ROTATIONAL SPECTRA AND STRUCTURE OF H_2S COMPLEXES: $Ar(H_2S)_2$ AND C_2H_4-H_2S

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Recently, we determined hydrogen bond radii for HF, HCl, HBr, HI, HCN, H_2O and HCCH, using the accurate structural data available from microwave spectroscopic studies on several B:HX complexes, where B is a hydrogen bond acceptor[a]. For H_2S, the available data is limited compared to other hydrogen bond donors listed above. Hence, a systematic investigation has been started on several H_2S complexes. Several transitions have been observed for Ar-$(H_2S)_2$ and C_2H_4-H_2S complexes. The rotational spectrum of C_2H_4-H_2S complex appears to be a composite of rotational spectra of the hydrogen bonded C_2H_4-H_2O and the van der Waals complex C_2H_4-Ar. Each transition is split in to four with a smaller splitting of about 0.14 MHz and a larger splitting of 1.67 MHz in (B+C)/2. The rotational constants for the strongest progression are A = 26(1) GHz; B = 1972.88(1) MHz and c = 1866.68(1) MHz. Assignment of Ar-$(H_2S)_2$ spectra is in progress. It was realized that the rotational spectrum for $(H_2S)_2$ complex has not been completely solved yet[b] and hence a 'revisit' started. Several more progressions have been assigned for this dimer now. The search for deuterated isotopomers was carried out by bubbling H_2S through D_2O and some new H_2O-H_2S transitions have been observed. During this talk, rotational spectra of all these complexes will be discussed.

[a] P. K. Mandal and E. Arunan J. Chem. Phys. 114, 3880 (2001)

[b] F. J. Lovas private communication