

1881
IR

C_4N_2

2-Butynedinitrile
Dicyanoacetylene
Acetylenedicarbonitrile

D_{ool}
 $N \equiv C - C \equiv C - C \equiv N$

r_0	\AA
$C \equiv N$	1.1606(50) ^{a)}
$C \equiv C$	1.2223(50) ^{a)}
$C - C$	1.3636(50) ^{a)}

Bond lengths transferred from the nitrile side of HC_5N predict a B_0 value extremely close to the experimental one (0.05%). A change of 0.0004 \AA in the distances is sufficient to reproduce the experimental B_0 . Therefore, the geometric parameters are well within 0.005 \AA of the transferred distances. This is further confirmed by *ab initio* predictions.

^{a)} Distances are taken from HC_5N .

Winther, F., Schönhoff, M., LePrince, R., Guarnieri, A., Bruget, D.N., McNaughton, D.: J.

Mol. Spectrosc. **152** (1992) 205

See also: McNaughton, D., Bruget, D.N.: J. Mol. Struct. **273** (1992) 11.

ED

r_{α}^0	$\text{\AA}^{\text{a)}}$
$C \equiv N$	1.161(5)
$C \equiv C$	1.198(11)
$C - C$	1.367(3)

The B_0 rotational constant derived from the ED bond lengths is nearly identical with the B_{av} value deduced from the Raman band-shape analysis.

The nozzle was at room temperature.

^{a)} Twice the estimated standard errors including a systematic error.

Brown, K.W., Nibler, J.W., Hedberg, K., Hedberg, L.: J. Phys. Chem. **93** (1989) 5679.