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Bis(tetramethylammonium) tetrachloridozincate(II), phase VI

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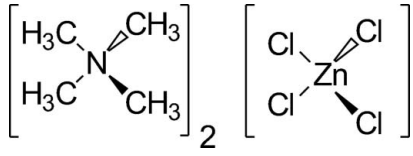
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(N–C) = 0.003 Å; R factor = 0.026; wR factor = 0.055; data-to-parameter ratio = 23.6.

Phase VI of bis(tetramethylammonium) tetrachlorozincate(II), $(C_4H_{12}N)_2[ZnCl_4]$, contains three formula units per asymmetric unit. Several short C—H···Cl contacts [2.70 (3) and 2.72 (4) Å] are observed, but they are believed to participate only in van der Waals interactions. The crystal studied exhibited inversion twinning.

Related literature

For related literature, see: Madariaga *et al.* (1987); Ruiz-Larrea *et al.* (1981); Wiesner *et al.* (1967); Zuñiga *et al.* (1989); Zhang & Bordwell (1994).



Experimental

Crystal data

$(C_4H_{12}N)_2[ZnCl_4]$
M_r = 355.46
Orthorhombic, $P2_12_12_1$
a = 8.9114 (18) Å
b = 15.105 (3) Å
c = 36.493 (7) Å
V = 4912.2 (17) Å^3
Z = 12
Mo $K\alpha$ radiation
μ = 2.13 mm^{-1}
T = 100.0 (2) K
0.36 × 0.24 × 0.04 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.512, T_{max} = 0.918
32538 measured reflections
9616 independent reflections
9039 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.055
S = 1.00
9616 reflections
407 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Absolute structure: Flack (1983), with 4218 Friedel pairs
Flack parameter: 0.611 (6)

Table 1
Selected geometric parameters (Å, °).

Zn1*A*—Cl4*A*	2.2645 (8)	Zn1*B*—Cl2*B*	2.2857 (8)
Zn1*A*—Cl2*A*	2.2743 (8)	Zn1*C*—Cl1*C*	2.2620 (8)
Zn1*A*—Cl1*A*	2.2807 (8)	Zn1*C*—Cl2*C*	2.2726 (8)
Zn1*A*—Cl3*A*	2.2836 (8)	Zn1*C*—Cl3*C*	2.2770 (8)
Zn1*B*—Cl1*B*	2.2677 (8)	Zn1*C*—Cl4*C*	2.2814 (8)
Zn1*B*—Cl4*B*	2.2709 (7)		
Zn1*B*—Cl3*B*	2.2797 (8)		
Cl4*A*—Zn1*A*—Cl2*A*	110.65 (3)	Cl4*B*—Zn1*B*—Cl2*B*	107.37 (3)
Cl4*A*—Zn1*A*—Cl1*A*	110.51 (3)	Cl3*B*—Zn1*B*—Cl2*B*	110.46 (3)
Cl2*A*—Zn1*A*—Cl1*A*	107.40 (3)	Cl1*C*—Zn1*C*—Cl2*C*	112.21 (3)
Cl4*A*—Zn1*A*—Cl3*A*	108.27 (3)	Cl1*C*—Zn1*C*—Cl3*C*	109.88 (3)
Cl2*A*—Zn1*A*—Cl3*A*	109.40 (3)	Cl2*C*—Zn1*C*—Cl3*C*	108.62 (3)
Cl1*A*—Zn1*A*—Cl3*A*	110.60 (3)	Cl1*C*—Zn1*C*—Cl4*C*	109.08 (3)
Cl1*B*—Zn1*B*—Cl4*B*	111.11 (3)	Cl2*C*—Zn1*C*—Cl4*C*	108.55 (3)
Cl1*B*—Zn1*B*—Cl3*B*	109.08 (3)	Cl3*C*—Zn1*C*—Cl4*C*	108.42 (3)
Cl4*B*—Zn1*B*—Cl3*B*	108.58 (3)		
Cl1*B*—Zn1*B*—Cl2*B*	110.23 (3)		

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2041).

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Acta Cryst. (2008). E**64**, m183 [https://doi.org/10.1107/S1600536807065828]

Bis(tetramethylammonium) tetrachloridozincate(II), phase VI

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S1. Comment

Bis(tetramethylammonium) tetrachlorozincate(II) undergoes five solid-solid phase transitions with decreasing temperature according to a calorimetric study by Ruiz-Larrea *et al.* (1981). The room temperature phase I crystallized in the space group *Pnma* with a = 12.276 (2), b = 8.998 (2), and c = 15.541 (2) Å (Wiesner *et al.*, 1967). Weak incommensurate lattice spots in phases II, III, and IV have shown that these two phases are small distortions of the room temperature phase (Madariaga *et al.*, 1987). Similarly, phase V was found to be an incommensurately modulated structure related to phase I (Zuñiga *et al.*, 1989).

No evidence of superlattice spots were observed in the frame data for phase VI. Short C—H···Cl contacts were observed, but because of the very large estimated pK_a of 42 for the protons of the cations (Zhang & Bordwell, 1994), it is unlikely that any of these contacts are weak hydrogen bonds. There were three formula units in the asymmetric unit of the cell (Fig. 1).

S2. Experimental

Single crystals of bis(tetramethylammonium) tetrachlorozincate(II) were grown by slow diffusion of diethyl ether into a methanol solution of $ZnCl_2$ and $N(CH_3)_4OH$ in a 1:3 mole ratio over the course of three days.

S3. Refinement

The methyl H atoms were initially located by geometry. The H atoms were then refined with distances of 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, but each methyl group was allowed to rotate freely about its N—C bond.

The refined Flack parameter indicated racemic twinning in the sample.

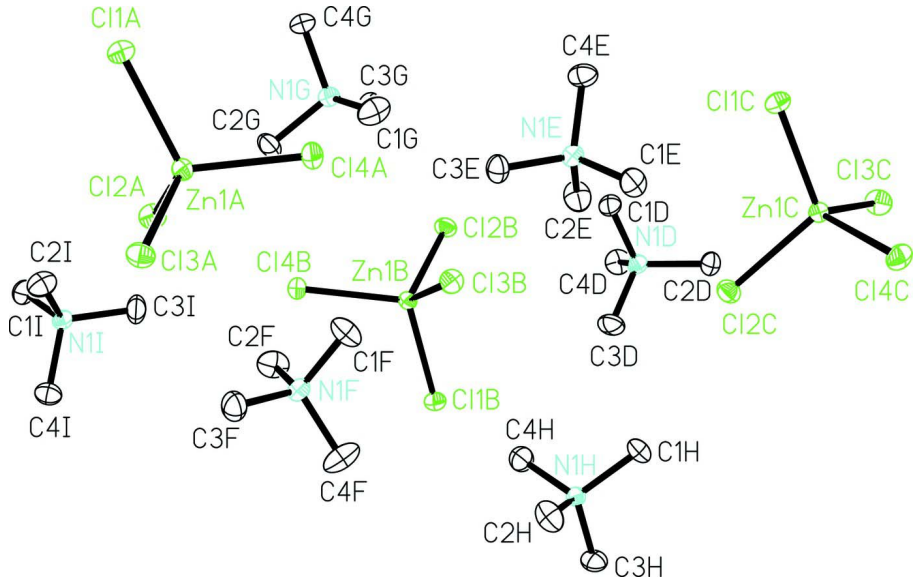

Figure 1

View of the unique atoms showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

bis(tetramethylammonium) tetrachlorozincate(II)

Crystal data

$(C_4H_{12}N)_2[ZnCl_4]$
$M_r = 355.46$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 8.9114\ (18)$ Å
$b = 15.105\ (3)$ Å
$c = 36.493\ (7)$ Å
$V = 4912.2\ (17)$ Å^3
$Z = 12$
$F(000) = 2208$
$D_x = 1.442$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6850 reflections
$\theta = 2.5–28.2°$
$\mu = 2.13$ mm^{-1}
$T = 100$ K
Plate, colourless
0.36 × 0.24 × 0.04 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
\ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.512$, $T_{max} = 0.918$
32538 measured reflections
9616 independent reflections
9039 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -10\rightarrow10$
$k = -18\rightarrow18$
$l = -44\rightarrow45$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.055$
$S = 1.00$
9616 reflections
407 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.022P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.611 (6)

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1A	0.22269 (3)	0.833130 (18)	0.249954 (7)	0.01451 (7)
Cl1A	0.27151 (7)	0.83942 (4)	0.311249 (16)	0.01927 (14)
Cl2A	0.42172 (7)	0.89470 (4)	0.220415 (17)	0.02094 (15)
Cl3A	0.01026 (7)	0.91090 (4)	0.236224 (17)	0.02043 (14)
Cl4A	0.18901 (8)	0.69109 (4)	0.231878 (17)	0.02295 (15)
Zn1B	0.80374 (3)	0.648812 (18)	0.085633 (7)	0.01432 (7)
Cl1B	0.78781 (7)	0.67180 (4)	0.024348 (16)	0.01814 (13)
Cl2B	0.99810 (7)	0.55514 (4)	0.098555 (17)	0.01982 (15)
Cl3B	0.58278 (8)	0.59089 (4)	0.106043 (18)	0.02098 (15)
Cl4B	0.84775 (8)	0.77752 (4)	0.115946 (17)	0.01842 (14)
Zn1C	0.27960 (3)	0.148178 (18)	0.084326 (7)	0.01390 (7)
Cl1C	0.30736 (7)	0.14537 (4)	0.145927 (16)	0.01915 (14)
Cl2C	0.32460 (8)	0.28462 (4)	0.060498 (18)	0.02114 (15)
Cl3C	0.44003 (8)	0.04975 (4)	0.057901 (18)	0.02362 (16)
Cl4C	0.04001 (7)	0.10798 (4)	0.069889 (17)	0.02188 (15)
N1D	0.7769 (2)	0.34272 (13)	0.04975 (5)	0.0161 (5)
C1D	0.7608 (3)	0.34836 (17)	0.09057 (6)	0.0214 (6)
H1D1	0.6561	0.3374	0.0974	0.032*
H1D2	0.7906	0.4075	0.0989	0.032*
H1D3	0.8253	0.3039	0.1021	0.032*
C2D	0.7222 (3)	0.25421 (16)	0.03673 (7)	0.0222 (6)
H2D1	0.7274	0.2518	0.0099	0.033*
H2D2	0.6181	0.2455	0.0446	0.033*
H2D3	0.7854	0.2074	0.0471	0.033*
C3D	0.6849 (3)	0.41380 (17)	0.03245 (7)	0.0268 (7)
H3D1	0.6954	0.4106	0.0058	0.040*
H3D2	0.7197	0.4717	0.0411	0.040*
H3D3	0.5793	0.4058	0.0391	0.040*
C4D	0.9376 (3)	0.35435 (19)	0.03958 (7)	0.0248 (6)
H4D1	0.9967	0.3053	0.0496	0.037*
H4D2	0.9747	0.4104	0.0496	0.037*
H4D3	0.9473	0.3550	0.0128	0.037*
N1E	0.2499 (2)	0.40749 (14)	0.17102 (5)	0.0148 (5)
C1E	0.1088 (3)	0.36434 (17)	0.15805 (8)	0.0252 (7)
H1E1	0.0675	0.3979	0.1374	0.038*

H1E2	0.0355	0.3631	0.1781	0.038*
H1E3	0.1306	0.3037	0.1502	0.038*
C2E	0.3602 (3)	0.41315 (18)	0.14052 (7)	0.0278 (7)
H2E1	0.3172	0.4477	0.1204	0.042*
H2E2	0.3842	0.3534	0.1318	0.042*
H2E3	0.4520	0.4420	0.1493	0.042*
C3E	0.2129 (3)	0.49855 (16)	0.18458 (7)	0.0218 (6)
H3E1	0.3047	0.5277	0.1931	0.033*
H3E2	0.1412	0.4943	0.2049	0.033*
H3E3	0.1685	0.5332	0.1646	0.033*
C4E	0.3153 (3)	0.35468 (17)	0.20164 (7)	0.0233 (6)
H4E1	0.3432	0.2958	0.1926	0.035*
H4E2	0.2410	0.3487	0.2213	0.035*
H4E3	0.4046	0.3848	0.2111	0.035*
N1F	0.2919 (3)	0.82358 (13)	0.11507 (5)	0.0179 (5)
C1F	0.2556 (3)	0.74168 (17)	0.13618 (8)	0.0279 (7)
H1F1	0.2800	0.7508	0.1621	0.042*
H1F2	0.3146	0.6921	0.1266	0.042*
H1F3	0.1485	0.7284	0.1337	0.042*
C2F	0.4559 (3)	0.84202 (19)	0.11789 (8)	0.0283 (7)
H2F1	0.4800	0.8957	0.1040	0.042*
H2F2	0.5124	0.7919	0.1079	0.042*
H2F3	0.4831	0.8506	0.1437	0.042*
C3F	0.2049 (3)	0.89951 (17)	0.13031 (8)	0.0284 (7)
H3F1	0.0973	0.8864	0.1288	0.043*
H3F2	0.2269	0.9530	0.1161	0.043*
H3F3	0.2332	0.9089	0.1560	0.043*
C4F	0.2506 (3)	0.8116 (2)	0.07569 (7)	0.0379 (8)
H4F1	0.2741	0.8658	0.0621	0.057*
H4F2	0.1429	0.7992	0.0738	0.057*
H4F3	0.3075	0.7620	0.0654	0.057*
N1G	0.7277 (2)	0.63485 (14)	0.21747 (5)	0.0161 (5)
C1G	0.5783 (3)	0.5939 (2)	0.21077 (8)	0.0304 (7)
H1G1	0.5017	0.6258	0.2248	0.046*
H1G2	0.5805	0.5318	0.2185	0.046*
H1G3	0.5544	0.5973	0.1846	0.046*
C2G	0.7243 (4)	0.73057 (17)	0.20696 (7)	0.0286 (7)
H2G1	0.8219	0.7576	0.2122	0.043*
H2G2	0.6461	0.7610	0.2210	0.043*
H2G3	0.7026	0.7359	0.1807	0.043*
C3G	0.8431 (3)	0.58795 (18)	0.19485 (7)	0.0244 (7)
H3G1	0.8174	0.5935	0.1688	0.037*
H3G2	0.8456	0.5252	0.2017	0.037*
H3G3	0.9419	0.6145	0.1992	0.037*
C4G	0.7650 (3)	0.62664 (18)	0.25733 (7)	0.0249 (7)
H4G1	0.6886	0.6574	0.2719	0.037*
H4G2	0.8634	0.6532	0.2620	0.037*
H4G3	0.7673	0.5639	0.2642	0.037*

N1H	0.2840 (2)	0.56575 (13)	−0.00491 (5)	0.0147 (5)
C1H	0.2778 (3)	0.46942 (16)	0.00445 (7)	0.0219 (6)
H1H1	0.2724	0.4624	0.0311	0.033*
H1H2	0.3682	0.4400	−0.0048	0.033*
H1H3	0.1889	0.4428	−0.0068	0.033*
C2H	0.1461 (3)	0.61057 (18)	0.00861 (8)	0.0264 (7)
H2H1	0.0579	0.5847	−0.0033	0.040*
H2H2	0.1515	0.6739	0.0029	0.040*
H2H3	0.1381	0.6027	0.0352	0.040*
C3H	0.2935 (3)	0.57694 (17)	−0.04539 (6)	0.0230 (6)
H3H1	0.3835	0.5470	−0.0546	0.035*
H3H2	0.2988	0.6401	−0.0513	0.035*
H3H3	0.2043	0.5510	−0.0569	0.035*
C4H	0.4208 (3)	0.60584 (18)	0.01198 (8)	0.0301 (7)
H4H1	0.5105	0.5767	0.0022	0.045*
H4H2	0.4172	0.5980	0.0386	0.045*
H4H3	0.4244	0.6692	0.0062	0.045*
N1I	0.7744 (2)	1.07188 (13)	0.16264 (5)	0.0150 (5)
C1I	0.9184 (3)	1.11122 (17)	0.17517 (7)	0.0216 (6)
H1I1	0.9615	1.0744	0.1946	0.032*
H1I2	0.9002	1.1710	0.1846	0.032*
H1I3	0.9886	1.1143	0.1545	0.032*
C2I	0.6673 (3)	1.06734 (18)	0.19391 (7)	0.0260 (7)
H2I1	0.7082	1.0285	0.2130	0.039*
H2I2	0.5711	1.0437	0.1854	0.039*
H2I3	0.6523	1.1268	0.2040	0.039*
C3I	0.8031 (4)	0.98137 (16)	0.14806 (7)	0.0286 (7)
H3I1	0.8714	0.9851	0.1271	0.043*
H3I2	0.7081	0.9547	0.1403	0.043*
H3I3	0.8487	0.9448	0.1672	0.043*
C4I	0.7082 (3)	1.12811 (17)	0.13312 (7)	0.0233 (6)
H4I1	0.7788	1.1323	0.1126	0.035*
H4I2	0.6880	1.1875	0.1428	0.035*
H4I3	0.6142	1.1014	0.1246	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1A	0.01419 (16)	0.01415 (15)	0.01521 (15)	0.00001 (13)	0.00065 (12)	0.00035 (12)
Cl1A	0.0185 (3)	0.0239 (3)	0.0154 (3)	−0.0007 (3)	−0.0014 (3)	0.0007 (3)
Cl2A	0.0165 (3)	0.0255 (4)	0.0209 (3)	−0.0037 (3)	0.0028 (3)	0.0024 (3)
Cl3A	0.0162 (3)	0.0223 (3)	0.0227 (3)	0.0038 (3)	−0.0018 (3)	0.0021 (3)
Cl4A	0.0318 (4)	0.0155 (3)	0.0215 (3)	−0.0028 (3)	−0.0004 (3)	−0.0019 (3)
Zn1B	0.01474 (15)	0.01379 (14)	0.01444 (14)	−0.00018 (13)	0.00038 (13)	0.00079 (12)
Cl1B	0.0189 (3)	0.0207 (3)	0.0149 (3)	0.0009 (3)	−0.0001 (3)	0.0016 (3)
Cl2B	0.0205 (4)	0.0189 (3)	0.0201 (3)	0.0046 (3)	−0.0015 (3)	0.0023 (3)
Cl3B	0.0177 (4)	0.0240 (3)	0.0212 (3)	−0.0048 (3)	0.0029 (3)	0.0013 (3)
Cl4B	0.0204 (4)	0.0157 (3)	0.0192 (3)	−0.0012 (3)	−0.0008 (3)	−0.0020 (3)

Zn1C	0.01250 (15)	0.01516 (14)	0.01404 (14)	0.00037 (13)	0.00063 (13)	−0.00004 (12)
Cl1C	0.0193 (3)	0.0243 (3)	0.0138 (3)	0.0011 (3)	−0.0003 (3)	−0.0010 (3)
Cl2C	0.0212 (4)	0.0187 (3)	0.0235 (3)	−0.0020 (3)	−0.0005 (3)	0.0038 (3)
Cl3C	0.0237 (4)	0.0247 (4)	0.0225 (3)	0.0072 (3)	0.0054 (3)	−0.0017 (3)
Cl4C	0.0145 (4)	0.0288 (4)	0.0224 (3)	−0.0039 (3)	−0.0024 (3)	−0.0007 (3)
N1D	0.0156 (11)	0.0178 (11)	0.0150 (11)	−0.0001 (10)	0.0002 (9)	−0.0003 (9)
C1D	0.0268 (16)	0.0229 (14)	0.0146 (13)	−0.0023 (12)	0.0036 (11)	−0.0007 (11)
C2D	0.0252 (16)	0.0192 (14)	0.0221 (15)	−0.0005 (13)	−0.0004 (13)	−0.0040 (11)
C3D	0.0293 (19)	0.0248 (15)	0.0262 (16)	0.0108 (14)	−0.0038 (14)	0.0033 (12)
C4D	0.0153 (15)	0.0317 (16)	0.0274 (15)	−0.0029 (13)	0.0060 (12)	0.0017 (13)
N1E	0.0126 (13)	0.0169 (11)	0.0150 (11)	0.0003 (9)	0.0010 (9)	−0.0013 (9)
C1E	0.0142 (15)	0.0238 (15)	0.0377 (17)	−0.0041 (12)	−0.0099 (13)	0.0033 (13)
C2E	0.0288 (18)	0.0265 (16)	0.0280 (16)	−0.0022 (14)	0.0104 (14)	−0.0014 (13)
C3E	0.0208 (16)	0.0181 (14)	0.0265 (15)	0.0017 (13)	−0.0006 (13)	−0.0041 (12)
C4E	0.0224 (16)	0.0277 (15)	0.0200 (14)	0.0081 (14)	−0.0014 (12)	0.0011 (12)
N1F	0.0177 (12)	0.0198 (11)	0.0163 (11)	−0.0004 (11)	−0.0012 (10)	−0.0019 (9)
C1F	0.0236 (17)	0.0210 (15)	0.0392 (18)	0.0014 (12)	0.0038 (14)	0.0097 (13)
C2F	0.0157 (15)	0.0356 (17)	0.0336 (16)	−0.0034 (14)	−0.0017 (12)	0.0066 (14)
C3F	0.0269 (17)	0.0231 (15)	0.0352 (17)	0.0040 (14)	−0.0053 (15)	−0.0052 (13)
C4F	0.035 (2)	0.060 (2)	0.0189 (16)	−0.0039 (16)	−0.0039 (13)	−0.0064 (15)
N1G	0.0156 (12)	0.0180 (11)	0.0146 (11)	0.0013 (10)	−0.0001 (9)	0.0000 (9)
C1G	0.0191 (16)	0.0458 (19)	0.0265 (16)	−0.0087 (15)	−0.0016 (13)	0.0008 (14)
C2G	0.044 (2)	0.0162 (14)	0.0253 (16)	0.0071 (14)	0.0024 (15)	0.0030 (12)
C3G	0.0211 (16)	0.0253 (15)	0.0269 (16)	0.0051 (13)	0.0043 (13)	−0.0059 (13)
C4G	0.0328 (18)	0.0256 (15)	0.0164 (14)	−0.0001 (13)	−0.0070 (12)	0.0015 (12)
N1H	0.0152 (12)	0.0142 (10)	0.0148 (11)	−0.0031 (10)	−0.0011 (10)	0.0020 (9)
C1H	0.0238 (16)	0.0156 (13)	0.0263 (15)	0.0000 (13)	0.0017 (13)	0.0049 (11)
C2H	0.0246 (17)	0.0232 (15)	0.0313 (16)	0.0063 (13)	0.0131 (13)	−0.0006 (13)
C3H	0.0274 (17)	0.0254 (15)	0.0163 (13)	−0.0005 (14)	0.0027 (13)	0.0053 (11)
C4H	0.0286 (18)	0.0240 (16)	0.0377 (18)	−0.0052 (14)	−0.0139 (14)	0.0024 (14)
N1I	0.0118 (11)	0.0180 (11)	0.0153 (11)	−0.0013 (9)	−0.0015 (9)	−0.0001 (9)
C1I	0.0171 (15)	0.0231 (15)	0.0246 (15)	−0.0039 (13)	−0.0024 (12)	−0.0027 (12)
C2I	0.0228 (17)	0.0345 (17)	0.0207 (15)	−0.0058 (14)	0.0032 (13)	0.0023 (13)
C3I	0.0325 (19)	0.0198 (14)	0.0336 (17)	0.0005 (14)	−0.0048 (15)	−0.0094 (13)
C4I	0.0198 (15)	0.0262 (15)	0.0238 (14)	0.0029 (13)	−0.0002 (13)	0.0043 (12)

Geometric parameters (Å, º)

Zn1A—Cl4A	2.2645 (8)	C3F—H3F1	0.9800
Zn1A—Cl2A	2.2743 (8)	C3F—H3F2	0.9800
Zn1A—Cl1A	2.2807 (8)	C3F—H3F3	0.9800
Zn1A—Cl3A	2.2836 (8)	C4F—H4F1	0.9800
Zn1B—Cl1B	2.2677 (8)	C4F—H4F2	0.9800
Zn1B—Cl4B	2.2709 (7)	C4F—H4F3	0.9800
Zn1B—Cl3B	2.2797 (8)	N1G—C1G	1.488 (3)
Zn1B—Cl2B	2.2857 (8)	N1G—C2G	1.496 (3)
Zn1C—Cl1C	2.2620 (8)	N1G—C3G	1.497 (3)
Zn1C—Cl2C	2.2726 (8)	N1G—C4G	1.497 (3)

Zn1C—Cl3C	2.2770 (8)	C1G—H1G1	0.9800
Zn1C—Cl4C	2.2814 (8)	C1G—H1G2	0.9800
N1D—C4D	1.490 (3)	C1G—H1G3	0.9800
N1D—C3D	1.491 (3)	C2G—H2G1	0.9800
N1D—C1D	1.499 (3)	C2G—H2G2	0.9800
N1D—C2D	1.500 (3)	C2G—H2G3	0.9800
C1D—H1D1	0.9800	C3G—H3G1	0.9800
C1D—H1D2	0.9800	C3G—H3G2	0.9800
C1D—H1D3	0.9800	C3G—H3G3	0.9800
C2D—H2D1	0.9800	C4G—H4G1	0.9800
C2D—H2D2	0.9800	C4G—H4G2	0.9800
C2D—H2D3	0.9800	C4G—H4G3	0.9800
C3D—H3D1	0.9800	N1H—C2H	1.487 (3)
C3D—H3D2	0.9800	N1H—C3H	1.489 (3)
C3D—H3D3	0.9800	N1H—C4H	1.494 (3)
C4D—H4D1	0.9800	N1H—C1H	1.496 (3)
C4D—H4D2	0.9800	C1H—H1H1	0.9800
C4D—H4D3	0.9800	C1H—H1H2	0.9800
N1E—C2E	1.488 (3)	C1H—H1H3	0.9800
N1E—C4E	1.491 (3)	C2H—H2H1	0.9800
N1E—C1E	1.494 (3)	C2H—H2H2	0.9800
N1E—C3E	1.498 (3)	C2H—H2H3	0.9800
C1E—H1E1	0.9800	C3H—H3H1	0.9800
C1E—H1E2	0.9800	C3H—H3H2	0.9800
C1E—H1E3	0.9800	C3H—H3H3	0.9800
C2E—H2E1	0.9800	C4H—H4H1	0.9800
C2E—H2E2	0.9800	C4H—H4H2	0.9800
C2E—H2E3	0.9800	C4H—H4H3	0.9800
C3E—H3E1	0.9800	N1I—C1I	1.486 (3)
C3E—H3E2	0.9800	N1I—C3I	1.489 (3)
C3E—H3E3	0.9800	N1I—C2I	1.490 (3)
C4E—H4E1	0.9800	N1I—C4I	1.493 (3)
C4E—H4E2	0.9800	C1I—H1I1	0.9800
C4E—H4E3	0.9800	C1I—H1I2	0.9800
N1F—C2F	1.491 (3)	C1I—H1I3	0.9800
N1F—C3F	1.492 (3)	C2I—H2I1	0.9800
N1F—C1F	1.493 (3)	C2I—H2I2	0.9800
N1F—C4F	1.494 (3)	C2I—H2I3	0.9800
C1F—H1F1	0.9800	C3I—H3I1	0.9800
C1F—H1F2	0.9800	C3I—H3I2	0.9800
C1F—H1F3	0.9800	C3I—H3I3	0.9800
C2F—H2F1	0.9800	C4I—H4I1	0.9800
C2F—H2F2	0.9800	C4I—H4I2	0.9800
C2F—H2F3	0.9800	C4I—H4I3	0.9800

Cl4A—Zn1A—Cl2A	110.65 (3)	N1F—C3F—H3F3	109.5
Cl4A—Zn1A—Cl1A	110.51 (3)	H3F1—C3F—H3F3	109.5
Cl2A—Zn1A—Cl1A	107.40 (3)	H3F2—C3F—H3F3	109.5

Cl4A—Zn1A—Cl3A	108.27 (3)	N1F—C4F—H4F1	109.5
Cl2A—Zn1A—Cl3A	109.40 (3)	N1F—C4F—H4F2	109.5
Cl1A—Zn1A—Cl3A	110.60 (3)	H4F1—C4F—H4F2	109.5
Cl1B—Zn1B—Cl4B	111.11 (3)	N1F—C4F—H4F3	109.5
Cl1B—Zn1B—Cl3B	109.08 (3)	H4F1—C4F—H4F3	109.5
Cl4B—Zn1B—Cl3B	108.58 (3)	H4F2—C4F—H4F3	109.5
Cl1B—Zn1B—Cl2B	110.23 (3)	C1G—N1G—C2G	109.9 (2)
Cl4B—Zn1B—Cl2B	107.37 (3)	C1G—N1G—C3G	109.1 (2)
Cl3B—Zn1B—Cl2B	110.46 (3)	C2G—N1G—C3G	109.3 (2)
Cl1C—Zn1C—Cl2C	112.21 (3)	C1G—N1G—C4G	108.9 (2)
Cl1C—Zn1C—Cl3C	109.88 (3)	C2G—N1G—C4G	109.50 (19)
Cl2C—Zn1C—Cl3C	108.62 (3)	C3G—N1G—C4G	110.1 (2)
Cl1C—Zn1C—Cl4C	109.08 (3)	N1G—C1G—H1G1	109.5
Cl2C—Zn1C—Cl4C	108.55 (3)	N1G—C1G—H1G2	109.5
Cl3C—Zn1C—Cl4C	108.42 (3)	H1G1—C1G—H1G2	109.5
C4D—N1D—C3D	109.7 (2)	N1G—C1G—H1G3	109.5
C4D—N1D—C1D	109.4 (2)	H1G1—C1G—H1G3	109.5
C3D—N1D—C1D	109.11 (19)	H1G2—C1G—H1G3	109.5
C4D—N1D—C2D	109.8 (2)	N1G—C2G—H2G1	109.5
C3D—N1D—C2D	109.2 (2)	N1G—C2G—H2G2	109.5
C1D—N1D—C2D	109.54 (19)	H2G1—C2G—H2G2	109.5
N1D—C1D—H1D1	109.5	N1G—C2G—H2G3	109.5
N1D—C1D—H1D2	109.5	H2G1—C2G—H2G3	109.5
H1D1—C1D—H1D2	109.5	H2G2—C2G—H2G3	109.5
N1D—C1D—H1D3	109.5	N1G—C3G—H3G1	109.5
H1D1—C1D—H1D3	109.5	N1G—C3G—H3G2	109.5
H1D2—C1D—H1D3	109.5	H3G1—C3G—H3G2	109.5
N1D—C2D—H2D1	109.5	N1G—C3G—H3G3	109.5
N1D—C2D—H2D2	109.5	H3G1—C3G—H3G3	109.5
H2D1—C2D—H2D2	109.5	H3G2—C3G—H3G3	109.5
N1D—C2D—H2D3	109.5	N1G—C4G—H4G1	109.5
H2D1—C2D—H2D3	109.5	N1G—C4G—H4G2	109.5
H2D2—C2D—H2D3	109.5	H4G1—C4G—H4G2	109.5
N1D—C3D—H3D1	109.5	N1G—C4G—H4G3	109.5
N1D—C3D—H3D2	109.5	H4G1—C4G—H4G3	109.5
H3D1—C3D—H3D2	109.5	H4G2—C4G—H4G3	109.5
N1D—C3D—H3D3	109.5	C2H—N1H—C3H	108.9 (2)
H3D1—C3D—H3D3	109.5	C2H—N1H—C4H	110.7 (2)
H3D2—C3D—H3D3	109.5	C3H—N1H—C4H	108.5 (2)
N1D—C4D—H4D1	109.5	C2H—N1H—C1H	109.7 (2)
N1D—C4D—H4D2	109.5	C3H—N1H—C1H	109.81 (19)
H4D1—C4D—H4D2	109.5	C4H—N1H—C1H	109.3 (2)
N1D—C4D—H4D3	109.5	N1H—C1H—H1H1	109.5
H4D1—C4D—H4D3	109.5	N1H—C1H—H1H2	109.5
H4D2—C4D—H4D3	109.5	H1H1—C1H—H1H2	109.5
C2E—N1E—C4E	109.5 (2)	N1H—C1H—H1H3	109.5
C2E—N1E—C1E	110.2 (2)	H1H1—C1H—H1H3	109.5
C4E—N1E—C1E	109.4 (2)	H1H2—C1H—H1H3	109.5

C2E—N1E—C3E	109.9 (2)	N1H—C2H—H2H1	109.5
C4E—N1E—C3E	109.25 (19)	N1H—C2H—H2H2	109.5
C1E—N1E—C3E	108.6 (2)	H2H1—C2H—H2H2	109.5
N1E—C1E—H1E1	109.5	N1H—C2H—H2H3	109.5
N1E—C1E—H1E2	109.5	H2H1—C2H—H2H3	109.5
H1E1—C1E—H1E2	109.5	H2H2—C2H—H2H3	109.5
N1E—C1E—H1E3	109.5	N1H—C3H—H3H1	109.5
H1E1—C1E—H1E3	109.5	N1H—C3H—H3H2	109.5
H1E2—C1E—H1E3	109.5	H3H1—C3H—H3H2	109.5
N1E—C2E—H2E1	109.5	N1H—C3H—H3H3	109.5
N1E—C2E—H2E2	109.5	H3H1—C3H—H3H3	109.5
H2E1—C2E—H2E2	109.5	H3H2—C3H—H3H3	109.5
N1E—C2E—H2E3	109.5	N1H—C4H—H4H1	109.5
H2E1—C2E—H2E3	109.5	N1H—C4H—H4H2	109.5
H2E2—C2E—H2E3	109.5	H4H1—C4H—H4H2	109.5
N1E—C3E—H3E1	109.5	N1H—C4H—H4H3	109.5
N1E—C3E—H3E2	109.5	H4H1—C4H—H4H3	109.5
H3E1—C3E—H3E2	109.5	H4H2—C4H—H4H3	109.5
N1E—C3E—H3E3	109.5	C1I—N1I—C3I	109.2 (2)
H3E1—C3E—H3E3	109.5	C1I—N1I—C2I	109.63 (19)
H3E2—C3E—H3E3	109.5	C3I—N1I—C2I	110.0 (2)
N1E—C4E—H4E1	109.5	C1I—N1I—C4I	109.6 (2)
N1E—C4E—H4E2	109.5	C3I—N1I—C4I	109.4 (2)
H4E1—C4E—H4E2	109.5	C2I—N1I—C4I	109.0 (2)
N1E—C4E—H4E3	109.5	N1I—C1I—H1I1	109.5
H4E1—C4E—H4E3	109.5	N1I—C1I—H1I2	109.5
H4E2—C4E—H4E3	109.5	H1I1—C1I—H1I2	109.5
C2F—N1F—C3F	109.9 (2)	N1I—C1I—H1I3	109.5
C2F—N1F—C1F	109.4 (2)	H1I1—C1I—H1I3	109.5
C3F—N1F—C1F	109.4 (2)	H1I2—C1I—H1I3	109.5
C2F—N1F—C4F	109.3 (2)	N1I—C2I—H2I1	109.5
C3F—N1F—C4F	108.9 (2)	N1I—C2I—H2I2	109.5
C1F—N1F—C4F	110.0 (2)	H2I1—C2I—H2I2	109.5
N1F—C1F—H1F1	109.5	N1I—C2I—H2I3	109.5
N1F—C1F—H1F2	109.5	H2I1—C2I—H2I3	109.5
H1F1—C1F—H1F2	109.5	H2I2—C2I—H2I3	109.5
N1F—C1F—H1F3	109.5	N1I—C3I—H3I1	109.5
H1F1—C1F—H1F3	109.5	N1I—C3I—H3I2	109.5
H1F2—C1F—H1F3	109.5	H3I1—C3I—H3I2	109.5
N1F—C2F—H2F1	109.5	N1I—C3I—H3I3	109.5
N1F—C2F—H2F2	109.5	H3I1—C3I—H3I3	109.5
H2F1—C2F—H2F2	109.5	H3I2—C3I—H3I3	109.5
N1F—C2F—H2F3	109.5	N1I—C4I—H4I1	109.5
H2F1—C2F—H2F3	109.5	N1I—C4I—H4I2	109.5
H2F2—C2F—H2F3	109.5	H4I1—C4I—H4I2	109.5
N1F—C3F—H3F1	109.5	N1I—C4I—H4I3	109.5
N1F—C3F—H3F2	109.5	H4I1—C4I—H4I3	109.5
H3F1—C3F—H3F2	109.5	H4I2—C4I—H4I3	109.5