

# Visualizing the mechanism of Unimolecular Nucleophilic Substitution Reaction of alkyl halide Molecule using Jmol

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## 1. Introduction

The term "nucleophilic substitution reaction" refers to a type of organic reaction in which one nucleophile substitutes another. It is quite similar to the typical displacement reactions seen in chemistry, in which a more reactive element replaces a less reactive element in its salt solution. The group that takes an electron pair and is displaced from carbon is known as the "leaving group," and the molecule on which substitution occurs is known as the "substrate." The leaving group is either a neutral molecule or an anion.

### 1.1 Unimolecular Nucleophilic Substitution Reaction

The unimolecular nucleophilic substitution ( $S_N1$ ) reaction mechanism proceeds in two steps. In the first step, the bond between the carbon atom and the leaving group breaks to produce a carbocation intermediate, an anionic leaving. In the second step, the carbocation reacts with the nucleophile to form the substitution product. The formation of a carbocation is the slow and rate determining step. The formation of a bond between the nucleophile and the carbocation occurs rapidly in the second step. The rate determining step involves only the substrate, the reaction is unimolecular. The rate of the reaction of the first step signifies the energy of activation required to form the carbocation intermediate. The rates of ( $S_N1$ ) reaction are determined by the stability of carbocation which is in the order  $3^\circ > 2^\circ > 1^\circ$ .



## 2. Objectives

- To draw the 3D structure of 2-Chloro 2-Methyl Propane molecule in Jmol interface
- Save the 3D structure of 2-Chloro 2-Methyl Propane molecule as .mol file
- To draw the 3D structure of planar carbocation intermediate in Jmol interface

- Save the 3D structure of planar carbocation intermediate as .mol file
- To draw the 3D structure of 2-Methyl Propane-2-ol molecule in Jmol interface
- Save the 3D structure of 2-Methyl Propane-2-ol molecule as .mol file
- Comparing the molecular electrostatic potential surfaces obtained using Jmol interface
- Importing the .mol file to the Energy Profile Diagram of  $S_N1$

### **3. Drawing the 3D structure of 2-Chloro 2-Methyl Propane molecule in Jmol interface**

- Open Jmol interface select the model kit menu
- Select carbon atom, it appears as methane molecule
- Click on H atom, it appears as ethane molecule
- Click on H atom, it appears propane
- Delete the H atom on second carbon, click on C atom, it appears isopropane
- Delete the H atom on second carbon, click on Cl atom, it appears 2-Chloro-2-Methyl Propane.

#### **4.1 Energy optimization of generated molecules in Jmol interface**

- Exit from the model kit menu
- Now right click on the molecule
- Select the option computation
- Then click optimize structure

### **4. Drawing the 3D structure of 2-Chloro-Propane-2-ol molecule in Jmol interface**

- Open Jmol interface select the model kit menu
- Select carbon atom, it appears as methane molecule
- Click on H atom, it appears as ethane molecule
- Click on H atom, it appears propane
- Delete the H atom on second carbon, click on C atom, it appears isopropane
- Delete the H atom on second carbon, click on O atom, it appears 2-Chloro-Propane -2-ol.
- Energy optimization of molecule (refer 4.1)

### **5. Getting the 3D structure of hydroxide ion from Get MOL in Jmol interface**

- Open Jmol interface select the file menu
- Click on Get MOL option from file menu, type hydroxide ion in the dialogue box
- Click ok, it appears hydroxide ion

## **4.2 Energy optimization of generated molecules in Jmol interface**

- Exit from the model kit menu
- Now right click on the molecule
- Select the option computation
- Then click optimize structure

## **4.3 Molecular electrostatic potential surface modification in Jmol interface**

- Exit from the model kit menu
- Now right click on the molecule
- Select the option surfaces
- Then click molecular electrostatic potential (range -0.1 0.1)

## **4.4 Save the 3D structure as .mol file**

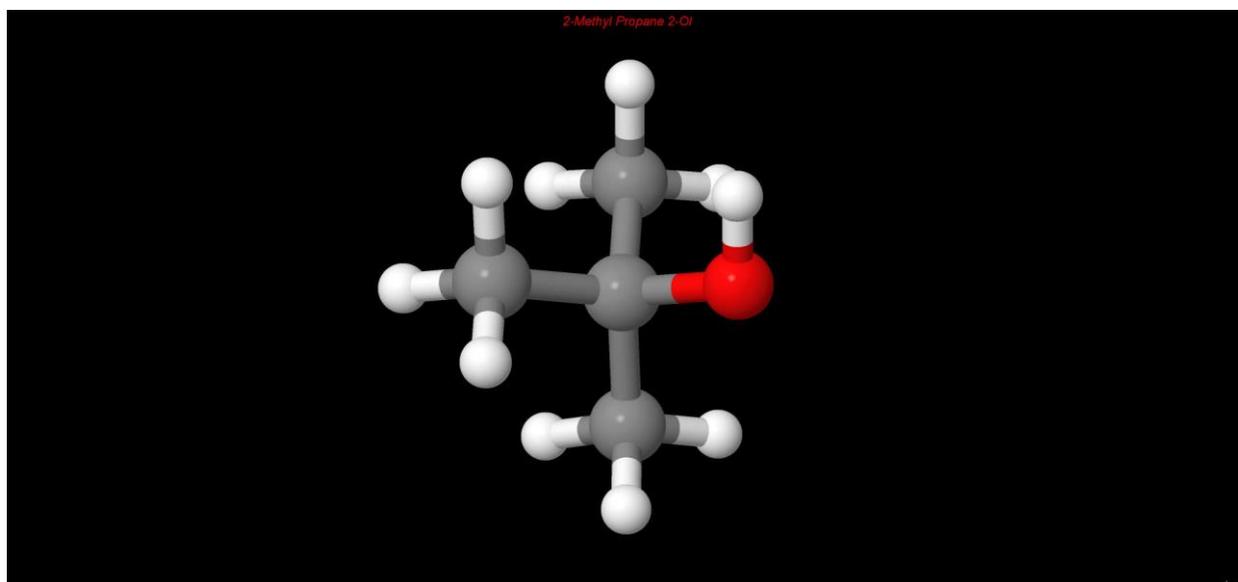
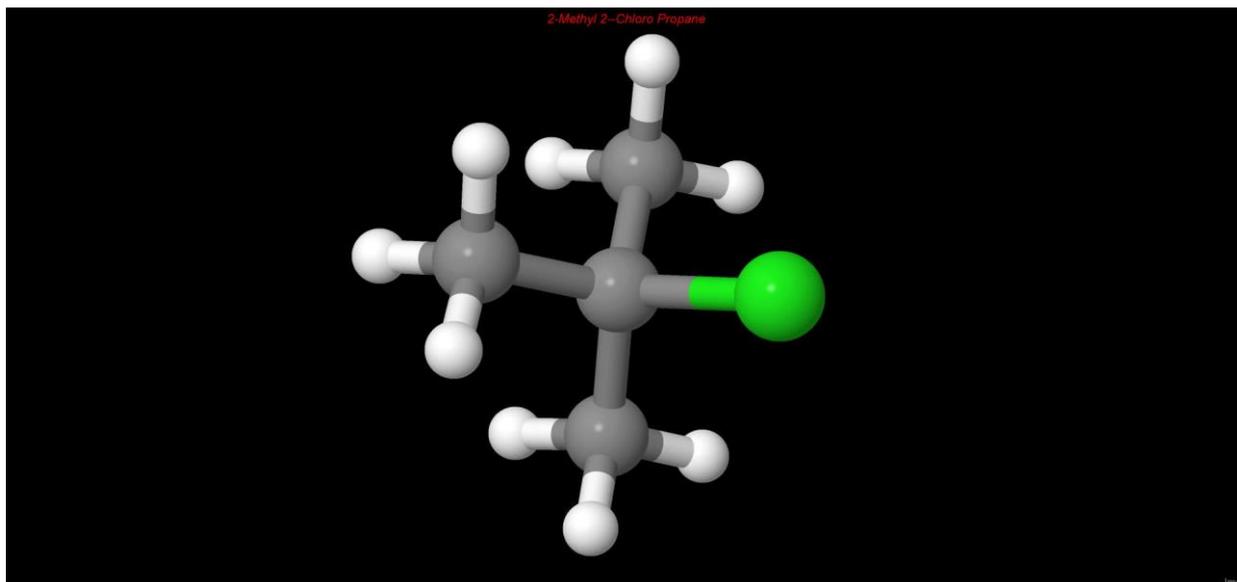
- Click the model kit menu
- In the drop down list select the last option
- Click on the save file option
- Now the structure is saved in the .mol format

## **6. Importing the .mol file to the Energy profile diagram**

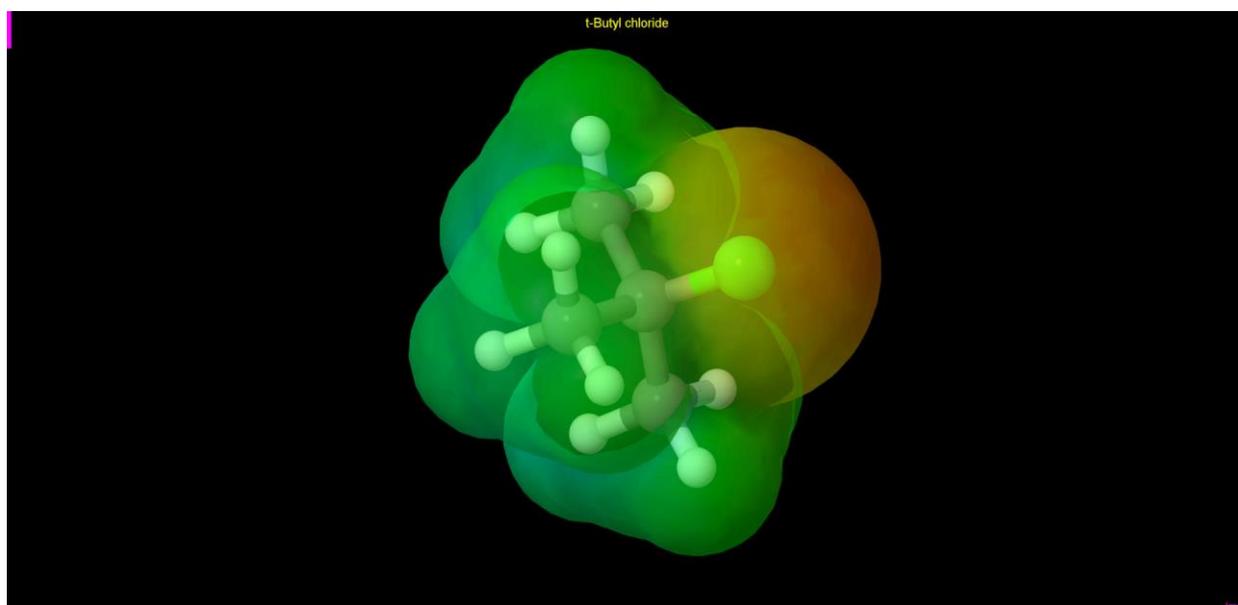
- Open the paint
- Draw the energy profile diagram
- Click on File menu-import molecule-select file type as mol
- Choose the .mol file saved already in the laptop/desktop
- Now the .mol file will be imported

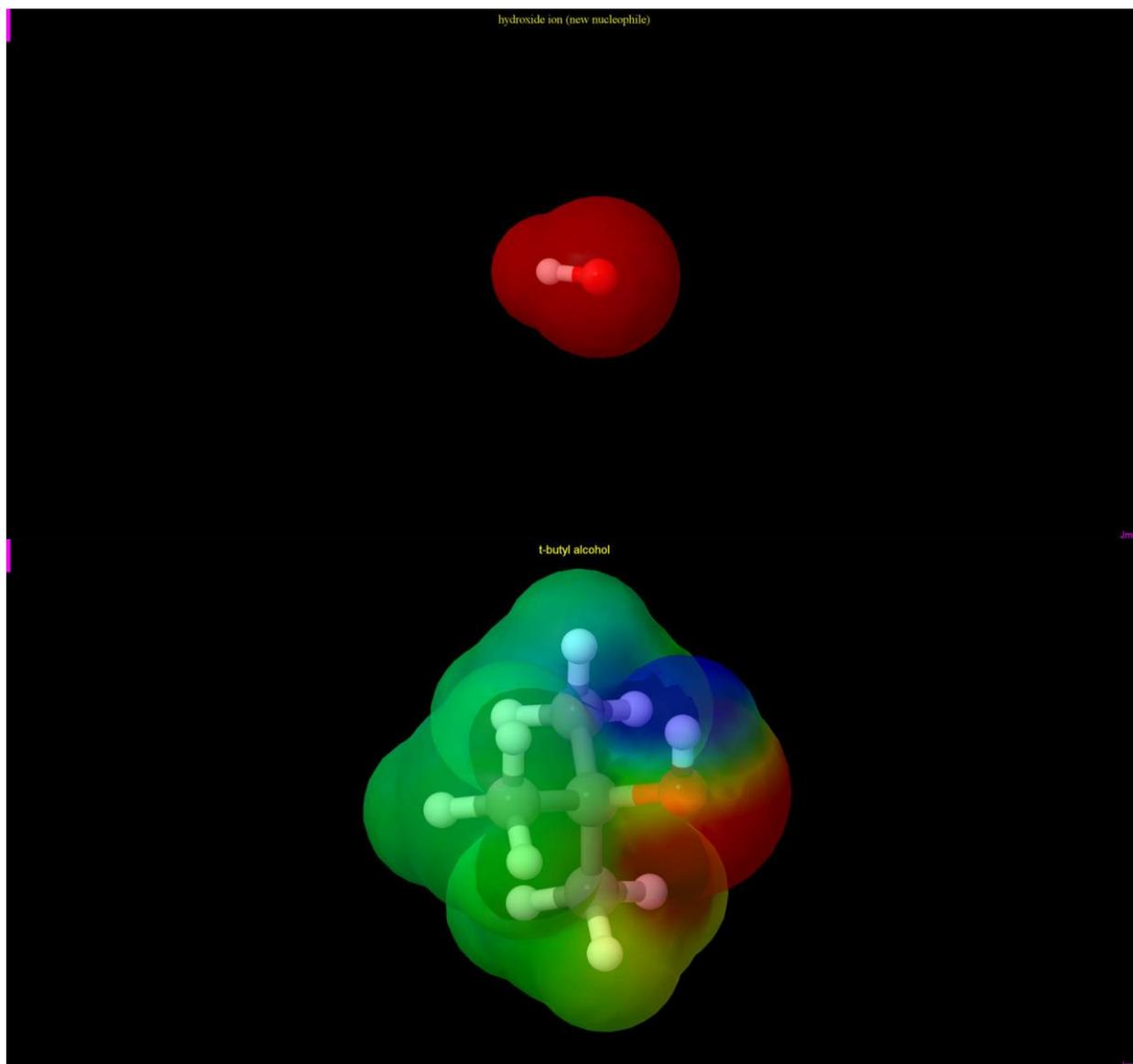
## **7. Comparing the .mol file to the Energy profile diagram**

- Open the paint
- Draw the energy profile diagram
- Click on File menu-import molecule-select file type as mol
- Choose the .mol file saved already in the laptop/desktop
- Now the .mol file will be imported

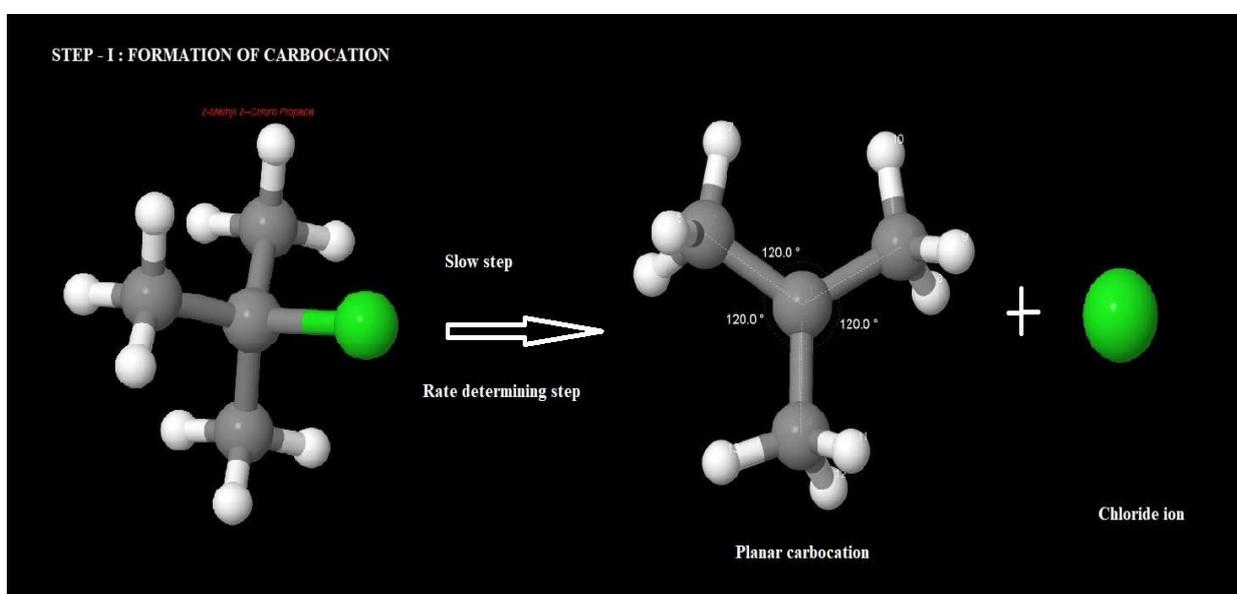


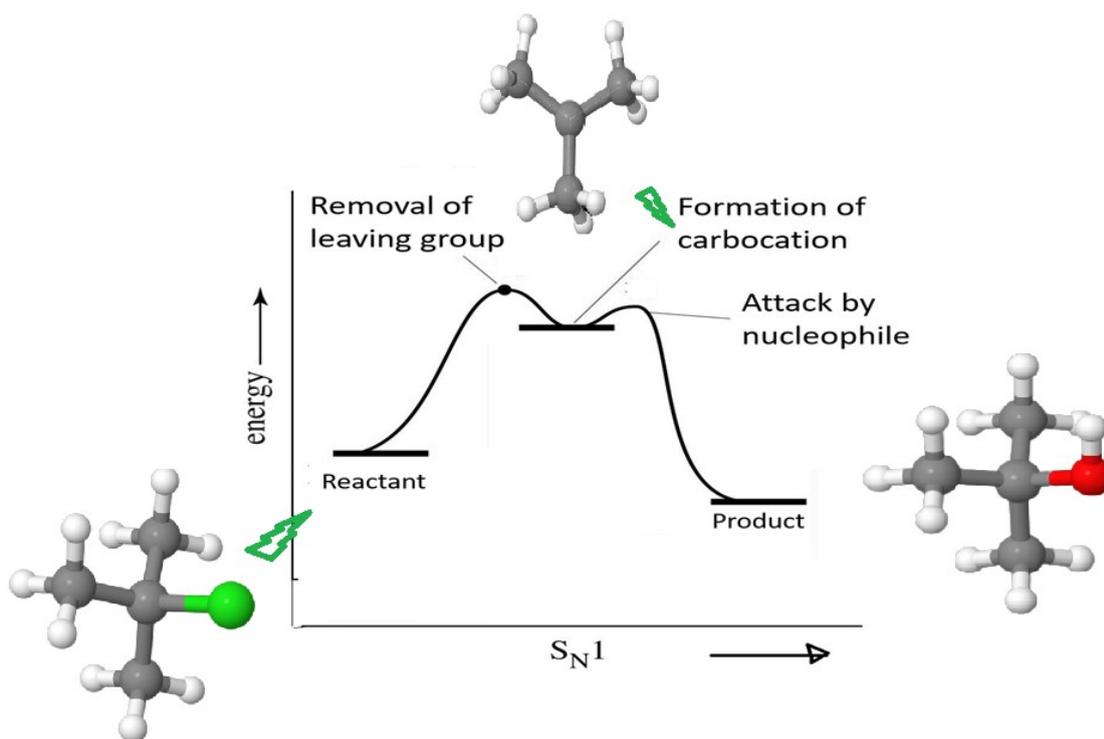
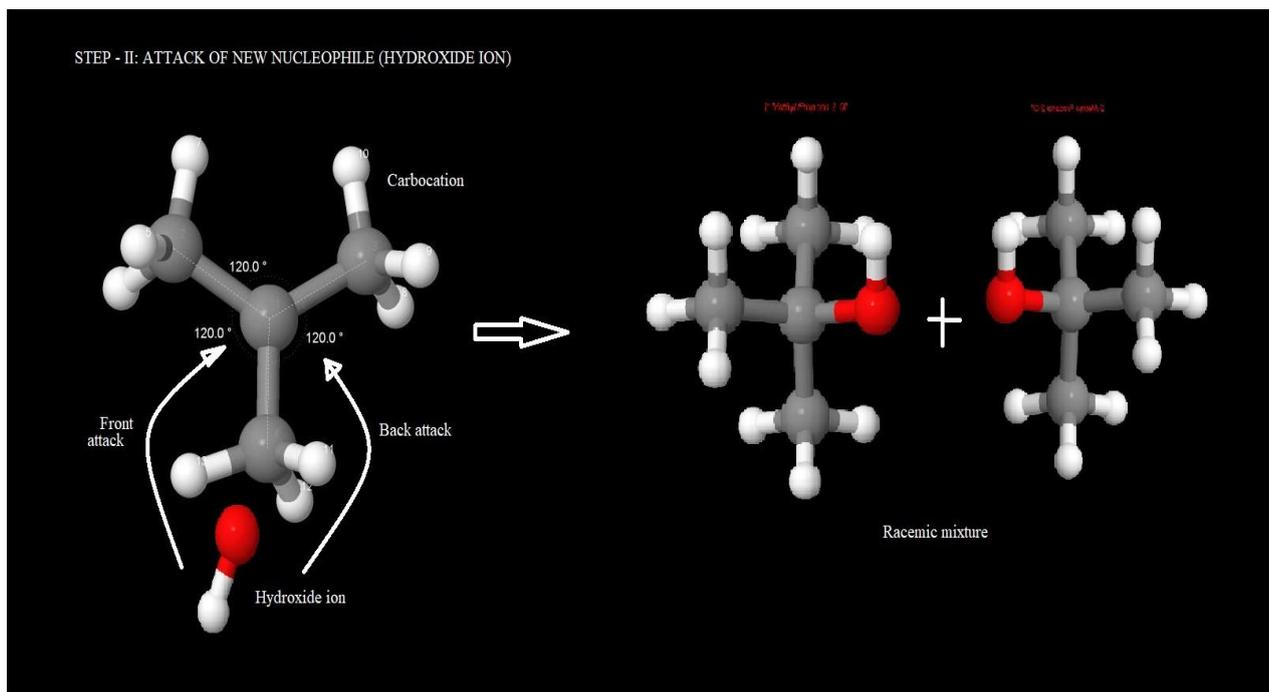
## SURFACES





## REACTION MECHANISM





**Energy profile diagram of unimolecular nucleophilic substitution reaction**

## **Acknowledgement**

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