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Intermolecular Hydrogen Bonding Effect on the VA and VCD Spectra of Lactic Acid in Water and in Methanol: Experimental and DFT Studies MARTIN LOSADA, HA TRAN, YUNJIE XU, University of Alberta — Understanding the structure, stability and formation of intermolecular H-bonded complexes involving chiral molecules on the molecular level is of crucial importance in life sciences. Carboxilic acids are well known for their strong intermolecular associations. Lactic acid (LA) is studied using vibrational absorption (VA) and vibrational circular dichroism (VCD) spectroscopic techniques to examine the effect of dimerization. Experimental results indicate that for LA in $CDCl_3$ solution, a complex equilibrium exists between the monomers and dimers. Furthermore, VCD spectroscopy was used to probe the solute-solute and solute-solvent H-bonding interactions of LA-water and LA-methanol complexes in solution phase. Geometry optimizations were carried out for LA monomer, LA dimer and both LA-$(H_2O)_n$ and LA-$(CH_3OH)_n$ complexes, with $n = 1, 2, 3$, using both B3PW91/6-311++G(d,p) and B3LYP/6-311++G(d,p) levels of theory. Some of these clusters were also investigated at the B3LYP/cc-pVTZ level. Detailed spectral simulations were performed in order to understand the dependence of the VA and VCD spectra on the specific binding characters. Three solvent models were exploited to evaluate solvent effects; a pure implicit continuum approach, a pure explicit model with up to three solvent molecules, and a combined approach.

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