ROTATIONAL SPECTRUM AND INTERNAL DYNAMICS OF THE Ne-H_2S VAN DER WAALS COMPLEX

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Rotational spectra of several isotopomers of the Ne-H_2S van der Waals dimer were measured in the frequency range from 4 to 22 GHz, using a pulsed molecular beam Fourier transform microwave spectrometer. Two K=0 progressions were recorded for the symmetrical isotopomers (with H_2S/D_2S). This doubling is attributed to an internal rotation motion of the H_2S moiety within the complex. The two states can be correlated to the 0_{00} and 1_{01} internal rotor states of free H_2S and D_2S. Only one K=0 progression was measured for Ne-DSH. The excited internal rotor state is no longer metastable since the symmetry constraints no longer apply. An anomalous isotope effect observed in Ar-H_2S, where the substitution of hydrogen by deuterium causes an increase in the ground state B rotational constant,[a] was not observed here, in agreement with the *ab initio* study by Dykstra and co-workers.[b] Nuclear quadrupole hyperfine structure was resolved or partially resolved for isotopomers containing ^{33}S and D, respectively, and the corresponding quadrupole coupling constants were determined. These were used to derive information about the intermolecular dynamics. The results are compared with those of Ar-H_2S and Ar-H_2O.

[a] H. S. Gutowsky, T. Emilsson, and E. Arunan, *J. Chem. Phys.* **106**, 5309 (1997).
[b] G. de Oliveria and C. Dykstra, *J. Chem. Phys.* **110**, 289 (1999).