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, \(J = \frac{1}{2} - \frac{3}{2}\), 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 \(ab\) \textit{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\(^b\).