A ROTATIONAL STUDY OF THE INTERACTIONS OF WATER WITH THE MONOTERPENOID CARVONE

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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 by plants to the atmosphere. Moreover, it is widely used as an odorant in household products, perfumes and cosmetics. Water is abundant in the atmosphere and in the mucus layer, and thus carvone interactions with water are of atmospheric and biological interest. We have studied the complexes of carvone with water using chirped pulse Fourier transform microwave spectroscopy in the 2-8 GHz frequency range. Supporting calculations have been carried out using MP2 and B3LYP-D3BJ 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]. Binding preferences are dictated by the formation of O–H···O and C–H···O hydrogen bonds. To visualise these interactions and gain further insight on their relative strength, non-covalent interaction and natural bond orbital analyses were performed. We will discuss our results in the context of other complexes formed by carvone.

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[2] D. Loru, A. Vigorito, A. F. M. Santos, J. Tang and M. E. Sanz, *PCCP*, **2019**, *21*, 26111-26116.