

ROTATIONAL SPECTRUM AND INTERNAL DYNAMICS OF THE Ne-H₂S VAN DER WAALS COMPLEX

YAQIAN LIU and WOLFGANG JÄGER, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada, T6G 2G2.*

Rotational spectra of several isotopomers of the Ne-H₂S 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 H₂S/D₂S). This doubling is attributed to an internal rotation motion of the H₂S moiety within the complex. The two states can be correlated to the 0_{00} and 1_{01} internal rotor states of free H₂S and D₂S. 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-H₂S, 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 ³³S 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-H₂S and Ar-H₂O.

^aH. S. Gutowsky, T. Emilsson, and E. Arunan, *J. Chem. Phys.* **106**, 5309 (1997).

^bG. de Oliveria and C. Dykstra, *J. Chem. Phys.* **110**, 289 (1999).