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Synthesis and structure of dichlorido{(*E*)-4-methyl-*N*′-[1-(pyridin-2-yl)ethylidene]benzohydrazide}-zinc(II)

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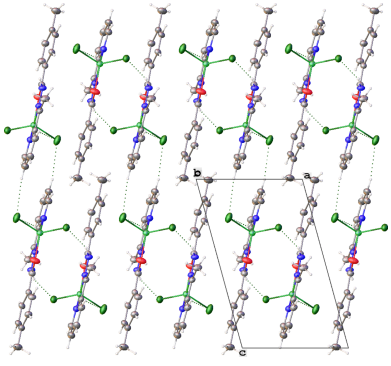
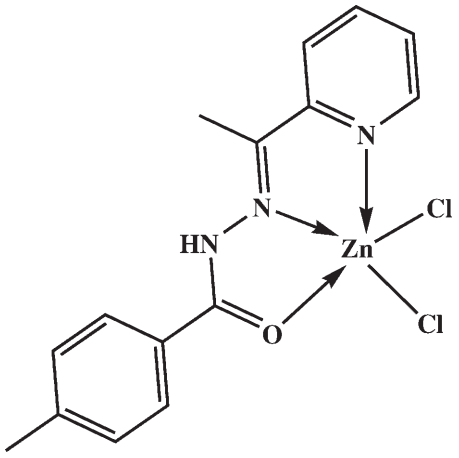
The ligand in the title complex, $[ZnCl_2(C_{15}H_{15}N_3O)]$, was obtained by a condensation reaction between *p*-tolyl hydrazide and 2-acetylpyridine. The ligand molecule bonds to the metal ion in a tridentate manner *via* its imino nitrogen atom, its carbonyl oxygen atom, and the nitrogen atom of the pyridine ring. The geometry of the coordination polyhedron around the zinc ion is intermediate between a trigonal bipyramid and a square pyramid, but closer to the latter. In the extended structure, pairwise N—H···Cl hydrogen bonds generate inversion dimers and very weak C—H···Cl interactions link the dimers into sheets.

1. Chemical context

In recent years, hydrazone derivatives containing a –C(=O)NHN=CH– moiety have attracted the attention of many chemists due to their diverse biological properties and large range of applications in medicinal chemistry (Mansi *et al.*, 2023; Socea *et al.*, 2022; Mali *et al.*, 2021). In their formal structures, hydrazine derivatives exhibit amido–iminol tautomerism (Polo-Cerón *et al.*, 2021; Jamadar *et al.*, 2012), with the amide form predominating in the solid state (Gamov *et al.*, 2019). Theoretically, acylhydrazone derivatives have four isomers, two of which are geometric isomers (*E*/*Z*) due to the rigid C=N double bond, and two are conformational isomers (*syn*/*anti*) due to rotation about the single N—N bond (Chen *et al.*, 2019; Dasgupta *et al.*, 2020). In a mixture of *E* and *Z* isomers, it has been shown that the *E* isomer predominates (Naskar *et al.*, 2011). In coordination chemistry, hydrazone-derived Schiff bases are effective ligands due to their ability to chelate metal ions and to lead to the formation of supramolecular structures *via* intermolecular interactions (Mondal *et al.*, 2013). Depending on reaction conditions such as pH, ligand concentration and the oxidation state of the metal ion involved, these types of Schiff bases coordinate with metal ions in their neutral amide form or in their iminolate form. As part of our studies in this area, we now describe the synthesis and structure of the title compound, $[Zn(C_{15}H_{15}N_3O)Cl_2]$ (**I**).





2. Structural commentary

Compound (**I**) crystallizes in the triclinic system with space group $P\overline{1}$. The molecular structure of (**I**) (Fig. 1) reveals a mononuclear complex in which the Zn^{2+} metal ion is penta-coordinated by a tridentate N,N,O-bonded ligand and two chloride ions: selected geometrical data are presented in Table 1. The bond angles around the metal ion reveal a notable distortion in the coordination sphere, particularly the bite angles N2—Zn1—N1 and N2—Zn1—O1, which are characteristic of the constraint imposed by chelation. The N1/C1/C6/N2/Zn1 chelate ring is a shallow envelope with Zn1 as the flap deviating by −0.228 (1) Å from the other atoms whereas the N2/N3/C8/O1/Zn1 ring is almost planar (r.m.s. deviation = 0.018 Å). The Addison τ parameter (Addison *et al.*, 1984) of 0.29 for the metal ion suggests a geometry intermediate between trigonal-pyramidal and square-based pyramidal but closer to the latter. Analysis of the ligand bond lengths confirms its coordination to the metal in the amide form. The C8═O1 distance of 1.233 (6) Å indicates that the C=O bond retains its double-bond character, ruling out iminolization. The distances N2—N3 = 1.370 (5) Å and C6—N2 = 1.287 (5) Å reflect electronic delocalization within the hydrazone fragment, while the nearly planar nature of the chelating system promotes π conjugation. Overall, the complex molecule has approximate local C_s symmetry.

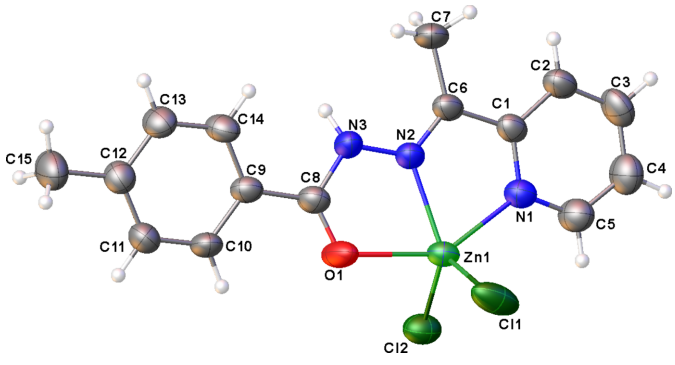


Figure 1
The molecular structure of (**I**) with displacement ellipsoids plotted at the 30% probability level.

Table 1
Selected geometric parameters (Å, °).

Zn1—Cl2	2.2348 (12)	Zn1—O1	2.260 (3)
Zn1—Cl1	2.2318 (13)	Zn1—N2	2.107 (3)
Zn1—N1	2.186 (4)		
Cl2—Zn1—O1	94.84 (11)	N1—Zn1—O1	145.35 (13)
Cl1—Zn1—Cl2	111.46 (5)	N2—Zn1—Cl2	127.98 (11)
Cl1—Zn1—O1	98.16 (13)	N2—Zn1—Cl1	120.03 (11)
N1—Zn1—Cl2	103.12 (11)	N2—Zn1—N1	73.64 (13)
N1—Zn1—Cl1	102.32 (11)	N2—Zn1—O1	71.95 (12)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···Cl2^{i}	0.87 (2)	2.40 (3)	3.214 (4)	156 (5)
C2—H2···Cl1^{ii}	0.93	2.93	3.649 (5)	136
C4—H4···Cl1^{iii}	0.93	2.98	3.888 (6)	165

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

3. Supramolecular features

In the extended structure of (**I**), pairwise N3—H3···Cl2 hydrogen bonds (Table 2) generate inversion dimers with an $R_2^2(10)$ graph-set descriptor. The dimers are linked by very weak C—H···Cl hydrogen bonds to form sheets lying parallel to the *bc* plane, which are further linked into a three-dimensional network (Figs. 2 and 3).

4. Database survey

We are not aware of any previous reports of the ligand reported here but similar ligands possessing O,N,N donor

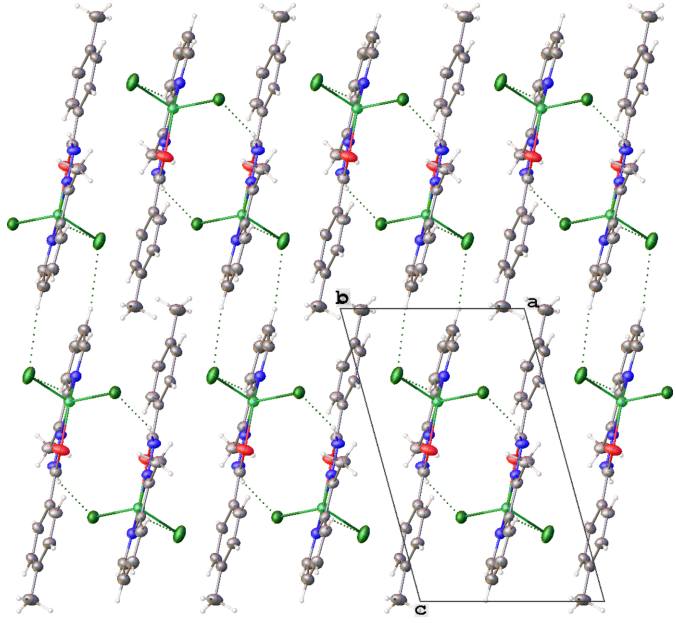


Figure 2
Hydrogen-bonded sheets lying parallel to the *bc* plane.

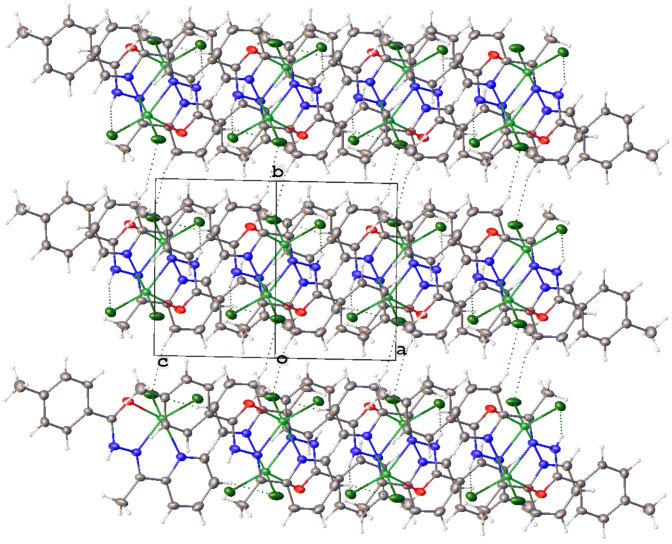


Figure 3
Hydrogen-bonded sheets lying parallel to the *ac* plane.

groups exist in the literature. For general background to hydrazones and their complexes, see Abubakar & Habu (2026). For similar ligands and their Ni^{II}, Zn^{II}, and V^{V} complexes, see Laila *et al.* (2026) and You *et al.* (2025).

5. Synthesis and crystallization

p-Tolyl hydrazide (1.5 g, 10 mmol) and 2-acetylpyridine in a 1:1 ratio in methanol, in the presence of a few drops of glacial acetic acid were heated to reflux for seven hours. After cooling and filtration, a white solid was obtained in 79% yield (m.p. = 449–451 K). FT-IR (ν, cm^{-1}): 3236 (NH); 1668 (C═O); 1609 (C═N) imine; 1525–1434 (C═C) aromatic; 1580 (C═N) pyridine; 1122 (N—N). ^{1}H NMR [$CDCl_3$, δ (ppm)]: 2.52 [3H, *s*, CH_3—C═N)pyridine]); 2.56 (3H, *s*, CH_3—Ar); 7.42 (2H, *d*, H—Ar); 7.66 (2H, *d*, H—Ar); 7.75 (1H, *d*, H—Ar); 7.91 (1H, *d*, H—Ar); 8.62 (1H, *m*, H—Ar); 8.75 (1H, *dd*, H—pyridine); 15.73 (1H, *s*, H—N). ^{13}C NMR [$CDCl_3$, δ (ppm)]: 164.47 (C═O); 153.55 (C═N), 147.38 (C—Ar); 142.92 (C—Ar); 142.28 (C—Ar); 137.97 (C—Ar); 131.14 (C—Ar); 129.36 (C—Ar); 127.64 (C—Ar); 124.20 (C—Ar); 124.06 (C—Ar); 22.65 (CH_3—Ar); 21.55 (CH_3—Ar). Calculated analysis for $C_{15}H_{15}N_3O$: C, 71.13; H, 5.97; N, 16.59%; found C, 71.18; H, 6.04; N, 16.63%. To a solution of the ligand (0.10 g, 0.4 mmol) in 15 ml of methanol, 0.4 mmol of $ZnCl_2$ was added. The mixture was refluxed for two h. Upon cooling, the resulting solution was filtered, and the filtrate was left to evaporate slowly at 298 K. After one week, colorless crystals of (**I**) suitable for X-ray diffraction were collected.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms attached to the amide group were located from difference-Fourier maps and refined. Other H atoms (CH, CH_3 groups) were geometrically optimized and refined as riding atoms with U_{iso}(H) = 1.2U_{eq}(C) (1.5 for CH_3).

Table 3
Experimental details.

Crystal data	
Chemical formula	$[ZnCl_2(C_{15}H_{15}N_3O)]$
M_r	389.57
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, *b*, *c* (Å)	7.7318 (6), 8.4484 (8), 12.8117 (11)
α, β, γ (°)	84.016 (7), 74.425 (7), 86.261 (7)
V (Å^3)	801.15 (12)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	1.87
Crystal size (mm)	0.26 × 0.03 × 0.02
Data collection	
Diffractometer	XtaLAB AFC12 (RINC): Kappa single
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.598, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19173, 3265, 2757
R_{int}	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.056, 0.169, 1.06
No. of reflections	3265
No. of parameters	204
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.54, −0.73

Computer programs: *CrysAlis PRO*a (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *OLEX2* 1.3 (Dolomanov *et al.*, 2009).

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Synthesis and structure of dichlorido{(*E*)-4-methyl-*N*′-[1-(pyridin-2-yl)ethylidene]benzohydrazide}zinc(II)

Mohamedou El Boukhary, Thierno Moussa Seck, Farba Bouyagui Tamboura, Ibrahima Elhadji Thiam, Aliou Hamady Barry, Pascal Retailleau and Mohamed Gaye

Computing details

Dichlorido{(*E*)-4-methyl-*N*′-[1-(pyridin-2-yl)ethylidene]benzohydrazide}zinc(II)

Crystal data

$[ZnCl_2(C_{15}H_{15}N_3O)]$
M_r = 389.57
Triclinic, $P\overline{1}$
a = 7.7318 (6) Å
b = 8.4484 (8) Å
c = 12.8117 (11) Å
α = 84.016 (7)°
β = 74.425 (7)°
γ = 86.261 (7)°
V = 801.15 (12) Å^3
Z = 2
$F(000)$ = 396.000
D_x = 1.615 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6354 reflections
θ = 3.7–29.1°
μ = 1.87 mm^{-1}
T = 293 K
Prismatic, yellow
0.26 × 0.03 × 0.02 mm

Data collection

XtaLAB AFC12 (RINC): Kappa single diffractometer
Radiation source: micro-focus sealed X-ray tube, Rigaku (Mo) X-ray Source
Mirror monochromator
Detector resolution: 5.8140 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2023)
T_{min} = 0.598, T_{max} = 1.000
19173 measured reflections
3265 independent reflections
2757 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 26.4°, θ_{min} = 3.7°
h = −9→9
k = −10→10
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.169
S = 1.06
3265 reflections
204 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1117P)^2 + 0.6932P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.38989 (7)	0.64352 (5)	0.31892 (4)	0.0429 (2)
Cl2	0.65189 (16)	0.76112 (14)	0.28753 (10)	0.0557 (3)
Cl1	0.2085 (2)	0.77878 (14)	0.22910 (14)	0.0738 (5)
N1	0.4632 (5)	0.4296 (4)	0.2319 (3)	0.0448 (8)
O1	0.2718 (6)	0.7383 (4)	0.4828 (3)	0.0691 (11)
N2	0.2932 (5)	0.4499 (4)	0.4327 (3)	0.0418 (8)
N3	0.2126 (6)	0.4816 (4)	0.5379 (3)	0.0483 (9)
H3	0.214 (7)	0.411 (5)	0.592 (3)	0.058*
C1	0.3935 (6)	0.2944 (5)	0.2879 (3)	0.0416 (9)
C9	0.1303 (6)	0.6744 (5)	0.6711 (3)	0.0419 (9)
C14	0.0322 (6)	0.5671 (5)	0.7500 (4)	0.0479 (10)
H14	0.018369	0.464954	0.733199	0.058*
C6	0.2975 (6)	0.3083 (5)	0.4033 (3)	0.0426 (9)
C8	0.2115 (6)	0.6369 (5)	0.5581 (4)	0.0457 (9)
C10	0.1503 (7)	0.8272 (5)	0.6982 (4)	0.0500 (10)
H10	0.216923	0.900526	0.646215	0.060*
C2	0.4114 (7)	0.1528 (5)	0.2398 (4)	0.0518 (11)
H2	0.360613	0.060866	0.279332	0.062*
C11	0.0715 (7)	0.8687 (6)	0.8015 (4)	0.0531 (11)
H11	0.085523	0.970784	0.818279	0.064*
C13	−0.0457 (6)	0.6108 (6)	0.8540 (4)	0.0518 (11)
H13	−0.111027	0.537309	0.906550	0.062*
C5	0.5538 (7)	0.4239 (6)	0.1288 (4)	0.0565 (11)
H5	0.603320	0.516982	0.090251	0.068*
C12	−0.0277 (6)	0.7636 (6)	0.8810 (4)	0.0487 (10)
C7	0.2165 (9)	0.1664 (6)	0.4756 (4)	0.0639 (14)
H7A	0.307863	0.105710	0.502040	0.096*
H7B	0.165939	0.101230	0.435135	0.096*
H7C	0.123837	0.201349	0.536005	0.096*
C3	0.5058 (8)	0.1507 (6)	0.1322 (4)	0.0609 (13)
H3A	0.519876	0.056798	0.098317	0.073*
C4	0.5788 (8)	0.2870 (7)	0.0753 (4)	0.0639 (13)
H4	0.643393	0.287701	0.002708	0.077*
C15	−0.1136 (9)	0.8107 (8)	0.9938 (4)	0.0754 (17)
H15A	−0.022367	0.818845	1.030978	0.113*
H15B	−0.196337	0.731666	1.033128	0.113*
H15C	−0.176888	0.911770	0.989505	0.113*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0526 (3)	0.0286 (3)	0.0467 (3)	−0.00524 (19)	−0.0127 (2)	0.00132 (19)
Cl2	0.0564 (7)	0.0472 (6)	0.0653 (7)	−0.0115 (5)	−0.0206 (5)	0.0042 (5)
Cl1	0.0821 (10)	0.0370 (6)	0.1211 (13)	−0.0027 (6)	−0.0620 (9)	0.0011 (7)
N1	0.050 (2)	0.0357 (18)	0.0482 (19)	−0.0026 (15)	−0.0133 (16)	−0.0020 (15)
O1	0.108 (3)	0.0326 (17)	0.0500 (18)	−0.0117 (17)	0.0096 (18)	−0.0026 (14)
N2	0.058 (2)	0.0295 (16)	0.0388 (17)	−0.0022 (14)	−0.0146 (15)	−0.0004 (13)
N3	0.076 (3)	0.0322 (18)	0.0353 (17)	−0.0046 (17)	−0.0121 (17)	−0.0009 (14)
C1	0.050 (2)	0.032 (2)	0.047 (2)	0.0004 (16)	−0.0218 (18)	−0.0030 (16)
C9	0.046 (2)	0.031 (2)	0.046 (2)	−0.0016 (16)	−0.0102 (17)	0.0012 (16)
C14	0.048 (2)	0.037 (2)	0.055 (2)	−0.0086 (18)	−0.0046 (19)	−0.0055 (18)
C6	0.056 (2)	0.0298 (19)	0.046 (2)	−0.0024 (17)	−0.0211 (18)	0.0012 (16)
C8	0.056 (3)	0.031 (2)	0.048 (2)	−0.0012 (17)	−0.0109 (19)	−0.0017 (17)
C10	0.074 (3)	0.030 (2)	0.044 (2)	−0.0095 (19)	−0.011 (2)	0.0032 (17)
C2	0.070 (3)	0.032 (2)	0.057 (3)	−0.0008 (19)	−0.023 (2)	−0.0031 (19)
C11	0.070 (3)	0.040 (2)	0.050 (2)	−0.008 (2)	−0.016 (2)	−0.0074 (19)
C13	0.050 (2)	0.051 (3)	0.049 (2)	−0.010 (2)	−0.0015 (19)	−0.004 (2)
C5	0.059 (3)	0.050 (3)	0.055 (3)	−0.002 (2)	−0.005 (2)	−0.005 (2)
C12	0.049 (2)	0.050 (3)	0.048 (2)	−0.0049 (19)	−0.0111 (19)	−0.0080 (19)
C7	0.104 (4)	0.034 (2)	0.053 (3)	−0.018 (2)	−0.020 (3)	0.006 (2)
C3	0.072 (3)	0.048 (3)	0.066 (3)	0.009 (2)	−0.019 (3)	−0.025 (2)
C4	0.064 (3)	0.070 (4)	0.054 (3)	0.004 (3)	−0.008 (2)	−0.016 (2)
C15	0.095 (4)	0.074 (4)	0.054 (3)	−0.017 (3)	−0.004 (3)	−0.020 (3)

Geometric parameters (Å, º)

Zn1—Cl2	2.2348 (12)	C10—H10	0.9300
Zn1—Cl1	2.2318 (13)	C10—C11	1.371 (7)
Zn1—N1	2.186 (4)	C2—H2	0.9300
Zn1—O1	2.260 (3)	C2—C3	1.378 (7)
Zn1—N2	2.107 (3)	C11—H11	0.9300
N1—C1	1.346 (6)	C11—C12	1.377 (7)
N1—C5	1.323 (6)	C13—H13	0.9300
O1—C8	1.233 (6)	C13—C12	1.396 (7)
N2—N3	1.370 (5)	C5—H5	0.9300
N2—C6	1.287 (5)	C5—C4	1.382 (8)
N3—H3	0.87 (2)	C12—C15	1.503 (7)
N3—C8	1.363 (5)	C7—H7A	0.9600
C1—C6	1.478 (6)	C7—H7B	0.9600
C1—C2	1.385 (6)	C7—H7C	0.9600
C9—C14	1.381 (6)	C3—H3A	0.9300
C9—C8	1.474 (6)	C3—C4	1.365 (8)
C9—C10	1.400 (6)	C4—H4	0.9300
C14—H14	0.9300	C15—H15A	0.9600
C14—C13	1.385 (7)	C15—H15B	0.9600
C6—C7	1.497 (6)	C15—H15C	0.9600

Cl2—Zn1—O1	94.84 (11)	C11—C10—C9	120.0 (4)
Cl1—Zn1—Cl2	111.46 (5)	C11—C10—H10	120.0
Cl1—Zn1—O1	98.16 (13)	C1—C2—H2	120.6
N1—Zn1—Cl2	103.12 (11)	C3—C2—C1	118.7 (5)
N1—Zn1—Cl1	102.32 (11)	C3—C2—H2	120.6
N1—Zn1—O1	145.35 (13)	C10—C11—H11	119.1
N2—Zn1—Cl2	127.98 (11)	C10—C11—C12	121.9 (4)
N2—Zn1—Cl1	120.03 (11)	C12—C11—H11	119.1
N2—Zn1—N1	73.64 (13)	C14—C13—H13	119.5
N2—Zn1—O1	71.95 (12)	C14—C13—C12	120.9 (4)
C1—N1—Zn1	115.1 (3)	C12—C13—H13	119.5
C5—N1—Zn1	126.4 (3)	N1—C5—H5	118.3
C5—N1—C1	118.2 (4)	N1—C5—C4	123.4 (5)
C8—O1—Zn1	115.2 (3)	C4—C5—H5	118.3
N3—N2—Zn1	117.7 (2)	C11—C12—C13	118.0 (4)
C6—N2—Zn1	121.3 (3)	C11—C12—C15	121.3 (5)
C6—N2—N3	120.8 (4)	C13—C12—C15	120.7 (5)
N2—N3—H3	121 (4)	C6—C7—H7A	109.5
C8—N3—N2	115.3 (3)	C6—C7—H7B	109.5
C8—N3—H3	117 (4)	C6—C7—H7C	109.5
N1—C1—C6	115.4 (4)	H7A—C7—H7B	109.5
N1—C1—C2	121.7 (4)	H7A—C7—H7C	109.5
C2—C1—C6	122.9 (4)	H7B—C7—H7C	109.5
C14—C9—C8	122.9 (4)	C2—C3—H3A	120.1
C14—C9—C10	118.9 (4)	C4—C3—C2	119.8 (4)
C10—C9—C8	118.2 (4)	C4—C3—H3A	120.1
C9—C14—H14	119.8	C5—C4—H4	121.0
C9—C14—C13	120.3 (4)	C3—C4—C5	118.1 (5)
C13—C14—H14	119.8	C3—C4—H4	121.0
N2—C6—C1	113.7 (4)	C12—C15—H15A	109.5
N2—C6—C7	125.3 (4)	C12—C15—H15B	109.5
C1—C6—C7	121.0 (4)	C12—C15—H15C	109.5
O1—C8—N3	119.8 (4)	H15A—C15—H15B	109.5
O1—C8—C9	123.5 (4)	H15A—C15—H15C	109.5
N3—C8—C9	116.7 (4)	H15B—C15—H15C	109.5
C9—C10—H10	120.0		

Zn1—N1—C1—C6	−7.2 (5)	C14—C9—C8—O1	166.9 (5)
Zn1—N1—C1—C2	172.8 (3)	C14—C9—C8—N3	−11.0 (7)
Zn1—N1—C5—C4	−172.6 (4)	C14—C9—C10—C11	−0.6 (7)
Zn1—O1—C8—N3	−2.7 (6)	C14—C13—C12—C11	−0.7 (7)
Zn1—O1—C8—C9	179.5 (3)	C14—C13—C12—C15	179.6 (5)
Zn1—N2—N3—C8	−2.8 (5)	C6—N2—N3—C8	−177.9 (4)
Zn1—N2—C6—C1	6.6 (5)	C6—C1—C2—C3	−178.9 (4)
Zn1—N2—C6—C7	−173.8 (4)	C8—C9—C14—C13	−177.9 (4)
N1—C1—C6—N2	0.8 (5)	C8—C9—C10—C11	177.7 (4)
N1—C1—C6—C7	−178.8 (4)	C10—C9—C14—C13	0.4 (7)

N1—C1—C2—C3	1.1 (7)	C10—C9—C8—O1	−11.4 (7)
N1—C5—C4—C3	0.0 (9)	C10—C9—C8—N3	170.7 (4)
N2—N3—C8—O1	3.7 (7)	C10—C11—C12—C13	0.4 (8)
N2—N3—C8—C9	−178.4 (4)	C10—C11—C12—C15	−179.9 (5)
N3—N2—C6—C1	−178.5 (4)	C2—C1—C6—N2	−179.2 (4)
N3—N2—C6—C7	1.0 (7)	C2—C1—C6—C7	1.2 (7)
C1—N1—C5—C4	0.8 (8)	C2—C3—C4—C5	−0.3 (8)
C1—C2—C3—C4	−0.3 (8)	C5—N1—C1—C6	178.7 (4)
C9—C14—C13—C12	0.3 (7)	C5—N1—C1—C2	−1.4 (6)
C9—C10—C11—C12	0.2 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···Cl2^{i}	0.87 (2)	2.40 (3)	3.214 (4)	156 (5)
C2—H2···Cl1^{ii}	0.93	2.93	3.649 (5)	136
C4—H4···Cl1^{iii}	0.93	2.98	3.888 (6)	165

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