

1075 **C₃H₂O** **Acetylene – carbon monoxide (1/1)** **C_{∞v}**
 IR (weakly bound complex) (effective symmetry class)
 HC≡CH · CO

r_0	Å
$R_{\text{cm}}(^{12}\text{CO})$	5.011(15) ^{a)}
$R_{\text{cm}}(^{13}\text{CO})$	4.989(15) ^{a)}

The structures of the two monomers were assumed to be unchanged on complex formation. The isotopic substitution confirms the linearity of the complex and the orientation of the CO unit.

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

Marshall, M.D., Kim, J., Hu, T.A., Sun, L.H., Muentner, J.S.: J. Chem. Phys. **94** (1991) 6334.
 Kawashima, Y., Nishizawa, K.: Chem. Phys. Lett. **253** (1996) 77.

MW

Species	$r_0(R_{\text{cm}})$ [Å] ^{a)}	$r_0(\text{H} \cdots \text{C})$ [Å] ^{a)}	k_s ^{b)} [N m ⁻¹]	$R_{\text{e,cm}}$ [Å] ^{a)}
HCCH · CO	5.0167(50)	2.7811(50)	1.713	4.9672(70)
H ¹³ CCH · CO	5.0391(50)	2.7818(50)	1.715	4.9903(70)
HC ¹³ CH · CO	4.9955(50)	2.7817(50)	1.729	4.9465(70)
HCCH · ¹³ CO	4.9953(50)	2.7812(50)	1.734	4.9463(70)
HCCH · C ¹⁸ O	5.0478(50)	2.7813(50)	1.718	4.9995(70)

Atom	a_s [Å]
C	-3.1888
C	-2.0181
C	1.8003
O	2.8825

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Stretching force constant of the intermolecular bond.

Germann, T.C., Tschopp, S.L., Gutowsky, H.S.: J. Chem. Phys. **97** (1992) 1619.
 Legon, A.C., Wallwork, A.L., Bevan, J.W., Wang, Z.: Chem. Phys. Lett. **180** (1991) 57.
 Roehrig, M.A., Kukolich, S.G.: Chem. Phys. Lett. **188** (1992) 232.