

1567
MW

C₄H₄O₃

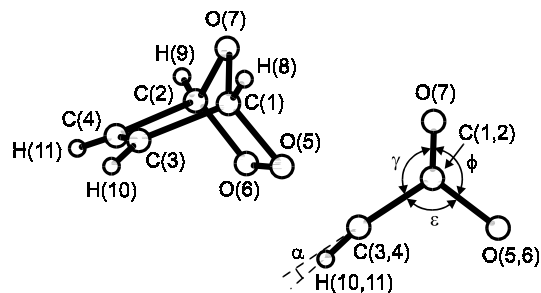
Cyclobutadiene ozonide
2,3,7-Trioxabicyclo[2.2.1]hept-5-ene

C_s

r_s	Å ^{a)}	θ_s	deg ^{a)}
C(1)–O(5)	1.435(2)	C(1)–C(3)–C(4)	103.2(2)
C(1)–O(7)	1.409(2)	C(1)–O(5)–O(6)	101.6(2)
C(1)–C(3)	1.538(2)	C(1)–O(7)–C(2)	93.8(2)
C(3)–C(4)	1.356(2)	C(3)–C(1)–O(5)	108.8(2)
O(5)–O(6)	1.480(2)	C(3)–C(1)–O(7)	103.2(2)
C(1)–H(8)	1.079(3)	O(7)–C(1)–O(5)	103.3(2)
C(3)–H(10)	1.067(3)	C(1)–C(3)–H(10)	126.7(3)
		C(4)–C(3)–H(10)	129.4(3)
		C(3)–C(1)–H(8)	109.1(3)
		O(5)–C(1)–H(8)	119.6(3)
		O(7)–C(1)–H(8)	114.5(3)
		γ	126.6(2)
		ε	109.3(2)
		ϕ	124.1(2)
		α	8.9(3)
		$\tau^b)$	32.0(3)



Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1,2)	−0.0174	±1.0291	−0.3368
C(3,4)	−1.2893	±0.6775	0.4525
O(5,6)	1.0768	±0.7402	0.5461
O(7)	0.0635	0.0	−1.2961
H(8,9)	−0.1215	±2.0202	−0.7499
H(10,11)	−1.9137	±1.3554	0.9900



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

^{b)} Dihedral angle H(8)–C(1)–C(3)–H(10).

Lorencak, P., Kuczkowski, R.L.: J. Phys. Chem. **93** (1989) 2276.