

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# Dichlorido(2,9-dimethoxy-1,10-phenanthroline- $\kappa^2N,N'$ )zinc(II)

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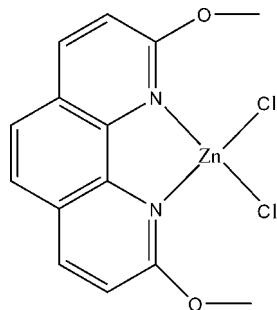
Received 13 June 2009; accepted 28 June 2009

 Key indicators: single-crystal X-ray study;  $T = 291$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.065; data-to-parameter ratio = 18.0.

In the crystal structure of the title compound,  $[ZnCl_2(C_{14}H_{12}N_2O_2)]$ , the  $Zn^{II}$  center is four-coordinated by two N atoms from one 2,9-dimethoxy-1,10-phenanthroline ligand and two Cl atoms. The coordination geometry is distorted tetrahedral, as the  $Zn-N$  bond distances are shorter than the  $Zn-Cl$  distances, and the  $Cl-Zn-N$  and  $Cl-Zn-Cl$  bond angles are much larger than the  $N-Zn-N$  angle. For the ligand, the O and C atoms of the methoxy groups are almost in the plane defined by the phenanthroline ring. The two O atoms deviate from the phenanthroline mean plane by 0.076 (2) and 0.084 (2) Å, and the two methyl C atoms deviate from the phenanthroline mean plane by 0.035 (3) and 0.361 (3) Å. There are medium  $\pi-\pi$  stacking interactions between two parallel phenanthroline rings with a centroid-centroid distance of 3.7860 (2) Å and a dihedral angle between the plane defined by the two parallel phenanthroline rings of 1.13 (5)°.

## Related literature

For background information, see: Majumder *et al.* (2006); Bie *et al.* (2006). For the synthesis, see: Pijper *et al.* (1984).



## Experimental

## Crystal data

 $[ZnCl_2(C_{14}H_{12}N_2O_2)]$   
 $M_r = 376.53$ 

 Monoclinic,  $P2_1/c$ 
 $a = 9.0494$  (8) Å

 $b = 10.3783$  (9) Å

 $c = 16.3517$  (14) Å

 $\beta = 99.022$  (1)°

 $V = 1516.7$  (2) Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 1.98$  mm<sup>-1</sup>
 $T = 291$  K

 $0.27 \times 0.14 \times 0.10$  mm

## Data collection

 Bruker APEXII CCD detector  
 diffractometer

 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)

 $T_{min} = 0.616$ ,  $T_{max} = 0.835$ 

9326 measured reflections

3465 independent reflections

 2917 reflections with  $I > 2\sigma(I)$ 
 $R_{int} = 0.017$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.025$ 
 $wR(F^2) = 0.065$ 
 $S = 1.03$ 

3465 reflections

192 parameters

H-atom parameters constrained

 $\Delta\rho_{max} = 0.30$  e Å<sup>-3</sup>
 $\Delta\rho_{min} = -0.25$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Zn1–N1	2.0659 (14)	Zn1–Cl1	2.2007 (6)
Zn1–N2	2.0911 (14)	Zn1–Cl2	2.2219 (6)
N1–Zn1–N2	80.58 (6)	N1–Zn1–Cl2	110.66 (4)
N1–Zn1–Cl1	113.27 (4)	N2–Zn1–Cl2	108.06 (4)
N2–Zn1–Cl1	120.54 (4)	Cl1–Zn1–Cl2	117.82 (2)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXL97* and *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXL97*.

We are grateful to Mrs Li for her assistance with the X-ray crystallographic analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2228).

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## supporting information

*Acta Cryst.* (2009). E65, m869 [doi:10.1107/S160053680902491X]

**Dichlorido(2,9-dimethoxy-1,10-phenanthroline- $\kappa^2N,N'$ )zinc(II)**

Cao-Yuan Niu, Hui Su, Lei Meng and Chun-Hong Kou

**S1. Comment**

The compound 1,10-phenanthroline was reported to be used to synthesize some potential strong luminescent materials with  $d^{10}$  metals. It can be predicted that the title compound that composed of a derivative of 1,10-phenanthroline and a  $d^{10}$  metal zinc would possess strong ligand to ligand or metal perturbed ligand to ligand emissions (Majumder *et al.*, 2006; Bie, *et al.*, 2006). 2,9-Dimethoxy-1,10-phenanthroline and 2,9-Diethoxy-1,10-phenanthroline as derivatives of 1,10-phenanthroline were synthesized at early time and they possess antimycoplasmal activity in the presence of copper (Pijper, *et al.*, 1984).

The title compound (I) is a mononuclear zinc(II) complex of 2,9-dimethoxy-1,10-phenanthroline (shown as Fig.1). The zinc metal centre is four coordinated to two nitrogen atoms (N1, N2) from the 1,10-phenanthroline ring and two independent chlorine atoms (Cl1, Cl2), defining a deformed tetrahedron coordination geometry around the metal center. The Zn—Cl bond distances are 2.2007 (6) and 2.2219 (6) Å, which are longer than the Zn—N bond distances from 2.0659 (14) to 2.0911 (14) Å. The Cl—Zn—N and Cl—Zn—Cl bond angles are at the range of 108.06 (4) to 120.54 (4) °, which are larger than that of N—Zn—N [80.58 (6)°]. Furthermore, there are medium  $\pi$ - $\pi$  stackings between two parallel phenanthroline rings from two symmetry-related monomers with the centroid-to-centroid distances of about 3.7860 (2) Å and dihedral angle of 1.13 (5) ° (Fig. 2). For the ligand, two methoxy groups are basically coplanar to the phenanthroline ring. Two oxygen atoms deviate from the phenanthroline plane by 0.076 (2) and 0.084 (2) Å, and two methyl carbon atoms deviate from the phenanthroline plane by 0.035 (3) and 0.361 (3) Å.

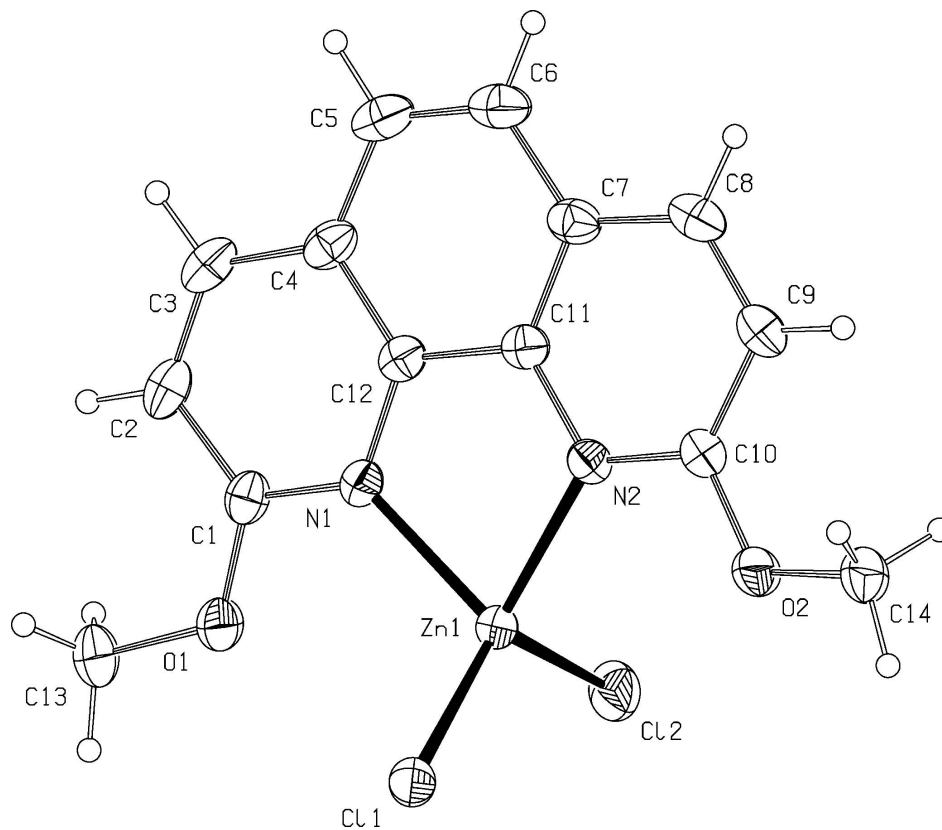
Three-dimensional supramolecular structure of the title compound is formed *via* the above-mentioned  $\pi$ - $\pi$  stackings and weak van der waals interactions. Some interesting packings along three crystallographic directions can be seen from Fig. 3.

**S2. Experimental**

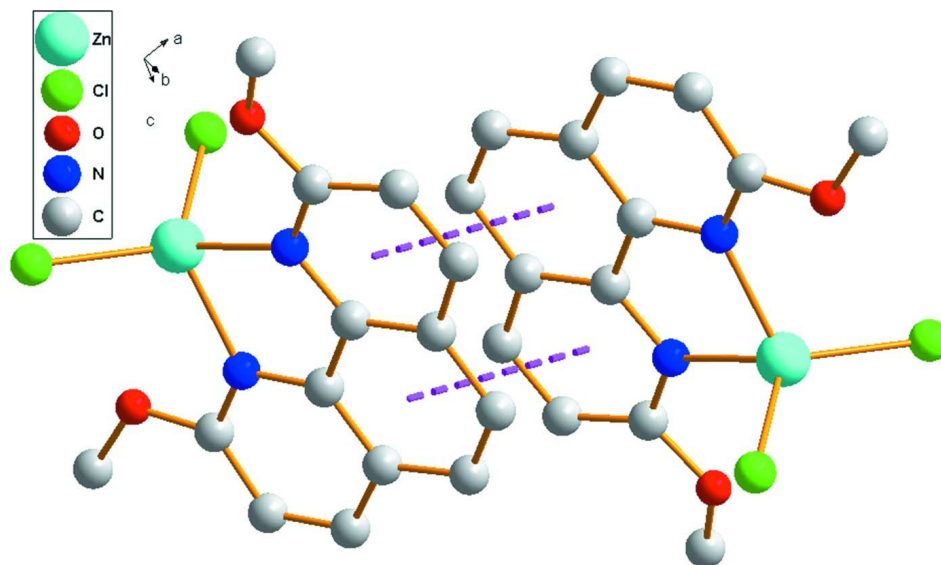
The organic ligand 2,9-dimethoxy-1,10-phenanthroline was prepared according to the procedure of literature (Pijper, *et al.*, 1984). The slow evaporation of mixture of the ligand (0.022 g, 0.1 mmol) and zinc dichloride (0.014 g, 0.1 mmol) in 30 ml *me* thanol afforded suitable colourless block crystals in about 7 days (yield 45%).

**S3. Refinement**

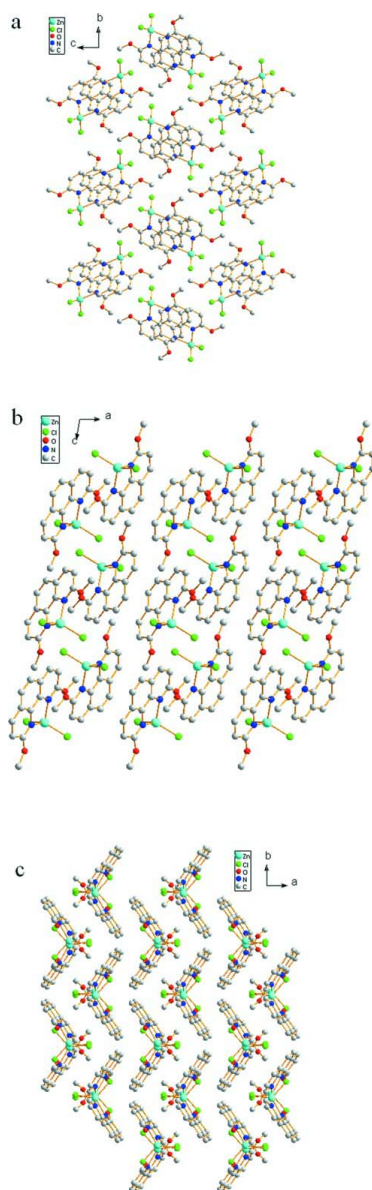
Carbon-bound H atoms were positioned geometrically and refined using a riding model [C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$  for aromatic H atoms; C—H = 0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$  for methyl H atoms;]. The final difference Fourier map had a highest peak at 0.85 Å from atom Cl2 and a deepest hole at 0.59 Å from atom Cl2, but were otherwise featureless.

**Figure 1**

A view of the  $\text{Zn}^{\text{II}}$  coordination environment in (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

**Figure 2**

Packing diagram showing the  $\pi$ - $\pi$  interaction (purple dotted line). All H atoms have been omitted for clarity.


**Figure 3**

Diagrams showing the three-dimensional packing forms along three crystallographic directions.

**Dichlorido(2,9-dimethoxy-1,10-phenanthroline- $\kappa^2N,N'$ )zinc(II)**
*Crystal data*

[ZnCl<sub>2</sub>(C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>)]

$M_r = 376.53$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 9.0494 (8) \text{ \AA}$

$b = 10.3783 (9) \text{ \AA}$

$c = 16.3517 (14) \text{ \AA}$

$\beta = 99.022 (1)^\circ$

$V = 1516.7 (2) \text{ \AA}^3$

$Z = 4$

$F(000) = 760$

$D_x = 1.649 \text{ Mg m}^{-3}$

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

Cell parameters from 4023 reflections

$\theta = 2.3\text{--}27.9^\circ$

$\mu = 1.98 \text{ mm}^{-1}$

$T = 291 \text{ K}$

Block, colorless

$0.27 \times 0.14 \times 0.10 \text{ mm}$

*Data collection*

Bruker APEXII CCD detector diffractometer	9326 measured reflections 3465 independent reflections
Radiation source: fine-focus sealed tube	2917 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.017$
$\varphi$ and $\omega$ scans	$\theta_{\text{max}} = 27.5^\circ$ , $\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7 \rightarrow 11$
$T_{\text{min}} = 0.616$ , $T_{\text{max}} = 0.835$	$k = -13 \rightarrow 13$
	$l = -21 \rightarrow 21$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H-atom parameters constrained
$wR(F^2) = 0.065$	$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 0.4767P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
3465 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
192 parameters	$\Delta\rho_{\text{max}} = 0.30 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.85210 (2)	0.73107 (2)	0.142693 (13)	0.03691 (8)
Cl1	1.07679 (6)	0.76186 (5)	0.21365 (3)	0.05122 (14)
Cl2	0.68839 (6)	0.89157 (5)	0.13748 (4)	0.05898 (15)
O1	0.99184 (17)	0.81556 (14)	-0.01403 (8)	0.0502 (3)
O2	0.71476 (16)	0.58258 (13)	0.28668 (8)	0.0481 (3)
N1	0.85558 (16)	0.65629 (14)	0.02592 (9)	0.0366 (3)
N2	0.73776 (16)	0.55838 (14)	0.15361 (9)	0.0360 (3)
C1	0.9193 (2)	0.70500 (19)	-0.03500 (11)	0.0405 (4)
C2	0.9063 (3)	0.6460 (2)	-0.11341 (12)	0.0502 (5)
H2	0.9523	0.6820	-0.1550	0.060*
C3	0.8256 (3)	0.5361 (2)	-0.12718 (12)	0.0519 (5)
H3	0.8160	0.4967	-0.1788	0.062*
C4	0.7557 (2)	0.48020 (19)	-0.06404 (12)	0.0447 (4)
C5	0.6660 (2)	0.3663 (2)	-0.07373 (14)	0.0548 (5)
H5	0.6523	0.3232	-0.1242	0.066*
C6	0.6011 (2)	0.3201 (2)	-0.01103 (14)	0.0540 (5)

H6	0.5415	0.2468	-0.0192	0.065*
C7	0.6228 (2)	0.38262 (18)	0.06829 (13)	0.0434 (4)
C8	0.5595 (2)	0.3401 (2)	0.13704 (14)	0.0500 (5)
H8	0.4985	0.2675	0.1319	0.060*
C9	0.5859 (2)	0.40325 (19)	0.21063 (13)	0.0464 (5)
H9	0.5437	0.3748	0.2557	0.056*
C10	0.6789 (2)	0.51305 (18)	0.21712 (12)	0.0391 (4)
C11	0.71040 (19)	0.49372 (17)	0.07990 (11)	0.0369 (4)
C12	0.7758 (2)	0.54491 (17)	0.01209 (11)	0.0367 (4)
C13	1.0711 (3)	0.8779 (2)	-0.07353 (13)	0.0554 (5)
H13A	1.1445	0.8199	-0.0891	0.083*
H13B	1.1199	0.9540	-0.0492	0.083*
H13C	1.0014	0.9013	-0.1217	0.083*
C14	0.6826 (3)	0.5280 (2)	0.36304 (12)	0.0536 (5)
H14A	0.5763	0.5196	0.3604	0.080*
H14B	0.7216	0.5834	0.4083	0.080*
H14C	0.7285	0.4447	0.3712	0.080*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn1	0.03791 (13)	0.03966 (13)	0.03454 (12)	-0.00516 (9)	0.01002 (9)	-0.00396 (8)
Cl1	0.0399 (3)	0.0714 (4)	0.0431 (3)	-0.0099 (2)	0.0087 (2)	-0.0143 (2)
Cl2	0.0501 (3)	0.0513 (3)	0.0795 (4)	0.0074 (2)	0.0226 (3)	-0.0024 (3)
O1	0.0623 (9)	0.0531 (8)	0.0391 (7)	-0.0104 (7)	0.0201 (6)	0.0019 (6)
O2	0.0561 (9)	0.0513 (8)	0.0389 (7)	-0.0155 (7)	0.0138 (6)	0.0014 (6)
N1	0.0378 (8)	0.0402 (9)	0.0323 (7)	0.0027 (6)	0.0071 (6)	-0.0009 (6)
N2	0.0342 (8)	0.0367 (8)	0.0370 (8)	-0.0032 (6)	0.0057 (6)	0.0017 (6)
C1	0.0419 (10)	0.0461 (11)	0.0342 (9)	0.0081 (8)	0.0083 (8)	0.0043 (8)
C2	0.0608 (13)	0.0582 (13)	0.0339 (10)	0.0133 (10)	0.0148 (9)	0.0022 (9)
C3	0.0647 (14)	0.0557 (13)	0.0348 (10)	0.0144 (11)	0.0057 (9)	-0.0088 (9)
C4	0.0468 (11)	0.0458 (11)	0.0392 (10)	0.0126 (9)	-0.0006 (8)	-0.0068 (8)
C5	0.0601 (13)	0.0487 (12)	0.0520 (12)	0.0071 (10)	-0.0030 (10)	-0.0183 (10)
C6	0.0510 (12)	0.0410 (11)	0.0661 (14)	-0.0020 (9)	-0.0028 (10)	-0.0123 (10)
C7	0.0364 (10)	0.0381 (10)	0.0530 (11)	0.0008 (8)	-0.0007 (8)	-0.0035 (8)
C8	0.0405 (11)	0.0411 (11)	0.0660 (14)	-0.0081 (9)	0.0011 (10)	0.0013 (10)
C9	0.0405 (11)	0.0448 (11)	0.0544 (12)	-0.0067 (8)	0.0087 (9)	0.0086 (9)
C10	0.0353 (9)	0.0400 (10)	0.0422 (10)	-0.0016 (7)	0.0065 (8)	0.0039 (8)
C11	0.0322 (9)	0.0356 (9)	0.0411 (9)	0.0038 (7)	0.0006 (7)	-0.0018 (7)
C12	0.0345 (9)	0.0377 (10)	0.0365 (9)	0.0072 (7)	0.0009 (7)	-0.0021 (7)
C13	0.0574 (13)	0.0644 (14)	0.0490 (12)	-0.0040 (11)	0.0226 (10)	0.0113 (10)
C14	0.0590 (13)	0.0624 (14)	0.0427 (11)	-0.0119 (11)	0.0179 (10)	0.0042 (9)

*Geometric parameters (Å, °)*

Zn1—N1	2.0659 (14)	C4—C5	1.429 (3)
Zn1—N2	2.0911 (14)	C5—C6	1.347 (3)
Zn1—Cl1	2.2007 (6)	C5—H5	0.9300

Zn1—C12	2.2219 (6)	C6—C7	1.436 (3)
O1—C1	1.340 (2)	C6—H6	0.9300
O1—C13	1.449 (2)	C7—C11	1.395 (3)
O2—C10	1.343 (2)	C7—C8	1.410 (3)
O2—C14	1.442 (2)	C8—C9	1.358 (3)
N1—C1	1.327 (2)	C8—H8	0.9300
N1—C12	1.363 (2)	C9—C10	1.411 (3)
N2—C10	1.325 (2)	C9—H9	0.9300
N2—C11	1.368 (2)	C11—C12	1.438 (3)
C1—C2	1.409 (3)	C13—H13A	0.9600
C2—C3	1.354 (3)	C13—H13B	0.9600
C2—H2	0.9300	C13—H13C	0.9600
C3—C4	1.417 (3)	C14—H14A	0.9600
C3—H3	0.9300	C14—H14B	0.9600
C4—C12	1.401 (3)	C14—H14C	0.9600
N1—Zn1—N2	80.58 (6)	C7—C6—H6	119.6
N1—Zn1—C11	113.27 (4)	C11—C7—C8	116.32 (18)
N2—Zn1—C11	120.54 (4)	C11—C7—C6	119.39 (19)
N1—Zn1—C12	110.66 (4)	C8—C7—C6	124.29 (19)
N2—Zn1—C12	108.06 (4)	C9—C8—C7	121.19 (18)
C11—Zn1—C12	117.82 (2)	C9—C8—H8	119.4
C1—O1—C13	119.03 (15)	C7—C8—H8	119.4
C10—O2—C14	117.89 (15)	C8—C9—C10	118.47 (19)
C1—N1—C12	118.68 (16)	C8—C9—H9	120.8
C1—N1—Zn1	128.47 (13)	C10—C9—H9	120.8
C12—N1—Zn1	112.80 (11)	N2—C10—O2	113.56 (16)
C10—N2—C11	118.48 (16)	N2—C10—C9	122.41 (18)
C10—N2—Zn1	129.50 (13)	O2—C10—C9	124.03 (17)
C11—N2—Zn1	111.65 (11)	N2—C11—C7	123.09 (17)
N1—C1—O1	112.80 (16)	N2—C11—C12	117.31 (16)
N1—C1—C2	122.24 (19)	C7—C11—C12	119.60 (17)
O1—C1—C2	124.95 (17)	N1—C12—C4	123.06 (17)
C3—C2—C1	118.91 (19)	N1—C12—C11	117.18 (15)
C3—C2—H2	120.5	C4—C12—C11	119.76 (17)
C1—C2—H2	120.5	O1—C13—H13A	109.5
C2—C3—C4	120.96 (18)	O1—C13—H13B	109.5
C2—C3—H3	119.5	H13A—C13—H13B	109.5
C4—C3—H3	119.5	O1—C13—H13C	109.5
C12—C4—C3	116.14 (19)	H13A—C13—H13C	109.5
C12—C4—C5	119.19 (19)	H13B—C13—H13C	109.5
C3—C4—C5	124.66 (18)	O2—C14—H14A	109.5
C6—C5—C4	121.18 (19)	O2—C14—H14B	109.5
C6—C5—H5	119.4	H14A—C14—H14B	109.5
C4—C5—H5	119.4	O2—C14—H14C	109.5
C5—C6—C7	120.8 (2)	H14A—C14—H14C	109.5
C5—C6—H6	119.6	H14B—C14—H14C	109.5

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N2—Zn1—N1—C1	-177.42 (16)	C7—C8—C9—C10	-0.1 (3)
Cl1—Zn1—N1—C1	-58.12 (16)	C11—N2—C10—O2	178.99 (16)
Cl2—Zn1—N1—C1	76.72 (16)	Zn1—N2—C10—O2	-8.7 (2)
N2—Zn1—N1—C12	5.17 (12)	C11—N2—C10—C9	-1.9 (3)
Cl1—Zn1—N1—C12	124.47 (11)	Zn1—N2—C10—C9	170.42 (14)
Cl2—Zn1—N1—C12	-100.69 (12)	C14—O2—C10—N2	-167.68 (17)
N1—Zn1—N2—C10	-179.01 (17)	C14—O2—C10—C9	13.3 (3)
Cl1—Zn1—N2—C10	69.45 (17)	C8—C9—C10—N2	1.8 (3)
Cl2—Zn1—N2—C10	-70.22 (16)	C8—C9—C10—O2	-179.18 (18)
N1—Zn1—N2—C11	-6.24 (12)	C10—N2—C11—C7	0.3 (3)
Cl1—Zn1—N2—C11	-117.78 (11)	Zn1—N2—C11—C7	-173.33 (14)
Cl2—Zn1—N2—C11	102.56 (11)	C10—N2—C11—C12	-179.91 (16)
C12—N1—C1—O1	178.81 (15)	Zn1—N2—C11—C12	6.43 (19)
Zn1—N1—C1—O1	1.5 (2)	C8—C7—C11—N2	1.3 (3)
C12—N1—C1—C2	0.5 (3)	C6—C7—C11—N2	-179.37 (17)
Zn1—N1—C1—C2	-176.81 (14)	C8—C7—C11—C12	-178.48 (17)
C13—O1—C1—N1	178.04 (17)	C6—C7—C11—C12	0.9 (3)
C13—O1—C1—C2	-3.7 (3)	C1—N1—C12—C4	-1.1 (3)
N1—C1—C2—C3	0.2 (3)	Zn1—N1—C12—C4	176.62 (14)
O1—C1—C2—C3	-177.93 (19)	C1—N1—C12—C11	178.97 (16)
C1—C2—C3—C4	-0.3 (3)	Zn1—N1—C12—C11	-3.35 (19)
C2—C3—C4—C12	-0.2 (3)	C3—C4—C12—N1	0.9 (3)
C2—C3—C4—C5	178.6 (2)	C5—C4—C12—N1	-177.93 (17)
C12—C4—C5—C6	-0.2 (3)	C3—C4—C12—C11	-179.10 (17)
C3—C4—C5—C6	-178.9 (2)	C5—C4—C12—C11	2.0 (3)
C4—C5—C6—C7	-1.4 (3)	N2—C11—C12—N1	-2.2 (2)
C5—C6—C7—C11	1.0 (3)	C7—C11—C12—N1	177.58 (16)
C5—C6—C7—C8	-179.7 (2)	N2—C11—C12—C4	177.84 (16)
C11—C7—C8—C9	-1.4 (3)	C7—C11—C12—C4	-2.4 (3)
C6—C7—C8—C9	179.3 (2)		

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