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[*N*,*N*′-Bis(4-chlorobenzyl)ethane-1,2-diamine]dichloridozinc(II)

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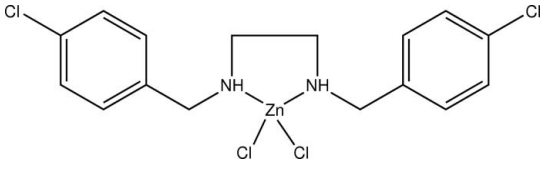
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.026 Å; R factor = 0.062; wR factor = 0.190; data-to-parameter ratio = 15.4.

In the title complex, $[ZnCl_2(C_{16}H_{18}Cl_2N_2)]$, the asymmetric unit contains one molecule and two half-molecules, which have similar geometric parameters; in the latter two molecules each Zn atom lies on a twofold rotation axis. The environment about each Zn^{II} atom is distorted tetrahedral with coordination of two terminal Cl atoms and two N atoms of the *N*,*N*′-bis(4-chlorobenzyl)ethane-1,2-diamine ligand. Four N—H···Cl hydrogen bonds link the molecules into a chain of $R_2^2(8)$ rings in the [001] direction.

Related literature

For related literature, see: Han *et al.* (2006); Bernstein *et al.* (1995).



Experimental

Crystal data

$[ZnCl_2(C_{16}H_{18}Cl_2N_2)]$
M_r = 445.49
Monoclinic, $C2$
a = 32.753 (3) Å
b = 6.9774 (1) Å
c = 21.365 (2) Å
β = 127.062 (2)°
V = 3896.2 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.81 mm^{-1}
T = 298 (2) K
0.56 × 0.43 × 0.40 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.431, T_{max} = 0.532 (expected range = 0.393–0.485)
9226 measured reflections
6408 independent reflections
4023 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.190
S = 1.06
6408 reflections
417 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −1.37 e Å^{-3}
Absolute structure: Flack (1983), 2750 Freidel pairs
Flack parameter: 0.02 (3)

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.056 (9)	Zn2—N3	2.04 (1)
Zn1—N2	2.081 (8)	Zn2—Cl5	2.224 (3)
Zn1—Cl2	2.202 (3)	Zn3—N4	2.06 (1)
Zn1—Cl1	2.232 (3)	Zn3—Cl7	2.205 (3)
N1—Zn1—N2	87.9 (4)	N1—Zn1—Cl1	111.2 (2)
N1—Zn1—Cl2	111.0 (3)	N2—Zn1—Cl1	110.4 (3)
N2—Zn1—Cl2	112.7 (2)	Cl2—Zn1—Cl1	119.4 (1)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl7	0.91	2.43	3.279 (9)	155
N2—H2···Cl5	0.91	2.46	3.328 (9)	161
N3—H3···Cl2^{i}	0.91	2.45	3.295 (9)	155
N4—H4···Cl1^{ii}	0.91	2.49	3.352 (9)	158

Symmetry codes: (i) $-x+1, y, -z+1$; (ii) $-x+1, y, -z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: BV2076).

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supplementary materials

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[*N*,*N*'-Bis(4-chlorobenzyl)ethane-1,2-diamine]dichloridozinc(II)

S.-P. Yang, L.-J. Han, D.-Q. Wang and H.-T. Xia

Comment

We have reported recently the crystal structure of a Zn^{II} complex (Han *et al.*, 2006). As part of our study of Zn^{II} complexes with diamine derivatives, we report here the crystal structure of a new Zn^{II} complex, dichloro-bis[*N*,*N*'-bis(4-chlorobenzyl)-1,2-ethanediamine]zinc(II), (I).

Complex (I) crystallizes in the monoclinic space group *C*2, with two half-molecules and one molecule in the asymmetric unit (Fig. 1). The central zinc ion is in a distorted tetrahedral environment (Fig.1), coordinated by two terminal Cl atoms and two N atoms of the *N*,*N*-bis(4-chlorobenzyl)ethane-1,2-diamine; the bond lengths and angles around the metal centre are listed in table 1. It can be seen that the molecules exhibit similar geometric values, the average values of the Zn—Cl and Zn—N bond lengths are 2.232 (3) Å and 2.06 (5) Å, respectively, which are similar to the Zn^{II} complex previously reported (Zn—Cl of 2.2213 (9) Å and Zn—N of 2.056 (2) Å; Han *et al.*, 2006); the average value of the dihedral angles enclosed by the N/Zn/N planes and Cl/Zn/Cl planes is 88.9 (4)°.

The molecules are linked by four N—H···Cl hydrogen bonds into a chain of $R_2^2(8)$ rings (Bernstein *et al.*, 1995) in the [0 0 1] direction (Table 2 and Fig. 2).

Experimental

To a solution containing *N*,*N*-bis(4-chlorobenzyl)ethane-1,2-diamine (1.53 g, 5 mmol) and ethanol (30 ml), a solution of zinc chloride (0.68 g, 5 mmol) and ethanol (10 ml) was added with stirring for 6 h at room temperature (298–300 K); the solid obtained was filtered off, washed successively with chloroform and ethanol, and dried at room temperature. Colourless crystals of (I) suitable for X-ray structure analysis were obtained by slow evaporation of a DMF-ethanol (1:10) solution containing the product over a period of two weeks (*M*.p.562– 564 K).

Refinement

All H atoms were located in difference Fourier maps and then treated as riding atoms, with C—H distances of 0.93 Å (aryl), 0.97 Å (methylene), N—H distances of 0.91 Å (amine), and with $U_{iso}(H) = 1.2U_{eq}(C,N)$ (aryl, methylene, amine).

Figures

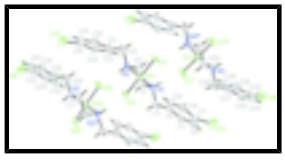


Fig. 1. The molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [symmetry code: (*)1 − *x*,*y*,1 − *z*(#)1 − *x*,*y*,-*z*].

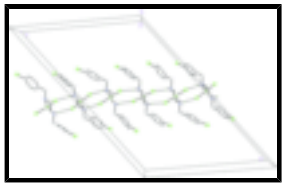


Fig. 2. A stereoview of part of the crystal structure of (I), showing the formation of a chain along [0 0 1]. For clarity, the H atoms have been omitted. Dashed lines indicate hydrogen bonds.[symmetry code: (i) −*x* + 1, *y*, −*z* + 1; (ii) −*x* + 1, *y*, −*z*].

[*N*,*N*'-Bis(4-chlorobenzyl)ethane-1,2-diamine]dichloridozinc(II)

Crystal data

$[ZnCl_2(C_{16}H_{18}Cl_2N_2)]$	F_{000} = 1808
M_r = 445.49	D_x = 1.519 Mg m^{-3}
Monoclinic, *C*2	Melting point: 562 K
Hall symbol: C 2y	Mo *K*α radiation λ = 0.71073 Å
a = 32.753 (3) Å	Cell parameters from 3365 reflections
b = 6.97740 (10) Å	θ = 3.0–28.0º
c = 21.365 (2) Å	μ = 1.81 mm^{-1}
β = 127.062 (2)º	*T* = 298 (2) K
V = 3896.2 (5) Å^3	Block, colourless
Z = 8	0.56 × 0.43 × 0.40 mm

Data collection

Bruker SMART CCD area-detector diffractometer	6408 independent reflections
Radiation source: fine-focus sealed tube	4023 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −38→36
T_{min} = 0.431, T_{max} = 0.532	*k* = −8→8
9226 measured reflections	*l* = −25→24

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.062	$w = 1/[\sigma^2(F_o^2) + (0.0962P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.190	$(\Delta/\sigma)_{max} < 0.001$
S = 1.06	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
6408 reflections	$\Delta\rho_{min}$ = −1.37 e Å^{-3}
417 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 2750 Freidel pairs

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Flack parameter: 0.02 (3)

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.48642 (5)	0.70473 (12)	0.23944 (6)	0.0384 (3)
Zn2	0.5000	0.4651 (2)	0.5000	0.0611 (6)
Zn3	0.5000	0.4662 (2)	0.0000	0.0707 (7)
Cl1	0.45178 (11)	0.8598 (4)	0.12650 (14)	0.0546 (7)
Cl2	0.52078 (11)	0.8701 (4)	0.34826 (14)	0.0518 (7)
Cl3	0.70480 (18)	1.0495 (10)	0.2570 (3)	0.139 (2)
Cl4	0.29475 (18)	1.0590 (10)	0.2786 (3)	0.145 (2)
Cl5	0.45931 (13)	0.3065 (4)	0.38706 (17)	0.0684 (9)
Cl6	0.30025 (18)	0.1189 (11)	0.5227 (4)	0.158 (2)
Cl7	0.52765 (15)	0.3038 (4)	0.10737 (18)	0.0762 (10)
Cl8	0.71047 (18)	0.1195 (11)	−0.0012 (3)	0.160 (2)
N1	0.5351 (3)	0.4920 (12)	0.2546 (5)	0.049 (2)
H1	0.5311	0.4789	0.2088	0.058*
N2	0.4373 (3)	0.4908 (12)	0.2256 (5)	0.044 (2)
H2	0.4432	0.4715	0.2726	0.053*
N3	0.4535 (4)	0.6760 (16)	0.4909 (6)	0.064 (3)
H3	0.4605	0.6891	0.5389	0.077*
N4	0.5505 (4)	0.6790 (15)	0.0209 (6)	0.063 (3)
H4	0.5479	0.6936	−0.0236	0.075*
C1	0.5143 (4)	0.3162 (18)	0.2659 (7)	0.056 (3)
H1A	0.5274	0.2027	0.2572	0.067*
H1B	0.5246	0.3120	0.3190	0.067*
C2	0.4577 (5)	0.3220 (16)	0.2089 (7)	0.058 (3)
H2A	0.4434	0.2047	0.2126	0.070*
H2B	0.4477	0.3315	0.1561	0.070*
C3	0.5902 (4)	0.5090 (19)	0.3189 (6)	0.061 (3)
H3A	0.6060	0.3838	0.3289	0.073*
H3B	0.5946	0.5489	0.3661	0.073*
C4	0.6180 (4)	0.6499 (17)	0.3023 (7)	0.057 (3)
C5	0.6617 (5)	0.595 (2)	0.3137 (8)	0.076 (4)

H5	0.6729	0.4689	0.3282	0.091*
C6	0.6916 (5)	0.729 (3)	0.3037 (9)	0.089 (4)
H6	0.7231	0.6956	0.3158	0.107*
C7	0.6727 (6)	0.886 (3)	0.2785 (9)	0.083 (4)
C8	0.6265 (5)	0.957 (2)	0.2605 (8)	0.077 (4)
H8	0.6138	1.0790	0.2404	0.093*
C9	0.6022 (5)	0.825 (2)	0.2762 (8)	0.071 (4)
H9	0.5720	0.8645	0.2674	0.085*
C10	0.3802 (4)	0.5216 (17)	0.1635 (7)	0.056 (3)
H10A	0.3743	0.5761	0.1169	0.067*
H10B	0.3628	0.3991	0.1494	0.067*
C11	0.3590 (4)	0.6512 (19)	0.1922 (7)	0.064 (4)
C12	0.3730 (5)	0.852 (2)	0.2072 (9)	0.083 (4)
H12	0.3948	0.8997	0.1968	0.099*
C13	0.3549 (5)	0.975 (3)	0.2369 (9)	0.093 (5)
H13	0.3662	1.1011	0.2505	0.111*
C14	0.3186 (5)	0.898 (3)	0.2448 (8)	0.079 (4)
C15	0.3041 (5)	0.717 (3)	0.2298 (8)	0.085 (4)
H15	0.2804	0.6750	0.2371	0.102*
C16	0.3226 (5)	0.586 (3)	0.2034 (8)	0.085 (4)
H16	0.3116	0.4592	0.1933	0.101*
C17	0.4722 (5)	0.855 (2)	0.4758 (7)	0.072 (4)
H17A	0.4583	0.8606	0.4209	0.087*
H17B	0.4606	0.9671	0.4878	0.087*
C18	0.3976 (5)	0.657 (2)	0.4330 (8)	0.088 (4)
H18A	0.3823	0.7826	0.4247	0.105*
H18B	0.3899	0.6160	0.3836	0.105*
C19	0.3736 (5)	0.523 (2)	0.4548 (8)	0.072 (4)
C20	0.3350 (6)	0.579 (3)	0.4544 (9)	0.094 (5)
H20	0.3229	0.7041	0.4390	0.113*
C21	0.3128 (5)	0.462 (3)	0.4756 (10)	0.106 (6)
H21	0.2863	0.5085	0.4758	0.127*
C22	0.3289 (5)	0.269 (3)	0.4977 (9)	0.090 (5)
C23	0.3691 (6)	0.220 (3)	0.5014 (8)	0.090 (4)
H23	0.3819	0.0960	0.5178	0.109*
C24	0.3921 (6)	0.335 (2)	0.4834 (9)	0.088 (4)
H24	0.4213	0.2934	0.4895	0.106*
C25	0.5291 (5)	0.8502 (19)	0.0300 (8)	0.074 (4)
H25A	0.5430	0.9633	0.0226	0.089*
H25B	0.5385	0.8543	0.0825	0.089*
C26	0.6038 (6)	0.653 (2)	0.0847 (8)	0.082 (4)
H26A	0.6062	0.6026	0.1291	0.099*
H26B	0.6198	0.7788	0.0998	0.099*
C27	0.6345 (6)	0.524 (2)	0.0703 (7)	0.075 (4)
C28	0.6200 (7)	0.334 (3)	0.0500 (9)	0.100 (5)
H28	0.5932	0.2862	0.0494	0.120*
C29	0.6454 (6)	0.207 (3)	0.0298 (8)	0.102 (5)
H29	0.6347	0.0808	0.0170	0.122*
C30	0.6831 (5)	0.266 (3)	0.0291 (8)	0.087 (5)

C31	0.6972 (6)	0.465 (3)	0.0448 (9)	0.101 (5)
H31	0.7218	0.5147	0.0406	0.121*
C32	0.6743 (6)	0.575 (3)	0.0654 (8)	0.094 (5)
H32	0.6858	0.7008	0.0783	0.113*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0618 (7)	0.0246 (6)	0.0328 (6)	−0.0039 (6)	0.0306 (5)	−0.0023 (5)
Zn2	0.1129 (16)	0.0341 (11)	0.0524 (11)	0.000	0.0584 (11)	0.000
Zn3	0.1457 (19)	0.0341 (11)	0.0649 (12)	0.000	0.0808 (14)	0.000
Cl1	0.091 (2)	0.0389 (15)	0.0399 (14)	0.0112 (13)	0.0425 (14)	0.0066 (11)
Cl2	0.0859 (18)	0.0366 (15)	0.0380 (13)	−0.0087 (12)	0.0401 (13)	−0.0056 (10)
Cl3	0.106 (3)	0.193 (5)	0.138 (4)	−0.057 (3)	0.083 (3)	0.003 (4)
Cl4	0.120 (3)	0.207 (6)	0.125 (3)	0.060 (4)	0.083 (3)	−0.003 (4)
Cl5	0.123 (3)	0.0428 (17)	0.0542 (16)	−0.0172 (15)	0.0614 (18)	−0.0119 (13)
Cl6	0.093 (3)	0.203 (6)	0.162 (5)	−0.042 (3)	0.069 (3)	0.016 (4)
Cl7	0.152 (3)	0.0445 (17)	0.0737 (19)	0.0237 (17)	0.090 (2)	0.0174 (14)
Cl8	0.098 (3)	0.223 (7)	0.133 (4)	0.066 (4)	0.056 (3)	0.009 (4)
N1	0.078 (6)	0.032 (5)	0.047 (5)	0.001 (4)	0.044 (5)	0.002 (4)
N2	0.076 (6)	0.025 (5)	0.052 (5)	−0.012 (4)	0.049 (5)	−0.004 (4)
N3	0.114 (8)	0.055 (7)	0.060 (6)	0.005 (6)	0.072 (6)	0.000 (5)
N4	0.117 (8)	0.042 (6)	0.057 (5)	0.003 (6)	0.067 (6)	0.006 (5)
C1	0.085 (8)	0.024 (6)	0.070 (7)	0.016 (6)	0.053 (7)	0.010 (6)
C2	0.096 (9)	0.024 (6)	0.073 (7)	−0.020 (5)	0.060 (7)	−0.012 (5)
C3	0.076 (8)	0.048 (7)	0.066 (7)	0.015 (6)	0.046 (7)	0.004 (6)
C4	0.063 (7)	0.050 (8)	0.073 (8)	0.006 (5)	0.048 (6)	−0.004 (5)
C5	0.075 (8)	0.072 (9)	0.091 (10)	0.013 (7)	0.056 (8)	0.004 (7)
C6	0.079 (9)	0.097 (12)	0.103 (11)	0.011 (10)	0.061 (8)	−0.003 (10)
C7	0.081 (10)	0.081 (12)	0.087 (10)	−0.028 (8)	0.051 (8)	−0.010 (8)
C8	0.073 (8)	0.063 (9)	0.103 (10)	−0.011 (7)	0.057 (8)	−0.002 (7)
C9	0.079 (9)	0.058 (9)	0.100 (10)	0.005 (6)	0.067 (8)	0.004 (7)
C10	0.067 (7)	0.046 (7)	0.064 (7)	−0.023 (5)	0.046 (6)	−0.016 (5)
C11	0.061 (7)	0.075 (11)	0.078 (8)	−0.015 (6)	0.053 (7)	−0.007 (6)
C12	0.073 (8)	0.076 (11)	0.105 (10)	−0.014 (7)	0.057 (8)	−0.013 (8)
C13	0.074 (8)	0.091 (12)	0.115 (11)	0.006 (9)	0.058 (8)	−0.021 (9)
C14	0.061 (8)	0.106 (13)	0.083 (9)	0.006 (8)	0.051 (7)	−0.004 (8)
C15	0.065 (7)	0.120 (13)	0.097 (10)	−0.001 (10)	0.062 (7)	−0.002 (11)
C16	0.072 (8)	0.086 (11)	0.094 (10)	−0.011 (8)	0.049 (8)	−0.006 (9)
C17	0.134 (10)	0.048 (8)	0.063 (8)	0.001 (7)	0.075 (8)	0.011 (6)
C18	0.100 (11)	0.074 (11)	0.074 (9)	0.008 (8)	0.044 (8)	0.005 (7)
C19	0.084 (9)	0.073 (10)	0.072 (8)	0.008 (7)	0.054 (7)	−0.006 (7)
C20	0.086 (10)	0.091 (12)	0.090 (11)	0.014 (9)	0.046 (9)	0.002 (9)
C21	0.076 (10)	0.112 (15)	0.109 (13)	0.015 (10)	0.044 (9)	−0.005 (11)
C22	0.076 (9)	0.100 (13)	0.096 (11)	−0.019 (8)	0.053 (8)	0.002 (9)
C23	0.099 (10)	0.089 (11)	0.096 (10)	−0.006 (10)	0.066 (9)	−0.004 (10)
C24	0.101 (11)	0.075 (11)	0.099 (11)	−0.002 (8)	0.066 (9)	0.006 (9)
C25	0.131 (10)	0.038 (8)	0.086 (9)	−0.002 (7)	0.083 (8)	−0.002 (7)

C26	0.128 (12)	0.057 (9)	0.076 (9)	−0.007 (7)	0.070 (9)	−0.006 (6)
C27	0.096 (10)	0.066 (10)	0.057 (7)	−0.009 (7)	0.043 (7)	0.002 (6)
C28	0.110 (12)	0.074 (11)	0.100 (11)	−0.002 (9)	0.055 (9)	−0.002 (9)
C29	0.102 (11)	0.086 (11)	0.089 (10)	0.003 (11)	0.043 (9)	−0.011 (10)
C30	0.068 (8)	0.101 (14)	0.068 (9)	0.018 (8)	0.028 (7)	0.011 (8)
C31	0.081 (10)	0.117 (16)	0.086 (10)	−0.004 (10)	0.041 (8)	0.011 (10)
C32	0.100 (11)	0.082 (11)	0.079 (9)	−0.018 (9)	0.043 (9)	0.005 (8)

Geometric parameters (Å, °)

Zn1—N1	2.056 (9)	C10—C11	1.48 (2)
Zn1—N2	2.081 (8)	C10—H10A	0.9700
Zn1—Cl2	2.202 (3)	C10—H10B	0.9700
Zn1—Cl1	2.232 (3)	C11—C16	1.43 (2)
Zn2—N3^{i}	2.04 (1)	C11—C12	1.45 (2)
Zn2—N3	2.04 (1)	C12—C13	1.40 (2)
Zn2—Cl5	2.224 (3)	C12—H12	0.9300
Zn2—Cl5^{i}	2.224 (3)	C13—C14	1.41 (2)
Zn3—N4	2.06 (1)	C13—H13	0.9300
Zn3—N4^{ii}	2.06 (1)	C14—C15	1.32 (2)
Zn3—Cl7^{ii}	2.205 (3)	C15—C16	1.39 (2)
Zn3—Cl7	2.205 (3)	C15—H15	0.9300
Cl3—C7	1.79 (2)	C16—H16	0.9300
Cl4—C14	1.75 (2)	C17—C17^{i}	1.45 (3)
Cl6—C22	1.69 (2)	C17—H17A	0.9700
Cl8—C30	1.72 (2)	C17—H17B	0.9700
N1—C3	1.48 (2)	C18—C19	1.47 (2)
N1—C1	1.49 (2)	C18—H18A	0.9700
N1—H1	0.9100	C18—H18B	0.9700
N2—C2	1.50 (1)	C19—C20	1.32 (2)
N2—C10	1.52 (2)	C19—C24	1.42 (2)
N2—H2	0.9100	C20—C21	1.34 (2)
N3—C18	1.47 (2)	C20—H20	0.9300
N3—C17	1.51 (2)	C21—C22	1.42 (2)
N3—H3	0.9100	C21—H21	0.9300
N4—C26	1.44 (2)	C22—C23	1.31 (2)
N4—C25	1.46 (2)	C23—C24	1.31 (2)
N4—H4	0.9100	C23—H23	0.9300
C1—C2	1.48 (2)	C24—H24	0.9300
C1—H1A	0.9700	C25—C25^{ii}	1.53 (3)
C1—H1B	0.9700	C25—H25A	0.9700
C2—H2A	0.9700	C25—H25B	0.9700
C2—H2B	0.9700	C26—C27	1.52 (2)
C3—C4	1.52 (2)	C26—H26A	0.9700
C3—H3A	0.9700	C26—H26B	0.9700
C3—H3B	0.9700	C27—C28	1.39 (2)
C4—C9	1.32 (2)	C27—C32	1.41 (2)
C4—C5	1.36 (2)	C28—C29	1.44 (2)

C5—C6	1.46 (2)	C28—H28	0.9300
C5—H5	0.9300	C29—C30	1.31 (2)
C6—C7	1.22 (2)	C29—H29	0.9300
C6—H6	0.9300	C30—C31	1.44 (2)
C7—C8	1.41 (2)	C31—C32	1.32 (2)
C8—C9	1.38 (2)	C31—H31	0.9300
C8—H8	0.9300	C32—H32	0.9300
C9—H9	0.9300		
N1—Zn1—N2	87.9 (4)	C11—C10—H10B	109.4
N1—Zn1—Cl2	111.0 (3)	N2—C10—H10B	109.4
N2—Zn1—Cl2	112.7 (2)	H10A—C10—H10B	108.0
N1—Zn1—Cl1	111.2 (2)	C16—C11—C12	117 (1)
N2—Zn1—Cl1	110.4 (3)	C16—C11—C10	122 (1)
Cl2—Zn1—Cl1	119.4 (1)	C12—C11—C10	121 (1)
N3^{i}—Zn2—N3	87.8 (6)	C13—C12—C11	122 (1)
N3^{i}—Zn2—Cl5	112.7 (3)	C13—C12—H12	118.9
N3—Zn2—Cl5	109.3 (3)	C11—C12—H12	118.9
N3^{i}—Zn2—Cl5^{i}	109.3 (3)	C12—C13—C14	116 (2)
N3—Zn2—Cl5^{i}	112.7 (3)	C12—C13—H13	121.9
Cl5—Zn2—Cl5^{i}	120.3 (2)	C14—C13—H13	121.9
N4—Zn3—N4^{ii}	87.8 (6)	C15—C14—C13	123 (1)
N4—Zn3—Cl7^{ii}	111.6 (3)	C15—C14—Cl4	122 (1)
N4^{ii}—Zn3—Cl7^{ii}	111.8 (3)	C13—C14—Cl4	115 (1)
N4—Zn3—Cl7	111.8 (3)	C14—C15—C16	123 (1)
N4^{ii}—Zn3—Cl7	111.6 (3)	C14—C15—H15	118.4
Cl7^{ii}—Zn3—Cl7	118.1 (2)	C16—C15—H15	118.4
C3—N1—C1	109.7 (9)	C15—C16—C11	118 (2)
C3—N1—Zn1	119.1 (7)	C15—C16—H16	121.0
C1—N1—Zn1	103.5 (6)	C11—C16—H16	121.0
C3—N1—H1	108.0	C17^{i}—C17—N3	110.2 (8)
C1—N1—H1	108.0	C17^{i}—C17—H17A	109.6
Zn1—N1—H1	108.0	N3—C17—H17A	109.6
C2—N2—C10	113.2 (8)	C17^{i}—C17—H17B	109.6
C2—N2—Zn1	100.3 (6)	N3—C17—H17B	109.6
C10—N2—Zn1	117.5 (7)	H17A—C17—H17B	108.1
C2—N2—H2	108.4	C19—C18—N3	115 (1)
C10—N2—H2	108.4	C19—C18—H18A	108.5
Zn1—N2—H2	108.4	N3—C18—H18A	108.5
C18—N3—C17	111 (1)	C19—C18—H18B	108.5
C18—N3—Zn2	119.6 (9)	N3—C18—H18B	108.5
C17—N3—Zn2	103.9 (7)	H18A—C18—H18B	107.5
C18—N3—H3	107.3	C20—C19—C24	116 (2)
C17—N3—H3	107.3	C20—C19—C18	120 (2)
Zn2—N3—H3	107.3	C24—C19—C18	124 (1)
C26—N4—C25	112 (1)	C19—C20—C21	122 (2)
C26—N4—Zn3	118.2 (8)	C19—C20—H20	119.1

C25—N4—Zn3	103.5 (7)	C21—C20—H20	119.1
C26—N4—H4	107.4	C20—C21—C22	122 (2)
C25—N4—H4	107.4	C20—C21—H21	119.3
Zn3—N4—H4	107.4	C22—C21—H21	119.3
C2—C1—N1	108.1 (9)	C23—C22—C21	115 (2)
C2—C1—H1A	110.1	C23—C22—Cl6	123 (2)
N1—C1—H1A	110.1	C21—C22—Cl6	122 (1)
C2—C1—H1B	110.1	C24—C23—C22	124 (2)
N1—C1—H1B	110.1	C24—C23—H23	118.2
H1A—C1—H1B	108.4	C22—C23—H23	118.2
C1—C2—N2	110.0 (9)	C23—C24—C19	122 (2)
C1—C2—H2A	109.7	C23—C24—H24	119.2
N2—C2—H2A	109.7	C19—C24—H24	119.2
C1—C2—H2B	109.7	N4—C25—C25^{ii}	110.2 (9)
N2—C2—H2B	109.7	N4—C25—H25A	109.6
H2A—C2—H2B	108.2	C25^{ii}—C25—H25A	109.6
N1—C3—C4	113.9 (9)	N4—C25—H25B	109.6
N1—C3—H3A	108.8	C25^{ii}—C25—H25B	109.6
C4—C3—H3A	108.8	H25A—C25—H25B	108.1
N1—C3—H3B	108.8	N4—C26—C27	117 (1)
C4—C3—H3B	108.8	N4—C26—H26A	108.0
H3A—C3—H3B	107.7	C27—C26—H26A	108.0
C9—C4—C5	116 (1)	N4—C26—H26B	108.0
C9—C4—C3	125 (1)	C27—C26—H26B	108.0
C5—C4—C3	119 (1)	H26A—C26—H26B	107.3
C4—C5—C6	121 (1)	C28—C27—C32	112 (2)
C4—C5—H5	119.3	C28—C27—C26	119 (2)
C6—C5—H5	119.3	C32—C27—C26	129 (2)
C7—C6—C5	116 (1)	C27—C28—C29	122 (2)
C7—C6—H6	122.1	C27—C28—H28	119.1
C5—C6—H6	122.1	C29—C28—H28	119.1
C6—C7—C8	128 (2)	C30—C29—C28	122 (2)
C6—C7—Cl3	118 (1)	C30—C29—H29	119.0
C8—C7—Cl3	114 (1)	C28—C29—H29	119.0
C9—C8—C7	112 (1)	C29—C30—C31	118 (2)
C9—C8—H8	123.8	C29—C30—Cl8	122 (2)
C7—C8—H8	123.8	C31—C30—Cl8	120 (2)
C4—C9—C8	126 (1)	C32—C31—C30	119 (2)
C4—C9—H9	117.1	C32—C31—H31	121.0
C8—C9—H9	117.1	C30—C31—H31	121.0
C11—C10—N2	111.3 (9)	C31—C32—C27	128 (2)
C11—C10—H10A	109.4	C31—C32—H32	116.0
N2—C10—H10A	109.4	C27—C32—H32	116.0
N2—Zn1—N1—C3	−134.9 (8)	N2—C10—C11—C16	−114.7 (13)
Cl2—Zn1—N1—C3	−21.4 (8)	N2—C10—C11—C12	67.6 (15)
Cl1—Zn1—N1—C3	114.0 (7)	C16—C11—C12—C13	5(2)
N2—Zn1—N1—C1	−12.8 (6)	C10—C11—C12—C13	−177.7 (13)
Cl2—Zn1—N1—C1	100.7 (6)	C11—C12—C13—C14	−5(2)

Cl1—Zn1—N1—C1	−123.9 (6)	C12—C13—C14—C15	4(2)
N1—Zn1—N2—C2	−17.5 (6)	C12—C13—C14—Cl4	−177.7 (11)
Cl2—Zn1—N2—C2	−129.3 (6)	C13—C14—C15—C16	−1(2)
Cl1—Zn1—N2—C2	94.4 (6)	Cl4—C14—C15—C16	−179.6 (11)
N1—Zn1—N2—C10	−140.6 (7)	C14—C15—C16—C11	0(2)
Cl2—Zn1—N2—C10	107.5 (7)	C12—C11—C16—C15	−2(2)
Cl1—Zn1—N2—C10	−28.8 (7)	C10—C11—C16—C15	−179.4 (12)
N3^{i}—Zn2—N3—C18	137.6 (10)	C18—N3—C17—C17^{i}	−170.1 (11)
Cl5—Zn2—N3—C18	24.3 (9)	Zn2—N3—C17—C17^{i}	−40.5 (12)
Cl5^{i}—Zn2—N3—C18	−112.4 (9)	C17—N3—C18—C19	−163.1 (11)
N3^{i}—Zn2—N3—C17	13.6 (5)	Zn2—N3—C18—C19	76.2 (13)
Cl5—Zn2—N3—C17	−99.8 (7)	N3—C18—C19—C20	126.6 (15)
Cl5^{i}—Zn2—N3—C17	123.6 (6)	N3—C18—C19—C24	−47.7 (19)
N4^{ii}—Zn3—N4—C26	139.5 (10)	C24—C19—C20—C21	−4(2)
Cl7^{ii}—Zn3—N4—C26	−107.9 (8)	C18—C19—C20—C21	−178.4 (14)
Cl7—Zn3—N4—C26	27.0 (9)	C19—C20—C21—C22	−2(3)
N4^{ii}—Zn3—N4—C25	14.4 (6)	C20—C21—C22—C23	5(2)
Cl7^{ii}—Zn3—N4—C25	127.1 (7)	C20—C21—C22—Cl6	−178.7 (13)
Cl7—Zn3—N4—C25	−98.0 (7)	C21—C22—C23—C24	−3(2)
C3—N1—C1—C2	170.1 (9)	Cl6—C22—C23—C24	−178.9 (13)
Zn1—N1—C1—C2	41.9 (10)	C22—C23—C24—C19	−3(3)
N1—C1—C2—N2	−63.3 (12)	C20—C19—C24—C23	6(2)
C10—N2—C2—C1	172.7 (9)	C18—C19—C24—C23	−179.4 (14)
Zn1—N2—C2—C1	46.6 (10)	C26—N4—C25—C25^{ii}	−169.0 (12)
C1—N1—C3—C4	164.5 (9)	Zn3—N4—C25—C25^{ii}	−40.3 (13)
Zn1—N1—C3—C4	−76.6 (10)	C25—N4—C26—C27	−160.0 (11)
N1—C3—C4—C9	48.9 (17)	Zn3—N4—C26—C27	79.5 (13)
N1—C3—C4—C5	−130.2 (12)	N4—C26—C27—C28	−59.8 (18)
C9—C4—C5—C6	5(2)	N4—C26—C27—C32	112.1 (16)
C3—C4—C5—C6	−175.9 (11)	C32—C27—C28—C29	2(2)
C4—C5—C6—C7	−6(2)	C26—C27—C28—C29	175.3 (13)
C5—C6—C7—C8	3(3)	C27—C28—C29—C30	0(2)
C5—C6—C7—Cl3	−174.8 (10)	C28—C29—C30—C31	−3(2)
C6—C7—C8—C9	1(2)	C28—C29—C30—Cl8	−175.6 (11)
Cl3—C7—C8—C9	178.6 (11)	C29—C30—C31—C32	5(2)
C5—C4—C9—C8	−1(2)	Cl8—C30—C31—C32	177.8 (12)
C3—C4—C9—C8	180.0 (12)	C30—C31—C32—C27	−4(3)
C7—C8—C9—C4	−2(2)	C28—C27—C32—C31	0(2)
C2—N2—C10—C11	164.1 (9)	C26—C27—C32—C31	−172.3 (15)
Zn1—N2—C10—C11	−79.6 (10)		

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

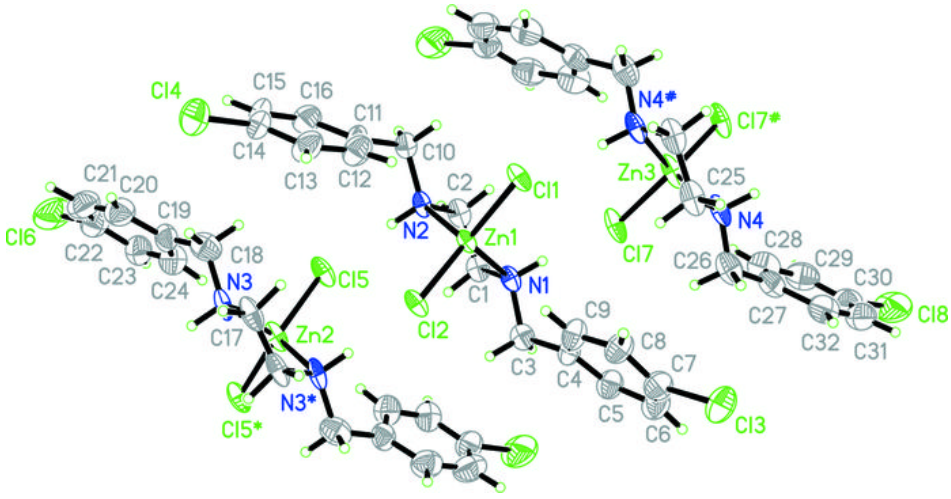
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl7	0.91	2.43	3.279 (9)	155
N2—H2···Cl5	0.91	2.46	3.328 (9)	161

N3—H3···Cl2^{i}	0.91	2.45	3.295 (9)	155
N4—H4···Cl1^{ii}	0.91	2.49	3.352 (9)	158

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

Fig. 1


Cl4
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C16
C11
C14
C13
C12
C10
C2
Cl1
N2
Zn1
Cl2
C1
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C21
C20
C19
Cl6
C22
C23
C24
C18
N3
Cl5
C17
Zn2
N3*
Cl5*
C9
C8
C7
C3
C4
C5
C6
Cl3
N4*
Cl7*
Zn3
C25
N4
Cl7
C26
C28
C29
C30
C27
C32
C31
Cl8

Fig. 2