

1285
MW

C₃H₆O₃

3-Methyl-1,2,4-trioxolane
Propylene ozonide

C₁

r_s	Å	θ_s	deg
O(4)–C(3)	1.423(18)	C(3)–O(4)–C(5)	104.6(6)
O(4)–C(5)	1.423(20)	O(4)–C(3)–O(2)	105.6(8)
O(2)–C(3)	1.399(14)	O(1)–C(5)–O(4)	105.7(4)
O(1)–C(5)	1.411(5)	C(3)–O(2)–O(1)	99.7(5)
O(1)–O(2)	1.471 ^{a)}	C(5)–O(1)–O(2)	99.2(3)
C(3)–H(7)	1.099(4)	O(4)–C(3)–H(7)	108.5(11)
C(5)–H(9)	1.091(5)	O(4)–C(5)–H(9)	109.9(7)
C(5)–H(8)	1.108(4)	O(2)–C(3)–H(7)	110.1(11)
C(6)–H(10,11,12)	1.09 ^{a)}	O(1)–C(5)–H(9)	110.7(5)
C(3)–C(6)	1.534(4)	O(4)–C(5)–H(9)	109.9(6)
		O(1)–C(5)–H(8)	105.9(4)
		O(4)–C(3)–C(6)	110.1(21)
		O(2)–C(3)–C(6)	108.3(17)
		C(6)–C(3)–H(7)	113.9(4)
		H(8)–C(5)–H(9)	114.3(3)
		C(3)–C(6)–H(10,11,12)	109.5 ^{a)}
		τ_1 ^{b) c)}	–41.0
		τ_2 ^{c) d)}	49.2
		τ_3 ^{c) e)}	–39.8
		τ_4 ^{c) f)}	15.5
		τ_5 ^{c) g)}	16.9

Atom	a_s [Å]	b_s [Å]	c_s [Å]
O(4)	–0.017	–1.1422	–0.1062
O(2)	–0.002	1.0880	0.1747
O(1)	–1.3719	0.6645	–0.1538
C(3)	0.7160	0.039	–0.4091
C(5)	–1.3037	–0.6757	0.2817
C(6)	2.1022	–0.018	0.2463
H(7)	0.7445	0.1617	–1.5010
H(8)	–2.0885	–1.2183	–0.2827
H(9)	–1.4093	–0.7349	1.3664

^{a)} Assumed.

^{b)} Dihedral angle O(4)–C(3)–O(2)–O(1).

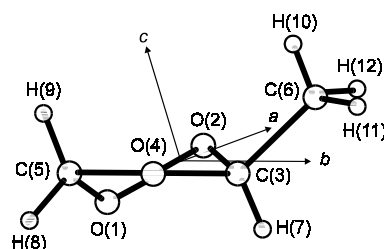
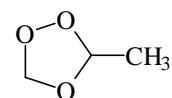
^{c)} Dependent parameters.

^{d)} Dihedral angle C(3)–O(2)–O(1)–C(5).

^{e)} Dihedral angle O(2)–O(1)–C(5)–O(4).

^{f)} Dihedral angle O(1)–C(5)–O(4)–C(3).

^{g)} Dihedral angle C(5)–O(4)–C(3)–O(2).



Lattimer, R.P., Kuczkowski, R.L., Gillies, C.W.: J. Am Chem. Soc. **96** (1974) 348.