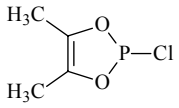
529 **$C_4H_6ClO_2P$** **2-Chloro-4,5-dimethyl-2*H*-1,3,2-dioxaphospholene** **C_s**

ED, MW, *ab initio* calculations

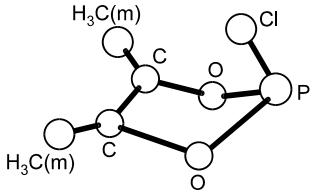
2-Chloro-4,5-dimethyl-1,3,2-dioxaphosphole



r_α^0 [a])	Å [b])	θ_α^0 [a])	deg [b])
P–O	1.633(3)	O–P–O	93.3(5)
O–C	1.415(7)	P–O–C	109.6(4)
C=C	1.329(10)	O–C=C	111.7(3)
P–Cl	2.101(6)	O–P–Cl	100.2(4)
C–C(m)	1.488(7)	C=C–C(m)	133.0(4)
C–H (average)	1.082(36)	C–C–H	109.8(24)
		Cl–P–O–C	82.6(5)
		φ [c])	18.7(8)

The ED data from [1] were reinvestigated. The refined structural parameters are in agreement with the results of RHF/6-31G* and MP2/6-31G* calculations except for the P–O bond length.
The temperature of the experiments was 328 K.

[a]) Vibrational corrections to r_a parameters were calculated taking into account nonlinear relations between the internal and Cartesian coordinates.
[b]) Uncertainties were unidentified, possibly estimated total errors.
[c]) Deviation of the OPO plane from the ring plane.



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MW

The height of the barrier to internal rotation of the methyl groups and the frequency of torsional vibrations were determined to be $V_{30} = V_{03} = 665$ cm^{-1} and $\nu = 167$ cm^{-1}, respectively.

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II/25C (3, 1632)