Nonempirical Quantum-Chemical Calculations of the Structure and Conformations of the 2,2-Dichloroethanal Molecule in the Lowest Excited Singlet State

V. A. Bataev, A. V. Kudich, A. V. Abramenkov, and I. A. Godunov

Moscow State University, Moscow, Russia

Received September 26, 2000

Abstract—The structure of the 2,2-dichloroethanal molecule ($CHCl_2CHO$) in the lowest excited singlet state was calculated by the nonempirical multiconfigurational self-consistent field method. The electron transition of $CHCl_2CHO$ from the ground to lowest excited singlet state is accompanied by rotation of the $CHCl_2$ group, and the carbonyl fragment becomes nonplanar. The potential energy surface for the excited $CHCl_2CHO$ molecule contains six minima corresponding to three pairs of enantiomers. This surface was used to solve torsion and inversion motion problems in the one-dimensional approximation and also two-dimensional torsion–inversion problem. Comparison of the results showed a relation between torsion and inversion motions.