

1114
ED, MW

C₃H₃NO

2-Oxopropanenitrile

Acetyl cyanide
Pyruvonnitrile

C_s
H₃C–C(O)–C≡N

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(3)–H	1.116(11)	H–C(3)–H	109.2(7)
C(2)–C(3)	1.518(9)	C(1)–C(2)–C(3)	114.2(9)
C(2)=O	1.208(9)	C(3)–C(2)=O	124.6(7)
C(1)–C(2)	1.477(8)	C(2)–C(1)≡N	179.2(22) ^{b)}
C(1)≡N	1.167(10)		

The measurements were made at room temperature.

^{a)} Estimated limits of error.

^{b)} The C≡N bond is *anti* to the C=O bond.

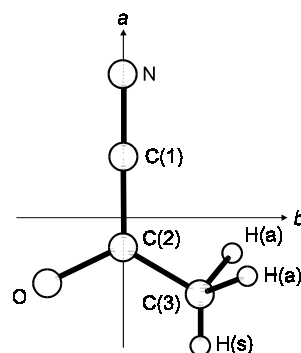
Sugie, M., Kuchitsu, K.: J. Mol. Struct. **20** (1974) 437.

MW

r_s	Å	θ_s	deg
C(3)–H(s)	1.083(4)	H(s)–C(3)–H(a)	111.1(21)
C(3)–H(a)	1.091(2)	H(a)–C(3)–H(a)	105.1(16)
C(2)–C(3)	1.476(14)	C(1)–C(2)–C(3)	119.6(18)
C(2)=O	1.245(6)	C(3)–C(2)=O	123.7(17)
C(1)–C(2)	1.457(16)	C(2)–C(1)≡N	176.2(43) ^{a)}
C(1)≡N	1.166(17)		

r_0	Å	θ_0	deg
C(3)–H(s)	1.102(13)	H(s)–C(3)–H(a)	109.5(14)
C(3)–H(a)	1.067(3)	H(a)–C(3)–H(a)	104.6(13)
C(2)–C(3)	1.488(22)	C(1)–C(2)–C(3)	114.2(15)
C(2)=O	1.218(24)	C(3)–C(2)=O	125.3(37)
C(1)–C(2)	1.489(49)	C(2)–C(1)≡N	180.0 ^{b)}
C(1)≡N	1.149(13)		

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(3)	–1.230	1.196	0.0
H(s)	–2.2991	1.0213	0.0
H(a)	–0.9293	1.7878	±0.8663
C(2)	–0.483	–0.076	0.0
O	–1.026	–1.196	0.0
C(1)	0.974	–0.054	0.0
N	2.126	0.122	0.0



The discrepancies between r_0 and r_s for some of the parameters may indicate the difficulties in locating C(2), C(1), and N atoms in the molecule. The same comment applies to the deviations of the r_s/r_0 structures from the r_g/θ_α structure, which is totally unaffected by such difficulties.

^{a)} Bent toward CH₃.

^{b)} Assumed.

Pandey, G.K., Andolfatto, M., Dreizler, H.: Z. Naturforsch. **32a** (1977) 1301.