

# Predicting the Conformational analysis of Dichloroethane using Jmol application and comparing the conformers

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## 1. Introduction

The term 'conformation' refers to any one of the infinite number of possible spatial arrangements of atoms or groups in a molecule that result from rotation of its constituent groups of atoms about (in most cases C-C) single bonds. Conformational isomerism is a form of stereoisomerism where interconversions of isomers are possible by rotations referring to single bonds. These isomers are termed as conformational isomers. Rotational energy acts as a barrier in the case of single-bond rotation. It has to be overcome to interconvert one conformer to another. The energy barrier must be small for Conformational Isomerism to occur.

Ethane is an organic chemical compound. It is a colourless and odourless gas at a standard temperature. Ethane molecule consists of seven sigma bonds. There will be a change in the shape of the molecule when there is a rotation of about six carbon-hydrogen bonds. But many possible differences occur when there is a rotation about the carbon-carbon bond..

## 2. Objectives

- ) To calculate the number of modes of vibrations in 2,2'-Dichloroethane molecule using the formula
- ) To draw the 3D structure of 2,2'-Dichloroethane molecule in Jmol interface
- ) Save the 3D structure of 2,2'-Dichloroethane molecule as .mol file
- ) Using tools in the modelkit menu to rotate bonds
- ) Script commands are used to rotate the specific bonds in a model
- ) Creating a models of anti, gauche and eclipsed conformers of 1,2-dichloroethane by rotating every 60° angle
- ) By comparing the stability of the conformers using energy profile diagram

#### 4. Drawing the 3D structure of Dichloroethane molecule in Jmol interface

- ) Open Jmol interface select the model kit menu
- ) Select carbon atom, it appears as methane molecule
- ) Select another methane molecule from model kit menu and attached to it
- ) Delete two H atom and drag to add two Cl atoms

#### 5. Energy minimization of Dichloroethane molecule in Jmol interface

- ) Exit from the model kit menu
- ) Now right click on the molecule
- ) Select the energy minimization
- ) Rotate the conformer using model kit menu

#### 6. Save the 3D structure as .mol file

- ) Click the model kit menu
- ) In the drop down list select the last option
- ) Click on the save file option
- ) Now the structure is saved in the .mol format

#### 7. Result

##### Analyzing the stability of conformers using energy level profile diagram

- ) Energy profile diagram drawn using X-axis - Torsional angle and Y-axis - Energy (kcal/mol)
- ) When the substituent's on the two carbons are directly in front of each other looking down the bond the conformation is *eclipsed*
- ) This is the highest energy conformation the molecule can adopt because every group in the front is experiencing torsional strain with the corresponding group in the back.

##### Staggered conformation

- ) When the substituents on the two carbons are the maximum distance from each other looking down the bond the conformation is *staggered*
- ) This is the lowest energy conformation the molecule can adopt because every group in the front is as far as possible from the corresponding group in the back. Because there are six groups around the C-C bond, the maximum dihedral angle is  $60^\circ$  ( $6 \times 60^\circ = 360^\circ$ ), which is the dihedral angle in this case.

### **Anti conformation**

- ) The antiperiplanar conformation (*anti*) is the staggered conformation where the two large groups are as far apart as possible.
- ) The dihedral angle between the two groups is  $180^\circ$ . There is no torsional strain and no steric strain. As a result, this is the most stable conformation.

### **Gauche Conformation**

- ) The *gauche* conformations are the staggered conformations where the two large groups are staggered close to each other.
- ) The dihedral angle between the two groups is  $60^\circ$ . There is a very small amount of steric strain and no torsional strain. As a result, these are the second most stable conformations.

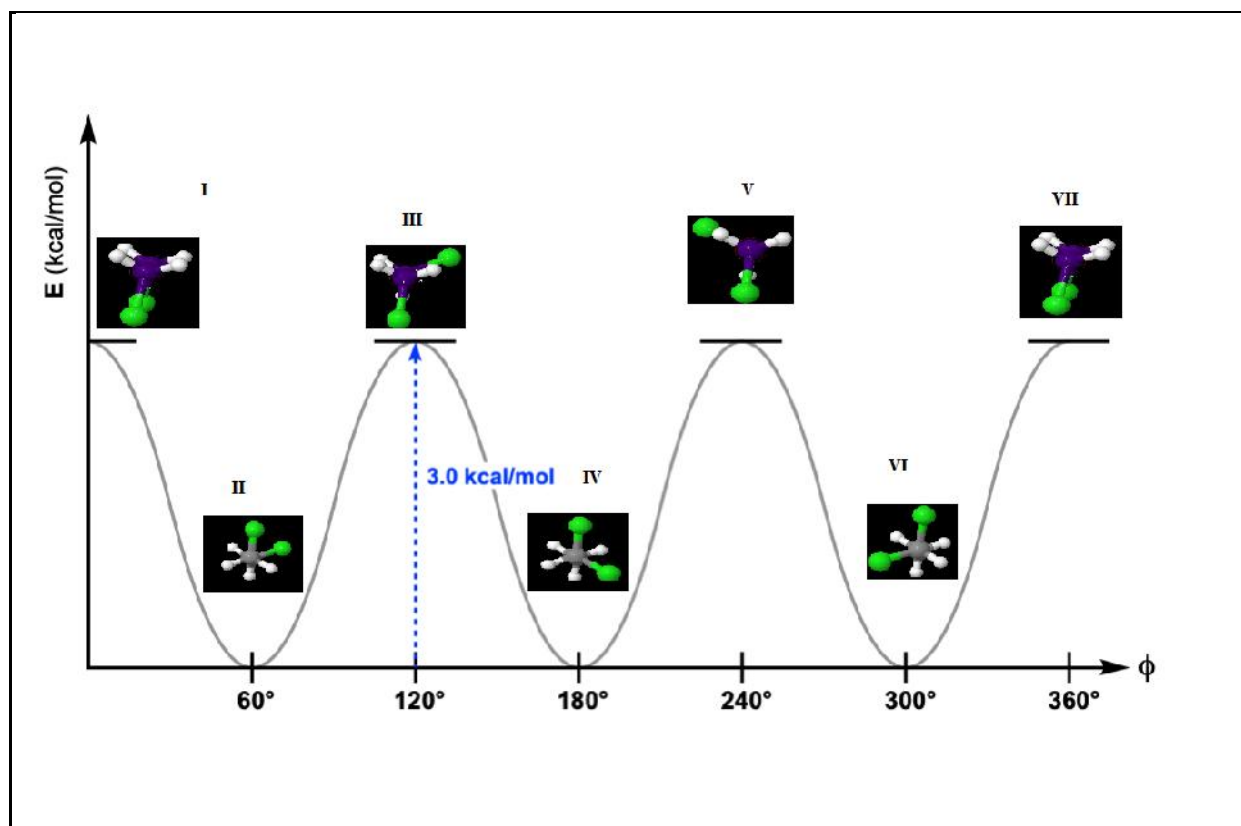
### **Partially eclipsed conformation**

- ) The “partially eclipsed” conformations are the eclipsed conformations where the two large groups are eclipsing the small groups. The dihedral angle between the two groups is  $120^\circ$  and these are the second least stable conformations.


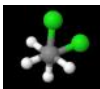
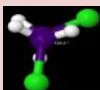
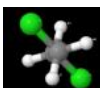

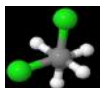

### **Fully eclipsed conformation**

- ) The “fully eclipsed” conformation is the eclipsed conformation where the two large groups are eclipsing each other.
- ) The dihedral angle between the two groups is  $0^\circ$ . There is torsional strain and steric strain. As a result, this is the least stable conformation.
- ) As the C-C bond is rotated the molecule transitions between staggered and eclipsed conformations. Since the different conformations experience different types and amounts of strain, they have different energy levels.
- ) The diagram shows that the first and last conformations are identical, with the bond having been rotated a full  $360^\circ$ .

8. Energy profile diagram for conformers



## Conformational analysis of Dichloroethane

S. No	Angle of rotation	Name of the conformer	Structure of conformer
I	0°	Fully eclipsed	
II	60°	Staggered (Gauch)	
III	120°	Partially eclipsed	
IV	180°	Staggered (Anti)	
V	240°	Partially eclipsed	
VI	300°	Staggered (Gauch)	
VII	360°	Fully eclipsed	

## Conclusion

Staggered conformation of ethane is most stable, while eclipsed conformation is least stable. Staggered form has the least torsional strain and the eclipsed form has the maximum torsional strain.

The Order of stability of these conformations is anti gauche partially eclipsed fully eclipsed.

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