Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dichlorido{*N*,*N*-dimethyl-*N*′-[1-(2-pyridyl)ethylidene]ethane-1,2-diamine-κ^3N,N',N''}zinc

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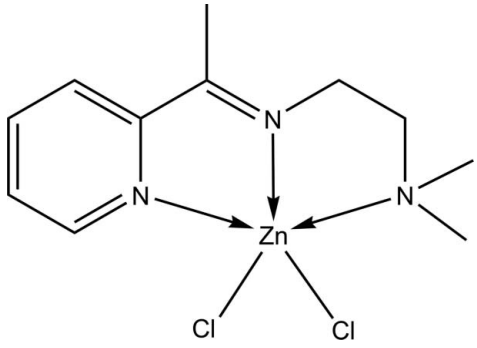
Received 26 June 2011; accepted 29 June 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.021; wR factor = 0.052; data-to-parameter ratio = 20.1.

The asymmetric unit of the title compound, $[ZnCl_2(C_{11}H_{17}N_3)]$, contains two independent pentacoordinate Zn^{II} complex molecules. In each molecule, the metal atom is coordinated by an *N*,*N*′,*N*″-tridenate Schiff base and two Cl atoms in a distorted square-pyramidal geometry. The two molecules differ little in their geometry, but more in their intermolecular interactions. In the crystal, adjacent molecules are connected *via* C—H···Cl interactions into a three-dimensional supramolecular structure. The network is supplemented by π–π interactions formed between the aromatic rings of pairs of the symmetry-related molecules [centroid–centroid distances = 3.6255 (10) and 3.7073 (10) Å]. The crystal lattice contains void spaces with a size of 52 Å^3.

Related literature

For the isotypic Mn(II) complex, see: Ikmal Hisham *et al.* (2011). For the crystal structures of similar $ZnCl_2$ complexes, see: Gourbatsis *et al.* (1999); Sun (2005). For a description of the geometry of five-coordinate metal complexes, see: Addison *et al.* (1984).



Experimental

Crystal data

$[ZnCl_2(C_{11}H_{17}N_3)]$
M_r = 327.55
Monoclinic, $P2_1/c$
a = 17.4849 (8) Å
b = 9.8161 (4) Å
c = 20.4264 (7) Å
β = 124.578 (3)°
V = 2886.6 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.05 mm^{-1}
T = 100 K
0.27 × 0.23 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.607, T_{max} = 0.748
20477 measured reflections
6294 independent reflections
5510 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.052
S = 1.04
6294 reflections
313 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···Cl2^{i}	0.95	2.79	3.6690 (17)	155
C8—H8A···Cl1^{ii}	0.99	2.63	3.5668 (16)	158
C8—H8B···Cl2^{iii}	0.99	2.73	3.6564 (16)	156
C11—H11A···Cl2^{iii}	0.98	2.77	3.6573 (17)	151
C15—H15···Cl2^{iv}	0.95	2.74	3.6347 (17)	157
C18—H18B···Cl1^{iv}	0.98	2.75	3.7227 (17)	175
C19—H19B···Cl4^{v}	0.99	2.82	3.8089 (16)	174

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

The authors thank the University of Malaya for funding this study (UMRG grant No. RG024/09BIO).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2444).

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supporting information

Acta Cryst. (2011). E**67**, m1027 [doi:10.1107/S1600536811025669]

Dichlorido{*N*,*N*-dimethyl-*N*′-[1-(2-pyridyl)ethylidene]ethane-1,2-diamine-κ^3N,N',N''}zinc

Nura Suleiman Gwaram, Hamid Khaledi and Hapipah Mohd Ali

S1. Comment

The crystal structure of the title Zn^{II} complex is isomorphous with that of the Mn^{II} analogue (Ikmal Hisham *et al.*, 2011). The asymmetric unit consists of two geometrically slightly different molecules; the weighted r.m.s. fit for the superposition of the non-H atoms in both molecules (after inversion) being 0.078 Å. The metal centers are five-coordinate in distorted square-pyramidal geometries, the apical positions being occupied by a chlorine atom. The Addison τ values (Addison *et al.*, 1984) for Zn1 and Zn2 molecules are 0.103 and 0.168, respectively. The Zn—Cl and Zn—N bond lengths are comparable to those reported for similar complexes (Gourbatsis *et al.*, 1999, Sun, 2005). In the crystal, the molecules are linked through C—H···Cl interactions (Table 1) into a three-dimensional polymeric structure and this is consolidated by π–π interactions formed between pairs of molecules [$Cg1\cdots Cg1^{i}$ = 3.6255 (10) Å; $Cg2\cdots Cg2^{ii}$ = 3.7073 (10) Å, where *Cg*1 and *Cg*2, are the centroids of the rings N1/C1—C5 and N4/C12—C16, for i: -*x*, -*y* + 1, -*z*; ii: -*x* + 1, -*y* + 1, -*z* + 1]. The lattice contains void spaces with the size of 52 $Å^3$ within which there is no evidence for included solvent.

S2. Experimental

A mixture of 2-acetylpyridine (0.20 g, 1.65 mmol) and *N*,*N*-dimethylethyldiamine (0.15 g, 1.65 mmol) in ethanol (20 ml) was refluxed for 2 hr followed by addition of a solution of zinc(II) chloride (0.225 g, 1.65 mmol) in the minimum amount of water. The resulting solution was refluxed for 30 min, and then set aside at room temperature. The colorless crystals of the title compound were obtained in a few days.

S3. Refinement

Hydrogen atoms were placed at calculated positions and refined as riding atoms with C—H distances of 0.95 (aryl), 0.98 (methyl) and 0.99 (methylene) Å, and *U*iso(H) set to 1.2 (1.5 for methyl) *U*eq(carrier atoms). The most disagreeable reflections with delta(F2)/ e.s.d. >10 were omitted (6 reflections).

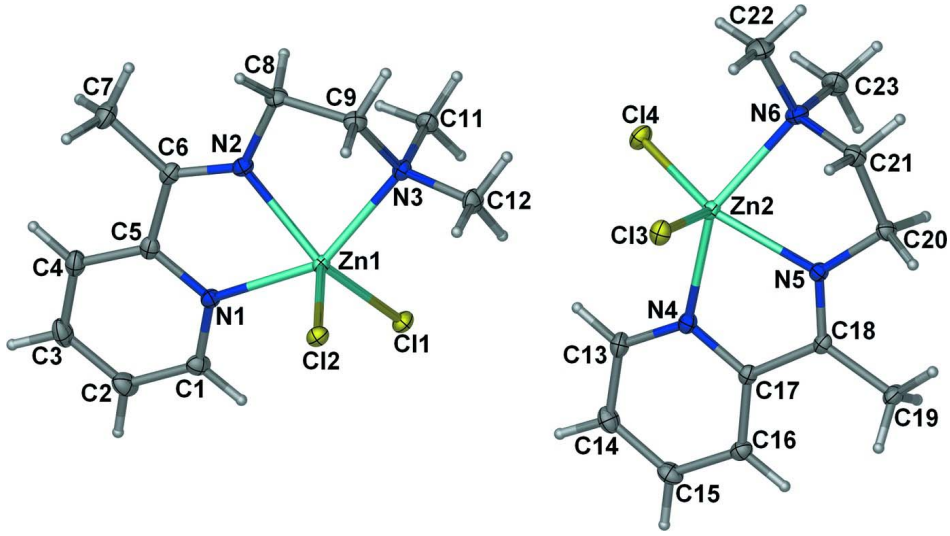

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Dichlorido{*N*,*N*-dimethyl-*N*′-[1-(2- pyridyl)ethylidene]ethane-1,2-diamine- κ^3N,N',N''}zinc

Crystal data

$[ZnCl_2(C_{11}H_{17}N_3)]$
$M_r = 327.55$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.4849\ (8)$ Å
$b = 9.8161\ (4)$ Å
$c = 20.4264\ (7)$ Å
$\beta = 124.578\ (3)°$
$V = 2886.6\ (2)$ Å^3
$Z = 8$
$F(000) = 1344$
$D_x = 1.507$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9925 reflections
$\theta = 2.4–30.6°$
$\mu = 2.05$ mm^{-1}
$T = 100$ K
Block, colorless
0.27 × 0.23 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.607$, $T_{max} = 0.748$
20477 measured reflections
6294 independent reflections
5510 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.0°$
$h = -22\rightarrow21$
$k = -12\rightarrow12$
$l = -26\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.052$
$S = 1.04$
6294 reflections
313 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

$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 0.9433P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-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 $F^2 > \sigma(F^2)$ 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	0.097383 (12)	0.523307 (18)	0.248455 (10)	0.01180 (5)
Cl1	0.22099 (3)	0.66993 (4)	0.31121 (2)	0.01561 (8)
Cl2	0.14396 (3)	0.31088 (4)	0.23943 (2)	0.01519 (8)
N1	0.03628 (9)	0.60104 (13)	0.12863 (8)	0.0139 (3)
N2	−0.04898 (9)	0.51386 (13)	0.19110 (8)	0.0141 (3)
N3	0.08663 (9)	0.49253 (13)	0.34845 (8)	0.0141 (3)
C1	0.08312 (12)	0.65350 (16)	0.10080 (10)	0.0181 (3)
H1	0.1487	0.6620	0.1358	0.022*
C2	0.03935 (13)	0.69606 (17)	0.02250 (10)	0.0225 (4)
H2	0.0745	0.7317	0.0041	0.027*
C3	−0.05605 (13)	0.68571 (18)	−0.02813 (10)	0.0238 (4)
H3	−0.0876	0.7140	−0.0820	0.029*
C4	−0.10510 (12)	0.63350 (17)	0.00065 (10)	0.0202 (3)
H4	−0.1709	0.6268	−0.0330	0.024*
C5	−0.05711 (11)	0.59111 (16)	0.07919 (9)	0.0156 (3)
C6	−0.10354 (11)	0.53702 (15)	0.11671 (10)	0.0153 (3)
C7	−0.20671 (12)	0.51654 (19)	0.06620 (11)	0.0247 (4)
H7A	−0.2272	0.4868	0.0997	0.037*
H7B	−0.2229	0.4469	0.0259	0.037*
H7C	−0.2375	0.6025	0.0400	0.037*
C8	−0.08002 (11)	0.46662 (16)	0.24024 (10)	0.0161 (3)
H8A	−0.1292	0.3968	0.2113	0.019*
H8B	−0.1056	0.5436	0.2534	0.019*
C9	0.00363 (11)	0.40623 (16)	0.31586 (9)	0.0167 (3)
H9A	−0.0107	0.3962	0.3560	0.020*
H9B	0.0166	0.3145	0.3043	0.020*
C10	0.16872 (11)	0.42164 (17)	0.41521 (9)	0.0196 (3)
H10A	0.2242	0.4774	0.4349	0.029*
H10B	0.1762	0.3336	0.3969	0.029*
H10C	0.1601	0.4069	0.4581	0.029*
C11	0.07513 (12)	0.62345 (17)	0.37716 (10)	0.0186 (3)
H11A	0.0239	0.6745	0.3324	0.028*

H11B	0.1326	0.6765	0.4015	0.028*
H11C	0.0613	0.6065	0.4167	0.028*
Zn2	0.381351 (12)	0.529056 (18)	0.644032 (11)	0.01293 (5)
Cl3	0.34646 (3)	0.30943 (4)	0.59819 (2)	0.01758 (8)
Cl4	0.27052 (3)	0.69499 (4)	0.58273 (2)	0.01882 (9)
N4	0.45804 (9)	0.59876 (13)	0.59532 (8)	0.0145 (3)
N5	0.52234 (9)	0.51339 (13)	0.73866 (8)	0.0130 (3)
N6	0.37431 (9)	0.51154 (13)	0.74869 (8)	0.0163 (3)
C12	0.42130 (12)	0.64614 (16)	0.52195 (10)	0.0182 (3)
H12	0.3558	0.6565	0.4872	0.022*
C13	0.47570 (12)	0.68075 (17)	0.49470 (10)	0.0205 (4)
H13	0.4477	0.7133	0.4420	0.025*
C14	0.57101 (12)	0.66722 (16)	0.54521 (10)	0.0198 (4)
H14	0.6095	0.6906	0.5279	0.024*
C15	0.60962 (11)	0.61874 (16)	0.62199 (10)	0.0161 (3)
H15	0.6750	0.6085	0.6580	0.019*
C16	0.55100 (11)	0.58562 (15)	0.64499 (9)	0.0130 (3)
C17	0.58544 (11)	0.53679 (15)	0.72681 (9)	0.0129 (3)
C18	0.68712 (11)	0.52205 (17)	0.78736 (10)	0.0181 (3)
H18A	0.7152	0.6124	0.8059	0.027*
H18B	0.7153	0.4753	0.7636	0.027*
H18C	0.6978	0.4688	0.8324	0.027*
C19	0.54256 (11)	0.46863 (16)	0.81533 (9)	0.0157 (3)
H19A	0.5678	0.5453	0.8536	0.019*
H19B	0.5891	0.3943	0.8374	0.019*
C20	0.45215 (11)	0.41849 (16)	0.80131 (10)	0.0172 (3)
H20A	0.4377	0.3267	0.7770	0.021*
H20B	0.4595	0.4110	0.8529	0.021*
C21	0.38747 (13)	0.64417 (17)	0.78738 (11)	0.0234 (4)
H21A	0.3349	0.7038	0.7516	0.035*
H21B	0.4451	0.6861	0.7997	0.035*
H21C	0.3912	0.6309	0.8367	0.035*
C22	0.28596 (12)	0.4513 (2)	0.72779 (11)	0.0263 (4)
H22A	0.2878	0.4376	0.7762	0.039*
H22B	0.2766	0.3634	0.7015	0.039*
H22C	0.2346	0.5127	0.6918	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01005 (10)	0.01180 (9)	0.01230 (9)	0.00035 (7)	0.00560 (8)	0.00060 (7)
Cl1	0.01217 (18)	0.01420 (18)	0.01770 (19)	−0.00150 (14)	0.00683 (16)	−0.00033 (14)
Cl2	0.01386 (19)	0.01249 (18)	0.01870 (19)	0.00000 (14)	0.00892 (16)	−0.00121 (14)
N1	0.0130 (7)	0.0136 (7)	0.0141 (6)	0.0031 (5)	0.0071 (6)	0.0012 (5)
N2	0.0132 (7)	0.0117 (6)	0.0175 (7)	0.0005 (5)	0.0088 (6)	−0.0004 (5)
N3	0.0128 (7)	0.0131 (6)	0.0142 (7)	0.0005 (5)	0.0064 (6)	0.0003 (5)
C1	0.0182 (9)	0.0167 (8)	0.0211 (8)	0.0044 (7)	0.0122 (7)	0.0029 (6)
C2	0.0274 (10)	0.0221 (9)	0.0227 (9)	0.0062 (7)	0.0170 (8)	0.0067 (7)

C3	0.0294 (10)	0.0232 (9)	0.0151 (8)	0.0067 (7)	0.0105 (8)	0.0033 (7)
C4	0.0188 (9)	0.0201 (9)	0.0158 (8)	0.0025 (7)	0.0062 (7)	−0.0008 (7)
C5	0.0161 (8)	0.0121 (8)	0.0153 (8)	0.0018 (6)	0.0068 (7)	−0.0023 (6)
C6	0.0137 (8)	0.0114 (7)	0.0179 (8)	0.0003 (6)	0.0072 (7)	−0.0017 (6)
C7	0.0150 (9)	0.0282 (10)	0.0222 (9)	−0.0020 (7)	0.0055 (8)	0.0009 (7)
C8	0.0147 (8)	0.0158 (8)	0.0198 (8)	−0.0029 (6)	0.0109 (7)	−0.0009 (6)
C9	0.0182 (9)	0.0144 (8)	0.0197 (8)	−0.0015 (6)	0.0120 (7)	0.0009 (6)
C10	0.0179 (9)	0.0203 (9)	0.0166 (8)	0.0038 (7)	0.0074 (7)	0.0048 (7)
C11	0.0186 (9)	0.0178 (8)	0.0189 (8)	0.0017 (7)	0.0103 (7)	−0.0035 (7)
Zn2	0.01031 (10)	0.01210 (9)	0.01425 (9)	−0.00008 (7)	0.00570 (8)	−0.00033 (7)
Cl3	0.0177 (2)	0.01292 (18)	0.01780 (19)	−0.00023 (15)	0.00746 (17)	−0.00134 (14)
Cl4	0.0140 (2)	0.01604 (19)	0.02074 (19)	0.00305 (15)	0.00643 (17)	0.00000 (15)
N4	0.0132 (7)	0.0133 (7)	0.0142 (7)	−0.0006 (5)	0.0062 (6)	−0.0007 (5)
N5	0.0126 (7)	0.0121 (6)	0.0138 (6)	0.0007 (5)	0.0071 (6)	0.0003 (5)
N6	0.0143 (7)	0.0154 (7)	0.0205 (7)	−0.0009 (5)	0.0107 (6)	−0.0018 (5)
C12	0.0157 (8)	0.0182 (8)	0.0147 (8)	0.0000 (7)	0.0051 (7)	0.0007 (6)
C13	0.0264 (10)	0.0181 (8)	0.0165 (8)	−0.0003 (7)	0.0118 (8)	0.0021 (6)
C14	0.0253 (9)	0.0179 (8)	0.0221 (9)	−0.0022 (7)	0.0168 (8)	0.0005 (7)
C15	0.0144 (8)	0.0151 (8)	0.0190 (8)	0.0005 (6)	0.0096 (7)	−0.0011 (6)
C16	0.0127 (8)	0.0102 (7)	0.0138 (7)	0.0012 (6)	0.0062 (7)	−0.0009 (6)
C17	0.0117 (8)	0.0097 (7)	0.0142 (8)	−0.0005 (6)	0.0055 (7)	−0.0021 (6)
C18	0.0124 (8)	0.0215 (9)	0.0184 (8)	0.0004 (7)	0.0075 (7)	0.0017 (7)
C19	0.0169 (8)	0.0165 (8)	0.0145 (8)	0.0020 (6)	0.0093 (7)	0.0027 (6)
C20	0.0196 (9)	0.0155 (8)	0.0177 (8)	0.0008 (7)	0.0113 (7)	0.0017 (6)
C21	0.0255 (10)	0.0216 (9)	0.0248 (9)	0.0036 (7)	0.0152 (8)	−0.0044 (7)
C22	0.0199 (10)	0.0327 (10)	0.0310 (10)	−0.0051 (8)	0.0173 (9)	−0.0013 (8)

Geometric parameters (Å, º)

Zn1—N2	2.1278 (13)	Zn2—N5	2.1044 (13)
Zn1—N3	2.1758 (13)	Zn2—N4	2.1842 (13)
Zn1—N1	2.1785 (13)	Zn2—N6	2.2166 (13)
Zn1—Cl2	2.2837 (4)	Zn2—Cl4	2.2852 (4)
Zn1—Cl1	2.2893 (4)	Zn2—Cl3	2.2910 (4)
N1—C1	1.337 (2)	N4—C12	1.335 (2)
N1—C5	1.351 (2)	N4—C16	1.348 (2)
N2—C6	1.275 (2)	N5—C17	1.2775 (19)
N2—C8	1.4612 (19)	N5—C19	1.4635 (19)
N3—C11	1.473 (2)	N6—C21	1.472 (2)
N3—C9	1.473 (2)	N6—C22	1.473 (2)
N3—C10	1.477 (2)	N6—C20	1.477 (2)
C1—C2	1.389 (2)	C12—C13	1.390 (2)
C1—H1	0.9500	C12—H12	0.9500
C2—C3	1.380 (3)	C13—C14	1.381 (2)
C2—H2	0.9500	C13—H13	0.9500
C3—C4	1.384 (2)	C14—C15	1.393 (2)
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.387 (2)	C15—C16	1.387 (2)

C4—H4	0.9500	C15—H15	0.9500
C5—C6	1.495 (2)	C16—C17	1.498 (2)
C6—C7	1.499 (2)	C17—C18	1.488 (2)
C7—H7A	0.9800	C18—H18A	0.9800
C7—H7B	0.9800	C18—H18B	0.9800
C7—H7C	0.9800	C18—H18C	0.9800
C8—C9	1.521 (2)	C19—C20	1.520 (2)
C8—H8A	0.9900	C19—H19A	0.9900
C8—H8B	0.9900	C19—H19B	0.9900
C9—H9A	0.9900	C20—H20A	0.9900
C9—H9B	0.9900	C20—H20B	0.9900
C10—H10A	0.9800	C21—H21A	0.9800
C10—H10B	0.9800	C21—H21B	0.9800
C10—H10C	0.9800	C21—H21C	0.9800
C11—H11A	0.9800	C22—H22A	0.9800
C11—H11B	0.9800	C22—H22B	0.9800
C11—H11C	0.9800	C22—H22C	0.9800

N2—Zn1—N3	78.06 (5)	N5—Zn2—N4	74.89 (5)
N2—Zn1—N1	74.15 (5)	N5—Zn2—N6	77.63 (5)
N3—Zn1—N1	148.73 (5)	N4—Zn2—N6	148.01 (5)
N2—Zn1—Cl2	106.76 (4)	N5—Zn2—Cl4	137.94 (4)
N3—Zn1—Cl2	100.01 (4)	N4—Zn2—Cl4	94.36 (4)
N1—Zn1—Cl2	101.48 (3)	N6—Zn2—Cl4	95.15 (4)
N2—Zn1—Cl1	142.56 (4)	N5—Zn2—Cl3	102.01 (4)
N3—Zn1—Cl1	96.82 (4)	N4—Zn2—Cl3	101.45 (4)
N1—Zn1—Cl1	96.55 (4)	N6—Zn2—Cl3	99.99 (4)
Cl2—Zn1—Cl1	110.650 (15)	Cl4—Zn2—Cl3	120.032 (16)
C1—N1—C5	118.83 (14)	C12—N4—C16	119.00 (13)
C1—N1—Zn1	125.76 (11)	C12—N4—Zn2	126.29 (11)
C5—N1—Zn1	115.39 (10)	C16—N4—Zn2	114.65 (10)
C6—N2—C8	123.84 (14)	C17—N5—C19	123.13 (14)
C6—N2—Zn1	120.07 (11)	C17—N5—Zn2	120.03 (11)
C8—N2—Zn1	115.79 (10)	C19—N5—Zn2	116.78 (10)
C11—N3—C9	111.07 (12)	C21—N6—C22	109.24 (13)
C11—N3—C10	108.91 (12)	C21—N6—C20	110.95 (13)
C9—N3—C10	109.76 (12)	C22—N6—C20	110.13 (13)
C11—N3—Zn1	110.89 (9)	C21—N6—Zn2	111.83 (10)
C9—N3—Zn1	104.09 (9)	C22—N6—Zn2	112.01 (11)
C10—N3—Zn1	112.07 (10)	C20—N6—Zn2	102.55 (9)
N1—C1—C2	122.36 (16)	N4—C12—C13	122.15 (16)
N1—C1—H1	118.8	N4—C12—H12	118.9
C2—C1—H1	118.8	C13—C12—H12	118.9
C3—C2—C1	118.86 (16)	C14—C13—C12	119.16 (15)
C3—C2—H2	120.6	C14—C13—H13	120.4
C1—C2—H2	120.6	C12—C13—H13	120.4
C2—C3—C4	119.06 (16)	C13—C14—C15	118.84 (15)
C2—C3—H3	120.5	C13—C14—H14	120.6

C4—C3—H3	120.5	C15—C14—H14	120.6
C3—C4—C5	119.25 (16)	C16—C15—C14	118.83 (15)
C3—C4—H4	120.4	C16—C15—H15	120.6
C5—C4—H4	120.4	C14—C15—H15	120.6
N1—C5—C4	121.63 (15)	N4—C16—C15	122.01 (14)
N1—C5—C6	114.84 (13)	N4—C16—C17	114.84 (13)
C4—C5—C6	123.48 (15)	C15—C16—C17	123.13 (14)
N2—C6—C5	114.69 (14)	N5—C17—C18	125.30 (14)
N2—C6—C7	126.21 (15)	N5—C17—C16	115.18 (14)
C5—C6—C7	119.10 (14)	C18—C17—C16	119.51 (13)
C6—C7—H7A	109.5	C17—C18—H18A	109.5
C6—C7—H7B	109.5	C17—C18—H18B	109.5
H7A—C7—H7B	109.5	H18A—C18—H18B	109.5
C6—C7—H7C	109.5	C17—C18—H18C	109.5
H7A—C7—H7C	109.5	H18A—C18—H18C	109.5
H7B—C7—H7C	109.5	H18B—C18—H18C	109.5
N2—C8—C9	107.67 (12)	N5—C19—C20	107.57 (13)
N2—C8—H8A	110.2	N5—C19—H19A	110.2
C9—C8—H8A	110.2	C20—C19—H19A	110.2
N2—C8—H8B	110.2	N5—C19—H19B	110.2
C9—C8—H8B	110.2	C20—C19—H19B	110.2
H8A—C8—H8B	108.5	H19A—C19—H19B	108.5
N3—C9—C8	111.57 (13)	N6—C20—C19	111.55 (13)
N3—C9—H9A	109.3	N6—C20—H20A	109.3
C8—C9—H9A	109.3	C19—C20—H20A	109.3
N3—C9—H9B	109.3	N6—C20—H20B	109.3
C8—C9—H9B	109.3	C19—C20—H20B	109.3
H9A—C9—H9B	108.0	H20A—C20—H20B	108.0
N3—C10—H10A	109.5	N6—C21—H21A	109.5
N3—C10—H10B	109.5	N6—C21—H21B	109.5
H10A—C10—H10B	109.5	H21A—C21—H21B	109.5
N3—C10—H10C	109.5	N6—C21—H21C	109.5
H10A—C10—H10C	109.5	H21A—C21—H21C	109.5
H10B—C10—H10C	109.5	H21B—C21—H21C	109.5
N3—C11—H11A	109.5	N6—C22—H22A	109.5
N3—C11—H11B	109.5	N6—C22—H22B	109.5
H11A—C11—H11B	109.5	H22A—C22—H22B	109.5
N3—C11—H11C	109.5	N6—C22—H22C	109.5
H11A—C11—H11C	109.5	H22A—C22—H22C	109.5
H11B—C11—H11C	109.5	H22B—C22—H22C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Cl2^{i}	0.95	2.79	3.6690 (17)	155
C8—H8*A*···Cl1^{ii}	0.99	2.63	3.5668 (16)	158
C8—H8*B*···Cl2^{iii}	0.99	2.73	3.6564 (16)	156
C11—H11*A*···Cl2^{iii}	0.98	2.77	3.6573 (17)	151

C15—H15···Cl2^{iv}	0.95	2.74	3.6347 (17)	157
C18—H18*B*···Cl1^{iv}	0.98	2.75	3.7227 (17)	175
C19—H19*B*···Cl4^{v}	0.99	2.82	3.8089 (16)	174

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