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

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Abstract

This work aims at predicting the conformational analysis of 1,2-Dichloroethane using Jmol and comparing the conformers. The 3D structure of 1,2-Dichloroethane molecule was drawn in the Jmol interface and energy minimization was done. The energy minimized 3D structure of 1,2-Dichloroethane molecule was saved as .mol file. This mol file was given as the source file and rotate this conformer by every 60° angle by model kit menu. By comparing the stability of the conformers using energy profile diagram and indicated that staggered conformation has the least torsional strain and minimum energy. Consequently, staggered conformation is more stable than eclipsed conformation on the basis of energy levels.

Keyword
Conformational analysis, 2-Chloroethane, Jmol, Energy profile, Torsional strain