Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Dihydridotetrakis(4-picoline-*N*)silicon dibromide chloroform hexasolvate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.008 Å
R factor = 0.054
wR factor = 0.148
Data-to-parameter ratio = 18.4

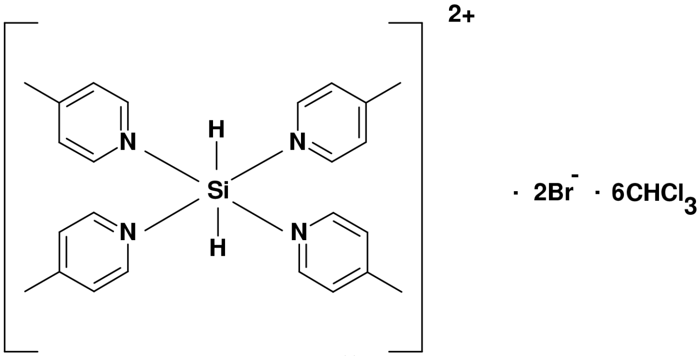
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[SiH_2(C_6H_7N)_4]Br_2 \cdot 6CHCl_3$ or $C_{24}H_{30}N_4Si^{2+} \cdot 2Br^- \cdot 6CHCl_3$, contains a hexacoordinated Si atom located on a crystallographic centre of inversion. The coordination of the Si atom can be described as a slightly distorted octahedron, with the 4-picoline ligands in the equatorial plane and the two H atoms occupying axial positions. The title compound is isomorphous with its analogue where the Br^- ions are substituted by Cl^- ions.

Received 23 January 2001
Accepted 31 January 2001
Online 13 February 2001

Comment

The title compound, (I), is isomorphous with its analogue where the Br^- ions are substituted by Cl^- ions (Stumpf & Bolte, 2001).



(I)

Experimental

The title compound was prepared as described by Faber (2000).

Crystal data

$C_{24}H_{30}N_4Si^{2+} \cdot 2Br^- \cdot 6CHCl_3$
M_r = 1278.64
Triclinic, $P\bar{1}$
a = 9.506 (1) Å
b = 11.337 (2) Å
c = 12.960 (2) Å
α = 92.28 (1)°
β = 104.06 (1)°
γ = 98.20 (1)°
V = 1337.0 (3) $Å^3$

Z = 1
D_x = 1.588 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 8192 reflections
θ = 1–25°
μ = 2.47 mm^{-1}
T = 173 (2) K
Needle, colourless
0.6 × 0.4 × 0.3 mm

Data collection

Siemens CCD three-circle diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.290, T_{max} = 0.477
15 431 measured reflections
4721 independent reflections
3954 reflections with $I > 2\sigma(I)$

R_{int} = 0.027
θ_{max} = 25.0°
h = −11 → 8
k = −13 → 13
l = −15 → 15
98 standard reflections
frequency: 1440 min
intensity decay: none

DOI: 101107/S1600536801002227

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.148$
$S = 1.03$
4721 reflections
256 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 3.3546P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.020$
$\Delta\rho_{\max} = 1.98$ e Å^{-3}
$\Delta\rho_{\min} = -0.75$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Si1—N1	1.958 (4)	Si1—N2	1.959 (5)
H1SI—Si1—N2	91 (2)	N1—Si1—N2	89.79 (17)

All H atoms bonded to C atoms were located by difference Fourier synthesis and refined with fixed individual displacement parameters [$U(\mathrm{H}) = 1.5U_{\mathrm{eq}}(\mathrm{C}_{\mathrm{methyl}})$ or $U(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{C})$] using a riding model with C—H(aromatic) = 0.95, C—H(methyl) = 0.98 or C—H(tertiary) = 1.00 Å. The methyl groups attached to the aromatic rings were allowed to rotate about their local threefold axis. The H atom bonded to Si was refined isotropically applying a restraint of 1.40 (1) Å to the Si—H distance

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97).

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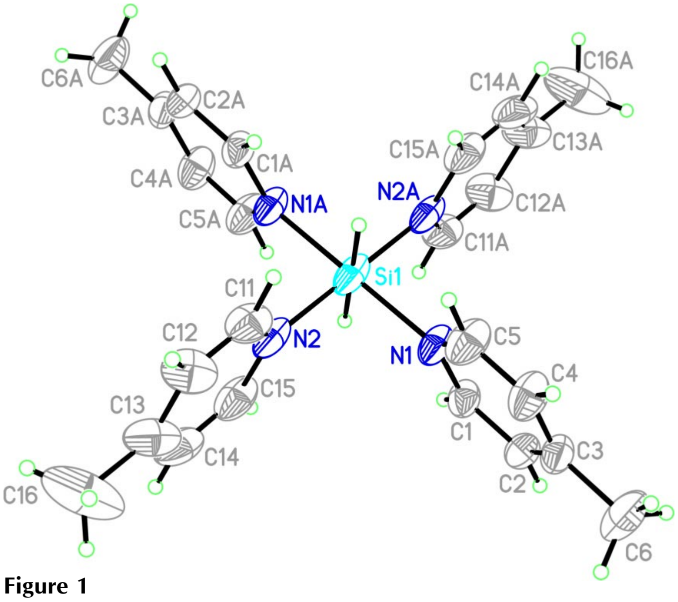

Figure 1
A perspective view of the cation of (I) with the atom-numbering scheme. Displacement ellipsoids are at the 50% probability level and H atoms are drawn as small spheres of arbitrary radii.

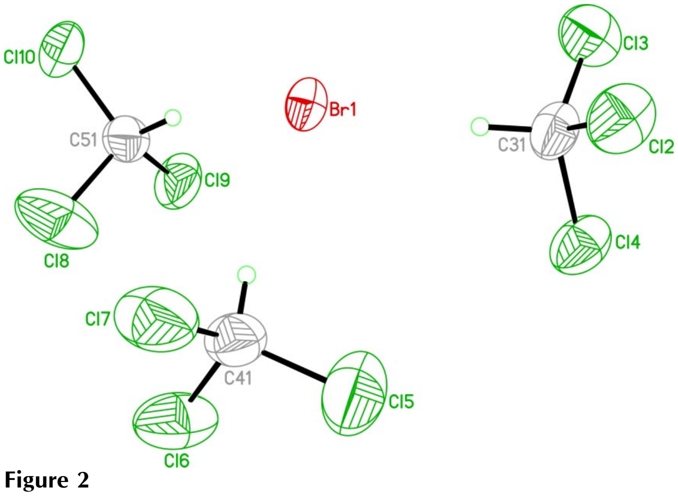

Figure 2
A perspective view of the anion and the solvent molecules of (I) with the atom-numbering scheme. Displacement ellipsoids are at the 50% probability level and H atoms are drawn as small spheres of arbitrary radii.