

STRUCTURES OF COMPLEXES OF CYCLOOCTANONE WITH WATER

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Water is present in the air with a concentration of up to 4 %, and also in the olfactory mucosa. Odorants are thus very likely to interact with water before reaching olfactory receptors. We have investigated the complexes of cyclooctanone with water as a first step towards understanding how larger macrocyclic odorants interact with water. Two complexes of the most abundant conformer of cyclooctanone with one water molecule, and two complexes with two water molecules have been characterised using chirped-pulse Fourier Transform Microwave (CP-FTMW) spectroscopy. In the cyclooctanone-H₂O complexes, water forms a O-H...O hydrogen bond with the carbonyl oxygen of cyclooctanone and two O...H-C hydrogen bonds with the -CH₂ groups in the cyclooctanone ring. In the cyclooctanone-(H₂O)₂ complexes, the second molecule of water binds primarily to the first molecule of water through hydrogen bonding, whilst also forming secondary interactions with the -CH₂ groups in the ring. The observation of all ¹³C isotopic species of the cyclooctanone ring in the complexes in their natural abundances, and of the ¹⁸O species using isotopically enriched water allowed us to calculate the experimental structures of the complexes.

