STRUCTURE AND DYNAMICS OF THE WEAKLY BOUND TRIMER $(H_2S)_2(H_2O)$ OBSERVED USING ROTATIONAL SPECTROSCOPY

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The weakly bound complex between two hydrogen sulfide molecules and one water molecule, $(H_2S)_2(H_2O)$, was identified from its rotational spectrum observed at conditions of supersonic expansion. The spectra of parent species were obtained using a chirped-pulse Fourier transform microwave spectrometer (Newcastle, UK). The isotopologues were identified with Balle-Flygare Fourier transform microwave spectrometer (Bangalore, India). Distinct physical properties of H_2O and H_2S under ambient settings have long been recognized as a result of their significantly different hydrogen-bonding capabilities. It has conclusively shown $(H_2S)_2$ is hydrogen-bonded similar to $(H_2O)_2$ at very low temperature[a]. The break with axial molecular symmetry and the simplified internal dynamics allowed us to investigate $(H_2S)_2(H_2O)$ at a level of structural detail that has not yet been possible for $(H_2O)_3$ and $(H_2S)_3$ with rotational spectroscopy due to their zero-dipole moment. The rotational spectrum of $(H_2S)_2(H_2O)$ shows a doubling of the lines, close to 1:3 relative intensity for the parent species, caused by the internal rotation of the H_2O moiety about its C_2 axis. Analysis of experimental results reveals that the three monomers are bound in a triangular arrangement through the S-H···S, O-H···S and S-H···O hydrogen bonds. The r_s and r_0 structural parameters have been evaluated, and the three heavy atom distances r_s(S-H···S)=4.067(2)Å, r_s(O-H···S)=3.412(11)Å and r_s(S-H···O)=3.454(11)Å are appreciably shorter than the respective distances in $(H_2S)_2$, *HOH*···SH_2 and *HSH*···OH_2[b]. The geometry contains numerous characteristics that indicate the cooperative nature of the intermolecular interaction. The experimental results for all observables determinable from the rotational spectrum are found to be in excellent agreement with *ab initio* predictions.

[a] A. Das, P. K. Mandal, F. J. Lovas, C. Medcraft, N. R. Walker, and E. Arunan. *Angewandte Chemie International Edition*, 2018, 57, 15199-15203.

[b] P. K. Mandal, Ph.D. Dissertation, Indian Institute of Science, 2005.