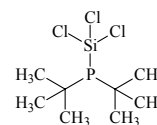


**853**      **C<sub>8</sub>H<sub>18</sub>Cl<sub>3</sub>PSi**ED, *ab initio*  
calculations**Di-*t*-butyl(trichlorosilyl)phosphine**

Bis(1,1-dimethylethyl)(trichlorosilyl)phosphine

**C<sub>1</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C–H	1.136(4)	C–C–H	109.2(9)
C–C	1.536(2)	P–C–C (mean)	109.2(4)
P–C (mean)	1.925(10)	P–Si–Cl (mean)	112.9(2)
Si–Cl	2.047(3)	C(6)–P–C(2) <sup>b)</sup>	110.6(13)
P–Si	2.250(12)	Si–P–C(6) <sup>b)</sup>	103.4(8)
		Si–P–C(2) <sup>b)</sup>	102.8(6)
		P–Si–Cl(3) <sup>b)</sup>	118.8(7)
		P–Si–Cl(4) <sup>b)</sup>	108.9(16)
		P–Si–Cl(5) <sup>b)</sup>	110.6(16)
		P–C(6)–C(7) <sup>b)</sup>	104.9(10)
		P–C(6)–C(8) <sup>b)</sup>	107.6(10)
		P–C(6)–C(9) <sup>b)</sup>	114.9(10)
		P–C(2)–C(3) <sup>b)</sup>	106.3(8)
		P–C(2)–C(4) <sup>b)</sup>	105.3(8)
		P–C(2)–C(5) <sup>b)</sup>	115.7(9)
		SiCl <sub>3</sub> torsion <sup>c)</sup>	194.1(15)
		tilt (SiCl <sub>3</sub> ) axial <sup>d)</sup>	6.0(6)
		tilt (SiCl <sub>3</sub> ) equat. <sup>d)</sup>	–0.5(19)
		twist (CH <sub>3</sub> ) <sup>e)</sup>	6.2(19)
		<i>t</i> -butyl torsion (mean) <sup>f)</sup>	18.1(21)
		<i>t</i> -butyl torsion (difference)	288.3(10)
		tilt ( <i>t</i> -butyl) axial (mean) <sup>g)</sup>	5.9(6)
		tilt ( <i>t</i> -butyl) equat. (mean) <sup>g)</sup>	–0.7(4)
		Cl(5)–Si–P–C(2) <sup>b)</sup>	–163.4(16)
		C(3)–C(2)–P–C(6) <sup>b)</sup>	–156.5(23)
		C(8)–C(6)–P–Si <sup>b)</sup>	–161.8(21)



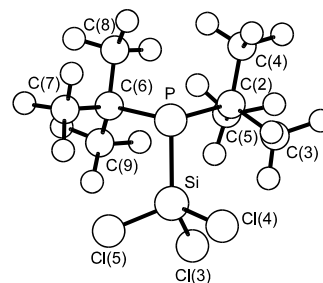
Local C<sub>3</sub> symmetry was assumed for the *t*-butyl and SiCl<sub>3</sub> groups. Local C<sub>3v</sub> symmetry and no tilt were assumed for methyl groups. Both *t*-butyl and SiCl<sub>3</sub> groups were found to be twisted *ca.* 17° from the perfectly staggered positions and tilted about 6° away from each other. See the original paper for more details of the relative orientations of the *t*-butyl groups. Values for geometrical restraints were taken from MP2/6-31G\* calculations. The nozzle temperature was *ca.* 448 K.

<sup>a)</sup> Uncertainties were unidentified, possibly estimated standard errors.

<sup>b)</sup> Dependent parameter.

<sup>c)</sup> Torsional angle of SiCl<sub>3</sub> group around the P–Si bond (*z* axis); zero degree when the Si–Cl(3) bond lies in the *xz* plane of a right-handed coordinate system with P at the origin; positive value for anticlockwise rotation when viewed down the axis from Si to P. The *x* axis is nearly in the direction of the phosphorous lone pair.

<sup>d)</sup> Axial and equatorial tilts of SiCl<sub>3</sub> group are anticlockwise rotations at Si atom about the axes parallel to the *y* axis and the *x* axis, respectively (see footnote c for definition of local coordinate system).



- <sup>e)</sup> Angle of torsion of C(methyl)–H bond around C–C(methyl) axis from the staggered position.
  - <sup>f)</sup> Angle of torsion of *t*-butyl group about P–C bond (*z* axis).
  - <sup>g)</sup> Axial and equatorial tilts of *t*-butyl group are rotations about the *y* axis and the *x* axis of the local coordinate system, respectively; positive axial tilt moves *t*-butyl group towards the phosphorus lone pair and equatorial tilt moves this group around the three-fold belt.
- du Mont, W.W., Müller, L., Martens, R., Papathomas, P.M., Smart, B.A., Robertson, H.E., Rankin, D.W.H.: Eur. J. Inorg. Chem. (1999) 1381.