THREE-DIMENSIONAL POTENTIAL ENERGY SURFACE OF Ar-OH

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All the pure rotational transitions in the ground state for Ar-OH and Ar-OD [a,b] and in the first excited state of the OH stretching vibration, v_{OH} = 1, for Ar-OH observed by Fourier-transform microwave spectroscopy, and rotation-vibration transitions observed by infrared spectroscopy [c] have been simultaneously analyzed to determine the potential energy surface of Ar-OH in the ground electronic state. A Schrödinger equation considering all the three-dimensional freedom of motion for an atom-diatom complex in the Jacobi coordinate, R, θ, and r, was numerically solved to obtain energies of the ro-vibrational levels using the discrete variable representation method. A three-dimensional potential energy surface is determined by a least-squares fitting using initial values of the potential parameters obtained by $ab\ initio$ calculations at the RCCSD(T)/aug-cc-pVTZ+bond functions level of theory. The P-level structures in the v_{OH} = 0 state observed by SEP spectroscopy [d], are well reproduced by the present potential energy surface. Dependence of the interaction energy between Ar and OH on the bond length of the OH monomer will be compared with that of the isovalent radical complex, Ar-SH [e].

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[a] Y. Ohshima, et al. *J. Chem. Phys.* **95**, 7001 1991.

[b] Y. Endo, et al. *Faraday Discuss. Chem. Soc.* **97**, 341 1994.

[c] R. T. Bonn, et al. *J. Chem. Phys.* **112**, 4942 2000.

[d] M. T. Berry, et al. *J. Chem. Phys.* **96**, 7890 1992.

[e] Y. Sumiyoshi, et al. *J. Chem. Phys.* **123**, 054325 2005.