Conformational analysis and vibrational assignments of 2,2,3,3-tetrafluoro-1-propanol CHF2CF2CH2OH as three-rotors system. Badawi Hassan M; Forner Wolfgang
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Abstract

The conformational stability of 2,2,3,3-tetrafluoro-1-propanol was investigated by DFT-B3LYP/6-311+G** and ab initio MP2/6-311+G** calculations. The calculated potential energy curves of the molecule at DFT-B3LYP level were consistent with five distinct minima that correspond to gauche(-)-gauche-gauche (G1gg), trans-trans-gauche (Ttg), trans-gauche-gauche (Tgg), trans-gauche-gauche(-) (Tgg1) and gauche(-)-gauche-trans (G1gt) conformers in the order of decreasing relative stability. The equilibrium constants for the conformational interconversion of 2,2,3,3-tetrafluoro-1-propanol were calculated and found to correspond to an equilibrium mixture of about 38% G1gg, 28% Ttg, 13% Tgg, 11% Tggt and 10% G1gt conformations at 298.15K. The vibrational frequencies of 2,2,3,3,-tetrafluoro-1-propanol in its five stable forms were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calculations and comparison with experimental data of the molecule.