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Bis(nitrato- κ O)(3-oxapentane-1,5-diamine- κ^3 N,O,N')zinc(II)

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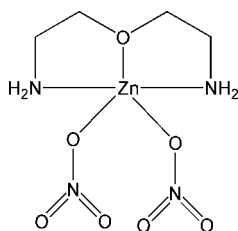
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.026; wR factor = 0.065; data-to-parameter ratio = 11.8.

In the title compound, $[\text{Zn}(\text{NO}_3)_2(\text{C}_4\text{H}_{12}\text{N}_2\text{O})]$, the Zn^{II} atom is N,O,N' -chelated by a 3-oxapentane-1,5-diamine ligand and is further coordinated by two nitrate anions in a distorted trigonal-bipyramidal geometry. Intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonding is present in the crystal structure. A short $\text{O}\cdots\text{O}$ contact of 2.816 (8) Å is observed between the nitrate anions of adjacent molecules.

Related literature

For polydentate amine ligands in metal complexes, see: Fanshawe *et al.* (2000). For applications of metal complexes with a tridentate amine ligand, see: Junk & Steed (2007). For a description of the geometry of complexes with five-coordinate metal atoms, see: Addison *et al.* (1984).



Experimental

Crystal data

$[\text{Zn}(\text{NO}_3)_2(\text{C}_4\text{H}_{12}\text{N}_2\text{O})]$ $a = 8.031$ (19) Å
 $M_r = 293.55$ $b = 8.034$ (19) Å
Triclinic, $P\bar{1}$ $c = 9.55$ (2) Å

$\alpha = 103.97$ (2)°
 $\beta = 101.90$ (2)°
 $\gamma = 115.879$ (18)°
 $V = 503$ (2) Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 2.48$ mm⁻¹
 $T = 296$ K
 $0.30 \times 0.28 \times 0.26$ mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
 $T_{\text{min}} = 0.524$, $T_{\text{max}} = 0.565$

2969 measured reflections
1712 independent reflections
1543 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.065$
 $S = 1.08$
1712 reflections

145 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.39$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{N1}-\text{H3A}\cdots\text{O2}^{\text{i}}$ | 0.90 | 2.39 | 3.217 (7) | 152 |
| $\text{N1}-\text{H3B}\cdots\text{O6}^{\text{ii}}$ | 0.90 | 2.51 | 3.168 (9) | 130 |
| $\text{N2}-\text{H2A}\cdots\text{O4}^{\text{iii}}$ | 0.90 | 2.42 | 3.058 (8) | 128 |
| $\text{N2}-\text{H2B}\cdots\text{O5}^{\text{iv}}$ | 0.90 | 2.41 | 3.201 (9) | 145 |
| $\text{N2}-\text{H2B}\cdots\text{O3}^{\text{iv}}$ | 0.90 | 2.49 | 3.106 (6) | 126 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x, y+1, z$; (iv) $-x+2, -y+2, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU5211).

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supporting information

Acta Cryst. (2011). E67, m764 [doi:10.1107/S1600536811018010]

Bis(nitrato- κ O)(3-oxapentane-1,5-diamine- κ^3 N,O,N')zinc(II)

Fei Jia, Fan Kou, Bin Liu, Bei-Bei Jia and Hui-Lu Wu

S1. Comment

Polydentate amine ligands generally coordinate to transition metal ions using all of the available nitrogen atoms as donors (Fanshawe *et al.*, 2000). Transition metal coordination complexes involving tridentate amines as ligands have attracted solid attention for their role as model compounds for bioinorganic systems, as building blocks in supramolecular assemblies and as catalysts (Junk & Steed, 2007). 3-oxapentane-1,5-diamine as the one of the classics of polyamines behaves as a tridentate ligand that can form three coordinative bonds with a metal atom through the lone pair electrons on two N atoms and one oxygen.

The Zn^{II} in the complex is N,O,N'-chelated by a 3-oxapentane-1,5-diamine ligand and is further coordinated by two nitrate anions. The coordination geometry of the Zn^{II} ion may be best described as distorted trigonal bipyramidal ($\tau = 2/3$). The parameter τ is defined as $(\beta - \alpha)/60$ [where $\beta = \text{O}(5)\text{-Zn}(1)\text{-O}(1)$, $\alpha = \text{N}(2)\text{-Zn}(1)\text{-N}(1)$] and its value varies from 0 (in regular square-base pyramidal) to 1 (in regular trigonal bipyramidal) (Addison *et al.*, 1984). The equatorial plane is occupied by two N atoms of the ligand, and one O atom of nitrate anions, whereas the Zn^{II} ion protrudes towards O5 by 0.337 Å from the plane of atoms N1/N2/O2. The axial positions are occupied by O1 and O5 atoms. The crystal structure is mainly stabilized by the intermolecular H-bond.

S2. Experimental

To a stirred solution of 3-oxapentane-1,5-diamine (0.104 g, 0.10 mmol) in EtOH (10 ml) was added Zn(NO₃)₂(H₂O)₆ (0.297 g, 0.1 mmol) in EtOH (5 ml). A white crystalline product formed rapidly. The precipitate was filtered off, washed with EtOH and *in vacuo*. The dried precipitate was dissolved in DMF resulting in a colourless solution. The crystals suitable for X-ray diffraction studies were obtained by ether diffusion into DMF after several days at room temperature. Yield, 0.115 g (28%). (found: C, 16.45; H, 3.99; N, 19.43. Calcd.: C, 16.37; H, 4.12; N, 19.09).

S3. Refinement

H atoms were placed in calculated positions with C—H = 0.97 and N—H = 0.90 Å, and refined in a riding-model approximation with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

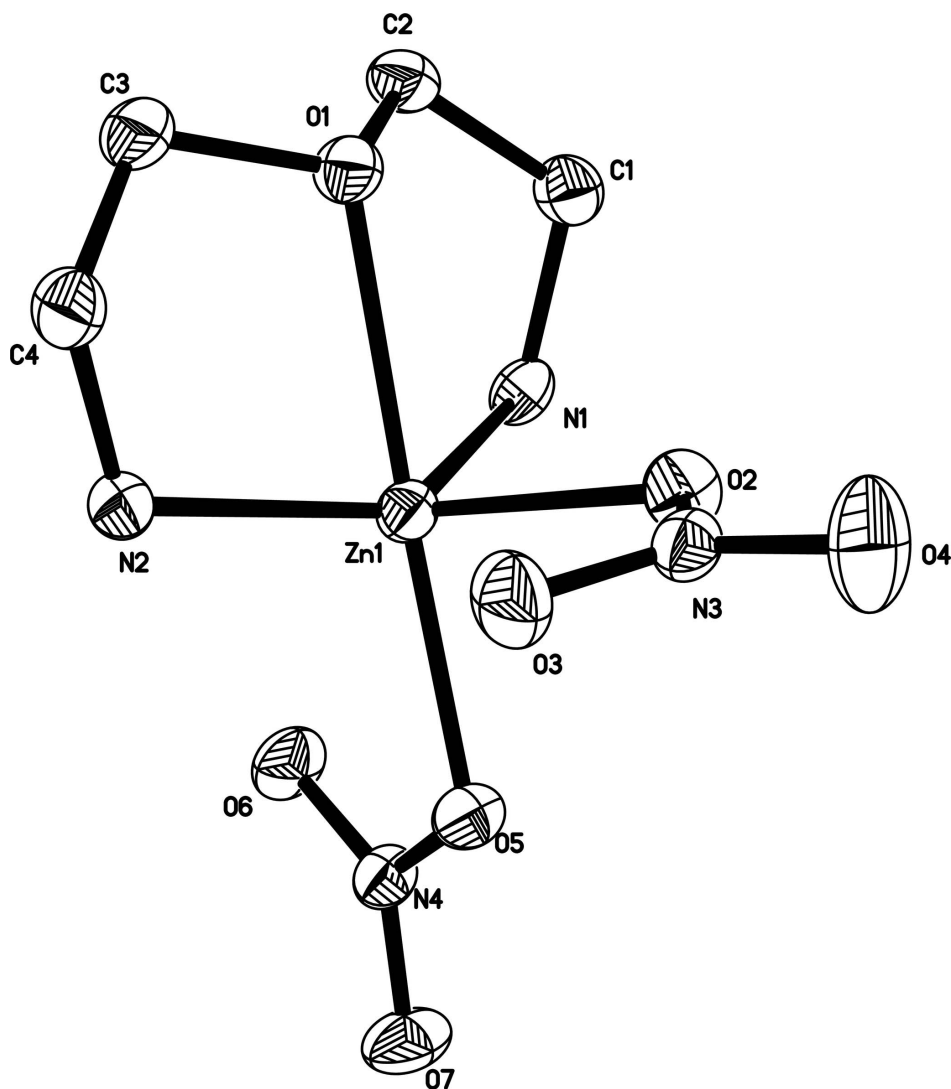


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

Bis(nitrato- κ O)(3-oxapentane-1,5-diamine- κ^3 N,O,N')zinc(II)

Crystal data

[Zn(NO₃)₂(C₄H₁₂N₂O)]

$M_r = 293.55$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.031(19) \text{ \AA}$

$b = 8.034(19) \text{ \AA}$

$c = 9.55(2) \text{ \AA}$

$\alpha = 103.97(2)^\circ$

$\beta = 101.90(2)^\circ$

$\gamma = 115.879(18)^\circ$

$V = 503(2) \text{ \AA}^3$

$Z = 2$

$F(000) = 300$

$D_x = 1.940 \text{ Mg m}^{-3}$

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

Cell parameters from 1744 reflections

$\theta = 2.4\text{--}26.2^\circ$

$\mu = 2.48 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colourless

$0.30 \times 0.28 \times 0.26 \text{ mm}$

Data collection

| | |
|--|--|
| Bruker SMART 1000 diffractometer | 2969 measured reflections 1712 independent reflections |
| Radiation source: fine-focus sealed tube | 1543 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{\text{int}} = 0.016$ |
| ω scans | $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2001) | $h = -9 \rightarrow 9$ |
| $T_{\text{min}} = 0.524$, $T_{\text{max}} = 0.565$ | $k = -9 \rightarrow 9$ |
| | $l = -11 \rightarrow 10$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.026$ | H-atom parameters constrained |
| $wR(F^2) = 0.065$ | $w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.3287P]$ |
| $S = 1.08$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 1712 reflections | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 145 parameters | $\Delta\rho_{\text{max}} = 0.39 \text{ e } \text{\AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\text{min}} = -0.30 \text{ e } \text{\AA}^{-3}$ |
| 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|------------|------------|----------------------------------|
| C1 | 0.1984 (4) | 0.4429 (4) | 0.1842 (4) | 0.0421 (7) |
| H4A | 0.0585 | 0.3840 | 0.1683 | 0.050* |
| H4B | 0.2276 | 0.3362 | 0.1631 | 0.050* |
| C2 | 0.2448 (4) | 0.5479 (4) | 0.0773 (3) | 0.0408 (7) |
| H3C | 0.1756 | 0.4536 | -0.0289 | 0.049* |
| H3D | 0.2044 | 0.6464 | 0.0907 | 0.049* |
| C3 | 0.5347 (5) | 0.8083 (5) | 0.0668 (4) | 0.0447 (8) |
| H1A | 0.4661 | 0.8816 | 0.0797 | 0.054* |
| H1B | 0.5209 | 0.7623 | -0.0409 | 0.054* |
| C4 | 0.7451 (5) | 0.9362 (5) | 0.1657 (4) | 0.0443 (8) |
| H2C | 0.8153 | 0.8670 | 0.1428 | 0.053* |
| H2D | 0.8031 | 1.0575 | 0.1449 | 0.053* |
| N1 | 0.3161 (3) | 0.5833 (4) | 0.3447 (3) | 0.0354 (5) |
| H3A | 0.3025 | 0.5149 | 0.4077 | 0.043* |
| H3B | 0.2702 | 0.6660 | 0.3699 | 0.043* |
| N2 | 0.7660 (3) | 0.9873 (3) | 0.3291 (3) | 0.0350 (5) |

| | | | | |
|-----|-------------|-------------|-------------|--------------|
| H2A | 0.7262 | 1.0754 | 0.3551 | 0.042* |
| H2B | 0.8947 | 1.0466 | 0.3874 | 0.042* |
| N3 | 0.8109 (4) | 0.5303 (3) | 0.3367 (3) | 0.0344 (5) |
| N4 | 0.7273 (4) | 0.9449 (3) | 0.6934 (3) | 0.0351 (6) |
| O1 | 0.4541 (3) | 0.6427 (3) | 0.1137 (2) | 0.0370 (5) |
| O2 | 0.6435 (3) | 0.5019 (3) | 0.3413 (2) | 0.0425 (5) |
| O3 | 0.9375 (3) | 0.6943 (3) | 0.3458 (3) | 0.0538 (6) |
| O4 | 0.8395 (4) | 0.3919 (4) | 0.3230 (4) | 0.0700 (8) |
| O5 | 0.7711 (3) | 0.8330 (3) | 0.6081 (2) | 0.0367 (5) |
| O6 | 0.6094 (3) | 0.9873 (3) | 0.6285 (3) | 0.0489 (6) |
| O7 | 0.8036 (4) | 1.0070 (4) | 0.8329 (2) | 0.0556 (6) |
| Zn1 | 0.60715 (5) | 0.74633 (5) | 0.37628 (4) | 0.03129 (12) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| C1 | 0.0341 (16) | 0.0388 (16) | 0.0448 (18) | 0.0122 (13) | 0.0134 (14) | 0.0155 (14) |
| C2 | 0.0346 (16) | 0.0391 (16) | 0.0352 (16) | 0.0135 (13) | 0.0052 (13) | 0.0097 (13) |
| C3 | 0.0485 (19) | 0.0457 (17) | 0.0352 (17) | 0.0162 (15) | 0.0176 (15) | 0.0209 (14) |
| C4 | 0.0460 (18) | 0.0410 (17) | 0.0428 (18) | 0.0156 (14) | 0.0213 (15) | 0.0196 (14) |
| N1 | 0.0376 (13) | 0.0451 (14) | 0.0364 (13) | 0.0247 (12) | 0.0195 (11) | 0.0232 (11) |
| N2 | 0.0336 (13) | 0.0318 (12) | 0.0356 (13) | 0.0148 (10) | 0.0092 (11) | 0.0129 (10) |
| N3 | 0.0433 (14) | 0.0363 (13) | 0.0311 (13) | 0.0245 (12) | 0.0157 (11) | 0.0145 (10) |
| N4 | 0.0397 (14) | 0.0386 (13) | 0.0337 (14) | 0.0239 (12) | 0.0139 (11) | 0.0162 (11) |
| O1 | 0.0351 (11) | 0.0374 (10) | 0.0339 (11) | 0.0131 (9) | 0.0137 (9) | 0.0159 (9) |
| O2 | 0.0388 (12) | 0.0442 (12) | 0.0500 (13) | 0.0251 (10) | 0.0185 (10) | 0.0165 (10) |
| O3 | 0.0541 (14) | 0.0401 (12) | 0.0583 (15) | 0.0136 (11) | 0.0231 (12) | 0.0227 (11) |
| O4 | 0.0750 (18) | 0.0592 (15) | 0.114 (2) | 0.0528 (15) | 0.0505 (17) | 0.0426 (16) |
| O5 | 0.0444 (12) | 0.0435 (11) | 0.0305 (10) | 0.0298 (10) | 0.0135 (9) | 0.0123 (9) |
| O6 | 0.0525 (13) | 0.0560 (13) | 0.0527 (14) | 0.0402 (12) | 0.0129 (11) | 0.0237 (11) |
| O7 | 0.0754 (17) | 0.0698 (15) | 0.0279 (12) | 0.0482 (14) | 0.0122 (11) | 0.0121 (11) |
| Zn1 | 0.03247 (19) | 0.03232 (19) | 0.03040 (19) | 0.01648 (14) | 0.01121 (14) | 0.01408 (14) |

Geometric parameters (Å, °)

| | | | |
|--------|-----------|--------|-----------|
| C1—N1 | 1.467 (4) | N1—H3A | 0.9000 |
| C1—C2 | 1.480 (5) | N1—H3B | 0.9000 |
| C1—H4A | 0.9700 | N2—Zn1 | 2.020 (4) |
| C1—H4B | 0.9700 | N2—H2A | 0.9000 |
| C2—O1 | 1.429 (5) | N2—H2B | 0.9000 |
| C2—H3C | 0.9700 | N3—O4 | 1.214 (4) |
| C2—H3D | 0.9700 | N3—O3 | 1.231 (4) |
| C3—O1 | 1.429 (4) | N3—O2 | 1.273 (4) |
| C3—C4 | 1.470 (5) | N4—O7 | 1.215 (4) |
| C3—H1A | 0.9700 | N4—O6 | 1.240 (3) |
| C3—H1B | 0.9700 | N4—O5 | 1.279 (3) |
| C4—N2 | 1.468 (5) | O1—Zn1 | 2.307 (5) |
| C4—H2C | 0.9700 | O2—Zn1 | 2.068 (5) |

| | | | |
|--------------|------------|--------------|--------------|
| C4—H2D | 0.9700 | O5—Zn1 | 2.091 (4) |
| N1—Zn1 | 2.029 (5) | | |
| N1—C1—C2 | 110.1 (3) | H3A—N1—H3B | 108.0 |
| N1—C1—H4A | 109.6 | C4—N2—Zn1 | 112.71 (19) |
| C2—C1—H4A | 109.6 | C4—N2—H2A | 109.1 |
| N1—C1—H4B | 109.6 | Zn1—N2—H2A | 109.1 |
| C2—C1—H4B | 109.6 | C4—N2—H2B | 109.1 |
| H4A—C1—H4B | 108.2 | Zn1—N2—H2B | 109.1 |
| O1—C2—C1 | 106.9 (2) | H2A—N2—H2B | 107.8 |
| O1—C2—H3C | 110.3 | O4—N3—O3 | 122.0 (3) |
| C1—C2—H3C | 110.3 | O4—N3—O2 | 117.9 (3) |
| O1—C2—H3D | 110.3 | O3—N3—O2 | 120.0 (3) |
| C1—C2—H3D | 110.3 | O7—N4—O6 | 122.9 (3) |
| H3C—C2—H3D | 108.6 | O7—N4—O5 | 119.3 (2) |
| O1—C3—C4 | 106.7 (3) | O6—N4—O5 | 117.8 (3) |
| O1—C3—H1A | 110.4 | C2—O1—C3 | 114.1 (2) |
| C4—C3—H1A | 110.4 | C2—O1—Zn1 | 108.81 (17) |
| O1—C3—H1B | 110.4 | C3—O1—Zn1 | 109.59 (19) |
| C4—C3—H1B | 110.4 | N3—O2—Zn1 | 116.47 (18) |
| H1A—C3—H1B | 108.6 | N4—O5—Zn1 | 109.2 (2) |
| N2—C4—C3 | 110.2 (3) | N2—Zn1—N1 | 133.42 (10) |
| N2—C4—H2C | 109.6 | N2—Zn1—O2 | 124.63 (18) |
| C3—C4—H2C | 109.6 | N1—Zn1—O2 | 93.24 (17) |
| N2—C4—H2D | 109.6 | N2—Zn1—O5 | 102.15 (13) |
| C3—C4—H2D | 109.6 | N1—Zn1—O5 | 107.77 (13) |
| H2C—C4—H2D | 108.1 | O2—Zn1—O5 | 84.95 (10) |
| C1—N1—Zn1 | 111.6 (2) | N2—Zn1—O1 | 76.61 (12) |
| C1—N1—H3A | 109.3 | N1—Zn1—O1 | 77.29 (11) |
| Zn1—N1—H3A | 109.3 | O2—Zn1—O1 | 90.28 (10) |
| C1—N1—H3B | 109.3 | O5—Zn1—O1 | 173.20 (8) |
| Zn1—N1—H3B | 109.3 | | |
| N1—C1—C2—O1 | 55.3 (3) | C1—N1—Zn1—O5 | -153.7 (2) |
| O1—C3—C4—N2 | -53.8 (3) | C1—N1—Zn1—O1 | 21.62 (19) |
| C2—C1—N1—Zn1 | -49.5 (3) | N3—O2—Zn1—N2 | 22.7 (2) |
| C3—C4—N2—Zn1 | 48.8 (3) | N3—O2—Zn1—N1 | 173.84 (19) |
| C1—C2—O1—C3 | -157.2 (2) | N3—O2—Zn1—O5 | -78.6 (2) |
| C1—C2—O1—Zn1 | -34.5 (3) | N3—O2—Zn1—O1 | 96.6 (2) |
| C4—C3—O1—C2 | 156.3 (3) | N4—O5—Zn1—N2 | 81.0 (3) |
| C4—C3—O1—Zn1 | 34.0 (3) | N4—O5—Zn1—N1 | -62.8 (2) |
| O4—N3—O2—Zn1 | 176.9 (2) | N4—O5—Zn1—O2 | -154.59 (18) |
| O3—N3—O2—Zn1 | -3.2 (3) | N4—O5—Zn1—O1 | 159.8 (5) |
| O7—N4—O5—Zn1 | 178.1 (2) | C2—O1—Zn1—N2 | -133.23 (19) |
| O6—N4—O5—Zn1 | -2.8 (3) | C3—O1—Zn1—N2 | -7.84 (19) |
| C4—N2—Zn1—N1 | -78.7 (2) | C2—O1—Zn1—N1 | 7.84 (17) |
| C4—N2—Zn1—O2 | 59.7 (2) | C3—O1—Zn1—N1 | 133.2 (2) |
| C4—N2—Zn1—O5 | 152.0 (2) | C2—O1—Zn1—O2 | 101.1 (2) |

| | | | |
|--------------|-----------|--------------|------------|
| C4—N2—Zn1—O1 | -21.2 (2) | C3—O1—Zn1—O2 | -133.5 (2) |
| C1—N1—Zn1—N2 | 78.9 (3) | C2—O1—Zn1—O5 | 146.5 (6) |
| C1—N1—Zn1—O2 | -67.9 (2) | C3—O1—Zn1—O5 | -88.1 (7) |

Hydrogen-bond geometry (Å, °)

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|----------------------------|------------|--------------|--------------|----------------|
| N1—H3A...O2 ⁱ | 0.90 | 2.39 | 3.217 (7) | 152 |
| N1—H3B...O6 ⁱⁱ | 0.90 | 2.51 | 3.168 (9) | 130 |
| N2—H2A...O4 ⁱⁱⁱ | 0.90 | 2.42 | 3.058 (8) | 128 |
| N2—H2B...O5 ^{iv} | 0.90 | 2.41 | 3.201 (9) | 145 |
| N2—H2B...O3 ^{iv} | 0.90 | 2.49 | 3.106 (6) | 126 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x, y+1, z$; (iv) $-x+2, -y+2, -z+1$.