

1157
MW, IR

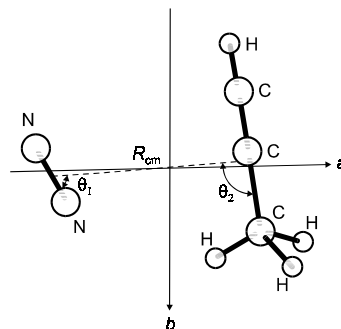


Methylacetylene – dinitrogen (1/1)
Propyne – dinitrogen (1/1)
(weakly bound complex)

C_s
(effective symmetry class)
H₃C–C≡CH · N₂

r_0	Å	θ_0	deg
R_{cm}	3.708(2)	θ_1	63.59(100) ^a
		θ_2	95.03(100) ^a

The structure of the complex is determined from the rotational constants of three isotopomers. There is free or almost free internal rotation of the propyne moiety. The molecular axes of C₃H₄ and N₂ are assumed to be coplanar. R_{cm} is the distance between the centers of mass of the subunits. θ_1 is the angle between the R_{cm} vector and the N₂ axis. θ_2 is the angle between the R_{cm} vector and the CCC axis. The structure of the subunits is assumed to be unchanged on complex formation.



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

Lovas, F.J., Fowler, P.W., Kisiel, Z., Tseng, S.-H., Beck, R.D., Eggers, D.F., Blake, T.A., Watts, R.O.: J. Chem. Phys. **100** (1994) 3415.