

catena-Poly[[bis(1-methylimidazole- κN^3)-zinc(II)]- μ -isophthalato- $\kappa^2 O^1:O^3$]

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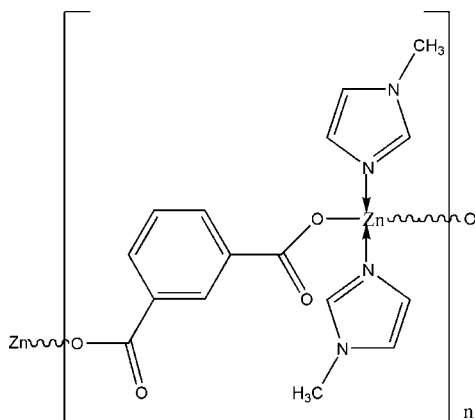
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.009$ Å; R factor = 0.068; wR factor = 0.207; data-to-parameter ratio = 13.5.

In the solid state, the title compound, $[Zn(C_8H_4O_4)(C_4H_6N_2)_2]_n$, exhibits the existence of polymeric zigzag chains extending along the a axis. Each Zn^{II} ion is coordinated by two N atoms [$Zn-N = 1.996$ (6) and 2.032 (5) Å] and two O atoms [$Zn-O = 1.930$ (4) and 1.976 (4) Å] in a distorted tetrahedral geometry. Weak $C-H \cdots O$ interactions contribute to the crystal packing stability.

Related literature

In the related zinc compound $[Zn(\text{isophthalato})(1-H\text{-imidazole})_2]$ (Yang *et al.*, 2002), the Zn^{II} ions also have a distorted tetrahedral environment.



Experimental

Crystal data

| | |
|--------------------------------|-----------------------------------|
| $[Zn(C_8H_4O_4)(C_4H_6N_2)_2]$ | $V = 3454.8$ (12) Å ³ |
| $M_r = 393.72$ | $Z = 8$ |
| Orthorhombic, $Pbca$ | Mo $K\alpha$ radiation |
| $a = 9.6820$ (19) Å | $\mu = 1.45$ mm ⁻¹ |
| $b = 13.224$ (3) Å | $T = 293$ (2) K |
| $c = 26.983$ (5) Å | $0.20 \times 0.10 \times 0.10$ mm |

Data collection

| | |
|-----------------------------------|--|
| Enraf-Nonius CAD-4 diffractometer | 2041 reflections with $I > 2\sigma(I)$ |
| Absorption correction: none | $R_{int} = 0.035$ |
| 3091 measured reflections | 3 standard reflections every 100 reflections |
| 2967 independent reflections | intensity decay: none |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.068$ | 40 restraints |
| $wR(F^2) = 0.207$ | H-atom parameters constrained |
| $S = 1.05$ | $\Delta\rho_{max} = 0.50$ e Å ⁻³ |
| 2967 reflections | $\Delta\rho_{min} = -0.61$ e Å ⁻³ |
| 220 parameters | |

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---------------------------|-------|--------------|--------------|----------------|
| $C1-H1A \cdots O3^i$ | 0.96 | 2.55 | 3.423 (10) | 150 |
| $C4-H4B \cdots O3^i$ | 0.93 | 2.31 | 3.150 (9) | 150 |
| $C11-H11A \cdots O2^{ii}$ | 0.93 | 2.54 | 3.457 (8) | 171 |

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

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2451).

References

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Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Yang, J., Zheng, S., Tao, J., Liu, G. & Chen, X. (2002). *Aust. J. Chem.* **55**, 741–744.

supplementary materials

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catena-Poly[[bis(1-methylimidazole- κN^3)zinc(II)]- μ -isophthalato- $\kappa^2 O^1:O^3$]

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Comment

In the title compound, (I) (Fig. 1), the zinc(II) centers are bridged by carboxylate groups of isophthalate ligands. Each Zn^{II} ion is coordinated by two N [Zn—N2 = 1.996 (6) Å, Zn—N4 = 2.032 (5) Å] and two O [Zn—O1 = 1.930 (4) Å, Zn—O4 = 1.976 (4) Å] atoms in a distorted tetrahedral geometry. All these values agree well with those observed in [Zn(isophthalato)(1-*H*-imidazole)₂] (Yang *et al.*, 2002). Each isophthalate dianion in (I) acts as a bidentate ligand to bridge two Zn^{II} atoms through two monodentate carboxylate groups, building a zigzag polymeric chain along the *a* axis. The metal–metal distance across each polymer backbone is 9.682 (7) Å.

In the crystal, weak C—H \cdots O interactions contribute to the crystal packing stability. In the corresponding zinc compound [Zn(isophthalato)(1-*H*-imidazole)₂] (Yang *et al.*, 2002), the Zn^{II} ions have a distorted tetrahedral environment.

Experimental

The reaction of ZnCl₂ (0.68 g, 5 mmol) with isophthalic acid (0.83 g, 5 mmol) in an aqueous-alcohol (3:1) solution (40 ml) at 363 K for 30 minutes produced a blue solution, to which 1-methylimidazole (0.82 g, 10 mmol) was added. The reaction solution was kept at room temperature after stirring for an hour at 333 K. Colourless crystals were obtained after a few days.

Refinement

H atoms were positioned geometrically (C—H = 0.93 or 0.96 Å) and allowed to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 times $U_{\text{eq}}(\text{C})$.

Figures

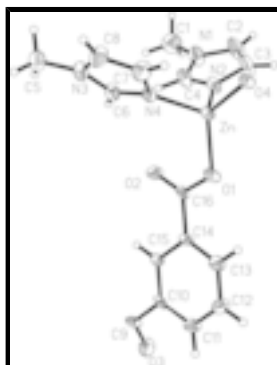


Fig. 1. A portion of the polymeric chain in (I) showing the atomic numbering and 30% probability displacement ellipsoids.

catena-Poly[[bis(1-methylimidazole- κ N³)zinc(II)]- μ -isophthalato- κ^2 O¹:O³]

Crystal data

| | |
|---|---|
| $[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_4\text{H}_6\text{N}_2)_2]$ | $F(000) = 1616$ |
| $M_r = 393.72$ | $D_x = 1.514 \text{ Mg m}^{-3}$ |
| Orthorhombic, <i>Pbca</i> | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: -P 2ac 2ab | Cell parameters from 25 reflections |
| $a = 9.6820 (19) \text{ \AA}$ | $\theta = 10\text{--}14^\circ$ |
| $b = 13.224 (3) \text{ \AA}$ | $\mu = 1.45 \text{ mm}^{-1}$ |
| $c = 26.983 (5) \text{ \AA}$ | $T = 293 \text{ K}$ |
| $V = 3454.8 (12) \text{ \AA}^3$ | Block, colourless |
| $Z = 8$ | $0.20 \times 0.10 \times 0.10 \text{ mm}$ |

Data collection

| | |
|---|--|
| Enraf–Nonius CAD-4 diffractometer | $R_{\text{int}} = 0.036$ |
| Radiation source: fine-focus sealed tube graphite | $\theta_{\text{max}} = 25.2^\circ$, $\theta_{\text{min}} = 1.5^\circ$ |
| ω scans | $h = 0 \rightarrow 11$ |
| 3091 measured reflections | $k = 0 \rightarrow 15$ |
| 2967 independent reflections | $l = 0 \rightarrow 32$ |
| 2041 reflections with $I > 2\sigma(I)$ | 3 standard reflections every 100 reflections |
| | intensity decay: none |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.068$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.207$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.1255P)^2]$ |
| 2967 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 220 parameters | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 40 restraints | $\Delta\rho_{\text{max}} = 0.50 \text{ e \AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.61 \text{ e \AA}^{-3}$ |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|-------------|--------------|----------------------------------|
| Zn | 0.18405 (6) | 0.12667 (5) | 0.12048 (3) | 0.0338 (3) |
| N1 | 0.1883 (6) | 0.3348 (5) | 0.2326 (2) | 0.0594 (17) |
| N2 | 0.1689 (5) | 0.2071 (4) | 0.1829 (2) | 0.0434 (13) |
| N3 | 0.2381 (6) | 0.3608 (4) | 0.0199 (2) | 0.0461 (14) |
| N4 | 0.1948 (5) | 0.2244 (4) | 0.06251 (18) | 0.0358 (12) |
| O1 | 0.3326 (4) | 0.0294 (4) | 0.11870 (16) | 0.0460 (12) |
| O2 | 0.4748 (4) | 0.1603 (3) | 0.12273 (18) | 0.0510 (13) |
| O3 | 1.0442 (4) | -0.0567 (4) | 0.1520 (2) | 0.0680 (16) |
| O4 | -0.0041 (4) | 0.0763 (3) | 0.10656 (16) | 0.0440 (11) |
| C1 | 0.2355 (10) | 0.4326 (6) | 0.2511 (3) | 0.081 |
| H1A | 0.3017 | 0.4605 | 0.2284 | 0.122* |
| H1B | 0.2777 | 0.4239 | 0.2830 | 0.122* |
| H1C | 0.1581 | 0.4776 | 0.2539 | 0.122* |
| C2 | 0.0944 (8) | 0.2711 (7) | 0.2534 (3) | 0.079 (3) |
| H2A | 0.0483 | 0.2798 | 0.2833 | 0.094* |
| C3 | 0.0821 (8) | 0.1945 (7) | 0.2223 (3) | 0.071 (2) |
| H3A | 0.0229 | 0.1399 | 0.2267 | 0.086* |
| C4 | 0.2306 (8) | 0.2910 (6) | 0.1911 (2) | 0.0523 (18) |
| H4B | 0.2976 | 0.3181 | 0.1703 | 0.063* |
| C5 | 0.2982 (8) | 0.4589 (5) | 0.0065 (3) | 0.060 (2) |
| H5A | 0.3727 | 0.4745 | 0.0288 | 0.089* |
| H5B | 0.2287 | 0.5104 | 0.0089 | 0.089* |
| H5C | 0.3326 | 0.4560 | -0.0268 | 0.089* |
| C6 | 0.2723 (6) | 0.3054 (5) | 0.0588 (2) | 0.0408 (15) |
| H6A | 0.3427 | 0.3218 | 0.0809 | 0.049* |
| C7 | 0.1029 (8) | 0.2310 (5) | 0.0239 (3) | 0.0568 (19) |
| H7A | 0.0326 | 0.1849 | 0.0175 | 0.068* |
| C8 | 0.1294 (8) | 0.3137 (5) | -0.0030 (3) | 0.059 (2) |
| H8A | 0.0835 | 0.3349 | -0.0315 | 0.070* |
| C9 | 0.9641 (6) | -0.0064 (5) | 0.1281 (2) | 0.0361 (14) |
| C10 | 0.8172 (5) | -0.0403 (5) | 0.1219 (2) | 0.0328 (14) |
| C11 | 0.7891 (7) | -0.1438 (5) | 0.1187 (2) | 0.0436 (16) |
| H11A | 0.8608 | -0.1907 | 0.1190 | 0.052* |
| C12 | 0.6544 (7) | -0.1755 (5) | 0.1151 (3) | 0.060 (2) |
| H12A | 0.6356 | -0.2443 | 0.1126 | 0.072* |
| C13 | 0.5473 (7) | -0.1080 (5) | 0.1151 (3) | 0.0510 (18) |
| H13A | 0.4572 | -0.1318 | 0.1121 | 0.061* |
| C14 | 0.5702 (5) | -0.0054 (4) | 0.1195 (2) | 0.0301 (12) |
| C15 | 0.7082 (5) | 0.0286 (4) | 0.1222 (2) | 0.0321 (13) |
| H15A | 0.7265 | 0.0975 | 0.1242 | 0.039* |

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C16 0.4545 (6) 0.0702 (5) 0.1210 (2) 0.0340 (14)

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|--------------|-------------|------------|
| Zn | 0.0166 (4) | 0.0401 (4) | 0.0446 (5) | 0.0005 (3) | -0.0007 (3) | 0.0023 (3) |
| N1 | 0.067 (4) | 0.058 (3) | 0.053 (3) | -0.018 (3) | 0.016 (3) | -0.013 (3) |
| N2 | 0.032 (3) | 0.056 (3) | 0.043 (3) | -0.008 (2) | 0.006 (2) | 0.001 (2) |
| N3 | 0.051 (3) | 0.052 (3) | 0.035 (3) | -0.008 (3) | 0.003 (3) | 0.003 (3) |
| N4 | 0.024 (2) | 0.043 (3) | 0.041 (3) | -0.009 (2) | -0.009 (2) | 0.006 (2) |
| O1 | 0.019 (2) | 0.057 (3) | 0.062 (3) | 0.004 (2) | 0.0020 (19) | 0.003 (2) |
| O2 | 0.021 (2) | 0.036 (2) | 0.096 (4) | -0.0011 (19) | -0.001 (2) | 0.004 (2) |
| O3 | 0.023 (2) | 0.075 (3) | 0.106 (4) | -0.001 (2) | -0.013 (3) | 0.041 (3) |
| O4 | 0.020 (2) | 0.049 (3) | 0.063 (3) | -0.0021 (19) | -0.004 (2) | 0.008 (2) |
| C1 | 0.081 | 0.081 | 0.081 | 0.000 | 0.000 | 0.000 |
| C2 | 0.068 (5) | 0.100 (6) | 0.068 (5) | -0.024 (4) | 0.038 (4) | -0.019 (4) |
| C3 | 0.064 (5) | 0.081 (5) | 0.069 (5) | -0.030 (4) | 0.031 (4) | -0.006 (4) |
| C4 | 0.052 (4) | 0.071 (4) | 0.033 (3) | -0.010 (3) | 0.015 (3) | -0.005 (3) |
| C5 | 0.069 (5) | 0.054 (4) | 0.056 (5) | -0.010 (4) | 0.008 (4) | 0.004 (4) |
| C6 | 0.034 (3) | 0.051 (4) | 0.037 (4) | -0.006 (3) | 0.001 (3) | 0.003 (3) |
| C7 | 0.053 (4) | 0.054 (4) | 0.063 (5) | -0.009 (4) | -0.017 (4) | 0.005 (4) |
| C8 | 0.061 (5) | 0.060 (5) | 0.054 (5) | -0.004 (4) | -0.017 (4) | 0.017 (4) |
| C9 | 0.017 (3) | 0.046 (3) | 0.045 (4) | 0.006 (3) | 0.000 (3) | -0.007 (3) |
| C10 | 0.011 (3) | 0.054 (4) | 0.033 (3) | -0.002 (2) | 0.002 (2) | 0.005 (3) |
| C11 | 0.026 (3) | 0.041 (4) | 0.064 (4) | 0.005 (3) | -0.006 (3) | -0.007 (3) |
| C12 | 0.029 (4) | 0.031 (3) | 0.119 (7) | -0.006 (3) | -0.005 (4) | -0.006 (4) |
| C13 | 0.024 (3) | 0.042 (4) | 0.087 (5) | -0.005 (3) | -0.002 (3) | -0.007 (3) |
| C14 | 0.015 (3) | 0.037 (3) | 0.038 (3) | 0.002 (2) | -0.004 (2) | 0.001 (3) |
| C15 | 0.017 (3) | 0.034 (3) | 0.046 (4) | -0.001 (2) | -0.002 (2) | 0.005 (3) |
| C16 | 0.012 (3) | 0.049 (4) | 0.041 (3) | 0.001 (3) | 0.001 (2) | 0.008 (3) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|------------|---------------------|-----------|
| Zn—O1 | 1.930 (4) | C3—H3A | 0.9300 |
| Zn—O4 | 1.976 (4) | C4—H4B | 0.9300 |
| Zn—N2 | 1.996 (6) | C5—H5A | 0.9600 |
| Zn—N4 | 2.032 (5) | C5—H5B | 0.9600 |
| N1—C4 | 1.327 (8) | C5—H5C | 0.9600 |
| N1—C2 | 1.360 (9) | C6—H6A | 0.9300 |
| N1—C1 | 1.459 (10) | C7—C8 | 1.339 (9) |
| N2—C4 | 1.279 (8) | C7—H7A | 0.9300 |
| N2—C3 | 1.367 (8) | C8—H8A | 0.9300 |
| N3—C6 | 1.322 (8) | C9—O4 ⁱⁱ | 1.277 (8) |
| N3—C8 | 1.371 (9) | C9—C10 | 1.501 (7) |
| N3—C5 | 1.468 (8) | C10—C15 | 1.395 (8) |
| N4—C6 | 1.311 (7) | C10—C11 | 1.399 (9) |
| N4—C7 | 1.372 (8) | C11—C12 | 1.373 (8) |
| O1—C16 | 1.299 (7) | C11—H11A | 0.9300 |

| | | | |
|------------------------|-------------|--------------------------|------------|
| O2—C16 | 1.209 (8) | C12—C13 | 1.368 (9) |
| O3—C9 | 1.207 (7) | C12—H12A | 0.9300 |
| O4—C9 ⁱ | 1.277 (8) | C13—C14 | 1.381 (8) |
| C1—H1A | 0.9600 | C13—H13A | 0.9300 |
| C1—H1B | 0.9600 | C14—C15 | 1.411 (7) |
| C1—H1C | 0.9600 | C14—C16 | 1.502 (8) |
| C2—C3 | 1.319 (11) | C15—H15A | 0.9300 |
| C2—H2A | 0.9300 | | |
| O1—Zn—O4 | 117.23 (19) | H5A—C5—H5B | 109.5 |
| O1—Zn—N2 | 115.5 (2) | N3—C5—H5C | 109.5 |
| O4—Zn—N2 | 105.80 (19) | H5A—C5—H5C | 109.5 |
| O1—Zn—N4 | 111.51 (19) | H5B—C5—H5C | 109.5 |
| O4—Zn—N4 | 96.63 (18) | N4—C6—N3 | 111.7 (6) |
| N2—Zn—N4 | 108.3 (2) | N4—C6—H6A | 124.2 |
| C4—N1—C2 | 106.5 (6) | N3—C6—H6A | 124.2 |
| C4—N1—C1 | 125.3 (7) | C8—C7—N4 | 109.9 (6) |
| C2—N1—C1 | 128.2 (7) | C8—C7—H7A | 125.1 |
| C4—N2—C3 | 104.9 (6) | N4—C7—H7A | 125.1 |
| C4—N2—Zn | 125.0 (5) | C7—C8—N3 | 105.8 (6) |
| C3—N2—Zn | 129.6 (5) | C7—C8—H8A | 127.1 |
| C6—N3—C8 | 107.4 (5) | N3—C8—H8A | 127.1 |
| C6—N3—C5 | 125.9 (6) | O3—C9—O4 ⁱⁱ | 124.1 (6) |
| C8—N3—C5 | 126.5 (6) | O3—C9—C10 | 120.2 (6) |
| C6—N4—C7 | 105.2 (5) | O4 ⁱⁱ —C9—C10 | 115.7 (5) |
| C6—N4—Zn | 127.4 (4) | C15—C10—C11 | 119.5 (5) |
| C7—N4—Zn | 126.2 (4) | C15—C10—C9 | 121.5 (6) |
| C16—O1—Zn | 113.5 (4) | C11—C10—C9 | 118.9 (5) |
| C9 ⁱ —O4—Zn | 115.1 (4) | C12—C11—C10 | 119.2 (6) |
| N1—C1—H1A | 109.5 | C12—C11—H11A | 120.4 |
| N1—C1—H1B | 109.5 | C10—C11—H11A | 120.4 |
| H1A—C1—H1B | 109.5 | C13—C12—C11 | 121.4 (6) |
| N1—C1—H1C | 109.5 | C13—C12—H12A | 119.3 |
| H1A—C1—H1C | 109.5 | C11—C12—H12A | 119.3 |
| H1B—C1—H1C | 109.5 | C12—C13—C14 | 121.2 (6) |
| C3—C2—N1 | 105.9 (7) | C12—C13—H13A | 119.4 |
| C3—C2—H2A | 127.0 | C14—C13—H13A | 119.4 |
| N1—C2—H2A | 127.0 | C13—C14—C15 | 118.0 (5) |
| C2—C3—N2 | 110.2 (7) | C13—C14—C16 | 122.4 (5) |
| C2—C3—H3A | 124.9 | C15—C14—C16 | 119.5 (5) |
| N2—C3—H3A | 124.9 | C10—C15—C14 | 120.5 (5) |
| N2—C4—N1 | 112.4 (6) | C10—C15—H15A | 119.7 |
| N2—C4—H4B | 123.8 | C14—C15—H15A | 119.7 |
| N1—C4—H4B | 123.8 | O2—C16—O1 | 124.0 (6) |
| N3—C5—H5A | 109.5 | O2—C16—C14 | 122.4 (5) |
| N3—C5—H5B | 109.5 | O1—C16—C14 | 113.6 (5) |
| O1—Zn—N2—C4 | 89.0 (6) | Zn—N4—C6—N3 | -169.7 (4) |
| O4—Zn—N2—C4 | -139.6 (6) | C8—N3—C6—N4 | 0.9 (8) |
| N4—Zn—N2—C4 | -36.9 (6) | C5—N3—C6—N4 | 176.2 (6) |

supplementary materials

| | | | |
|--------------------------|------------|------------------------------|------------|
| O1—Zn—N2—C3 | -100.1 (7) | C6—N4—C7—C8 | 1.9 (8) |
| O4—Zn—N2—C3 | 31.4 (7) | Zn—N4—C7—C8 | 170.1 (5) |
| N4—Zn—N2—C3 | 134.1 (7) | N4—C7—C8—N3 | -1.4 (9) |
| O1—Zn—N4—C6 | -81.7 (5) | C6—N3—C8—C7 | 0.3 (9) |
| O4—Zn—N4—C6 | 155.6 (5) | C5—N3—C8—C7 | -175.0 (6) |
| N2—Zn—N4—C6 | 46.5 (6) | O3—C9—C10—C15 | 141.9 (7) |
| O1—Zn—N4—C7 | 112.7 (6) | O4 ⁱⁱ —C9—C10—C15 | -38.6 (9) |
| O4—Zn—N4—C7 | -10.0 (6) | O3—C9—C10—C11 | -34.3 (9) |
| N2—Zn—N4—C7 | -119.1 (6) | O4 ⁱⁱ —C9—C10—C11 | 145.2 (6) |
| O4—Zn—O1—C16 | 170.5 (4) | C15—C10—C11—C12 | 1.0 (10) |
| N2—Zn—O1—C16 | -63.7 (4) | C9—C10—C11—C12 | 177.3 (6) |
| N4—Zn—O1—C16 | 60.4 (4) | C10—C11—C12—C13 | -0.7 (12) |
| O1—Zn—O4—C9 ⁱ | 44.5 (5) | C11—C12—C13—C14 | -1.0 (12) |
| N2—Zn—O4—C9 ⁱ | -86.0 (4) | C12—C13—C14—C15 | 2.4 (11) |
| N4—Zn—O4—C9 ⁱ | 162.9 (4) | C12—C13—C14—C16 | -178.4 (6) |
| C4—N1—C2—C3 | -2.1 (10) | C11—C10—C15—C14 | 0.3 (9) |
| C1—N1—C2—C3 | 177.6 (8) | C9—C10—C15—C14 | -175.9 (5) |
| N1—C2—C3—N2 | 1.5 (11) | C13—C14—C15—C10 | -2.0 (10) |
| C4—N2—C3—C2 | -0.2 (10) | C16—C14—C15—C10 | 178.7 (5) |
| Zn—N2—C3—C2 | -172.6 (6) | Zn—O1—C16—O2 | -1.8 (8) |
| C3—N2—C4—N1 | -1.2 (9) | Zn—O1—C16—C14 | -180.0 (4) |
| Zn—N2—C4—N1 | 171.6 (5) | C13—C14—C16—O2 | -176.8 (7) |
| C2—N1—C4—N2 | 2.1 (9) | C15—C14—C16—O2 | 2.4 (9) |
| C1—N1—C4—N2 | -177.6 (7) | C13—C14—C16—O1 | 1.4 (8) |
| C7—N4—C6—N3 | -1.7 (7) | C15—C14—C16—O1 | -179.4 (5) |

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

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|-------|-------------|-------------|---------------|
| C1—H1A \cdots O3 ⁱⁱⁱ | 0.96 | 2.55 | 3.423 (10) | 150 |
| C4—H4B \cdots O3 ⁱⁱⁱ | 0.93 | 2.31 | 3.150 (9) | 150 |
| C11—H11A \cdots O2 ^{iv} | 0.93 | 2.54 | 3.457 (8) | 171 |

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

Fig. 1

