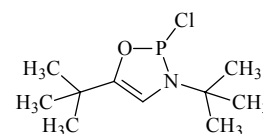


892 C₁₀H₁₉ClNOPED, *ab initio* and DFT
calculations**3,5-Di-*t*-butyl-2-chloro-2,3-dihydro-[1,3,2]oxazaphosphole C₁**2-Chloro-3,5-bis(1,1-dimethylethyl)-
2,3-dihydro-1,3,2-oxazaphosphole

r_a	\AA^a	θ_a	deg^a
P–Cl	2.177(6)	O–P–N	94.5(12)
P–O	1.657(10)	P–N–C(4)	108.7(19)
P–N	1.698(15)	C–N–C ^b	121.7(21)
C–O ^b	1.392(27)	C(5)=C(4)–N	112.2(28)
C(4)=C(5)	1.348(16)	C(4)=C(5)–O	115.0(23)
N–C(4)	1.398(13)	P–O–C ^b	108.8(15)
N–C(7)	1.474(13)	O–P–Cl	99.1(10)
$\Delta(\text{N–C})^c$	0.072(39)	N–P–Cl	101.1(8)
C–C(methyl)	1.557(5)	P–N–C(7)	129.6(11)
C(5)–C(8)	1.510(5)	C(4)=C(5)–C(8)	134.6(24)
$\Delta(\text{C–C})^d$	0.036 ^e	N–C–C(methyl)	109.3(8)
C–H	1.091(5)	C–C–C(methyl)	109.3(8)
		C(methyl)–C–C(methyl) ^b	109.6(8)
		τ_1^f	8.4(16)
		τ_2^g	139.9(30)
		τ_3^h	120.3(131)

Local C_{3v} symmetry was assumed for the methyl and *t*-butyl groups. The molecule was found to have a P-envelope conformation with the axial orientation of the P–Cl bond. The temperature of the measurements was 60 °C.

^a) Three times the estimated standard errors.

^b) Dependent parameter.

^c) $r_\alpha[\text{N–C}(7)] - r_\alpha[\text{N–C}(4)]$.

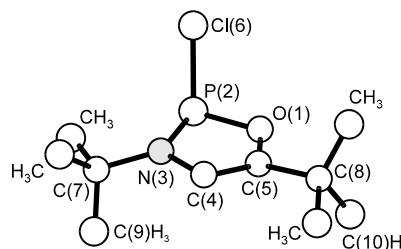
^d) $r_\alpha[\text{C–C(methyl)}] - r_\alpha[\text{C}(5)–\text{C}(8)]$.

^e) Assumed at the value from MP2/6-31G** and B3PW91/6-31G** calculations.

^f) Torsional angle O–P–N–C(4).

^g) Torsional angle C(9)–C(7)–N–P.

^h) Torsional angle C(10)–C(8)–C(5)=C(4).



Naumov, V.A., Dakkouri, M., Ziatdinova, R.N., Oberhammer, H.: Mendelev Comm. (1999) 225.