

catena-Poly[[tetraqua(μ -4,4'-bipyridine- κ^2 N:N')zinc(II)] fumarate tetrahydrate]

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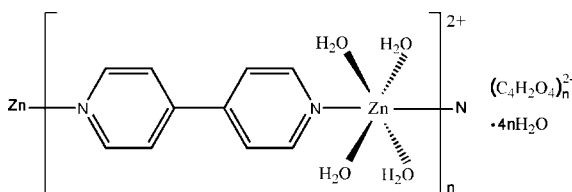
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.041; wR factor = 0.113; data-to-parameter ratio = 14.2.

In the title compound, $\{[\text{Zn}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4](\text{C}_4\text{H}_2\text{O}_4) \cdot 4\text{H}_2\text{O}\}_n$, the Zn^{II} atom is coordinated by two N atoms from two μ -4,4'-bipyridine ligands and four water molecules in a distorted octahedral geometry. The coordination unit is extended through the Zn–N bond, leading to a one-dimensional cationic chain. A twofold rotation axis passes through the Zn atom and along the axis of the 4,4'-bipyridine ligand. Each uncoordinated water molecule acts as both hydrogen-bond donor and acceptor. A three-dimensional network is constructed through hydrogen bonds involving water molecules and fumarate dianions.

Related literature

For related literature, see: Lu *et al.* (2006); Moulton & Zaworotko (2001); Nordell *et al.* (2003); Wagner *et al.* (2002); Wen *et al.* (2005); Yaghi *et al.* (1997); Zaworotko (2001); Zhou *et al.* (2007).



Experimental

Crystal data

$[\text{Zn}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4](\text{C}_4\text{H}_2\text{O}_4) \cdot 4\text{H}_2\text{O}$

$M_r = 479.74$

Monoclinic, $C2/c$

$a = 17.094$ (5) Å

$b = 11.394$ (3) Å

$c = 13.082$ (6) Å

$\beta = 126.652$ (2)°

$V = 2044.3$ (12) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.26$ mm⁻¹

$T = 293$ (2) K

$0.39 \times 0.28 \times 0.26$ mm

Data collection

Bruker SMART APEXII CCD
area-detector diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.626$, $T_{\text{max}} = 0.712$

7538 measured reflections
1907 independent reflections
1724 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.112$

$S = 1.09$

1907 reflections

134 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.98$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.86$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|--------------------------|-------------|--------------------------|------------|
| Zn1–O2 | 2.0697 (18) | Zn1–N1 | 2.146 (3) |
| Zn1–N2 ⁱ | 2.133 (3) | Zn1–O1 | 2.186 (2) |
| O2 ⁱⁱ –Zn1–O2 | 179.01 (9) | O2–Zn1–O1 | 88.01 (7) |
| O2–Zn1–N2 ⁱ | 89.50 (4) | N2 ⁱ –Zn1–O1 | 89.21 (4) |
| O2–Zn1–N1 | 90.50 (4) | N1–Zn1–O1 | 90.79 (4) |
| O2–Zn1–O1 ⁱⁱ | 91.97 (7) | O1 ⁱⁱ –Zn1–O1 | 178.43 (8) |

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

Table 2

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|-----------------------------------|-------|--------------|--------------|----------------|
| O1–H1W \cdots O3 ⁱⁱⁱ | 0.83 | 1.93 | 2.757 (2) | 173 |
| O1–H2W \cdots O4 ^{iv} | 0.83 | 2.01 | 2.835 (3) | 172 |
| O2–H3W \cdots O3 | 0.83 | 1.91 | 2.732 (2) | 172 |
| O2–H4W \cdots O6 ^v | 0.82 | 1.83 | 2.623 (3) | 162 |
| O3–H5W \cdots O5 | 0.83 | 1.88 | 2.707 (3) | 173 |
| O3–H6W \cdots O4 ^{iv} | 0.82 | 2.10 | 2.911 (3) | 172 |
| O4–H7W \cdots O6 ^v | 0.83 | 2.00 | 2.832 (3) | 175 |
| O4–H8W \cdots O5 | 0.83 | 1.99 | 2.811 (3) | 169 |

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

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: HY2122).

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supplementary materials

Acta Cryst. (2008). E64, m662-m663 [doi:10.1107/S1600536808009227]

***catena*-Poly[[tetraqua(μ -4,4'-bipyridine- κ^2 N:N')zinc(II)] fumarate tetrahydrate]**

Y. Tian, Y.-P. Wu, D.-S. Li, H. Wang and J.-W. Wang

Comment

Coordination polymer networks represent a result of applying supramolecular concepts to the design of new functional solids and are well exemplified by compounds in which transition metal centers (nodes) are connected by linear bidentate organic ligands (spacer groups) such as 4,4'-bipyridine (Lu *et al.*, 2006; Nordell *et al.*, 2003; Wagner *et al.*, 2002; Wen *et al.*, 2005; Yaghi *et al.*, 1997; Zhou *et al.*, 2007). These supramolecular structures are of interest as they provide opportunity for generating open framework compounds with controllable cavity sizes and they therefore have the potential to exhibit porosity and/or encapsulate guest molecules (Moulton & Zaworotko, 2001; Zaworotko, 2001).

The title compound consists of one $[\text{Zn}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4]^{2+}$ cation, one fumarate dianion and four lattice water molecules (Fig. 1). Each Zn^{II} atom is six-coordinated in an octahedral geometry with four O atoms of four water molecules in the equatorial plane and two N atoms from two μ -4,4'-bipyridine ligands in the axial sites, resulting a one-dimensional cationic chain along the *b*-axis. The two pyridyl rings of 4,4'-bipyridine present a torsion angle of 10.0 (2)°.

Each lattice water molecule acts as both hydrogen-bond donor and acceptor. In the crystal structure, the cationic chains are arranged parallel to the *bc* plane with the fumarate dianions and lattice water molecules located between the sheets composed of the chains. A three-dimensional supramolecular network is formed by hydrogen-bonding interactions involving the water molecules and fumarate dianions (Fig. 2).

Experimental

A mixture of $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.030 g, 0.1 mmol), 4,4'-bipyridine (0.016 g, 0.1 mmol), mercaptosuccinic acid (0.015 g, 0.1 mmol), NaOH (0.008 g, 0.2 mmol) and distilled water (10 ml) was sealed in a 25 ml Teflon-lined stainless autoclave and heated at 433 K for 72 h under autogenous pressure. After slowly cooling to room temperature, yellow block-like crystals of the title compound suitable for X-ray analysis were obtained from the reaction mixture by filtration.

Refinement

H atoms of the water molecules were located in a difference Fourier map and fixed in the refinements with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The remaining H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

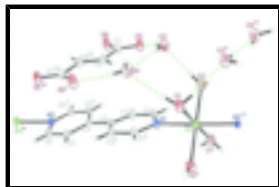


Fig. 1. The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $1 - x, y, 3/2 - z$; (ii) $1/2 - x, 3/2 - y, 1 - z$; (iii) $x, -1 + y, z$; (iv) $x, 1 + y, z$; (v) $1/2 - x, 1/2 - y, 1 - z$; (vi) $1/2 - x, -1/2 + y, 3/2 - z$.]

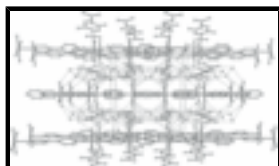


Fig. 2. A view of the three-dimensional network in the title compound, viewed down the a axis.

catena-Poly[[tetraaqua(μ -4,4'-bipyridine- $\kappa^2N:N'$)zinc(II)] fumarate tetrahydrate]

Crystal data

$[\text{Zn}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_4](\text{C}_4\text{H}_2\text{O}_4)\cdot 4\text{H}_2\text{O}$

$M_r = 479.74$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 17.094 (5) \text{ \AA}$

$b = 11.394 (3) \text{ \AA}$

$c = 13.082 (6) \text{ \AA}$

$\beta = 126.652 (2)^\circ$

$V = 2044.3 (12) \text{ \AA}^3$

$Z = 4$

$F_{000} = 1000$

$D_x = 1.559 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3920 reflections

$\theta = 2.3\text{--}28.2^\circ$

$\mu = 1.27 \text{ mm}^{-1}$

$T = 293 (2) \text{ K}$

Block, colorless

$0.39 \times 0.28 \times 0.26 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2) \text{ K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.626, T_{\max} = 0.712$

7538 measured reflections

1907 independent reflections

1724 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\text{max}} = 25.5^\circ$

$\theta_{\text{min}} = 2.3^\circ$

$h = -20 \rightarrow 20$

$k = -13 \rightarrow 13$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

| | |
|--|--|
| $R[F^2 > 2\sigma(F^2)] = 0.040$ | $w = 1/[\sigma^2(F_o^2) + (0.0789P)^2 + 0.2551P]$ |
| $wR(F^2) = 0.112$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.09$ | $(\Delta/\sigma)_{\max} < 0.001$ |
| 1907 reflections | $\Delta\rho_{\max} = 0.99 \text{ e } \text{\AA}^{-3}$ |
| 134 parameters | $\Delta\rho_{\min} = -0.86 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: SHELXL97 (Sheldrick, 2008) |
| Secondary atom site location: difference Fourier map | Extinction coefficient: 0 |

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| Zn1 | 0.5000 | 0.27603 (3) | 0.7500 | 0.02705 (18) |
| O1 | 0.41826 (14) | 0.27340 (13) | 0.54278 (17) | 0.0358 (4) |
| H1W | 0.3814 | 0.2172 | 0.5259 | 0.054* |
| H2W | 0.3864 | 0.3328 | 0.5041 | 0.054* |
| O2 | 0.36784 (13) | 0.27446 (13) | 0.72328 (17) | 0.0358 (4) |
| H3W | 0.3232 | 0.3120 | 0.6610 | 0.054* |
| H4W | 0.3621 | 0.2706 | 0.7812 | 0.054* |
| O3 | 0.21520 (12) | 0.40439 (15) | 0.53213 (15) | 0.0396 (4) |
| H5W | 0.2070 | 0.4658 | 0.5581 | 0.059* |
| H6W | 0.2331 | 0.4167 | 0.4872 | 0.059* |
| O4 | 0.29343 (13) | 0.53785 (16) | 0.89255 (16) | 0.0454 (5) |
| H7W | 0.3041 | 0.4667 | 0.8933 | 0.068* |
| H8W | 0.2635 | 0.5646 | 0.8191 | 0.068* |
| O5 | 0.19945 (14) | 0.59997 (17) | 0.63613 (17) | 0.0437 (4) |
| O6 | 0.17990 (18) | 0.79445 (17) | 0.6206 (2) | 0.0499 (5) |
| N1 | 0.5000 | 0.4644 (2) | 0.7500 | 0.0305 (6) |
| N2 | 0.5000 | 1.0888 (2) | 0.7500 | 0.0281 (6) |
| C1 | 0.47776 (19) | 0.5262 (2) | 0.8170 (2) | 0.0375 (6) |
| H1A | 0.4613 | 0.4854 | 0.8633 | 0.045* |
| C2 | 0.47816 (19) | 0.6469 (2) | 0.8206 (2) | 0.0352 (5) |
| H2A | 0.4638 | 0.6856 | 0.8702 | 0.042* |
| C3 | 0.5000 | 0.7114 (3) | 0.7500 | 0.0288 (7) |
| C4 | 0.5000 | 0.8413 (3) | 0.7500 | 0.0286 (7) |
| C5 | 0.5361 (2) | 0.9065 (2) | 0.6958 (3) | 0.0378 (6) |
| H5 | 0.5612 | 0.8681 | 0.6584 | 0.045* |
| C6 | 0.53453 (18) | 1.0269 (2) | 0.6974 (2) | 0.0358 (5) |
| H6 | 0.5587 | 1.0677 | 0.6601 | 0.043* |
| C7 | 0.20633 (18) | 0.6996 (2) | 0.6001 (2) | 0.0330 (5) |
| C8 | 0.24700 (18) | 0.7029 (2) | 0.5263 (2) | 0.0355 (5) |
| H8 | 0.2699 | 0.6328 | 0.5167 | 0.043* |

Atomic displacement parameters (\AA^2)

| | | | | | |
|----------|----------|----------|----------|----------|----------|
| U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----------|----------|----------|----------|----------|----------|

supplementary materials

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| Zn1 | 0.0401 (3) | 0.0197 (3) | 0.0348 (3) | 0.000 | 0.0296 (2) | 0.000 |
| O1 | 0.0500 (10) | 0.0311 (10) | 0.0364 (9) | -0.0015 (6) | 0.0313 (8) | 0.0004 (6) |
| O2 | 0.0455 (10) | 0.0390 (11) | 0.0419 (10) | 0.0077 (7) | 0.0362 (8) | 0.0091 (7) |
| O3 | 0.0540 (10) | 0.0334 (9) | 0.0408 (9) | -0.0009 (7) | 0.0334 (8) | -0.0006 (7) |
| O4 | 0.0691 (12) | 0.0338 (10) | 0.0394 (10) | 0.0009 (8) | 0.0357 (9) | 0.0017 (7) |
| O5 | 0.0722 (12) | 0.0362 (10) | 0.0497 (10) | -0.0015 (9) | 0.0509 (10) | 0.0025 (8) |
| O6 | 0.0879 (15) | 0.0365 (10) | 0.0668 (13) | -0.0006 (9) | 0.0685 (13) | 0.0000 (9) |
| N1 | 0.0468 (15) | 0.0214 (13) | 0.0374 (14) | 0.000 | 0.0327 (13) | 0.000 |
| N2 | 0.0357 (13) | 0.0213 (13) | 0.0346 (14) | 0.000 | 0.0250 (12) | 0.000 |
| C1 | 0.0596 (15) | 0.0256 (12) | 0.0471 (14) | -0.0003 (11) | 0.0424 (13) | 0.0025 (11) |
| C2 | 0.0574 (14) | 0.0249 (11) | 0.0435 (13) | 0.0034 (10) | 0.0410 (12) | -0.0010 (10) |
| C3 | 0.0341 (16) | 0.0228 (17) | 0.0319 (16) | 0.000 | 0.0211 (14) | 0.000 |
| C4 | 0.0354 (15) | 0.0247 (16) | 0.0308 (15) | 0.000 | 0.0224 (13) | 0.000 |
| C5 | 0.0595 (15) | 0.0249 (12) | 0.0547 (15) | 0.0010 (11) | 0.0480 (13) | -0.0029 (11) |
| C6 | 0.0528 (13) | 0.0271 (12) | 0.0489 (14) | 0.0000 (10) | 0.0418 (12) | 0.0019 (10) |
| C7 | 0.0462 (13) | 0.0339 (12) | 0.0312 (11) | -0.0023 (10) | 0.0297 (11) | -0.0014 (10) |
| C8 | 0.0528 (14) | 0.0326 (11) | 0.0401 (13) | 0.0016 (10) | 0.0381 (12) | -0.0007 (10) |

Geometric parameters (Å, °)

| | | | |
|---------------------------------------|-------------|--|-------------|
| Zn1—O2 ⁱ | 2.0697 (18) | N2—C6 | 1.344 (3) |
| Zn1—O2 | 2.0697 (18) | N2—C6 ⁱ | 1.344 (3) |
| Zn1—N2 ⁱⁱ | 2.133 (3) | N2—Zn1 ⁱⁱⁱ | 2.133 (3) |
| Zn1—N1 | 2.146 (3) | C1—C2 | 1.376 (3) |
| Zn1—O1 ⁱ | 2.186 (2) | C1—H1A | 0.9300 |
| Zn1—O1 | 2.186 (2) | C2—C3 | 1.394 (3) |
| O1—H1W | 0.8300 | C2—H2A | 0.9300 |
| O1—H2W | 0.8259 | C3—C2 ⁱ | 1.394 (3) |
| O2—H3W | 0.8283 | C3—C4 | 1.480 (5) |
| O2—H4W | 0.8210 | C4—C5 | 1.400 (3) |
| O3—H5W | 0.8263 | C4—C5 ⁱ | 1.400 (3) |
| O3—H6W | 0.8200 | C5—C6 | 1.372 (4) |
| O4—H7W | 0.8299 | C5—H5 | 0.9300 |
| O4—H8W | 0.8315 | C6—H6 | 0.9300 |
| O5—C7 | 1.261 (3) | C7—C8 | 1.490 (3) |
| O6—C7 | 1.261 (3) | C8—C8 ^{iv} | 1.312 (5) |
| N1—C1 ⁱ | 1.345 (3) | C8—H8 | 0.9300 |
| N1—C1 | 1.345 (3) | | |
| O2 ⁱ —Zn1—O2 | 179.01 (9) | C6—N2—Zn1 ⁱⁱⁱ | 121.70 (14) |
| O2 ⁱ —Zn1—N2 ⁱⁱ | 89.50 (4) | C6 ⁱ —N2—Zn1 ⁱⁱⁱ | 121.70 (14) |
| O2—Zn1—N2 ⁱⁱ | 89.50 (4) | N1—C1—C2 | 123.2 (2) |
| O2 ⁱ —Zn1—N1 | 90.50 (4) | N1—C1—H1A | 118.4 |
| O2—Zn1—N1 | 90.50 (4) | C2—C1—H1A | 118.4 |
| N2 ⁱⁱ —Zn1—N1 | 179.999 (1) | C1—C2—C3 | 120.1 (2) |
| O2 ⁱ —Zn1—O1 ⁱ | 88.01 (7) | C1—C2—H2A | 119.9 |
| O2—Zn1—O1 ⁱ | 91.97 (7) | C3—C2—H2A | 119.9 |

| | | | |
|---|--------------|--|-------------|
| N2 ⁱⁱ —Zn1—O1 ⁱ | 89.21 (4) | C2 ⁱ —C3—C2 | 116.4 (3) |
| N1—Zn1—O1 ⁱ | 90.79 (4) | C2 ⁱ —C3—C4 | 121.79 (14) |
| O2 ⁱ —Zn1—O1 | 91.98 (7) | C2—C3—C4 | 121.79 (14) |
| O2—Zn1—O1 | 88.01 (7) | C5—C4—C5 ⁱ | 115.9 (3) |
| N2 ⁱⁱ —Zn1—O1 | 89.21 (4) | C5—C4—C3 | 122.05 (15) |
| N1—Zn1—O1 | 90.79 (4) | C5 ⁱ —C4—C3 | 122.05 (15) |
| O1 ⁱ —Zn1—O1 | 178.43 (8) | C6—C5—C4 | 120.3 (2) |
| Zn1—O1—H1W | 99.4 | C6—C5—H5 | 119.9 |
| Zn1—O1—H2W | 116.6 | C4—C5—H5 | 119.9 |
| H1W—O1—H2W | 110.6 | N2—C6—C5 | 123.5 (2) |
| Zn1—O2—H3W | 115.7 | N2—C6—H6 | 118.3 |
| Zn1—O2—H4W | 124.3 | C5—C6—H6 | 118.3 |
| H3W—O2—H4W | 112.8 | O6—C7—O5 | 124.5 (2) |
| H5W—O3—H6W | 112.2 | O6—C7—C8 | 118.8 (2) |
| H7W—O4—H8W | 110.5 | O5—C7—C8 | 116.7 (2) |
| C1 ⁱ —N1—C1 | 116.8 (3) | C8 ^{iv} —C8—C7 | 124.9 (3) |
| C1 ⁱ —N1—Zn1 | 121.60 (14) | C8 ^{iv} —C8—H8 | 117.5 |
| C1—N1—Zn1 | 121.60 (14) | C7—C8—H8 | 117.5 |
| C6—N2—C6 ⁱ | 116.6 (3) | | |
| O2 ⁱ —Zn1—N1—C1 ⁱ | 45.69 (14) | C1—C2—C3—C4 | 179.23 (18) |
| O2—Zn1—N1—C1 ⁱ | -134.31 (14) | C2 ⁱ —C3—C4—C5 | -10.02 (17) |
| O1 ⁱ —Zn1—N1—C1 ⁱ | 133.71 (14) | C2—C3—C4—C5 | 169.98 (17) |
| O1—Zn1—N1—C1 ⁱ | -46.29 (14) | C2 ⁱ —C3—C4—C5 ⁱ | 169.97 (17) |
| O2 ⁱ —Zn1—N1—C1 | -134.31 (14) | C2—C3—C4—C5 ⁱ | -10.02 (17) |
| O2—Zn1—N1—C1 | 45.69 (14) | C5 ⁱ —C4—C5—C6 | -0.19 (18) |
| O1 ⁱ —Zn1—N1—C1 | -46.29 (15) | C3—C4—C5—C6 | 179.81 (18) |
| O1—Zn1—N1—C1 | 133.70 (15) | C6 ⁱ —N2—C6—C5 | -0.21 (19) |
| C1 ⁱ —N1—C1—C2 | -0.83 (19) | Zn1 ⁱⁱⁱ —N2—C6—C5 | 179.80 (19) |
| Zn1—N1—C1—C2 | 179.17 (19) | C4—C5—C6—N2 | 0.4 (4) |
| N1—C1—C2—C3 | 1.6 (4) | O6—C7—C8—C8 ^{iv} | -3.9 (5) |
| C1—C2—C3—C2 ⁱ | -0.77 (18) | O5—C7—C8—C8 ^{iv} | 174.9 (3) |

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| O1—H1W \cdots O3 ^v | 0.83 | 1.93 | 2.757 (2) | 173 |
| O1—H2W \cdots O4 ^{vi} | 0.83 | 2.01 | 2.835 (3) | 172 |
| O2—H3W \cdots O3 | 0.83 | 1.91 | 2.732 (2) | 172 |
| O2—H4W \cdots O6 ^{vii} | 0.82 | 1.83 | 2.623 (3) | 162 |
| O3—H5W \cdots O5 | 0.83 | 1.88 | 2.707 (3) | 173 |
| O3—H6W \cdots O4 ^{vi} | 0.82 | 2.10 | 2.911 (3) | 172 |
| O4—H7W \cdots O6 ^{vii} | 0.83 | 2.00 | 2.832 (3) | 175 |
| O4—H8W \cdots O5 | 0.83 | 1.99 | 2.811 (3) | 169 |

supplementary materials

Symmetry codes: (v) $-x+1/2, -y+1/2, -z+1$; (vi) $x, -y+1, z-1/2$; (vii) $-x+1/2, y-1/2, -z+3/2$.

Fig. 1

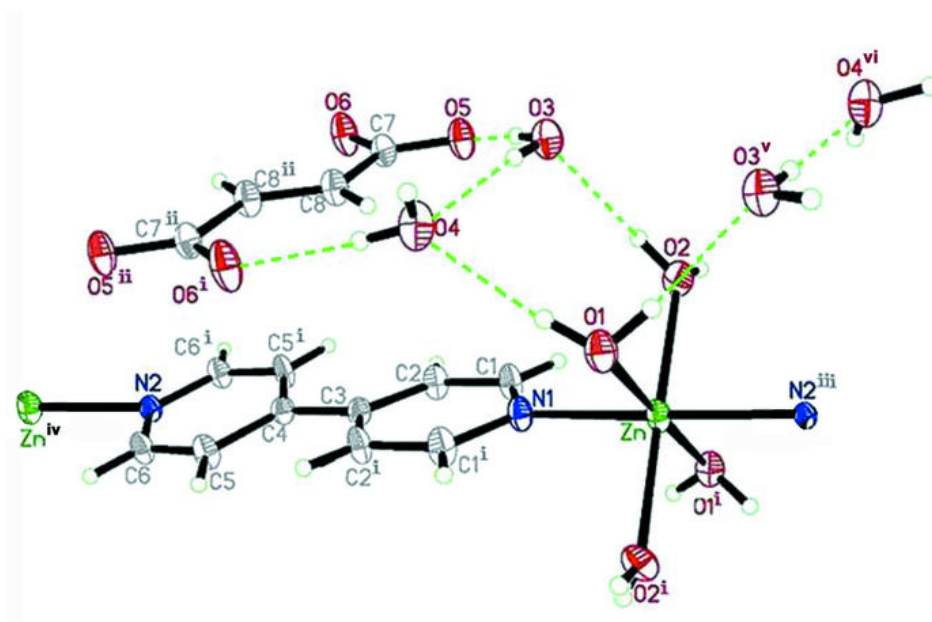


Fig. 2

