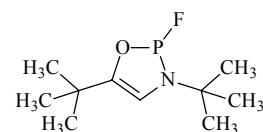


893 C₁₀H₁₉FNOPED, *ab initio*
calculations**3,5-Bis(1,1-dimethylethyl)-2-fluoro-2,3-dihydro-
1,3,2-oxazaphosphole**3,5-Di-*t*-butyl-2-fluoro-2,3-
dihydro-1,3,2-oxazaphospholeC₁

r_a	\AA^a	θ_a	deg^a
P–F	1.641(11)	O–P–N	92.7(11)
P–O	1.645(9)	P–N–C(4)	107.5(12)
P–N	1.706(9)	C(5)=C(4)–N	112.4(16)
$\Delta(\text{P–N, O})^b$	0.061(20) ^c	C(4)=C(5)–O	113.0(18)
C(4)=C(5)	1.344 ^d	P–O–C	112.1(20)
N–C(4)	1.435(9)	P–N–C(7)	125.1(19)
N–C(7)	1.494(9)	C–N–C	119.9(19)
$\Delta(\text{N–C})^e$	0.059 ^e	$\Delta(\text{C–N–C, P})^f$	5.2 ^e
C–O	1.365(9)	O–P–F	102.5(20)
C–C(methyl) ^g	1.542(3)	N–P–F	105.1(20)
C(5)–C(6)	1.513(3)	$\Delta(\text{F–P–N, O})^h$	2.6(11) ^e
$\Delta(\text{C–C})^i$	0.029 ^e	C(4)=C(5)–C	131.4(42)
C–H	1.095(4)	N–C–C(methyl)	110.6(11)
		C–C–C(methyl)	110.6(11)
		C(methyl)–C(6,7)–C(methyl) ^g	108.4(11)
		C(4)–N–P–O	13.2(54)
		C(8)–C(7)–N–P	144.7(60)
		C(9)–C(6)–C(5)=C(4)	126.1(98)

Local C_{3v} symmetry was assumed for the methyl and *t*-butyl groups. The N=C=C–O moiety was assumed to be planar. The diheterophospholene ring was found to have a P-envelope conformation with axial orientation of the P–F bond. The *t*-butyl group bonded to N is pseudoequatorial.

The measurements were made at 40 °C.

^a) Three times the estimated standard errors.

^b) [P–N] – [P–O].

^c) Constrained to the value from HF/3-21G* calculations.

^d) Assumed.

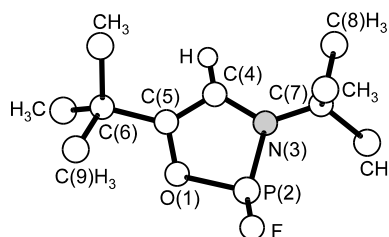
^e) [N–C(7)] – [N–C(4)].

^f) [P–N–C(7)] – [C–N–C].

^g) Mean value.

^h) [N–P–F] – [O–P–F].

ⁱ) [C–C(methyl)] – [C(5)–C(6)].



Naumov, V.A., Dakkouri, M., Ziatdinova, R.N., Oberhammer, H.: *Mendeleev Commun.* (1998) 89.