

## Structure Data of Free Polyatomic Molecules

197 MW	<b>C<sub>2</sub>H<sub>2</sub>Ar</b>	<b>Acetylene – argon (1/1)</b>		<b>C<sub>2v</sub></b> (effective symmetry class) (large-amplitude motion) H–C≡C–H · Ar
		Ethyne – argon (1/1) (weakly bound complex)		
	Isotopic species	<i>r</i> <sub>0</sub> ( <i>R</i> <sub>cm</sub> ) [Å] <sup>a) b)</sup>	<i>r</i> <sub>0</sub> ( <i>R</i> <sub>cm</sub> ) [Å] <sup>a) c)</sup>	
	Ar · HCCH	4.046(5)	4.039(5)	
	Ar · DCCD	4.046(5)	4.042(5)	
	Ar · H <sup>13</sup> C <sup>13</sup> CH	4.041(5)	4.036(5)	
	Ar · DCCH		4.038(5)	
	Ar · H <sup>13</sup> C <sup>12</sup> CH		4.037(5)	

A semirigid rotor model was employed to obtain the rotational and centrifugal distortion constants, which were in turn used to extract structural information about the complex. The unusually large standard deviations of the spectroscopic fits are indicators of large-amplitude internal motions of the acetylene subunit. Separate fits of the individual  $K$ -stacks yielded lower standard deviations, and their results were used to interpret some of the unusual spectroscopic observations.

<sup>a)</sup> Uncertainties were not estimated in the original paper.

<sup>b)</sup> Calculated using  $R_{\text{cm}} = [(k/\mu)(1/C - 1/b)]^{1/2}$ , where  $b$  denotes the rotational constant of acetylene.

<sup>c)</sup> Calculated using pseudodiatomic expression:  $R_{\text{cm}} = [(k/\mu)(2/(B + C))]^{1/2}$ .

Liu, Y., Jäger, W.: J. Mol. Spectrosc. **205** (2001) 177.

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