes. This special stability is due to a unique conformation it adopts. The most stable conformation of cyclohexane is called the "chair" conformation, since it somewhat resembles a chair. In the chair conformation of cyclohexane, all the carbons are at 109.5° bond angles, so no angle strain applies. The hydrogens on adjacent carbons are also arranged in a perfect staggered conformation that makes the ring free of torsional strain as well. This will be illustrated more clearly later when we learn about the Newman projection of the chair conformation. Properties of the chair conformation In the chair conformation of cyclohexane, the twelve C-H bonds can be divided into two categories based on the orientations, which are axial ("a") and equatorial ("e"). In the structure below, the six red-coloured bonds are axial, and the six blue-coloured bonds are equatorial. Axial bonds are vertical and perpendicular to the average plane of the ring, while the equatorial bonds are more "flat" and extend from the perimeter of the ring. For both "a" and "e", they can either point up (above the ring), or point down (below the ring). The trending of "a" and "e" bonds in the chair conformation can be summarized as: Each carbon has one "a" bond and one "e" bond; if one bond points up (above the ring), the other has to point down (below the ring) For the same type of bonds, the orientation up (above the ring) and down (below the ring) alternates from one carbon to the adjacent carbon, meaning if a certain carbon has a (up), then the adjacent carbon must have a (down) For the twelve C-H bonds: 3a (up), 3a (down), 3e (up), and 3e (down). How to draw the chair conformation It is important to understand and recognize all the bonds in the chair conformation, and you are also expected to be able to draw the conformation correctly and quickly. The procedure is: Draw two parallel lines of the same length that both point slightly down (if connected, they would form a parallelogram with an internal angle of about 60°/120°). Connect the right ending points of the two lines with a "V" shape so that the vertex of the V points to the upper right. Connect the left starting points of the two lines with another "V" shape so that the vertex of the V points to the bottom left. Add up all of the "a" bonds on each carbon as the vertical lines, and follow the alternating trend on adjacent carbons. Add all of the "e" bonds by following the trend in which on a certain carbon, if an "a" bond points up, then an "e" bond must point down, and vice versa. Also notice that the "e" bond is parallel to the C-C bond which is one bond away, as shown below.



The "green e" is parallel to the "green C-C bond", and the "blue e" is parallel to the "blue C-C bond". (It is more challenging to draw "e" bonds, and following the above trend makes it easier). It is highly recommended that a molecular model set is used as a study tool in this section. Assemble a cyclohexane ring with the model and become familiar with all the bonds in the chair conformation. Practice makes perfect! A lot of practice is required to become skilled in drawing and understanding the chair conformation. Ring flipping When a cyclohexane ring undergoes a chair-chair conformation conversion, this is known as ring flipping. Ring flipping comes from C-C bond rotation, but since all of the bonds are limited within the ring, the rotation can only partially occur, which leads to the ring "flipping". Cyclohexane rapidly interconverts between two stable chair conformations because of the ease of bond rotation. The energy barrier is about 45 kJ/mol, and the thermal energies of the molecules at room temperature are high enough to cause about 1 million interconversions to occur per second. For cyclohexane, the ring after flipping still appears almost identical to the original ring, but some changes happen on the C-H bonds. Specifically, all the "a" bonds become "e" bonds, and all the "e" bonds become "a" bonds; however, their relative positions in terms of the ring, up or down, remain the same. The ring flipping is shown in the equation below. Compare the carbon with the same numbering in the two structures to see what happened to the bonds due to ring flipping. Taking C #1 as an example, you will notice that the red a (up) converted to a red e (down), and the blue e (up) converted to a blue a (down) after ring flipping. Summary of ring flipping for chair conformation: This is NOT rotation, but ring flipping. The two structures are conformation isomers (or conformers). All "a" bonds become "e" bonds and all "e" bonds become "a" bonds. These two conformations are equivalent for the cyclohexane ring itself (without any substituents), with the same energy level. A molecular model is very useful for understanding ring flipping.

Newman projection of the chair conformation The chair conformation is strain-free, with all the C-H bonds in a staggered position. However, it is not easy to see the staggered conformation in the drawings we have so far, and a Newman projection helps for this purpose. To draw Newman projections for the chair conformation of cyclohexane, we also need to pick up the C-C bonds to view along, just as we did for alkanes. Since there are a total of six C-C bonds, we will pick two of them, and these two need to be parallel to each other. For the chair conformation example here, the two blue parallel C-C bonds, C1-C2 and C5-C4, are chosen for viewing. (There are 3 pairs of parallel bonds in the chair conformation, and any pair can be chosen with the resulting Newman projection looking the same). For the C1-C2 bond, C1 is the "front" carbon and C2 is the "rear" carbon.



For the C5-C4 bond, C5 is the "front" carbon and C4 is the "rear" carbon. These two bonds will be represented by two "Newman projections" we are familiar with (two circle things), and each represents two carbons, as shown below: Keep in mind that there are a total of six carbons in the ring, and the drawing above only shows four of them with C3 and C6 being left out. Additionally, the two "separated" Newman projections above are actually connected to both C3 and C6, so the overall Newman projection of the chair conformation of cyclohexane looks like this: The staggered conformation of hydrogens is clearly shown in the Newman projection here! Notes for Newman projections of the chair conformation (refer to the drawing below): The "a" or "e" bonds on four carbons (C1, C2, C4 and C5) are shown explicitly, while the bonds on C3 and C6 are just shown as CH2. The vertical red C-H bonds are the "a" bonds, and the "flat" blue C-H bonds are the "e" bonds. The dashed line in the drawing below can be regarded as the average plane of the ring. Those above the line are the bonds that point up (above the ring), and those below the line are the bonds that point down (below the ring). Other conformation of cyclohexane The chair conformation is the most stable one with the lowest energy, but it is not the only conformation for cyclohexane. During the ring flipping from one chair conformation to another, the ring goes through several other conformations, and we will only briefly discuss the boat conformation here. Figure 4.3a Boat conformation of cyclohexane The boat conformation comes from partial C-C bond rotations (only flipping one carbon up to convert the chair to a boat) of the chair conformation, and all the carbons still have 109.5° bond angles, so there are no angle strains. However, the hydrogens on the base of the boat are all in eclipsed positions, so there are torsional strains. This can be illustrated by the Newman projection below. The Newman projection is drawn by viewing along C6-C5 and C2-C3 bonds of the above boat conformation. Figure 4.3b Newman projection of boat conformation Other than that, the two hydrogen atoms on C1 and C4 are very close to each other and cause steric strain. This is also called the "flagpole" interaction of the boat conformation. The two types of strains make the boat conformation have considerably higher energy (about 30 kJ/mol) than the chair conformation.