# metal-organic compounds

# trans-Diaquabis[5-carboxy-4-carboxyl-ato-2-(4-pyridinio)-1H-imidazol-1-ido-κ²N³,O⁴]zinc(II)

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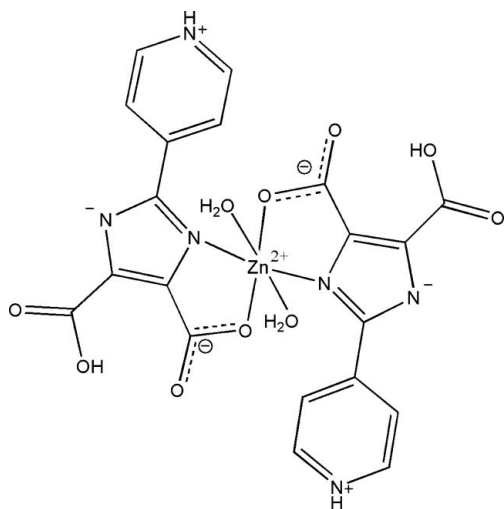Correspondence e-mail: lixia@hncj.edu.cn

In the title complex, $[Zn(C_{10}H_6N_3O_4)_2(H_2O)_2]$, the $Zn^{II}$ atom is located on a twofold rotation axis and is coordinated by two trans-positioned $N,O$-bidentate and zwitterionic 5-carboxy-4-carboxylato-2-(4-pyridinio)-1H-imidazol-1-ide ($H_2PIDC^-$) ligands and two water molecules, defining a distorted octahedral environment. The complete solid-state structure can be described as a three-dimensional supramolecular framework, stabilized by extensive hydrogen-bonding inter-actions involving the coordinated water molecules, uncoordin-ated imidazole N atom, protonated pyridine N and carboxylate O atoms of the $H_2PIDC^-$ ligands.

## Related literature

For related structures, see: Li, Liu et al. (2009); Li, Wu et al. (2009). For the preparation of 2-(pyridin-4-yl)-1H-imidazole-4,5-dicarboxylic acid, see: Sun et al. (2006).



## Experimental

### Crystal data

| | |
|---|---|
| $[Zn(C_{10}H_6N_3O_4)_2(H_2O)_2]$ | $V$ = 2003.7 (4) Å³ |
| $M_r$ = 565.76 | $Z$ = 4 |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation |
| $a$ = 7.4138 (9) Å | $\mu$ = 1.31 mm⁻¹ |
| $b$ = 20.204 (3) Å | $T$ = 173 K |
| $c$ = 13.4778 (17) Å | 0.27 × 0.17 × 0.10 mm |
| $\beta$ = 97.008 (1)° | |

### Data collection

| | |
|---|---|
| Rigaku Mercury CCD diffractometer | 9235 measured reflections |
| Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000) | 2488 independent reflections |
| $T_{min}$ = 0.754, $T_{max}$ = 0.878 | 1957 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.031 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.031 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.090 | |
| $S$ = 1.04 | $\Delta\rho_{max}$ = 0.34 e Å⁻³ |
| 2488 reflections | $\Delta\rho_{min}$ = −0.37 e Å⁻³ |
| 178 parameters | |
| 1 restraint | |

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

| | | | |
|---|---|---|---|
| Zn1—O2 | 2.0713 (15) | Zn1—N1 | 2.1592 (17) |
| Zn1—O1 | 2.1407 (18) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$B$···N2[i] | 0.82 (3) | 2.08 (3) | 2.898 (3) | 178 (3) |
| N3—H3···O5[ii] | 0.88 | 1.89 | 2.755 (2) | 169 |
| O4—H4$A$···O3 | 0.89 (2) | 1.58 (2) | 2.459 (2) | 173 (3) |

Symmetry codes: (i) $-x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (ii) $-x - \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2196).

## References

Li, X., Liu, W., Wu, B.-L. & Zhang, H.-Y. (2009). *Acta Cryst.* E**65**, m820–m821.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sun, T., Ma, J.-P., Huang, R.-Q. & Dong, Y.-B. (2006). *Acta Cryst.* E**62**, o2751–o2752.

**supplementary materials**

## *trans*-Diaquabis[5-carboxy-4-carboxylato-2-(4-pyridinio)-1*H*-imidazol-1-ido-$\kappa^2N^3,O^4$]zinc(II)

## X. Li, L.-Z. Du, B.-L. Wu and H.-Y. Zhang

### Comment

Multifunctional connector 2-(pyridin-4-yl)-1*H*-imidazole-4,5-dicarboxylate acid ($H_3$PIDC), a rigid N-heterocyclic carboxylate, has great potential for coordinative interactions and hydrogen bonding, showing more interesting traits in the construction of MOFs. It can be successively deprotonated to generate various species with different proton numbers, and hence may result in a large diversity of supramolecular architectures. Very recently, we have reported several supramolecular architectures (Li, Wu *et al.*, 2009; Li, Liu *et al.*, 2009) base on ligand 2-(pyridin-4-yl)-1*H*-imidazole-4,5-dicarboxylic acid. As an extension of our previous investigations, we have isolated a new Zn(II) complex, $[Zn(H_2PIDC)_2(H_2O)_2]$, (I), by the reaction of $H_3$PIDC and Zn(II) diacetate under the hydrothermal condition. We report here the single-crystal structure of this complex.

As shown in Fig. 1, the molecule of (I) is a discrete neutral monomer, in which the Zn atom resides on a crystallographic inversion centre and the asymmetric unit contains one-half of the $[Zn(H_2PIDC)_2(H_2O)_2]$ formula unit. Each Zn atom is six-coordinated by $N_2O_4$ with two chelating rings from two $H_2PIDC$ ligands arranged symmetrically in the equatorial plane and two water molecules occupying the apical sites, showing a distorted octahedral geometry (Table 1). In this complex, one carboxyl group and imidazole group are deprotonated and the pyridyl group is protonated, and the ligand bears a formal charge of -1, and the uncoordinated carboxylate atoms O3 and O4 form an intramolecular hydrogen bond (Table 2). All non-H atoms in the imidazole-4,5-dicarboxyl group are nearly coplanar [the mean deviation is 0.075 (3) Å], and the dihedral angle between imidazole group and pyridine group is 11.4 (2) °.

A three-dimensional supramolecular network is constructed *via* hydrogen-bonding interactions involving the coordinated water molecules, uncoordinated imidazole N atom, protonated pyridine N and carboxylate O atoms of the $H_2PIDC^-$ ligands (Table 2 and Fig. 2).

### Experimental

A mixture of zinc diacetate dihydrate (0.022 g, 0.1 mmol), 2-(pyridin-4-yl)-1*H*-imidazole-4,5-dicarboxylic acid (0.024 g, 0.1 mmol) (Sun *et al.*, 2006), NaOH (0.004 g, 0.1 mmol) and water (10 ml) was sealed into a Teflon-lined stainless autoclave and heated at 413 K for 3 days, then cooled to room temperature gradually and colourless block crystals of (I) were obtained. Analysis calculated for $C_{20}H_{16}ZnN_6O_{10}$: C 42.46, H 2.85, N 14.85; found: C 42.82, H 2.73, N 14.70.

### Refinement

H atoms attached to N and O atoms were located in a difference Fourier maps and refined as riding in their as-found relative positions, with $U_{iso}(H) = 1.5U_{eq}(O,N)$. Other H atoms were positioned geometrically with C—H = 0.95 Å and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C)$.
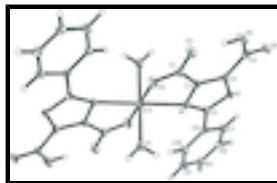
# supplementary materials

**Figures**



Fig. 1. A view of the molecular of (I), showing the atom-labelling scheme and displacement ellipsoids at the 30% probability level.
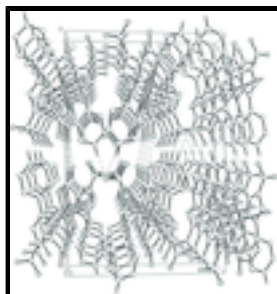


Fig. 2. The crystal packing of (I), showing the three-dimensional hydrogen-bonding network, H atoms have been omited for clarity.

**$trans$-Diaquabis[5-carboxy-4-carboxylato-2-(4-pyridinio)-1$H$- imidazol-1-ido-$\kappa^2 N^3,O^4$]zinc(II)**

*Crystal data*

| | |
|---|---|
| [Zn(C$_{10}$H$_6$N$_3$O$_4$)$_2$(H$_2$O)$_2$] | $F(000) = 1152$ |
| $M_r = 565.76$ | $D_x = 1.875$ Mg m$^{-3}$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 7.4138 (9)$ Å | $\theta = 2.5–28.3°$ |
| $b = 20.204 (3)$ Å | $\mu = 1.31$ mm$^{-1}$ |
| $c = 13.4778 (17)$ Å | $T = 173$ K |
| $\beta = 97.008 (1)°$ | Block, colorless |
| $V = 2003.7 (4)$ Å$^3$ | $0.27 \times 0.17 \times 0.10$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Rigaku Mercury CCD diffractometer | 2488 independent reflections |
| Radiation source: fine-focus sealed tube | 1957 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.031$ |
| ω scan | $\theta_{max} = 28.3°$, $\theta_{min} = 2.5°$ |
| Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000) | $h = -9\rightarrow9$ |
| $T_{min} = 0.754$, $T_{max} = 0.878$ | $k = -26\rightarrow26$ |
| 9235 measured reflections | $l = -17\rightarrow17$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.090$

$S = 1.04$

2488 reflections

178 parameters

1 restraint

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

$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 2.1588P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.34$ e Å$^{-3}$

$\Delta\rho_{min} = -0.37$ 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.

**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 (Å$^2$)*

|  | *x* | *y* | *z* | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.2500 | 0.2500 | 0.5000 | 0.02158 (12) |
| O1 | 0.1031 (3) | 0.21527 (11) | 0.36331 (14) | 0.0405 (5) |
| N1 | −0.0003 (2) | 0.26283 (8) | 0.56460 (13) | 0.0181 (3) |
| C1 | 0.0872 (3) | 0.37351 (10) | 0.51444 (16) | 0.0230 (4) |
| O2 | 0.1956 (2) | 0.34788 (7) | 0.46161 (13) | 0.0296 (4) |
| N2 | −0.2095 (2) | 0.28420 (8) | 0.67035 (13) | 0.0204 (4) |
| C2 | −0.2007 (3) | 0.40644 (10) | 0.68011 (17) | 0.0239 (4) |
| O3 | 0.0612 (2) | 0.43586 (7) | 0.51721 (13) | 0.0355 (4) |
| N3 | −0.2067 (3) | 0.03644 (9) | 0.68078 (15) | 0.0283 (4) |
| H3 | −0.2203 | −0.0056 | 0.6953 | 0.034* |
| C3 | −0.0184 (3) | 0.32960 (9) | 0.57348 (15) | 0.0184 (4) |
| O4 | −0.1528 (3) | 0.46001 (7) | 0.63823 (14) | 0.0368 (4) |
| C4 | −0.1451 (3) | 0.34251 (9) | 0.63948 (15) | 0.0192 (4) |
| O5 | −0.2869 (2) | 0.40756 (8) | 0.75300 (12) | 0.0322 (4) |
| C5 | −0.1194 (3) | 0.23786 (9) | 0.62332 (15) | 0.0184 (4) |
| C6 | −0.1542 (3) | 0.16745 (9) | 0.63892 (15) | 0.0180 (4) |
| C7 | −0.2469 (3) | 0.14843 (10) | 0.71861 (17) | 0.0250 (5) |
| H7 | −0.2949 | 0.1811 | 0.7587 | 0.030* |
| C8 | −0.2687 (3) | 0.08256 (11) | 0.73901 (17) | 0.0278 (5) |
| H8 | −0.3279 | 0.0698 | 0.7946 | 0.033* |
| C9 | −0.1247 (3) | 0.05237 (11) | 0.60116 (18) | 0.0311 (5) |
| H9 | −0.0866 | 0.0184 | 0.5597 | 0.037* |

| C10 | −0.0947 (3) | 0.11772 (10) | 0.57857 (17) | 0.0251 (5) |
| H10 | −0.0343 | 0.1288 | 0.5226 | 0.030* |
| H1B | −0.008 (4) | 0.2148 (13) | 0.353 (2) | 0.030* |
| H1A | 0.135 (4) | 0.1903 (13) | 0.324 (2) | 0.030* |
| H4A | −0.080 (3) | 0.4538 (12) | 0.5916 (16) | 0.030* |

*Atomic displacement parameters (Å$^2$)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0248 (2) | 0.01734 (18) | 0.0245 (2) | 0.00358 (13) | 0.01053 (13) | 0.00102 (13) |
| O1 | 0.0245 (9) | 0.0669 (14) | 0.0305 (10) | 0.0044 (9) | 0.0054 (8) | −0.0200 (9) |
| N1 | 0.0208 (8) | 0.0139 (8) | 0.0206 (8) | 0.0008 (6) | 0.0066 (7) | 0.0011 (6) |
| C1 | 0.0266 (11) | 0.0175 (10) | 0.0261 (11) | 0.0015 (8) | 0.0088 (9) | 0.0026 (8) |
| O2 | 0.0361 (9) | 0.0201 (7) | 0.0366 (9) | 0.0046 (7) | 0.0203 (7) | 0.0067 (7) |
| N2 | 0.0216 (9) | 0.0161 (8) | 0.0250 (9) | −0.0002 (7) | 0.0085 (7) | −0.0004 (7) |
| C2 | 0.0263 (11) | 0.0184 (10) | 0.0280 (11) | 0.0016 (8) | 0.0077 (9) | −0.0012 (8) |
| O3 | 0.0493 (11) | 0.0144 (7) | 0.0482 (11) | 0.0022 (7) | 0.0275 (9) | 0.0071 (7) |
| N3 | 0.0356 (11) | 0.0140 (8) | 0.0359 (11) | −0.0042 (7) | 0.0074 (8) | 0.0035 (7) |
| C3 | 0.0209 (10) | 0.0140 (9) | 0.0212 (10) | 0.0006 (7) | 0.0063 (8) | 0.0004 (7) |
| O4 | 0.0576 (12) | 0.0155 (7) | 0.0430 (10) | 0.0036 (7) | 0.0291 (9) | −0.0001 (7) |
| C4 | 0.0222 (10) | 0.0144 (9) | 0.0220 (10) | 0.0007 (7) | 0.0062 (8) | 0.0013 (7) |
| O5 | 0.0417 (10) | 0.0220 (8) | 0.0370 (9) | 0.0018 (7) | 0.0215 (8) | −0.0053 (7) |
| C5 | 0.0204 (10) | 0.0153 (9) | 0.0199 (10) | −0.0008 (7) | 0.0045 (8) | 0.0015 (7) |
| C6 | 0.0186 (10) | 0.0145 (9) | 0.0213 (10) | −0.0013 (7) | 0.0034 (8) | 0.0016 (7) |
| C7 | 0.0309 (12) | 0.0183 (10) | 0.0275 (11) | −0.0017 (8) | 0.0101 (9) | −0.0008 (8) |
| C8 | 0.0324 (12) | 0.0239 (11) | 0.0287 (12) | −0.0055 (9) | 0.0109 (10) | 0.0054 (9) |
| C9 | 0.0411 (14) | 0.0190 (10) | 0.0353 (13) | −0.0016 (9) | 0.0137 (10) | −0.0037 (9) |
| C10 | 0.0312 (12) | 0.0195 (10) | 0.0266 (11) | −0.0023 (8) | 0.0115 (9) | −0.0011 (8) |

*Geometric parameters (Å, °)*

| Zn1—O2 | 2.0713 (15) | C2—O4 | 1.290 (3) |
|---|---|---|---|
| Zn1—O2$^i$ | 2.0713 (15) | C2—C4 | 1.481 (3) |
| Zn1—O1 | 2.1407 (18) | N3—C9 | 1.336 (3) |
| Zn1—O1$^i$ | 2.1407 (18) | N3—C8 | 1.335 (3) |
| Zn1—N1$^i$ | 2.1592 (17) | N3—H3 | 0.8800 |
| Zn1—N1 | 2.1592 (17) | C3—C4 | 1.395 (3) |
| O1—H1B | 0.82 (3) | O4—H4A | 0.885 (16) |
| O1—H1A | 0.78 (3) | C5—C6 | 1.466 (2) |
| N1—C5 | 1.353 (3) | C6—C7 | 1.398 (3) |
| N1—C3 | 1.362 (2) | C6—C10 | 1.397 (3) |
| C1—O2 | 1.249 (3) | C7—C8 | 1.372 (3) |
| C1—O3 | 1.276 (2) | C7—H7 | 0.9500 |
| C1—C3 | 1.478 (3) | C8—H8 | 0.9500 |
| N2—C5 | 1.352 (3) | C9—C10 | 1.379 (3) |
| N2—C4 | 1.355 (2) | C9—H9 | 0.9500 |
| C2—O5 | 1.236 (3) | C10—H10 | 0.9500 |
| O2—Zn1—O2$^i$ | 180.0 | C9—N3—C8 | 121.80 (19) |

| | | | |
|---|---|---|---|
| O2—Zn1—O1 | 92.00 (8) | C9—N3—H3 | 119.1 |
| O2$^i$—Zn1—O1 | 88.00 (8) | C8—N3—H3 | 119.1 |
| O2—Zn1—O1$^i$ | 88.00 (8) | N1—C3—C4 | 108.82 (17) |
| O2$^i$—Zn1—O1$^i$ | 92.00 (8) | N1—C3—C1 | 118.85 (17) |
| O1—Zn1—O1$^i$ | 180.0 | C4—C3—C1 | 132.32 (18) |
| O2—Zn1—N1$^i$ | 99.47 (6) | C2—O4—H4A | 114.6 (16) |
| O2$^i$—Zn1—N1$^i$ | 80.53 (6) | N2—C4—C3 | 108.85 (17) |
| O1—Zn1—N1$^i$ | 89.17 (7) | N2—C4—C2 | 121.34 (18) |
| O1$^i$—Zn1—N1$^i$ | 90.83 (7) | C3—C4—C2 | 129.67 (18) |
| O2—Zn1—N1 | 80.53 (6) | N1—C5—N2 | 114.27 (17) |
| O2$^i$—Zn1—N1 | 99.47 (6) | N1—C5—C6 | 125.79 (18) |
| O1—Zn1—N1 | 90.83 (7) | N2—C5—C6 | 119.94 (18) |
| O1$^i$—Zn1—N1 | 89.17 (7) | C7—C6—C10 | 117.99 (18) |
| N1$^i$—Zn1—N1 | 180.0 | C7—C6—C5 | 119.26 (18) |
| Zn1—O1—H1B | 123.2 (19) | C10—C6—C5 | 122.73 (18) |
| Zn1—O1—H1A | 129 (2) | C8—C7—C6 | 120.1 (2) |
| H1B—O1—H1A | 105 (3) | C8—C7—H7 | 120.0 |
| C5—N1—C3 | 103.85 (16) | C6—C7—H7 | 120.0 |
| C5—N1—Zn1 | 147.69 (13) | N3—C8—C7 | 120.1 (2) |
| C3—N1—Zn1 | 104.67 (12) | N3—C8—H8 | 119.9 |
| O2—C1—O3 | 122.40 (19) | C7—C8—H8 | 119.9 |
| O2—C1—C3 | 118.55 (18) | N3—C9—C10 | 120.6 (2) |
| O3—C1—C3 | 119.02 (18) | N3—C9—H9 | 119.7 |
| C1—O2—Zn1 | 111.87 (13) | C10—C9—H9 | 119.7 |
| C5—N2—C4 | 104.20 (17) | C9—C10—C6 | 119.3 (2) |
| O5—C2—O4 | 121.93 (19) | C9—C10—H10 | 120.4 |
| O5—C2—C4 | 120.28 (19) | C6—C10—H10 | 120.4 |
| O4—C2—C4 | 117.77 (19) | | |
| O2—Zn1—N1—C5 | −170.7 (3) | N1—C3—C4—N2 | −1.3 (2) |
| O2$^i$—Zn1—N1—C5 | 9.3 (3) | C1—C3—C4—N2 | 177.0 (2) |
| O1—Zn1—N1—C5 | 97.4 (3) | N1—C3—C4—C2 | 174.4 (2) |
| O1$^i$—Zn1—N1—C5 | −82.6 (3) | C1—C3—C4—C2 | −7.3 (4) |
| N1$^i$—Zn1—N1—C5 | 37 (16) | O5—C2—C4—N2 | 10.2 (3) |
| O2—Zn1—N1—C3 | −19.40 (13) | O4—C2—C4—N2 | −171.3 (2) |
| O2$^i$—Zn1—N1—C3 | 160.60 (13) | O5—C2—C4—C3 | −165.1 (2) |
| O1—Zn1—N1—C3 | −111.28 (14) | O4—C2—C4—C3 | 13.5 (4) |
| O1$^i$—Zn1—N1—C3 | 68.72 (14) | C3—N1—C5—N2 | −1.2 (2) |
| N1$^i$—Zn1—N1—C3 | −171 (100) | Zn1—N1—C5—N2 | 150.2 (2) |
| O3—C1—O2—Zn1 | 166.35 (18) | C3—N1—C5—C6 | 179.3 (2) |
| C3—C1—O2—Zn1 | −15.4 (3) | Zn1—N1—C5—C6 | −29.3 (4) |
| O2$^i$—Zn1—O2—C1 | 24 (100) | C4—N2—C5—N1 | 0.4 (2) |
| O1—Zn1—O2—C1 | 110.06 (17) | C4—N2—C5—C6 | 179.97 (19) |
| O1$^i$—Zn1—O2—C1 | −69.94 (17) | N1—C5—C6—C7 | 164.9 (2) |
| N1$^i$—Zn1—O2—C1 | −160.45 (16) | N2—C5—C6—C7 | −14.7 (3) |
| N1—Zn1—O2—C1 | 19.55 (16) | N1—C5—C6—C10 | −13.6 (3) |

| | | | |
|---|---|---|---|
| C5—N1—C3—C4 | 1.5 (2) | N2—C5—C6—C10 | 166.9 (2) |
| Zn1—N1—C3—C4 | −163.20 (14) | C10—C6—C7—C8 | 3.5 (3) |
| C5—N1—C3—C1 | −177.10 (19) | C5—C6—C7—C8 | −175.1 (2) |
| Zn1—N1—C3—C1 | 18.2 (2) | C9—N3—C8—C7 | −0.8 (4) |
| O2—C1—C3—N1 | −3.1 (3) | C6—C7—C8—N3 | −2.2 (3) |
| O3—C1—C3—N1 | 175.2 (2) | C8—N3—C9—C10 | 2.6 (4) |
| O2—C1—C3—C4 | 178.8 (2) | N3—C9—C10—C6 | −1.2 (4) |
| O3—C1—C3—C4 | −3.0 (4) | C7—C6—C10—C9 | −1.8 (3) |
| C5—N2—C4—C3 | 0.6 (2) | C5—C6—C10—C9 | 176.7 (2) |
| C5—N2—C4—C2 | −175.55 (19) | | |

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

*Hydrogen-bond geometry (Å, °)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| O1—H1B···N2[ii] | 0.82 (3) | 2.08 (3) | 2.898 (3) | 178 (3) |
| N3—H3···O5[iii] | 0.88 | 1.89 | 2.755 (2) | 169. |
| O4—H4A···O3 | 0.89 (2) | 1.58 (2) | 2.459 (2) | 173 (3) |

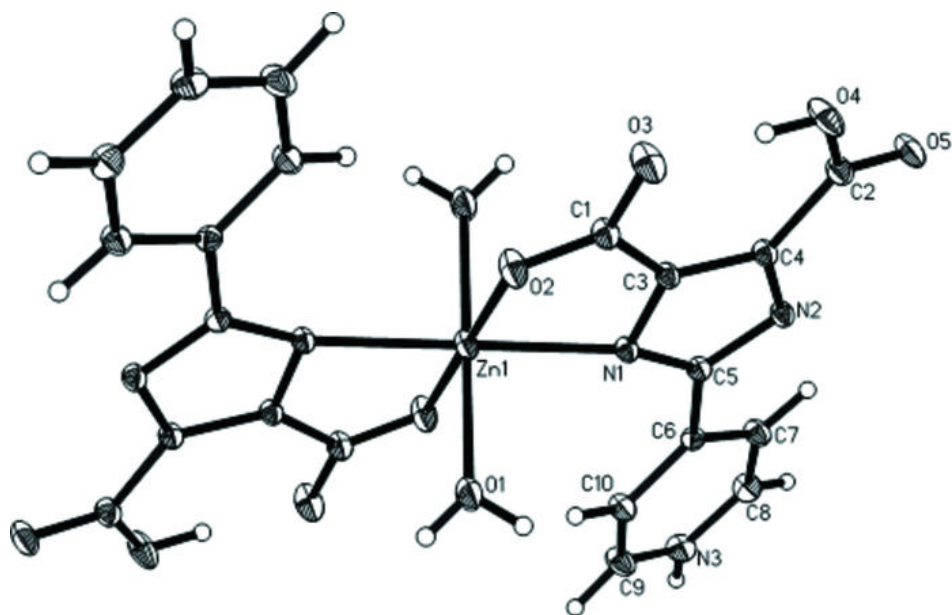Symmetry codes: (ii) $-x-1/2, -y+1/2, -z+1$; (iii) $-x-1/2, y-1/2, -z+3/2$.

**Fig. 1**

**Fig. 2**