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Decachlorocyclopentasilanes coordinated by pairs of chloride anions, with different cations, but the same solvent molecules

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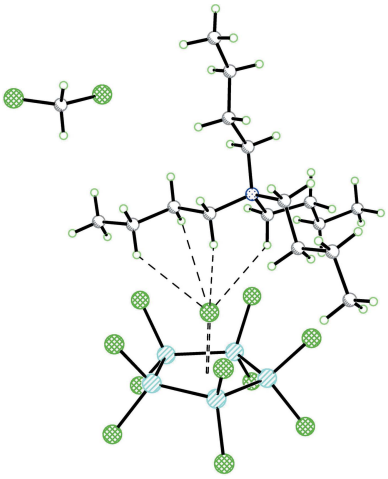
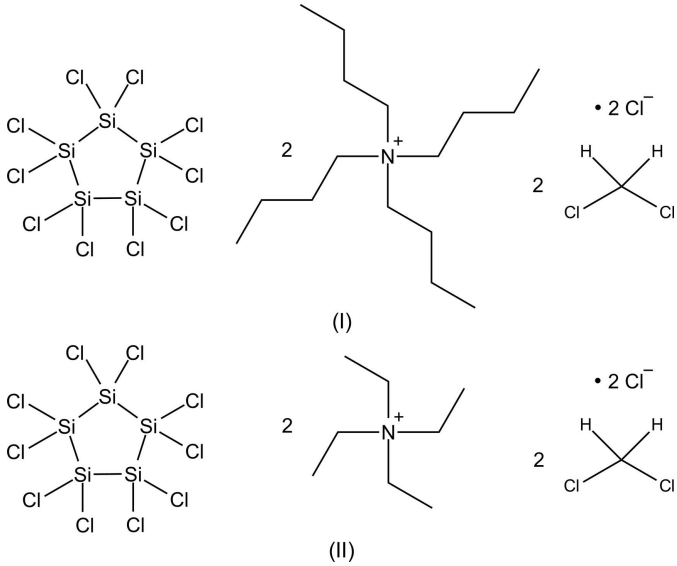
Supporting information: this article has supporting information at journals.iucr.org/e

We have determined the crystal structures of two decachlorocyclopentasilanes, namely bis(tetra-*n*-butylammonium) dichloride decachlorocyclopentasilane dichloromethane disolvate, $2C_{16}H_{36}N^{+}\cdot 2Cl^{-}\cdot Si_5Cl_{10}\cdot 2CH_2Cl_2$, (I), and bis(tetraethylammonium) dichloride decachlorocyclopentasilane dichloromethane disolvate, $2C_8H_{20}N^{+}\cdot 2Cl^{-}\cdot Si_5Cl_{10}\cdot 2CH_2Cl_2$, (II), both of which crystallize with discrete cations, anions, and solvent molecules. In (I), the complete decachlorocyclopentasilane ring is generated by a crystallographic twofold rotation axis. In (II), one cation is located on a general position and the other two are disordered about centres of inversion. These are the first structures featuring the structural motif of a five-membered cyclopentasilane ring coordinated from both sides by a chloride ion. The extended structures of (I) and (II) feature numerous C—H···Cl interactions. In (II), the N atoms are located on centres of inversion and as a result, the ethylene chains are disordered over equally occupied orientations.

1. Chemical context

The title compounds are the first known halide diadducts of the long-known perchlorinated cyclopentasilane Si_5Cl_{10} (Hengge & Kovar, 1977). Their structures can be seen as inverse-sandwich complexes, in which two chloride ions lie above and below the planar five-membered silicon ring.





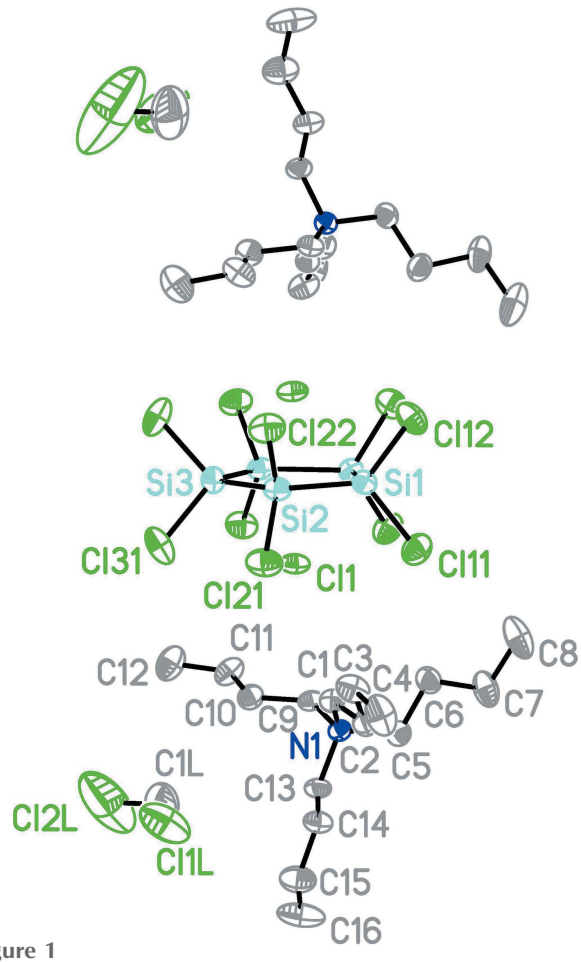


Figure 1
Perspective view of (I) with displacement ellipsoids drawn at the 50% probability level. For clarity, H atoms are omitted and only the symmetry independent molecules are labelled. Atoms without labels are generated by the symmetry operator $-x+1, y, -z+\frac{3}{2}$.

In the recent years, new and facile synthetic protocols for the Cl^- diadduct $[Si_6Cl_{14}]^{2-}$ of dodecachlorocyclohexasilane have been developed. It can either be prepared through the chloride-induced disproportionation of Si_2Cl_6, which leads directly to $[Si_6Cl_{14}]^{2-}$ (Tillmann *et al.*, 2012, 2014; Tillmann, Moxter *et al.*, 2015), or the Lewis acidic uncomplexed Si_6Cl_{12} can be used as the starting material. In the latter case, mere addition of soluble chloride salts $[R_4N]Cl$ (R = *n*Bu or Et) leads to the formation of $[Si_6Cl_{14}]^{2-}$ (Dai *et al.*, 2010). Given this background, it was of interest to investigate the Lewis acidity and ability of Si_5Cl_{10} to bind Cl^- ions.

2. Structural commentary

Bis(tetra-*n*-butylammonium) dichloride decachlorocyclopentasilane dichloromethane disolvate, $2C_{16}H_{36}N^+\cdot 2Cl^-\cdot Si_5Cl_{10}\cdot 2CH_2Cl_2$, (I), crystallizes with discrete cations, anions, and solvent molecules (Fig. 1). The five-membered decachlorocyclopentasilane ring is located on a twofold rotation axis. The Si—Cl bond lengths range from 2.081 (3) Å for Si2—Cl21 to 2.100 (3) Å for Si2—Cl22. The Si—Si bond lengths do not vary markedly: they range from 2.339 (3) Å (Si1—Si2) to 2.347 (3) Å (Si2—Si3).

The almost planar ring (r.m.s. deviation 0.002 Å) is coordinated by two chloride anions located above and below the ring. The distances of the chloride ions to the Si atoms [Cl1···Si1 2.907 (3), Cl1···Si2 2.914 (3), Cl1···Si3 2.930 (3) Å,] show that the chloride ions are located almost exactly above the centroid of the ring [distance Cl1···*Cg* = 2.1434 (16) Å].

Bis(tetraethylammonium) dichloride decachlorocyclopentasilane dichloromethane disolvate, $2C_8H_{20}N^+\cdot 2Cl^-\cdot Si_5Cl_{10}\cdot 2CH_2Cl_2$, (II), crystallizes as (I) with discrete cations, anions, and solvent molecules (Fig. 2). The Si—Cl bonds again lie in a quite narrow range [2.0805 (9) Å (Si1—Cl12) to 2.1102 (8) Å (Si2—Cl22)] and the Si—Si bond lengths are also very similar [2.3386 (8) Å (Si1—Si2) to 2.3473 (7) Å (Si4—Si5)].

The five-membered decachlorocyclopentasilane ring is almost planar (r.m.s. deviation = 0.017 Å) and coordinated by two chloride anions located above and below the ring with a Cl···*Cg* distance of 2.1781 (5) Å for Cl1 and 2.1237 (5) Å for Cl2. The Cl···Si distances range from 2.9381 (7) Å (Cl1···Si5) to 2.9645 (7) Å (Cl1···Si2) and from 2.8759 (8) Å (Cl2···Si2) to 2.9510 (7) Å (Cl2···Si5). Since the Cl···Si distances have a broader range for Cl2, it can be said that this ion is slightly displaced from a position directly over the ring centroid.

It is interesting to note that (I) and (II) have – apart from the different cations – the same molecular stoichiometry, *i.e.* one Si_5Cl_{10} ring coordinated by two chloride anions, two cations and two solvent dichloromethane molecules. However, since (I) has twofold rotation symmetry, there are only half of the chemical entities in the asymmetric unit.

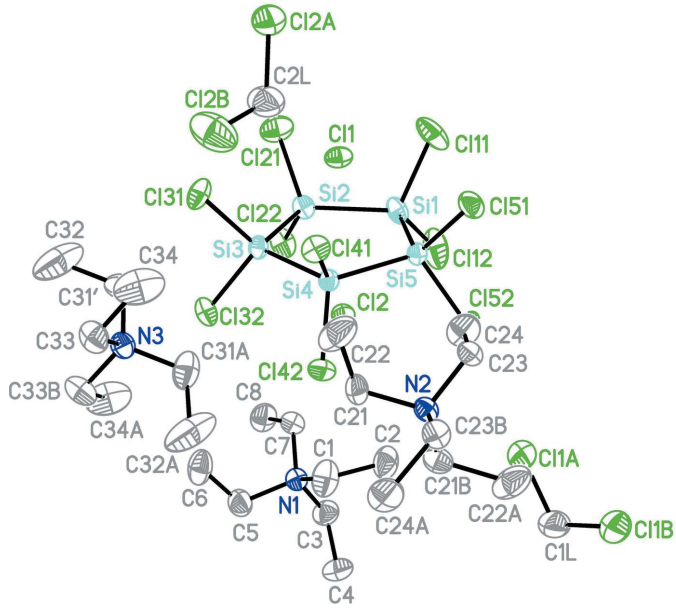


Figure 2
Perspective view of (II) with displacement ellipsoids drawn at the 50% probability level. For clarity, H atoms are omitted and only one of the two disordered sites of the tetraethylammonium cations are shown.

Table 1
Hydrogen-bond geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···Cl1	0.99	2.88	3.686 (7)	139
C2—H2A···Cl31^{i}	0.99	2.89	3.596 (8)	129
C5—H5A···Cl22^{ii}	0.99	2.99	3.945 (7)	163
C9—H9B···Cl1	0.99	2.91	3.652 (7)	132
C1L—H1L1···Cl12^{ii}	0.99	2.96	3.528 (13)	119

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···Cl42	0.99	2.99	3.829 (3)	144
C2—H2C···Cl2	0.98	2.95	3.753 (3)	139
C3—H3A···Cl52^{i}	0.99	2.79	3.643 (3)	144
C3—H3B···Cl2B^{ii}	0.99	2.98	3.804 (3)	142
C5—H5B···Cl22^{iii}	0.99	2.89	3.850 (3)	165
C6—H6B···Cl21^{iii}	0.98	2.86	3.630 (3)	136
C7—H7A···Cl2	0.99	2.86	3.394 (2)	115
C22—H22C···Cl51^{iv}	0.98	2.89	3.847 (4)	165
C22—H22E···Cl41	0.98	2.90	3.859 (3)	165
C23—H23B···Cl1^{iv}	0.99	2.98	3.465 (4)	111
C23′—H23C···Cl42	0.99	2.87	3.497 (4)	122
C24—H24C···Cl41	0.98	2.84	3.793 (3)	164
C24—H24E···Cl51^{iv}	0.98	2.81	3.771 (3)	165
C24—H24F···Cl2A^{iv}	0.98	2.92	3.778 (3)	147
C31′—H31C···Cl31	0.99	2.95	3.434 (5)	111
C32—H32F···Cl21^{v}	0.98	2.76	3.584 (4)	142
C33—H33A···Cl32^{vi}	0.99	2.94	3.515 (4)	118
C33′—H33D···Cl41	0.99	2.98	3.630 (5)	124
C34—H34A···Cl1B^{vii}	0.98	2.93	3.556 (3)	123
C34—H34C···Cl2B	0.98	2.89	3.716 (4)	142
C34—H34A···Cl1B^{vii}	0.98	2.93	3.556 (3)	123
C1L—H1L1···Cl12^{i}	0.99	2.90	3.421 (3)	114
C2L—H2L2···Cl41	0.99	2.96	3.465 (3)	113

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x, y, z-1$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z+1$; (v) $-x+1, -y+2, -z+1$; (vi) $-x, -y+2, -z+1$; (vii) $-x, -y+1, -z+1$.

3. Supramolecular features

The components of (I) and (II) are linked by a plethora of C—H···Cl contacts (Tables 1 and 2, respectively); in particular the chloride ions are surrounded by C—H groups. For an example, see Fig. 3. As a result of the disorder of the N2 and N3 cations in (II), a plot showing the coordination of the Cl ions looks extremely crowded and is therefore omitted.

4. Database survey

The present structures are the first examples of a decachlorocyclopentasilane ring coordinated by two anions. There are only two structures of a decachlorocyclopentasilane ring in the CSD (Version 5.38 of November 2016 plus three updates; Groom *et al.*, 2016), namely decachlorocyclopentasilane 4-methylbenzonitrile solvate (refcode ELAFON; Dai *et al.*, 2010) and decachlorocyclopentasilane acetonitrile solvate (ELAFIH; Dai *et al.*, 2010). In both of them, the decachlorocyclopentasilane ring is almost planar (0.017 Å for ELAFON and 0.001 Å for ELAFIH) and shows almost no variation in the Si—Si (2.358–2.368 Å for ELAFON and 2.342–2.349 Å for ELAFIH) and Si—Cl (2.030–2.059 Å for ELAFON and 2.034– 2.038 Å for ELAFIH) bond lengths.

Table 3
Mean values (Å) of Si—Si, Si—Cl bond lengths and Cl/N···Cg contacts in the title compounds and related structures.

X = Cl for (I) and (II) and X = N for ELAFON and ELAFIH. The row for Si_6Cl_{12} contains data for dichloride dodecachlorohexasilanes (Tillmann, Lerner & Bolte, 2015).

Structure	Si—Si	Si—Cl	X···Cg
(I)	2.342	2.092	2.143
(II)	2.344	2.092	2.151
ELAFON	2.363	2.049	2.174
ELAFIH	2.348	2.036	2.234
Si_6Cl_{12}	2.322	2.078	1.90

The distance of the N atom to the centroid of the ring is 2.152 and 2.196 Å for ELAFON and 2.234 Å for ELAFIH. This difference could be due to the steric demand of the benzene ring in ELAFIH. The N···Cg distances are in the same range as the Cl···Cg distances in (I) and (II).

Mean values of the structural parameters of the four compared structures and dichloride dodecachlorocyclohexasilanes (Tillmann, Lerner & Bolte, 2015) are compiled in Table 3. It is remarkable that the Si—Si and Si—Cl bond

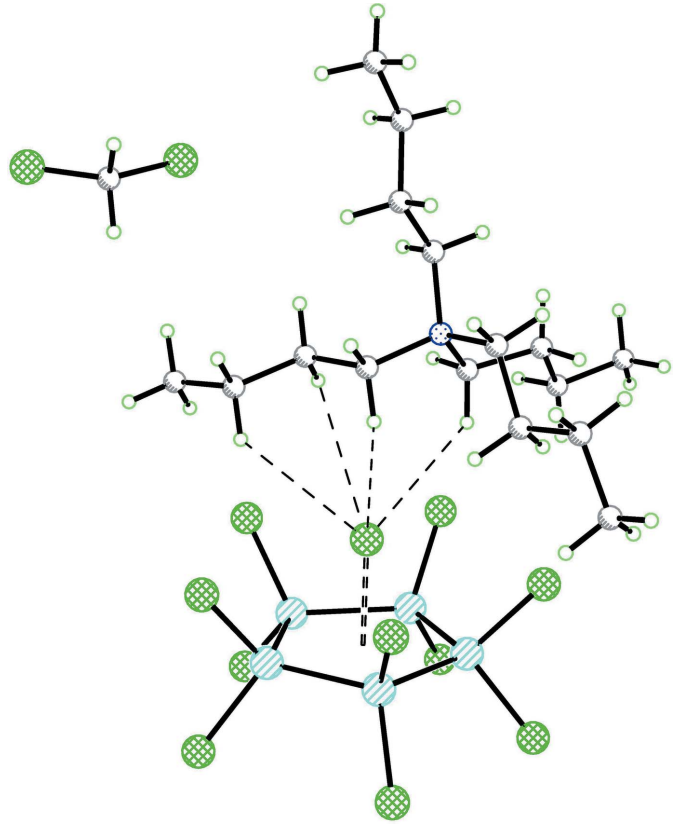


Figure 3
Perspective view of (I) showing the environment of the Cl anion. The contact to the centre of the five-membered ring is drawn as an open dashed bond. H···Cl contacts less than 3.5 Å are drawn as dashed lines.

Table 4
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$2C_{16}H_{36}N^+\cdot 2Cl^-\cdot Si_5Cl_{10}\cdot 2CH_2Cl_2$	$2C_8H_{20}N^+\cdot 2Cl^-\cdot Si_5Cl_{10}\cdot 2CH_2Cl_2$
M_r	1220.61	996.20
Crystal system, space group	Monoclinic, *C*2/*c*	Triclinic, $P\overline{1}$
Temperature (K)	173	173
a, *b*, *c* (Å)	20.9091 (15), 15.7423 (7), 19.8734 (16)	10.3596 (4), 13.9612 (5), 16.0205 (6)
α, β, γ (°)	90, 112.451 (6), 90	89.959 (3), 72.484 (3), 79.534 (3)
V (Å^3)	6045.7 (7)	2169.29 (15)
Z	4	2
Radiation type	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.85	1.17
Crystal size (mm)	0.27 × 0.16 × 0.12	0.23 × 0.23 × 0.20
Data collection		
Diffractometer	Stoe IPDS II two-circle	Stoe IPDS II two-circle
Absorption correction	Multi-scan (*X-AREA*; Stoe & Cie, 2001)	Multi-scan (*X-AREA*; Stoe & Cie, 2001)
T_{min}, T_{max}	0.543, 1.000	0.408, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32650, 5699, 4428	62962, 13044, 11976
R_{int}	0.060	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.612	0.715
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.103, 0.199, 1.15	0.048, 0.131, 1.08
No. of reflections	5699	13044
No. of parameters	258	409
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.50, −1.46	0.87, −0.84

Computer programs: *X-AREA* (Stoe & Cie, 2001), *XP* in *SHELXTL-Plus* and *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

lengths do not vary significantly between the five and six-membered Si rings, but the Cl···*Cg* distance in the dodecachlorocyclohexasilanes is significantly shorter than for decachlorocyclopentasilane. This might be due to the fact that the Cl ligands form a narrower cone in five- compared to six-membered rings.

5. Synthesis and crystallization

The addition of a solution of $[R_4N]Cl$ (*R* = *n*Bu or Et) in CH_2Cl_2 at 195 K to a solution of Si_5Cl_{10} in CH_2Cl_2 furnished the Cl^- diadducts $[R_4N]_2[Si_5Cl_{12}]$ (*R* = *n*Bu or Et) (Fig. 4). Crystals of $[R_4N]_2[Si_5Cl_{12}]$ (*R* = *n*Bu or Et) could be harvested after storage of the reaction solution for one week at 195 K in 89% and 93% yield, respectively. Both adducts are stable in the solid phase under inert conditions. However, in solution a rapid transformation of $[n\mathrm{Bu_4N}]_2[Si_5Cl_{12}]$ to $[n\mathrm{Bu_4N}]_2[Si_6Cl_{14}]$ and $[n\mathrm{Bu_4N}]_2[Si_7Cl_{16}]$ (Fig. 5) can be observed *via* ^{29}Si NMR spectroscopy (for the NMR spectrum see Fig. S1 in the Supporting information), while $[Et_4N]_2[Si_5Cl_{12}]$ is not soluble.

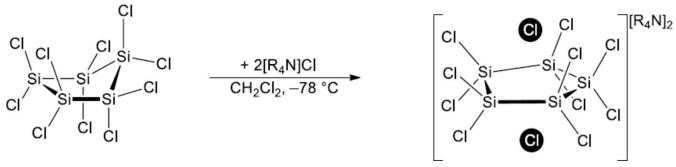


Figure 4
Synthesis of $[R_4N]_2[Si_5Cl_{12}]$ (*R* = *n*Bu or Et).

For comparison, a ^{29}Si CP/MAS NMR spectrum of single crystals of $[n\mathrm{Bu_4N}]_2[Si_5Cl_{12}]$ was recorded (Fig. S2 in the Supporting information).

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 4. H atoms were refined using a riding model, with C_{methyl}—H = 0.98 Å or $C_{methylene}$—H = 0.99 Å and with $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$ or $1.2U_{eq}(C)$.

The Cl atoms of the dichloromethane solvent molecule in (I) have rather large displacement ellipsoids, but since no valid disorder model for splitting this molecule could be found, refinement with enlarged ADPs was preferred. In (II), atoms N2 and N3 are located on centres of inversion. As a result, the ethylene chains are disordered over equally occupied orientations.

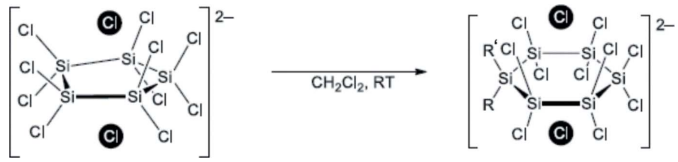


Figure 5
Transformation of $[n\mathrm{Bu_4N}]_2[Si_5Cl_{12}]$ (I) to $[n\mathrm{Bu_4N}]_2[Si_6Cl_{14}]$ (*R* = *R*′ = Cl) and $[n\mathrm{Bu_4N}]_2[Si_7Cl_{16}]$ (*R* = Cl; *R*′ = $SiCl_3$).

Acknowledgements

The authors wish to thank Johanna Becker-Baldus for the recording of the ^{29}Si CP/MAS NMR spectrum.

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supporting information

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Decachlorocyclopentasilanes coordinated by pairs of chloride anions, with different cations, but the same solvent molecules

Maximilian Moxter, Julian Teichmann, Hans-Wolfram Lerner, Michael Bolte and Matthias Wagner

Computing details

For both structures, data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA* (Stoe & Cie, 2001); data reduction: *X-AREA* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

Bis(tetra-*n*-butylammonium) dichloride decachlorocyclopentasilane dichloromethane disolvate (I)

Crystal data

$2C_{16}H_{36}N^+\cdot 2Cl^-\cdot Si_5Cl_{10}\cdot 2CH_2Cl_2$
M_r = 1220.61
Monoclinic, *C*2/*c*
a = 20.9091 (15) Å
b = 15.7423 (7) Å
c = 19.8734 (16) Å
β = 112.451 (6)°
V = 6045.7 (7) Å^3
Z = 4
F(000) = 2544
D_x = 1.341 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 30920 reflections
θ = 3.3–25.8°
μ = 0.85 mm^{-1}
T = 173 K
Needle, colourless
0.27 × 0.16 × 0.12 mm

Data collection

Stoe IPDS II two-circle diffractometer
Radiation source: Genix 3D I*μ*S microfocus X-ray source
ω scans
Absorption correction: multi-scan (X-AREA; Stoe & Cie, 2001)
T_{min} = 0.543, T_{max} = 1.000
32650 measured reflections
5699 independent reflections
4428 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 25.8°, θ_{min} = 3.3°
h = −25→25
k = −18→19
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.103
$wR(F^2)$ = 0.199
S = 1.15
5699 reflections
258 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0209P)^2 + 98.7944P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.50 e Å^{-3}
$\Delta\rho_{min}$ = −1.46 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.44920 (9)	0.65838 (13)	0.63371 (9)	0.0392 (4)
Si1	0.55353 (9)	0.75962 (13)	0.74394 (10)	0.0312 (4)
Si2	0.58692 (10)	0.61853 (14)	0.73977 (10)	0.0329 (4)
Si3	0.5000	0.53144 (19)	0.7500	0.0368 (7)
Cl11	0.55030 (11)	0.83349 (15)	0.65484 (12)	0.0536 (5)
Cl12	0.62942 (10)	0.82642 (15)	0.82814 (12)	0.0535 (6)
Cl21	0.60720 (11)	0.58866 (16)	0.64782 (11)	0.0534 (6)
Cl22	0.68493 (9)	0.59548 (15)	0.82099 (11)	0.0499 (5)
Cl31	0.46207 (13)	0.44593 (15)	0.66352 (15)	0.0667 (7)
N1	0.3868 (3)	0.7205 (4)	0.4082 (3)	0.0278 (12)
C1	0.4614 (3)	0.6993 (5)	0.4564 (4)	0.0309 (15)
H1A	0.4668	0.6368	0.4578	0.037*
H1B	0.4699	0.7185	0.5065	0.037*
C2	0.5172 (4)	0.7380 (5)	0.4335 (4)	0.0373 (17)
H2A	0.5102	0.7188	0.3838	0.045*
H2B	0.5135	0.8008	0.4329	0.045*
C3	0.5881 (4)	0.7115 (6)	0.4859 (4)	0.047 (2)
H3A	0.5894	0.6489	0.4913	0.056*
H3B	0.5969	0.7367	0.5343	0.056*
C4	0.6455 (4)	0.7395 (6)	0.4601 (6)	0.060 (3)
H4A	0.6905	0.7210	0.4956	0.090*
H4B	0.6375	0.7137	0.4127	0.090*
H4C	0.6450	0.8015	0.4557	0.090*
C5	0.3758 (4)	0.8156 (5)	0.3999 (4)	0.0351 (16)
H5A	0.3258	0.8265	0.3728	0.042*
H5B	0.4007	0.8374	0.3700	0.042*
C6	0.3994 (4)	0.8659 (5)	0.4706 (4)	0.0440 (19)
H6A	0.3744	0.8457	0.5010	0.053*
H6B	0.4495	0.8568	0.4981	0.053*
C7	0.3852 (4)	0.9597 (5)	0.4545 (5)	0.055 (2)
H7A	0.3348	0.9685	0.4288	0.066*
H7B	0.4082	0.9787	0.4219	0.066*
C8	0.4110 (5)	1.0135 (6)	0.5234 (6)	0.078 (3)
H8A	0.4008	1.0734	0.5104	0.116*
H8B	0.3877	0.9957	0.5554	0.116*
H8C	0.4611	1.0059	0.5485	0.116*
C9	0.3385 (3)	0.6853 (5)	0.4418 (4)	0.0303 (15)
H9A	0.2910	0.7045	0.4120	0.036*
H9B	0.3513	0.7107	0.4908	0.036*

C10	0.3372 (4)	0.5894 (5)	0.4494 (4)	0.0396 (17)
H10A	0.3273	0.5623	0.4015	0.047*
H10B	0.3830	0.5693	0.4835	0.047*
C11	0.2824 (4)	0.5642 (5)	0.4778 (4)	0.044 (2)
H11A	0.2364	0.5815	0.4420	0.053*
H11B	0.2906	0.5951	0.5237	0.053*
C12	0.2818 (4)	0.4698 (6)	0.4915 (5)	0.059 (2)
H12A	0.2455	0.4567	0.5097	0.088*
H12B	0.2727	0.4389	0.4459	0.088*
H12C	0.3268	0.4525	0.5276	0.088*
C13	0.3714 (4)	0.6817 (5)	0.3333 (3)	0.0348 (16)
H13A	0.4026	0.7085	0.3125	0.042*
H13B	0.3834	0.6206	0.3400	0.042*
C14	0.2978 (4)	0.6896 (6)	0.2779 (4)	0.0412 (18)
H14A	0.2839	0.7501	0.2711	0.049*
H14B	0.2657	0.6589	0.2953	0.049*
C15	0.2940 (4)	0.6515 (7)	0.2051 (4)	0.057 (2)
H15A	0.3294	0.6789	0.1907	0.068*
H15B	0.3049	0.5901	0.2118	0.068*
C16	0.2249 (5)	0.6627 (9)	0.1459 (5)	0.083 (4)
H16A	0.2251	0.6375	0.1009	0.124*
H16B	0.1898	0.6346	0.1594	0.124*
H16C	0.2143	0.7234	0.1383	0.124*
C1L	0.1235 (8)	0.4569 (8)	0.2807 (9)	0.110 (5)
H1L1	0.1317	0.4857	0.3275	0.132*
H1L2	0.0904	0.4924	0.2416	0.132*
Cl1L	0.19998 (18)	0.4539 (3)	0.2681 (2)	0.1200 (15)
Cl2L	0.0881 (5)	0.3685 (5)	0.2810 (5)	0.294 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0321 (9)	0.0584 (12)	0.0230 (8)	−0.0037 (9)	0.0059 (7)	−0.0024 (8)
Si1	0.0233 (9)	0.0364 (11)	0.0327 (10)	−0.0031 (8)	0.0092 (8)	−0.0029 (8)
Si2	0.0281 (9)	0.0417 (12)	0.0302 (10)	0.0050 (9)	0.0124 (8)	−0.0018 (9)
Si3	0.0373 (15)	0.0330 (16)	0.0421 (16)	0.000	0.0174 (13)	0.000
Cl11	0.0498 (11)	0.0575 (14)	0.0576 (13)	−0.0087 (10)	0.0251 (10)	0.0109 (11)
Cl12	0.0345 (10)	0.0572 (14)	0.0600 (13)	−0.0137 (9)	0.0082 (9)	−0.0193 (11)
Cl21	0.0526 (12)	0.0739 (15)	0.0441 (11)	0.0101 (11)	0.0302 (10)	−0.0056 (10)
Cl22	0.0276 (9)	0.0708 (15)	0.0470 (11)	0.0139 (9)	0.0095 (8)	0.0056 (10)
Cl31	0.0663 (15)	0.0501 (13)	0.0859 (18)	−0.0109 (12)	0.0315 (13)	−0.0313 (13)
N1	0.027 (3)	0.032 (3)	0.028 (3)	0.003 (2)	0.014 (2)	0.002 (2)
C1	0.025 (3)	0.036 (4)	0.030 (4)	0.002 (3)	0.009 (3)	0.000 (3)
C2	0.044 (4)	0.035 (4)	0.039 (4)	−0.006 (3)	0.023 (3)	−0.005 (3)
C3	0.030 (4)	0.065 (6)	0.045 (4)	−0.006 (4)	0.014 (3)	−0.011 (4)
C4	0.045 (5)	0.054 (6)	0.096 (7)	−0.011 (4)	0.043 (5)	−0.018 (5)
C5	0.032 (4)	0.035 (4)	0.040 (4)	0.009 (3)	0.015 (3)	0.003 (3)
C6	0.052 (5)	0.039 (4)	0.046 (4)	0.001 (4)	0.024 (4)	−0.007 (4)

C7	0.042 (5)	0.038 (5)	0.082 (7)	0.005 (4)	0.020 (4)	−0.012 (4)
C8	0.063 (6)	0.052 (6)	0.116 (9)	−0.004 (5)	0.033 (6)	−0.034 (6)
C9	0.024 (3)	0.042 (4)	0.025 (3)	0.000 (3)	0.010 (3)	0.003 (3)
C10	0.039 (4)	0.043 (4)	0.041 (4)	−0.002 (4)	0.019 (3)	0.003 (4)
C11	0.028 (4)	0.057 (5)	0.049 (5)	0.001 (4)	0.016 (3)	0.016 (4)
C12	0.043 (5)	0.059 (6)	0.079 (7)	−0.005 (4)	0.027 (5)	0.019 (5)
C13	0.040 (4)	0.043 (4)	0.025 (3)	0.004 (3)	0.017 (3)	−0.002 (3)
C14	0.036 (4)	0.055 (5)	0.030 (4)	−0.003 (4)	0.010 (3)	−0.005 (3)
C15	0.044 (5)	0.082 (7)	0.045 (5)	0.005 (5)	0.018 (4)	−0.005 (5)
C16	0.056 (6)	0.150 (12)	0.035 (5)	0.004 (7)	0.009 (4)	−0.019 (6)
C1L	0.143 (13)	0.077 (9)	0.149 (13)	0.017 (9)	0.100 (11)	−0.003 (9)
Cl1L	0.087 (2)	0.168 (4)	0.114 (3)	−0.022 (2)	0.048 (2)	−0.065 (3)
Cl2L	0.471 (12)	0.237 (7)	0.350 (10)	−0.225 (8)	0.355 (10)	−0.183 (7)

Geometric parameters (Å, º)

Si1—Cl12	2.097 (3)	C7—H7A	0.9900
Si1—Cl11	2.098 (3)	C7—H7B	0.9900
Si1—Si2	2.339 (3)	C8—H8A	0.9800
Si1—Si1^{i}	2.341 (4)	C8—H8B	0.9800
Si2—Cl21	2.081 (3)	C8—H8C	0.9800
Si2—Cl22	2.100 (3)	C9—C10	1.519 (10)
Si2—Si3	2.347 (3)	C9—H9A	0.9900
Si3—Cl31	2.086 (3)	C9—H9B	0.9900
Si3—Cl31^{i}	2.086 (3)	C10—C11	1.509 (9)
Si3—Si2^{i}	2.347 (3)	C10—H10A	0.9900
N1—C9	1.513 (8)	C10—H10B	0.9900
N1—C5	1.515 (9)	C11—C12	1.513 (12)
N1—C1	1.523 (8)	C11—H11A	0.9900
N1—C13	1.525 (8)	C11—H11B	0.9900
C1—C2	1.531 (9)	C12—H12A	0.9800
C1—H1A	0.9900	C12—H12B	0.9800
C1—H1B	0.9900	C12—H12C	0.9800
C2—C3	1.510 (10)	C13—C14	1.518 (10)
C2—H2A	0.9900	C13—H13A	0.9900
C2—H2B	0.9900	C13—H13B	0.9900
C3—C4	1.538 (10)	C14—C15	1.539 (10)
C3—H3A	0.9900	C14—H14A	0.9900
C3—H3B	0.9900	C14—H14B	0.9900
C4—H4A	0.9800	C15—C16	1.485 (12)
C4—H4B	0.9800	C15—H15A	0.9900
C4—H4C	0.9800	C15—H15B	0.9900
C5—C6	1.521 (10)	C16—H16A	0.9800
C5—H5A	0.9900	C16—H16B	0.9800
C5—H5B	0.9900	C16—H16C	0.9800
C6—C7	1.516 (11)	C1L—Cl2L	1.578 (14)
C6—H6A	0.9900	C1L—Cl1L	1.711 (13)
C6—H6B	0.9900	C1L—H1L1	0.9900

C7—C8	1.522 (13)	C1L—H1L2	0.9900
Cl12—Si1—Cl11	99.57 (12)	C6—C7—H7B	109.2
Cl12—Si1—Si2	111.06 (11)	C8—C7—H7B	109.2
Cl11—Si1—Si2	114.22 (11)	H7A—C7—H7B	107.9
Cl12—Si1—Si1^{i}	112.32 (12)	C7—C8—H8A	109.5
Cl11—Si1—Si1^{i}	111.28 (12)	C7—C8—H8B	109.5
Si2—Si1—Si1^{i}	108.28 (6)	H8A—C8—H8B	109.5
Cl21—Si2—Cl22	99.76 (11)	C7—C8—H8C	109.5
Cl21—Si2—Si1	114.16 (12)	H8A—C8—H8C	109.5
Cl22—Si2—Si1	110.71 (12)	H8B—C8—H8C	109.5
Cl21—Si2—Si3	111.61 (12)	N1—C9—C10	116.6 (6)
Cl22—Si2—Si3	113.15 (11)	N1—C9—H9A	108.1
Si1—Si2—Si3	107.47 (10)	C10—C9—H9A	108.1
Cl31—Si3—Cl31^{i}	99.6 (2)	N1—C9—H9B	108.1
Cl31—Si3—Si2	111.65 (9)	C10—C9—H9B	108.1
Cl31^{i}—Si3—Si2	112.64 (9)	H9A—C9—H9B	107.3
Cl31—Si3—Si2^{i}	112.64 (9)	C11—C10—C9	110.0 (6)
Cl31^{i}—Si3—Si2^{i}	111.65 (9)	C11—C10—H10A	109.7
Si2—Si3—Si2^{i}	108.50 (16)	C9—C10—H10A	109.7
C9—N1—C5	108.1 (5)	C11—C10—H10B	109.7
C9—N1—C1	109.8 (5)	C9—C10—H10B	109.7
C5—N1—C1	111.2 (5)	H10A—C10—H10B	108.2
C9—N1—C13	110.9 (5)	C10—C11—C12	112.6 (7)
C5—N1—C13	108.8 (5)	C10—C11—H11A	109.1
C1—N1—C13	108.0 (5)	C12—C11—H11A	109.1
N1—C1—C2	116.1 (6)	C10—C11—H11B	109.1
N1—C1—H1A	108.3	C12—C11—H11B	109.1
C2—C1—H1A	108.3	H11A—C11—H11B	107.8
N1—C1—H1B	108.3	C11—C12—H12A	109.5
C2—C1—H1B	108.3	C11—C12—H12B	109.5
H1A—C1—H1B	107.4	H12A—C12—H12B	109.5
C3—C2—C1	110.1 (6)	C11—C12—H12C	109.5
C3—C2—H2A	109.6	H12A—C12—H12C	109.5
C1—C2—H2A	109.6	H12B—C12—H12C	109.5
C3—C2—H2B	109.6	C14—C13—N1	116.9 (6)
C1—C2—H2B	109.6	C14—C13—H13A	108.1
H2A—C2—H2B	108.1	N1—C13—H13A	108.1
C2—C3—C4	112.1 (7)	C14—C13—H13B	108.1
C2—C3—H3A	109.2	N1—C13—H13B	108.1
C4—C3—H3A	109.2	H13A—C13—H13B	107.3
C2—C3—H3B	109.2	C13—C14—C15	108.9 (6)
C4—C3—H3B	109.2	C13—C14—H14A	109.9
H3A—C3—H3B	107.9	C15—C14—H14A	109.9
C3—C4—H4A	109.5	C13—C14—H14B	109.9
C3—C4—H4B	109.5	C15—C14—H14B	109.9
H4A—C4—H4B	109.5	H14A—C14—H14B	108.3
C3—C4—H4C	109.5	C16—C15—C14	112.5 (7)

H4A—C4—H4C	109.5	C16—C15—H15A	109.1
H4B—C4—H4C	109.5	C14—C15—H15A	109.1
N1—C5—C6	115.6 (6)	C16—C15—H15B	109.1
N1—C5—H5A	108.4	C14—C15—H15B	109.1
C6—C5—H5A	108.4	H15A—C15—H15B	107.8
N1—C5—H5B	108.4	C15—C16—H16A	109.5
C6—C5—H5B	108.4	C15—C16—H16B	109.5
H5A—C5—H5B	107.4	H16A—C16—H16B	109.5
C7—C6—C5	110.1 (7)	C15—C16—H16C	109.5
C7—C6—H6A	109.6	H16A—C16—H16C	109.5
C5—C6—H6A	109.6	H16B—C16—H16C	109.5
C7—C6—H6B	109.6	Cl2L—C1L—Cl1L	116.2 (8)
C5—C6—H6B	109.6	Cl2L—C1L—H1L1	108.2
H6A—C6—H6B	108.2	Cl1L—C1L—H1L1	108.2
C6—C7—C8	112.3 (8)	Cl2L—C1L—H1L2	108.2
C6—C7—H7A	109.2	Cl1L—C1L—H1L2	108.2
C8—C7—H7A	109.2	H1L1—C1L—H1L2	107.4
C9—N1—C1—C2	−174.3 (6)	C5—N1—C9—C10	175.4 (6)
C5—N1—C1—C2	−54.8 (7)	C1—N1—C9—C10	−63.2 (7)
C13—N1—C1—C2	64.6 (7)	C13—N1—C9—C10	56.1 (8)
N1—C1—C2—C3	−179.8 (6)	N1—C9—C10—C11	−175.2 (6)
C1—C2—C3—C4	172.9 (7)	C9—C10—C11—C12	−176.1 (7)
C9—N1—C5—C6	68.4 (7)	C9—N1—C13—C14	55.2 (8)
C1—N1—C5—C6	−52.2 (7)	C5—N1—C13—C14	−63.6 (8)
C13—N1—C5—C6	−171.0 (6)	C1—N1—C13—C14	175.6 (6)
N1—C5—C6—C7	−179.9 (6)	N1—C13—C14—C15	176.8 (7)
C5—C6—C7—C8	−177.3 (7)	C13—C14—C15—C16	−175.4 (9)

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···Cl1	0.99	2.88	3.686 (7)	139
C2—H2*A*···Cl31^{ii}	0.99	2.89	3.596 (8)	129
C5—H5*A*···Cl22^{iii}	0.99	2.99	3.945 (7)	163
C9—H9*B*···Cl1	0.99	2.91	3.652 (7)	132
C1*L*—H1*L*1···Cl12^{iii}	0.99	2.96	3.528 (13)	119

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1/2, −*y*+3/2, *z*−1/2.

Bis(tetraethylammonium) dichloride decachlorocyclopentasilane dichloromethane disolvate (II)

Crystal data

$2C_8H_{20}N^+·2Cl^-·Si_5Cl_{10}·2CH_2Cl_2$
M_r = 996.20
Triclinic, $P\overline{1}$
a = 10.3596 (4) Å
b = 13.9612 (5) Å
c = 16.0205 (6) Å
α = 89.959 (3)°
β = 72.484 (3)°
γ = 79.534 (3)°
V = 2169.29 (15) Å^3

$Z = 2$
$F(000) = 1016$
$D_x = 1.525$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 153722 reflections
$\theta = 3.3$–$30.8°$
$\mu = 1.17$ mm^{-1}
$T = 173$ K
Block, colourless
0.23 × 0.23 × 0.20 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: multi-scan (X-AREA; Stoe & Cie, 2001)
$T_{min} = 0.408$, $T_{max} = 1.000$
62962 measured reflections
13044 independent reflections
11976 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 30.5°$, $\theta_{min} = 3.4°$
$h = -14 \rightarrow 14$
$k = -19 \rightarrow 19$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.131$
$S = 1.08$
13044 reflections
409 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 1.6519P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.87$ e Å^{-3}
$\Delta\rho_{min} = -0.84$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.68362 (5)	0.71247 (4)	0.37887 (3)	0.03357 (10)	
Cl2	0.55394 (6)	0.71721 (4)	0.14756 (3)	0.03425 (11)	
Si1	0.79603 (6)	0.63165 (4)	0.19539 (4)	0.03316 (12)	
Si2	0.74595 (6)	0.80223 (4)	0.20699 (4)	0.02939 (11)	
Si3	0.51729 (5)	0.85241 (4)	0.29623 (3)	0.02570 (10)	
Si4	0.42527 (5)	0.71172 (4)	0.33588 (3)	0.02431 (10)	
Si5	0.59853 (6)	0.57465 (4)	0.27696 (4)	0.02724 (11)	
Cl11	0.97197 (6)	0.57714 (6)	0.23162 (6)	0.0628 (2)	
Cl12	0.86579 (9)	0.57414 (5)	0.06642 (4)	0.0632 (2)	
Cl21	0.88627 (7)	0.86092 (6)	0.25209 (5)	0.05179 (16)	
Cl22	0.78501 (6)	0.86177 (4)	0.08273 (4)	0.04303 (13)	
Cl31	0.49581 (7)	0.94164 (4)	0.40573 (4)	0.04399 (13)	
Cl32	0.39997 (6)	0.94686 (4)	0.23306 (4)	0.04020 (12)	
Cl41	0.33929 (5)	0.71094 (4)	0.47227 (3)	0.03436 (10)	
Cl42	0.24659 (5)	0.71209 (4)	0.29964 (4)	0.03703 (11)	
Cl51	0.63586 (6)	0.47736 (4)	0.36927 (4)	0.04057 (12)	
Cl52	0.53223 (8)	0.48498 (4)	0.20041 (4)	0.04831 (15)	

N1	0.27041 (18)	0.79721 (13)	−0.00541 (11)	0.0299 (3)	
C1	0.2204 (4)	0.7299 (2)	0.06657 (18)	0.0551 (7)	
H1A	0.1238	0.7262	0.0717	0.066*	
H1B	0.2206	0.7590	0.1228	0.066*	
C2	0.3050 (4)	0.62647 (19)	0.0530 (2)	0.0551 (7)	
H2A	0.2656	0.5882	0.1024	0.083*	
H2B	0.3034	0.5959	−0.0016	0.083*	
H2C	0.4004	0.6288	0.0497	0.083*	
C3	0.2867 (3)	0.7533 (2)	−0.09498 (16)	0.0438 (5)	
H3A	0.3641	0.6966	−0.1089	0.053*	
H3B	0.3126	0.8021	−0.1387	0.053*	
C4	0.1610 (4)	0.7201 (3)	−0.1052 (3)	0.0648 (9)	
H4A	0.1816	0.6928	−0.1651	0.097*	
H4B	0.1357	0.6701	−0.0636	0.097*	
H4C	0.0842	0.7759	−0.0934	0.097*	
C5	0.1640 (3)	0.89268 (19)	0.0117 (2)	0.0470 (6)	
H5A	0.1863	0.9314	−0.0407	0.056*	
H5B	0.0721	0.8767	0.0192	0.056*	
C6	0.1555 (3)	0.9554 (2)	0.0910 (2)	0.0545 (7)	
H6A	0.0852	1.0145	0.0967	0.082*	
H6B	0.1306	0.9187	0.1438	0.082*	
H6C	0.2451	0.9736	0.0837	0.082*	
C7	0.4085 (3)	0.81784 (18)	−0.00349 (18)	0.0412 (5)	
H7A	0.3980	0.8424	0.0566	0.049*	
H7B	0.4756	0.7554	−0.0155	0.049*	
C8	0.4683 (3)	0.8892 (2)	−0.0662 (2)	0.0517 (6)	
H8A	0.5568	0.8970	−0.0594	0.078*	
H8B	0.4826	0.8651	−0.1264	0.078*	
H8C	0.4048	0.9523	−0.0540	0.078*	
N2	0.0000	0.5000	0.5000	0.0260 (4)	
C21	−0.0005 (4)	0.6091 (3)	0.5117 (3)	0.0331 (8)	0.5
H21A	−0.0855	0.6483	0.5040	0.040*	0.5
H21B	0.0800	0.6270	0.4675	0.040*	0.5
C21′	0.0128 (5)	0.5139 (3)	0.5909 (3)	0.0350 (8)	0.5
H21C	0.1013	0.4755	0.5941	0.042*	0.5
H21D	−0.0633	0.4912	0.6352	0.042*	0.5
C22	0.0063 (3)	0.6300 (3)	0.6105 (2)	0.0638 (9)	
H22A	0.0061	0.6994	0.6197	0.096*	0.5
H22B	−0.0740	0.6122	0.6536	0.096*	0.5
H22C	0.0908	0.5910	0.6173	0.096*	0.5
H22D	0.0144	0.6403	0.6690	0.096*	0.5
H22E	0.0823	0.6518	0.5665	0.096*	0.5
H22F	−0.0818	0.6675	0.6075	0.096*	0.5
C23	0.1319 (4)	0.4394 (3)	0.5085 (3)	0.0294 (7)	0.5
H23A	0.1285	0.3693	0.5040	0.035*	0.5
H23B	0.1411	0.4544	0.5666	0.035*	0.5
C23′	0.1182 (4)	0.5289 (3)	0.4300 (3)	0.0321 (7)	0.5
H23C	0.1196	0.5986	0.4398	0.039*	0.5

H23D	0.1063	0.5197	0.3717	0.039*	0.5
C24	0.2624 (2)	0.4624 (2)	0.4327 (2)	0.0533 (7)	
H24A	0.3471	0.4228	0.4389	0.080*	0.5
H24B	0.2538	0.4467	0.3753	0.080*	0.5
H24C	0.2662	0.5317	0.4377	0.080*	0.5
H24D	0.3391	0.4813	0.3871	0.080*	0.5
H24E	0.2743	0.4723	0.4903	0.080*	0.5
H24F	0.2610	0.3935	0.4224	0.080*	0.5
N3	0.0000	1.0000	0.5000	0.0324 (5)	
C31	−0.0124 (7)	1.0998 (4)	0.5376 (4)	0.0522 (13)	0.5
H31A	−0.0599	1.1032	0.6015	0.063*	0.5
H31B	−0.0684	1.1477	0.5106	0.063*	0.5
C31′	0.1452 (5)	1.0189 (5)	0.4881 (4)	0.0509 (13)	0.5
H31C	0.2003	1.0076	0.4255	0.061*	0.5
H31D	0.1910	0.9729	0.5221	0.061*	0.5
C32	0.1392 (6)	1.1271 (4)	0.5199 (3)	0.0956 (17)	
H32A	0.1294	1.1930	0.5450	0.143*	0.5
H32B	0.1941	1.0803	0.5474	0.143*	0.5
H32C	0.1855	1.1246	0.4566	0.143*	0.5
H32D	0.2330	1.1379	0.5118	0.143*	0.5
H32E	0.0951	1.1727	0.4856	0.143*	0.5
H32F	0.0857	1.1380	0.5821	0.143*	0.5
C33	−0.0905 (5)	1.0176 (4)	0.5927 (3)	0.0412 (10)	0.5
H33A	−0.1850	1.0092	0.5967	0.049*	0.5
H33B	−0.0952	1.0851	0.6140	0.049*	0.5
C33′	0.0691 (5)	0.9243 (4)	0.5529 (3)	0.0459 (11)	0.5
H33C	0.1629	0.9350	0.5479	0.055*	0.5
H33D	0.0765	0.8572	0.5296	0.055*	0.5
C34	−0.0250 (4)	0.9384 (3)	0.6531 (2)	0.0724 (11)	
H34A	−0.0833	0.9490	0.7144	0.109*	0.5
H34B	−0.0212	0.8719	0.6318	0.109*	0.5
H34C	0.0683	0.9475	0.6490	0.109*	0.5
H34D	0.0162	0.8916	0.6879	0.109*	0.5
H34E	−0.0314	1.0050	0.6756	0.109*	0.5
H34F	−0.1175	0.9274	0.6574	0.109*	0.5
C1L	0.1880 (4)	0.3162 (2)	0.1144 (2)	0.0565 (7)	
H1L1	0.2330	0.2960	0.0516	0.068*	
H1L2	0.0997	0.3611	0.1200	0.068*	
Cl1A	0.29537 (8)	0.37721 (5)	0.15334 (6)	0.05663 (17)	
Cl1B	0.15522 (9)	0.21224 (6)	0.17452 (6)	0.05883 (18)	
C2L	0.4865 (4)	0.7900 (3)	0.6208 (2)	0.0642 (8)	
H2L1	0.5201	0.8228	0.5657	0.077*	
H2L2	0.4831	0.7222	0.6050	0.077*	
Cl2A	0.60192 (10)	0.78831 (6)	0.68194 (6)	0.0634 (2)	
Cl2B	0.32076 (10)	0.85079 (10)	0.67916 (6)	0.0828 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0361 (2)	0.0429 (3)	0.0274 (2)	−0.01369 (19)	−0.01464 (17)	0.00581 (17)
Cl2	0.0424 (3)	0.0357 (2)	0.0271 (2)	−0.00201 (19)	−0.01742 (18)	−0.00062 (16)
Si1	0.0284 (2)	0.0311 (3)	0.0307 (3)	0.0042 (2)	−0.0012 (2)	0.0051 (2)
Si2	0.0258 (2)	0.0307 (3)	0.0279 (2)	−0.00452 (19)	−0.00314 (19)	0.00405 (19)
Si3	0.0266 (2)	0.0229 (2)	0.0245 (2)	−0.00328 (17)	−0.00405 (18)	−0.00117 (17)
Si4	0.0239 (2)	0.0234 (2)	0.0246 (2)	−0.00303 (17)	−0.00662 (17)	−0.00054 (16)
Si5	0.0287 (2)	0.0228 (2)	0.0295 (2)	−0.00127 (18)	−0.00988 (19)	−0.00119 (18)
Cl11	0.0288 (3)	0.0663 (4)	0.0855 (5)	0.0061 (3)	−0.0147 (3)	0.0272 (4)
Cl12	0.0766 (5)	0.0475 (3)	0.0344 (3)	0.0162 (3)	0.0127 (3)	−0.0050 (2)
Cl21	0.0423 (3)	0.0669 (4)	0.0530 (3)	−0.0301 (3)	−0.0132 (3)	0.0083 (3)
Cl22	0.0427 (3)	0.0432 (3)	0.0342 (2)	−0.0043 (2)	−0.0008 (2)	0.0144 (2)
Cl31	0.0582 (3)	0.0344 (2)	0.0360 (3)	−0.0095 (2)	−0.0090 (2)	−0.0121 (2)
Cl32	0.0410 (3)	0.0302 (2)	0.0445 (3)	0.00368 (19)	−0.0119 (2)	0.00648 (19)
Cl41	0.0336 (2)	0.0416 (3)	0.0253 (2)	−0.01096 (19)	−0.00306 (17)	0.00253 (17)
Cl42	0.0285 (2)	0.0429 (3)	0.0433 (3)	−0.00619 (18)	−0.01663 (19)	0.0021 (2)
Cl51	0.0404 (3)	0.0343 (2)	0.0516 (3)	−0.0089 (2)	−0.0198 (2)	0.0174 (2)
Cl52	0.0629 (4)	0.0337 (3)	0.0529 (3)	−0.0081 (2)	−0.0251 (3)	−0.0133 (2)
N1	0.0310 (8)	0.0304 (8)	0.0275 (7)	−0.0052 (6)	−0.0080 (6)	0.0030 (6)
C1	0.0746 (19)	0.0423 (13)	0.0395 (12)	−0.0160 (13)	−0.0016 (12)	0.0076 (10)
C2	0.085 (2)	0.0343 (12)	0.0522 (15)	−0.0151 (13)	−0.0287 (15)	0.0117 (10)
C3	0.0530 (14)	0.0456 (12)	0.0365 (11)	−0.0105 (10)	−0.0187 (10)	−0.0010 (9)
C4	0.069 (2)	0.0598 (18)	0.087 (2)	−0.0171 (15)	−0.0524 (19)	−0.0019 (16)
C5	0.0357 (11)	0.0378 (12)	0.0634 (16)	−0.0041 (9)	−0.0110 (11)	0.0002 (11)
C6	0.0512 (15)	0.0407 (13)	0.0554 (15)	−0.0079 (11)	0.0070 (12)	−0.0096 (11)
C7	0.0378 (11)	0.0392 (11)	0.0498 (13)	−0.0028 (9)	−0.0208 (10)	0.0006 (9)
C8	0.0378 (12)	0.0480 (14)	0.0643 (17)	−0.0150 (10)	−0.0042 (11)	−0.0017 (12)
N2	0.0230 (9)	0.0267 (10)	0.0268 (10)	−0.0036 (8)	−0.0063 (8)	0.0051 (8)
C21	0.0329 (18)	0.0228 (16)	0.040 (2)	−0.0042 (14)	−0.0058 (16)	0.0055 (14)
C21′	0.0330 (19)	0.043 (2)	0.0293 (17)	−0.0049 (16)	−0.0108 (15)	0.0050 (15)
C22	0.0471 (15)	0.073 (2)	0.0663 (19)	−0.0141 (14)	−0.0078 (13)	−0.0342 (16)
C23	0.0252 (16)	0.0297 (17)	0.0327 (17)	−0.0030 (13)	−0.0095 (14)	0.0056 (14)
C23′	0.0275 (17)	0.0336 (18)	0.0322 (18)	−0.0082 (14)	−0.0031 (14)	0.0067 (14)
C24	0.0240 (9)	0.0589 (16)	0.0671 (17)	−0.0074 (10)	0.0005 (10)	−0.0163 (13)
N3	0.0243 (10)	0.0345 (12)	0.0329 (11)	0.0000 (9)	−0.0037 (9)	−0.0037 (9)
C31	0.072 (4)	0.037 (2)	0.040 (2)	−0.006 (2)	−0.009 (2)	−0.0055 (19)
C31′	0.030 (2)	0.081 (4)	0.043 (3)	−0.015 (2)	−0.0107 (18)	0.013 (2)
C32	0.146 (4)	0.103 (3)	0.080 (3)	−0.084 (3)	−0.061 (3)	0.023 (2)
C33	0.034 (2)	0.049 (2)	0.0292 (18)	0.0039 (18)	0.0004 (16)	−0.0031 (17)
C33′	0.033 (2)	0.055 (3)	0.045 (2)	0.0018 (19)	−0.0118 (19)	0.009 (2)
C34	0.083 (2)	0.110 (3)	0.0381 (14)	−0.048 (2)	−0.0207 (15)	0.0216 (16)
C1L	0.0620 (17)	0.0570 (16)	0.0647 (18)	−0.0176 (14)	−0.0369 (15)	0.0150 (13)
Cl1A	0.0500 (3)	0.0452 (3)	0.0797 (5)	−0.0104 (3)	−0.0265 (3)	0.0018 (3)
Cl1B	0.0613 (4)	0.0527 (4)	0.0685 (5)	−0.0195 (3)	−0.0237 (4)	0.0092 (3)
C2L	0.0639 (19)	0.078 (2)	0.0503 (16)	0.0043 (16)	−0.0266 (14)	−0.0118 (15)
Cl2A	0.0746 (5)	0.0622 (4)	0.0588 (4)	0.0015 (4)	−0.0367 (4)	−0.0093 (3)

Cl2B	0.0612 (5)	0.1170 (9)	0.0576 (5)	0.0084 (5)	−0.0143 (4)	0.0110 (5)

Geometric parameters (Å, º)

Si1—Cl12	2.0805 (9)	C22—H22B	0.9800
Si1—Cl11	2.0906 (9)	C22—H22C	0.9800
Si1—Si2	2.3386 (8)	C22—H22D	0.9800
Si1—Si5	2.3469 (8)	C22—H22E	0.9800
Si2—Cl21	2.0910 (8)	C22—H22F	0.9800
Si2—Cl22	2.1102 (8)	C23—C24	1.604 (5)
Si2—Si3	2.3465 (7)	C23—H23A	0.9900
Si3—Cl31	2.0849 (7)	C23—H23B	0.9900
Si3—Cl32	2.0967 (8)	C23′—C24	1.622 (5)
Si3—Si4	2.3419 (7)	C23′—H23C	0.9900
Si4—Cl41	2.0977 (7)	C23′—H23D	0.9900
Si4—Cl42	2.0993 (7)	C24—H24A	0.9800
Si4—Si5	2.3473 (7)	C24—H24B	0.9800
Si5—Cl51	2.0814 (7)	C24—H24C	0.9800
Si5—Cl52	2.0890 (8)	C24—H24D	0.9800
N1—C3	1.510 (3)	C24—H24E	0.9800
N1—C1	1.516 (3)	C24—H24F	0.9800
N1—C7	1.519 (3)	N3—C31^{ii}	1.487 (5)
N1—C5	1.533 (3)	N3—C31	1.487 (5)
C1—C2	1.526 (4)	N3—C33^{ii}	1.491 (4)
C1—H1A	0.9900	N3—C33	1.491 (4)
C1—H1B	0.9900	N3—C31′^{ii}	1.530 (5)
C2—H2A	0.9800	N3—C31′	1.530 (5)
C2—H2B	0.9800	N3—C33′^{ii}	1.561 (5)
C2—H2C	0.9800	N3—C33′	1.561 (5)
C3—C4	1.511 (4)	C31—C32	1.625 (8)
C3—H3A	0.9900	C31—H31A	0.9900
C3—H3B	0.9900	C31—H31B	0.9900
C4—H4A	0.9800	C31′—C32	1.579 (8)
C4—H4B	0.9800	C31′—H31C	0.9900
C4—H4C	0.9800	C31′—H31D	0.9900
C5—C6	1.514 (4)	C32—H32A	0.9800
C5—H5A	0.9900	C32—H32B	0.9800
C5—H5B	0.9900	C32—H32C	0.9800
C6—H6A	0.9800	C32—H32D	0.9800
C6—H6B	0.9800	C32—H32E	0.9800
C6—H6C	0.9800	C32—H32F	0.9800
C7—C8	1.495 (4)	C33—C34	1.656 (6)
C7—H7A	0.9900	C33—H33A	0.9900
C7—H7B	0.9900	C33—H33B	0.9900
C8—H8A	0.9800	C33′—C34	1.599 (6)
C8—H8B	0.9800	C33′—H33C	0.9900
C8—H8C	0.9800	C33′—H33D	0.9900
N2—C23′^{i}	1.508 (4)	C34—H34A	0.9800

N2—C23′	1.508 (4)	C34—H34B	0.9800
N2—C23^{i}	1.514 (4)	C34—H34C	0.9800
N2—C23	1.514 (4)	C34—H34D	0.9800
N2—C21′^{i}	1.517 (4)	C34—H34E	0.9800
N2—C21′	1.517 (4)	C34—H34F	0.9800
N2—C21	1.533 (4)	C1L—Cl1A	1.765 (3)
N2—C21^{i}	1.533 (4)	C1L—Cl1B	1.769 (3)
C21—C22	1.633 (6)	C1L—H1L1	0.9900
C21—H21A	0.9900	C1L—H1L2	0.9900
C21—H21B	0.9900	C2L—Cl2B	1.746 (4)
C21′—C22	1.636 (6)	C2L—Cl2A	1.757 (3)
C21′—H21C	0.9900	C2L—H2L1	0.9900
C21′—H21D	0.9900	C2L—H2L2	0.9900
C22—H22A	0.9800		

Cl12—Si1—Cl11	98.50 (4)	C21—C22—H22A	109.5
Cl12—Si1—Si2	113.28 (3)	C21—C22—H22B	109.5
Cl11—Si1—Si2	111.32 (4)	H22A—C22—H22B	109.5
Cl12—Si1—Si5	111.49 (4)	C21—C22—H22C	109.5
Cl11—Si1—Si5	113.90 (4)	H22A—C22—H22C	109.5
Si2—Si1—Si5	108.23 (3)	H22B—C22—H22C	109.5
Cl21—Si2—Cl22	98.77 (4)	C21′—C22—H22D	109.5
Cl21—Si2—Si1	112.27 (4)	C21′—C22—H22E	109.5
Cl22—Si2—Si1	111.72 (3)	H22D—C22—H22E	109.5
Cl21—Si2—Si3	112.69 (3)	C21′—C22—H22F	109.5
Cl22—Si2—Si3	113.01 (3)	H22D—C22—H22F	109.5
Si1—Si2—Si3	108.26 (3)	H22E—C22—H22F	109.5
Cl31—Si3—Cl32	100.07 (3)	N2—C23—C24	110.3 (3)
Cl31—Si3—Si4	111.69 (3)	N2—C23—H23A	109.6
Cl32—Si3—Si4	111.61 (3)	C24—C23—H23A	109.6
Cl31—Si3—Si2	114.12 (3)	N2—C23—H23B	109.6
Cl32—Si3—Si2	111.88 (3)	C24—C23—H23B	109.6
Si4—Si3—Si2	107.47 (3)	H23A—C23—H23B	108.1
Cl41—Si4—Cl42	98.87 (3)	N2—C23′—C24	109.6 (3)
Cl41—Si4—Si3	111.22 (3)	N2—C23′—H23C	109.7
Cl42—Si4—Si3	112.22 (3)	C24—C23′—H23C	109.7
Cl41—Si4—Si5	112.75 (3)	N2—C23′—H23D	109.7
Cl42—Si4—Si5	113.01 (3)	C24—C23′—H23D	109.7
Si3—Si4—Si5	108.60 (3)	H23C—C23′—H23D	108.2
Cl51—Si5—Cl52	99.88 (3)	C23—C24—H24A	109.5
Cl51—Si5—Si1	113.02 (3)	C23—C24—H24B	109.5
Cl52—Si5—Si1	112.15 (3)	H24A—C24—H24B	109.5
Cl51—Si5—Si4	114.27 (3)	C23—C24—H24C	109.5
Cl52—Si5—Si4	110.11 (3)	H24A—C24—H24C	109.5
Si1—Si5—Si4	107.38 (3)	H24B—C24—H24C	109.5
C3—N1—C1	111.90 (19)	C23′—C24—H24D	109.5
C3—N1—C7	108.98 (18)	C23′—C24—H24E	109.5
C1—N1—C7	109.2 (2)	H24D—C24—H24E	109.5

C3—N1—C5	108.79 (19)	C23′—C24—H24F	109.5
C1—N1—C5	108.2 (2)	H24D—C24—H24F	109.5
C7—N1—C5	109.76 (17)	H24E—C24—H24F	109.5
N1—C1—C2	115.0 (2)	C31^{ii}—N3—C31	180.0 (4)
N1—C1—H1A	108.5	C31^{ii}—N3—C33^{ii}	66.3 (3)
C2—C1—H1A	108.5	C31—N3—C33^{ii}	113.7 (3)
N1—C1—H1B	108.5	C31^{ii}—N3—C33	113.7 (3)
C2—C1—H1B	108.5	C31—N3—C33	66.3 (3)
H1A—C1—H1B	107.5	C33^{ii}—N3—C33	180.0
C1—C2—H2A	109.5	C31′^{ii}—N3—C31′	180.0 (7)
C1—C2—H2B	109.5	C31′^{ii}—N3—C33′^{ii}	72.4 (3)
H2A—C2—H2B	109.5	C31′—N3—C33′^{ii}	107.6 (3)
C1—C2—H2C	109.5	C31′^{ii}—N3—C33′	107.6 (3)
H2A—C2—H2C	109.5	C31′—N3—C33′	72.4 (3)
H2B—C2—H2C	109.5	C33′^{ii}—N3—C33′	180.0 (3)
N1—C3—C4	115.5 (2)	N3—C31—C32	110.4 (4)
N1—C3—H3A	108.4	N3—C31—H31A	109.6
C4—C3—H3A	108.4	C32—C31—H31A	109.6
N1—C3—H3B	108.4	N3—C31—H31B	109.6
C4—C3—H3B	108.4	C32—C31—H31B	109.6
H3A—C3—H3B	107.5	H31A—C31—H31B	108.1
C3—C4—H4A	109.5	N3—C31′—C32	110.7 (4)
C3—C4—H4B	109.5	N3—C31′—H31C	109.5
H4A—C4—H4B	109.5	C32—C31′—H31C	109.5
C3—C4—H4C	109.5	N3—C31′—H31D	109.5
H4A—C4—H4C	109.5	C32—C31′—H31D	109.5
H4B—C4—H4C	109.5	H31C—C31′—H31D	108.1
C6—C5—N1	115.2 (2)	C31—C32—H32A	109.5
C6—C5—H5A	108.5	C31—C32—H32B	109.5
N1—C5—H5A	108.5	H32A—C32—H32B	109.5
C6—C5—H5B	108.5	C31—C32—H32C	109.5
N1—C5—H5B	108.5	H32A—C32—H32C	109.5
H5A—C5—H5B	107.5	H32B—C32—H32C	109.5
C5—C6—H6A	109.5	C31′—C32—H32D	109.5
C5—C6—H6B	109.5	C31′—C32—H32E	109.5
H6A—C6—H6B	109.5	H32D—C32—H32E	109.5
C5—C6—H6C	109.5	C31′—C32—H32F	109.5
H6A—C6—H6C	109.5	H32D—C32—H32F	109.5
H6B—C6—H6C	109.5	H32E—C32—H32F	109.5
C8—C7—N1	116.3 (2)	N3—C33—C34	108.3 (3)
C8—C7—H7A	108.2	N3—C33—H33A	110.0
N1—C7—H7A	108.2	C34—C33—H33A	110.0
C8—C7—H7B	108.2	N3—C33—H33B	110.0
N1—C7—H7B	108.2	C34—C33—H33B	110.0
H7A—C7—H7B	107.4	H33A—C33—H33B	108.4
C7—C8—H8A	109.5	N3—C33′—C34	107.8 (3)
C7—C8—H8B	109.5	N3—C33′—H33C	110.1
H8A—C8—H8B	109.5	C34—C33′—H33C	110.1

C7—C8—H8C	109.5	N3—C33′—H33D	110.1
H8A—C8—H8C	109.5	C34—C33′—H33D	110.1
H8B—C8—H8C	109.5	H33C—C33′—H33D	108.5
C23′^{i}—N2—C23′	180.0	C33—C34—H34A	109.5
C23^{i}—N2—C23	180.0 (3)	C33—C34—H34B	109.5
C23′^{i}—N2—C21′^{i}	111.7 (2)	H34A—C34—H34B	109.5
C23′—N2—C21′^{i}	68.3 (2)	C33—C34—H34C	109.5
C23′^{i}—N2—C21′	68.3 (2)	H34A—C34—H34C	109.5
C23′—N2—C21′	111.7 (2)	H34B—C34—H34C	109.5
C21′^{i}—N2—C21′	180.0	C33′—C34—H34D	109.5
C23^{i}—N2—C21	69.5 (2)	C33′—C34—H34E	109.5
C23—N2—C21	110.5 (2)	H34D—C34—H34E	109.5
C23^{i}—N2—C21^{i}	110.5 (2)	C33′—C34—H34F	109.5
C23—N2—C21^{i}	69.5 (2)	H34D—C34—H34F	109.5
C21—N2—C21^{i}	180.0 (4)	H34E—C34—H34F	109.5
N2—C21—C22	107.8 (3)	Cl1A—C1L—Cl1B	110.64 (16)
N2—C21—H21A	110.2	Cl1A—C1L—H1L1	109.5
C22—C21—H21A	110.2	Cl1B—C1L—H1L1	109.5
N2—C21—H21B	110.2	Cl1A—C1L—H1L2	109.5
C22—C21—H21B	110.2	Cl1B—C1L—H1L2	109.5
H21A—C21—H21B	108.5	H1L1—C1L—H1L2	108.1
N2—C21′—C22	108.4 (3)	Cl2B—C2L—Cl2A	111.70 (18)
N2—C21′—H21C	110.0	Cl2B—C2L—H2L1	109.3
C22—C21′—H21C	110.0	Cl2A—C2L—H2L1	109.3
N2—C21′—H21D	110.0	Cl2B—C2L—H2L2	109.3
C22—C21′—H21D	110.0	Cl2A—C2L—H2L2	109.3
H21C—C21′—H21D	108.4	H2L1—C2L—H2L2	107.9
C3—N1—C1—C2	52.6 (3)	C23′^{i}—N2—C21′—C22	−117.4 (3)
C7—N1—C1—C2	−68.1 (3)	C23′—N2—C21′—C22	62.6 (3)
C5—N1—C1—C2	172.4 (3)	C21—N2—C23—C24	−62.3 (3)
C1—N1—C3—C4	53.9 (3)	C21^{i}—N2—C23—C24	117.7 (3)
C7—N1—C3—C4	174.8 (2)	C21′^{i}—N2—C23′—C24	−119.9 (3)
C5—N1—C3—C4	−65.6 (3)	C21′—N2—C23′—C24	60.1 (3)
C3—N1—C5—C6	−168.9 (2)	C33^{ii}—N3—C31—C32	−49.5 (5)
C1—N1—C5—C6	69.3 (3)	C33—N3—C31—C32	130.5 (5)
C7—N1—C5—C6	−49.8 (3)	C33′^{ii}—N3—C31′—C32	57.8 (4)
C3—N1—C7—C8	61.8 (3)	C33′—N3—C31′—C32	−122.2 (4)
C1—N1—C7—C8	−175.7 (2)	C31^{ii}—N3—C33—C34	60.0 (5)
C5—N1—C7—C8	−57.2 (3)	C31—N3—C33—C34	−120.0 (5)
C23^{i}—N2—C21—C22	118.2 (3)	C31′^{ii}—N3—C33′—C34	−58.6 (5)
C23—N2—C21—C22	−61.8 (3)	C31′—N3—C33′—C34	121.4 (5)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···Cl42	0.99	2.99	3.829 (3)	144

C2—H2*C*···Cl2	0.98	2.95	3.753 (3)	139
C3—H3*A*···Cl52^{iii}	0.99	2.79	3.643 (3)	144
C3—H3*B*···Cl2*B*^{iv}	0.99	2.98	3.804 (3)	142
C5—H5*B*···Cl22^{v}	0.99	2.89	3.850 (3)	165
C6—H6*B*···Cl21^{v}	0.98	2.86	3.630 (3)	136
C7—H7*A*···Cl2	0.99	2.86	3.394 (2)	115
C22—H22*C*···Cl51^{vi}	0.98	2.89	3.847 (4)	165
C22—H22*E*···Cl41	0.98	2.90	3.859 (3)	165
C23—H23*B*···Cl1^{vi}	0.99	2.98	3.465 (4)	111
C23′—H23*C*···Cl42	0.99	2.87	3.497 (4)	122
C24—H24*C*···Cl41	0.98	2.84	3.793 (3)	164
C24—H24*E*···Cl51^{vi}	0.98	2.81	3.771 (3)	165
C24—H24*F*···Cl2*A*^{vi}	0.98	2.92	3.778 (3)	147
C31′—H31*C*···Cl31	0.99	2.95	3.434 (5)	111
C32—H32*F*···Cl21^{vii}	0.98	2.76	3.584 (4)	142
C33—H33*A*···Cl32^{ii}	0.99	2.94	3.515 (4)	118
C33′—H33*D*···Cl41	0.99	2.98	3.630 (5)	124
C34—H34*A*···Cl1*B*^{i}	0.98	2.93	3.556 (3)	123
C34—H34*C*···Cl2*B*	0.98	2.89	3.716 (4)	142
C34—H34*A*···Cl1*B*^{i}	0.98	2.93	3.556 (3)	123
C1*L*—H1*L*1···Cl12^{iii}	0.99	2.90	3.421 (3)	114
C2*L*—H2*L*2···Cl41	0.99	2.96	3.465 (3)	113

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*, −*y*+2, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*; (iv) *x*, *y*, *z*−1; (v) *x*−1, *y*, *z*; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) −*x*+1, −*y*+2, −*z*+1.