CARBONYL STRETCHING RO-VIBRATIONAL AND PURE ROTATIONAL SPECTRA OF METHYL LACTATE

N. BORHO and Y. Xu, *Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Canada*.

Methyl lactate ($COOCH_3CHCH_3OH$) has recently attracted attention due to its specific self-assembly in the gas phase[a]. Here, we investigate the pure rotational and ro-vibrational carbonyl stretching spectra of methyl lactate monomer in order to pursue further high resolution studies of methyl lactate aggregates.

The lowest energy conformer of methyl lactate stabilized via an intramolecular OH$\cdots$O=C hydrogen bond was detected with a Fourier Transform microwave spectrometer in a supersonic beam environment. From 119 microwave transitions observed, we derived the ground state rotational and centrifugal distortion constants. The tunneling splittings due to the internal rotation of the ester methyl group were observed and analyzed with the program XIAM[b]. We determined the barrier height of the ester methyl torsion to be 4.81 ± 0.01 kJ mol^{-1}. The ro-vibrational spectrum in the carbonyl frequency region (1750 to 1760 cm^{-1}) was recorded using a rapid scanning diode laser spectrometer and will be presented.

---

[a] N. Borho and M. A. Suhm, *Org. Biomol. Chem.*, 2003, **1**, 4351

[b] H. Hartwig and H. Dreizler, *Z. Naturforschung*, 1996, **51a**, 923.