

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Dichloridobis[2-(1-hydrazinylidene-ethyl)pyrazine- κN^1]zinc

Li-li Liang, Meng Li,* Jia-cheng Liu and Yun Wei

College of Chemistry and Chemical Engineering, Northwest Normal University,
Lanzhou 730070, People's Republic of China
Correspondence e-mail: jcliu8@nwnu.edu.cn

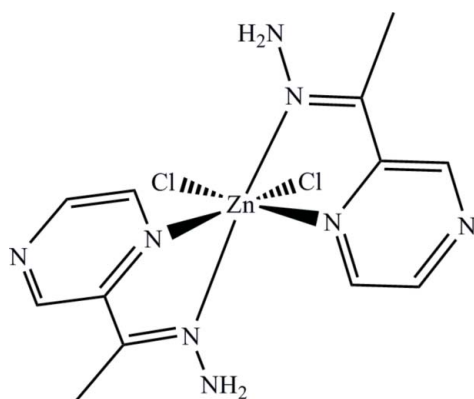
Received 30 March 2012; accepted 16 April 2012

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.029; wR factor = 0.078; data-to-parameter ratio = 18.5.

In the structure of the title complex, $[\text{ZnCl}_2(\text{C}_6\text{H}_8\text{N}_4)_2]$, the Zn^{II} atom has a distorted octahedral geometry. Two *cis* Cl^- ions and four N atoms belonging to two different 2-(1-hydrazinylideneethyl)pyrazine ligands coordinate the Zn^{II} atom, forming two five-membered $\text{Zn}-\text{N}-\text{C}-\text{C}-\text{N}$ rings. The dihedral angle between the planes of these metallocycles is $88.13(4)^\circ$. The organic ligands are essentially planar (r.m.s. deviations from planarity = 0.072 and 0.040 Å). Inter-molecular $\text{N}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{Cl}$ interactions join the molecules into a three-dimensional framework.

Related literature

For the biochemical applications of complexes based on ligands containing pyrazine, see: Ha *et al.* (1999); Blackstock *et al.* (2000); Adams *et al.* (2002); Lee *et al.* (2012). For the preparation of the ligand, see: Stadler *et al.* (2010).



Experimental

Crystal data

 $[\text{ZnCl}_2(\text{C}_6\text{H}_8\text{N}_4)_2]$ $M_r = 408.60$

Monoclinic, $P2_1/n$
 $a = 8.4289(8)$ Å
 $b = 15.1128(14)$ Å
 $c = 13.4196(13)$ Å
 $\beta = 104.077(1)^\circ$
 $V = 1658.1(3)$ Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.81$ mm⁻¹
 $T = 296$ K
 $0.20 \times 0.18 \times 0.15$ mm

Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2008)
 $T_{\min} = 0.713$, $T_{\max} = 0.773$

11576 measured reflections
4132 independent reflections
3456 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.078$
 $S = 1.03$
4132 reflections
223 parameters
4 restraints

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{\text{max}} = 0.42$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N8}-\text{H2N8}\cdots\text{Cl1}$	0.86 (2)	2.73 (2)	3.400 (2)	137 (2)
$\text{N8}-\text{H2N8}\cdots\text{N1}^{\text{i}}$	0.86 (2)	2.60 (2)	3.165 (3)	124 (2)
$\text{N4}-\text{H2N4}\cdots\text{Cl2}$	0.83 (2)	2.60 (2)	3.250 (2)	137 (2)
$\text{N4}-\text{H1N4}\cdots\text{Cl1}^{\text{ii}}$	0.81 (2)	2.66 (2)	3.4429 (19)	165 (2)

Symmetry codes: (i) $x - 1, y, z$; (ii) $-x + 2, -y, -z + 2$.

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

We are thankful for the support of this study by the National Natural Science Foundation of China (No. 20871099 and J0730425) and Gansu provincial Natural Science Foundation of China (No. 0710RJZA113).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2404).

References

- Adams, T. B., Doull, J. & Feron, V. J. (2002). *Food Chem. Toxicol.* **40**, 429–451.
Blackstock, A. W., Acostamadiedo, J. & Lesser, G. (2000). *Clin. Lung Cancer*, **2**, 62–66.
Bruker (2008). SADABS, SAINT-Plus and APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
Ha, T. G., Jang, J. J. & Kim, S. G. (1999). *Chem. Biol. Interact.* **121**, 209–222.
Lee, S. E., Chung, H. & Kim, Y. S. (2012). *Food Chem.* **131**, 1248–1254.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Stadler, A. M., Puntoriero, F., Nastasi, F., Campagna, S. & Lehn, J. M. (2010). *Chem. Eur. J.* **16**, 5645–5660.

supporting information

Acta Cryst. (2012). E68, m710 [https://doi.org/10.1107/S1600536812016418]

Dichloridobis[2-(1-hydrazinylideneethyl)pyrazine- κ N¹]zinc**Li-li Liang, Meng Li, Jia-cheng Liu and Yun Wei****S1. Comment**

Pyrazine and its derivatives have received considerable attention and interest in the field of biochemistry. Such research has been focused on drugs (Ha *et al.*, 1999; Blackstock *et al.*, 2000), flavor ingredients (Adams *et al.*, 2002), and enzymatic modification (Lee *et al.*, 2012). In this paper, a new Zn^{II} complex, dichlorido-bis[2-(1-hydrazonethyl)pyrazine]zinc(II), is described.

The crystal of the title compound, [ZnCl₂(C₆H₈N₄)₂], consists of two Cl⁻ ions, two N atoms from two different pyrazines (N2, N6) and other two imine N atoms (N3, N7), forming a distorted octahedron (Fig. 1). The equatorial plane of the octahedron is occupied by Cl1, N2, N6 and Cl2, the four atoms are almost coplanar, with the dihedral angle of 13.28 (1)°. Atoms N3, N7 are in the axial positions of the octahedron. The distances between N3, N7 and Zn^{II} (2.158 (1) Å, 2.164 (1) Å) are shorter than those of N2, N6 of the equatorial plane with Zn^{II} (2.244 (1) Å, 2.258 (2) Å).

As shown in the packing diagram (Fig. 2), a three-dimensional framework is formed by intermolecular N—H⋯N and N—H⋯Cl interactions.

S2. Experimental

2-(1-hydrazinylideneethyl)pyrazine (Stadler *et al.*, 2010) (0.1 mmol, 0.0136 g) was dissolved in 20 ml absolute ethanol, then ZnCl₂·2H₂O (0.2 mmol, 0.0268 g) was added, and after 0.5 h of stirring at 333 K, the mixture was filtered and held at room temperature to allow slow evaporation of solvent. Shiny pale yellow crystals suitable for X-ray diffraction were collected after one week (Yield = 64%).

S3. Refinement

H atoms of the pyrazine ring were placed in calculated positions, with C—H = 0.93 Å, and refined using riding mode, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of the methyl group were located in difference Fourier maps and included as part of a rigid rotor, with C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C methyl})$. H atoms of the NH₂ groups were refined subject to a variable distance restraint that refined to N—H = 0.83 (2) Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$.

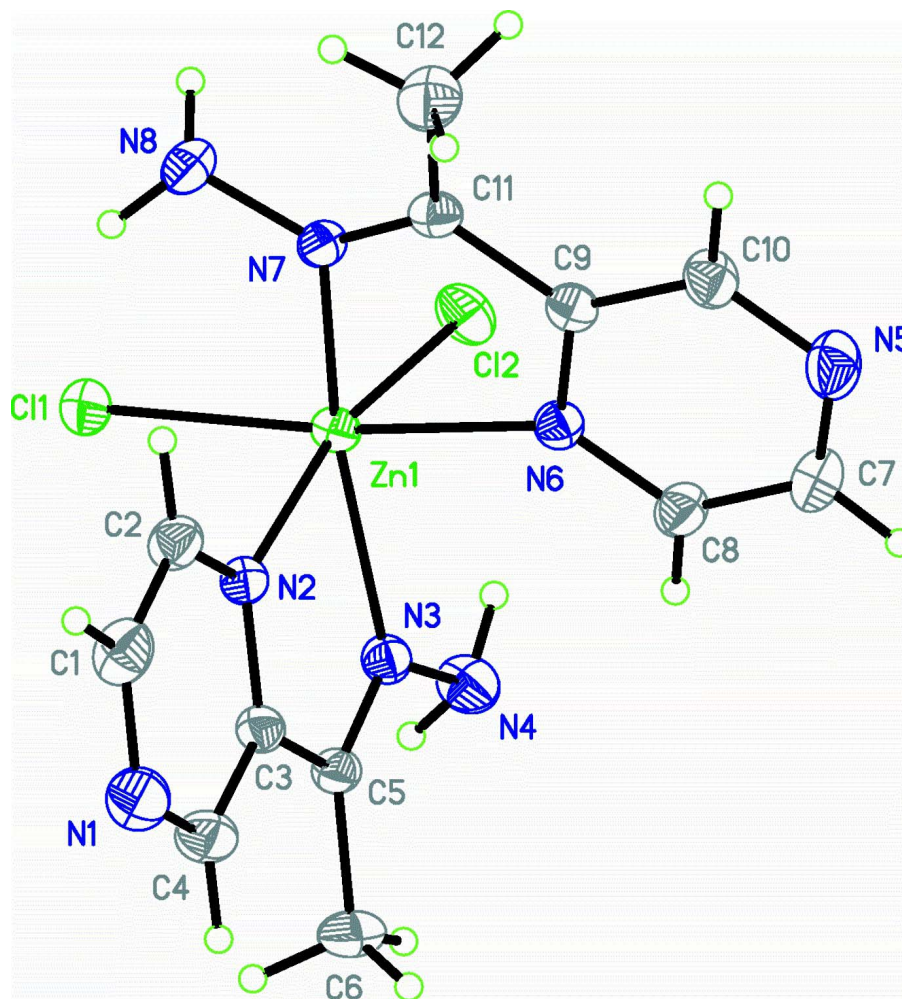


Figure 1

The crystal structure of the title complex. Ellipsoids are drawn at the 50% probability level. Hydrogen atoms are depicted as small spheres of arbitrary radius.

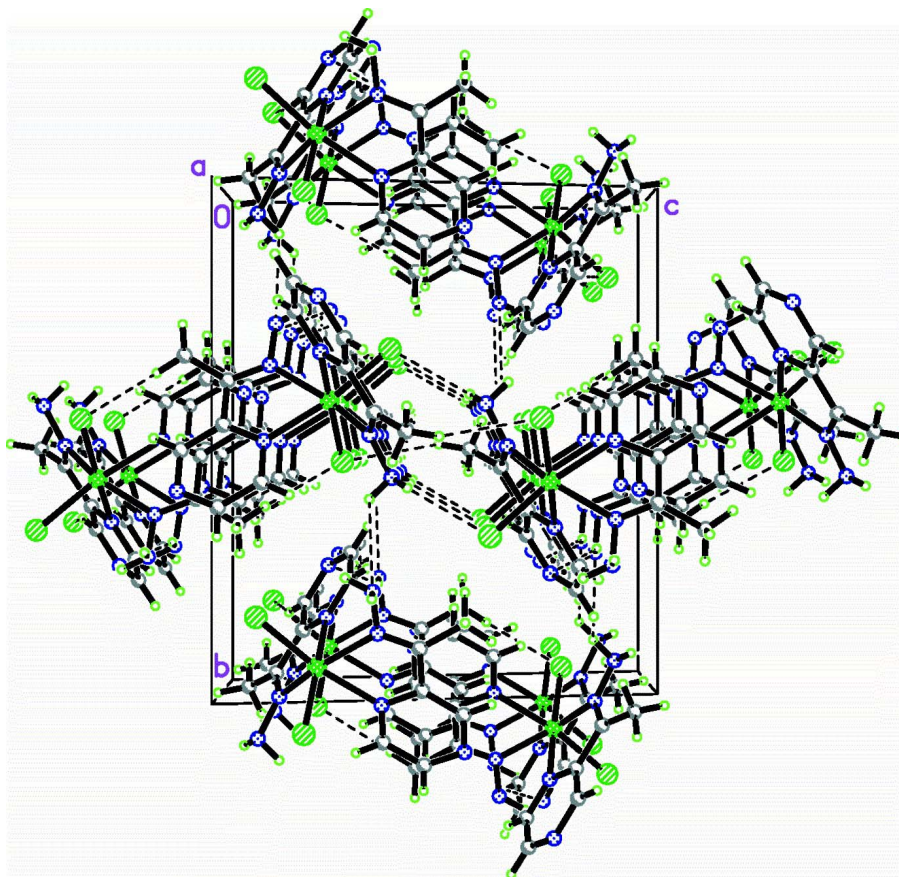


Figure 2

The packing diagram of the title complex, viewed along the *a* axis. Intermolecular interactions are shown as dashed lines.

Dichloridobis[2-(1-hydrazinylideneethyl)pyrazine- κN^1]zinc

Crystal data

$[\text{ZnCl}_2(\text{C}_6\text{H}_8\text{N}_4)_2]$

$M_r = 408.60$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 8.4289\ (8)\ \text{\AA}$

$b = 15.1128\ (14)\ \text{\AA}$

$c = 13.4196\ (13)\ \text{\AA}$

$\beta = 104.077\ (1)^\circ$

$V = 1658.1\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 832$

$D_x = 1.637\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 4411 reflections

$\theta = 2.7\text{--}28.2^\circ$

$\mu = 1.81\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, colourless

$0.20 \times 0.18 \times 0.15\ \text{mm}$

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\min} = 0.713$, $T_{\max} = 0.773$

11576 measured reflections

4132 independent reflections

3456 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -10 \rightarrow 11$

$k = -18 \rightarrow 20$

$l = -9 \rightarrow 17$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.029$ $wR(F^2) = 0.078$ $S = 1.03$

4132 reflections

223 parameters

4 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.3057P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.009$ $\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$ *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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.79801 (2)	0.074400 (13)	0.764996 (15)	0.03098 (8)
Cl1	0.74457 (6)	0.17192 (3)	0.89354 (4)	0.04074 (12)
Cl2	0.61902 (6)	−0.03984 (4)	0.78802 (4)	0.04526 (13)
N1	1.2922 (2)	0.25410 (13)	0.75292 (16)	0.0535 (5)
N2	1.00732 (17)	0.16076 (10)	0.75046 (11)	0.0322 (3)
N3	1.01610 (18)	0.01092 (10)	0.85368 (11)	0.0331 (3)
N4	1.0037 (3)	−0.06823 (12)	0.89868 (16)	0.0478 (5)
H1N4	1.076 (3)	−0.0850 (16)	0.9461 (18)	0.057*
H2N4	0.909 (3)	−0.0860 (17)	0.892 (2)	0.057*
N5	0.8091 (3)	−0.09261 (13)	0.44379 (15)	0.0533 (5)
N6	0.82991 (18)	−0.00119 (10)	0.62587 (11)	0.0327 (3)
N7	0.65102 (18)	0.14165 (10)	0.63190 (12)	0.0330 (3)
N8	0.5788 (2)	0.22084 (12)	0.64252 (16)	0.0473 (4)
H1N8	0.493 (3)	0.2340 (17)	0.5969 (17)	0.057*
H2N8	0.568 (3)	0.2228 (17)	0.7042 (15)	0.057*
C1	1.1478 (3)	0.28105 (15)	0.69904 (19)	0.0508 (5)
H1	1.1414	0.3328	0.6607	0.061*
C2	1.0057 (2)	0.23502 (12)	0.69773 (16)	0.0405 (4)
H2	0.9065	0.2567	0.6589	0.049*
C3	1.1533 (2)	0.13197 (12)	0.80650 (14)	0.0329 (4)
C4	1.2941 (2)	0.18004 (14)	0.80619 (18)	0.0459 (5)
H4	1.3939	0.1593	0.8451	0.055*
C5	1.1551 (2)	0.05001 (13)	0.86525 (14)	0.0333 (4)
C6	1.3119 (2)	0.01689 (16)	0.93253 (16)	0.0478 (5)

H6A	1.2922	−0.0376	0.9643	0.072*
H6B	1.3546	0.0600	0.9847	0.072*
H6C	1.3894	0.0070	0.8919	0.072*
C7	0.9003 (3)	−0.12098 (14)	0.53299 (17)	0.0476 (5)
H7	0.9594	−0.1731	0.5344	0.057*
C8	0.9103 (3)	−0.07594 (12)	0.62350 (17)	0.0405 (4)
H8	0.9752	−0.0986	0.6843	0.049*
C9	0.7363 (2)	0.02954 (12)	0.53650 (14)	0.0321 (4)
C10	0.7270 (3)	−0.01761 (14)	0.44637 (15)	0.0433 (5)
H10	0.6608	0.0040	0.3854	0.052*
C11	0.6464 (2)	0.11247 (12)	0.54143 (14)	0.0332 (4)
C12	0.5611 (3)	0.15970 (16)	0.44551 (17)	0.0542 (6)
H12A	0.4486	0.1689	0.4459	0.081*
H12B	0.5671	0.1247	0.3868	0.081*
H12C	0.6128	0.2159	0.4422	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02815 (12)	0.03323 (12)	0.02997 (12)	−0.00097 (8)	0.00402 (8)	0.00062 (8)
Cl1	0.0421 (2)	0.0393 (3)	0.0413 (3)	0.00117 (19)	0.01106 (19)	−0.00545 (19)
Cl2	0.0444 (3)	0.0473 (3)	0.0443 (3)	−0.0159 (2)	0.0113 (2)	−0.0026 (2)
N1	0.0427 (10)	0.0487 (11)	0.0738 (14)	−0.0098 (8)	0.0232 (10)	−0.0013 (9)
N2	0.0295 (7)	0.0318 (7)	0.0353 (8)	−0.0001 (6)	0.0078 (6)	−0.0032 (6)
N3	0.0339 (8)	0.0326 (8)	0.0309 (8)	0.0006 (6)	0.0044 (6)	0.0015 (6)
N4	0.0466 (11)	0.0423 (10)	0.0485 (11)	−0.0012 (8)	−0.0003 (9)	0.0142 (8)
N5	0.0660 (13)	0.0522 (11)	0.0441 (11)	0.0055 (9)	0.0181 (9)	−0.0093 (8)
N6	0.0328 (8)	0.0319 (8)	0.0326 (8)	0.0006 (6)	0.0064 (6)	0.0008 (6)
N7	0.0286 (7)	0.0313 (7)	0.0390 (9)	0.0020 (6)	0.0081 (6)	0.0001 (6)
N8	0.0458 (10)	0.0413 (10)	0.0545 (11)	0.0136 (8)	0.0115 (9)	0.0010 (8)
C1	0.0531 (13)	0.0376 (11)	0.0671 (15)	−0.0016 (9)	0.0250 (11)	0.0061 (10)
C2	0.0400 (10)	0.0351 (10)	0.0466 (11)	0.0033 (8)	0.0110 (8)	0.0030 (8)
C3	0.0275 (8)	0.0381 (10)	0.0334 (9)	−0.0009 (7)	0.0084 (7)	−0.0060 (7)
C4	0.0317 (10)	0.0515 (12)	0.0557 (13)	−0.0047 (9)	0.0130 (9)	−0.0018 (10)
C5	0.0290 (9)	0.0412 (10)	0.0284 (9)	0.0034 (7)	0.0047 (7)	−0.0043 (7)
C6	0.0331 (10)	0.0616 (14)	0.0448 (12)	0.0089 (9)	0.0018 (9)	0.0065 (10)
C7	0.0530 (13)	0.0399 (11)	0.0527 (13)	0.0083 (9)	0.0185 (10)	−0.0033 (9)
C8	0.0412 (11)	0.0369 (10)	0.0432 (11)	0.0056 (8)	0.0098 (9)	0.0018 (8)
C9	0.0300 (8)	0.0349 (9)	0.0319 (9)	−0.0030 (7)	0.0083 (7)	0.0019 (7)
C10	0.0498 (12)	0.0462 (11)	0.0330 (10)	0.0011 (9)	0.0079 (9)	−0.0016 (8)
C11	0.0293 (9)	0.0340 (9)	0.0343 (9)	−0.0004 (7)	0.0042 (7)	0.0054 (7)
C12	0.0656 (15)	0.0501 (13)	0.0408 (12)	0.0119 (11)	0.0011 (10)	0.0117 (9)

Geometric parameters (Å, °)

Zn1—N3	2.1568 (15)	N8—H2N8	0.857 (18)
Zn1—N7	2.1637 (15)	C1—C2	1.382 (3)
Zn1—N2	2.2408 (15)	C1—H1	0.9300

Zn1—N6	2.2600 (15)	C2—H2	0.9300
Zn1—Cl2	2.3620 (5)	C3—C4	1.392 (3)
Zn1—Cl1	2.3934 (5)	C3—C5	1.466 (3)
N1—C1	1.320 (3)	C4—H4	0.9300
N1—C4	1.326 (3)	C5—C6	1.493 (3)
N2—C2	1.325 (2)	C6—H6A	0.9600
N2—C3	1.349 (2)	C6—H6B	0.9600
N3—C5	1.288 (2)	C6—H6C	0.9600
N3—N4	1.355 (2)	C7—C8	1.377 (3)
N4—H1N4	0.806 (19)	C7—H7	0.9300
N4—H2N4	0.827 (19)	C8—H8	0.9300
N5—C7	1.326 (3)	C9—C10	1.389 (3)
N5—C10	1.333 (3)	C9—C11	1.474 (3)
N6—C8	1.322 (2)	C10—H10	0.9300
N6—C9	1.348 (2)	C11—C12	1.494 (3)
N7—C11	1.283 (2)	C12—H12A	0.9600
N7—N8	1.366 (2)	C12—H12B	0.9600
N8—H1N8	0.850 (19)	C12—H12C	0.9600
N3—Zn1—N7	154.76 (6)	N2—C2—H2	119.2
N3—Zn1—N2	73.96 (6)	C1—C2—H2	119.2
N7—Zn1—N2	87.67 (5)	N2—C3—C4	119.51 (18)
N3—Zn1—N6	88.53 (6)	N2—C3—C5	117.46 (16)
N7—Zn1—N6	73.43 (6)	C4—C3—C5	123.03 (17)
N2—Zn1—N6	88.17 (5)	N1—C4—C3	122.96 (19)
N3—Zn1—Cl2	95.08 (4)	N1—C4—H4	118.5
N7—Zn1—Cl2	101.28 (4)	C3—C4—H4	118.5
N2—Zn1—Cl2	168.11 (4)	N3—C5—C3	115.63 (15)
N6—Zn1—Cl2	86.94 (4)	N3—C5—C6	124.36 (18)
N3—Zn1—Cl1	99.25 (4)	C3—C5—C6	120.01 (17)
N7—Zn1—Cl1	97.78 (4)	C5—C6—H6A	109.5
N2—Zn1—Cl1	89.67 (4)	C5—C6—H6B	109.5
N6—Zn1—Cl1	171.02 (4)	H6A—C6—H6B	109.5
Cl2—Zn1—Cl1	96.76 (2)	C5—C6—H6C	109.5
C1—N1—C4	116.34 (18)	H6A—C6—H6C	109.5
C2—N2—C3	117.43 (16)	H6B—C6—H6C	109.5
C2—N2—Zn1	129.32 (13)	N5—C7—C8	122.3 (2)
C3—N2—Zn1	113.23 (12)	N5—C7—H7	118.9
C5—N3—N4	121.17 (16)	C8—C7—H7	118.9
C5—N3—Zn1	119.41 (12)	N6—C8—C7	121.45 (19)
N4—N3—Zn1	119.40 (13)	N6—C8—H8	119.3
N3—N4—H1N4	120.3 (19)	C7—C8—H8	119.3
N3—N4—H2N4	114.6 (18)	N6—C9—C10	119.67 (18)
H1N4—N4—H2N4	120 (3)	N6—C9—C11	116.67 (16)
C7—N5—C10	116.23 (18)	C10—C9—C11	123.65 (17)
C8—N6—C9	117.76 (17)	N5—C10—C9	122.61 (19)
C8—N6—Zn1	128.07 (13)	N5—C10—H10	118.7
C9—N6—Zn1	113.55 (12)	C9—C10—H10	118.7

C11—N7—N8	119.22 (16)	N7—C11—C9	115.91 (15)
C11—N7—Zn1	119.93 (12)	N7—C11—C12	123.24 (18)
N8—N7—Zn1	120.38 (13)	C9—C11—C12	120.81 (18)
N7—N8—H1N8	117.0 (17)	C11—C12—H12A	109.5
N7—N8—H2N8	106.8 (17)	C11—C12—H12B	109.5
H1N8—N8—H2N8	114 (2)	H12A—C12—H12B	109.5
N1—C1—C2	122.2 (2)	C11—C12—H12C	109.5
N1—C1—H1	118.9	H12A—C12—H12C	109.5
C2—C1—H1	118.9	H12B—C12—H12C	109.5
N2—C2—C1	121.55 (19)		
N3—Zn1—N2—C2	178.63 (17)	C4—N1—C1—C2	0.0 (3)
N7—Zn1—N2—C2	16.15 (17)	C3—N2—C2—C1	0.6 (3)
N6—Zn1—N2—C2	89.63 (17)	Zn1—N2—C2—C1	178.73 (15)
Cl2—Zn1—N2—C2	155.39 (16)	N1—C1—C2—N2	−0.3 (3)
Cl1—Zn1—N2—C2	−81.65 (16)	C2—N2—C3—C4	−0.5 (3)
N3—Zn1—N2—C3	−3.15 (12)	Zn1—N2—C3—C4	−178.93 (14)
N7—Zn1—N2—C3	−165.63 (13)	C2—N2—C3—C5	179.72 (16)
N6—Zn1—N2—C3	−92.15 (13)	Zn1—N2—C3—C5	1.3 (2)
Cl2—Zn1—N2—C3	−26.4 (3)	C1—N1—C4—C3	0.1 (3)
Cl1—Zn1—N2—C3	96.57 (12)	N2—C3—C4—N1	0.1 (3)
N7—Zn1—N3—C5	50.1 (2)	C5—C3—C4—N1	179.9 (2)
N2—Zn1—N3—C5	5.20 (13)	N4—N3—C5—C3	175.73 (17)
N6—Zn1—N3—C5	93.72 (14)	Zn1—N3—C5—C3	−6.2 (2)
Cl2—Zn1—N3—C5	−179.49 (13)	N4—N3—C5—C6	−4.0 (3)
Cl1—Zn1—N3—C5	−81.77 (14)	Zn1—N3—C5—C6	174.13 (15)
N7—Zn1—N3—N4	−131.82 (16)	N2—C3—C5—N3	3.1 (3)
N2—Zn1—N3—N4	−176.68 (16)	C4—C3—C5—N3	−176.72 (18)
N6—Zn1—N3—N4	−88.16 (15)	N2—C3—C5—C6	−177.23 (17)
Cl2—Zn1—N3—N4	−1.36 (15)	C4—C3—C5—C6	3.0 (3)
Cl1—Zn1—N3—N4	96.35 (15)	C10—N5—C7—C8	0.0 (3)
N3—Zn1—N6—C8	23.01 (17)	C9—N6—C8—C7	0.4 (3)
N7—Zn1—N6—C8	−174.88 (17)	Zn1—N6—C8—C7	170.70 (15)
N2—Zn1—N6—C8	97.01 (17)	N5—C7—C8—N6	−0.5 (3)
Cl2—Zn1—N6—C8	−72.15 (16)	C8—N6—C9—C10	0.3 (3)
N3—Zn1—N6—C9	−166.32 (13)	Zn1—N6—C9—C10	−171.45 (14)
N7—Zn1—N6—C9	−4.21 (12)	C8—N6—C9—C11	179.32 (17)
N2—Zn1—N6—C9	−92.33 (13)	Zn1—N6—C9—C11	7.6 (2)
Cl2—Zn1—N6—C9	98.51 (12)	C7—N5—C10—C9	0.7 (3)
N3—Zn1—N7—C11	46.0 (2)	N6—C9—C10—N5	−0.8 (3)
N2—Zn1—N7—C11	88.76 (14)	C11—C9—C10—N5	−179.8 (2)
N6—Zn1—N7—C11	−0.03 (14)	N8—N7—C11—C9	176.15 (16)
Cl2—Zn1—N7—C11	−83.36 (14)	Zn1—N7—C11—C9	4.0 (2)
Cl1—Zn1—N7—C11	178.11 (14)	N8—N7—C11—C12	−1.8 (3)
N3—Zn1—N7—N8	−126.06 (16)	Zn1—N7—C11—C12	−174.00 (16)
N2—Zn1—N7—N8	−83.33 (14)	N6—C9—C11—N7	−7.9 (2)
N6—Zn1—N7—N8	−172.11 (15)	C10—C9—C11—N7	171.15 (18)
Cl2—Zn1—N7—N8	104.55 (14)	N6—C9—C11—C12	170.15 (18)

Cl1—Zn1—N7—N8	6.02 (14)	C10—C9—C11—C12	−10.8 (3)
---------------	-----------	----------------	-----------

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N8—H2N8···Cl1	0.86 (2)	2.73 (2)	3.400 (2)	137 (2)
N8—H2N8···N1 ⁱ	0.86 (2)	2.60 (2)	3.165 (3)	124 (2)
N4—H2N4···Cl2	0.83 (2)	2.60 (2)	3.250 (2)	137 (2)
N4—H1N4···Cl1 ⁱⁱ	0.81 (2)	2.66 (2)	3.4429 (19)	165 (2)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y, -z+2$.