

Structures and dynamics of acrolein-(H₂O)_n clusters revealed by MW spectroscopy and *ab initio* calculation

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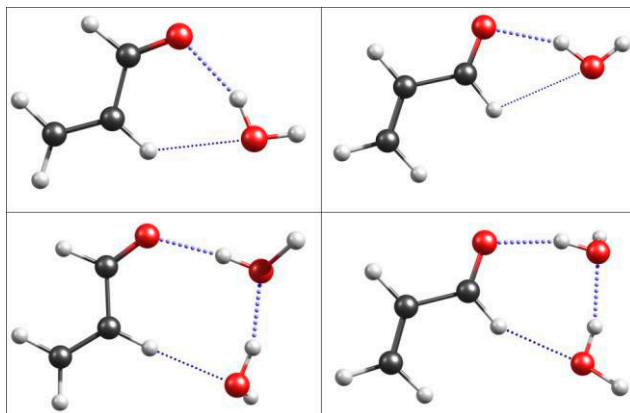
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We present a rotational study of the interaction between the simplest unsaturated aldehyde Acrolein (ACR) and water (W) by using cavity based coaxial pulsed jet Fourier transform microwave spectroscopy. The rotational spectra of two conformers of the dimer ACR-W and two conformers of the trimer ACR-W₂ were identified in the frequency range 6.5–18.5 GHz.^[1]

Acrolein is present only as *trans* isomer in all the assigned clusters which agrees with the preference of *ab initio* predictions. ACR is linked with one or two water molecules through the OH...O hydrogen bond (HB) and the C_αH...O/C_βH...O weak HB.

The ¹³C and ¹⁸O monosubstituted isotopologues of ACR-W and the ¹⁸O species of A-W₂ have been also assigned. The spectroscopy intensity of the clusters including acrolein-¹⁸O increased dramatically when we seeded normal acrolein and H₂¹⁸O in the sample. This implies that the exchange of the O atoms between acrolein and water happened. The *ab initio* calculation helped us to explore the reaction pathways.



Discovering the conformations of formamide complexes and formamide–water clusters by microwave spectroscopy

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We have recorded the broadband microwave spectra (2–8 GHz) of pure formamide (¹⁴N and ¹⁵N isotopologues) and mixtures of formamide and water using a chirped-pulse Fourier transform microwave spectrometer. The structures of several clusters of the formamide trimer have been identified using the rotational parameters determined for the different isotopologues detected. In the formamide–water spectra, two complexes, F-(H₂O)₄ and F₂-(H₂O)₂, have been identified from the rotational and quadrupole coupling constants. We present the predicted conformational landscape of complexes and the preliminary results obtained.

Does the structure of the polycyclic aromatic hydrocarbon impact the aggregation of water on its surface? Fluorene vs acenaphthene

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Polycyclic aromatic hydrocarbons (PAHs) are thought to be ubiquitous in the interstellar medium, and as such they would play a key role in everything from complex organic molecule formation to the formation of ice grains. In the event of ice grain formation, PAH-water interactions would be of importance. In this investigation we aim to study the onset of these interactions using chirped pulse Fourier transform microwave (CP-FTMW) spectroscopy. Fluorene, which was previously studied [1], and its complexes with water were measured. Transitions for ¹³C species of the monomer were observed, as well as the ¹⁸O isotopologues of the water complexes. This allowed for the structural analysis of the species to be performed. These structures will be compared to the previously studied acenaphthene (Ace) and Ace-(H₂O)_n (n=1-4)[2]. As in the Ace-water study, we have observed up to three water molecules complexed with fluorene. In this talk we will present these findings and the structural differences between the two PAH-water systems.

[1] Thorwirth, S., Theulé, P., Gottlieb, C.A., McCarthy, M.C., Thaddeus, P. *Astrophys. J.*, 2007, 662, 1309.

[2] Steber, A.L., Pérez, C., Temelso, B., Shields, G.C., Rijs, A.M., Pate, B.H., Kisiel, Z., Schnell, M. *J. Phys. Chem. Lett.*, 2017, 8, 5744.

Characterization of microsolvated 15C5 crown ether from broadband rotational spectroscopy

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15-crown-5 ether (15C5) and its complexes with water generated in a supersonic jet have been studied using broadband Fourier transform microwave spectroscopy. The most stable form of the crown ether not previously reported, to complete a total of nine isolated forms, has been detected. In addition, two 1:1 and two 1:2 clusters have been observed. The clusters structures have been unambiguously identified through the observation of water ¹⁸O isotopologue spectra and a detailed analysis of the rotational parameters. The structures of all the clusters show that at least one water molecule, located close to the axis of the ring, interacts through two simultaneous hydrogen bonds to the endocyclic oxygen atoms. This interaction reshapes the 15C5 ring to reduce its rich conformational panorama to only two open structures, related to those found in complexes with LiS⁺ or Na⁺ ions. In the most intense 1:2 form, the two water molecules repeat the same interaction scheme in both sides of the ring while in the second one the water molecules lie on the same side of the ring.