3-DIMENSIONAL POTENTIAL ENERGY SURFACE OF THE Ar-SH COMPLEX

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All the pure rotational transitions reported in the previous studies,[a,b] and recently observed rotation vibration transitions, P = 1/2 - 3/2, for Ar-SH[c] and Ar-SD have been simultaneously analyzed to determine an intermolecular potential energy surface of Ar-SH in the ground state. In the analysis, the SH vibration was explicitly considered to calculate ro-vibrational energies of the complex on a 3-dimensional intermolecular potential energy surface (3D-IPS), where *ab initio* calculations at the RCCSD(T)/aug-cc-pVTZ + BF level of theory have been performed to facilitate the results as initial values for the least-squares analysis. The determined 3D-IPS was able to fit all the pure-rotational and ro-vibrational data for Ar-SH and Ar-SD without introducing empirical correction terms required in the previous study.[b]

[a] Y. Sumiyoshi, et al. *J. Chem. Phys.* **113**, 10121 2000.
[b] Y. Sumiyoshi, et al. *J. Mol. Spectrosc.* **222**, 22 2003.
[c] Y. Sumiyoshi, et al. *Talk TH11, 59th Ohio State University International Symposium on Molecular Spectroscopy, 2004.*