

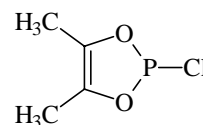
1632
MW

C₄H₆ClO₂P

2-Chloro-4,5-dimethyl-1,3,2-dioxaphosphole

C_s

r_s	Å
C=C	1.345(8)
C(ring)–C(methyl)	1.424(8)
C(methyl)...C(methyl)	3.320(6)
C(methyl)...C(ring)	2.548(5)
Cl...C(methyl)	4.471(3)
Cl...C(ring)	3.319(6)

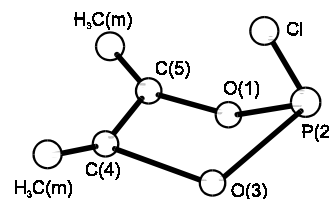


Galeev, R.V., Gunderova, L.N., Garipova, G.R., Mamleev, A.Kh., Pozdeev, N.M., Varand, O.L., Proskurnina, M.V., Khaikin, L.S.: Proc. Spie **1811** (1992) 235.

ED

r_a	Å ^{a)}	θ_a	deg ^{a)}
C=C	1.327(30)	O–P–O	95.0(8)
P–O	1.615(4)	P–O–C	108.5(10)
O–C	1.377(2)	O–C=C	112.5(8)
P–Cl	2.073(3)	O–P–Cl	98.9(3)
C(4,5)–C(m)	1.485(10)	C=C–C(m)	131.0(15)
C–H	1.090(8)	C–C–H	112.5(24)
		φ^b	16.0(10)
		O–P–O–C	15.6(11)
		P–O–C=C	11.3(8)
		O–C=C–O	0.0 ^{c)}
		Cl–P–O–C	84.2(11)

The molecule has an envelope conformation with a tricoordinated P atom in the flap. The P–Cl bond occupies an axial position.
The nozzle temperature was 55(5) °C.



^{a)} Three times the estimated standard errors.

^{b)} Dihedral angle between the OPO and OCCO planes.

^{c)} Assumed.

Khaikin, L.S., Smirnov, V.V., Proskurnina, M.V., Golubinskii, A.V., Vilkov, L.V., Zefirov, N.S.: Dokl. Akad. Nauk SSSR **296** (1987) 169; Proc. Acad. Sd. USSR (Engl. Transl.) **296** (1987) 863.