

1121
MW

C₃H₃NO₂

Methyl cyanoformate

C_s
N≡C–C(O)–OCH₃

r_0	Å
C≡N	1.153(7)
C(1)–C(2)	1.487(40)
C=O	1.209(31)
C(2)–O	1.310(23)
O–C(3)	1.447(6)
C–H(1)	1.073(11)
C–H(2,3)	1.074(27)

r_0^c	Å
C≡N	1.154(9)
C(1)–C(2)	1.477(47)
C=O	1.215(42)
C(2)–O	1.310(32)
O–C(3)	1.448(9)
C–H(1)	1.086 ^d
C–H(2,3)	1.088 ^d

r_s	Å
C≡N	1.155(7)
C(1)–C(2)	1.479(40)
C=O	1.217(31)
C(2)–O	1.311(23)
O–C(3)	1.447(6)
C–H(1)	1.074(11)
C–H(2,3)	1.074(27)

θ_0	deg
C(2)–C≡N	178.1(15)
C(1)–C(2)=O	120.8(27)
C(1)–C(2)–O	110.3(20) ^a
O=C–O	128.9(39)
C(2)–O–C(3)	114.0(15)
O–C(3)–H(1)	105.2(6)
O–C(3)–H(2,3)	110.3(2)
H(1)–C(3)–H(2,3)	111.2(19) ^a
H(2)–C(3)–H(3)	108.6(40) ^a
H(2)–O–C(3)–H(1) ^b	120.0(25)

θ_0^c	deg
C(2)–C≡N	178.3(22)
C(1)–C(2)=O	121.0(33)
C(1)–C(2)–O	110.6(27) ^a
O=C–O	128.4(44)
C(2)–O–C(3)	114.1(19)
O–C(3)–H(1)	106.8 ^d
O–C(3)–H(2,3)	111.5 ^d
H(1)–C(3)–H(2,3)	109.8 ^d
H(2)–C(3)–H(3)	107.4 ^d
H(2)–O–C(3)–H(1) ^b	120.0 ^d

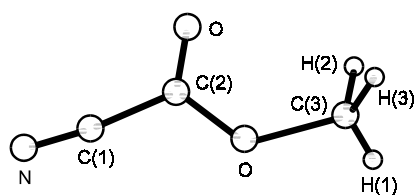
θ_s	deg
C(2)–C≡N	178.1(15)
C(1)–C(2)=O	121.2(27)
C(1)–C(2)–O	110.5(20) ^a
O=C–O	128.3(39)
C(2)–O–C(3)	114.3(15)
O–C(3)–H(1)	105.2(6)
O–C(3)–H(2,3)	109.7(2)
H(1)–C(3)–H(2,3)	109.9(19)
H(2)–C(3)–H(3)	112.2(40)
H(2)–O–C(3)–H(1) ^b	118.1(25)

^a) Dependent parameter.

^b) Dihedral angle.

^c) Heavy atom structure fit.

^d) Fixed value.



Durig, J.R., Groner, P., Lin, J., van der Veken, B.J.: J. Chem. Phys. **96** (1992) 8062.