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# Diaquabis[4-(dimethylamino)benzoato-$\kappa O$]bis(nicotinamide-$\kappa N^1$)zinc(II) dihydrate

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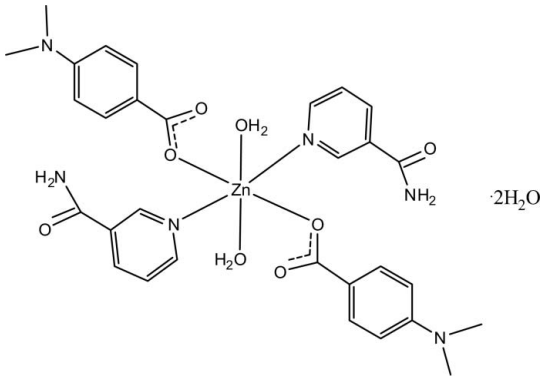
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.026; $wR$ factor = 0.068; data-to-parameter ratio = 16.6.

In the centrosymmetric title structure, $[Zn(C_9H_{10}NO_2)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$, the $Zn^{II}$ cation, located on an inversion center, is coordinated by two 4-(methylamino)benzoate anions, two nicotinamide ligands and two water molecules in a slightly distorted octahedral geometry. The dihedral angle between the carboxylate group and the attached benzene ring is 3.09 (9)°, while the pyridine and benzene rings are oriented at a dihedral angle of 77.10 (4)°. The uncoordinated water molecule is linked to nicotinamide ligands by O—H···O hydrogen bonds. In the crystal, intermolecular N—H···O, O—H···O and C—H···O hydrogen bonds link the molecules into a three-dimensional network. A weak N—H···$\pi$ interaction also occurs.

## Related literature

For niacin, see: Krishnamachari (1974). For *N*,*N*-diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (1996, 2009*a*,*b*,*c*); Hökelek & Necefoğlu (1998); Necefoğlu *et al.* (2010*a*,*b*).




## Experimental

### Crystal data

$[Zn(C_9H_{10}NO_2)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$
$M_r$ = 710.07
Triclinic, $P\overline{1}$
$a$ = 8.1810 (2) Å
$b$ = 9.9877 (2) Å
$c$ = 10.1982 (3) Å
$\alpha$ = 76.141 (2)°
$\beta$ = 88.894 (3)°
$\gamma$ = 78.200 (2)°
$V$ = 791.55 (4) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.84 mm$^{-1}$
$T$ = 100 K
0.40 × 0.24 × 0.18 mm

### Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.783, $T_{max}$ = 0.856
14586 measured reflections
3975 independent reflections
3725 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.068
$S$ = 1.05
3975 reflections
240 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Zn1—O1 | 2.0442 (9) | Zn1—N1 | 2.1963 (10) |
| Zn1—O4 | 2.1503 (11) | | |

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

*Cg*1 is the centroid of the C2–C7 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H21···O5$^{i}$ | 0.85 (2) | 2.05 (2) | 2.8826 (19) | 169.3 (2) |
| O4—H41···O2$^{ii}$ | 0.78 (2) | 2.00 (2) | 2.7370 (16) | 159 (2) |
| O4—H42···O3$^{iii}$ | 0.81 (2) | 1.96 (2) | 2.7681 (15) | 175.1 (2) |
| O5—H51···O2 | 0.85 (3) | 2.02 (3) | 2.8732 (19) | 174 (3) |
| O5—H52···O2$^{iv}$ | 0.81 (3) | 2.11 (3) | 2.9150 (18) | 173 (2) |
| C13—H13···O4$^{v}$ | 0.93 | 2.52 | 3.4422 (19) | 170 |
| N2—H22···*Cg*1$^{ii}$ | 0.829 (19) | 2.79 (2) | 3.5200 (15) | 147.9 (2) |

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

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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5088).

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# supporting information

*Acta Cryst.* (2010). E**66**, m1636–m1637 [https://doi.org/10.1107/S1600536810046854]

## Diaquabis[4-(dimethylamino)benzoato-$\kappa O$]bis(nicotinamide-$\kappa N^1$)zinc(II) dihydrate

**Tuncer Hökelek, Ertuğrul Gazi Sağlam, Barış Tercan, Özgür Aybirdi and Hacali Necefoğlu**

### S1. Comment

As a part of our ongoing investigation on transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

The title compound, (I), is a mononuclear complex, where the $Zn^{II}$ ion is located on a crystallographic inversion center. The asymmetric unit contains one 4-(methylamino)benzoate (PMAB) anion, one nicotinamide (NA) ligand, one coordinated and one uncoordinated water molecules, all ligands are monodentate (Fig. 1). The crystal structures of some NA and/or DENA complexes of $Cu^{II}$, $Co^{II}$, $Ni^{II}$, $Mn^{II}$ and $Zn^{II}$ ions, $[Cu(C_7H_5O_2)_2(C_{10}H_{14}N_2O)_2]$, (II) (Hökelek *et al.*, 1996), $[Cu_2(C_8H_7O_2)_4(C_6H_6N_2O)_2]$, (III) (Necefoğlu *et al.*, 2010*a*), $[Co(C_6H_6N_2O)_2(C_7H_4NO_4)_2(H_2O)_2]$, (IV) (Hökelek & Necefoğlu, 1998), $[Ni(C_7H_4ClO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, (V) (Hökelek *et al.*, 2009*a*), $[Ni(C_8H_7O_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, (VI) (Necefoğlu *et al.*, 2010*b*), $[Mn(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$, (VII) (Hökelek *et al.*, 2009*b*) and $[Zn(C_7H_4BrO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, (VIII) (Hökelek *et al.*, 2009*c*) have also been reported. In (II), two benzoate ions are coordinated to the Cu atom as bidentate ligands, while in other structures all ligands being monodentate.

The four O atoms (O1, O4, and the symmetry-related atoms, O1′, O4′) in the equatorial plane around the $Zn^{II}$ ion form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the NA ligands (N1, N1′) in the axial positions (Fig. 1). The near equality of the C1—O1 [1.2691 (16) Å] and C1—O2 [1.2624 (17) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds. The average Zn—O bond length is 2.0973 (10) Å (Table 1), and the $Zn^{II}$ ion is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by -0.8557 (1) Å. The dihedral angle between the planar carboxylate group and the benzene ring A (C2—C7) is 3.09 (9)°, while that between rings A and B (N1/C10—C14) is 77.10 (4)°. The uncoordinated water molecules are linked to the NA ligands by O—H···O hydrogen bonds (Table 2 and Fig. 1).

In the crystal structure, intermolecular N—H···O, O—H···O, and C—H···O hydrogen bonds (Table 2) link the molecules into a three-dimensional network, in which they may be effective in the stabilization of the structure. There also exists a weak N-H···$\pi$ interaction (Table 2).

### S2. Experimental

The title compound was prepared by the reaction of $ZnSO_4.H_2O$ (0.90 g, 5 mmol) in $H_2O$ (50 ml) and nicotinamide (1.22 g, 10 mmol) in $H_2O$ (30 ml) with sodium 4-dimethylaminobenzoate (1.88 g, 10 mmol) in $H_2O$ (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving colorless single crystals.

## S3. Refinement

Atoms H21, H22 (for $NH_2$) and H41, H42, H51, H52 (for $H_2O$) were located in a difference Fourier map and refined isotropically. The remaining H atoms were positioned geometrically with C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl H and $x = 1.2$ for aromatic H atoms.

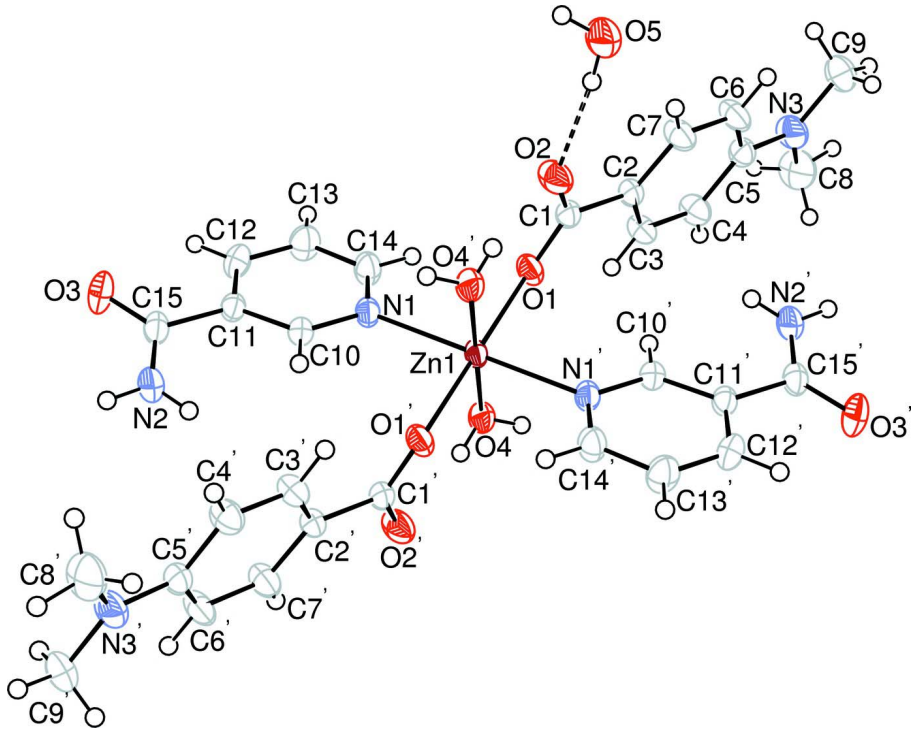


**Figure 1**

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Primed atoms are generated by the symmetry operator: (′) -*x*, -*y*, -*z*. Only one of the crystal water molecules is shown [dashed line indicates the O—H···O hydrogen-bond].

**Diaquabis[4-(dimethylamino)benzoato-$\kappa O$]bis(nicotinamide-$\kappa N^1$)zinc(II) dihydrate**

*Crystal data*

$[Zn(C_9H_{10}NO_2)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 710.07$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.1810$ (2) Å
$b = 9.9877$ (2) Å
$c = 10.1982$ (3) Å
$\alpha = 76.141$ (2)°
$\beta = 88.894$ (3)°
$\gamma = 78.200$ (2)°
$V = 791.55$ (4) Å$^3$
$Z = 1$
$F(000) = 372$
$D_x = 1.490$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7854 reflections
$\theta = 2.6$–$28.4$°
$\mu = 0.84$ mm$^{-1}$
$T = 100$ K
Block, colorless
0.40 × 0.24 × 0.18 mm

*Data collection*

Bruker Kappa APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.783, $T_{max}$ = 0.856
14586 measured reflections
3975 independent reflections
3725 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020
$\theta_{max}$ = 28.5°, $\theta_{min}$ = 2.1°
$h$ = −10→10
$k$ = −13→13
$l$ = −13→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.068
$S$ = 1.05
3975 reflections
240 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2 + 0.2491P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 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 | 0.0000 | 0.0000 | 0.0000 | 0.02409 (7) |
| O1 | 0.14766 (12) | −0.13955 (9) | 0.15299 (10) | 0.0301 (2) |
| O2 | 0.01781 (15) | −0.12085 (10) | 0.34423 (11) | 0.0406 (3) |
| O3 | 0.22843 (14) | 0.63006 (10) | −0.11818 (13) | 0.0428 (3) |
| O4 | 0.16532 (13) | −0.08200 (11) | −0.14162 (11) | 0.0305 (2) |
| H41 | 0.128 (3) | −0.035 (2) | −0.211 (2) | 0.057 (6)* |
| H42 | 0.179 (3) | −0.165 (2) | −0.138 (2) | 0.052 (6)* |
| O5 | −0.1009 (2) | −0.13619 (14) | 0.61334 (15) | 0.0543 (3) |
| H51 | −0.070 (3) | −0.136 (3) | 0.533 (3) | 0.083 (9)* |
| H52 | −0.086 (3) | −0.063 (3) | 0.628 (2) | 0.069 (7)* |
| N1 | 0.15651 (14) | 0.15584 (11) | −0.00723 (11) | 0.0266 (2) |
| N2 | 0.00655 (17) | 0.58552 (13) | −0.21424 (13) | 0.0355 (3) |
| H21 | −0.027 (2) | 0.671 (2) | −0.2554 (18) | 0.040 (5)* |
| H22 | −0.047 (2) | 0.529 (2) | −0.2306 (19) | 0.041 (5)* |
| N3 | 0.45941 (17) | −0.75023 (13) | 0.50923 (14) | 0.0395 (3) |

| | | | | |
|---|---|---|---|---|
| C1 | 0.11626 (17) | −0.18927 (13) | 0.27526 (13) | 0.0272 (3) |
| C2 | 0.20133 (16) | −0.33741 (13) | 0.33617 (13) | 0.0261 (3) |
| C3 | 0.31531 (17) | −0.41206 (14) | 0.26313 (14) | 0.0314 (3) |
| H3 | 0.3353 | −0.3688 | 0.1746 | 0.038* |
| C4 | 0.39964 (18) | −0.54815 (15) | 0.31784 (15) | 0.0341 (3) |
| H4 | 0.4749 | −0.5949 | 0.2659 | 0.041* |
| C5 | 0.37268 (17) | −0.61713 (13) | 0.45193 (14) | 0.0300 (3) |
| C6 | 0.2540 (2) | −0.54300 (15) | 0.52383 (15) | 0.0373 (3) |
| H6 | 0.2304 | −0.5866 | 0.6114 | 0.045* |
| C7 | 0.1715 (2) | −0.40668 (15) | 0.46724 (14) | 0.0347 (3) |
| H7 | 0.0943 | −0.3600 | 0.5178 | 0.042* |
| C8 | 0.5794 (3) | −0.82465 (18) | 0.4327 (2) | 0.0539 (5) |
| H8A | 0.6301 | −0.9151 | 0.4886 | 0.081* |
| H8B | 0.6640 | −0.7712 | 0.4028 | 0.081* |
| H8C | 0.5241 | −0.8373 | 0.3557 | 0.081* |
| C9 | 0.4290 (2) | −0.82016 (16) | 0.64594 (18) | 0.0481 (4) |
| H9A | 0.5045 | −0.9100 | 0.6712 | 0.072* |
| H9B | 0.3160 | −0.8336 | 0.6515 | 0.072* |
| H9C | 0.4464 | −0.7633 | 0.7061 | 0.072* |
| C10 | 0.10521 (16) | 0.29304 (13) | −0.06636 (13) | 0.0254 (2) |
| H10 | −0.0026 | 0.3238 | −0.1040 | 0.030* |
| C11 | 0.20513 (16) | 0.39157 (13) | −0.07418 (13) | 0.0255 (2) |
| C12 | 0.36499 (18) | 0.34448 (15) | −0.01643 (16) | 0.0333 (3) |
| H12 | 0.4347 | 0.4076 | −0.0181 | 0.040* |
| C13 | 0.41990 (18) | 0.20295 (16) | 0.04360 (17) | 0.0384 (3) |
| H13 | 0.5273 | 0.1692 | 0.0816 | 0.046* |
| C14 | 0.31197 (18) | 0.11262 (14) | 0.04593 (15) | 0.0335 (3) |
| H14 | 0.3491 | 0.0174 | 0.0863 | 0.040* |
| C15 | 0.14646 (17) | 0.54593 (13) | −0.13868 (14) | 0.0290 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.02776 (11) | 0.01681 (10) | 0.02584 (11) | −0.00591 (7) | −0.00232 (8) | −0.00020 (7) |
| O1 | 0.0319 (5) | 0.0245 (4) | 0.0288 (5) | −0.0056 (4) | −0.0030 (4) | 0.0035 (4) |
| O2 | 0.0583 (7) | 0.0255 (5) | 0.0311 (5) | 0.0038 (4) | 0.0011 (5) | −0.0040 (4) |
| O3 | 0.0468 (6) | 0.0225 (5) | 0.0621 (7) | −0.0132 (4) | 0.0022 (5) | −0.0111 (5) |
| O4 | 0.0348 (5) | 0.0206 (4) | 0.0342 (6) | −0.0030 (4) | −0.0019 (4) | −0.0046 (4) |
| O5 | 0.0850 (10) | 0.0309 (6) | 0.0437 (8) | −0.0101 (6) | −0.0006 (7) | −0.0043 (5) |
| N1 | 0.0290 (5) | 0.0203 (5) | 0.0297 (6) | −0.0068 (4) | −0.0013 (4) | −0.0029 (4) |
| N2 | 0.0466 (7) | 0.0213 (5) | 0.0367 (7) | −0.0077 (5) | −0.0003 (5) | −0.0024 (5) |
| N3 | 0.0471 (7) | 0.0252 (6) | 0.0382 (7) | 0.0033 (5) | −0.0064 (6) | −0.0005 (5) |
| C1 | 0.0325 (6) | 0.0206 (5) | 0.0275 (6) | −0.0065 (5) | −0.0063 (5) | −0.0023 (5) |
| C2 | 0.0303 (6) | 0.0206 (5) | 0.0255 (6) | −0.0049 (5) | −0.0032 (5) | −0.0017 (5) |
| C3 | 0.0349 (7) | 0.0297 (6) | 0.0254 (6) | −0.0046 (5) | 0.0014 (5) | −0.0003 (5) |
| C4 | 0.0359 (7) | 0.0300 (7) | 0.0316 (7) | 0.0012 (5) | 0.0029 (5) | −0.0050 (5) |
| C5 | 0.0329 (7) | 0.0224 (6) | 0.0320 (7) | −0.0036 (5) | −0.0062 (5) | −0.0025 (5) |
| C6 | 0.0497 (9) | 0.0280 (7) | 0.0263 (7) | −0.0015 (6) | 0.0031 (6) | 0.0030 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.0440 (8) | 0.0270 (6) | 0.0273 (7) | 0.0007 (6) | 0.0048 (6) | −0.0023 (5) |
| C8 | 0.0595 (11) | 0.0315 (8) | 0.0609 (11) | 0.0102 (7) | −0.0030 (9) | −0.0085 (7) |
| C9 | 0.0647 (11) | 0.0267 (7) | 0.0436 (9) | −0.0036 (7) | −0.0102 (8) | 0.0054 (6) |
| C10 | 0.0279 (6) | 0.0217 (5) | 0.0267 (6) | −0.0062 (5) | 0.0004 (5) | −0.0050 (5) |
| C11 | 0.0320 (6) | 0.0212 (5) | 0.0254 (6) | −0.0085 (5) | 0.0062 (5) | −0.0076 (5) |
| C12 | 0.0322 (7) | 0.0300 (6) | 0.0423 (8) | −0.0145 (5) | 0.0037 (6) | −0.0110 (6) |
| C13 | 0.0299 (7) | 0.0349 (7) | 0.0494 (9) | −0.0081 (6) | −0.0076 (6) | −0.0067 (6) |
| C14 | 0.0325 (7) | 0.0240 (6) | 0.0409 (8) | −0.0053 (5) | −0.0053 (6) | −0.0016 (5) |
| C15 | 0.0373 (7) | 0.0209 (6) | 0.0304 (7) | −0.0086 (5) | 0.0107 (5) | −0.0078 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—O1 | 2.0442 (9) | C3—C4 | 1.3795 (19) |
| Zn1—O1$^{i}$ | 2.0442 (9) | C3—H3 | 0.9300 |
| Zn1—O4 | 2.1503 (11) | C4—H4 | 0.9300 |
| Zn1—O4$^{i}$ | 2.1503 (11) | C5—C4 | 1.411 (2) |
| Zn1—N1 | 2.1963 (10) | C5—C6 | 1.403 (2) |
| Zn1—N1$^{i}$ | 2.1963 (10) | C6—H6 | 0.9300 |
| O1—C1 | 1.2691 (16) | C7—C6 | 1.3802 (19) |
| O2—C1 | 1.2624 (17) | C7—H7 | 0.9300 |
| O3—C15 | 1.2327 (17) | C8—H8A | 0.9600 |
| O4—H41 | 0.78 (2) | C8—H8B | 0.9600 |
| O4—H42 | 0.81 (2) | C8—H8C | 0.9600 |
| O5—H51 | 0.85 (3) | C9—H9A | 0.9600 |
| O5—H52 | 0.81 (3) | C9—H9B | 0.9600 |
| N1—C10 | 1.3402 (15) | C9—H9C | 0.9600 |
| N1—C14 | 1.3371 (17) | C10—C11 | 1.3900 (17) |
| N2—C15 | 1.3279 (19) | C10—H10 | 0.9300 |
| N2—H21 | 0.845 (19) | C11—C12 | 1.3871 (19) |
| N2—H22 | 0.829 (19) | C12—C13 | 1.382 (2) |
| N3—C5 | 1.3675 (17) | C12—H12 | 0.9300 |
| N3—C8 | 1.440 (2) | C13—H13 | 0.9300 |
| N3—C9 | 1.444 (2) | C14—C13 | 1.3816 (19) |
| C1—C2 | 1.4881 (17) | C14—H14 | 0.9300 |
| C2—C3 | 1.3911 (19) | C15—C11 | 1.5045 (17) |
| C2—C7 | 1.3923 (19) | | |
| | | | |
| O1$^{i}$—Zn1—O1 | 180.00 (9) | C5—C4—H4 | 119.7 |
| O1—Zn1—O4 | 88.47 (4) | N3—C5—C4 | 121.30 (13) |
| O1$^{i}$—Zn1—O4 | 91.53 (4) | N3—C5—C6 | 121.57 (13) |
| O1—Zn1—O4$^{i}$ | 91.53 (4) | C6—C5—C4 | 117.13 (12) |
| O1$^{i}$—Zn1—O4$^{i}$ | 88.47 (4) | C5—C6—H6 | 119.4 |
| O1—Zn1—N1 | 90.96 (4) | C7—C6—C5 | 121.30 (13) |
| O1$^{i}$—Zn1—N1 | 89.04 (4) | C7—C6—H6 | 119.4 |
| O1—Zn1—N1$^{i}$ | 89.04 (4) | C2—C7—H7 | 119.2 |
| O1$^{i}$—Zn1—N1$^{i}$ | 90.96 (4) | C6—C7—C2 | 121.51 (14) |
| O4—Zn1—O4$^{i}$ | 180.00 (8) | C6—C7—H7 | 119.2 |
| O4—Zn1—N1 | 87.36 (4) | N3—C8—H8A | 109.5 |

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| O4$^{i}$—Zn1—N1 | 92.64 (4) | N3—C8—H8B | 109.5 |
| O4—Zn1—N1$^{i}$ | 92.64 (4) | N3—C8—H8C | 109.5 |
| O4$^{i}$—Zn1—N1$^{i}$ | 87.36 (4) | H8A—C8—H8B | 109.5 |
| N1$^{i}$—Zn1—N1 | 180.0 | H8A—C8—H8C | 109.5 |
| C1—O1—Zn1 | 130.87 (9) | H8B—C8—H8C | 109.5 |
| Zn1—O4—H41 | 102.7 (16) | N3—C9—H9A | 109.5 |
| Zn1—O4—H42 | 117.8 (15) | N3—C9—H9B | 109.5 |
| H42—O4—H41 | 113 (2) | N3—C9—H9C | 109.5 |
| H52—O5—H51 | 106 (2) | H9A—C9—H9B | 109.5 |
| C10—N1—Zn1 | 122.97 (8) | H9A—C9—H9C | 109.5 |
| C14—N1—Zn1 | 119.13 (8) | H9B—C9—H9C | 109.5 |
| C14—N1—C10 | 117.87 (11) | N1—C10—C11 | 123.24 (12) |
| C15—N2—H21 | 120.5 (12) | N1—C10—H10 | 118.4 |
| C15—N2—H22 | 123.3 (13) | C11—C10—H10 | 118.4 |
| H21—N2—H22 | 115.9 (17) | C10—C11—C15 | 123.17 (12) |
| C5—N3—C8 | 120.47 (14) | C12—C11—C10 | 117.79 (11) |
| C5—N3—C9 | 120.68 (14) | C12—C11—C15 | 119.02 (11) |
| C8—N3—C9 | 118.82 (13) | C11—C12—H12 | 120.3 |
| O1—C1—C2 | 116.26 (12) | C13—C12—C11 | 119.49 (12) |
| O2—C1—O1 | 123.66 (11) | C13—C12—H12 | 120.3 |
| O2—C1—C2 | 120.08 (12) | C12—C13—H13 | 120.7 |
| C3—C2—C1 | 120.65 (12) | C14—C13—C12 | 118.62 (13) |
| C3—C2—C7 | 117.35 (12) | C14—C13—H13 | 120.7 |
| C7—C2—C1 | 122.00 (12) | N1—C14—C13 | 122.98 (12) |
| C2—C3—H3 | 118.9 | N1—C14—H14 | 118.5 |
| C4—C3—C2 | 122.10 (13) | C13—C14—H14 | 118.5 |
| C4—C3—H3 | 118.9 | O3—C15—N2 | 122.89 (13) |
| C3—C4—C5 | 120.56 (13) | O3—C15—C11 | 119.01 (13) |
| C3—C4—H4 | 119.7 | N2—C15—C11 | 118.10 (12) |

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| O4—Zn1—O1—C1 | −158.28 (11) | O1—C1—C2—C7 | −176.86 (13) |
| O4$^{i}$—Zn1—O1—C1 | 21.72 (11) | O2—C1—C2—C3 | −177.34 (13) |
| N1—Zn1—O1—C1 | 114.39 (11) | O2—C1—C2—C7 | 2.4 (2) |
| N1$^{i}$—Zn1—O1—C1 | −65.61 (11) | C1—C2—C3—C4 | 178.22 (13) |
| O1—Zn1—N1—C14 | 19.82 (11) | C7—C2—C3—C4 | −1.5 (2) |
| O1$^{i}$—Zn1—N1—C14 | −160.18 (11) | C1—C2—C7—C6 | −178.48 (14) |
| O1—Zn1—N1—C10 | −162.18 (11) | C3—C2—C7—C6 | 1.3 (2) |
| O1$^{i}$—Zn1—N1—C10 | 17.82 (11) | C2—C3—C4—C5 | −0.1 (2) |
| O4—Zn1—N1—C10 | 109.39 (11) | N3—C5—C4—C3 | −177.74 (14) |
| O4$^{i}$—Zn1—N1—C10 | −70.61 (11) | C6—C5—C4—C3 | 1.9 (2) |
| O4—Zn1—N1—C14 | −68.60 (11) | N3—C5—C6—C7 | 177.47 (15) |
| O4$^{i}$—Zn1—N1—C14 | 111.40 (11) | C4—C5—C6—C7 | −2.2 (2) |
| Zn1—O1—C1—O2 | −33.61 (19) | C2—C7—C6—C5 | 0.6 (2) |
| Zn1—O1—C1—C2 | 145.62 (9) | N1—C10—C11—C12 | −0.6 (2) |
| Zn1—N1—C10—C11 | −178.36 (9) | N1—C10—C11—C15 | −179.02 (12) |
| C14—N1—C10—C11 | −0.3 (2) | C10—C11—C12—C13 | 1.3 (2) |
| Zn1—N1—C14—C13 | 178.79 (12) | C15—C11—C12—C13 | 179.73 (14) |
| C10—N1—C14—C13 | 0.7 (2) | C11—C12—C13—C14 | −1.0 (2) |

| | | | |
|---|---|---|---|
| C8—N3—C5—C4 | −1.0 (2) | N1—C14—C13—C12 | 0.0 (3) |
| C8—N3—C5—C6 | 179.36 (15) | O3—C15—C11—C10 | 165.58 (13) |
| C9—N3—C5—C4 | −179.22 (15) | O3—C15—C11—C12 | −12.8 (2) |
| C9—N3—C5—C6 | 1.1 (2) | N2—C15—C11—C10 | −13.6 (2) |
| O1—C1—C2—C3 | 3.40 (18) | N2—C15—C11—C12 | 168.04 (13) |

Symmetry code: (i) −*x*, −*y*, −*z*.

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C2–C7 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H21···O5$^{ii}$ | 0.85 (2) | 2.05 (2) | 2.8826 (19) | 169.3 (2) |
| O4—H41···O2$^{i}$ | 0.78 (2) | 2.00 (2) | 2.7370 (16) | 159 (2) |
| O4—H42···O3$^{iii}$ | 0.81 (2) | 1.96 (2) | 2.7681 (15) | 175.1 (2) |
| O5—H51···O2 | 0.85 (3) | 2.02 (3) | 2.8732 (19) | 174 (3) |
| O5—H52···O2$^{iv}$ | 0.81 (3) | 2.11 (3) | 2.9150 (18) | 173 (2) |
| C13—H13···O4$^{v}$ | 0.93 | 2.52 | 3.4422 (19) | 170 |
| N2—H22···*Cg*1$^{i}$ | 0.829 (19) | 2.79 (2) | 3.5200 (15) | 147.9 (2) |

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