STRUCTURE OF MICROSOLVATED VERBENONE DETERMINED BY MICROWAVE FOURIER TRANSFORM SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS

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Verbenone ($C_{10}H_{14}O$) is a bicyclic ketone terpene. It is one of the products of oxidation of α-pinene in the troposphere. It may have a significant role in the formation of secondary organic aerosols, in particular through its ability to interact with water molecules.Verbenone is almost insoluble in water so it is therefore important to understand how this type of molecules interacts with water.

The rotational spectrum of verbenone and the determination of its r_s and r_0 molecular structures were recently investigated [a]. This work deals with the study of its hydrates. Water is expected to form a primary hydrogen bond with the carbonyl group of verbenone, and the hydrogen atoms of the -CH_3 or -CH_2 groups may form weak interactions with the lone pairs of the water oxygen to stabilize different hydrates. The structures of two monohydrates, two dihydrates and four trihydrates of verbenone were optimized at the DFT B3LYP-D3BJ / def2-TZVP and *ab initio* MP2 / 6-311++G(d,p) levels, before searching for their rotational signatures, using a supersonic expansion coupled to a cavity-based Fourier transform microwave spectrometer working in the 2 - 20 GHz frequency range. We were able to analyse the spectra of the expected two mono- and two dihydrates, and of the lowest energy conformer of the trihydrate. We also analysed the spectra of the water-^{18}O substituted species using ^{18}O labeled water. For each hydrate, the sets of rotational constants were used to calculate the substitution coordinates of the water oxygen atoms and an effective r_0 structure of the water arrangements of water around the molecule of verbenone.

The present work was funded by the French ANR Labex CaPPA through the PIA (contract ANR-11-LABX-0005-01), by the Regional Council Hauts de France, by the European Funds for Regional Economic Development, and by the French Ministère de l'Enseignement Supérieur et de la Recherche. It is a contribution to the CPER research Project CLIMIBIO.

[a] F. E. Marshall, G. Sedo, C. West, B. H. Pate, S. M. Allpress, C. J. Evans, P. D. Godfrey, D. McNaughton and G. S. Grubbs, *J. Mol. Spectrosc.* **342**, 109 - 115 (2017).