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# (5,5′-Dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)-(1-naphthylacetato-$\kappa O$)(1-naphthylacetato-$\kappa^2O,O'$)zinc hemihydrate

**Li-Li Ji,[a] Jian-She Liu[a]* and Wen-Dong Song[b]**

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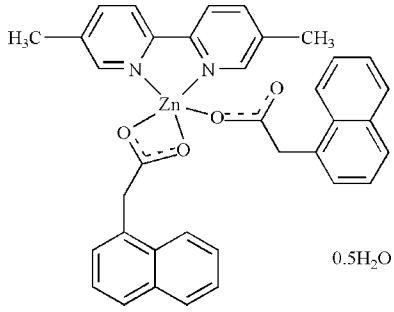
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.044; $wR$ factor = 0.106; data-to-parameter ratio = 13.5.

In the title compound, $[Zn(C_{12}H_9O_2)_2(C_{12}H_{12}N_2)]\cdot0.5H_2O$, the water molecule lies on a twofold rotation axis. The $Zn^{II}$ atom is coordinated by three O atoms from two 1-naphthylacetate ligands, one monodentate and the other asymmetric bidentate chelate, and two N atoms from a 5,5′-dimethyl-2,2′-bipyridine ligand, giving an irregular environment. In the crystal, the complex molecules are interlinked through the water molecule by $O-H\cdots O_{carboxylate}$ hydrogen bonds, together with weak $C-H\cdots O$ and bipyridine ring $\pi$–$\pi$ stacking interactions [ring centroid separation = 3.761 (2) Å], giving a two-dimensional network structure.

## Related literature

For background to self-assembly of supramolecular architectures based on naphthylcarboxylate ligands, see: Kong *et al.* (2009); Li *et al.* (2009). The Zn—O distance in the second ligand [2.417 (3) Å] suggests a non-negligible (bidentate) interaction, see: Guilera & Steed (1999).




## Experimental

### Crystal data

$[Zn(C_{12}H_9O_2)_2(C_{12}H_{12}N_2)]\cdot0.5H_2O$
$M_r$ = 629.00
Monoclinic, $C2/c$
$a$ = 32.212 (7) Å
$b$ = 8.2668 (17) Å
$c$ = 25.314 (5) Å
$\beta$ = 117.865 (4)°
$V$ = 5959 (2) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.87 mm$^{-1}$
$T$ = 296 K
0.30 × 0.28 × 0.21 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.756, $T_{max}$ = 0.819
21468 measured reflections
5325 independent reflections
3566 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.106
$S$ = 0.99
5325 reflections
395 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.30 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H5···O1 | 0.82 | 2.21 | 2.948 (3) | 150 |
| C8—H8$A$···O4$^{i}$ | 0.93 | 2.59 | 3.515 (6) | 171 |

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

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: *SHELXL97*.

The authors acknowledge Donghua University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2105).

## References

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# supporting information

*Acta Cryst.* (2011). E**67**, m606 [doi:10.1107/S1600536811013353]

# (5,5′-Dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)(1-naphthylacetato-$\kappa O$)(1-naphthylacetato-$\kappa^2O,O'$)zinc hemihydrate

**Li-Li Ji, Jian-She Liu and Wen-Dong Song**

## S1. Comment

Self-assembly of supramolecular architectures based on naphthylcarboxylate ligands has attracted much attention during recent decades (Kong *et al.*, 2009; Li *et al.*, 2009). However, to our knowledge, 1-naphthylacetic acid has not been used as a potential building block in the construction of supramolecular architectures. Herein we report the structure of the title compound, the mixed ligand complex $[(C_{12}H_{12}N_2)(C_{12}H_9O_2)_2]_2 \cdot 0.5H_2O$ (I), from the reaction of zinc nitrate with 1-naphthylacetic acid and 5,5′-dimethyl-2,2′-bipyridyrine in a basic aqueous solution.

The asymmetric unit in (I) (Fig. 1) consists of one $Zn^{II}$ complex unit and a water molecule which lies on a two-fold rotation axis (Fig. 1). The five-coordinate Zn centre comprises three O atoms from two 1-naphthylacetate ligands and two N atoms from a 5,5′-dimethyl-2,2′-bipyridyrine ligand. There are two coordination modes for the 1-naphthylacetate ligands in the structure: one monodentate the other asymmetric bidentate chelate. The Zn1-O4 distance in the second ligand [2.417 (3) Å] suggests a non-negligible (bidentate) interaction (Guilera & Steed, 1999) whereas the Zn1—O5 distance in the first ligand [2.587 (3)] is considered beyond the distance maximum for a bidentate interaction. In the crystal, the supramolecular network is stabilized by water O—H···$O_{carboxyl}$, hydrogen bonds together with weak intermolecular aromatic C8—H···$O_{carboxyl}$ interactions (Table 1), giving a two-dimensional network structure. In addition the inter-ring separation between the pyridine rings of two adjacent 5,5′-dimethyl-2,2′-bipyridine ligands is 3.761 (2) Å, indicating weak $\pi$-$\pi$ stacking interactions (Fig. 2).

## S2. Experimental

A mixture of 1-naphthylacetic acid (0.110 g, 0.5 mmol), 5,5′-dimethyl-2,2′-bipyridine (0.092 g, 0.5 mmol), zinc nitrate hexahydrate (0.075 g, 0.25 mmol), NaOH (0.08 g, 0.2 mmol) and water (10 ml) was placed in a 23 ml Teflon-lined reactor, which was heated to 423 K for 3 days, and then cooled to room temperature at a rate of 10 K $h^{-1}$. The colorless crystals obtained were washed with water and dried in air (yield 47% based on zinc).

## S3. Refinement

All H atoms were located from difference maps, and were treated as riding atoms with O—H = 0.82 Å and C—H = 0.93, 0.96 and 0.97 Å, for aryl, methyl and methine groups respectively, and with $U_{iso}(H) = 1.5U_{eq}$ (methyl C-atoms) and $1.2U_{eq}$(non-methyl C-atoms or water O-atom).

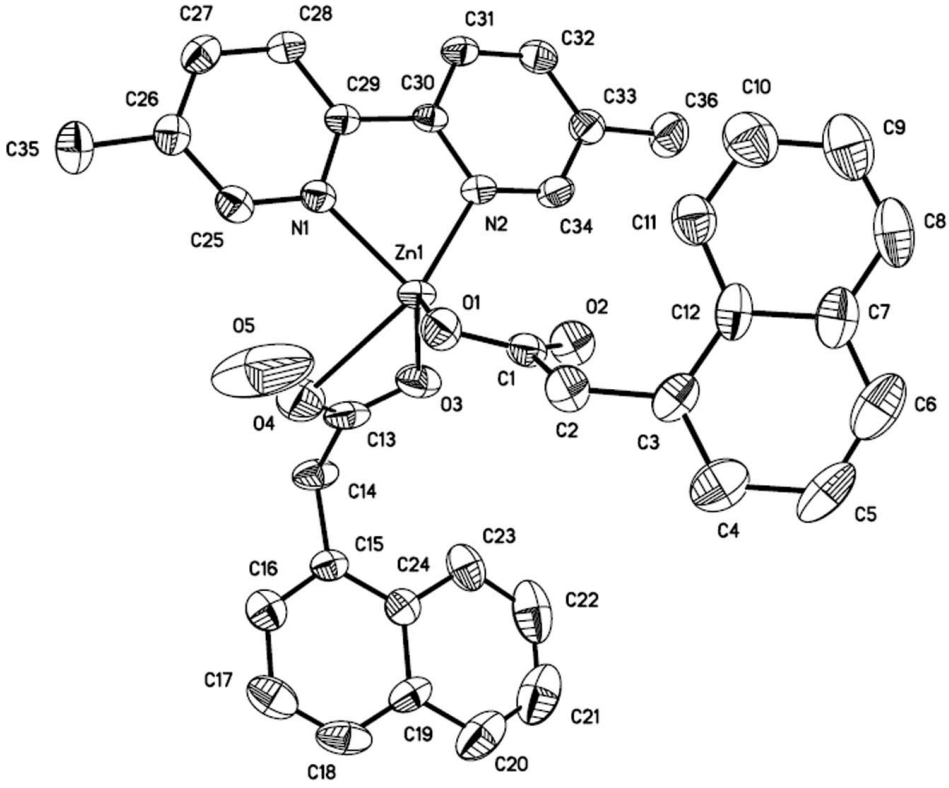


**Figure 1**

The structure of the title compound, showing the atom numbering scheme. The water molecule of solvation (O5) lies on a twofold rotation axis. Non-H atoms are shown with 30% probability displacement ellipsoids and H atoms are omitted.

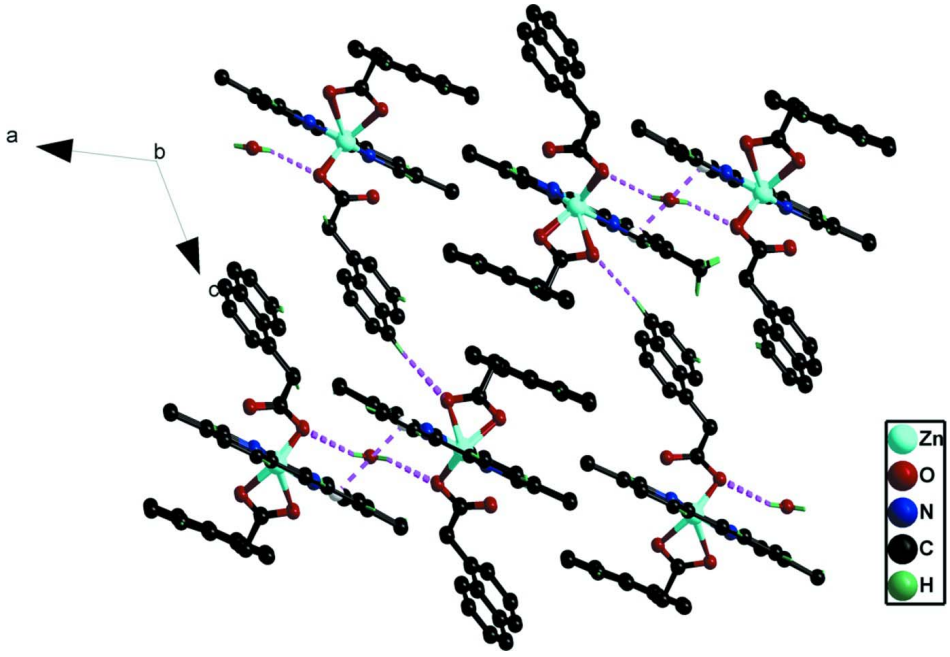


**Figure 2**

A view of the three-dimensional network in (I) showing O—H···O, C—H···O and $\pi$-$\pi$ stacking interactions as dashed lines.

**(5,5′-Dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)(1-naphthylacetato-$\kappa O$)(1-naphthylacetato-$\kappa^2O,O'$)zinc hemihydrate**

*Crystal data*

$[Zn(C_{12}H_9O_2)_2(C_{12}H_{12}N_2)]\cdot 0.5H_2O$
$M_r = 629.00$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 32.212$ (7) Å
$b = 8.2668$ (17) Å
$c = 25.314$ (5) Å
$\beta = 117.865$ (4)°
$V = 5959$ (2) Å$^3$
$Z = 8$
$F(000) = 2616$
$D_x = 1.402$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5837 reflections
$\theta = 2.8$–$27.9°$
$\mu = 0.87$ mm$^{-1}$
$T = 296$ K
Block, colorless
0.30 × 0.28 × 0.21 mm

*Data collection*

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.756$, $T_{max} = 0.819$
21468 measured reflections
5325 independent reflections
3566 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 25.2°$, $\theta_{min} = 2.6°$
$h = -38\rightarrow38$
$k = -9\rightarrow9$
$l = -30\rightarrow30$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.106$
$S = 0.99$
5325 reflections
395 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 11.176P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.020$
$\Delta\rho_{max} = 0.45$ e Å$^{-3}$
$\Delta\rho_{min} = -0.30$ 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.

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.120445 (14) | 0.34832 (5) | 0.280713 (17) | 0.04660 (14) |
| O1 | 0.07142 (9) | 0.4782 (3) | 0.21694 (10) | 0.0619 (6) |
| O2 | 0.12780 (10) | 0.4724 (3) | 0.19164 (11) | 0.0687 (7) |
| O3 | 0.18066 (9) | 0.4490 (3) | 0.34162 (11) | 0.0691 (7) |

| | | | | |
|---|---|---|---|---|
| O4 | 0.12345 (12) | 0.5188 (4) | 0.35996 (13) | 0.0879 (10) |
| N1 | 0.08321 (9) | 0.1801 (3) | 0.30436 (11) | 0.0448 (7) |
| N2 | 0.14254 (9) | 0.1318 (3) | 0.26096 (11) | 0.0442 (6) |
| C1 | 0.08888 (14) | 0.5173 (4) | 0.18284 (15) | 0.0533 (9) |
| C2 | 0.05863 (14) | 0.6281 (5) | 0.13114 (16) | 0.0660 (11) |
| H2A | 0.0269 | 0.5856 | 0.1120 | 0.079* |
| H2B | 0.0576 | 0.7335 | 0.1473 | 0.079* |
| C3 | 0.07433 (12) | 0.6504 (5) | 0.08408 (17) | 0.0647 (11) |
| C4 | 0.09184 (16) | 0.7942 (6) | 0.0771 (2) | 0.0952 (16) |
| H4A | 0.0946 | 0.8806 | 0.1021 | 0.114* |
| C5 | 0.10634 (18) | 0.8141 (8) | 0.0303 (3) | 0.107 (2) |
| H5A | 0.1182 | 0.9118 | 0.0249 | 0.129* |
| C6 | 0.10167 (19) | 0.6813 (9) | −0.0053 (3) | 0.108 (2) |
| H6A | 0.1106 | 0.6928 | −0.0350 | 0.130* |
| C7 | 0.08495 (14) | 0.5357 (7) | 0.00033 (18) | 0.0784 (12) |
| C8 | 0.08172 (16) | 0.4032 (8) | −0.03669 (19) | 0.0912 (16) |
| H8A | 0.0905 | 0.4142 | −0.0667 | 0.109* |
| C9 | 0.06576 (19) | 0.2613 (9) | −0.0279 (2) | 0.1072 (19) |
| H9A | 0.0644 | 0.1735 | −0.0516 | 0.129* |
| C10 | 0.05146 (17) | 0.2409 (8) | 0.0143 (2) | 0.1002 (16) |
| H10A | 0.0402 | 0.1408 | 0.0187 | 0.120* |
| C11 | 0.05356 (14) | 0.3666 (6) | 0.05021 (18) | 0.0737 (12) |
| H11A | 0.0433 | 0.3512 | 0.0786 | 0.088* |
| C12 | 0.07062 (12) | 0.5175 (6) | 0.04549 (15) | 0.0641 (11) |
| C13 | 0.16592 (17) | 0.5149 (4) | 0.37445 (16) | 0.0638 (11) |
| C14 | 0.20119 (15) | 0.5898 (5) | 0.43349 (15) | 0.0676 (12) |
| H14A | 0.1916 | 0.5664 | 0.4638 | 0.081* |
| H14B | 0.2317 | 0.5409 | 0.4460 | 0.081* |
| C15 | 0.20519 (12) | 0.7702 (4) | 0.42897 (13) | 0.0492 (9) |
| C16 | 0.17724 (13) | 0.8677 (6) | 0.44192 (16) | 0.0655 (11) |
| H16A | 0.1560 | 0.8203 | 0.4525 | 0.079* |
| C17 | 0.17903 (17) | 1.0338 (6) | 0.44005 (19) | 0.0818 (14) |
| H17A | 0.1594 | 1.0964 | 0.4495 | 0.098* |
| C18 | 0.20899 (19) | 1.1047 (5) | 0.42461 (18) | 0.0820 (14) |
| H18A | 0.2097 | 1.2170 | 0.4230 | 0.098* |
| C19 | 0.23921 (14) | 1.0145 (5) | 0.41079 (15) | 0.0629 (11) |
| C20 | 0.2712 (2) | 1.0871 (8) | 0.3958 (2) | 0.1019 (19) |
| H20A | 0.2722 | 1.1993 | 0.3938 | 0.122* |
| C21 | 0.3005 (2) | 0.9985 (12) | 0.3841 (2) | 0.116 (2) |
| H21A | 0.3211 | 1.0504 | 0.3734 | 0.140* |
| C22 | 0.30117 (18) | 0.8311 (11) | 0.3874 (2) | 0.111 (2) |
| H22A | 0.3229 | 0.7723 | 0.3807 | 0.133* |
| C23 | 0.26923 (15) | 0.7514 (7) | 0.40089 (16) | 0.0795 (13) |
| H23A | 0.2687 | 0.6390 | 0.4018 | 0.095* |
| C24 | 0.23771 (12) | 0.8422 (5) | 0.41318 (13) | 0.0525 (9) |
| C25 | 0.05275 (12) | 0.2135 (5) | 0.32507 (14) | 0.0537 (9) |
| H25A | 0.0477 | 0.3213 | 0.3308 | 0.064* |
| C26 | 0.02851 (12) | 0.0962 (5) | 0.33832 (14) | 0.0535 (9) |

| | | | | |
|---|---|---|---|---|
| C27 | 0.03634 (12) | −0.0623 (5) | 0.32856 (15) | 0.0577 (10) |
| H27A | 0.0202 | −0.1448 | 0.3361 | 0.069* |
| C28 | 0.06785 (12) | −0.0999 (4) | 0.30777 (15) | 0.0514 (9) |
| H28A | 0.0733 | −0.2070 | 0.3015 | 0.062* |
| C29 | 0.09120 (11) | 0.0246 (4) | 0.29648 (13) | 0.0412 (7) |
| C30 | 0.12614 (11) | −0.0026 (4) | 0.27505 (13) | 0.0401 (7) |
| C31 | 0.14199 (12) | −0.1536 (4) | 0.26986 (14) | 0.0496 (8) |
| H31A | 0.1304 | −0.2456 | 0.2795 | 0.060* |
| C32 | 0.17511 (12) | −0.1673 (5) | 0.25029 (15) | 0.0571 (9) |
| H32A | 0.1859 | −0.2690 | 0.2467 | 0.069* |
| C33 | 0.19239 (13) | −0.0319 (5) | 0.23602 (16) | 0.0575 (9) |
| C34 | 0.17446 (12) | 0.1158 (4) | 0.24173 (16) | 0.0537 (9) |
| H34A | 0.1853 | 0.2089 | 0.2316 | 0.064* |
| C35 | −0.00465 (14) | 0.1416 (6) | 0.36237 (18) | 0.0762 (12) |
| H35A | −0.0321 | 0.0742 | 0.3444 | 0.114* |
| H35B | −0.0137 | 0.2529 | 0.3532 | 0.114* |
| H35C | 0.0106 | 0.1267 | 0.4049 | 0.114* |
| C36 | 0.22968 (16) | −0.0420 (6) | 0.2159 (2) | 0.0877 (14) |
| H36A | 0.2215 | −0.1249 | 0.1862 | 0.131* |
| H36B | 0.2594 | −0.0675 | 0.2495 | 0.131* |
| H36C | 0.2319 | 0.0601 | 0.1993 | 0.131* |
| O5 | 0.0000 | 0.5928 (8) | 0.2500 | 0.233 (5) |
| H5 | 0.0203 | 0.5336 | 0.2496 | 0.350* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0513 (2) | 0.0329 (2) | 0.0490 (2) | −0.0034 (2) | 0.01794 (17) | −0.00328 (19) |
| O1 | 0.0735 (16) | 0.0611 (17) | 0.0491 (13) | 0.0086 (12) | 0.0271 (12) | 0.0098 (11) |
| O2 | 0.0709 (18) | 0.0643 (18) | 0.0627 (16) | 0.0214 (15) | 0.0243 (14) | 0.0167 (14) |
| O3 | 0.0811 (19) | 0.0525 (17) | 0.0566 (15) | −0.0065 (14) | 0.0180 (15) | −0.0072 (13) |
| O4 | 0.087 (2) | 0.093 (2) | 0.0689 (18) | −0.030 (2) | 0.0246 (17) | −0.0223 (17) |
| N1 | 0.0496 (16) | 0.0399 (17) | 0.0419 (14) | 0.0014 (13) | 0.0189 (13) | −0.0009 (12) |
| N2 | 0.0438 (15) | 0.0358 (16) | 0.0497 (15) | −0.0030 (13) | 0.0191 (13) | −0.0008 (13) |
| C1 | 0.073 (3) | 0.039 (2) | 0.0403 (19) | 0.0021 (19) | 0.0200 (19) | −0.0002 (16) |
| C2 | 0.073 (3) | 0.064 (3) | 0.057 (2) | 0.021 (2) | 0.027 (2) | 0.014 (2) |
| C3 | 0.052 (2) | 0.067 (3) | 0.064 (2) | 0.014 (2) | 0.0175 (19) | 0.033 (2) |
| C4 | 0.088 (3) | 0.080 (4) | 0.097 (4) | 0.015 (3) | 0.027 (3) | 0.035 (3) |
| C5 | 0.091 (4) | 0.102 (5) | 0.125 (5) | 0.003 (3) | 0.048 (4) | 0.065 (4) |
| C6 | 0.085 (4) | 0.127 (6) | 0.109 (4) | 0.017 (4) | 0.043 (3) | 0.064 (4) |
| C7 | 0.059 (3) | 0.112 (4) | 0.061 (3) | 0.021 (3) | 0.026 (2) | 0.028 (2) |
| C8 | 0.071 (3) | 0.152 (5) | 0.050 (2) | 0.031 (3) | 0.028 (2) | 0.014 (3) |
| C9 | 0.095 (4) | 0.149 (6) | 0.066 (3) | 0.017 (4) | 0.028 (3) | −0.002 (4) |
| C10 | 0.090 (4) | 0.114 (5) | 0.083 (3) | −0.006 (3) | 0.029 (3) | −0.014 (3) |
| C11 | 0.067 (3) | 0.090 (3) | 0.061 (2) | 0.002 (3) | 0.028 (2) | 0.000 (3) |
| C12 | 0.045 (2) | 0.102 (4) | 0.042 (2) | 0.018 (2) | 0.0176 (17) | 0.022 (2) |
| C13 | 0.091 (3) | 0.035 (2) | 0.042 (2) | −0.013 (2) | 0.011 (2) | 0.0039 (17) |
| C14 | 0.089 (3) | 0.047 (2) | 0.0400 (19) | −0.020 (2) | 0.0077 (19) | −0.0006 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.052 (2) | 0.046 (2) | 0.0334 (17) | −0.0076 (17) | 0.0067 (16) | −0.0008 (15) |
| C16 | 0.055 (2) | 0.077 (3) | 0.051 (2) | −0.002 (2) | 0.0142 (18) | −0.008 (2) |
| C17 | 0.075 (3) | 0.074 (3) | 0.073 (3) | 0.021 (3) | 0.014 (2) | −0.011 (3) |
| C18 | 0.099 (4) | 0.044 (2) | 0.061 (3) | 0.008 (3) | 0.003 (3) | 0.003 (2) |
| C19 | 0.064 (3) | 0.059 (3) | 0.044 (2) | −0.019 (2) | 0.0076 (19) | 0.0078 (18) |
| C20 | 0.092 (4) | 0.118 (5) | 0.067 (3) | −0.045 (4) | 0.013 (3) | 0.015 (3) |
| C21 | 0.076 (4) | 0.185 (8) | 0.075 (4) | −0.045 (5) | 0.025 (3) | 0.006 (5) |
| C22 | 0.065 (3) | 0.198 (8) | 0.064 (3) | 0.002 (4) | 0.025 (2) | −0.019 (4) |
| C23 | 0.070 (3) | 0.109 (4) | 0.050 (2) | 0.004 (3) | 0.020 (2) | −0.015 (2) |
| C24 | 0.0480 (19) | 0.064 (2) | 0.0318 (16) | −0.0043 (19) | 0.0071 (15) | −0.0030 (17) |
| C25 | 0.058 (2) | 0.050 (2) | 0.050 (2) | 0.0059 (18) | 0.0224 (18) | −0.0012 (17) |
| C26 | 0.049 (2) | 0.064 (3) | 0.0421 (19) | 0.0022 (18) | 0.0167 (17) | 0.0041 (17) |
| C27 | 0.053 (2) | 0.062 (3) | 0.053 (2) | −0.0085 (19) | 0.0199 (18) | 0.0090 (19) |
| C28 | 0.052 (2) | 0.040 (2) | 0.058 (2) | −0.0038 (16) | 0.0228 (18) | 0.0003 (16) |
| C29 | 0.0428 (19) | 0.0373 (18) | 0.0340 (16) | −0.0004 (15) | 0.0101 (14) | 0.0013 (14) |
| C30 | 0.0405 (18) | 0.0328 (17) | 0.0363 (16) | −0.0014 (14) | 0.0091 (14) | −0.0019 (14) |
| C31 | 0.057 (2) | 0.0340 (18) | 0.0529 (19) | −0.0014 (17) | 0.0214 (17) | 0.0010 (17) |
| C32 | 0.062 (2) | 0.044 (2) | 0.065 (2) | 0.0070 (19) | 0.0292 (19) | −0.0030 (18) |
| C33 | 0.060 (2) | 0.053 (2) | 0.064 (2) | 0.0037 (19) | 0.032 (2) | −0.0004 (19) |
| C34 | 0.055 (2) | 0.043 (2) | 0.066 (2) | −0.0055 (17) | 0.0298 (19) | 0.0020 (17) |
| C35 | 0.070 (3) | 0.095 (3) | 0.076 (3) | 0.014 (3) | 0.045 (2) | 0.010 (3) |
| C36 | 0.098 (3) | 0.076 (3) | 0.122 (4) | 0.015 (3) | 0.079 (3) | 0.010 (3) |
| O5 | 0.134 (5) | 0.083 (5) | 0.495 (15) | 0.000 | 0.157 (8) | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—O1 | 1.967 (2) | C16—C17 | 1.376 (6) |
| Zn1—O3 | 2.009 (3) | C16—H16A | 0.9300 |
| Zn1—N2 | 2.072 (3) | C17—C18 | 1.334 (6) |
| Zn1—N1 | 2.098 (3) | C17—H17A | 0.9300 |
| Zn1—O4 | 2.416 (3) | C18—C19 | 1.394 (6) |
| O1—C1 | 1.273 (4) | C18—H18A | 0.9300 |
| O2—C1 | 1.224 (4) | C19—C20 | 1.391 (6) |
| O3—C13 | 1.258 (5) | C19—C24 | 1.427 (5) |
| O4—C13 | 1.240 (5) | C20—C21 | 1.333 (8) |
| N1—C29 | 1.344 (4) | C20—H20A | 0.9300 |
| N1—C25 | 1.340 (4) | C21—C22 | 1.386 (9) |
| N2—C34 | 1.334 (4) | C21—H21A | 0.9300 |
| N2—C30 | 1.348 (4) | C22—C23 | 1.392 (7) |
| C1—C2 | 1.520 (5) | C22—H22A | 0.9300 |
| C2—C3 | 1.507 (5) | C23—C24 | 1.410 (5) |
| C2—H2A | 0.9700 | C23—H23A | 0.9300 |
| C2—H2B | 0.9700 | C25—C26 | 1.381 (5) |
| C3—C4 | 1.363 (6) | C25—H25A | 0.9300 |
| C3—C12 | 1.437 (6) | C26—C27 | 1.378 (5) |
| C4—C5 | 1.470 (7) | C26—C35 | 1.503 (5) |
| C4—H4A | 0.9300 | C27—C28 | 1.379 (5) |
| C5—C6 | 1.383 (8) | C27—H27A | 0.9300 |

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|---|---|---|---|
| C5—H5A | 0.9300 | C28—C29 | 1.381 (4) |
| C6—C7 | 1.352 (7) | C28—H28A | 0.9300 |
| C6—H6A | 0.9300 | C29—C30 | 1.477 (4) |
| C7—C8 | 1.414 (7) | C30—C31 | 1.378 (4) |
| C7—C12 | 1.427 (5) | C31—C32 | 1.375 (5) |
| C8—C9 | 1.340 (8) | C31—H31A | 0.9300 |
| C8—H8A | 0.9300 | C32—C33 | 1.372 (5) |
| C9—C10 | 1.356 (7) | C32—H32A | 0.9300 |
| C9—H9A | 0.9300 | C33—C34 | 1.387 (5) |
| C10—C11 | 1.362 (6) | C33—C36 | 1.509 (5) |
| C10—H10A | 0.9300 | C34—H34A | 0.9300 |
| C11—C12 | 1.391 (6) | C35—H35A | 0.9600 |
| C11—H11A | 0.9300 | C35—H35B | 0.9600 |
| C13—C14 | 1.523 (5) | C35—H35C | 0.9600 |
| C14—C15 | 1.505 (5) | C36—H36A | 0.9600 |
| C14—H14A | 0.9700 | C36—H36B | 0.9600 |
| C14—H14B | 0.9700 | C36—H36C | 0.9600 |
| C15—C16 | 1.358 (5) | O5—H5 | 0.8199 |
| C15—C24 | 1.415 (5) | | |

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|---|---|---|---|
| O1—Zn1—O3 | 121.37 (11) | C15—C16—C17 | 122.7 (4) |
| O1—Zn1—N2 | 120.53 (10) | C15—C16—H16A | 118.6 |
| O3—Zn1—N2 | 103.04 (11) | C17—C16—H16A | 118.6 |
| O1—Zn1—N1 | 104.43 (11) | C18—C17—C16 | 119.7 (5) |
| O3—Zn1—N1 | 122.09 (10) | C18—C17—H17A | 120.1 |
| N2—Zn1—N1 | 78.64 (11) | C16—C17—H17A | 120.1 |
| O1—Zn1—O4 | 93.91 (11) | C17—C18—C19 | 121.6 (4) |
| O3—Zn1—O4 | 58.10 (11) | C17—C18—H18A | 119.2 |
| N2—Zn1—O4 | 145.01 (11) | C19—C18—H18A | 119.2 |
| N1—Zn1—O4 | 87.49 (11) | C20—C19—C18 | 122.1 (5) |
| C1—O1—Zn1 | 104.8 (2) | C20—C19—C24 | 119.1 (5) |
| C13—O3—Zn1 | 99.2 (3) | C18—C19—C24 | 118.8 (4) |
| C13—O4—Zn1 | 80.9 (2) | C21—C20—C19 | 121.1 (6) |
| C29—N1—C25 | 118.7 (3) | C21—C20—H20A | 119.5 |
| C29—N1—Zn1 | 114.6 (2) | C19—C20—H20A | 119.5 |
| C25—N1—Zn1 | 126.6 (2) | C20—C21—C22 | 121.8 (6) |
| C34—N2—C30 | 118.6 (3) | C20—C21—H21A | 119.1 |
| C34—N2—Zn1 | 125.8 (2) | C22—C21—H21A | 119.1 |
| C30—N2—Zn1 | 115.3 (2) | C21—C22—C23 | 119.8 (6) |
| O2—C1—O1 | 122.7 (3) | C21—C22—H22A | 120.1 |
| O2—C1—C2 | 122.0 (3) | C23—C22—H22A | 120.1 |
| O1—C1—C2 | 115.4 (3) | C22—C23—C24 | 119.5 (5) |
| C3—C2—C1 | 115.9 (3) | C22—C23—H23A | 120.2 |
| C3—C2—H2A | 108.3 | C24—C23—H23A | 120.2 |
| C1—C2—H2A | 108.3 | C23—C24—C15 | 122.9 (4) |
| C3—C2—H2B | 108.3 | C23—C24—C19 | 118.7 (4) |
| C1—C2—H2B | 108.3 | C15—C24—C19 | 118.4 (4) |
| H2A—C2—H2B | 107.4 | N1—C25—C26 | 123.5 (3) |

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|---|---|---|---|
| C4—C3—C12 | 119.1 (4) | N1—C25—H25A | 118.3 |
| C4—C3—C2 | 121.5 (5) | C26—C25—H25A | 118.3 |
| C12—C3—C2 | 119.4 (4) | C27—C26—C25 | 116.9 (3) |
| C3—C4—C5 | 120.6 (5) | C27—C26—C35 | 122.3 (4) |
| C3—C4—H4A | 119.7 | C25—C26—C35 | 120.8 (4) |
| C5—C4—H4A | 119.7 | C26—C27—C28 | 120.8 (4) |
| C6—C5—C4 | 117.2 (5) | C26—C27—H27A | 119.6 |
| C6—C5—H5A | 121.4 | C28—C27—H27A | 119.6 |
| C4—C5—H5A | 121.4 | C27—C28—C29 | 118.7 (3) |
| C7—C6—C5 | 124.4 (6) | C27—C28—H28A | 120.7 |
| C7—C6—H6A | 117.8 | C29—C28—H28A | 120.7 |
| C5—C6—H6A | 117.8 | N1—C29—C28 | 121.4 (3) |
| C6—C7—C8 | 122.0 (5) | N1—C29—C30 | 115.6 (3) |
| C6—C7—C12 | 118.1 (5) | C28—C29—C30 | 123.0 (3) |
| C8—C7—C12 | 119.9 (5) | N2—C30—C31 | 120.9 (3) |
| C9—C8—C7 | 118.9 (5) | N2—C30—C29 | 115.6 (3) |
| C9—C8—H8A | 120.6 | C31—C30—C29 | 123.5 (3) |
| C7—C8—H8A | 120.6 | C32—C31—C30 | 119.6 (3) |
| C8—C9—C10 | 122.6 (6) | C32—C31—H31A | 120.2 |
| C8—C9—H9A | 118.7 | C30—C31—H31A | 120.2 |
| C10—C9—H9A | 118.7 | C31—C32—C33 | 120.4 (4) |
| C9—C10—C11 | 120.1 (6) | C31—C32—H32A | 119.8 |
| C9—C10—H10A | 120.0 | C33—C32—H32A | 119.8 |
| C11—C10—H10A | 120.0 | C32—C33—C34 | 116.8 (3) |
| C10—C11—C12 | 121.7 (5) | C32—C33—C36 | 121.9 (4) |
| C10—C11—H11A | 119.1 | C34—C33—C36 | 121.3 (4) |
| C12—C11—H11A | 119.1 | N2—C34—C33 | 123.8 (3) |
| C11—C12—C7 | 116.9 (5) | N2—C34—H34A | 118.1 |
| C11—C12—C3 | 122.5 (4) | C33—C34—H34A | 118.1 |
| C7—C12—C3 | 120.6 (4) | C26—C35—H35A | 109.5 |
| O4—C13—O3 | 121.4 (4) | C26—C35—H35B | 109.5 |
| O4—C13—C14 | 119.6 (4) | H35A—C35—H35B | 109.5 |
| O3—C13—C14 | 119.1 (4) | C26—C35—H35C | 109.5 |
| C15—C14—C13 | 112.3 (3) | H35A—C35—H35C | 109.5 |
| C15—C14—H14A | 109.1 | H35B—C35—H35C | 109.5 |
| C13—C14—H14A | 109.1 | C33—C36—H36A | 109.5 |
| C15—C14—H14B | 109.1 | C33—C36—H36B | 109.5 |
| C13—C14—H14B | 109.1 | H36A—C36—H36B | 109.5 |
| H14A—C14—H14B | 107.9 | C33—C36—H36C | 109.5 |
| C16—C15—C24 | 118.7 (4) | H36A—C36—H36C | 109.5 |
| C16—C15—C14 | 118.7 (4) | H36B—C36—H36C | 109.5 |
| C24—C15—C14 | 122.6 (4) | | |

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|---|---|---|---|
| O3—Zn1—O1—C1 | 69.3 (3) | Zn1—O3—C13—O4 | −7.8 (4) |
| N2—Zn1—O1—C1 | −62.5 (3) | Zn1—O3—C13—C14 | 171.6 (3) |
| N1—Zn1—O1—C1 | −147.6 (2) | O4—C13—C14—C15 | −81.9 (5) |
| O4—Zn1—O1—C1 | 124.0 (2) | O3—C13—C14—C15 | 98.7 (4) |
| O1—Zn1—O3—C13 | 77.4 (2) | C13—C14—C15—C16 | 91.5 (4) |

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|---|---|---|---|
| N2—Zn1—O3—C13 | −143.8 (2) | C13—C14—C15—C24 | −90.0 (5) |
| N1—Zn1—O3—C13 | −59.2 (3) | C24—C15—C16—C17 | 0.3 (5) |
| O4—Zn1—O3—C13 | 4.0 (2) | C14—C15—C16—C17 | 178.8 (3) |
| O1—Zn1—O4—C13 | −128.9 (2) | C15—C16—C17—C18 | 0.5 (6) |
| O3—Zn1—O4—C13 | −4.1 (2) | C16—C17—C18—C19 | −0.7 (6) |
| N2—Zn1—O4—C13 | 60.8 (3) | C17—C18—C19—C20 | −178.7 (4) |
| N1—Zn1—O4—C13 | 126.8 (2) | C17—C18—C19—C24 | 0.2 (6) |
| O1—Zn1—N1—C29 | 119.4 (2) | C18—C19—C20—C21 | 178.4 (4) |
| O3—Zn1—N1—C29 | −97.9 (2) | C24—C19—C20—C21 | −0.5 (6) |
| N2—Zn1—N1—C29 | 0.5 (2) | C19—C20—C21—C22 | −1.2 (8) |
| O4—Zn1—N1—C29 | −147.2 (2) | C20—C21—C22—C23 | 2.7 (8) |
| O1—Zn1—N1—C25 | −59.6 (3) | C21—C22—C23—C24 | −2.4 (7) |
| O3—Zn1—N1—C25 | 83.1 (3) | C22—C23—C24—C15 | −178.1 (3) |
| N2—Zn1—N1—C25 | −178.5 (3) | C22—C23—C24—C19 | 0.7 (5) |
| O4—Zn1—N1—C25 | 33.8 (3) | C16—C15—C24—C23 | 177.9 (3) |
| O1—Zn1—N2—C34 | 83.3 (3) | C14—C15—C24—C23 | −0.5 (5) |
| O3—Zn1—N2—C34 | −55.9 (3) | C16—C15—C24—C19 | −0.8 (4) |
| N1—Zn1—N2—C34 | −176.6 (3) | C14—C15—C24—C19 | −179.3 (3) |
| O4—Zn1—N2—C34 | −108.0 (3) | C20—C19—C24—C23 | 0.8 (5) |
| O1—Zn1—N2—C30 | −103.9 (2) | C18—C19—C24—C23 | −178.2 (3) |
| O3—Zn1—N2—C30 | 116.9 (2) | C20—C19—C24—C15 | 179.5 (3) |
| N1—Zn1—N2—C30 | −3.7 (2) | C18—C19—C24—C15 | 0.6 (5) |
| O4—Zn1—N2—C30 | 64.9 (3) | C29—N1—C25—C26 | −0.7 (5) |
| Zn1—O1—C1—O2 | 1.7 (4) | Zn1—N1—C25—C26 | 178.3 (2) |
| Zn1—O1—C1—C2 | −176.5 (3) | N1—C25—C26—C27 | −0.8 (5) |
| O2—C1—C2—C3 | 12.7 (6) | N1—C25—C26—C35 | 179.0 (3) |
| O1—C1—C2—C3 | −169.0 (3) | C25—C26—C27—C28 | 1.4 (5) |
| C1—C2—C3—C4 | −110.8 (4) | C35—C26—C27—C28 | −178.5 (3) |
| C1—C2—C3—C12 | 69.5 (5) | C26—C27—C28—C29 | −0.5 (5) |
| C12—C3—C4—C5 | 0.6 (6) | C25—N1—C29—C28 | 1.7 (4) |
| C2—C3—C4—C5 | −179.2 (4) | Zn1—N1—C29—C28 | −177.4 (2) |
| C3—C4—C5—C6 | −0.4 (7) | C25—N1—C29—C30 | −178.4 (3) |
| C4—C5—C6—C7 | −0.3 (8) | Zn1—N1—C29—C30 | 2.5 (3) |
| C5—C6—C7—C8 | −178.9 (5) | C27—C28—C29—N1 | −1.1 (5) |
| C5—C6—C7—C12 | 0.7 (8) | C27—C28—C29—C30 | 179.0 (3) |
| C6—C7—C8—C9 | 178.6 (5) | C34—N2—C30—C31 | 0.1 (4) |
| C12—C7—C8—C9 | −1.0 (7) | Zn1—N2—C30—C31 | −173.3 (2) |
| C7—C8—C9—C10 | 1.7 (8) | C34—N2—C30—C29 | 179.5 (3) |
| C8—C9—C10—C11 | −0.8 (8) | Zn1—N2—C30—C29 | 6.1 (3) |
| C9—C10—C11—C12 | −0.7 (7) | N1—C29—C30—N2 | −5.7 (4) |
| C10—C11—C12—C7 | 1.3 (6) | C28—C29—C30—N2 | 174.1 (3) |
| C10—C11—C12—C3 | −178.2 (4) | N1—C29—C30—C31 | 173.7 (3) |
| C6—C7—C12—C11 | 180.0 (4) | C28—C29—C30—C31 | −6.5 (5) |
| C8—C7—C12—C11 | −0.4 (6) | N2—C30—C31—C32 | 0.3 (5) |
| C6—C7—C12—C3 | −0.5 (6) | C29—C30—C31—C32 | −179.1 (3) |
| C8—C7—C12—C3 | 179.1 (4) | C30—C31—C32—C33 | 0.0 (5) |
| C4—C3—C12—C11 | 179.4 (4) | C31—C32—C33—C34 | −0.7 (5) |
| C2—C3—C12—C11 | −0.9 (5) | C31—C32—C33—C36 | 178.4 (4) |

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|---|---|---|---|
| C4—C3—C12—C7 | −0.1 (6) | C30—N2—C34—C33 | −0.8 (5) |
| C2—C3—C12—C7 | 179.6 (3) | Zn1—N2—C34—C33 | 171.8 (3) |
| Zn1—O4—C13—O3 | 6.5 (3) | C32—C33—C34—N2 | 1.1 (5) |
| Zn1—O4—C13—C14 | −172.9 (3) | C36—C33—C34—N2 | −177.9 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5···O1 | 0.82 | 2.21 | 2.948 (3) | 150 |
| C8—H8*A*···O4$^{i}$ | 0.93 | 2.59 | 3.515 (6) | 171 |

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