THE CHIRPED-PULSE AND CAVITY BASED FTMW SPECTROSCOPY OF THE METHYL LACTATE-WATER AND METHYL LACTATE-DEUTERIUM OXIDE DIMERS

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The delicate competition between the inter- and intramolecular hydrogen-bonding in the complex consisting of a chiral alpha-hydroxy ester, methyl lactate, and water, has been studied using rotational spectroscopy and high level ab initio calculations. Extensive ab initio calculations have been performed to locate all possible low energy conformers of the methyl lactate-water contact pair and *five* lowest energy conformers have been identified. The most stable conformer forms a seven membered ring with two intermolecular hydrogen bonds: one between the alcoholic hydroxy group of methyl lactate and the oxygen of the water molecule and the other between the hydrogen of water and the oxygen of the carbonyl group. Broadband scans for the rotational spectra of these conformers have been carried out using a newly built chirped-pulse FTMW instrument and the final frequency measurements with a cavity based FTMW instrument. Spectral assignments have been made for the lowest energy conformer of methyl lactate-H_2O and D_2O. The hyperfine splitting and the source of the splitting will be discussed.