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

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Abstract

This work aims at visualizing the possible unimoleculecular nucleophilic substitution reaction mechanism of 2-Chloro 2-Methyl Propane molecule. The 3D structure of 2-Chloro 2-Methyl Propane molecule was drawn in the Jmol interface and energy minimization, molecular electrostatic potential surfaces modifications were done. The energy minimized 3D structure of 2-Chloro 2-Methyl Propane molecule was saved as. mol file. This. mol file was given as the source file for identifying the electron rich center where the nucleophilic substitution will occur. The.mol images are incorporated in the energy profile diagram to learn the formation of carbocation intermediate in the first step. Also, the nucleophilic attack of hydroxide ion on t-butyl carbocation intermediate to produce t-butyl alcohol.

Keyword

unimoleculecular nucleophilic substitution, Jmol, t-butyl alcohol