Crystal structure of 1,1,2,2-tetra-*tert*-butyl-1,2-dichlorodisilane, $[(C_4H_9)_2ClSi]_2$

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Source of material: The reaction of tetrachloromethane with tetra-*tert*-butyldisilene furnished the title compound, which is also smoothly accessible by chlorination of 1,1,2,2-tetra-*tert*-butyldisilane, see ref. 1.

The crystal structure analysis reveals that the title compound adopts the *gauche* conformation. The most conspicuous feature is the Si–Si bond length of 246.8(1) pm which is markedly longer than that of the normal single bond length (234 pm, see ref. 2).

$C_{16}H_{36}Cl_2Si_2$, orthorhombic, *Pbcn* (No. 60), $a = 7.995(1)$ Å, $b = 14.904(2)$ Å, $c = 17.965(2)$ Å, $V = 2140.7$ Å³, $Z = 4$, $R(F) = 0.044$, $R_w(F) = 0.046$.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow plate, size 0.75 x 0.75 x 0.45 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	4.10 cm ⁻¹
Diffractometer:	AXS P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	2461
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	92
Program:	SHELXTL-plus

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(11A)	8d	0.1579(4)	0.0769(2)	0.0364(1)	0.08
H(11B)	8d	0.2902(4)	0.0038(2)	0.0583(1)	0.08
H(11C)	8d	0.3221(4)	0.1048(2)	0.0781(1)	0.08
H(12A)	8d	0.2326(3)	0.0093(2)	0.2527(1)	0.08
H(12B)	8d	0.3672(3)	0.0644(2)	0.2086(1)	0.08
H(12C)	8d	0.3353(3)	-0.0366(2)	0.1888(1)	0.08
H(13A)	8d	-0.0349(4)	-0.0417(2)	0.1854(1)	0.08
H(13B)	8d	0.0810(4)	-0.0851(2)	0.1249(1)	0.08
H(13C)	8d	-0.0563(4)	-0.0156(2)	0.1014(1)	0.08
H(21A)	8d	-0.0443(4)	0.3351(2)	0.1288(2)	0.08
H(21B)	8d	-0.1873(4)	0.3132(2)	0.1856(2)	0.08
H(21C)	8d	-0.2301(4)	0.3290(2)	0.1014(2)	0.08
H(22A)	8d	0.0263(4)	0.2223(2)	0.0292(1)	0.08
H(22B)	8d	-0.1631(4)	0.2222(2)	0.0067(1)	0.08
H(22C)	8d	-0.0723(4)	0.1315(2)	0.0247(1)	0.08
H(23A)	8d	-0.2851(3)	0.0952(2)	0.1226(2)	0.08
H(23B)	8d	-0.3760(3)	0.1835(2)	0.0978(2)	0.08
H(23C)	8d	-0.3332(3)	0.1678(2)	0.1820(2)	0.08

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Cl(1)	8d	0.23895(8)	0.24687(4)	0.17665(4)	0.0631(4)	0.0629(4)	0.0722(4)	-0.0239(3)	0.0079(3)	0.0022(3)
Si(1)	8d	0.04182(6)	0.15382(4)	0.18389(3)	0.0374(3)	0.0389(3)	0.0399(3)	-0.0007(2)	-0.0002(2)	0.0012(2)
C(1)	8d	0.1486(3)	0.0461(2)	0.1488(1)	0.048(1)	0.049(1)	0.046(1)	0.006(1)	-0.001(1)	-0.006(1)
C(2)	8d	-0.1280(3)	0.2035(2)	0.1203(1)	0.051(1)	0.060(1)	0.049(1)	0.007(1)	-0.004(1)	0.011(1)
C(11)	8d	0.2383(4)	0.0590(2)	0.0733(1)	0.070(2)	0.087(2)	0.057(1)	0.013(2)	0.013(1)	-0.010(1)
C(12)	8d	0.2838(3)	0.0183(2)	0.2049(1)	0.054(1)	0.068(2)	0.067(1)	0.020(1)	-0.007(1)	-0.010(1)
C(13)	8d	0.0229(4)	-0.0315(2)	0.1393(1)	0.078(2)	0.053(1)	0.062(1)	0.001(1)	-0.004(1)	-0.016(1)

Table 3. (Continued)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(21)	8 <i>d</i>	−0.1491(4)	0.3048(2)	0.1354(2)	0.104(2)	0.066(2)	0.087(2)	0.032(2)	−0.004(2)	0.021(2)
C(22)	8 <i>d</i>	−0.0800(4)	0.1940(2)	0.0373(1)	0.077(2)	0.106(2)	0.050(1)	0.013(2)	−0.006(1)	0.018(2)
C(23)	8 <i>d</i>	−0.2960(3)	0.1584(2)	0.1318(2)	0.047(1)	0.107(2)	0.072(2)	0.007(2)	−0.015(1)	0.020(2)

References

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