

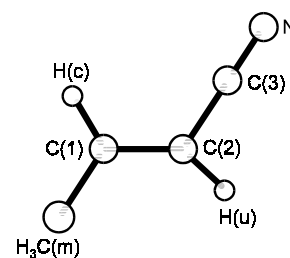
1589
MW

C₄H₅N

(E)-2-Butenenitrile
Crotononitrile

C_s
H₃C–CH=CH–C≡N

$r_e^a)$	$\text{\AA}^b)$	$\theta_e^a)$	$\text{deg}^b)$
C(3)≡N	1.158(3)	C(1)=C(2)–C(3)	122.1(3)
C(1)=C(2)	1.339(5)	C(2)=C(1)–C(m)	123.8(5)
C(2)–C(3)	1.430(3)	C(1)=C(2)–H(u)	121.1(3)
C(1)–C(m)	1.491(5)	C(2)=C(1)–H(c)	118.6(5)
C(2)–H(u)	1.083(5)	C(1)–C(m)–H(s)	111.3(5)
C(1)–H(c)	1.085(5)	C(1)–C(m)–H(a)	110.5(5)
C(m)–H(s)	1.089(5)	C(2)–C(3)≡N	179.4(5)
C(m)–H(a)	1.091(5)	C(2)=C(1)–C(m)–H(a)	120.8(5)



^{a)} A near-equilibrium structure was estimated using offsets derived empirically.

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

Lesarri, A.G., Cosleou, J., Li, X., Wlodarczak, G., Demaison, J.: J. Mol. Spectrosc. **172** (1995) 520.