

1534
MW

C₄H₄

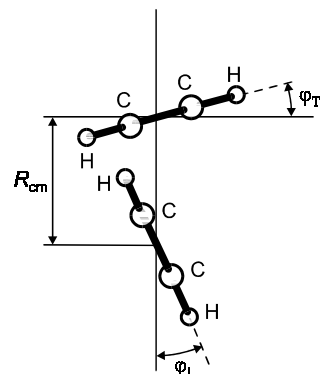
Acetylene dimer
(weakly bound complex)

C_s
(effective symmetry class)
HC≡CH · HC≡CH

r_0	Å	θ_0	deg
R_{cm}	4.38(2)	φ_T	27(2)
		φ_L	0 ^{a)}

^{a)} Assumed.

Prichard, D.G., Nandi, R.N., Muentner, J.S.: J. Chem. Phys. **89** (1988) 115.



IR, MW

r_0	Å ^{a)}
R_{cm}	4.404(20)

The complex has a T-shaped structure with interconversion tunneling between four isoenergetic hydrogen-bonded minima. The barrier to the tunneling is quite small (33.2 cm⁻¹). The structure of the monomer units was assumed to be unchanged in the complex.

^{a)} Uncertainty was not given in the original paper.

Fraser, G.T., Suenram, R.D., Lovas, F.J., Pine, A.S., Hougen, J.T., Lafferty, W.J., Muentner, J.S.: J. Chem. Phys. **89** (1988) 6028.

See also:

Ohshima, Y., Matsumoto, Y., Takami, M., Kuchitsu, K.: Chem. Phys. Lett. **147** (1988) 1.

Ohshima, Y., Matsumoto, Y., Takami, M., Kuchitsu, K.: Chem. Phys. Lett. **152** (1988) 116.