

1068
MW

$\text{C}_3\text{H}_2\text{N}_2$

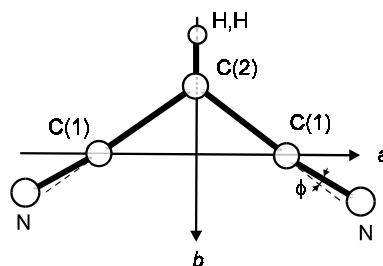
Propanedinitrile
Malononitrile

C_{2v}
 $\text{CH}_2(\text{CN})_2$

r_{av}	Å	θ_{av}	deg
C–C	1.4593(20)	C–C≡N	180 – 1.4(3)
C≡N	1.1602(19)	C–C–C/2	56.25(16)
C–H	1.1090(22)	H–C–H/2	53.47(21)

$r_{\text{m}}^{\text{p} \text{ a})}$	Å	$\theta_{\text{m}}^{\text{p} \text{ a})}$	deg
C–C	1.454(2)	C–C≡N	180 – 2.2(4)
C≡N	1.152(3)	C–C–C/2	56.0(2)
C–H	1.103(3)	H–C–H/2	53.7(2)

Atom	a_{m}^{p} [Å]	b_{m}^{p} [Å]	c_{m}^{p} [Å]
N	±2.1849	–0.5423	0.0
C(1)	±1.2055	0.0649	0.0
C(2)	0.0	0.8786	0.0
H	0.0	1.5313	±0.8894



The authors of [2] state that the r_{m}^{p} structure given in [1] is not very accurate and that the $r_{\text{e}}(\text{C–H})$ value is more probably near 1.088 Å than near 1.103 Å.

^{a)} Multiple isotope substitution structure.

[1] Randell, J., Cox, A.P., Merke, I., Dreizler, H.: J. Chem. Soc., Faraday Trans. **86** (1990) 1981.

[2] Demaison, J., Wlodarczak, G.: Struct. Chem. **5** (1994) 57.