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# Bis(μ-2,2′-oxydibenzoato-κ⁴O,O′:O″,O‴)bis[(4,4′-dimethyl-2,2′-bipyridine-κ²N,N′)zinc(II)] dihydrate

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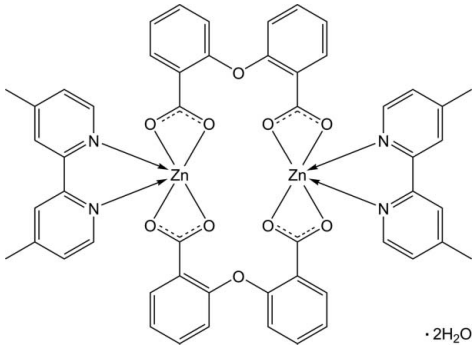
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean σ(C–C) = 0.007 Å; $R$ factor = 0.058; $wR$ factor = 0.124; data-to-parameter ratio = 14.1.

In the title compound, $[Zn_2(C_{14}H_8O_5)_2(C_{12}H_{12}N_2)_2]\cdot 2H_2O$, the $Zn^{II}$ atom exhibits a distorted octahedral coordination geometry, defined by two N atoms from one 4,4′-dimethyl-2,2′-bipyridine ligand and four O atoms from two bridging 2,2′-oxydibenzoate ligands. The molecule is a centrosymmetric dimer. π–π Stacking interactions are observed between the 4,4′-dimethyl-2,2′-bipyridine ligands, with a centroid–centroid distance of 3.649 (2) Å.

## Related literature

For related literature, see: Allen *et al.* (1987); Zhang *et al.* (2008).




## Experimental

### Crystal data

$[Zn_2(C_{14}H_8O_5)_2(C_{12}H_{12}N_2)_2]\cdot 2H_2O$
$M_r$ = 1047.65
Triclinic, $P\overline{1}$
$a$ = 10.425 (2) Å
$b$ = 10.866 (2) Å
$c$ = 11.960 (2) Å
α = 68.413 (4)°
β = 66.721 (3)°
γ = 78.348 (4)°
$V$ = 1154.7 (4) Å³
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 1.11 mm$^{-1}$
$T$ = 293 (2) K
0.20 × 0.16 × 0.15 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.808, $T_{max}$ = 0.851
6797 measured reflections
4484 independent reflections
3788 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.123
$S$ = 1.16
4484 reflections
318 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—O2 | 2.006 (3) | Zn1—N1 | 2.086 (3) |
| Zn1—O4$^{i}$ | 2.053 (4) | Zn1—O5$^{i}$ | 2.295 (5) |
| Zn1—N2 | 2.059 (3) | Zn1—O3 | 2.495 (4) |
| | | | |
| O2—Zn1—O4$^{i}$ | 100.39 (14) | N2—Zn1—O5$^{i}$ | 108.05 (15) |
| O2—Zn1—N2 | 100.84 (13) | N1—Zn1—O5$^{i}$ | 98.21 (12) |
| O4$^{i}$—Zn1—N2 | 96.86 (14) | O2—Zn1—O3 | 56.84 (11) |
| O2—Zn1—N1 | 106.07 (12) | O4$^{i}$—Zn1—O3 | 99.09 (14) |
| O4$^{i}$—Zn1—N1 | 153.52 (14) | N2—Zn1—O3 | 154.58 (12) |
| N2—Zn1—N1 | 79.25 (11) | N1—Zn1—O3 | 94.60 (12) |
| O2—Zn1—O5$^{i}$ | 145.16 (14) | O5$^{i}$—Zn1—O3 | 97.20 (14) |
| O4$^{i}$—Zn1—O5$^{i}$ | 57.76 (14) | | |

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$WA$···O3 | 0.85 | 2.04 | 2.845 (5) | 158 |
| O1$W$—H1$WB$···O5$^{i}$ | 0.85 | 2.07 | 2.876 (6) | 158 |

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

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2127).

## References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, W., Yao, L. & Tao, R. (2008). *Acta Cryst.* E**64**, m169.

# supporting information

*Acta Cryst.* (2008). E**64**, m697 [doi:10.1107/S1600536808010271]

# Bis(*μ*-2,2′-oxydibenzoato-$\kappa^4O,O':O'',O'''$)bis[(4,4′-dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)zinc(II)] dihydrate

**Hong Cui, Wen-Juan Li and Ruo-Jie Tao**

## S1. Comment

As part of our ongoing studies (Zhang *et al.*, 2008), we synthesized the title compound and report here its crystal structure.

The bond lengths and angles of the title compound are within normal ranges (Allen *et al.*, 1987) (Table 1). Intermolecular hydrogen bonds are formed between the water molecule and the carboxylate groups (Fig. 1; Table 2). The molecule is centrosymmetric with an inversion center located at the midpoint of the Zn1 and Zn1$^{i}$ atoms [symmetry code (i): 1 - *x*, 2 - *y*, 1 - *z*]. The asymmetric unit thus contains one-half molecule. The Zn$^{II}$ atom exhibits a distorted octahedral coordination geometry, defined by two N atoms from one 4,4′-dimethyl-2,2′-bipyridine (dbpy) ligand and four O atoms from two 2,2′-oxydibenzoate (odb) ligands. The two carboxylate groups of each odb ligand coordinate to two different Zn atoms.

The *π*–*π* stacking interactions between the aromatic rings of the dbpy ligands are observed, with a centroid–centroid distance of 3.649 (2)Å [Fig. 2; *Cg*1 = the centroid of N1$^{ii}$, C15$^{ii}$, C16$^{ii}$, C17$^{ii}$, C19$^{ii}$, C20$^{ii}$ and *Cg*2 = the centroid of N2, C21, C22, C23, C25, C26; symmetry code: (ii) 2 - *x*, 2 - *y*, 1 - *z*].

## S2. Experimental

The title compound was synthesized hydrothermally in a Teflon-lined autoclave (23 ml) by heating a mixture of $H_2$odb (0.052 g, 0.2 mmol), dbpy (0.037 g, 0.2 mmol), $Zn(NO_3)_2.6H_2O$ (0.059 g, 0.2 mmol) and one drop of $Et_3N$ (pH = 8~9) in water (10 ml) at 393 K for 3 d. Colorless single crystals were collected in 56% yield based on Zn.

## S3. Refinement

H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic) and 0.96 (methyl) Å and with $U_{iso}$(H) = 1.2(1.5 for methyl groups)$U_{eq}$(C). The H atoms of the water molecule were located from a difference Fourier map and fixed in the final refinements with $U_{iso}$(H) = 1.2$U_{eq}$(O).

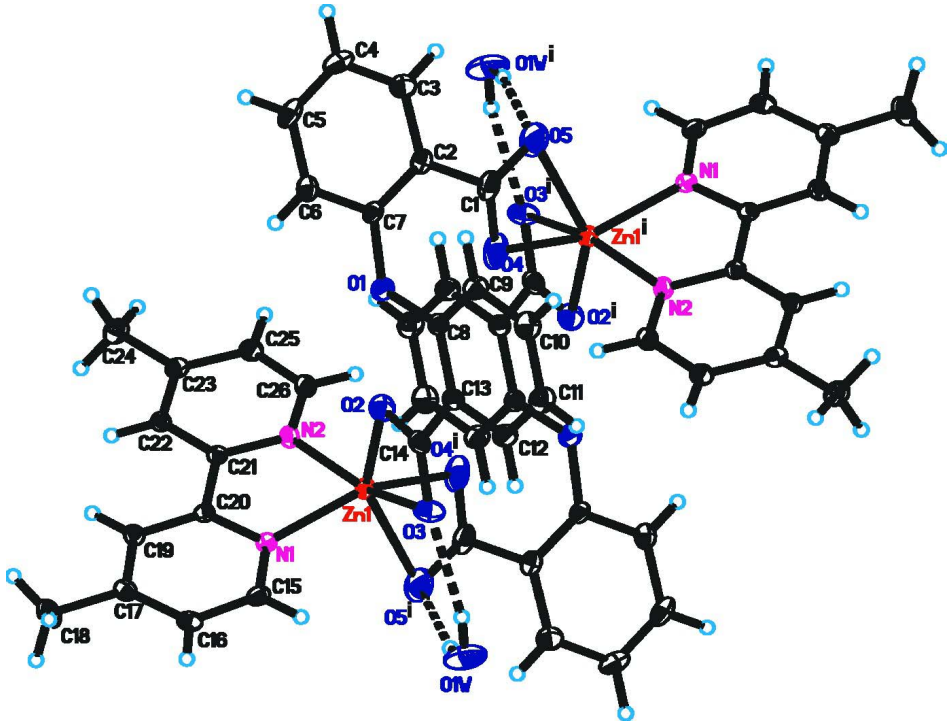


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 20% probability level. Hydrogen bonds are indicated by dashed lines. [Symmetry code (i): 1 - *x*, 2 - *y*, 1 - *z*.]

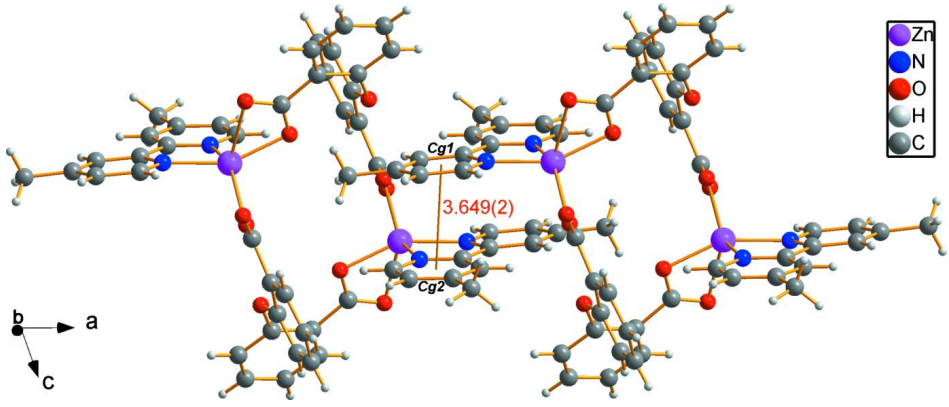


**Figure 2**

A view of the crystal packing, showing the $\pi$–$\pi$ stacking interaction.

**Bis(*μ*-2,2′-oxydibenzoato- $\kappa^4O,O':O'',O'''$)*β*is[(4,4′-dimethyl-2,2′- bipyridine-$\kappa^2N,N'$)zinc(II)] dihydrate**

*Crystal data*

$[Zn_2(C_{14}H_8O_5)_2(C_{12}H_{12}N_2)_2]\cdot 2H_2O$
$M_r$ = 1047.65
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 10.425 (2) Å
$b$ = 10.866 (2) Å
$c$ = 11.960 (2) Å
$\alpha$ = 68.413 (4)°
$\beta$ = 66.721 (3)°
$\gamma$ = 78.348 (4)°
$V$ = 1154.7 (4) Å$^3$
$Z$ = 1
$F$(000) = 540
$D_x$ = 1.507 Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2731 reflections
$\theta$ = 2.3–27.8°
$\mu$ = 1.11 mm$^{-1}$
$T$ = 293 K
Block, colorless
0.20 × 0.16 × 0.15 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.809, $T_{max}$ = 0.851
6797 measured reflections
4484 independent reflections
3788 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.0°
$h$ = −12→12
$k$ = −13→13
$l$ = −10→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.123
$S$ = 1.16
4484 reflections
318 parameters
0 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 1.1151P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.79 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 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.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.69886 (4) | 0.81936 (4) | 0.62615 (4) | 0.02963 (15) |
| N1 | 0.8962 (3) | 0.7397 (3) | 0.6331 (3) | 0.0290 (7) |
| N2 | 0.7562 (3) | 0.9615 (3) | 0.6702 (3) | 0.0294 (7) |
| O1 | 0.7872 (3) | 1.0671 (3) | 0.1966 (3) | 0.0402 (7) |
| O2 | 0.7264 (3) | 0.9119 (3) | 0.4398 (3) | 0.0476 (7) |
| O3 | 0.7021 (4) | 0.7032 (3) | 0.4797 (3) | 0.0653 (10) |
| O4 | 0.5135 (3) | 1.1471 (4) | 0.2926 (4) | 0.0723 (11) |
| O5 | 0.4336 (4) | 1.3253 (4) | 0.1854 (5) | 0.0931 (15) |
| O1W | 0.6185 (5) | 0.4727 (3) | 0.6971 (4) | 0.0904 (14) |
| H1WA | 0.6406 | 0.5286 | 0.6219 | 0.109* |
| H1WB | 0.6035 | 0.5144 | 0.7494 | 0.109* |
| C1 | 0.5330 (5) | 1.2495 (5) | 0.1998 (6) | 0.0507 (12) |
| C2 | 0.6804 (4) | 1.2853 (4) | 0.1109 (4) | 0.0366 (9) |
| C3 | 0.7046 (5) | 1.4153 (4) | 0.0292 (5) | 0.0474 (11) |
| H3 | 0.6285 | 1.4758 | 0.0235 | 0.057* |

| | | | | |
|---|---|---|---|---|
| C4 | 0.8373 (5) | 1.4565 (4) | −0.0429 (5) | 0.0522 (12) |
| H4 | 0.8506 | 1.5438 | −0.0965 | 0.063* |
| C5 | 0.9501 (5) | 1.3685 (5) | −0.0355 (4) | 0.0497 (12) |
| H5 | 1.0402 | 1.3968 | −0.0825 | 0.060* |
| C6 | 0.9309 (4) | 1.2378 (4) | 0.0413 (4) | 0.0400 (10) |
| H6 | 1.0078 | 1.1776 | 0.0441 | 0.048* |
| C7 | 0.7965 (4) | 1.1970 (4) | 0.1141 (4) | 0.0305 (8) |
| C8 | 0.7349 (4) | 0.9736 (3) | 0.1771 (4) | 0.0311 (8) |
| C9 | 0.7182 (4) | 0.9954 (4) | 0.0613 (4) | 0.0395 (10) |
| H9 | 0.7370 | 1.0770 | −0.0029 | 0.047* |
| C10 | 0.6740 (5) | 0.8971 (4) | 0.0415 (4) | 0.0469 (11) |
| H10 | 0.6611 | 0.9133 | −0.0354 | 0.056* |
| C11 | 0.6487 (5) | 0.7745 (4) | 0.1344 (5) | 0.0485 (11) |
| H11 | 0.6212 | 0.7071 | 0.1200 | 0.058* |
| C12 | 0.6650 (4) | 0.7535 (4) | 0.2488 (5) | 0.0432 (10) |
| H12 | 0.6476 | 0.6707 | 0.3113 | 0.052* |
| C13 | 0.7062 (4) | 0.8508 (4) | 0.2750 (4) | 0.0325 (8) |
| C14 | 0.7124 (4) | 0.8198 (4) | 0.4060 (4) | 0.0401 (10) |
| C15 | 0.9622 (4) | 0.6263 (3) | 0.6140 (4) | 0.0360 (9) |
| H15 | 0.9129 | 0.5688 | 0.6071 | 0.043* |
| C16 | 1.0999 (4) | 0.5905 (4) | 0.6042 (4) | 0.0375 (9) |
| H16 | 1.1412 | 0.5100 | 0.5917 | 0.045* |
| C17 | 1.1763 (4) | 0.6746 (4) | 0.6130 (4) | 0.0347 (9) |
| C18 | 1.3281 (5) | 0.6431 (5) | 0.5984 (6) | 0.0558 (13) |
| H18A | 1.3359 | 0.5799 | 0.6768 | 0.084* |
| H18B | 1.3699 | 0.7228 | 0.5796 | 0.084* |
| H18C | 1.3756 | 0.6065 | 0.5295 | 0.084* |
| C19 | 1.1067 (4) | 0.7924 (3) | 0.6351 (4) | 0.0311 (8) |
| H19 | 1.1540 | 0.8513 | 0.6425 | 0.037* |
| C20 | 0.9681 (4) | 0.8214 (3) | 0.6458 (3) | 0.0260 (8) |
| C21 | 0.8882 (4) | 0.9448 (3) | 0.6701 (3) | 0.0258 (7) |
| C22 | 0.9417 (4) | 1.0362 (3) | 0.6920 (3) | 0.0285 (8) |
| H22 | 1.0326 | 1.0222 | 0.6923 | 0.034* |
| C23 | 0.8611 (4) | 1.1487 (3) | 0.7136 (4) | 0.0329 (9) |
| C24 | 0.9184 (5) | 1.2489 (4) | 0.7370 (5) | 0.0450 (11) |
| H24A | 0.9678 | 1.2041 | 0.7953 | 0.068* |
| H24B | 0.8428 | 1.3055 | 0.7737 | 0.068* |
| H24C | 0.9812 | 1.3013 | 0.6572 | 0.068* |
| C25 | 0.7257 (4) | 1.1644 (4) | 0.7143 (4) | 0.0368 (9) |
| H25 | 0.6680 | 1.2384 | 0.7288 | 0.044* |
| C26 | 0.6775 (4) | 1.0689 (4) | 0.6931 (4) | 0.0371 (9) |
| H26 | 0.5860 | 1.0798 | 0.6949 | 0.045* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0253 (2) | 0.0322 (2) | 0.0321 (3) | −0.00478 (16) | −0.00982 (19) | −0.01000 (19) |
| N1 | 0.0305 (17) | 0.0258 (15) | 0.0303 (17) | −0.0043 (12) | −0.0116 (15) | −0.0061 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.0243 (16) | 0.0322 (15) | 0.0351 (18) | −0.0003 (12) | −0.0112 (14) | −0.0144 (14) |
| O1 | 0.0490 (18) | 0.0403 (15) | 0.0358 (16) | −0.0131 (13) | −0.0210 (14) | −0.0053 (13) |
| O2 | 0.0485 (19) | 0.0604 (19) | 0.0336 (16) | −0.0092 (15) | −0.0156 (15) | −0.0106 (15) |
| O3 | 0.076 (2) | 0.0526 (19) | 0.053 (2) | −0.0105 (17) | −0.033 (2) | 0.0133 (17) |
| O4 | 0.040 (2) | 0.113 (3) | 0.051 (2) | −0.034 (2) | −0.0021 (17) | −0.013 (2) |
| O5 | 0.040 (2) | 0.069 (2) | 0.155 (5) | 0.0009 (18) | −0.023 (3) | −0.034 (3) |
| O1W | 0.115 (4) | 0.0360 (18) | 0.091 (3) | 0.000 (2) | −0.016 (3) | −0.014 (2) |
| C1 | 0.033 (3) | 0.051 (3) | 0.078 (4) | −0.005 (2) | −0.013 (3) | −0.038 (3) |
| C2 | 0.031 (2) | 0.042 (2) | 0.039 (2) | −0.0068 (17) | −0.0070 (19) | −0.0184 (19) |
| C3 | 0.051 (3) | 0.038 (2) | 0.053 (3) | −0.0012 (19) | −0.019 (2) | −0.015 (2) |
| C4 | 0.073 (4) | 0.037 (2) | 0.042 (3) | −0.021 (2) | −0.014 (3) | −0.006 (2) |
| C5 | 0.048 (3) | 0.061 (3) | 0.038 (2) | −0.032 (2) | −0.001 (2) | −0.015 (2) |
| C6 | 0.030 (2) | 0.051 (2) | 0.039 (2) | −0.0054 (18) | −0.0098 (19) | −0.016 (2) |
| C7 | 0.034 (2) | 0.0351 (19) | 0.0239 (19) | −0.0122 (16) | −0.0099 (17) | −0.0072 (16) |
| C8 | 0.0245 (19) | 0.0331 (19) | 0.035 (2) | −0.0020 (15) | −0.0083 (17) | −0.0120 (17) |
| C9 | 0.047 (3) | 0.042 (2) | 0.027 (2) | −0.0101 (19) | −0.012 (2) | −0.0077 (18) |
| C10 | 0.052 (3) | 0.057 (3) | 0.041 (3) | −0.004 (2) | −0.017 (2) | −0.025 (2) |
| C11 | 0.051 (3) | 0.042 (2) | 0.060 (3) | −0.003 (2) | −0.019 (2) | −0.026 (2) |
| C12 | 0.035 (2) | 0.034 (2) | 0.053 (3) | 0.0008 (17) | −0.011 (2) | −0.012 (2) |
| C13 | 0.027 (2) | 0.0325 (19) | 0.034 (2) | 0.0011 (15) | −0.0090 (18) | −0.0096 (17) |
| C14 | 0.024 (2) | 0.050 (2) | 0.034 (2) | −0.0015 (17) | −0.0089 (18) | −0.002 (2) |
| C15 | 0.043 (2) | 0.0257 (18) | 0.040 (2) | −0.0070 (16) | −0.015 (2) | −0.0086 (17) |
| C16 | 0.043 (2) | 0.0263 (18) | 0.042 (2) | 0.0070 (16) | −0.016 (2) | −0.0138 (18) |
| C17 | 0.033 (2) | 0.036 (2) | 0.035 (2) | 0.0031 (16) | −0.0127 (18) | −0.0122 (18) |
| C18 | 0.039 (3) | 0.055 (3) | 0.085 (4) | 0.018 (2) | −0.031 (3) | −0.036 (3) |
| C19 | 0.032 (2) | 0.0329 (19) | 0.032 (2) | 0.0001 (15) | −0.0148 (18) | −0.0115 (17) |
| C20 | 0.0282 (19) | 0.0241 (16) | 0.0236 (18) | −0.0021 (14) | −0.0077 (16) | −0.0068 (15) |
| C21 | 0.0258 (19) | 0.0260 (17) | 0.0230 (18) | −0.0020 (14) | −0.0065 (16) | −0.0071 (15) |
| C22 | 0.028 (2) | 0.0301 (18) | 0.0272 (19) | −0.0025 (15) | −0.0100 (17) | −0.0080 (16) |
| C23 | 0.039 (2) | 0.0294 (18) | 0.029 (2) | −0.0051 (16) | −0.0103 (18) | −0.0085 (17) |
| C24 | 0.052 (3) | 0.038 (2) | 0.053 (3) | −0.0059 (19) | −0.017 (2) | −0.023 (2) |
| C25 | 0.035 (2) | 0.0309 (19) | 0.044 (2) | 0.0037 (16) | −0.013 (2) | −0.0149 (19) |
| C26 | 0.027 (2) | 0.034 (2) | 0.051 (3) | 0.0043 (16) | −0.014 (2) | −0.0168 (19) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—O2 | 2.006 (3) | C8—C13 | 1.405 (5) |
| Zn1—O4$^{i}$ | 2.053 (4) | C9—C10 | 1.370 (6) |
| Zn1—N2 | 2.059 (3) | C9—H9 | 0.9300 |
| Zn1—N1 | 2.086 (3) | C10—C11 | 1.379 (6) |
| Zn1—O5$^{i}$ | 2.295 (5) | C10—H10 | 0.9300 |
| Zn1—O3 | 2.495 (4) | C11—C12 | 1.375 (6) |
| N1—C15 | 1.335 (5) | C11—H11 | 0.9300 |
| N1—C20 | 1.353 (4) | C12—C13 | 1.391 (5) |
| N2—C26 | 1.335 (5) | C12—H12 | 0.9300 |
| N2—C21 | 1.350 (4) | C13—C14 | 1.501 (6) |
| O1—C8 | 1.372 (4) | C15—C16 | 1.378 (5) |
| O1—C7 | 1.389 (4) | C15—H15 | 0.9300 |

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| O2—C14 | 1.261 (5) | C16—C17 | 1.383 (5) |
| O3—C14 | 1.246 (5) | C16—H16 | 0.9300 |
| O4—C1 | 1.231 (6) | C17—C19 | 1.399 (5) |
| O4—Zn1$^{i}$ | 2.053 (4) | C17—C18 | 1.503 (5) |
| O5—C1 | 1.214 (5) | C18—H18A | 0.9600 |
| O5—Zn1$^{i}$ | 2.295 (5) | C18—H18B | 0.9600 |
| O1W—H1WA | 0.8500 | C18—H18C | 0.9600 |
| O1W—H1WB | 0.8500 | C19—C20 | 1.380 (5) |
| C1—C2 | 1.512 (6) | C19—H19 | 0.9300 |
| C1—Zn1$^{i}$ | 2.519 (5) | C20—C21 | 1.489 (5) |
| C2—C7 | 1.389 (5) | C21—C22 | 1.378 (5) |
| C2—C3 | 1.395 (6) | C22—C23 | 1.383 (5) |
| C3—C4 | 1.372 (6) | C22—H22 | 0.9300 |
| C3—H3 | 0.9300 | C23—C25 | 1.385 (5) |
| C4—C5 | 1.367 (7) | C23—C24 | 1.497 (5) |
| C4—H4 | 0.9300 | C24—H24A | 0.9600 |
| C5—C6 | 1.382 (6) | C24—H24B | 0.9600 |
| C5—H5 | 0.9300 | C24—H24C | 0.9600 |
| C6—C7 | 1.386 (5) | C25—C26 | 1.377 (5) |
| C6—H6 | 0.9300 | C25—H25 | 0.9300 |
| C8—C9 | 1.392 (5) | C26—H26 | 0.9300 |

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| O2—Zn1—O4$^{i}$ | 100.39 (14) | C10—C9—C8 | 120.3 (4) |
| O2—Zn1—N2 | 100.84 (13) | C10—C9—H9 | 119.8 |
| O4$^{i}$—Zn1—N2 | 96.86 (14) | C8—C9—H9 | 119.8 |
| O2—Zn1—N1 | 106.07 (12) | C9—C10—C11 | 120.7 (4) |
| O4$^{i}$—Zn1—N1 | 153.52 (14) | C9—C10—H10 | 119.7 |
| N2—Zn1—N1 | 79.25 (11) | C11—C10—H10 | 119.7 |
| O2—Zn1—O5$^{i}$ | 145.16 (14) | C12—C11—C10 | 118.8 (4) |
| O4$^{i}$—Zn1—O5$^{i}$ | 57.76 (14) | C12—C11—H11 | 120.6 |
| N2—Zn1—O5$^{i}$ | 108.05 (15) | C10—C11—H11 | 120.6 |
| N1—Zn1—O5$^{i}$ | 98.21 (12) | C11—C12—C13 | 122.8 (4) |
| O2—Zn1—O3 | 56.84 (11) | C11—C12—H12 | 118.6 |
| O4$^{i}$—Zn1—O3 | 99.09 (14) | C13—C12—H12 | 118.6 |
| N2—Zn1—O3 | 154.58 (12) | C12—C13—C8 | 117.0 (4) |
| N1—Zn1—O3 | 94.60 (12) | C12—C13—C14 | 118.4 (4) |
| O5$^{i}$—Zn1—O3 | 97.20 (14) | C8—C13—C14 | 124.6 (4) |
| O2—Zn1—C1$^{i}$ | 124.65 (15) | O3—C14—O2 | 121.3 (4) |
| O4$^{i}$—Zn1—C1$^{i}$ | 29.03 (14) | O3—C14—C13 | 119.1 (4) |
| N2—Zn1—C1$^{i}$ | 104.76 (13) | O2—C14—C13 | 119.6 (3) |
| N1—Zn1—C1$^{i}$ | 126.34 (15) | N1—C15—C16 | 123.2 (3) |
| O5$^{i}$—Zn1—C1$^{i}$ | 28.74 (14) | N1—C15—H15 | 118.4 |
| O3—Zn1—C1$^{i}$ | 98.76 (13) | C16—C15—H15 | 118.4 |
| C15—N1—C20 | 117.9 (3) | C15—C16—C17 | 119.7 (3) |
| C15—N1—Zn1 | 127.7 (2) | C15—C16—H16 | 120.1 |
| C20—N1—Zn1 | 114.0 (2) | C17—C16—H16 | 120.1 |
| C26—N2—C21 | 118.4 (3) | C16—C17—C19 | 117.2 (3) |
| C26—N2—Zn1 | 126.0 (2) | C16—C17—C18 | 122.2 (4) |

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| C21—N2—Zn1 | 115.5 (2) | C19—C17—C18 | 120.7 (4) |
| C8—O1—C7 | 121.0 (3) | C17—C18—H18A | 109.5 |
| C14—O2—Zn1 | 101.8 (3) | C17—C18—H18B | 109.5 |
| C14—O3—Zn1 | 79.6 (3) | H18A—C18—H18B | 109.5 |
| C1—O4—Zn1$^{i}$ | 97.0 (3) | C17—C18—H18C | 109.5 |
| C1—O5—Zn1$^{i}$ | 85.9 (4) | H18A—C18—H18C | 109.5 |
| H1WA—O1W—H1WB | 107.7 | H18B—C18—H18C | 109.5 |
| O5—C1—O4 | 119.3 (5) | C20—C19—C17 | 120.1 (3) |
| O5—C1—C2 | 120.5 (5) | C20—C19—H19 | 119.9 |
| O4—C1—C2 | 120.1 (4) | C17—C19—H19 | 119.9 |
| O5—C1—Zn1$^{i}$ | 65.3 (3) | N1—C20—C19 | 121.8 (3) |
| O4—C1—Zn1$^{i}$ | 54.0 (3) | N1—C20—C21 | 115.6 (3) |
| C2—C1—Zn1$^{i}$ | 171.7 (4) | C19—C20—C21 | 122.7 (3) |
| C7—C2—C3 | 117.3 (4) | N2—C21—C22 | 121.3 (3) |
| C7—C2—C1 | 122.8 (4) | N2—C21—C20 | 115.0 (3) |
| C3—C2—C1 | 119.6 (4) | C22—C21—C20 | 123.7 (3) |
| C4—C3—C2 | 122.0 (4) | C21—C22—C23 | 120.4 (3) |
| C4—C3—H3 | 119.0 | C21—C22—H22 | 119.8 |
| C2—C3—H3 | 119.0 | C23—C22—H22 | 119.8 |
| C5—C4—C3 | 119.6 (4) | C22—C23—C25 | 117.8 (3) |
| C5—C4—H4 | 120.2 | C22—C23—C24 | 120.9 (3) |
| C3—C4—H4 | 120.2 | C25—C23—C24 | 121.4 (4) |
| C4—C5—C6 | 120.4 (4) | C23—C24—H24A | 109.5 |
| C4—C5—H5 | 119.8 | C23—C24—H24B | 109.5 |
| C6—C5—H5 | 119.8 | H24A—C24—H24B | 109.5 |
| C5—C6—C7 | 119.6 (4) | C23—C24—H24C | 109.5 |
| C5—C6—H6 | 120.2 | H24A—C24—H24C | 109.5 |
| C7—C6—H6 | 120.2 | H24B—C24—H24C | 109.5 |
| C6—C7—O1 | 115.8 (3) | C26—C25—C23 | 119.2 (4) |
| C6—C7—C2 | 121.0 (4) | C26—C25—H25 | 120.4 |
| O1—C7—C2 | 123.0 (3) | C23—C25—H25 | 120.4 |
| O1—C8—C9 | 121.5 (3) | N2—C26—C25 | 122.9 (3) |
| O1—C8—C13 | 118.0 (3) | N2—C26—H26 | 118.5 |
| C9—C8—C13 | 120.3 (3) | C25—C26—H26 | 118.5 |

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| O2—Zn1—N1—C15 | −82.0 (3) | C1—C2—C7—C6 | −172.7 (4) |
| O4$^{i}$—Zn1—N1—C15 | 95.9 (4) | C3—C2—C7—O1 | 176.2 (3) |
| N2—Zn1—N1—C15 | 179.7 (3) | C1—C2—C7—O1 | 1.9 (6) |
| O5$^{i}$—Zn1—N1—C15 | 72.7 (3) | C7—O1—C8—C9 | 14.3 (6) |
| O3—Zn1—N1—C15 | −25.3 (3) | C7—O1—C8—C13 | −169.4 (3) |
| C1$^{i}$—Zn1—N1—C15 | 79.1 (4) | O1—C8—C9—C10 | 175.9 (4) |
| O2—Zn1—N1—C20 | 90.9 (3) | C13—C8—C9—C10 | −0.3 (6) |
| O4$^{i}$—Zn1—N1—C20 | −91.2 (4) | C8—C9—C10—C11 | −1.5 (7) |
| N2—Zn1—N1—C20 | −7.4 (2) | C9—C10—C11—C12 | 1.7 (7) |
| O5$^{i}$—Zn1—N1—C20 | −114.4 (3) | C10—C11—C12—C13 | −0.1 (7) |
| O3—Zn1—N1—C20 | 147.7 (3) | C11—C12—C13—C8 | −1.6 (6) |
| C1$^{i}$—Zn1—N1—C20 | −107.9 (3) | C11—C12—C13—C14 | 176.4 (4) |
| O2—Zn1—N2—C26 | 78.6 (3) | O1—C8—C13—C12 | −174.5 (3) |

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| O4$^{i}$—Zn1—N2—C26 | −23.5 (4) | C9—C8—C13—C12 | 1.8 (6) |
| N1—Zn1—N2—C26 | −176.9 (3) | O1—C8—C13—C14 | 7.6 (6) |
| O5$^{i}$—Zn1—N2—C26 | −81.7 (3) | C9—C8—C13—C14 | −176.1 (4) |
| O3—Zn1—N2—C26 | 105.1 (4) | Zn1—O3—C14—O2 | 6.0 (4) |
| C1$^{i}$—Zn1—N2—C26 | −51.9 (4) | Zn1—O3—C14—C13 | −173.3 (3) |
| O2—Zn1—N2—C21 | −98.6 (3) | Zn1—O2—C14—O3 | −7.5 (5) |
| O4$^{i}$—Zn1—N2—C21 | 159.4 (3) | Zn1—O2—C14—C13 | 171.8 (3) |
| N1—Zn1—N2—C21 | 5.9 (3) | C12—C13—C14—O3 | 11.0 (6) |
| O5$^{i}$—Zn1—N2—C21 | 101.1 (3) | C8—C13—C14—O3 | −171.1 (4) |
| O3—Zn1—N2—C21 | −72.0 (4) | C12—C13—C14—O2 | −168.3 (4) |
| C1$^{i}$—Zn1—N2—C21 | 130.9 (3) | C8—C13—C14—O2 | 9.6 (6) |
| O4$^{i}$—Zn1—O2—C14 | −90.3 (3) | C20—N1—C15—C16 | −1.4 (6) |
| N2—Zn1—O2—C14 | 170.5 (2) | Zn1—N1—C15—C16 | 171.3 (3) |
| N1—Zn1—O2—C14 | 88.7 (3) | N1—C15—C16—C17 | −0.6 (6) |
| O5$^{i}$—Zn1—O2—C14 | −43.6 (4) | C15—C16—C17—C19 | 1.6 (6) |
| O3—Zn1—O2—C14 | 3.8 (2) | C15—C16—C17—C18 | −177.8 (4) |
| C1$^{i}$—Zn1—O2—C14 | −72.9 (3) | C16—C17—C19—C20 | −0.7 (6) |
| O2—Zn1—O3—C14 | −3.8 (2) | C18—C17—C19—C20 | 178.8 (4) |
| O4$^{i}$—Zn1—O3—C14 | 92.7 (3) | C15—N1—C20—C19 | 2.4 (5) |
| N2—Zn1—O3—C14 | −35.5 (4) | Zn1—N1—C20—C19 | −171.3 (3) |
| N1—Zn1—O3—C14 | −110.0 (2) | C15—N1—C20—C21 | −178.6 (3) |
| O5$^{i}$—Zn1—O3—C14 | 151.1 (2) | Zn1—N1—C20—C21 | 7.8 (4) |
| C1$^{i}$—Zn1—O3—C14 | 122.1 (3) | C17—C19—C20—N1 | −1.4 (6) |
| Zn1$^{i}$—O5—C1—O4 | 1.9 (5) | C17—C19—C20—C21 | 179.6 (3) |
| Zn1$^{i}$—O5—C1—C2 | −173.3 (4) | C26—N2—C21—C22 | −0.5 (5) |
| Zn1$^{i}$—O4—C1—O5 | −2.1 (5) | Zn1—N2—C21—C22 | 176.9 (3) |
| Zn1$^{i}$—O4—C1—C2 | 173.1 (3) | C26—N2—C21—C20 | 179.0 (3) |
| O5—C1—C2—C7 | −172.9 (5) | Zn1—N2—C21—C20 | −3.6 (4) |
| O4—C1—C2—C7 | 12.0 (7) | N1—C20—C21—N2 | −2.9 (5) |
| O5—C1—C2—C3 | 12.9 (7) | C19—C20—C21—N2 | 176.2 (3) |
| O4—C1—C2—C3 | −162.2 (4) | N1—C20—C21—C22 | 176.6 (3) |
| C7—C2—C3—C4 | −1.7 (7) | C19—C20—C21—C22 | −4.3 (6) |
| C1—C2—C3—C4 | 172.8 (4) | N2—C21—C22—C23 | −0.6 (6) |
| C2—C3—C4—C5 | 0.1 (7) | C20—C21—C22—C23 | 179.9 (3) |
| C3—C4—C5—C6 | 1.8 (7) | C21—C22—C23—C25 | 1.0 (6) |
| C4—C5—C6—C7 | −1.9 (7) | C21—C22—C23—C24 | −179.8 (4) |
| C5—C6—C7—O1 | −174.8 (4) | C22—C23—C25—C26 | −0.3 (6) |
| C5—C6—C7—C2 | 0.2 (6) | C24—C23—C25—C26 | −179.5 (4) |
| C8—O1—C7—C6 | −113.1 (4) | C21—N2—C26—C25 | 1.2 (6) |
| C8—O1—C7—C2 | 72.0 (5) | Zn1—N2—C26—C25 | −175.9 (3) |
| C3—C2—C7—C6 | 1.6 (6) | C23—C25—C26—N2 | −0.8 (6) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*WA*···O3 | 0.85 | 2.04 | 2.845 (5) | 158 |

| | | | | |
|---|---|---|---|---|
| O1*W*—H1*WB*···O5$^{i}$ | 0.85 | 2.07 | 2.876 (6) | 158 |

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