

<b>28</b>	<b>ArHS</b>	<b>Argon – monohydrogen monosulfide (1/1)</b>	<b>C<sub>∞v</sub></b>
MW, <i>ab initio</i>		Argon – sulfanyl (1/1)	(effective symmetry class)
calculations		(weakly bound complex)	(large-amplitude motion)
			Ar · SH

$$\frac{r_0}{R_{\text{cm}}} \frac{\text{\AA}^{\text{a)}}}{3.791(2)^{\text{b)}}}$$

A two-dimensional intermolecular potential energy surface for the Ar · SH (<sup>2</sup>Π<sub>i</sub>) complex has been derived from a least-squares fitting of the observed rotational transitions, where several parameters are constrained to the values from RCCSD(T)/aug-cc-pVQZ calculations. The average potential is fairly isotropic with two shallow minima corresponding to the linear Ar · SH and Ar · HS configurations, of which the former is 7.2 cm<sup>-1</sup> more stable than the latter. The vibrational ground state is located above the barrier of only *ca.* 20 cm<sup>-1</sup> between the two minima, and its wavefunction is widely spread along the bending coordinate.

<sup>a)</sup> Uncertainty was not estimated in the original paper.

<sup>b)</sup> In the Ar · SH global minimum configuration.

Sumiyoshi, Y., Endo, Y., Ohshima, Y.: J. Chem. Phys. **113** (2000) 10121.

## LIF

State	$\tilde{X}^2\Pi$	$\tilde{A}^2\Sigma^+$
Energy [eV]	0.00	
$r_0(\text{Ar}\dots\text{H}) [\text{\AA}]$	2.9002	2.062
$r_0(\text{Ar}\dots\text{D}) [\text{\AA}]$	2.8992	2.005

A mixture of *ca.* 1% H<sub>2</sub>S/D<sub>2</sub>S in helium to which 1...5% of argon was added, was expanded into a vacuum chamber and radicals were produced by laser photolysis. Fluorescence was excited by a probe laser derived from a CW dye laser which was pulse amplified and frequency doubled. By scanning the dye laser, spectra of the Ar · SH/SD radicals were obtained. Rotational analysis provided molecular constants from which structural information was derived. In both the  $\tilde{X}^2\Pi$  and  $\tilde{A}^2\Sigma^+$  states the Ar · SH van der Waals complex is best described as a nearly free SH whose rotation is slightly hindered by the presence of the Ar atom.

Carter, C.C., Miller, T.A.: J. Chem. Phys. **107** (1997) 3447.

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