

ROTATIONAL SPECTROSCOPY AND CONFORMATIONAL SPACE OF GLYCEROL DIMERS

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Glycerol ($\text{CH}_2\text{OHCHOHCH}_2\text{OH}$) is a colorless, odorless, and viscous liquid with a sweet taste and is widely used in food and drug industry. This polyol compound with three hydroxyl groups is capable of taking on many different intra- and intermolecular hydrogen bonding topologies, leading to highly complex conformational spaces for its monomer and dimer. Rotational spectra of five of its monomeric conformers had been reported before.[1],[2] In the current study, we apply CREST, a conformer-rotamer ensemble sampling tool developed by the Grimme group,[3] together with DFT calculations to systematically explore the conformational spaces of its monomer and dimer. Rotational spectra of glycerol in the 1-12 GHz range were recorded using a chirped-pulse Fourier transform microwave spectrometer and analyzed. Rotational transitions of several conformers of the binary glycerol complex were assigned. The structure-energy relationships of the conformers of the glycerol dimer and the corresponding monomer will be discussed.

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[3] S. Grimme, *J. Chem. Theory Comput.* 2019, 15, 2847.