ETHANOL TRIMER CONFIGURATIONS REVEALED BY CP-FTMW SPECTROSCOPY AND COMPUTATIONAL CALCULATIONS

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The study of hydrogen-bonded complexes in the gas phase aims to advance our knowledge of the intermolecular forces at play in these systems. To this end, ethanol clusters are of particular interest as archetypes of the interplay between hydrogen bonding and London dispersion forces. Here we present an investigation into the preferred isomers of ethanol trimer using computational methods in combination with broadband chirped-pulse Fourier transform microwave spectroscopy. The potential energy surface of ethanol trimer has been investigated through DFT and *ab initio* calculations, showing that the –OH groups forms a hydrogen bonded cyclic structure in the lower-energy isomers. From the analysis of the rotational spectrum, four distinct rotamers of ethanol trimer have been detected. All rotamers display O-H$\cdots$O hydrogen bonds between the three hydroxyl groups, where each hydroxyl group simultaneously acts as hydrogen bond donor and acceptor.