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{Bis[2-(3,4-methylenedioxybenzylamino)ethyl]amine}dichloridozinc(II) hemihydrate

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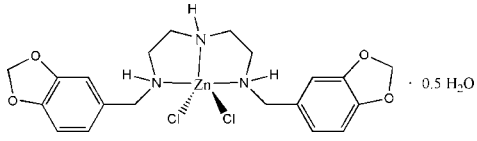
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.017 Å; disorder in solvent or counterion; R factor = 0.104; wR factor = 0.277; data-to-parameter ratio = 14.3.

In the title compound, $[ZnCl_2(C_{20}H_{25}N_3O_4)]\cdot 0.5H_2O$, the Zn^{II} ion assumes a trigonal bipyramidal coordination geometry formed by a tridentate amine ligand and two Cl^- anions. The tridentate amine ligand chelates the Zn^{II} ion in a meridional configuration. The extensive hydrogen-bonding network helps to stabilize the crystal structure.

Related literature

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



Experimental

Crystal data

$[ZnCl_2(C_{20}H_{25}N_3O_4)]\cdot 0.5H_2O$
M_r = 516.71
Monoclinic, $P2_1/c$
a = 24.042 (3) Å
b = 13.0193 (18) Å
c = 7.2678 (14) Å
β = 94.934 (2)°
V = 2266.5 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 298 (2) K
0.57 × 0.15 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.513, T_{max} = 0.855
11175 measured reflections
4003 independent reflections
2735 reflections with $I > 2\sigma(I)$
R_{int} = 0.077

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.104
$wR(F^2)$ = 0.277
S = 1.12
4003 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—Cl1	2.275 (3)	Zn1—N2	2.141 (8)
Zn1—Cl2	2.361 (3)	Zn1—N3	2.121 (9)
Zn1—N1	2.183 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.91	2.37	3.216 (12)	155
N2—H2···O5	0.91	2.19	3.03 (2)	155
N3—H3···Cl1^{ii}	0.91	2.58	3.459 (9)	162
O5—H5*A*···Cl2	0.85	2.25	3.10 (2)	173
O5—H5*B*···Cl2^{iii}	0.85	2.20	3.05 (2)	173
C8—H8*B*···Cl2^{iv}	0.97	2.74	3.713 (14)	175
C15—H15···O5	0.93	2.56	3.35 (2)	143
C20—H20*B*···O5^{iii}	0.97	2.50	3.44 (2)	164

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

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: XU2337).

References

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supplementary materials

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{Bis[2-(3,4-methylenedioxybenzylamino)ethyl]amine}dichloridozinc(II) hemihydrate

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Comment

We have reported recently the crystyl structure of a Zn^{II} complex (Han *et al.*, 2006). As part of our study of the Zn^{II} complexes with the diamine derives, we report here the crystal structure of a new Zn^{II} complex.

The title complex is a mononuclear compound, and the central zinc ion is five-coordinated by two Cl^{-} ions and three N atoms from a tridentate ligand *N*,*N*'-bis[(3,4-methylenedioxybenzyl)-2,2'-diaminodiethyl]amine (Fig. 1). The tridentate ligand chelates to the Zn^{II} ion in a meridional configuration. The coordination geometry around the Zn^{II} ion is a distorted trigonal bipyramid. The Zn—Cl and Zn—N bond lengths (Table 1) are slightly longer than those found in the related Zn^{II} complex (Han *et al.*, 2006).

The extensive hydrogen bonding network helps to stabilize the crystal structure (Table. 2).

Experimental

The ethanol solution (20 ml) of *N*,*N*'-bis[(3,4-methylenedioxybenzyl)-2,2'-diaminodiethyl]amine (1.86 g, 5 mmol) was mixed with the ethanol solution (30 ml) of zinc chloride (1.36 g, 10 mmol), the mixture was stirred for 4 h at 340 K. The crude solid obtained was filtered off and washed successively with ethanol. Single crystals of the title compound were obtained by slow evaporation of a DMF-chloroform-ethanol (1:5:10) solution of the crude product over a period of three weeks.

Refinement

H atoms were placed in calculated positions with C—H = 0.93 (aromatic), 0.97 (methylene), N—H = 0.91 and O—H = 0.82 Å, and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}$(carrier). Site occupancy factor for O5 atom was refined and converged to 0.529 (3), in the final cycles of refinement it was fixed as 0.5. The crystal quality is poor, the accuracy of the structure determination is low. The highest peak in difference Fourier map is 2.1 Å apart from C18 atom.

Figures

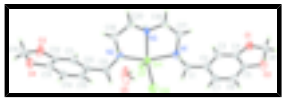


Fig. 1. The molecule of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

{Bis[2-(3,4-methylenedioxybenzylamino)ethyl]amine}dichloridozinc(II) hemihydrate

Crystal data

$[ZnCl_2(C_{20}H_{25}N_3O_4)]\cdot 0.5H_2O$ $F_{000} = 1068$

M_r = 516.71	D_x = 1.514 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 504-506 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 24.042 (3) Å	Cell parameters from 2613 reflections
b = 13.0193 (18) Å	θ = 3.0–22.0º
c = 7.2678 (14) Å	μ = 1.35 mm^{-1}
β = 94.934 (2)º	T = 298 (2) K
V = 2266.5 (6) Å^3	Prism, colorless
Z = 4	0.57 × 0.15 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4003 independent reflections
Radiation source: fine-focus sealed tube	2735 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.077
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −27→28
T_{min} = 0.513, T_{max} = 0.855	k = −11→15
11175 measured reflections	l = −8→8

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.104	H-atom parameters constrained
$wR(F^2)$ = 0.277	$w = 1/[\sigma^2(F_o^2) + (0.0881P)^2 + 21.9915P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max} < 0.001$
4003 reflections	$\Delta\rho_{max}$ = 1.46 e Å^{-3}
280 parameters	$\Delta\rho_{min}$ = −0.58 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 calculat-

ing *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}	Occ. (<1)
Zn1	0.25115 (5)	0.52956 (9)	0.26489 (17)	0.0442 (4)	
Cl1	0.22268 (12)	0.6661 (2)	0.0855 (4)	0.0546 (7)	
Cl2	0.28847 (14)	0.3967 (3)	0.0916 (6)	0.0838 (11)	
N1	0.3374 (3)	0.5641 (7)	0.3637 (12)	0.049 (2)	
H1	0.3545	0.5030	0.3920	0.058*	
N2	0.1760 (4)	0.4473 (7)	0.3044 (12)	0.049 (2)	
H2	0.1863	0.3821	0.3374	0.059*	
N3	0.2405 (3)	0.5717 (7)	0.5416 (12)	0.048 (2)	
H3	0.2278	0.6376	0.5380	0.058*	
O1	0.5505 (3)	0.7611 (6)	0.4817 (13)	0.068 (2)	
O2	0.6010 (3)	0.6208 (7)	0.4070 (13)	0.067 (2)	
O3	−0.0658 (4)	0.3908 (7)	0.2274 (16)	0.086 (3)	
O4	−0.0591 (3)	0.2137 (7)	0.2272 (13)	0.071 (2)	
O5	0.2238 (8)	0.2319 (15)	0.295 (4)	0.118 (10)	0.50
H5A	0.2440	0.2756	0.2449	0.141*	0.50
H5B	0.2443	0.1989	0.3760	0.141*	0.50
C1	0.3688 (5)	0.6133 (10)	0.2204 (16)	0.062 (3)	
H1A	0.3567	0.6842	0.2052	0.074*	
H1B	0.3600	0.5784	0.1037	0.074*	
C2	0.4317 (5)	0.6111 (10)	0.2678 (16)	0.057 (3)	
C3	0.4591 (5)	0.6960 (8)	0.3597 (16)	0.055 (3)	
H3A	0.4395	0.7541	0.3912	0.067*	
C4	0.5154 (4)	0.6885 (8)	0.3996 (16)	0.050 (3)	
C5	0.5446 (4)	0.6027 (9)	0.3560 (15)	0.050 (3)	
C6	0.5194 (5)	0.5227 (9)	0.2668 (16)	0.055 (3)	
H6	0.5397	0.4654	0.2358	0.066*	
C7	0.4631 (5)	0.5277 (9)	0.2231 (17)	0.060 (3)	
H7	0.4454	0.4728	0.1608	0.073*	
C8	0.6019 (5)	0.7118 (11)	0.521 (2)	0.076 (4)	
H8A	0.6071	0.6934	0.6504	0.091*	
H8B	0.6322	0.7568	0.4925	0.091*	
C9	0.1359 (5)	0.4388 (9)	0.1357 (16)	0.058 (3)	
H9A	0.1554	0.4092	0.0369	0.070*	
H9B	0.1242	0.5074	0.0975	0.070*	
C10	0.0845 (5)	0.3750 (9)	0.1598 (16)	0.054 (3)	
C11	0.0345 (5)	0.4233 (9)	0.1839 (17)	0.060 (3)	
H11	0.0317	0.4945	0.1858	0.072*	
C12	−0.0115 (4)	0.3608 (9)	0.2050 (16)	0.056 (3)	
C13	−0.0067 (4)	0.2563 (9)	0.2025 (17)	0.055 (3)	
C14	0.0417 (5)	0.2097 (9)	0.1823 (17)	0.057 (3)	
H14	0.0441	0.1384	0.1812	0.068*	
C15	0.0885 (5)	0.2694 (10)	0.1631 (17)	0.059 (3)	

H15	0.1228	0.2380	0.1524	0.071*
C16	−0.0944 (5)	0.2985 (10)	0.252 (2)	0.069 (3)
H16A	−0.1270	0.2948	0.1642	0.083*
H16B	−0.1069	0.2966	0.3756	0.083*
C17	0.3368 (5)	0.6222 (10)	0.5386 (17)	0.060 (3)
H17A	0.3736	0.6213	0.6049	0.072*
H17B	0.3264	0.6931	0.5130	0.072*
C18	0.2957 (5)	0.5732 (11)	0.6514 (17)	0.066 (3)
H18A	0.3073	0.5037	0.6836	0.079*
H18B	0.2930	0.6116	0.7647	0.079*
C19	0.1509 (5)	0.4926 (10)	0.4628 (17)	0.061 (3)
H19A	0.1227	0.4469	0.5045	0.073*
H19B	0.1333	0.5575	0.4276	0.073*
C20	0.1968 (5)	0.5093 (10)	0.6158 (16)	0.060 (3)
H20A	0.1821	0.5443	0.7189	0.072*
H20B	0.2121	0.4438	0.6591	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0434 (6)	0.0455 (7)	0.0439 (7)	0.0000 (6)	0.0041 (5)	0.0023 (6)
Cl1	0.0561 (16)	0.0485 (15)	0.0583 (18)	0.0004 (12)	0.0004 (13)	0.0091 (13)
Cl2	0.070 (2)	0.071 (2)	0.112 (3)	0.0116 (17)	0.0176 (19)	−0.034 (2)
N1	0.045 (5)	0.045 (5)	0.056 (6)	−0.003 (4)	0.008 (4)	0.004 (4)
N2	0.048 (5)	0.044 (5)	0.056 (6)	−0.003 (4)	0.011 (4)	−0.003 (4)
N3	0.030 (4)	0.065 (6)	0.048 (5)	−0.005 (4)	−0.007 (4)	0.017 (4)
O1	0.056 (5)	0.056 (5)	0.095 (7)	−0.012 (4)	0.015 (5)	−0.008 (5)
O2	0.054 (5)	0.067 (5)	0.081 (6)	−0.002 (4)	0.003 (4)	0.005 (5)
O3	0.056 (5)	0.068 (6)	0.135 (9)	0.003 (5)	0.017 (5)	−0.004 (6)
O4	0.049 (5)	0.069 (6)	0.095 (7)	−0.016 (4)	0.009 (4)	−0.006 (5)
O5	0.061 (12)	0.068 (12)	0.22 (3)	−0.001 (10)	−0.028 (15)	0.059 (16)
C1	0.067 (7)	0.075 (8)	0.044 (7)	−0.005 (6)	0.010 (6)	0.021 (6)
C2	0.052 (6)	0.063 (7)	0.055 (7)	−0.006 (6)	0.004 (5)	0.013 (6)
C3	0.066 (7)	0.039 (6)	0.061 (8)	0.002 (5)	0.002 (6)	0.000 (5)
C4	0.050 (6)	0.044 (6)	0.057 (7)	−0.011 (5)	0.003 (5)	0.009 (5)
C5	0.040 (6)	0.056 (7)	0.055 (7)	−0.001 (5)	0.012 (5)	0.009 (6)
C6	0.063 (7)	0.049 (7)	0.055 (7)	0.003 (6)	0.009 (6)	0.002 (6)
C7	0.064 (8)	0.060 (8)	0.058 (7)	−0.018 (6)	0.006 (6)	0.004 (6)
C8	0.056 (8)	0.077 (9)	0.092 (11)	−0.018 (7)	−0.004 (7)	0.004 (8)
C9	0.067 (7)	0.062 (7)	0.047 (7)	−0.006 (6)	0.012 (6)	0.004 (6)
C10	0.058 (7)	0.052 (7)	0.051 (7)	−0.011 (6)	0.000 (5)	0.004 (5)
C11	0.069 (8)	0.039 (6)	0.072 (8)	−0.009 (6)	−0.002 (6)	0.001 (6)
C12	0.047 (6)	0.059 (7)	0.060 (8)	0.000 (5)	0.002 (5)	0.004 (6)
C13	0.045 (6)	0.055 (7)	0.063 (8)	−0.009 (5)	−0.007 (5)	−0.007 (6)
C14	0.060 (7)	0.047 (6)	0.063 (8)	0.003 (6)	0.001 (6)	−0.003 (6)
C15	0.050 (6)	0.065 (8)	0.060 (8)	0.000 (6)	−0.002 (5)	−0.007 (6)
C16	0.052 (7)	0.078 (9)	0.077 (9)	−0.003 (7)	0.001 (6)	−0.007 (7)
C17	0.048 (6)	0.063 (7)	0.069 (8)	−0.002 (6)	0.002 (6)	−0.010 (6)

C18	0.055 (7)	0.089 (9)	0.051 (7)	−0.003 (7)	−0.011 (6)	−0.006 (7)
C19	0.049 (6)	0.073 (8)	0.063 (8)	−0.002 (6)	0.016 (6)	−0.001 (6)
C20	0.059 (7)	0.069 (8)	0.055 (7)	0.001 (6)	0.025 (6)	−0.002 (6)

Geometric parameters (Å, °)

Zn1—Cl1	2.275 (3)	C4—C5	1.371 (15)
Zn1—Cl2	2.361 (3)	C5—C6	1.344 (15)
Zn1—N1	2.183 (8)	C6—C7	1.363 (16)
Zn1—N2	2.141 (8)	C6—H6	0.9300
Zn1—N3	2.121 (9)	C7—H7	0.9300
N1—C1	1.483 (13)	C8—H8A	0.9700
N1—C17	1.481 (14)	C8—H8B	0.9700
N1—H1	0.9100	C9—C10	1.512 (15)
N2—C19	1.468 (14)	C9—H9A	0.9700
N2—C9	1.497 (14)	C9—H9B	0.9700
N2—H2	0.9100	C10—C11	1.381 (16)
N3—C20	1.467 (13)	C10—C15	1.379 (16)
N3—C18	1.487 (13)	C11—C12	1.392 (16)
N3—H3	0.9100	C11—H11	0.9300
O1—C4	1.369 (13)	C12—C13	1.366 (16)
O1—C8	1.400 (15)	C13—C14	1.332 (16)
O2—C5	1.395 (13)	C14—C15	1.384 (16)
O2—C8	1.444 (16)	C14—H14	0.9300
O3—C12	1.385 (13)	C15—H15	0.9300
O3—C16	1.404 (15)	C16—H16A	0.9700
O4—C13	1.402 (13)	C16—H16B	0.9700
O4—C16	1.415 (15)	C17—C18	1.482 (17)
O5—H5A	0.8505	C17—H17A	0.9700
O5—H5B	0.8504	C17—H17B	0.9700
C1—C2	1.521 (16)	C18—H18A	0.9700
C1—H1A	0.9700	C18—H18B	0.9700
C1—H1B	0.9700	C19—C20	1.514 (16)
C2—C7	1.378 (17)	C19—H19A	0.9700
C2—C3	1.425 (16)	C19—H19B	0.9700
C3—C4	1.363 (15)	C20—H20A	0.9700
C3—H3A	0.9300	C20—H20B	0.9700
N3—Zn1—N2	80.2 (3)	O2—C8—H8A	110.3
N3—Zn1—N1	79.8 (3)	O1—C8—H8B	110.3
N2—Zn1—N1	148.0 (3)	O2—C8—H8B	110.3
N3—Zn1—Cl1	106.6 (3)	H8A—C8—H8B	108.6
N2—Zn1—Cl1	104.6 (3)	N2—C9—C10	114.9 (9)
N1—Zn1—Cl1	104.9 (2)	N2—C9—H9A	108.5
N3—Zn1—Cl2	141.0 (3)	C10—C9—H9A	108.5
N2—Zn1—Cl2	93.9 (3)	N2—C9—H9B	108.5
N1—Zn1—Cl2	86.1 (3)	C10—C9—H9B	108.5
Cl1—Zn1—Cl2	112.09 (14)	H9A—C9—H9B	107.5
C1—N1—C17	115.2 (9)	C11—C10—C15	120.8 (11)
C1—N1—Zn1	112.6 (7)	C11—C10—C9	119.6 (10)

C17—N1—Zn1	107.9 (6)	C15—C10—C9	119.6 (11)
C1—N1—H1	106.9	C10—C11—C12	117.1 (10)
C17—N1—H1	106.9	C10—C11—H11	121.4
Zn1—N1—H1	106.9	C12—C11—H11	121.4
C19—N2—C9	113.1 (9)	C13—C12—O3	111.3 (10)
C19—N2—Zn1	108.2 (7)	C13—C12—C11	120.8 (11)
C9—N2—Zn1	114.7 (7)	O3—C12—C11	127.8 (11)
C19—N2—H2	106.8	C14—C13—C12	122.1 (11)
C9—N2—H2	106.8	C14—C13—O4	129.6 (11)
Zn1—N2—H2	106.8	C12—C13—O4	108.3 (10)
C20—N3—C18	116.3 (9)	C13—C14—C15	118.7 (11)
C20—N3—Zn1	110.7 (7)	C13—C14—H14	120.6
C18—N3—Zn1	109.8 (7)	C15—C14—H14	120.6
C20—N3—H3	106.5	C10—C15—C14	120.4 (11)
C18—N3—H3	106.5	C10—C15—H15	119.8
Zn1—N3—H3	106.5	C14—C15—H15	119.8
C4—O1—C8	105.8 (9)	O3—C16—O4	110.1 (9)
C5—O2—C8	104.9 (9)	O3—C16—H16A	109.6
C12—O3—C16	104.6 (9)	O4—C16—H16A	109.6
C13—O4—C16	105.3 (9)	O3—C16—H16B	109.6
H5A—O5—H5B	108.5	O4—C16—H16B	109.6
N1—C1—C2	112.8 (9)	H16A—C16—H16B	108.1
N1—C1—H1A	109.0	C18—C17—N1	108.2 (10)
C2—C1—H1A	109.0	C18—C17—H17A	110.1
N1—C1—H1B	109.0	N1—C17—H17A	110.1
C2—C1—H1B	109.0	C18—C17—H17B	110.1
H1A—C1—H1B	107.8	N1—C17—H17B	110.1
C7—C2—C3	118.7 (10)	H17A—C17—H17B	108.4
C7—C2—C1	121.2 (11)	N3—C18—C17	108.3 (10)
C3—C2—C1	120.2 (11)	N3—C18—H18A	110.0
C4—C3—C2	117.1 (11)	C17—C18—H18A	110.0
C4—C3—H3A	121.5	N3—C18—H18B	110.0
C2—C3—H3A	121.5	C17—C18—H18B	110.0
C3—C4—O1	127.3 (11)	H18A—C18—H18B	108.4
C3—C4—C5	121.9 (10)	N2—C19—C20	108.1 (9)
O1—C4—C5	110.8 (9)	N2—C19—H19A	110.1
C6—C5—C4	121.6 (10)	C20—C19—H19A	110.1
C6—C5—O2	130.4 (10)	N2—C19—H19B	110.1
C4—C5—O2	107.9 (10)	C20—C19—H19B	110.1
C5—C6—C7	118.2 (11)	H19A—C19—H19B	108.4
C5—C6—H6	120.9	N3—C20—C19	108.0 (9)
C7—C6—H6	120.9	N3—C20—H20A	110.1
C6—C7—C2	122.5 (11)	C19—C20—H20A	110.1
C6—C7—H7	118.8	N3—C20—H20B	110.1
C2—C7—H7	118.8	C19—C20—H20B	110.1
O1—C8—O2	106.9 (10)	H20A—C20—H20B	108.4
O1—C8—H8A	110.3		
N3—Zn1—N1—C1	−143.6 (8)	C4—C5—C6—C7	−1.3 (17)
N2—Zn1—N1—C1	164.1 (8)	O2—C5—C6—C7	−175.6 (11)

Cl1—Zn1—N1—C1	−39.0 (8)	C5—C6—C7—C2	−0.3 (18)
Cl2—Zn1—N1—C1	72.9 (8)	C3—C2—C7—C6	1.3 (18)
N3—Zn1—N1—C17	−15.4 (7)	C1—C2—C7—C6	−178.7 (11)
N2—Zn1—N1—C17	−67.7 (10)	C4—O1—C8—O2	18.4 (13)
Cl1—Zn1—N1—C17	89.3 (7)	C5—O2—C8—O1	−19.4 (13)
Cl2—Zn1—N1—C17	−158.9 (7)	C19—N2—C9—C10	−59.0 (13)
N3—Zn1—N2—C19	19.0 (7)	Zn1—N2—C9—C10	176.3 (8)
N1—Zn1—N2—C19	71.2 (10)	N2—C9—C10—C11	101.8 (13)
Cl1—Zn1—N2—C19	−85.8 (7)	N2—C9—C10—C15	−76.2 (14)
Cl2—Zn1—N2—C19	160.1 (7)	C15—C10—C11—C12	−2.1 (18)
N3—Zn1—N2—C9	146.3 (8)	C9—C10—C11—C12	179.9 (10)
N1—Zn1—N2—C9	−161.5 (7)	C16—O3—C12—C13	4.1 (14)
Cl1—Zn1—N2—C9	41.5 (8)	C16—O3—C12—C11	−176.9 (13)
Cl2—Zn1—N2—C9	−72.5 (7)	C10—C11—C12—C13	0.2 (18)
N2—Zn1—N3—C20	10.7 (7)	C10—C11—C12—O3	−178.7 (12)
N1—Zn1—N3—C20	−144.1 (8)	O3—C12—C13—C14	180.0 (11)
Cl1—Zn1—N3—C20	113.2 (7)	C11—C12—C13—C14	1(2)
Cl2—Zn1—N3—C20	−73.4 (8)	O3—C12—C13—O4	−1.1 (14)
N2—Zn1—N3—C18	140.4 (8)	C11—C12—C13—O4	179.8 (11)
N1—Zn1—N3—C18	−14.4 (8)	C16—O4—C13—C14	176.4 (13)
Cl1—Zn1—N3—C18	−117.1 (7)	C16—O4—C13—C12	−2.4 (13)
Cl2—Zn1—N3—C18	56.2 (9)	C12—C13—C14—C15	−0.1 (19)
C17—N1—C1—C2	71.4 (13)	O4—C13—C14—C15	−178.8 (12)
Zn1—N1—C1—C2	−164.2 (8)	C11—C10—C15—C14	3.0 (19)
N1—C1—C2—C7	86.2 (14)	C9—C10—C15—C14	−179.1 (11)
N1—C1—C2—C3	−93.9 (13)	C13—C14—C15—C10	−1.8 (18)
C7—C2—C3—C4	−0.7 (17)	C12—O3—C16—O4	−5.6 (14)
C1—C2—C3—C4	179.4 (10)	C13—O4—C16—O3	5.0 (14)
C2—C3—C4—O1	178.0 (11)	C1—N1—C17—C18	169.6 (10)
C2—C3—C4—C5	−0.8 (17)	Zn1—N1—C17—C18	42.8 (11)
C8—O1—C4—C3	170.4 (12)	C20—N3—C18—C17	169.0 (10)
C8—O1—C4—C5	−10.7 (13)	Zn1—N3—C18—C17	42.4 (12)
C3—C4—C5—C6	1.9 (18)	N1—C17—C18—N3	−57.0 (13)
O1—C4—C5—C6	−177.1 (10)	C9—N2—C19—C20	−173.0 (9)
C3—C4—C5—O2	177.4 (10)	Zn1—N2—C19—C20	−44.8 (11)
O1—C4—C5—O2	−1.6 (13)	C18—N3—C20—C19	−163.9 (10)
C8—O2—C5—C6	−172.2 (12)	Zn1—N3—C20—C19	−37.8 (11)
C8—O2—C5—C4	12.8 (12)	N2—C19—C20—N3	55.1 (13)

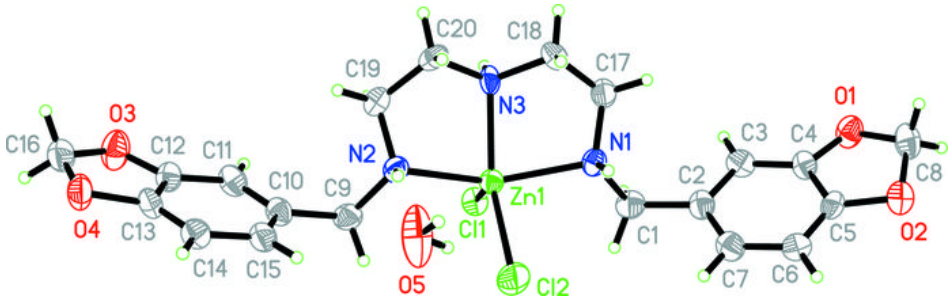
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.91	2.37	3.216 (12)	155
N2—H2···O5	0.91	2.19	3.03 (2)	155
N3—H3···Cl1^{ii}	0.91	2.58	3.459 (9)	162
O5—H5A···Cl2	0.85	2.25	3.10 (2)	173
O5—H5B···Cl2^{iii}	0.85	2.20	3.05 (2)	173
C8—H8B···Cl2^{iv}	0.97	2.74	3.713 (14)	175

C15—H15···O5	0.93	2.56	3.35 (2)	143
C20—H20B···O5^{iii}	0.97	2.50	3.44 (2)	164

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

Fig. 1


C20
C18
C19
C17
N3
O3
C16
C12
C11
N2
N1
O1
C3
C4
C10
C9
Zn1
C2
C8
O4
C13
Cl1
C1
C5
O2
C14
C15
O5
Cl2
C7
C6