CHARACTERIZATION OF THE CARVONE MONOHYDRATE COMPLEX: A ROTATIONAL STUDY

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Carvone ($C_{10}H_{14}O$, 5-isopropenyl-2-methyl-2-cyclohexenone) is one of the most abundant monoterpenoids. It is present in many essential oils, and released to the atmosphere by both natural and anthropogenic sources. Water is abundant in the atmosphere and in the mucus layer, and thus carvone interactions with water are of atmospheric and biological interest. Utilising a chirped-pulse Fourier transform microwave spectrometer in the 2-8 GHz frequency range we have studied the carvone monohydrate complex. Supporting calculations have been carried out using both DFT and ab initio methods. Eight different isomers of carvone-(H_2O) have been observed and identified based on the comparison between their experimental and theoretical rotational constants and the observation of the ^{18}O water isotopologues. Water forms complexes with all observed conformations of carvone in the gas phase. [1], [2] The binding preferences are dictated by the formation of O–H$\cdots$O and C–H$\cdots$O hydrogen bonds. To visualise these interactions and gain further insight on their relative strength, non-covalent interaction, natural bond orbital and SAPT analyses were performed.

[1] doi:10.1007s11224-012-0142-8, Ramón Avilés Moreno, Juan and R. Huet, Thérése and López González, J, Struct Chem., **24**, 1163–70, (2013).

[2] doi:10.1039/C9CP05264J, D. Loru, A. Vigorito, A. F. M. Santos J. Tang, M. E. Sanz, Physical Chemistry Chemical Physics, **21(47)**, 26111-26116, (2019)