Conformations of Pyrrolidinium Ion Studied by Molecular Orbital Calculations

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Ab initio HF/6-31G(d, p) and density functional theory B3LYP/6-31G(d, p) calculations were carried out to investigate the conformations of pyrrolidinium ion. Two conformations, corresponding to twisted (C2) and envelope (Cs) forms were optimized. Vibrational analysis showed that the twisted form is at a local minimum point and the envelope form at a saddle point. The energy difference between the conformations is ca. 2 kJ mol^{-1}.

Key words: Pyrrolidinium Ion; Conformation; HF; DFT.