

# THE COMPLICATED CONFORMATIONAL LANDSCAPES OF TETRAHYDRO-2-FUROIC DIMER AND MONOHYDRATE: BROADBAND ROTATIONAL SPECTRA AND COMPREHENSIVE CONFORMATIONAL SEARCHES

FAN XIE, NATHAN A. SEIFERT, MATTHIAS HEGER, WOLFGANG JÄGER, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada.*

Tetrahydro-2-furoic acid (THFA), a chiral carboxylic acid which is often used as a precursor in syntheses of pharmaceuticals, exhibits a complex conformational landscape in its monomeric form.<sup>1</sup> Detailed analyses of its conformational distribution and conversion barriers using rotational spectroscopy and theoretical modeling were reported recently.<sup>1</sup> In the current study, we focus on investigating how intermolecular interactions with water and THFA itself influence the aforementioned conformational preference. A large number of initial conformational geometries were generated using a semiempirical tight-binding (TB) quantum chemistry code, GFN-xTB, designed for prediction of equilibrium structural properties, such as geometries, vibrational frequencies, and non-covalent interactions.<sup>2</sup> The final geometry optimizations were carried out at the B3LYP-D3(BJ)/def2-TZVP, B3LYP-D3(BJ)/6-311++G(2d,p), and MP2/6-311G++(2d,p) levels of theory. Very interestingly, in the THFA monohydrate, the two monohydrates observed contain the most stable THFA monomeric conformer and are ranked the ninth and tenth in terms of their relative energy ordering. On the other hand, the THFA dimer observed contains the third most stable monomeric conformers. We interpret the observed phenomena in terms of the conformational conversion barriers and conformational cooling effects.