INTERMOLECULAR POTENTIAL ENERGY SURFACES FOR THE Rg-SH ($\tilde{X}\ ^2\Pi_i$) COMPLEXES (Rg:Ne,Kr) STUDIED BY FTMW SPECTROSCOPY

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Rare gas-SH complexes are interesting species because various phenomena caused by the unquenched spin and angular momenta exist. In the present study, we have observed pure rotational spectra of Ne-SH and Kr-SH in the ground state by FTMW spectroscopy. R-branch transitions in the lower spin component ($\Omega = 3/2$) for the linear $^2\Pi_i$ radical were observed for $J'' = 1.5 - 4.5$ in the $11 - 25$ GHz region for Ne-SH, and for $J'' = 1.5 - 6.5$ in the $5 - 17$ GHz region for Kr-SH, respectively. In these spectra P-type doublings and hyperfine splittings associated with the H nuclei have been observed. Although the spectral pattern of Kr-SH is relatively regular, that of Ne-SH is fairly irregular with the J dependence of the P-type doubling very different from other Rg-SH or Rg-OH species. In the present analysis, we used a program system explicitly taking into account of the large amplitude stretching and bending motions coupled with the fine and hyperfine structure. We were able to determine intermolecular potential energy surfaces(IPS) for both of the species. We have obtained systematic information on the intermolecular interaction, and compared it with that of Ar-SH[a]. The average potential turned out to be fairly shallow and isotropic, especially for Ne-SH, and this may be the source of the irregular spectral pattern of Ne-SH.

[a] Y. Sumiyoshi, Y.Ohshima, and Y. Endo, J. Chem. Phys. 113, 10121 (2000).