ROTATION-TUNNELING SPECTRA OF CHIRAL METHYL LACTATE DIMERS

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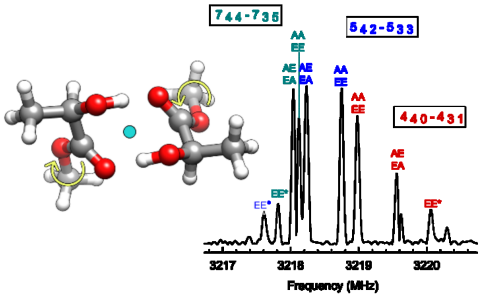
Methyl lactate, one of the simplest chiral esters, has been an iconic system for chiral recognition study in the past decades[1,2]. The methyl lactate monomer has the ability to form a strong intramolecular hydrogen bond between the hydroxy group and carbonyl group and its aggregates show a robust competition between intra- and intermolecular hydrogen bonding interactions[3,4]. Understanding its self-aggregation process is a fundamental step to draw a comprehensive picture of the conformational behavior of chiral α-hydroxy ketones, a ubiquitous structural unit found in natural products and pharmaceutical industries.

In the current study, we applied chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW) to detect homochiral and heterochiral binary aggregates of methyl lactate in the range of 2-6 GHz. Rotational spectra of several binary conformers of methyl lactate were assigned, aided by a conformational searching tool, CREST[5], and subsequent DFT calculations. The internal rotation of methyl rotors generated fine splitting structures of the rotational transition. This allows us to catch a glimpse of the symmetric geometry of the homochiral dimers. (see the figure)



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