MULTIPLE WATER CONFIGURATIONS IN FENCHONE$\cdots(H_2O)_{1-6}$ HYDRATES REVEALED BY ROTATIONAL SPECTROSCOPY

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Fenchone is a bicyclic monoterpenoid that is released to the atmosphere by natural and anthropogenic sources, where it interacts with other atmospheric molecules such as water. Here we present the investigation of the hydrates of fenchone $C_{10}H_{16}O\cdots(H_2O)_n$ (n = 1-6) by microwave spectroscopy, in the frequency range 2 to 20 GHz, and computational calculations[1]. Several isomers of each hydrated complex have been observed and their rotational and centrifugal distortion constants determined. For fenchone$\cdots(H_2O)_{1-4}$ complexes, observation of the ^{18}O isotopologues allowed us to determine the location of the oxygen atoms of water and the configuration of water molecules around fenchone. Water binds to fenchone through O–H$\cdots$O and C–H$\cdots$O hydrogen bonds. In the mono-, di- and trihydrates water molecules arrange in open chains around fenchone, while for the higher order hydrates water molecules adopt distorted tetramer, pentamer and hexamer configurations. The various configurations as well as the relevant intermolecular interactions, and their modelling by computational methods, will be discussed.

[1] M. Chrayteh, E. Burevschi, D. Loru, T. R. Huet, P. Dréan, M. E. Sanz, *PCCP*, 23, 20686 (2021).