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Chlorotrimethylsilane

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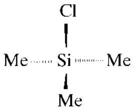
The title compound, C_3H_9ClSi, is liquid at room temperature. It was crystallized *in situ* on the diffractometer in a cold N_2 gas stream, forming a single crystal. The $(CH_3)_3SiCl$ molecule lies on a crystallographic mirror plane. The bond distances are Si—Cl 2.0863 (9) Å and Si—C 1.843 (3) and 1.845 (3) Å.

Comment

Alkylchlorosilanes such as $(CH_3)_3SiCl$, $(CH_3)_2SiCl_2$ and CH_3SiCl_3 are useful monomers in macromolecular organosilicon chemistry. Hydrolyzation of these chloromethylsilanes yields linear siloxanes and in this reaction the title compound, $(CH_3)_3SiCl$, (I), functions as a terminal chain group. However, crystal structure determinations of these important industrial chemical compounds have not previously been carried out. Here, the crystal structure of the first member of the chloromethylsilanes, chlorotrimethylsilane, (I), is reported.



$$\mathrm{Me{-}\overset{\overset{\textstyle Cl}{|}}{\underset{\underset{\textstyle Me}{|}}{Si}}{-}Me}$$

(I)

The title compound is liquid at room temperature and melts at 176 K, so a single crystal was grown at that temperature using the technique described below. Compound (I) crystallizes in the monoclinic space group $P2_1/m$, the molecule occupying a special position on the crystallographic mirror plane (see Fig. 1). The Cl, Si and one C atom, plus one H atom, lie in that plane. There is no indication of rotational disorder of the methyl groups.

The C—Si bond lengths of 1.843 (3) and 1.845 (3) Å are comparable with the corresponding bond lengths obtained by the structure determinations of 2,5-dichloro-2,5-dimethyl-2,5-disilahexane [1.848 (2) and 1.862 (2) Å; Ovchinnikov *et al.*, 1985], chlorotricyclohexylsilane [1.871 (3) and 1.875 (2) Å; Lindfors *et al.*, 1998] and chlorotriphenylsilane [1.852 (3) and 1.871 (2) Å; Lobkovskii *et al.*, 1981]. The Cl—Si bond length of 2.0863 (9) Å in (I) can also be compared with that of the cited investigations of chlorinated silanes [2.074 (1) (Lobkovskii *et al.*, 1981), 2.091 (1) (Ovchinnikov *et al.*, 1985) and 2.087 (1) Å (Lindfors *et al.*, 1998)].

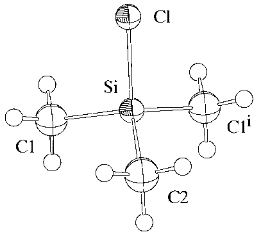


Figure 1
The molecular structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms are drawn as spheres of arbitrary radius [symmetry code: (i) $x, \frac{1}{2} - y, z$].

The C—Si—C bond angles [111.9 (1) and 112.6 (2)°] are larger than tetrahedral, while the C—Si—Cl angles [106.6 (1) and 106.9 (1)°] are significantly smaller than tetrahedral. In contrast with the polymeric crystal structure of $(CH_3)_3SnCl$ (Hossain *et al.*, 1979; Lefferts *et al.*, 1982), which exhibits short intermolecular Sn···Cl contacts of 3.269 (2) Å with a coordination number of 4+1 for the Sn atom, compound (I) is obviously tetracoordinated, with intermolecular Si···Cl contacts of 4.206 (2) Å. This is larger than the sum of the van der Waals radii (3.9 Å) for Si and Cl. Thus, the linear Cl—Si—Cl chain of the chlorotrimethylsilane structure [intermolecular Cl—Si—Cl angle of 179.9 (2)°] is comparable with the linear Cl—Sn—Cl chain in the $(CH_3)_3SnCl$ crystal.

Experimental

The title compound was condensed into a small thin-walled glass tube of 0.3 mm diameter, filling 4 mm at its tip. It was then sealed off to a length of 30 mm and fixed to an arcless and heat-insulated goniometer head, using which the sample was placed in the centre of a four-circle X-ray diffractometer equipped with an integrated N_2 gas stream cooling device of in-house construction (Dietrich & Dierks, 1970). The crystal was grown *in situ* in the cold N_2 gas stream by a process similar to pulling a single crystal from the molten substance, applying an electronically controlled coil of heating wire around the sample glass tube. It was cooled down further for the measurement.

Crystal data

C_3H_9ClSi
$M_r = 108.64$
Monoclinic, $P2_1/m$
$a = 6.2920 (10)$ Å
$b = 7.7350 (10)$ Å
$c = 6.745 (3)$ Å
$\beta = 90.800 (10)°$
$V = 328.24 (16)$ Å^3
$Z = 2$

$D_x = 1.099$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 126 reflections
$\theta = 8.0–17.3°$
$\mu = 0.626$ mm^{-1}
$T = 157$ K
Cylinder, colourless
0.8 × 0.3 × 0.3 mm

Table 1
Selected geometric parameters (Å, °).

Si—C1	1.843 (3)	Si—Cl	2.0863 (9)
Si—C2	1.845 (3)		
C1—Si—C1^i	112.6 (2)	C1—Si—Cl	106.57 (9)
C1—Si—C2	111.87 (11)	C2—Si—Cl	106.92 (12)

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

Data collection

Siemens four-circle single-crystal X-ray diffractometer with an open χ-circle of 100° and an integrated N_2 gas stream cooling device
ω–2θ scans; $\Delta\omega = 1.38° + 0.52° \times \tan\omega$
Absorption correction: analytical (the cylinder was approximated by an octagonal prism)
$T_{\min} = 0.853$, $T_{\max} = 0.864$

1216 measured reflections
971 independent reflections
689 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 31.01°$
$h = -3 \rightarrow 8$
$k = -10 \rightarrow 9$
$l = -9 \rightarrow 9$
4 standard reflections
frequency: 70 min
intensity decay: 45%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.096$
$S = 1.122$
971 reflections
47 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 0.0947P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.45$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

The C—H bond distances are in the range 0.90 (4)–1.00 (5)Å.

Data collection: Stoe software (Stoe & Cie, 1990*a*); cell refinement: Stoe software; data reduction: Stoe routine *REDUC* (Stoe & Cie, 1990*b*); program(s) used to solve structure: *SHELXS*90 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1971); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1303). Services for accessing these data are described at the back of the journal.

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122 Jürgen Buschmann *et al.* • C_3H_9ClSi *Acta Cryst.* (2000). C**56**, 121–122