CONFORMATIONAL ANALYSIS OF 3,4,5-TRIFLUOROBENZOIC ACID AND PROTON TUNNELING IN THE COMPLEX OF 3,4,5-TRIFLUOROBENZOIC ACID AND FORMIC ACID

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The potential energy surfaces of the 3,4,5-trifluorobenzoic acid monomer were scanned along C-C-C=O and O=C-O-H dihedral angles at the B3LYP/6-311G level to analyze its conformational landscape. Two conformations were identified and reoptimized at the B3LYP/aug-cc-pVTZ and MP2/aug-cc-pVTZ levels. The geometries of the relevant conformers are rationalized regarding the interactions between the carboxylic group and the substituted fluorine atoms. Only the planar global minimum conformation of the monomer was observed experimentally. The rotational spectra were recorded using a chirped pulse Fourier transform spectrometer in the frequency range of 6 – 12.5 GHz and analyzed for both the monomer and its complex with formic acid. The spectra of the parent, seven ^{13}C, and one deuterium singly substituted isotopologues of the monomer were analyzed and fitted to measurement accuracy for a semi-rigid asymmetric top molecule. Theoretical and spectroscopic studies were performed on the complex formed by 3,4,5-trifluorobenzoic acid and formic acid, which undergoes double proton transfer. Proton tunneling is a widely studied phenomenon that is present in various biological and chemical processes. The rotational constants, centrifugal distortion constants, and tunneling energy difference were determined for the 3,4,5-trifluorobenzoic acid and formic acid complex. The complex prefers a co-planar structure. The tunneling splittings are due to the concerted proton transfer of the two carboxylic hydrogens. The proton tunneling process in this complex will be compared to related complexes. The agreement between the calculated and experimental parameters is very good for both the monomer and the complex.