Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dichlorido{2-[3-(dimethylammonio)-propyliminomethyl]phenolato}zinc(II) hemihydrate

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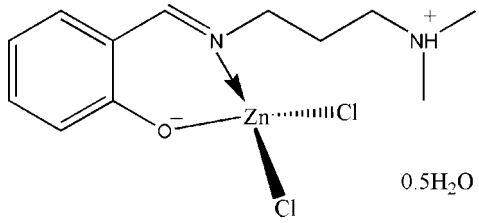
Received 14 October 2008; accepted 17 October 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.041; wR factor = 0.103; data-to-parameter ratio = 16.6.

The title complex, $[ZnCl_2(C_{12}H_{18}N_2O)]\cdot 0.5H_2O$, is a mononuclear zinc(II) compound derived from the zwitterionic form of the Schiff base 2-[3-(dimethylamino)propyliminomethyl]-phenol. The Zn^{II} atom is four-coordinated by the imine N and the phenolate O atoms of the Schiff base ligand, and by two chloride ions, in a distorted tetrahedral coordination geometry. The dimethylammonio group is disordered over two positions with site occupancies of 0.51 (3) and 0.49 (3). In the asymmetric unit, there is also a disordered water molecule with a partial occupancy of 0.5. In the crystal structure, the water molecules are linked to the Schiff base complex molecules through intermolecular N—H···O hydrogen bonds. Molecules are further linked through additional intermolecular N—H···O hydrogen bonds, forming chains running along the b axis.

Related literature

For a general background on the chemistry of Schiff base complexes, see: Ali *et al.* (2008); Biswas *et al.* (2008); Chen *et al.* (2008); Darensbourg & Frantz (2007); Habibi *et al.* (2007); Kawamoto *et al.* (2008); Lipscomb & Sträter (1996); Tomat *et al.* (2007); Wu *et al.* (2008); Yuan *et al.* (2007). For related structures, see: Zhu & Yang (2008*a*,*b*,*c*,*d*); Qiu (2006*a*,*b*); Wei *et al.* (2007); Zhu *et al.* (2007).



Experimental

Crystal data

$[ZnCl_2(C_{12}H_{18}N_2O)]\cdot 0.5H_2O$
M_r = 351.58
Orthorhombic, $Pna2_1$
a = 13.335 (2) Å
b = 16.384 (2) Å
c = 7.212 (1) Å
V = 1575.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 298 (2) K
0.23 × 0.23 × 0.22 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.650, T_{max} = 0.661
12635 measured reflections
3426 independent reflections
2915 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
S = 1.08
3426 reflections
206 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983), 1569 Friedel pairs
Flack parameter: 0.03 (2)

Table 1
Selected bond lengths (Å).

Zn1—O1	1.954 (3)	Zn1—Cl1	2.2182 (13)
Zn1—N1	2.003 (4)	Zn1—Cl2	2.2692 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2′—H2′A···O1^{i}	0.91	1.88	2.762 (14)	164
N2—H2C···O1^{i}	0.91	1.87	2.773 (12)	170

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2256).

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supporting information

Acta Cryst. (2008). E**64**, m1456–m1457 [doi:10.1107/S1600536808033977]

Dichlorido{2-[3-(dimethylammonio)propyliminomethyl]phenolato}zinc(II) hemihydrate

Xue-Wen Zhu

S1. Comment

Schiff bases have widely been used as versatile ligands in coordination chemistry (Biswas *et al.*, 2008; Wu *et al.*, 2008; Kawamoto *et al.*, 2008; Ali *et al.*, 2008; Habibi *et al.*, 2007), and their metal complexes are of great interest in many fields (Chen *et al.*, 2008; Yuan *et al.*, 2007; Tomat *et al.*, 2007; Darensbourg & Frantz, 2007). Zinc(II) is an important element in biological systems and functions as an active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase where it is in a hard-donor coordination environment of nitrogen and oxygen ligands (Lipscomb & Sträter, 1996). Recently, we have reported some Schiff base complexes (Zhu & Yang, 2008*a*,*b*,*c*,*d*). In this paper, the synthesis and structural characterization of a new zinc(II) complex (Fig. 1) of the Schiff base ligand 2-[(3-dimethylaminopropylimino)methyl]phenol is reported.

The zinc(II) atom in the title compound is four-coordinated by the imine N and phenolate O atoms of the zwitterionic form of the Schiff base ligand, and by two Cl^- ions in a tetrahedral coordination geometry. The coordinate bond lengths (Table 1) are typical and comparable to the corresponding values observed in other similar zinc(II) Schiff base complexes (Zhu *et al.*, 2007; Wei *et al.*, 2007; Qiu, 2006*a*,*b*).

In the crystal structure, the water molecules are linked to the Schiff base complex molecules through intermolecular N–H···O hydrogen bonds (Table 2). The molecules are further linked through intermolecular N–H···O hydrogen bonds (Table 2), forming chains running along the *b* axis (Fig. 2).

S2. Experimental

The Schiff base compound was prepared by the condensation of equimolar amounts of salicylaldehyde with *N*,*N*-dimethylpropane-1,3-diamine in a methanol solution. The complex was prepared by the following method: to an anhydrous methanol solution (5 ml) of $ZnCl_2$ (13.7 mg, 0.1 mmol) was added a methanol solution (10 ml) of the Schiff base compound (20.6 mg, 0.1 mmol) with stirring. The mixture was stirred for 30 min at room temperature and filtered. Upon keeping the filtrate in air for a few days, colourless block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

S3. Refinement

H atoms bound to C and N atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H distances in the range 0.93–0.97 Å, N–H distances of 0.91 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N) and 1.5U_{eq}(methyl C). The dimethylammmonium group is disordered over two distinct sites, with occupancies of 0.51 (3) and 0.49 (3), respectively. The lattice water molecule is also disordered, with an occupancy restrained to 0.50. The water H atoms were placed at calculated positions and refined with the O—H and H···H lengths constrained to 0.85 (1) and 1.37 (2) Å, respectively, and with the isotropic thermal parameter fixed at 0.08 Å^2.

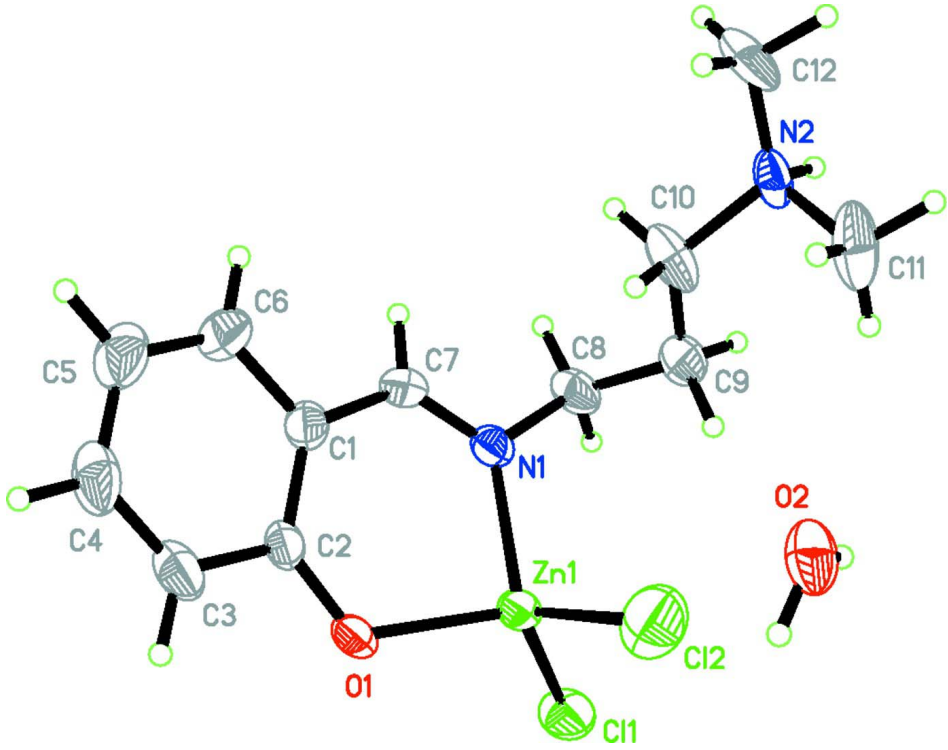

Figure 1

The molecular structure of the title compound with ellipsoids drawn at the 30% probability level. Only the major component of disorder is shown.

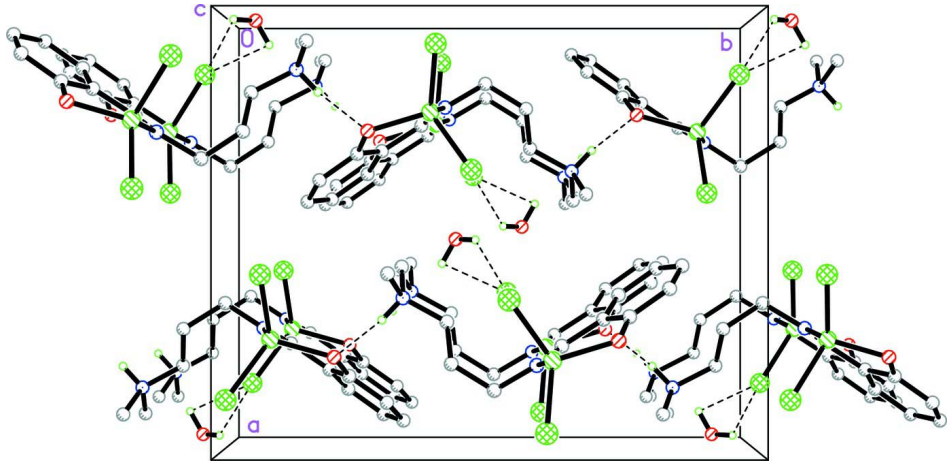

Figure 2

The crystal packing of the title compound viewed along the *c* axis. Hydrogen atoms not involved in hydrogen bonding interactions (dashed lines) are omitted for clarity. Only the major component of disorder is shown.

Dichlorido{2-[3-(dimethylammonio)propyliminomethyl]phenolato}zinc(II) hemihydrate

Crystal data

$[ZnCl_2(C_{12}H_{18}N_2O)]\cdot 0.5H_2O$
$M_r = 351.58$

Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n

a = 13.335 (2) Å
b = 16.384 (2) Å
c = 7.212 (1) Å
V = 1575.7 (4) Å^3
Z = 4
F(000) = 724
D_x = 1.482 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3872 reflections
θ = 2.4–25.3°
μ = 1.89 mm^{-1}
T = 298 K
Block, colorless
0.23 × 0.23 × 0.22 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.650, T_{max} = 0.661

12635 measured reflections
3426 independent reflections
2915 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.0°, θ_{min} = 2.0°
h = −17→17
k = −20→20
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
S = 1.08
3426 reflections
206 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0381P)^2 + 0.643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983), 1569 Friedel pairs
Absolute structure parameter: 0.03 (2)

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.

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 $F^2 > 2$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}	Occ. (<1)
Zn1	0.73458 (3)	1.10664 (2)	1.00222 (10)	0.04900 (15)	
Cl1	0.59091 (11)	1.09513 (7)	1.1550 (2)	0.0746 (4)	
Cl2	0.86270 (14)	1.03257 (11)	1.1229 (3)	0.1022 (5)	
N1	0.7159 (3)	1.0824 (2)	0.7323 (5)	0.0449 (7)	
O1	0.7749 (2)	1.21988 (16)	0.9610 (4)	0.0563 (8)	
O2	0.9856 (5)	0.9368 (4)	0.1435 (12)	0.0704 (18)	0.50
C1	0.8128 (3)	1.2011 (2)	0.6371 (6)	0.0488 (9)	
C2	0.8218 (3)	1.2425 (2)	0.8055 (6)	0.0464 (9)	

C3	0.8817 (4)	1.3118 (3)	0.8081 (9)	0.0656 (13)	
H3	0.8897	1.3401	0.9189	0.079*	
C4	0.9288 (4)	1.3393 (3)	0.6546 (10)	0.0783 (16)	
H4	0.9668	1.3868	0.6615	0.094*	
C5	0.9217 (4)	1.2989 (3)	0.4892 (11)	0.0835 (17)	
H5	0.9564	1.3172	0.3853	0.100*	
C6	0.8631 (4)	1.2317 (3)	0.4807 (8)	0.0736 (14)	
H6	0.8558	1.2049	0.3678	0.088*	
C7	0.7537 (3)	1.1280 (3)	0.6068 (6)	0.0506 (10)	
H7	0.7423	1.1129	0.4843	0.061*	
C8	0.6601 (3)	1.0080 (2)	0.6728 (7)	0.0575 (11)	
H8A	0.5968	1.0053	0.7389	0.069*	
H8B	0.6455	1.0117	0.5413	0.069*	
C9	0.7184 (4)	0.9327 (3)	0.7093 (7)	0.0674 (13)	
H9A	0.6748	0.8858	0.6947	0.081*	
H9B	0.7419	0.9335	0.8365	0.081*	
N2	0.8576 (13)	0.8452 (7)	0.543 (2)	0.055 (4)	0.51 (3)
H2C	0.8090	0.8071	0.5247	0.066*	0.51 (3)
C10	0.8059 (4)	0.9240 (3)	0.5831 (9)	0.0800 (18)	0.51 (3)
H10A	0.8570	0.9608	0.6296	0.096*	0.51 (3)
H10B	0.7849	0.9456	0.4641	0.096*	0.51 (3)
C11	0.9122 (17)	0.8214 (9)	0.713 (4)	0.091 (8)	0.51 (3)
H11A	0.8683	0.8257	0.8176	0.137*	0.51 (3)
H11B	0.9687	0.8569	0.7296	0.137*	0.51 (3)
H11C	0.9351	0.7661	0.7008	0.137*	0.51 (3)
C12	0.9244 (10)	0.8403 (9)	0.389 (3)	0.082 (6)	0.51 (3)
H12A	0.9523	0.7864	0.3816	0.123*	0.51 (3)
H12B	0.9775	0.8793	0.4036	0.123*	0.51 (3)
H12C	0.8883	0.8519	0.2765	0.123*	0.51 (3)
N2′	0.8443 (12)	0.8327 (9)	0.641 (4)	0.071 (5)	0.49 (3)
H2′A	0.7970	0.7970	0.5998	0.085*	0.49 (3)
C10′	0.8059 (4)	0.9240 (3)	0.5831 (9)	0.0800 (18)	0.49 (3)
H10C	0.8566	0.9650	0.6072	0.096*	0.49 (3)
H10D	0.7860	0.9265	0.4538	0.096*	0.49 (3)
C11′	0.8661 (16)	0.8106 (11)	0.824 (4)	0.101 (8)	0.49 (3)
H11D	0.8812	0.7534	0.8288	0.152*	0.49 (3)
H11E	0.8091	0.8220	0.9010	0.152*	0.49 (3)
H11F	0.9228	0.8413	0.8668	0.152*	0.49 (3)
C12′	0.9351 (17)	0.8164 (14)	0.534 (6)	0.139 (12)	0.49 (3)
H12D	0.9592	0.7626	0.5629	0.209*	0.49 (3)
H12E	0.9855	0.8559	0.5658	0.209*	0.49 (3)
H12F	0.9203	0.8199	0.4044	0.209*	0.49 (3)
H2A	0.984 (7)	0.973 (5)	0.228 (11)	0.080*	0.50
H2B	0.930 (4)	0.911 (5)	0.146 (15)	0.080*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0640 (3)	0.0390 (2)	0.0440 (2)	−0.00734 (18)	0.0112 (3)	−0.0061 (3)
Cl1	0.0750 (8)	0.0720 (8)	0.0768 (8)	−0.0113 (6)	0.0324 (7)	−0.0094 (6)
Cl2	0.1140 (13)	0.1004 (11)	0.0921 (11)	−0.0145 (9)	−0.0136 (10)	0.0143 (9)
N1	0.0476 (18)	0.0393 (16)	0.0478 (18)	0.0030 (14)	0.0062 (15)	−0.0058 (14)
O1	0.0774 (18)	0.0361 (12)	0.055 (2)	−0.0102 (12)	0.0190 (14)	−0.0142 (12)
O2	0.056 (4)	0.054 (4)	0.102 (6)	0.011 (3)	0.005 (4)	0.015 (4)
C1	0.052 (2)	0.0417 (19)	0.053 (2)	0.0019 (17)	0.0052 (18)	0.0038 (18)
C2	0.051 (2)	0.0308 (17)	0.058 (2)	−0.0004 (16)	0.0125 (19)	0.0006 (16)
C3	0.067 (3)	0.042 (2)	0.088 (4)	−0.008 (2)	0.011 (3)	−0.014 (2)
C4	0.064 (3)	0.048 (2)	0.123 (5)	−0.009 (2)	0.031 (3)	0.009 (3)
C5	0.079 (3)	0.072 (3)	0.100 (4)	0.002 (2)	0.041 (4)	0.019 (4)
C6	0.088 (3)	0.070 (3)	0.063 (3)	0.001 (2)	0.030 (3)	0.010 (3)
C7	0.062 (3)	0.049 (2)	0.041 (2)	−0.0007 (18)	0.0022 (19)	−0.0092 (19)
C8	0.059 (3)	0.046 (2)	0.068 (3)	−0.0111 (19)	0.001 (2)	−0.018 (2)
C9	0.098 (4)	0.043 (2)	0.061 (3)	−0.021 (2)	−0.006 (3)	−0.010 (2)
N2	0.070 (7)	0.026 (3)	0.069 (9)	−0.004 (3)	−0.020 (7)	−0.001 (5)
C10	0.078 (3)	0.037 (2)	0.124 (5)	−0.002 (2)	−0.008 (3)	−0.020 (3)
C11	0.085 (14)	0.052 (7)	0.136 (19)	0.000 (7)	−0.051 (14)	0.024 (9)
C12	0.072 (8)	0.049 (7)	0.125 (14)	0.020 (5)	0.017 (9)	−0.028 (7)
N2′	0.067 (8)	0.044 (7)	0.101 (14)	0.004 (5)	−0.006 (9)	−0.029 (8)
C10′	0.078 (3)	0.037 (2)	0.124 (5)	−0.002 (2)	−0.008 (3)	−0.020 (3)
C11′	0.094 (12)	0.051 (8)	0.16 (2)	0.014 (8)	−0.054 (13)	−0.027 (10)
C12′	0.094 (12)	0.127 (16)	0.20 (4)	0.010 (12)	0.068 (19)	−0.002 (19)

Geometric parameters (Å, º)

Zn1—O1	1.954 (3)	C9—C10	1.487 (8)
Zn1—N1	2.003 (4)	C9—H9A	0.9700
Zn1—Cl1	2.2182 (13)	C9—H9B	0.9700
Zn1—Cl2	2.2692 (18)	N2—C12	1.430 (19)
N1—C7	1.277 (6)	N2—C11	1.47 (2)
N1—C8	1.491 (5)	N2—C10	1.491 (15)
O1—C2	1.336 (5)	N2—H2C	0.9100
O2—H2A	0.852 (10)	C10—H10A	0.9700
O2—H2B	0.848 (10)	C10—H10B	0.9700
C1—C2	1.396 (6)	C11—H11A	0.9600
C1—C6	1.405 (6)	C11—H11B	0.9600
C1—C7	1.451 (6)	C11—H11C	0.9600
C2—C3	1.389 (6)	C12—H12A	0.9600
C3—C4	1.350 (8)	C12—H12B	0.9600
C3—H3	0.9300	C12—H12C	0.9600
C4—C5	1.368 (9)	N2′—C11′	1.40 (3)
C4—H4	0.9300	N2′—C12′	1.46 (2)
C5—C6	1.352 (7)	N2′—H2′A	0.9100
C5—H5	0.9300	C11′—H11D	0.9600

C6—H6	0.9300	C11′—H11E	0.9600
C7—H7	0.9300	C11′—H11F	0.9600
C8—C9	1.481 (7)	C12′—H12D	0.9600
C8—H8A	0.9700	C12′—H12E	0.9600
C8—H8B	0.9700	C12′—H12F	0.9600
O1—Zn1—N1	94.29 (13)	C10—C9—H9B	109.1
O1—Zn1—Cl1	113.19 (9)	H9A—C9—H9B	107.8
N1—Zn1—Cl1	111.04 (11)	C12—N2—C11	108.9 (14)
O1—Zn1—Cl2	111.03 (11)	C12—N2—C10	119.2 (9)
N1—Zn1—Cl2	111.10 (11)	C11—N2—C10	107.3 (12)
Cl1—Zn1—Cl2	114.48 (7)	C12—N2—H2C	106.9
C7—N1—C8	118.1 (4)	C11—N2—H2C	106.9
C7—N1—Zn1	121.6 (3)	C10—N2—H2C	106.9
C8—N1—Zn1	120.3 (3)	C9—C10—N2	124.4 (8)
C2—O1—Zn1	121.3 (2)	C9—C10—H10A	106.2
H2A—O2—H2B	108 (3)	N2—C10—H10A	106.2
C2—C1—C6	119.0 (4)	C9—C10—H10B	106.2
C2—C1—C7	125.4 (4)	N2—C10—H10B	106.2
C6—C1—C7	115.6 (4)	H10A—C10—H10B	106.4
O1—C2—C3	119.0 (4)	N2—C11—H11A	109.5
O1—C2—C1	123.7 (3)	N2—C11—H11B	109.5
C3—C2—C1	117.2 (4)	H11A—C11—H11B	109.5
C4—C3—C2	122.0 (5)	N2—C11—H11C	109.5
C4—C3—H3	119.0	H11A—C11—H11C	109.5
C2—C3—H3	119.0	H11B—C11—H11C	109.5
C3—C4—C5	121.4 (5)	N2—C12—H12A	109.5
C3—C4—H4	119.3	N2—C12—H12B	109.5
C5—C4—H4	119.3	H12A—C12—H12B	109.5
C6—C5—C4	118.3 (5)	N2—C12—H12C	109.5
C6—C5—H5	120.8	H12A—C12—H12C	109.5
C4—C5—H5	120.8	H12B—C12—H12C	109.5
C5—C6—C1	122.0 (6)	C11′—N2′—C12′	106.1 (19)
C5—C6—H6	119.0	C11′—N2′—H2′A	106.6
C1—C6—H6	119.0	C12′—N2′—H2′A	106.6
N1—C7—C1	126.2 (4)	N2′—C11′—H11D	109.5
N1—C7—H7	116.9	N2′—C11′—H11E	109.5
C1—C7—H7	116.9	H11D—C11′—H11E	109.5
C9—C8—N1	111.5 (4)	N2′—C11′—H11F	109.5
C9—C8—H8A	109.3	H11D—C11′—H11F	109.5
N1—C8—H8A	109.3	H11E—C11′—H11F	109.5
C9—C8—H8B	109.3	N2′—C12′—H12D	109.5
N1—C8—H8B	109.3	N2′—C12′—H12E	109.5
H8A—C8—H8B	108.0	H12D—C12′—H12E	109.5
C8—C9—C10	112.6 (4)	N2′—C12′—H12F	109.5
C8—C9—H9A	109.1	H12D—C12′—H12F	109.5
C10—C9—H9A	109.1	H12E—C12′—H12F	109.5
C8—C9—H9B	109.1		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2′—H2′*A*···O1^{i}	0.91	1.88	2.762 (14)	164
N2—H2*C*···O1^{i}	0.91	1.87	2.773 (12)	170

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