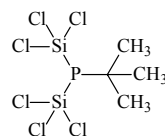


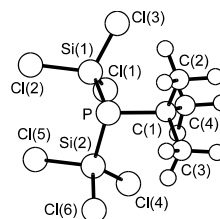
579  $\text{C}_4\text{H}_9\text{Cl}_6\text{PSi}_2$ ED, *ab initio*  
calculations*(t*-Butyl)bis(trichlorosilyl)phosphine $\text{C}_1$ 

$r_a$	$\text{\AA}^a$	$\theta_a$	$\text{deg}^a$
C–H	1.129(15)	C–C–H	111.8(5)
P–C	1.906(6)	P–C–C <sup>b</sup>	109.7(6)
C–C	1.565(6)	P–Si–Cl <sup>b</sup>	111.1(2)
P–Si	2.210(5)	C–P–Si <sup>b</sup>	104.7(7)
Si–Cl	2.032(1)	P–C(1)–C(2)	105.9(7)
		P–C(1)–C(4)	115.1(9)
		P–C(1)–C(3)	107.9(8)
		C(2)–C(1)–C(4)	109.7(14)
		C(2)–C(1)–C(3)	108.0(13)
		C(4)–C(1)–C(3)	109.9(17)
		P–Si(1)–Cl(1)	116.3(5)
		P–Si(1)–Cl(2)	107.5(8)
		P–Si(1)–Cl(3)	109.4(7)
		Cl(1)–Si(1)–Cl(2)	107.3(9)
		Cl(1)–Si(1)–Cl(3)	107.2(9)
		Cl(2)–Si(1)–Cl(3)	108.6(17)
		P–Si(2)–Cl(4)	117.4(5)
		P–Si(2)–Cl(5)	106.8(6)
		P–Si(2)–Cl(6)	109.3(6)
		Cl(4)–Si(2)–Cl(5)	108.8(10)
		Cl(4)–Si(2)–Cl(6)	107.6(10)
		Cl(5)–Si(2)–Cl(6)	106.6(17)
		C(2)–C(1)–P–Si(1,2) <sup>b</sup>	127.6(4)
		$\Delta[\text{C}(2)\text{--C}(1)\text{--P--Si}]^c$	81.2(17)
		$\tau(\text{CH}_3)^d$	–63.6(20)
		Cl(1,4)–Si–P–C(1) <sup>b</sup>	52.9(12)
		$\Delta[\text{Cl}(1,4)\text{--Si--P--C}(1)]^e$	30.8(10)



Some refining parameters and/or their differences were restrained to the values from MP2/6-31G\* calculations. The angles at the Si and C(1) atoms were found to vary from 105.9(7) to 117.4(5)°, indicating that the three groups are greatly distorted from regular tetrahedral geometry. The *t*-butyl group was found to tilt in the direction of the lone pair of P atom with virtually no equatorial tilt. One SiCl<sub>3</sub> group is tilted towards the *t*-butyl group and one tilted away, both with axial and equatorial components. According to results of HF/6-31G\* calculations, the fully staggered C<sub>s</sub> conformation is a saddle point and 26.7 kJ mol<sup>–1</sup> higher in energy than the C<sub>1</sub> conformer.

The nozzle temperature was 435 K.



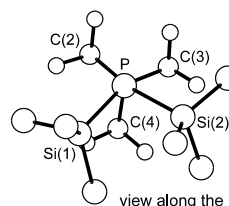
<sup>a</sup>) Estimated standard errors.

<sup>b</sup>) Mean value.

<sup>c</sup>) [C(2)–C(1)–P–Si(1)] – [C(2)–C(1)–P–Si(2)].

<sup>d</sup>) Torsional angle around the local C<sub>3</sub> axis, zero position when the P–C and C–H bonds are eclipsed.

<sup>e</sup>) [Cl(1)–Si–P–C(1)] – [Cl(4)–Si–P–C(1)].



view along the P–C bond

Hinchley, S.L., Robertson, H.E., Rankin, D.W.H., du Mont, W.-W.: J. Chem. Soc., Dalton Trans. (2002) 3787.