MOLECULAR RECOGNITION IN OLFACTION: INTERACTIONS OF THE ODORANT CARVONE WITH ETHANOL

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Non-covalent interactions are vitally important for molecular recognition in many biological and chemical processes. Understanding the interplay between intra- and intermolecular forces is crucial for advancing our knowledge on these events and how they are influenced by slight changes. Here we report the interactions of the common odorant carvone with ethanol, a mimic to the amino acid side chain serine. It has been studied through combination of chirped-pulse Fourier transform microwave spectroscopy and computational calculations, including density functional theory and ab initio methods. Seven carvone-ethanol complexes have been observed showing an O$\cdots$H-O primary bond between the carbonyl group of carvone, acting as a hydrogen bond acceptor, and the hydroxyl group of ethanol as the hydrogen bond donor. Secondary C-H$\cdots$O dispersion interactions anchoring ethanol to carvone are also established. Changes in the conformational preferences of the monomers upon complexation will be discussed.