

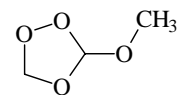
1289
MW

C₃H₆O₄

3-Methoxy-1,2,4-trioxolane

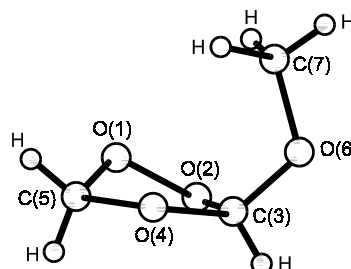
C₁

r_0	Å	θ_0	deg
C(3)–O(4)	1.418(8)	C(3)–O(4)–C(5)	105.8(4)
C(3)–O(2)	1.416(9)	O(4)–C(5)–O(1)	103.5(3)
C(3)–O(6)	1.367(7)	C(5)–O(1)–O(2)	99.2(2)
C(7)–O(6)	1.442(5)	O(1)–O(2)–C(3)	103.1(3)
C(5)–O(1)	1.407(5)	O(2)–C(3)–O(4)	105.8(5)
C(5)–O(4)	1.429(5)	O(4)–C(3)–O(6)	111.1(5)
O(1)–O(2)	1.472(4)	O(2)–C(3)–O(6)	115.3(7)
		C(5)–O(1)–O(2)–C(3)	–44.2
		O(1)–O(2)–C(3)–O(6)	–97.1
		O(4)–C(3)–O(6)–C(7)	–60.7
		O(2)–C(3)–O(4)–C(5)	1.8



r_s	Å	θ_s	deg
C(3)–O(4)	1.394(7)	C(3)–O(4)–C(5)	105.8(3)
C(3)–O(2)	1.406(5)	O(4)–C(5)–O(1)	103.6(2)
C(3)–O(6)	1.387(6)	C(5)–O(1)–O(2)	99.0(2)
C(7)–O(6)	1.427(5)	O(1)–O(2)–C(3)	102.6(2)
C(5)–O(1)	1.406(4)	O(2)–C(3)–O(4)	106.9(4)
C(5)–O(4)	1.430(4)	O(4)–C(3)–O(6)	111.6(4)
O(1)–O(2)	1.474(4)	O(2)–C(3)–O(6)	114.4(4)
		C(5)–O(1)–O(2)–C(3) ^{a)}	–43.8
		O(1)–O(2)–C(3)–O(6) ^{a)}	–97.6
		O(4)–C(3)–O(6)–C(7) ^{a)}	–60.8
		O(2)–C(3)–O(4)–C(5) ^{a)}	1.1

Atom	a_s [Å]	b_s [Å]	c_s [Å]
O(1)	1.1626	0.9115	–0.4017
O(2)	0.4402	0.8295	0.8826
C(3)	–0.2701	–0.3764	0.7583
O(4)	0.4467	–1.1800	–0.1259
C(5)	1.6023	–0.4195	–0.4926
O(6)	–1.5894	–0.2252	0.3567
C(7)	–1.7832	0.3867	–0.9181
H(8)	–0.3582	–0.8154	1.7575
H(9)	2.4129	–0.6317	0.1748
H(10)	1.8446	–0.6076	–1.5381



^{a)} Dependent parameters.

LaBarge, M.S., Keul, H., Kuczkowski, R.L., Wallasch, M., Cremer, D.: J. Am. Chem. Soc. **110** (1988) 2081.