CONFORMATIONAL LANDSCAPES OF 2-FUROIC ACID MONOMERS AND DIMERS BY ROTATIONAL SPECTROSCOPY AND DFT CALCULATIONS

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2-furoic acid (FA), a heterocyclic carboxylic acid, is a significant precursor of esters, acrylic chloride, and acid anhydride, and is often used for medical purpose, for example in an orally active antidiabetic vanadyl complex.1 FA monomer may exist in a number of possible conformations based on the orientation of the COOH group with the ring O atom and on the relative orientation of the C=O and OH in the COOH group. Some of these possible conformations were investigated before.2 In this work, we studied conformational landscapes of the FA monomer and dimer by using a chirped pulse Fourier transform microwave (FTMW) spectrometer and DFT calculations. Conformational searches were performed to identify possible conformations using a conformer-rotamer ensemble sampling tool (CREST).3 The resulting candidates were further optimized at the B3LYP-D3(BJ)/def2-TZVP level of theory. Three FA conformers and four (FA)2 conformers 2-furoic acid dimers were predicted. Experimentally, rotational spectra of three monomeric conformers and two binary conformers were assigned. Two other FA dimers predicted have zero electric dipole moments. Detailed analyses of the double proton tunneling motion and conformational conversion barriers will also be presented.

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