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BENZOIC ACID MICROSOLVATION IN GAS PHASE BY ROTATIONAL SPECTROSCOPY: STRUCTURE AND COOPERATIVE EFFECTS

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Gas-phase hydration of carboxylic acids, such as benzoic acid (C_6H_5COOH, BzAc), is crucial for a better understanding of biochemical processes in condensed phases. Despite its interest only a microwave rotational study of its monohydrated complex has been reported so far.[i] Herein, we present our investigation of higher-order benzoic acid hydrates, generated in a supersonic jet expansion and characterized using broadband chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW). We have identified several new benzoic acid hydrates in the gas phase: BzAc-W_{2-5} and $BzAc_2$-W. Additionally, we detected spectra for all ^{13}C monosubstituted isotopologues of BzAc, and the $H_2^{18}O$ monosubstituted isotopologues for BzAc-W_2 and $BzAc_2$-W, which enabled the determination of their Kraitchman substitution structure. Furthermore, we extended the measurements for the reported species across the 2–8 GHz frequency range. The BzAc-W_3 spectrum reveals a tunneling splitting between two equivalent non-planar forms, analyzed using a Coriolis-coupled two-states Hamiltonian to determine the vibrational energy spacing. Our experimental results have been complemented with theoretical calculations, providing a deeper understanding of the forces stabilizing these complexes and exploring the relationship between hydration number, structure, and cooperative effects.

[i] E. G. Schnitzler and W. Jäger, The benzoic acid–water complex: a potential atmospheric nucleation precursor studied using microwave spectroscopy and ab initio calculations, Phys. Chem. Chem. Phys., 16(6), 2305-2314, 2014. DOI: 10.1039/C3CP54486A.

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Early-career researchers´ workshop

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