TOWARDS SOLVATION OF A CHIRAL ALPHA-HYDROXY ESTER: BROADBAND CHIRP AND NARROW BAND CAVITY FOUIRIER TRANSFORM MICROWAVE SPECTROSCOPY OF METHYL LACTATE-WATER CLUSTERS

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Methyl lactate (ML), a chiral alpha-hydroxy ester, has attracted much attention as a prototype system in studies of chirality transfer,[1] solvation effects on chiroptical signatures,[2] and chirality recognition.[3] It has multiple functional groups which can serve both as a hydrogen donor and acceptor. By applying rotational spectroscopy and high level ab initio calculations, we examine the delicate competition between inter- and intramolecular hydrogen-bonding in the ML-water clusters. Broadband rotational spectra obtained with a chirp Fourier transform microwave (FTMW) spectrometer, reveal that the insertion conformations are the most favourable ones in the binary and ternary solvated complexes. In the insertion conformations, the water molecule(s) inserts itself (themselves) into the existing intramolecular hydrogen-bonded ring formed between the alcoholic hydroxyl group and the oxygen of the carbonyl group of ML. The final frequency measurements have been carried out using a cavity based FTMW instrument where internal rotation splittings due to the ester methyl group have also been detected. A number of insertion conformers with subtle structural differences for both the binary and ternary complexes have been identified theoretically. The interconversion dynamics of these conformers and the identification of the most favorable conformers will be discussed.

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