

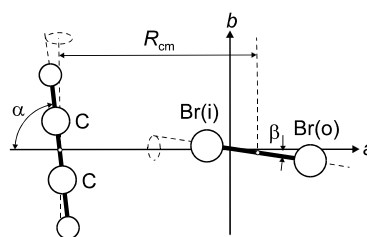
204
MW**C₂H₂Br₂****Acetylene – dibromine (1/1)**Ethyne – dibromine (1/1)
(weakly bound complex)**C_{2v}**(effective symmetry class)
(large-amplitude motion)HC≡CH · Br₂

Isotopic species	$r_0(R_{\text{cm}})$ [Å]	$r_0[\text{cm} \dots \text{Br(i)}]^{\text{a}}$ [Å]	$\theta_0(\alpha)$ [deg] ^b	$\theta_0(\beta)$ [deg] ^b
C ₂ H ₂ · ⁷⁹ Br ⁷⁹ Br	4.2789(25)	3.1333(25)	67.2(25)	5.5(5)
C ₂ H ₂ · ⁷⁹ Br ⁸¹ Br	4.2889(26)	3.1330(26)	68.2(26)	5.5(5)
C ₂ H ₂ · ⁸¹ Br ⁷⁹ Br	4.2600(25)	3.1327(25)	67.7(25)	5.5(5)
C ₂ H ₂ · ⁸¹ Br ⁸¹ Br	4.2743(28)	3.1327(28)	66.8(26)	5.5(5)

The complex possesses a T-shaped geometry at equilibrium with a zero-point distance of 3.144 Å between the center of the C≡C bond and the inner bromine atom. The intermolecular stretching force constant is 7.74 N m⁻¹.

^a) cm denotes the center of mass of the acetylene.

^b) See figure for the definition. Average value.



Davey, J.B., Legon, A.C.: Chem. Phys. Lett. **350** (2001) 39.