CHIRPED-PULSE AND CAVITY BASED FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF THE METHYL LACTATE-AMMONIA ADDUCT

JAVIX THOMAS, OLEKSANDR SUKHORUKOV, WOLFGANG JAEGER and YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Canada*.

The hydrogen bonded complex of ammonia with methyl lactate, a chiral alpha-hydroxyester, has been studied using rotational spectroscopy and high level ab initio calculations. Previous studies showed that methyl lactate can exist in a number of conformers. However, only the most stable one which has an intramolecular hydrogen bonded ring formed with its alcoholic hydroxyl and its carbonyl oxygen atom was detected experimentally An extensive ab initio search has been performed to locate all possible low energy conformers of the methyl lactate-ammonia contact pair. Five lowest energy conformers have been identified at the MP2/6-311++G(d,p) level. The lowest energy conformer favors an insertion arrangement, where ammonia is inserted into the existing intramolecular hydrogen bonded ring in the most stable methyl lactate conformer. Broadband scans for the rotational spectra of possible binary conformers have been carried out using a chirped-pulse Fourier transform microwave (FTMW) instrument. The most stable binary adduct was identified and assigned. The final frequency measurements have been done with a cavity based FTMW instrument. The spectrum observed shows complicated fine and hyperfine splitting patterns, likely due to the internal rotations of the methyl groups of methyl lactate and that of ammonia, as well as the 14N quadrupolar nucleus. The binary adduct with 15NH3 has also been studied to simplify the splitting pattern and to aid the assignments of the extensive splittings. The isotopic data and the fine and hyperfine structures will be discussed in terms of internal rotation dynamics and geometry of the hydrogen bonded adduct.