

Structure Data of Free Polyatomic Molecules

200 IR	$\text{C}_2\text{H}_2\text{Br}^-$	Ethyne – bromide (1/1) (weakly bound complex)	$\text{C}_{\infty v}$
			(effective symmetry class) (large-amplitude motion) $\text{HC}\equiv\text{CH} \cdot \text{Br}^-$

State	$R_{\text{cm}} [\text{\AA}]^{\text{a}}$	$r(\text{H}\dots\text{Br}) [\text{\AA}]^{\text{a}}$
$\nu=0$	4.11(3)	2.45(5)
$\nu_3=1$	4.07(3)	2.41(5)

The structure was determined from the rotationally resolved IR predissociation spectrum of the C–H fundamentals. The geometry of the ethyne subunit was assumed to be unchanged upon complexation.

^a) Uncertainties were not given in the original paper.

Wild, D.A., Milley, P.J., Loh, Z.M., Wolyneć, P.P., Weiser, P.S., Bieske, E.J.: J. Chem. Phys. **113** (2000) 1075.