Conformational and Vibrational Analysis of 2,4-, 2,5- and 2,6-Difluorobenzaldehydes by ab initio Hartree-Fock and Density Functional Theory Calculations

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Z. Naturforsch. **63a,** 175 – 182 (2008); received August 10, 2007

The optimized molecular structures, vibrational frequencies and corresponding vibrational assignments of the two planar O-*cis* and O-*trans* rotomers of 2,4-, 2,5- and 2,6-difluorobenzaldehyde have been calculated using ab initio Hartree-Fock (HF) and density functional theory (B3LYP) methods with the 6-311++G(d,p) basis set level. The calculations were adapted to the C_S symmetries of all the molecules. The O-*trans* rotomers with lower energy of all the compounds have been found as preferential rotomers in the ground state. The mean vibrational deviations between the vibrational frequency values of the two conformers of all the compounds have been shown to increase while the relative energies increase, and so it has been concluded that the higher the relative energy between the two conformers the bigger is the mean vibrational deviation.

Key words: Difluorobenzaldehydes; Conformers; Vibrations; IR Spectra; Raman Spectra; HF; DFT.