STRUCTURAL CHARACTERISATION OF FENCHONE AND ITS COMPLEXES WITH ETHANOL BY BROADBAND ROTATIONAL SPECTROSCOPY

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Although significant advances in understanding the human olfactory system have taken place over the last two decades, detailed information on how the interactions between odorants and olfactory receptors occur at the molecular level is still lacking. To achieve a better understanding on the molecular mechanisms involved in olfaction, we are investigating several odorants and their interactions with mimics of amino acid residues in olfactory receptors.

We present here the structural characterisation of fenchone ($C_{10}H_{16}O$) and its complexes with ethanol (to mimic the side chain of serine) using a 2-8 GHz chirped-pulse Fourier transform microwave spectrometer built at King's College London. The rotational spectrum of the parent species and all the ^{13}C and ^{18}O isotopologues of fenchone was observed, and from the experimental rotational constants the substitution (r_0) and effective (r_s) structures of fenchone were determined. The rotational spectrum of fenchone-ethanol was observed by adding ethanol to the carrier gas and passing the mixture through a receptacle with fenchone. Several 1:1 complexes of fenchone-ethanol have been identified in the rotational spectrum. In all the complexes the ethanol molecule binds to the carbonyl group through an O-H$\cdots$O hydrogen bond.