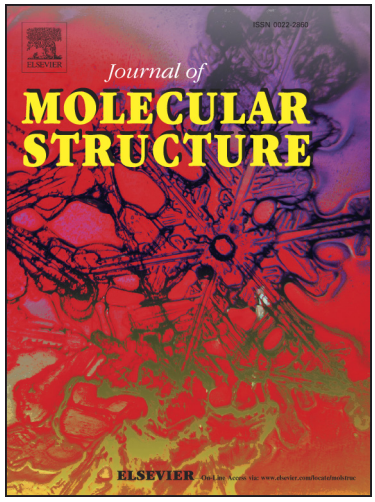

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Investigation of intermolecular hydrogen bonding in 2, 3, 4, 5, 6 Pentafluorobenzoic acid through molecular structure and vibrational analysis - A DFT Approach

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Abstract

The density functional theory (DFT) and Hatree-Fock (HF) method was performed at 6–311++G** level to derive the equilibrium geometry, vibrational wavenumbers, infrared intensities and Raman scattering activities of 2,3,4,5,6 pentafluorobenzoic acid molecule (PFBA). The conformer study of the monomer PFBA was also undertaken. The possibility of intermolecular hydrogen bonding and the dimeric form of the molecule was predicted using vibrational analysis of the monomer. The effects of molecular association through O–H· · O hydrogen bonding have been described in the dimer structure using geometrical structure analysis, Natural bond orbital analysis (NBO), Molecular electrostatic potential (MEP) maps and Mulliken charge analysis.

Keywords: Pentafluorobenzoic acid, DFT, vibrational analysis, intermolecular hydrogen bonding

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