UNLOCKING THE MYSTERIES OF ETHANOL TRIMER THROUGH BROADBAND ROTATIONAL SPECTROSCOPY AND COMPUTATIONAL STUDIES

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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 of the conformational preferences of ethanol trimer using computational methods in combination with broadband rotational spectroscopy. The potential energy surface of ethanol trimer has been investigated through DFT and ab initio calculations and the lower-energy conformations are predicted to have the -OH groups forming a hydrogen bonded cyclic structure. From the analysis of the rotational spectrum, four complexes of ethanol trimer have been identified, arising from four distinct families dependant on the monomer conformation. All isomers display O-H$\cdots$O hydrogen bonds between the three hydroxyl groups, where each hydroxyl group simultaneously acts as hydrogen bond donor and acceptor. In all complexes the O-H$\cdots$O bonds form a six membered ring and the -CH_2CH_3 tails of ethanol arrange themselves above and below the plane, simultaneously maximising van der Waals interactions and minimising steric repulsion. The potential energy surface, assignment and conformational preferences of ethanol trimer will be discussed.