

Bis(4-methoxybenzoato)- κ^2O,O' ; κO -bis(nicotinamide- κN^1)zinc(II)

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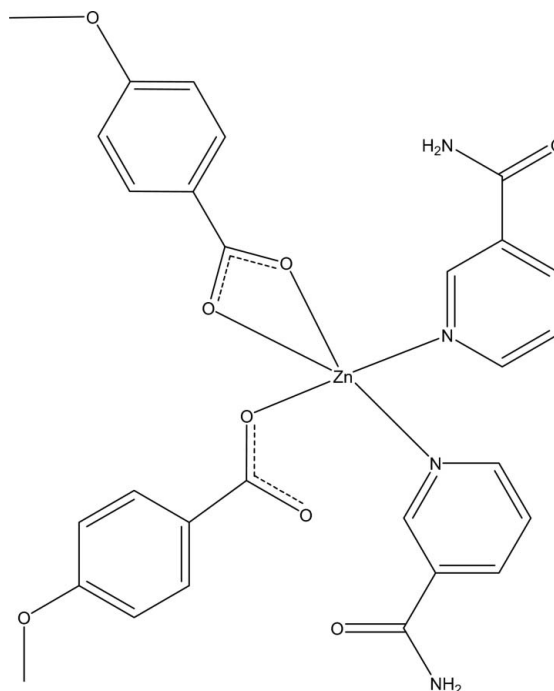
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.037; wR factor = 0.092; data-to-parameter ratio = 17.3.

The asymmetric unit of the title complex, $[Zn(C_8H_7O_3)_2(C_6H_6N_2O)_2]$, contains three crystallographically independent molecules with similar configurations. The Zn^{II} cation is coordinated by two N atoms of two nicotinamide ligands and three O atoms from two 4-methoxybenzoate anions in a distorted trigonal-bipyramidal geometry. In each independent molecule, one $Zn-O$ bond distance [2.5181 (12), 2.5931 (12) and 2.4085 (12) Å for the three molecules] is significantly longer than the other two. In the crystal structure, extensive $N-H \cdots O$ and $C-H \cdots O$ hydrogen bonding links the molecules into a three-dimensional network. $\pi-\pi$ contacts between the pyridine rings and between the pyridine and benzene rings [centroid-centroid distances = 3.7655 (9) and 3.8453 (10) Å, respectively] further stabilize the crystal structure.

Related literature

Nicotinamide is a form of niacin; for background to niacin, see: Krishnamachari (1974). For N,N -diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Greenaway *et al.* (1984); Hökelek *et al.* (2009*a,b*, 2010*a,b,c,d*).



Experimental

Crystal data

$[Zn(C_8H_7O_3)_2(C_6H_6N_2O)_2]$

$M_r = 611.92$

Triclinic, $P\bar{1}$

$a = 10.6828$ (2) Å

$b = 16.6230$ (3) Å

$c = 23.8011$ (4) Å

$\alpha = 77.050$ (2)°

$\beta = 85.654$ (3)°

$\gamma = 78.526$ (2)°

$V = 4034.63$ (13) Å³

$Z = 6$

Mo $K\alpha$ radiation

$\mu = 0.97$ mm⁻¹

$T = 100$ K

$0.26 \times 0.24 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.776$, $T_{\max} = 0.823$

72134 measured reflections

20155 independent reflections

14979 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.092$

$S = 1.03$

20155 reflections

1162 parameters

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.42$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.46$ e Å⁻³

Table 1

Selected bond lengths (Å).

| | | | |
|---------|-------------|---------|-------------|
| Zn1—O1 | 2.5181 (12) | Zn2—N5 | 2.0536 (15) |
| Zn1—O2 | 1.9631 (12) | Zn2—N7 | 2.0669 (14) |
| Zn1—O5 | 1.9392 (12) | Zn3—O17 | 2.4085 (12) |
| Zn1—N1 | 2.0793 (15) | Zn3—O18 | 1.9987 (12) |
| Zn1—N3 | 2.0561 (14) | Zn3—O21 | 1.9436 (12) |
| Zn2—O9 | 1.9523 (12) | Zn3—N9 | 2.0840 (14) |
| Zn2—O10 | 2.5931 (12) | Zn3—N11 | 2.0613 (14) |
| Zn2—O13 | 1.9317 (12) | | |

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

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|----------------------------------------|-------------|---------------|-----------------------|-------------------------|
| N2—H2 <i>A</i> ...O24 ⁱ | 0.82 (2) | 2.16 (2) | 2.966 (2) | 168.8 (2) |
| N2—H2 <i>B</i> ...O4 ⁱⁱ | 0.84 (2) | 2.16 (2) | 2.991 (2) | 176.6 (2) |
| N4—H4 <i>A</i> ...O17 ⁱⁱⁱ | 0.83 (2) | 2.08 (2) | 2.903 (2) | 169.4 (2) |
| N4—H4 <i>B</i> ...O16 ^{iv} | 0.85 (2) | 2.59 (2) | 3.152 (2) | 125.0 (2) |
| N4—H4 <i>B</i> ...O19 ^v | 0.85 (2) | 2.52 (2) | 3.225 (2) | 141.3 (2) |
| N6—H6 <i>A</i> ...O23 ^{vi} | 0.78 (2) | 2.40 (2) | 3.073 (2) | 146 (2) |
| N6—H6 <i>B</i> ...O10 ^{vii} | 0.86 (2) | 2.11 (2) | 2.959 (2) | 170.3 (2) |
| N8—H8 <i>D</i> ...O8 ^{iv} | 0.79 (2) | 2.13 (2) | 2.909 (2) | 166 (2) |
| N8—H8 <i>E</i> ...O20 ^{viii} | 0.87 (2) | 2.19 (2) | 3.058 (2) | 174.8 (2) |
| N10—H10 <i>A</i> ...O12 ^{ix} | 0.87 (2) | 2.21 (2) | 3.077 (2) | 172 (2) |
| N10—H10 <i>B</i> ...O15 ^{vi} | 0.84 (2) | 2.10 (2) | 2.917 (2) | 162.8 (2) |
| N12—H12 <i>A</i> ...O11 ⁱⁱⁱ | 0.83 (2) | 2.55 (2) | 3.268 (2) | 145 (2) |
| N12—H12 <i>B</i> ...O1 ⁱⁱⁱ | 0.87 (2) | 2.07 (2) | 2.940 (2) | 171.9 (2) |

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

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: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (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: XU5015).

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supplementary materials

Acta Cryst. (2010). E66, m1135-m1136 [doi:10.1107/S1600536810032885]

Bis(4-methoxybenzoato)- κ^2O,O' ; κO -bis(nicotinamide- κN^1)zinc(II)

T. Hökelek, G. Saka, B. Tercan, E. Tenlik and H. Necefoglu

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 monomeric complex, and its asymmetric unit contains three crystallographically independent molecules. The Zn^{II} centers are coordinated by three O atoms from two 4-methoxybenzoate ligands, which act in different modes—monodentate and bidentate, respectively, and N atoms of the nicotinamide ligands (Fig. 1). So that, all three independent molecules are five-coordinated in distorted trigonal-bipyramidal geometry. The structures of similar complexes of Cu^{II}, Co^{II}, Ni^{II} and Zn^{II} ions, [Cu(C₈H₇O₂)₂(C₆H₆N₂O)₂].2(H₂O), (II) (Hökelek *et al.*, 2010*a*), [Co(C₈H₇O₃)₂(C₆H₆N₂O)(H₂O)₂], (III) (Hökelek *et al.*, 2010*b*), [Co(C₈H₇O₃)₂(C₆H₆N₂O)₂(H₂O)₂].2H₂O, (IV) (Hökelek *et al.*, 2010*c*), [Ni(C₈H₇O₃)₂(C₆H₆N₂O)₂(H₂O)₂].2H₂O, (V) (Hökelek *et al.*, 2010*d*), [Zn(C₈H₈NO₂)₂(C₆H₆N₂O)₂].H₂O, (VI) (Hökelek *et al.*, 2009*a*) and [Zn(C₉H₁₀NO₂)₂(C₆H₆N₂O)₂(H₂O)₂], (VII) (Hökelek *et al.*, 2009*b*) have also been determined.

In the title compound (Fig. 1), the average Zn—O bond length is 2.1387 (12) Å (Table 1) and the Zn atoms are displaced out of the least-squares planes of the carboxylate groups: Zn1 by -0.0684 (2) Å and -0.1173 (2) Å from (O1/C1/O2) and (O4/C9/O5), Zn2 by -0.0104 (2) Å and 0.1363 (2) Å from (O9/C29/O10) and (O12/C37/O13) and Zn3 by 0.0517 (2) and -0.0728 (2) Å from (O17/C57/O18) and (O20/C65/O21), respectively. The dihedral angles between the planar carboxylate groups and the adjacent benzene rings A (C2—C7), B (C10—C15), E (C30—C35), F (C38—C43), I (C58—C63) and J (C66—C71) are 4.72 (8), 5.90 (15), 1.88 (13), 1.44 (9), 3.66 (9) and 9.14 (12) °, respectively, while those between rings A, B, C (N1/C17—C21), D (N3/C23—C27), E, F, G (N5/C45—C49), H (N7/C51—C55), I, J, K (N9/C73—C77) and L (N11/C79—C83) are A/B = 83.56 (6), A/C = 20.47 (6), A/D = 79.71 (5), B/C = 82.66 (5), B/D = 14.74 (5), C/D = 74.07 (5), E/F = 80.00 (6), E/G = 69.70 (5), E/H = 21.71 (5), F/G = 10.67 (5), F/H = 77.31 (6), G/H = 66.72 (5), I/J = 79.56 (6), I/K = 24.86 (5), I/L = 83.23 (5), J/K = 71.13 (6), J/L = 5.72 (6) and K/L = 72.72 (6) °.

In (I), the O1—Zn1—O2, O9—Zn2—O10 and O17—Zn3—O18 angles are 57.53 (5)°, 56.19 (5) and 59.04 (4)°, respectively. The corresponding O—M—O (where M is a metal) angles are 60.32 (4)° in (III), 59.02 (8)° in (VI), 60.03 (6)° in (VII) and 55.2 (1)° in [Cu(Asp)₂(py)₂] (where Asp is acetylsalicylate and py is pyridine) [(VIII); Greenaway *et al.*, 1984].

In the crystal structure, intramolecular C—H···O and intermolecular N—H···O and C—H···O hydrogen bonds (Table 2) link the molecules into a three-dimensional network. The π — π contacts between the pyridine rings and between the pyridine and benzene rings, Cg4—Cg12ⁱ and Cg4—Cg2ⁱⁱ [symmetry codes: (i) $x - 1, y + 1, z$, (ii) $1 - x, 1 - y, 1 - z$, where Cg2, Cg4 and Cg12 are the centroids of the rings B (C10—C15), D (N3/C23—C27) and L (N11/C79—C83), respectively] may also stabilize the structure, with centroid-centroid distances of 3.7655 (9) and 3.8453 (10) Å, respectively.

Experimental

The title compound was prepared by the reaction of ZnSO₄·H₂O (1.80 g, 10 mmol) in H₂O (50 ml) and NA (2.44 g, 20 mmol) in H₂O (50 ml) with sodium 4-methoxybenzoate (3.48 g, 20 mmol) in H₂O (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving colorless single crystals.

Refinement

H atoms of NH₂ groups were located in difference Fourier maps 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, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl H and $x = 1.2$ for aromatic H atoms.

Figures

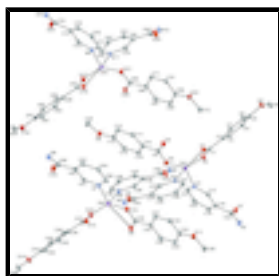


Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

Bis(4-methoxybenzoato)- κ^2O,O' ; κO -bis(nicotinamide- κN^1)zinc(II)

Crystal data

[Zn(C₈H₇O₃)₂(C₆H₆N₂O)₂]

$M_r = 611.92$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 10.6828(2)$ Å

$b = 16.6230(3)$ Å

$c = 23.8011(4)$ Å

$\alpha = 77.050(2)^\circ$

$\beta = 85.654(3)^\circ$

$\gamma = 78.526(2)^\circ$

$V = 4034.63(13)$ Å³

$Z = 6$

$F(000) = 1896$

$D_x = 1.511$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9864 reflections

$\theta = 2.5\text{--}28.1^\circ$

$\mu = 0.97$ mm⁻¹

$T = 100$ K

Block, colorless

$0.26 \times 0.24 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

20155 independent reflections

14979 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

φ and ω scans $\theta_{\max} = 28.5^\circ$, $\theta_{\min} = 0.9^\circ$
 Absorption correction: multi-scan $h = -14 \rightarrow 13$
 (SADABS; Bruker, 2005)
 $T_{\min} = 0.776$, $T_{\max} = 0.823$ $k = -20 \rightarrow 22$
 72134 measured reflections $l = -31 \rightarrow 29$

Refinement

Refinement on F^2 Primary atom site location: structure-invariant direct methods
 Least-squares matrix: full Secondary atom site location: difference Fourier map
 $R[F^2 > 2\sigma(F^2)] = 0.037$ Hydrogen site location: inferred from neighbouring sites
 $wR(F^2) = 0.092$ H atoms treated by a mixture of independent and constrained refinement
 $S = 1.03$ $w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.1789P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 20155 reflections $(\Delta/\sigma)_{\max} = 0.006$
 1162 parameters $\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$
 0 restraints $\Delta\rho_{\min} = -0.46 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|--------------|----------------------------------|
| Zn1 | 0.313492 (18) | 0.366125 (12) | 0.622308 (9) | 0.01588 (6) |
| Zn2 | 0.352863 (19) | 0.301859 (12) | 1.053489 (9) | 0.01722 (6) |
| Zn3 | 0.976026 (18) | 1.016176 (12) | 0.288848 (9) | 0.01588 (6) |
| O1 | 0.39085 (11) | 0.33289 (7) | 0.72375 (5) | 0.0209 (3) |
| O2 | 0.22139 (11) | 0.30695 (8) | 0.68818 (5) | 0.0208 (3) |
| O3 | 0.15524 (12) | 0.13733 (8) | 0.95436 (5) | 0.0250 (3) |
| O4 | 0.17745 (11) | 0.52611 (8) | 0.62504 (5) | 0.0216 (3) |
| O5 | 0.37345 (11) | 0.47164 (7) | 0.59757 (5) | 0.0208 (3) |
| O6 | 0.43183 (11) | 0.84998 (7) | 0.52950 (5) | 0.0204 (3) |
| O7 | 0.25931 (12) | 0.53514 (9) | 0.40279 (6) | 0.0322 (4) |
| O8 | 0.47812 (11) | 0.03835 (7) | 0.61971 (6) | 0.0224 (3) |
| O9 | 0.45314 (11) | 0.36051 (8) | 0.99141 (5) | 0.0223 (3) |

supplementary materials

| | | | | |
|------|---------------|--------------|-------------|------------|
| O10 | 0.27624 (11) | 0.35992 (8) | 0.94883 (5) | 0.0222 (3) |
| O11 | 0.59603 (11) | 0.54610 (8) | 0.73967 (5) | 0.0232 (3) |
| O12 | 0.47687 (12) | 0.14356 (8) | 1.04057 (5) | 0.0236 (3) |
| O13 | 0.28361 (11) | 0.19987 (7) | 1.07052 (5) | 0.0214 (3) |
| O14 | 0.20753 (11) | -0.17617 (7) | 1.12763 (6) | 0.0227 (3) |
| O15 | 0.20039 (12) | 0.63532 (8) | 1.02430 (6) | 0.0291 (3) |
| O16 | 0.40959 (12) | 0.11180 (8) | 1.26802 (6) | 0.0282 (3) |
| O17 | 1.04363 (11) | 0.97596 (8) | 0.38711 (5) | 0.0210 (3) |
| O18 | 0.87293 (11) | 0.95390 (8) | 0.35102 (5) | 0.0212 (3) |
| O19 | 0.78586 (12) | 0.80368 (8) | 0.61939 (5) | 0.0224 (3) |
| O20 | 0.85139 (11) | 1.17047 (7) | 0.30187 (5) | 0.0217 (3) |
| O21 | 1.04437 (11) | 1.11930 (7) | 0.26900 (5) | 0.0208 (3) |
| O22 | 1.09807 (11) | 1.49966 (7) | 0.21544 (6) | 0.0240 (3) |
| O23 | 0.92177 (12) | 1.20096 (8) | 0.07362 (6) | 0.0262 (3) |
| O24 | 1.12752 (11) | 0.68778 (7) | 0.28666 (6) | 0.0232 (3) |
| N1 | 0.19882 (13) | 0.37139 (9) | 0.55429 (6) | 0.0171 (3) |
| N2 | 0.06975 (16) | 0.53483 (11) | 0.36749 (7) | 0.0219 (4) |
| H2A | 0.0786 (17) | 0.5760 (12) | 0.3421 (8) | 0.019 (5)* |
| H2B | -0.0003 (18) | 0.5187 (11) | 0.3709 (8) | 0.018 (5)* |
| N3 | 0.48010 (13) | 0.28705 (9) | 0.60648 (6) | 0.0158 (3) |
| N4 | 0.69315 (16) | 0.00035 (10) | 0.61994 (7) | 0.0200 (4) |
| H4A | 0.7647 (18) | 0.0139 (11) | 0.6166 (8) | 0.016 (5)* |
| H4B | 0.6860 (18) | -0.0506 (13) | 0.6320 (8) | 0.025 (6)* |
| N5 | 0.19293 (13) | 0.38451 (9) | 1.07177 (6) | 0.0170 (3) |
| N6 | -0.01415 (17) | 0.67577 (11) | 1.03019 (8) | 0.0244 (4) |
| H6A | -0.0070 (19) | 0.7202 (13) | 1.0129 (9) | 0.030 (6)* |
| H6B | -0.086 (2) | 0.6600 (12) | 1.0391 (9) | 0.030 (6)* |
| N7 | 0.47047 (13) | 0.28584 (9) | 1.12176 (6) | 0.0176 (3) |
| N8 | 0.60015 (16) | 0.10780 (11) | 1.30460 (7) | 0.0208 (4) |
| H8D | 0.5895 (18) | 0.0675 (12) | 1.3282 (9) | 0.026 (6)* |
| H8E | 0.6731 (19) | 0.1242 (12) | 1.3019 (8) | 0.026 (6)* |
| N9 | 0.85885 (13) | 1.02845 (9) | 0.22012 (6) | 0.0168 (3) |
| N10 | 0.72992 (16) | 1.20652 (11) | 0.03746 (7) | 0.0223 (4) |
| H10A | 0.6560 (19) | 1.1910 (12) | 0.0412 (8) | 0.027 (6)* |
| H10B | 0.7391 (19) | 1.2516 (13) | 0.0144 (9) | 0.029 (6)* |
| N11 | 1.13843 (13) | 0.93611 (9) | 0.26882 (6) | 0.0153 (3) |
| N12 | 1.34124 (16) | 0.64813 (10) | 0.27654 (7) | 0.0224 (4) |
| H12A | 1.333 (2) | 0.5981 (14) | 0.2854 (9) | 0.044 (7)* |
| H12B | 1.418 (2) | 0.6591 (12) | 0.2761 (9) | 0.029 (6)* |
| C1 | 0.29193 (16) | 0.30146 (10) | 0.73072 (8) | 0.0170 (4) |
| C2 | 0.25311 (16) | 0.25679 (10) | 0.78890 (8) | 0.0171 (4) |
| C3 | 0.13826 (16) | 0.22777 (10) | 0.79820 (8) | 0.0175 (4) |
| H3 | 0.0854 | 0.2353 | 0.7674 | 0.021* |
| C4 | 0.10110 (17) | 0.18752 (11) | 0.85301 (8) | 0.0192 (4) |
| H4 | 0.0238 | 0.1687 | 0.8588 | 0.023* |
| C5 | 0.18076 (17) | 0.17579 (11) | 0.89893 (8) | 0.0192 (4) |
| C6 | 0.29574 (17) | 0.20519 (11) | 0.89017 (8) | 0.0217 (4) |
| H6 | 0.3485 | 0.1978 | 0.9210 | 0.026* |
| C7 | 0.33092 (17) | 0.24513 (11) | 0.83587 (8) | 0.0199 (4) |

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|------|--------------|--------------|-------------|------------|
| H7 | 0.4076 | 0.2647 | 0.8303 | 0.024* |
| C8 | 0.04683 (19) | 0.09769 (13) | 0.96477 (8) | 0.0313 (5) |
| H8A | 0.0421 | 0.0703 | 1.0047 | 0.047* |
| H8B | 0.0545 | 0.0568 | 0.9413 | 0.047* |
| H8C | -0.0293 | 0.1392 | 0.9553 | 0.047* |
| C9 | 0.28465 (16) | 0.53433 (11) | 0.60331 (7) | 0.0166 (4) |
| C10 | 0.31871 (16) | 0.61930 (10) | 0.58207 (7) | 0.0153 (4) |
| C11 | 0.43776 (16) | 0.62713 (11) | 0.55511 (7) | 0.0169 (4) |
| H11 | 0.4943 | 0.5795 | 0.5488 | 0.020* |
| C12 | 0.47221 (16) | 0.70479 (11) | 0.53776 (7) | 0.0168 (4) |
| H12 | 0.5514 | 0.7094 | 0.5195 | 0.020* |
| C13 | 0.38835 (16) | 0.77638 (11) | 0.54759 (7) | 0.0164 (4) |
| C14 | 0.26949 (16) | 0.76976 (11) | 0.57452 (8) | 0.0177 (4) |
| H14 | 0.2134 | 0.8174 | 0.5813 | 0.021* |
| C15 | 0.23561 (16) | 0.69100 (11) | 0.59123 (8) | 0.0184 (4) |
| H15 | 0.1559 | 0.6864 | 0.6088 | 0.022* |
| C16 | 0.34915 (17) | 0.92627 (11) | 0.53688 (8) | 0.0229 (4) |
| H16A | 0.3944 | 0.9721 | 0.5256 | 0.034* |
| H16B | 0.3214 | 0.9211 | 0.5766 | 0.034* |
| H16C | 0.2762 | 0.9367 | 0.5133 | 0.034* |
| C17 | 0.21054 (16) | 0.42806 (11) | 0.50529 (8) | 0.0178 (4) |
| H17 | 0.2712 | 0.4618 | 0.5031 | 0.021* |
| C18 | 0.13687 (16) | 0.43897 (11) | 0.45768 (8) | 0.0174 (4) |
| C19 | 0.04810 (17) | 0.38722 (11) | 0.46058 (8) | 0.0191 (4) |
| H19 | -0.0024 | 0.3923 | 0.4294 | 0.023* |
| C20 | 0.03620 (17) | 0.32754 (11) | 0.51122 (8) | 0.0202 (4) |
| H20 | -0.0216 | 0.2916 | 0.5141 | 0.024* |
| C21 | 0.11107 (16) | 0.32237 (11) | 0.55697 (8) | 0.0189 (4) |
| H21 | 0.1007 | 0.2836 | 0.5910 | 0.023* |
| C22 | 0.16008 (17) | 0.50751 (11) | 0.40618 (8) | 0.0206 (4) |
| C23 | 0.48424 (16) | 0.20469 (10) | 0.61163 (7) | 0.0159 (4) |
| H23 | 0.4084 | 0.1843 | 0.6200 | 0.019* |
| C24 | 0.59610 (16) | 0.14823 (11) | 0.60509 (7) | 0.0155 (4) |
| C25 | 0.70925 (16) | 0.17920 (11) | 0.59214 (7) | 0.0169 (4) |
| H25 | 0.7861 | 0.1433 | 0.5873 | 0.020* |
| C26 | 0.70518 (16) | 0.26460 (11) | 0.58660 (7) | 0.0184 (4) |
| H26 | 0.7795 | 0.2866 | 0.5778 | 0.022* |
| C27 | 0.59038 (16) | 0.31657 (11) | 0.59423 (7) | 0.0169 (4) |
| H27 | 0.5887 | 0.3736 | 0.5909 | 0.020* |
| C28 | 0.58516 (17) | 0.05697 (11) | 0.61515 (7) | 0.0169 (4) |
| C29 | 0.38364 (17) | 0.37940 (10) | 0.94675 (8) | 0.0177 (4) |
| C30 | 0.43568 (16) | 0.42607 (10) | 0.89192 (7) | 0.0160 (4) |
| C31 | 0.36663 (17) | 0.44726 (11) | 0.84179 (8) | 0.0188 (4) |
| H31 | 0.2860 | 0.4337 | 0.8430 | 0.023* |
| C32 | 0.41565 (16) | 0.48819 (11) | 0.79010 (8) | 0.0188 (4) |
| H32 | 0.3682 | 0.5024 | 0.7570 | 0.023* |
| C33 | 0.53688 (17) | 0.50788 (10) | 0.78834 (7) | 0.0163 (4) |
| C34 | 0.60823 (16) | 0.48612 (10) | 0.83812 (7) | 0.0175 (4) |
| H34 | 0.6895 | 0.4988 | 0.8368 | 0.021* |

supplementary materials

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|------|---------------|---------------|-------------|------------|
| C35 | 0.55725 (16) | 0.44565 (10) | 0.88937 (7) | 0.0165 (4) |
| H35 | 0.6047 | 0.4313 | 0.9225 | 0.020* |
| C36 | 0.52520 (18) | 0.57312 (12) | 0.68812 (8) | 0.0254 (4) |
| H36A | 0.5777 | 0.5979 | 0.6571 | 0.038* |
| H36B | 0.4508 | 0.6139 | 0.6939 | 0.038* |
| H36C | 0.4995 | 0.5257 | 0.6786 | 0.038* |
| C37 | 0.36803 (17) | 0.13662 (11) | 1.06136 (8) | 0.0189 (4) |
| C38 | 0.32856 (16) | 0.05274 (11) | 1.07873 (7) | 0.0167 (4) |
| C39 | 0.41094 (17) | -0.01964 (11) | 1.07027 (8) | 0.0203 (4) |
| H39 | 0.4922 | -0.0159 | 1.0541 | 0.024* |
| C40 | 0.37452 (17) | -0.09777 (11) | 1.08548 (8) | 0.0210 (4) |
| H40 | 0.4304 | -0.1457 | 1.0792 | 0.025* |
| C41 | 0.25362 (17) | -0.10318 (11) | 1.11019 (7) | 0.0181 (4) |
| C42 | 0.16967 (17) | -0.03088 (11) | 1.11905 (8) | 0.0194 (4) |
| H42 | 0.0888 | -0.0347 | 1.1357 | 0.023* |
| C43 | 0.20675 (16) | 0.04611 (11) | 1.10317 (7) | 0.0188 (4) |
| H43 | 0.1502 | 0.0942 | 1.1088 | 0.023* |
| C44 | 0.29057 (18) | -0.25313 (11) | 1.12221 (8) | 0.0251 (4) |
| H44A | 0.2447 | -0.2987 | 1.1335 | 0.038* |
| H44B | 0.3620 | -0.2630 | 1.1466 | 0.038* |
| H44C | 0.3207 | -0.2494 | 1.0828 | 0.038* |
| C45 | 0.19034 (17) | 0.46750 (11) | 1.05576 (7) | 0.0171 (4) |
| H45 | 0.2657 | 0.4857 | 1.0415 | 0.021* |
| C46 | 0.08131 (17) | 0.52752 (11) | 1.05929 (7) | 0.0178 (4) |
| C47 | -0.03127 (17) | 0.49980 (11) | 1.08085 (7) | 0.0204 (4) |
| H47 | -0.1066 | 0.5380 | 1.0838 | 0.025* |
| C48 | -0.02866 (18) | 0.41400 (12) | 1.09786 (8) | 0.0234 (4) |
| H48 | -0.1024 | 0.3941 | 1.1128 | 0.028* |
| C49 | 0.08380 (17) | 0.35845 (11) | 1.09249 (7) | 0.0202 (4) |
| H49 | 0.0842 | 0.3011 | 1.1036 | 0.024* |
| C50 | 0.09297 (17) | 0.61805 (11) | 1.03675 (8) | 0.0198 (4) |
| C51 | 0.45678 (16) | 0.22669 (11) | 1.16912 (8) | 0.0177 (4) |
| H51 | 0.3920 | 0.1962 | 1.1705 | 0.021* |
| C52 | 0.53452 (16) | 0.20865 (10) | 1.21624 (7) | 0.0167 (4) |
| C53 | 0.62936 (16) | 0.25576 (11) | 1.21433 (8) | 0.0188 (4) |
| H53 | 0.6828 | 0.2458 | 1.2452 | 0.023* |
| C54 | 0.64308 (17) | 0.31808 (11) | 1.16553 (8) | 0.0213 (4) |
| H54 | 0.7051 | 0.3508 | 1.1636 | 0.026* |
| C55 | 0.56339 (17) | 0.33059 (11) | 1.12013 (8) | 0.0191 (4) |
| H55 | 0.5742 | 0.3714 | 1.0872 | 0.023* |
| C56 | 0.50987 (17) | 0.13816 (11) | 1.26563 (8) | 0.0179 (4) |
| C57 | 0.94215 (16) | 0.94761 (10) | 0.39389 (8) | 0.0166 (4) |
| C58 | 0.89959 (16) | 0.90683 (10) | 0.45261 (7) | 0.0152 (4) |
| C59 | 0.78302 (16) | 0.88017 (10) | 0.46149 (7) | 0.0157 (4) |
| H59 | 0.7322 | 0.8861 | 0.4302 | 0.019* |
| C60 | 0.74133 (16) | 0.84458 (10) | 0.51674 (7) | 0.0166 (4) |
| H60 | 0.6633 | 0.8268 | 0.5224 | 0.020* |
| C61 | 0.81757 (16) | 0.83602 (10) | 0.56327 (7) | 0.0172 (4) |
| C62 | 0.93411 (16) | 0.86335 (11) | 0.55479 (8) | 0.0195 (4) |

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|------|--------------|--------------|-------------|------------|
| H62 | 0.9846 | 0.8580 | 0.5861 | 0.023* |
| C63 | 0.97440 (16) | 0.89826 (11) | 0.49998 (8) | 0.0178 (4) |
| H63 | 1.0523 | 0.9163 | 0.4945 | 0.021* |
| C64 | 0.67921 (18) | 0.76180 (12) | 0.62958 (8) | 0.0271 (5) |
| H64A | 0.6727 | 0.7362 | 0.6698 | 0.041* |
| H64B | 0.6908 | 0.7193 | 0.6072 | 0.041* |
| H64C | 0.6024 | 0.8018 | 0.6186 | 0.041* |
| C65 | 0.95912 (17) | 1.18050 (11) | 0.27986 (7) | 0.0177 (4) |
| C66 | 0.99348 (16) | 1.26563 (11) | 0.26387 (7) | 0.0169 (4) |
| C67 | 0.90216 (17) | 1.33733 (11) | 0.26628 (7) | 0.0181 (4) |
| H67 | 0.8189 | 1.3319 | 0.2785 | 0.022* |
| C68 | 0.93296 (16) | 1.41685 (11) | 0.25075 (8) | 0.0189 (4) |
| H68 | 0.8709 | 1.4643 | 0.2523 | 0.023* |
| C69 | 1.05760 (17) | 1.42473 (11) | 0.23278 (8) | 0.0180 (4) |
| C70 | 1.15106 (17) | 1.35321 (11) | 0.23154 (8) | 0.0198 (4) |
| H70 | 1.2349 | 1.3586 | 0.2206 | 0.024* |
| C71 | 1.11896 (16) | 1.27463 (11) | 0.24661 (8) | 0.0188 (4) |
| H71 | 1.1813 | 1.2272 | 0.2453 | 0.023* |
| C72 | 1.00517 (17) | 1.57534 (11) | 0.21247 (9) | 0.0245 (4) |
| H72A | 1.0469 | 1.6229 | 0.2015 | 0.037* |
| H72B | 0.9628 | 1.5753 | 0.2495 | 0.037* |
| H72C | 0.9435 | 1.5786 | 0.1844 | 0.037* |
| C73 | 0.87123 (16) | 1.08805 (11) | 0.17289 (7) | 0.0169 (4) |
| H73 | 0.9327 | 1.1208 | 0.1723 | 0.020* |
| C74 | 0.79723 (16) | 1.10346 (11) | 0.12490 (8) | 0.0172 (4) |
| C75 | 0.70755 (17) | 1.05289 (11) | 0.12522 (8) | 0.0205 (4) |
| H75 | 0.6567 | 1.0610 | 0.0936 | 0.025* |
| C76 | 0.69568 (17) | 0.98979 (11) | 0.17394 (8) | 0.0219 (4) |
| H76 | 0.6377 | 0.9545 | 0.1750 | 0.026* |
| C77 | 0.77072 (17) | 0.98031 (11) | 0.22049 (8) | 0.0198 (4) |
| H77 | 0.7602 | 0.9393 | 0.2533 | 0.024* |
| C78 | 0.82090 (17) | 1.17471 (11) | 0.07594 (8) | 0.0193 (4) |
| C79 | 1.13973 (16) | 0.85400 (10) | 0.27480 (7) | 0.0156 (4) |
| H79 | 1.0632 | 0.8348 | 0.2844 | 0.019* |
| C80 | 1.24907 (16) | 0.79606 (11) | 0.26748 (7) | 0.0156 (4) |
| C81 | 1.36362 (16) | 0.82537 (11) | 0.25309 (7) | 0.0173 (4) |
| H81 | 1.4392 | 0.7884 | 0.2480 | 0.021* |
| C82 | 1.36265 (17) | 0.91065 (11) | 0.24646 (8) | 0.0193 (4) |
| H82 | 1.4377 | 0.9316 | 0.2366 | 0.023* |
| C83 | 1.24980 (16) | 0.96386 (11) | 0.25458 (7) | 0.0177 (4) |
| H83 | 1.2500 | 1.0209 | 0.2501 | 0.021* |
| C84 | 1.23519 (17) | 0.70559 (11) | 0.27787 (7) | 0.0172 (4) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Zn1 | 0.01463 (11) | 0.01483 (11) | 0.01738 (11) | -0.00357 (8) | -0.00069 (8) | -0.00097 (8) |
| Zn2 | 0.01614 (11) | 0.01688 (11) | 0.01665 (11) | -0.00394 (8) | -0.00134 (8) | 0.00155 (8) |

supplementary materials

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|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Zn3 | 0.01497 (11) | 0.01439 (11) | 0.01705 (11) | -0.00305 (8) | -0.00064 (8) | -0.00048 (8) |
| O1 | 0.0182 (7) | 0.0227 (7) | 0.0227 (7) | -0.0074 (5) | 0.0011 (5) | -0.0044 (5) |
| O2 | 0.0184 (7) | 0.0254 (7) | 0.0176 (7) | -0.0066 (5) | -0.0026 (5) | 0.0002 (5) |
| O3 | 0.0288 (8) | 0.0297 (8) | 0.0163 (7) | -0.0102 (6) | -0.0039 (6) | 0.0010 (6) |
| O4 | 0.0180 (7) | 0.0222 (7) | 0.0244 (7) | -0.0080 (5) | 0.0000 (6) | -0.0009 (6) |
| O5 | 0.0181 (7) | 0.0144 (6) | 0.0288 (7) | -0.0035 (5) | -0.0015 (6) | -0.0014 (5) |
| O6 | 0.0178 (7) | 0.0141 (6) | 0.0287 (7) | -0.0043 (5) | -0.0002 (6) | -0.0025 (5) |
| O7 | 0.0256 (8) | 0.0415 (9) | 0.0287 (8) | -0.0206 (7) | -0.0077 (6) | 0.0091 (7) |
| O8 | 0.0179 (7) | 0.0176 (7) | 0.0303 (8) | -0.0066 (5) | -0.0077 (6) | 0.0027 (6) |
| O9 | 0.0195 (7) | 0.0278 (7) | 0.0166 (7) | -0.0064 (5) | -0.0022 (5) | 0.0038 (5) |
| O10 | 0.0198 (7) | 0.0244 (7) | 0.0229 (7) | -0.0081 (6) | 0.0013 (6) | -0.0032 (6) |
| O11 | 0.0238 (7) | 0.0303 (7) | 0.0142 (7) | -0.0113 (6) | -0.0039 (5) | 0.0044 (6) |
| O12 | 0.0196 (7) | 0.0251 (7) | 0.0251 (7) | -0.0079 (6) | 0.0011 (6) | -0.0010 (6) |
| O13 | 0.0209 (7) | 0.0168 (7) | 0.0261 (7) | -0.0048 (5) | -0.0014 (6) | -0.0023 (5) |
| O14 | 0.0211 (7) | 0.0166 (7) | 0.0301 (8) | -0.0047 (5) | -0.0024 (6) | -0.0028 (6) |
| O15 | 0.0203 (7) | 0.0210 (7) | 0.0440 (9) | -0.0067 (6) | -0.0133 (6) | 0.0041 (6) |
| O16 | 0.0225 (7) | 0.0347 (8) | 0.0258 (8) | -0.0159 (6) | -0.0057 (6) | 0.0079 (6) |
| O17 | 0.0176 (7) | 0.0227 (7) | 0.0233 (7) | -0.0071 (5) | 0.0015 (5) | -0.0040 (6) |
| O18 | 0.0193 (7) | 0.0253 (7) | 0.0174 (7) | -0.0066 (5) | -0.0031 (5) | 0.0019 (5) |
| O19 | 0.0248 (7) | 0.0285 (7) | 0.0143 (7) | -0.0104 (6) | -0.0018 (5) | -0.0005 (5) |
| O20 | 0.0196 (7) | 0.0217 (7) | 0.0240 (7) | -0.0092 (5) | 0.0005 (6) | -0.0014 (6) |
| O21 | 0.0204 (7) | 0.0145 (6) | 0.0268 (7) | -0.0038 (5) | 0.0002 (6) | -0.0029 (5) |
| O22 | 0.0191 (7) | 0.0133 (6) | 0.0380 (8) | -0.0040 (5) | -0.0010 (6) | -0.0013 (6) |
| O23 | 0.0192 (7) | 0.0313 (8) | 0.0250 (7) | -0.0100 (6) | -0.0036 (6) | 0.0058 (6) |
| O24 | 0.0188 (7) | 0.0172 (7) | 0.0332 (8) | -0.0063 (5) | -0.0049 (6) | -0.0011 (6) |
| N1 | 0.0155 (8) | 0.0151 (8) | 0.0196 (8) | -0.0022 (6) | -0.0006 (6) | -0.0021 (6) |
| N2 | 0.0202 (9) | 0.0230 (9) | 0.0210 (9) | -0.0110 (7) | -0.0041 (7) | 0.0057 (7) |
| N3 | 0.0163 (8) | 0.0166 (8) | 0.0143 (8) | -0.0036 (6) | -0.0013 (6) | -0.0019 (6) |
| N4 | 0.0187 (9) | 0.0136 (8) | 0.0280 (9) | -0.0049 (7) | -0.0031 (7) | -0.0025 (7) |
| N5 | 0.0172 (8) | 0.0188 (8) | 0.0145 (8) | -0.0049 (6) | -0.0014 (6) | -0.0010 (6) |
| N6 | 0.0223 (10) | 0.0179 (9) | 0.0324 (10) | -0.0046 (7) | -0.0048 (8) | -0.0018 (8) |
| N7 | 0.0171 (8) | 0.0164 (8) | 0.0181 (8) | -0.0033 (6) | -0.0003 (6) | -0.0010 (6) |
| N8 | 0.0182 (9) | 0.0215 (9) | 0.0206 (9) | -0.0075 (7) | -0.0040 (7) | 0.0045 (7) |
| N9 | 0.0166 (8) | 0.0155 (8) | 0.0176 (8) | -0.0015 (6) | 0.0009 (6) | -0.0039 (6) |
| N10 | 0.0194 (9) | 0.0228 (9) | 0.0218 (9) | -0.0052 (7) | -0.0026 (7) | 0.0031 (7) |
| N11 | 0.0158 (8) | 0.0158 (8) | 0.0139 (7) | -0.0040 (6) | -0.0019 (6) | -0.0009 (6) |
| N12 | 0.0188 (9) | 0.0146 (9) | 0.0334 (10) | -0.0025 (7) | -0.0010 (7) | -0.0045 (7) |
| C1 | 0.0151 (9) | 0.0138 (9) | 0.0207 (10) | -0.0008 (7) | 0.0016 (7) | -0.0036 (7) |
| C2 | 0.0161 (9) | 0.0155 (9) | 0.0192 (9) | -0.0017 (7) | 0.0009 (7) | -0.0042 (7) |
| C3 | 0.0174 (9) | 0.0147 (9) | 0.0193 (10) | -0.0024 (7) | -0.0024 (7) | -0.0012 (7) |
| C4 | 0.0167 (9) | 0.0183 (9) | 0.0219 (10) | -0.0046 (7) | -0.0005 (8) | -0.0020 (8) |
| C5 | 0.0241 (10) | 0.0155 (9) | 0.0164 (9) | -0.0018 (7) | 0.0004 (8) | -0.0020 (7) |
| C6 | 0.0205 (10) | 0.0250 (10) | 0.0199 (10) | -0.0017 (8) | -0.0058 (8) | -0.0061 (8) |
| C7 | 0.0148 (9) | 0.0233 (10) | 0.0216 (10) | -0.0034 (7) | -0.0013 (8) | -0.0047 (8) |
| C8 | 0.0406 (13) | 0.0351 (12) | 0.0193 (10) | -0.0185 (10) | -0.0015 (9) | 0.0025 (9) |
| C9 | 0.0173 (10) | 0.0179 (9) | 0.0149 (9) | -0.0048 (7) | -0.0049 (7) | -0.0014 (7) |
| C10 | 0.0152 (9) | 0.0160 (9) | 0.0145 (9) | -0.0025 (7) | -0.0046 (7) | -0.0016 (7) |
| C11 | 0.0179 (9) | 0.0157 (9) | 0.0160 (9) | -0.0004 (7) | -0.0034 (7) | -0.0026 (7) |
| C12 | 0.0148 (9) | 0.0207 (9) | 0.0150 (9) | -0.0050 (7) | -0.0006 (7) | -0.0025 (7) |

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|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C13 | 0.0170 (9) | 0.0161 (9) | 0.0162 (9) | -0.0041 (7) | -0.0060 (7) | -0.0012 (7) |
| C14 | 0.0155 (9) | 0.0159 (9) | 0.0209 (10) | 0.0006 (7) | -0.0028 (7) | -0.0046 (7) |
| C15 | 0.0128 (9) | 0.0217 (10) | 0.0199 (10) | -0.0036 (7) | -0.0012 (7) | -0.0023 (8) |
| C16 | 0.0241 (10) | 0.0161 (9) | 0.0276 (11) | -0.0014 (8) | -0.0042 (8) | -0.0037 (8) |
| C17 | 0.0145 (9) | 0.0182 (9) | 0.0207 (10) | -0.0042 (7) | 0.0008 (7) | -0.0039 (7) |
| C18 | 0.0146 (9) | 0.0182 (9) | 0.0185 (9) | -0.0027 (7) | 0.0014 (7) | -0.0029 (7) |
| C19 | 0.0184 (10) | 0.0188 (9) | 0.0203 (10) | -0.0037 (7) | -0.0022 (8) | -0.0036 (8) |
| C20 | 0.0193 (10) | 0.0171 (9) | 0.0249 (10) | -0.0075 (7) | -0.0016 (8) | -0.0023 (8) |
| C21 | 0.0204 (10) | 0.0160 (9) | 0.0182 (9) | -0.0022 (7) | -0.0008 (8) | -0.0004 (7) |
| C22 | 0.0217 (10) | 0.0235 (10) | 0.0164 (9) | -0.0072 (8) | -0.0006 (8) | -0.0014 (8) |
| C23 | 0.0165 (9) | 0.0157 (9) | 0.0150 (9) | -0.0055 (7) | -0.0032 (7) | 0.0007 (7) |
| C24 | 0.0171 (9) | 0.0186 (9) | 0.0104 (8) | -0.0043 (7) | -0.0026 (7) | -0.0011 (7) |
| C25 | 0.0130 (9) | 0.0204 (9) | 0.0162 (9) | -0.0019 (7) | -0.0015 (7) | -0.0026 (7) |
| C26 | 0.0155 (9) | 0.0212 (10) | 0.0191 (10) | -0.0085 (7) | -0.0013 (7) | -0.0009 (7) |
| C27 | 0.0199 (10) | 0.0141 (9) | 0.0173 (9) | -0.0063 (7) | -0.0023 (7) | -0.0010 (7) |
| C28 | 0.0188 (10) | 0.0183 (9) | 0.0137 (9) | -0.0045 (7) | -0.0036 (7) | -0.0013 (7) |
| C29 | 0.0180 (10) | 0.0141 (9) | 0.0197 (10) | -0.0020 (7) | 0.0003 (8) | -0.0021 (7) |
| C30 | 0.0170 (9) | 0.0151 (9) | 0.0161 (9) | -0.0032 (7) | -0.0002 (7) | -0.0034 (7) |
| C31 | 0.0154 (9) | 0.0199 (9) | 0.0210 (10) | -0.0046 (7) | -0.0031 (8) | -0.0021 (8) |
| C32 | 0.0164 (9) | 0.0224 (10) | 0.0172 (9) | -0.0024 (7) | -0.0054 (7) | -0.0030 (7) |
| C33 | 0.0205 (10) | 0.0146 (9) | 0.0129 (9) | -0.0035 (7) | -0.0007 (7) | -0.0008 (7) |
| C34 | 0.0130 (9) | 0.0186 (9) | 0.0213 (10) | -0.0054 (7) | -0.0027 (7) | -0.0023 (7) |
| C35 | 0.0188 (9) | 0.0145 (9) | 0.0157 (9) | -0.0018 (7) | -0.0064 (7) | -0.0015 (7) |
| C36 | 0.0297 (11) | 0.0282 (11) | 0.0153 (10) | -0.0064 (9) | -0.0056 (8) | 0.0044 (8) |
| C37 | 0.0200 (10) | 0.0216 (10) | 0.0152 (9) | -0.0055 (8) | -0.0043 (8) | -0.0018 (7) |
| C38 | 0.0154 (9) | 0.0197 (9) | 0.0145 (9) | -0.0036 (7) | -0.0031 (7) | -0.0018 (7) |
| C39 | 0.0157 (9) | 0.0242 (10) | 0.0195 (10) | -0.0029 (8) | 0.0006 (8) | -0.0026 (8) |
| C40 | 0.0186 (10) | 0.0196 (10) | 0.0233 (10) | 0.0005 (8) | -0.0006 (8) | -0.0053 (8) |
| C41 | 0.0215 (10) | 0.0174 (9) | 0.0158 (9) | -0.0057 (7) | -0.0053 (8) | -0.0011 (7) |
| C42 | 0.0155 (9) | 0.0232 (10) | 0.0198 (10) | -0.0055 (7) | -0.0004 (7) | -0.0034 (8) |
| C43 | 0.0168 (9) | 0.0197 (9) | 0.0197 (10) | -0.0002 (7) | -0.0031 (7) | -0.0059 (8) |
| C44 | 0.0308 (11) | 0.0176 (10) | 0.0267 (11) | -0.0040 (8) | -0.0031 (9) | -0.0039 (8) |
| C45 | 0.0169 (9) | 0.0201 (9) | 0.0144 (9) | -0.0056 (7) | -0.0035 (7) | -0.0011 (7) |
| C46 | 0.0210 (10) | 0.0206 (9) | 0.0136 (9) | -0.0054 (8) | -0.0056 (7) | -0.0045 (7) |
| C47 | 0.0188 (10) | 0.0254 (10) | 0.0159 (9) | -0.0025 (8) | -0.0002 (8) | -0.0033 (8) |
| C48 | 0.0190 (10) | 0.0264 (10) | 0.0224 (10) | -0.0078 (8) | 0.0041 (8) | 0.0012 (8) |
| C49 | 0.0221 (10) | 0.0199 (10) | 0.0170 (9) | -0.0071 (8) | 0.0001 (8) | 0.0019 (7) |
| C50 | 0.0203 (10) | 0.0205 (10) | 0.0191 (10) | -0.0040 (8) | -0.0081 (8) | -0.0025 (8) |
| C51 | 0.0145 (9) | 0.0175 (9) | 0.0205 (10) | -0.0034 (7) | 0.0000 (7) | -0.0029 (7) |
| C52 | 0.0161 (9) | 0.0152 (9) | 0.0175 (9) | -0.0015 (7) | 0.0004 (7) | -0.0025 (7) |
| C53 | 0.0178 (10) | 0.0194 (9) | 0.0191 (10) | -0.0032 (7) | -0.0031 (8) | -0.0035 (7) |
| C54 | 0.0208 (10) | 0.0183 (10) | 0.0261 (11) | -0.0081 (8) | -0.0001 (8) | -0.0035 (8) |
| C55 | 0.0227 (10) | 0.0126 (9) | 0.0208 (10) | -0.0039 (7) | 0.0008 (8) | -0.0010 (7) |
| C56 | 0.0171 (10) | 0.0195 (9) | 0.0164 (9) | -0.0043 (7) | 0.0009 (7) | -0.0024 (7) |
| C57 | 0.0153 (9) | 0.0129 (9) | 0.0199 (10) | -0.0002 (7) | -0.0003 (7) | -0.0024 (7) |
| C58 | 0.0138 (9) | 0.0130 (9) | 0.0181 (9) | -0.0018 (7) | -0.0010 (7) | -0.0022 (7) |
| C59 | 0.0160 (9) | 0.0138 (9) | 0.0159 (9) | -0.0014 (7) | -0.0044 (7) | -0.0004 (7) |
| C60 | 0.0132 (9) | 0.0164 (9) | 0.0196 (10) | -0.0030 (7) | -0.0012 (7) | -0.0022 (7) |
| C61 | 0.0196 (10) | 0.0151 (9) | 0.0159 (9) | -0.0018 (7) | 0.0009 (7) | -0.0028 (7) |

supplementary materials

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|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C62 | 0.0164 (10) | 0.0233 (10) | 0.0183 (10) | -0.0020 (7) | -0.0048 (7) | -0.0032 (8) |
| C63 | 0.0130 (9) | 0.0195 (9) | 0.0216 (10) | -0.0041 (7) | -0.0009 (7) | -0.0047 (8) |
| C64 | 0.0304 (11) | 0.0342 (12) | 0.0176 (10) | -0.0156 (9) | 0.0001 (8) | 0.0007 (8) |
| C65 | 0.0185 (10) | 0.0194 (9) | 0.0150 (9) | -0.0042 (8) | -0.0048 (7) | -0.0011 (7) |
| C66 | 0.0175 (9) | 0.0181 (9) | 0.0155 (9) | -0.0037 (7) | -0.0035 (7) | -0.0030 (7) |
| C67 | 0.0140 (9) | 0.0215 (10) | 0.0189 (9) | -0.0027 (7) | -0.0002 (7) | -0.0053 (8) |
| C68 | 0.0158 (9) | 0.0180 (9) | 0.0221 (10) | -0.0004 (7) | -0.0018 (8) | -0.0047 (8) |
| C69 | 0.0187 (10) | 0.0160 (9) | 0.0198 (10) | -0.0043 (7) | -0.0033 (8) | -0.0027 (7) |
| C70 | 0.0131 (9) | 0.0211 (10) | 0.0245 (10) | -0.0043 (7) | -0.0003 (8) | -0.0028 (8) |
| C71 | 0.0167 (10) | 0.0170 (9) | 0.0216 (10) | -0.0001 (7) | -0.0036 (8) | -0.0037 (7) |
| C72 | 0.0236 (11) | 0.0140 (9) | 0.0347 (12) | -0.0013 (8) | -0.0061 (9) | -0.0032 (8) |
| C73 | 0.0136 (9) | 0.0169 (9) | 0.0189 (9) | -0.0026 (7) | 0.0010 (7) | -0.0023 (7) |
| C74 | 0.0147 (9) | 0.0181 (9) | 0.0175 (9) | -0.0014 (7) | 0.0010 (7) | -0.0031 (7) |
| C75 | 0.0185 (10) | 0.0240 (10) | 0.0183 (10) | -0.0021 (8) | -0.0008 (8) | -0.0049 (8) |
| C76 | 0.0210 (10) | 0.0212 (10) | 0.0254 (11) | -0.0085 (8) | 0.0013 (8) | -0.0055 (8) |
| C77 | 0.0211 (10) | 0.0168 (9) | 0.0205 (10) | -0.0044 (7) | 0.0009 (8) | -0.0018 (7) |
| C78 | 0.0179 (10) | 0.0221 (10) | 0.0160 (9) | -0.0016 (8) | 0.0018 (7) | -0.0028 (7) |
| C79 | 0.0153 (9) | 0.0169 (9) | 0.0152 (9) | -0.0059 (7) | -0.0024 (7) | -0.0015 (7) |
| C80 | 0.0185 (9) | 0.0171 (9) | 0.0112 (9) | -0.0039 (7) | -0.0028 (7) | -0.0017 (7) |
| C81 | 0.0158 (9) | 0.0188 (9) | 0.0167 (9) | -0.0015 (7) | -0.0014 (7) | -0.0037 (7) |
| C82 | 0.0161 (9) | 0.0227 (10) | 0.0193 (10) | -0.0079 (7) | -0.0001 (7) | -0.0013 (8) |
| C83 | 0.0219 (10) | 0.0148 (9) | 0.0160 (9) | -0.0059 (7) | -0.0012 (7) | 0.0000 (7) |
| C84 | 0.0188 (10) | 0.0170 (9) | 0.0153 (9) | -0.0028 (7) | -0.0042 (7) | -0.0018 (7) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|---------|-----------|
| Zn1—O1 | 2.5181 (12) | C21—H21 | 0.9300 |
| Zn1—O2 | 1.9631 (12) | C23—N3 | 1.339 (2) |
| Zn1—O5 | 1.9392 (12) | C23—C24 | 1.387 (2) |
| Zn1—N1 | 2.0793 (15) | C23—H23 | 0.9300 |
| Zn1—N3 | 2.0561 (14) | C25—C24 | 1.393 (2) |
| Zn2—O9 | 1.9523 (12) | C25—C26 | 1.388 (2) |
| Zn2—O10 | 2.5931 (12) | C25—H25 | 0.9300 |
| Zn2—O13 | 1.9317 (12) | C26—H26 | 0.9300 |
| Zn2—N5 | 2.0536 (15) | C27—C26 | 1.378 (2) |
| Zn2—N7 | 2.0669 (14) | C27—H27 | 0.9300 |
| Zn3—O17 | 2.4085 (12) | C28—C24 | 1.509 (2) |
| Zn3—O18 | 1.9987 (12) | C29—C30 | 1.491 (2) |
| Zn3—O21 | 1.9436 (12) | C30—C35 | 1.394 (2) |
| Zn3—N9 | 2.0840 (14) | C31—C30 | 1.391 (2) |
| Zn3—N11 | 2.0613 (14) | C31—C32 | 1.386 (2) |
| O2—C1 | 1.284 (2) | C31—H31 | 0.9300 |
| O3—C5 | 1.364 (2) | C32—H32 | 0.9300 |
| O3—C8 | 1.423 (2) | C33—C32 | 1.393 (2) |
| O4—C9 | 1.240 (2) | C33—C34 | 1.397 (2) |
| O5—C9 | 1.287 (2) | C34—H34 | 0.9300 |
| O6—C13 | 1.363 (2) | C35—C34 | 1.384 (2) |
| O6—C16 | 1.432 (2) | C35—H35 | 0.9300 |
| O7—C22 | 1.227 (2) | C36—O11 | 1.428 (2) |

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|----------|-------------|----------|-----------|
| O8—C28 | 1.234 (2) | C36—H36A | 0.9600 |
| O9—C29 | 1.287 (2) | C36—H36B | 0.9600 |
| O10—C29 | 1.247 (2) | C36—H36C | 0.9600 |
| O11—C33 | 1.3653 (19) | C37—C38 | 1.497 (2) |
| O12—C37 | 1.245 (2) | C38—C39 | 1.387 (2) |
| O13—C37 | 1.289 (2) | C38—C43 | 1.399 (2) |
| O14—C41 | 1.367 (2) | C39—H39 | 0.9300 |
| O14—C44 | 1.430 (2) | C40—C39 | 1.392 (2) |
| O15—C50 | 1.236 (2) | C40—C41 | 1.389 (2) |
| O16—C56 | 1.228 (2) | C40—H40 | 0.9300 |
| O17—C57 | 1.251 (2) | C41—C42 | 1.396 (2) |
| O18—C57 | 1.279 (2) | C42—H42 | 0.9300 |
| O19—C64 | 1.428 (2) | C43—C42 | 1.378 (2) |
| O20—C65 | 1.254 (2) | C43—H43 | 0.9300 |
| O21—C65 | 1.282 (2) | C44—H44A | 0.9600 |
| O22—C69 | 1.366 (2) | C44—H44B | 0.9600 |
| O22—C72 | 1.431 (2) | C44—H44C | 0.9600 |
| O23—C78 | 1.234 (2) | C45—H45 | 0.9300 |
| O24—C84 | 1.235 (2) | C46—C45 | 1.386 (2) |
| N1—C17 | 1.340 (2) | C46—C47 | 1.394 (2) |
| N1—C21 | 1.348 (2) | C46—C50 | 1.507 (2) |
| N2—C22 | 1.326 (2) | C47—H47 | 0.9300 |
| N2—H2A | 0.821 (19) | C48—C49 | 1.379 (2) |
| N2—H2B | 0.836 (19) | C48—C47 | 1.388 (2) |
| N3—C27 | 1.352 (2) | C48—H48 | 0.9300 |
| N4—C28 | 1.330 (2) | C49—H49 | 0.9300 |
| N4—H4A | 0.832 (18) | C51—C52 | 1.389 (2) |
| N4—H4B | 0.85 (2) | C51—H51 | 0.9300 |
| N5—C45 | 1.341 (2) | C52—C53 | 1.391 (2) |
| N5—C49 | 1.345 (2) | C53—H53 | 0.9300 |
| N6—C50 | 1.333 (2) | C54—C53 | 1.392 (2) |
| N6—H6A | 0.78 (2) | C54—C55 | 1.380 (2) |
| N6—H6B | 0.86 (2) | C54—H54 | 0.9300 |
| N7—C51 | 1.340 (2) | C55—H55 | 0.9300 |
| N7—C55 | 1.347 (2) | C56—C52 | 1.511 (2) |
| N8—C56 | 1.333 (2) | C57—C58 | 1.490 (2) |
| N8—H8D | 0.79 (2) | C59—C58 | 1.389 (2) |
| N8—H8E | 0.87 (2) | C59—C60 | 1.395 (2) |
| N9—C77 | 1.350 (2) | C59—H59 | 0.9300 |
| N10—C78 | 1.333 (2) | C60—H60 | 0.9300 |
| N10—H10A | 0.87 (2) | C61—O19 | 1.368 (2) |
| N10—H10B | 0.84 (2) | C61—C60 | 1.389 (2) |
| N11—C79 | 1.338 (2) | C62—C61 | 1.394 (2) |
| N11—C83 | 1.353 (2) | C62—C63 | 1.378 (2) |
| N12—C84 | 1.332 (2) | C62—H62 | 0.9300 |
| N12—H12A | 0.83 (2) | C63—C58 | 1.396 (2) |
| N12—H12B | 0.87 (2) | C63—H63 | 0.9300 |
| C1—O1 | 1.254 (2) | C64—H64A | 0.9600 |
| C1—C2 | 1.489 (2) | C64—H64B | 0.9600 |

supplementary materials

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| C2—C3 | 1.391 (2) | C64—H64C | 0.9600 |
| C2—C7 | 1.399 (2) | C65—C66 | 1.492 (2) |
| C3—H3 | 0.9300 | C66—C71 | 1.399 (2) |
| C4—C5 | 1.392 (2) | C67—C66 | 1.391 (2) |
| C4—C3 | 1.394 (2) | C67—H67 | 0.9300 |
| C4—H4 | 0.9300 | C68—C67 | 1.388 (2) |
| C6—C5 | 1.395 (2) | C68—C69 | 1.390 (2) |
| C6—C7 | 1.376 (2) | C68—H68 | 0.9300 |
| C6—H6 | 0.9300 | C70—C69 | 1.396 (2) |
| C7—H7 | 0.9300 | C70—C71 | 1.379 (2) |
| C8—H8A | 0.9600 | C70—H70 | 0.9300 |
| C8—H8B | 0.9600 | C71—H71 | 0.9300 |
| C8—H8C | 0.9600 | C72—H72A | 0.9600 |
| C9—C10 | 1.496 (2) | C72—H72B | 0.9600 |
| C10—C11 | 1.397 (2) | C72—H72C | 0.9600 |
| C11—C12 | 1.378 (2) | C73—N9 | 1.339 (2) |
| C11—H11 | 0.9300 | C73—C74 | 1.386 (2) |
| C12—H12 | 0.9300 | C73—H73 | 0.9300 |
| C13—C12 | 1.394 (2) | C74—C75 | 1.393 (2) |
| C13—C14 | 1.391 (2) | C74—C78 | 1.510 (2) |
| C14—C15 | 1.392 (2) | C75—H75 | 0.9300 |
| C14—H14 | 0.9300 | C76—C75 | 1.395 (2) |
| C15—C10 | 1.386 (2) | C76—C77 | 1.379 (2) |
| C15—H15 | 0.9300 | C76—H76 | 0.9300 |
| C16—H16A | 0.9600 | C77—H77 | 0.9300 |
| C16—H16B | 0.9600 | C79—C80 | 1.385 (2) |
| C16—H16C | 0.9600 | C79—H79 | 0.9300 |
| C17—H17 | 0.9300 | C80—C81 | 1.397 (2) |
| C18—C17 | 1.387 (2) | C80—C84 | 1.504 (2) |
| C18—C19 | 1.390 (2) | C81—H81 | 0.9300 |
| C18—C22 | 1.517 (2) | C82—C81 | 1.389 (2) |
| C19—C20 | 1.394 (2) | C82—C83 | 1.375 (2) |
| C19—H19 | 0.9300 | C82—H82 | 0.9300 |
| C20—C21 | 1.377 (2) | C83—H83 | 0.9300 |
| C20—H20 | 0.9300 | | |
| O1—Zn1—O2 | 57.53 (5) | C31—C30—C35 | 118.79 (16) |
| O2—Zn1—N1 | 101.78 (5) | C35—C30—C29 | 120.46 (15) |
| O2—Zn1—N3 | 108.48 (5) | C30—C31—H31 | 119.4 |
| O2—Zn1—C1 | 29.07 (5) | C32—C31—C30 | 121.29 (16) |
| O5—Zn1—O2 | 139.19 (5) | C32—C31—H31 | 119.4 |
| O5—Zn1—N1 | 100.95 (5) | C31—C32—C33 | 119.24 (16) |
| O5—Zn1—N3 | 98.11 (5) | C31—C32—H32 | 120.4 |
| O5—Zn1—C1 | 119.75 (5) | C33—C32—H32 | 120.4 |
| N1—Zn1—C1 | 130.84 (6) | O11—C33—C32 | 124.34 (16) |
| N3—Zn1—N1 | 104.19 (6) | O11—C33—C34 | 115.38 (15) |
| N3—Zn1—C1 | 96.55 (5) | C32—C33—C34 | 120.24 (16) |
| O9—Zn2—O10 | 56.19 (5) | C35—C34—C33 | 119.60 (16) |
| O9—Zn2—N5 | 109.00 (5) | C35—C34—H34 | 120.2 |
| O9—Zn2—N7 | 99.89 (5) | C33—C34—H34 | 120.2 |

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|-------------|-------------|---------------|-------------|
| O13—Zn2—O9 | 137.57 (6) | C30—C35—H35 | 119.6 |
| O13—Zn2—N5 | 99.17 (6) | C34—C35—C30 | 120.83 (16) |
| O13—Zn2—N7 | 103.00 (5) | C34—C35—H35 | 119.6 |
| N5—Zn2—N7 | 104.55 (6) | O11—C36—H36A | 109.5 |
| O17—Zn3—C57 | 29.18 (5) | O11—C36—H36B | 109.5 |
| O18—Zn3—O17 | 59.04 (4) | O11—C36—H36C | 109.5 |
| O18—Zn3—N9 | 98.24 (5) | H36A—C36—H36B | 109.5 |
| O18—Zn3—N11 | 109.87 (5) | H36A—C36—H36C | 109.5 |
| O18—Zn3—C57 | 29.86 (5) | H36B—C36—H36C | 109.5 |
| O21—Zn3—O17 | 96.15 (5) | O12—C37—O13 | 122.84 (17) |
| O21—Zn3—O18 | 140.66 (5) | O12—C37—C38 | 121.36 (16) |
| O21—Zn3—N9 | 102.61 (5) | O13—C37—C38 | 115.78 (16) |
| O21—Zn3—N11 | 97.49 (5) | C39—C38—C37 | 120.88 (16) |
| O21—Zn3—C57 | 119.88 (6) | C39—C38—C43 | 118.66 (16) |
| N9—Zn3—O17 | 157.26 (5) | C43—C38—C37 | 120.45 (16) |
| N9—Zn3—C57 | 128.09 (6) | C38—C39—C40 | 121.34 (17) |
| N11—Zn3—O17 | 86.98 (5) | C38—C39—H39 | 119.3 |
| N11—Zn3—N9 | 102.99 (5) | C40—C39—H39 | 119.3 |
| N11—Zn3—C57 | 99.72 (5) | C39—C40—H40 | 120.4 |
| C1—O2—Zn1 | 102.95 (10) | C41—C40—C39 | 119.14 (17) |
| C5—O3—C8 | 117.49 (14) | C41—C40—H40 | 120.4 |
| C9—O5—Zn1 | 111.31 (11) | O14—C41—C40 | 124.63 (16) |
| C13—O6—C16 | 118.41 (14) | O14—C41—C42 | 115.19 (16) |
| C29—O9—Zn2 | 105.34 (11) | C40—C41—C42 | 120.18 (17) |
| C33—O11—C36 | 117.70 (14) | C41—C42—H42 | 120.0 |
| C37—O13—Zn2 | 111.31 (11) | C43—C42—C41 | 119.93 (17) |
| C41—O14—C44 | 118.14 (14) | C43—C42—H42 | 120.0 |
| C57—O17—Zn3 | 81.06 (10) | C42—C43—C38 | 120.74 (17) |
| C57—O18—Zn3 | 99.02 (10) | C42—C43—H43 | 119.6 |
| C61—O19—C64 | 117.23 (14) | C38—C43—H43 | 119.6 |
| C65—O21—Zn3 | 109.51 (11) | O14—C44—H44A | 109.5 |
| C69—O22—C72 | 118.16 (14) | O14—C44—H44B | 109.5 |
| C17—N1—Zn1 | 118.23 (12) | O14—C44—H44C | 109.5 |
| C17—N1—C21 | 117.89 (15) | H44A—C44—H44B | 109.5 |
| C21—N1—Zn1 | 123.86 (12) | H44A—C44—H44C | 109.5 |
| C22—N2—H2B | 124.0 (13) | H44B—C44—H44C | 109.5 |
| C22—N2—H2A | 116.6 (13) | N5—C45—C46 | 123.50 (16) |
| H2B—N2—H2A | 118.4 (18) | N5—C45—H45 | 118.3 |
| C23—N3—Zn1 | 121.31 (12) | C46—C45—H45 | 118.3 |
| C23—N3—C27 | 118.34 (15) | C45—C46—C47 | 117.95 (17) |
| C27—N3—Zn1 | 120.21 (11) | C45—C46—C50 | 116.88 (16) |
| C28—N4—H4A | 122.3 (12) | C47—C46—C50 | 125.11 (16) |
| C28—N4—H4B | 116.6 (13) | C46—C47—H47 | 120.7 |
| H4A—N4—H4B | 120.4 (18) | C48—C47—C46 | 118.69 (17) |
| C45—N5—Zn2 | 119.73 (12) | C48—C47—H47 | 120.7 |
| C45—N5—C49 | 118.06 (15) | C47—C48—H48 | 120.2 |
| C49—N5—Zn2 | 121.60 (12) | C49—C48—C47 | 119.64 (17) |
| C50—N6—H6A | 115.9 (15) | C49—C48—H48 | 120.2 |
| C50—N6—H6B | 119.0 (14) | N5—C49—C48 | 122.15 (17) |

supplementary materials

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| H6B—N6—H6A | 124 (2) | N5—C49—H49 | 118.9 |
| C51—N7—Zn2 | 118.84 (12) | C48—C49—H49 | 118.9 |
| C51—N7—C55 | 118.26 (15) | O15—C50—N6 | 123.07 (18) |
| C55—N7—Zn2 | 122.87 (12) | O15—C50—C46 | 118.91 (16) |
| C56—N8—H8E | 123.6 (13) | N6—C50—C46 | 118.00 (17) |
| C56—N8—H8D | 115.9 (15) | N7—C51—C52 | 123.23 (16) |
| H8E—N8—H8D | 119.6 (19) | N7—C51—H51 | 118.4 |
| C73—N9—Zn3 | 117.99 (12) | C52—C51—H51 | 118.4 |
| C73—N9—C77 | 118.04 (15) | C51—C52—C53 | 118.03 (16) |
| C77—N9—Zn3 | 123.97 (12) | C51—C52—C56 | 116.96 (15) |
| C78—N10—H10A | 122.7 (13) | C53—C52—C56 | 125.01 (16) |
| C78—N10—H10B | 115.6 (14) | C52—C53—C54 | 119.05 (16) |
| H10A—N10—H10B | 119.6 (19) | C52—C53—H53 | 120.5 |
| C79—N11—C83 | 118.10 (15) | C54—C53—H53 | 120.5 |
| C79—N11—Zn3 | 120.99 (11) | C53—C54—H54 | 120.5 |
| C83—N11—Zn3 | 120.61 (11) | C55—C54—C53 | 119.09 (17) |
| C84—N12—H12B | 123.2 (13) | C55—C54—H54 | 120.5 |
| C84—N12—H12A | 116.8 (15) | N7—C55—C54 | 122.33 (16) |
| H12B—N12—H12A | 117.9 (19) | N7—C55—H55 | 118.8 |
| O1—C1—Zn1 | 73.24 (10) | C54—C55—H55 | 118.8 |
| O1—C1—O2 | 121.19 (16) | O16—C56—N8 | 123.52 (17) |
| O1—C1—C2 | 120.57 (16) | O16—C56—C52 | 119.29 (16) |
| O2—C1—Zn1 | 47.98 (8) | N8—C56—C52 | 117.19 (16) |
| O2—C1—C2 | 118.23 (15) | O17—C57—Zn3 | 69.76 (10) |
| C2—C1—Zn1 | 166.13 (13) | O17—C57—O18 | 120.86 (16) |
| C3—C2—C1 | 121.20 (16) | O17—C57—C58 | 120.06 (16) |
| C3—C2—C7 | 118.62 (16) | O18—C57—Zn3 | 51.12 (8) |
| C7—C2—C1 | 120.16 (16) | O18—C57—C58 | 119.07 (15) |
| C2—C3—C4 | 120.98 (16) | C58—C57—Zn3 | 170.01 (12) |
| C2—C3—H3 | 119.5 | C59—C58—C57 | 120.79 (15) |
| C4—C3—H3 | 119.5 | C59—C58—C63 | 119.04 (16) |
| C3—C4—H4 | 120.3 | C63—C58—C57 | 120.11 (15) |
| C5—C4—C3 | 119.36 (16) | C58—C59—C60 | 120.75 (16) |
| C5—C4—H4 | 120.3 | C58—C59—H59 | 119.6 |
| O3—C5—C4 | 124.87 (16) | C60—C59—H59 | 119.6 |
| O3—C5—C6 | 114.99 (16) | C59—C60—H60 | 120.3 |
| C4—C5—C6 | 120.13 (17) | C61—C60—C59 | 119.34 (16) |
| C5—C6—H6 | 120.1 | C61—C60—H60 | 120.3 |
| C7—C6—C5 | 119.87 (17) | O19—C61—C60 | 124.66 (16) |
| C7—C6—H6 | 120.1 | O19—C61—C62 | 115.07 (15) |
| C2—C7—H7 | 119.5 | C60—C61—C62 | 120.25 (16) |
| C6—C7—C2 | 121.04 (17) | C61—C62—H62 | 120.1 |
| C6—C7—H7 | 119.5 | C63—C62—C61 | 119.86 (16) |
| O3—C8—H8A | 109.5 | C63—C62—H62 | 120.1 |
| O3—C8—H8B | 109.5 | C58—C63—H63 | 119.6 |
| O3—C8—H8C | 109.5 | C62—C63—C58 | 120.74 (16) |
| H8A—C8—H8B | 109.5 | C62—C63—H63 | 119.6 |
| H8A—C8—H8C | 109.5 | O19—C64—H64A | 109.5 |
| H8B—C8—H8C | 109.5 | O19—C64—H64B | 109.5 |

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| O4—C9—O5 | 123.06 (16) | H64A—C64—H64B | 109.5 |
| O4—C9—C10 | 121.34 (16) | O19—C64—H64C | 109.5 |
| O5—C9—C10 | 115.60 (15) | H64A—C64—H64C | 109.5 |
| C11—C10—C9 | 120.26 (15) | H64B—C64—H64C | 109.5 |
| C15—C10—C9 | 120.76 (16) | O20—C65—O21 | 122.42 (16) |
| C15—C10—C11 | 118.91 (16) | O20—C65—C66 | 121.08 (16) |
| C10—C11—H11 | 119.7 | O21—C65—C66 | 116.49 (16) |
| C12—C11—C10 | 120.66 (16) | C67—C66—C71 | 118.74 (16) |
| C12—C11—H11 | 119.7 | C67—C66—C65 | 120.88 (16) |
| C11—C12—C13 | 119.96 (17) | C71—C66—C65 | 120.38 (16) |
| C11—C12—H12 | 120.0 | C66—C67—H67 | 119.4 |
| C13—C12—H12 | 120.0 | C68—C67—C66 | 121.24 (17) |
| O6—C13—C12 | 115.50 (15) | C68—C67—H67 | 119.4 |
| O6—C13—C14 | 124.33 (16) | C67—C68—C69 | 119.25 (16) |
| C14—C13—C12 | 120.18 (16) | C67—C68—H68 | 120.4 |
| C13—C14—C15 | 119.16 (16) | C69—C68—H68 | 120.4 |
| C13—C14—H14 | 120.4 | O22—C69—C68 | 124.29 (16) |
| C15—C14—H14 | 120.4 | O22—C69—C70 | 115.54 (16) |
| C10—C15—C14 | 121.13 (17) | C68—C69—C70 | 120.16 (16) |
| C10—C15—H15 | 119.4 | C69—C70—H70 | 120.0 |
| C14—C15—H15 | 119.4 | C71—C70—C69 | 119.99 (17) |
| O6—C16—H16A | 109.5 | C71—C70—H70 | 120.0 |
| O6—C16—H16B | 109.5 | C66—C71—H71 | 119.7 |
| O6—C16—H16C | 109.5 | C70—C71—C66 | 120.59 (16) |
| H16A—C16—H16B | 109.5 | C70—C71—H71 | 119.7 |
| H16A—C16—H16C | 109.5 | O22—C72—H72A | 109.5 |
| H16B—C16—H16C | 109.5 | O22—C72—H72B | 109.5 |
| N1—C17—C18 | 123.41 (16) | O22—C72—H72C | 109.5 |
| N1—C17—H17 | 118.3 | H72A—C72—H72B | 109.5 |
| C18—C17—H17 | 118.3 | H72A—C72—H72C | 109.5 |
| C17—C18—C19 | 118.21 (16) | H72B—C72—H72C | 109.5 |
| C17—C18—C22 | 116.65 (15) | N9—C73—C74 | 123.42 (16) |
| C19—C18—C22 | 125.14 (16) | N9—C73—H73 | 118.3 |
| C18—C19—C20 | 118.71 (17) | C74—C73—H73 | 118.3 |
| C18—C19—H19 | 120.6 | C73—C74—C75 | 118.29 (16) |
| C20—C19—H19 | 120.6 | C73—C74—C78 | 116.66 (16) |
| C19—C20—H20 | 120.4 | C75—C74—C78 | 125.05 (16) |
| C21—C20—C19 | 119.23 (17) | C74—C75—C76 | 118.54 (17) |
| C21—C20—H20 | 120.4 | C74—C75—H75 | 120.7 |
| N1—C21—C20 | 122.51 (16) | C76—C75—H75 | 120.7 |
| N1—C21—H21 | 118.7 | C75—C76—H76 | 120.3 |
| C20—C21—H21 | 118.7 | C77—C76—C75 | 119.37 (17) |
| O7—C22—N2 | 123.73 (17) | C77—C76—H76 | 120.3 |
| O7—C22—C18 | 118.95 (16) | N9—C77—C76 | 122.30 (17) |
| N2—C22—C18 | 117.31 (16) | N9—C77—H77 | 118.8 |
| N3—C23—C24 | 123.22 (16) | C76—C77—H77 | 118.8 |
| N3—C23—H23 | 118.4 | O23—C78—N10 | 123.34 (17) |
| C24—C23—H23 | 118.4 | O23—C78—C74 | 119.05 (16) |
| C23—C24—C25 | 118.11 (16) | N10—C78—C74 | 117.61 (16) |

supplementary materials

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| C23—C24—C28 | 116.50 (15) | N11—C79—C80 | 123.44 (16) |
| C25—C24—C28 | 125.34 (16) | N11—C79—H79 | 118.3 |
| C24—C25—H25 | 120.6 | C80—C79—H79 | 118.3 |
| C26—C25—C24 | 118.80 (16) | C79—C80—C81 | 117.96 (16) |
| C26—C25—H25 | 120.6 | C79—C80—C84 | 116.83 (15) |
| C25—C26—H26 | 120.2 | C81—C80—C84 | 125.17 (16) |
| C27—C26—C25 | 119.64 (16) | C80—C81—H81 | 120.6 |
| C27—C26—H26 | 120.2 | C82—C81—C80 | 118.84 (16) |
| N3—C27—C26 | 121.90 (16) | C82—C81—H81 | 120.6 |
| N3—C27—H27 | 119.1 | C81—C82—H82 | 120.3 |
| C26—C27—H27 | 119.1 | C83—C82—C81 | 119.44 (16) |
| O8—C28—N4 | 123.41 (17) | C83—C82—H82 | 120.3 |
| O8—C28—C24 | 119.13 (15) | N11—C83—C82 | 122.22 (16) |
| N4—C28—C24 | 117.44 (16) | N11—C83—H83 | 118.9 |
| O9—C29—C30 | 117.64 (15) | C82—C83—H83 | 118.9 |
| O10—C29—O9 | 121.72 (16) | O24—C84—N12 | 123.03 (17) |
| O10—C29—C30 | 120.64 (16) | O24—C84—C80 | 119.32 (16) |
| C31—C30—C29 | 120.68 (16) | N12—C84—C80 | 117.64 (16) |
| O5—Zn1—O2—C1 | -58.62 (13) | C1—C2—C7—C6 | 178.95 (16) |
| N1—Zn1—O2—C1 | 178.80 (10) | C3—C2—C7—C6 | 0.6 (3) |
| N3—Zn1—O2—C1 | 69.30 (11) | C5—C4—C3—C2 | -0.4 (3) |
| O2—Zn1—O5—C9 | -48.85 (14) | C3—C4—C5—O3 | -179.89 (16) |
| N1—Zn1—O5—C9 | 73.99 (12) | C3—C4—C5—C6 | 0.9 (3) |
| N3—Zn1—O5—C9 | -179.76 (11) | C7—C6—C5—O3 | -179.91 (16) |
| C1—Zn1—O5—C9 | -77.39 (12) | C7—C6—C5—C4 | -0.6 (3) |
| O2—Zn1—N1—C17 | 160.84 (12) | C5—C6—C7—C2 | -0.1 (3) |
| O2—Zn1—N1—C21 | -17.59 (15) | O4—C9—C10—C11 | -176.73 (16) |
| O5—Zn1—N1—C17 | 14.96 (13) | O4—C9—C10—C15 | 6.4 (3) |
| O5—Zn1—N1—C21 | -163.47 (14) | O5—C9—C10—C11 | 3.4 (2) |
| N3—Zn1—N1—C17 | -86.41 (13) | O5—C9—C10—C15 | -173.43 (15) |
| N3—Zn1—N1—C21 | 95.16 (14) | C9—C10—C11—C12 | -177.03 (15) |
| C1—Zn1—N1—C17 | 161.61 (11) | C15—C10—C11—C12 | -0.1 (3) |
| C1—Zn1—N1—C21 | -16.81 (17) | C10—C11—C12—C13 | 0.6 (3) |
| O2—Zn1—N3—C23 | 38.12 (14) | O6—C13—C12—C11 | 179.24 (15) |
| O2—Zn1—N3—C27 | -137.51 (12) | C14—C13—C12—C11 | -0.5 (3) |
| O5—Zn1—N3—C23 | -173.27 (13) | O6—C13—C14—C15 | -179.87 (16) |
| O5—Zn1—N3—C27 | 11.10 (13) | C12—C13—C14—C15 | -0.2 (3) |
| N1—Zn1—N3—C23 | -69.74 (13) | C13—C14—C15—C10 | 0.7 (3) |
| N1—Zn1—N3—C27 | 114.64 (13) | C14—C15—C10—C9 | 176.34 (16) |
| C1—Zn1—N3—C23 | 65.34 (13) | C14—C15—C10—C11 | -0.6 (3) |
| C1—Zn1—N3—C27 | -110.29 (13) | C19—C18—C17—N1 | -1.4 (3) |
| O2—Zn1—C1—O1 | -178.16 (17) | C22—C18—C17—N1 | 178.48 (16) |
| O2—Zn1—C1—C2 | 7.0 (5) | C17—C18—C19—C20 | 0.7 (3) |
| O5—Zn1—C1—O1 | -38.16 (11) | C22—C18—C19—C20 | -179.14 (17) |
| O5—Zn1—C1—O2 | 140.01 (10) | C17—C18—C22—O7 | 17.5 (3) |
| O5—Zn1—C1—C2 | 147.1 (5) | C17—C18—C22—N2 | -161.67 (17) |
| N1—Zn1—C1—O1 | -179.72 (9) | C19—C18—C22—O7 | -162.65 (18) |
| N1—Zn1—C1—O2 | -1.56 (13) | C19—C18—C22—N2 | 18.1 (3) |
| N1—Zn1—C1—C2 | 5.5 (5) | C18—C19—C20—C21 | 0.9 (3) |

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| N3—Zn1—C1—O1 | 65.10 (10) | C19—C20—C21—N1 | -2.0 (3) |
| N3—Zn1—C1—O2 | -116.74 (11) | C24—C23—N3—C27 | 0.1 (2) |
| N3—Zn1—C1—C2 | -109.7 (5) | C24—C23—N3—Zn1 | -175.63 (12) |
| O13—Zn2—O9—C29 | 62.59 (13) | N3—C23—C24—C25 | -0.4 (3) |
| N5—Zn2—O9—C29 | -66.21 (12) | N3—C23—C24—C28 | 177.12 (15) |
| N7—Zn2—O9—C29 | -175.47 (11) | C26—C25—C24—C23 | 0.2 (2) |
| O9—Zn2—O13—C37 | 47.40 (14) | C26—C25—C24—C28 | -177.09 (16) |
| N5—Zn2—O13—C37 | 179.12 (12) | C24—C25—C26—C27 | 0.3 (3) |
| N7—Zn2—O13—C37 | -73.52 (12) | N3—C27—C26—C25 | -0.7 (3) |
| O9—Zn2—N5—C45 | -19.92 (14) | O8—C28—C24—C23 | 10.9 (2) |
| O9—Zn2—N5—C49 | 151.00 (13) | O8—C28—C24—C25 | -171.69 (17) |
| O13—Zn2—N5—C45 | -167.74 (12) | N4—C28—C24—C23 | -167.57 (16) |
| O13—Zn2—N5—C49 | 3.18 (14) | N4—C28—C24—C25 | 9.8 (3) |
| N7—Zn2—N5—C45 | 86.16 (13) | O9—C29—C30—C31 | 178.91 (16) |
| N7—Zn2—N5—C49 | -102.92 (13) | O9—C29—C30—C35 | 2.1 (2) |
| O9—Zn2—N7—C51 | -160.13 (13) | O10—C29—C30—C31 | -1.3 (3) |
| O9—Zn2—N7—C55 | 17.74 (15) | O10—C29—C30—C35 | -178.18 (16) |
| O13—Zn2—N7—C51 | -16.11 (14) | C29—C30—C35—C34 | 177.52 (16) |
| O13—Zn2—N7—C55 | 161.75 (13) | C31—C30—C35—C34 | 0.6 (3) |
| N5—Zn2—N7—C51 | 87.12 (13) | C32—C31—C30—C29 | -177.86 (16) |
| N5—Zn2—N7—C55 | -95.01 (14) | C32—C31—C30—C35 | -1.0 (3) |
| O18—Zn3—O17—C57 | -0.80 (10) | C30—C31—C32—C33 | 0.5 (3) |
| O21—Zn3—O17—C57 | 146.61 (10) | O11—C33—C32—C31 | 178.25 (16) |
| N9—Zn3—O17—C57 | 0.99 (18) | C34—C33—C32—C31 | 0.3 (3) |
| N11—Zn3—O17—C57 | -116.18 (10) | O11—C33—C34—C35 | -178.77 (15) |
| O17—Zn3—O18—C57 | 0.78 (9) | C32—C33—C34—C35 | -0.7 (3) |
| O21—Zn3—O18—C57 | -56.88 (13) | C30—C35—C34—C33 | 0.2 (3) |
| N9—Zn3—O18—C57 | -178.52 (10) | O12—C37—C38—C39 | -2.3 (3) |
| N11—Zn3—O18—C57 | 74.39 (11) | O12—C37—C38—C43 | 178.60 (16) |
| O17—Zn3—O21—C65 | -90.17 (11) | O13—C37—C38—C39 | 179.20 (16) |
| O18—Zn3—O21—C65 | -43.40 (15) | O13—C37—C38—C43 | 0.1 (2) |
| N9—Zn3—O21—C65 | 76.90 (12) | C37—C38—C39—C40 | -179.05 (16) |
| N11—Zn3—O21—C65 | -177.93 (11) | C43—C38—C39—C40 | 0.1 (3) |
| C57—Zn3—O21—C65 | -72.15 (12) | C37—C38—C43—C42 | 179.77 (16) |
| O17—Zn3—N9—C73 | 158.69 (12) | C39—C38—C43—C42 | 0.6 (3) |
| O17—Zn3—N9—C77 | -20.9 (2) | C41—C40—C39—C38 | -0.7 (3) |
| O18—Zn3—N9—C73 | 160.23 (12) | C39—C40—C41—O14 | -179.09 (16) |
| O18—Zn3—N9—C77 | -19.33 (14) | C39—C40—C41—C42 | 0.6 (3) |
| O21—Zn3—N9—C73 | 13.80 (13) | O14—C41—C42—C43 | 179.81 (15) |
| O21—Zn3—N9—C77 | -165.76 (13) | C40—C41—C42—C43 | 0.1 (3) |
| N11—Zn3—N9—C73 | -87.07 (13) | C38—C43—C42—C41 | -0.7 (3) |
| N11—Zn3—N9—C77 | 93.37 (14) | C47—C46—C45—N5 | 0.2 (3) |
| C57—Zn3—N9—C73 | 159.30 (11) | C50—C46—C45—N5 | -177.00 (15) |
| C57—Zn3—N9—C77 | -20.27 (17) | C45—C46—C47—C48 | 0.3 (3) |
| O17—Zn3—N11—C79 | 84.93 (13) | C50—C46—C47—C48 | 177.26 (16) |
| O17—Zn3—N11—C83 | -88.69 (13) | C45—C46—C50—O15 | -10.4 (2) |
| O18—Zn3—N11—C79 | 29.46 (14) | C45—C46—C50—N6 | 168.43 (17) |
| O18—Zn3—N11—C83 | -144.16 (12) | C47—C46—C50—O15 | 172.62 (17) |
| O21—Zn3—N11—C79 | -179.26 (12) | C47—C46—C50—N6 | -8.6 (3) |

supplementary materials

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| O21—Zn3—N11—C83 | 7.12 (13) | C49—C48—C47—C46 | -0.8 (3) |
| N9—Zn3—N11—C79 | -74.41 (13) | C47—C48—C49—N5 | 0.8 (3) |
| N9—Zn3—N11—C83 | 111.97 (13) | N7—C51—C52—C53 | 1.4 (3) |
| C57—Zn3—N11—C79 | 58.58 (13) | N7—C51—C52—C56 | -178.01 (16) |
| C57—Zn3—N11—C83 | -115.05 (13) | C51—C52—C53—C54 | -0.5 (3) |
| O17—Zn3—C57—O18 | -178.63 (17) | C56—C52—C53—C54 | 178.83 (16) |
| O18—Zn3—C57—O17 | 178.63 (17) | C55—C54—C53—C52 | -0.9 (3) |
| O21—Zn3—C57—O17 | -39.13 (11) | C53—C54—C55—N7 | 1.5 (3) |
| O21—Zn3—C57—O18 | 142.24 (10) | O16—C56—C52—C51 | -14.7 (3) |
| N9—Zn3—C57—O17 | -179.52 (9) | O16—C56—C52—C53 | 165.98 (18) |
| N9—Zn3—C57—O18 | 1.86 (13) | N8—C56—C52—C51 | 165.20 (17) |
| N11—Zn3—C57—O17 | 65.40 (10) | N8—C56—C52—C53 | -14.1 (3) |
| N11—Zn3—C57—O18 | -113.23 (10) | O17—C57—C58—C59 | 175.59 (16) |
| Zn1—O2—C1—O1 | 2.06 (19) | O17—C57—C58—C63 | -1.6 (2) |
| Zn1—O2—C1—C2 | -178.09 (12) | O18—C57—C58—C59 | -3.6 (2) |
| C8—O3—C5—C4 | 7.7 (3) | O18—C57—C58—C63 | 179.17 (15) |
| C8—O3—C5—C6 | -173.03 (16) | C60—C59—C58—C57 | -177.83 (15) |
| Zn1—O5—C9—O4 | 3.7 (2) | C60—C59—C58—C63 | -0.6 (2) |
| Zn1—O5—C9—C10 | -176.46 (11) | C58—C59—C60—C61 | 0.1 (3) |
| C16—O6—C13—C12 | 178.37 (15) | C60—C61—O19—C64 | 12.2 (2) |
| C16—O6—C13—C14 | -2.0 (2) | C62—C61—O19—C64 | -169.53 (16) |
| Zn2—O9—C29—O10 | -0.3 (2) | O19—C61—C60—C59 | 178.68 (16) |
| Zn2—O9—C29—C30 | 179.44 (12) | C62—C61—C60—C59 | 0.5 (3) |
| C36—O11—C33—C32 | 4.8 (2) | C63—C62—C61—O19 | -178.98 (15) |
| C36—O11—C33—C34 | -177.21 (15) | C63—C62—C61—C60 | -0.6 (3) |
| Zn2—O13—C37—O12 | -4.3 (2) | C61—C62—C63—C58 | 0.1 (3) |
| Zn2—O13—C37—C38 | 174.17 (11) | C62—C63—C58—C57 | 177.72 (16) |
| C44—O14—C41—C40 | 2.5 (3) | C62—C63—C58—C59 | 0.5 (3) |
| C44—O14—C41—C42 | -177.25 (15) | O21—C65—C66—C67 | 170.90 (16) |
| Zn3—O17—C57—O18 | 1.24 (15) | O21—C65—C66—C71 | -9.7 (2) |
| Zn3—O17—C57—C58 | -177.97 (15) | O20—C65—C66—C67 | -8.0 (3) |
| Zn3—O18—C57—O17 | -1.50 (18) | O20—C65—C66—C71 | 171.43 (16) |
| Zn3—O18—C57—C58 | 177.72 (13) | C65—C66—C71—C70 | 179.70 (16) |
| Zn3—O21—C65—O20 | 2.3 (2) | C67—C66—C71—C70 | -0.9 (3) |
| Zn3—O21—C65—C66 | -176.59 (11) | C68—C67—C66—C65 | -179.13 (16) |
| C72—O22—C69—C68 | -3.6 (3) | C68—C67—C66—C71 | 1.4 (3) |
| C72—O22—C69—C70 | 176.33 (16) | C69—C68—C67—C66 | -0.4 (3) |
| C21—N1—C17—C18 | 0.4 (3) | C67—C68—C69—O22 | 178.65 (16) |
| Zn1—N1—C17—C18 | -178.16 (13) | C67—C68—C69—C70 | -1.3 (3) |
| Zn1—N1—C21—C20 | 179.77 (13) | C71—C70—C69—O22 | -178.09 (16) |
| C17—N1—C21—C20 | 1.3 (3) | C71—C70—C69—C68 | 1.8 (3) |
| Zn1—N3—C27—C26 | 176.25 (13) | C69—C70—C71—C66 | -0.8 (3) |
| C23—N3—C27—C26 | 0.5 (2) | C74—C73—N9—C77 | 0.9 (3) |
| Zn2—N5—C45—C46 | 171.01 (13) | C74—C73—N9—Zn3 | -178.69 (13) |
| C49—N5—C45—C46 | -0.2 (3) | N9—C73—C74—C75 | -1.7 (3) |
| Zn2—N5—C49—C48 | -171.37 (14) | N9—C73—C74—C78 | 178.28 (16) |
| C45—N5—C49—C48 | -0.3 (3) | C73—C74—C75—C76 | 0.6 (3) |
| Zn2—N7—C51—C52 | 177.20 (13) | C78—C74—C75—C76 | -179.40 (16) |
| C55—N7—C51—C52 | -0.8 (3) | C73—C74—C78—O23 | 18.3 (3) |

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|-----------------|--------------|-----------------|--------------|
| Zn2—N7—C55—C54 | -178.59 (13) | C73—C74—C78—N10 | -161.14 (17) |
| C51—N7—C55—C54 | -0.7 (3) | C75—C74—C78—O23 | -161.71 (18) |
| Zn3—N9—C77—C76 | -179.39 (13) | C75—C74—C78—N10 | 18.8 (3) |
| C73—N9—C77—C76 | 1.0 (3) | C77—C76—C75—C74 | 1.2 (3) |
| Zn3—N11—C79—C80 | -173.43 (13) | C75—C76—C77—N9 | -2.1 (3) |
| C83—N11—C79—C80 | 0.4 (2) | N11—C79—C80—C81 | 0.0 (3) |
| Zn3—N11—C83—C82 | 173.53 (13) | N11—C79—C80—C84 | 177.85 (15) |
| C79—N11—C83—C82 | -0.3 (2) | C79—C80—C81—C82 | -0.4 (2) |
| Zn1—C1—C2—C3 | -11.2 (6) | C84—C80—C81—C82 | -178.06 (16) |
| Zn1—C1—C2—C7 | 170.4 (4) | C79—C80—C84—O24 | 7.0 (2) |
| O1—C1—C2—C3 | 174.56 (16) | C79—C80—C84—N12 | -173.62 (16) |
| O1—C1—C2—C7 | -3.8 (3) | C81—C80—C84—O24 | -175.31 (17) |
| O2—C1—C2—C3 | -5.3 (2) | C81—C80—C84—N12 | 4.1 (3) |
| O2—C1—C2—C7 | 176.36 (15) | C83—C82—C81—C80 | 0.5 (3) |
| C1—C2—C3—C4 | -178.65 (16) | C81—C82—C83—N11 | -0.1 (3) |
| C7—C2—C3—C4 | -0.3 (3) | | |

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

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|--------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N2—H2A \cdots O24 ⁱ | 0.82 (2) | 2.16 (2) | 2.966 (2) | 168.8 (2) |
| N2—H2B \cdots O4 ⁱⁱ | 0.84 (2) | 2.16 (2) | 2.991 (2) | 176.6 (2) |
| N4—H4A \cdots O17 ⁱⁱⁱ | 0.83 (2) | 2.08 (2) | 2.903 (2) | 169.4 (2) |
| N4—H4B \cdots O16 ^{iv} | 0.85 (2) | 2.59 (2) | 3.152 (2) | 125.0 (2) |
| N4—H4B \cdots O19 ^v | 0.85 (2) | 2.52 (2) | 3.225 (2) | 141.3 (2) |
| N6—H6A \cdots O23 ^{vi} | 0.78 (2) | 2.40 (2) | 3.073 (2) | 146 (2) |
| N6—H6B \cdots O10 ^{vii} | 0.86 (2) | 2.11 (2) | 2.959 (2) | 170.3 (2) |
| N8—H8D \cdots O8 ^{iv} | 0.79 (2) | 2.13 (2) | 2.909 (2) | 166 (2) |
| N8—H8E \cdots O20 ^{viii} | 0.87 (2) | 2.19 (2) | 3.058 (2) | 174.8 (2) |
| N10—H10A \cdots O12 ^{ix} | 0.87 (2) | 2.21 (2) | 3.077 (2) | 172 (2) |
| N10—H10B \cdots O15 ^{vi} | 0.84 (2) | 2.10 (2) | 2.917 (2) | 162.8 (2) |
| N12—H12A \cdots O11 ⁱⁱⁱ | 0.83 (2) | 2.55 (2) | 3.268 (2) | 145 (2) |
| N12—H12B \cdots O1 ⁱⁱⁱ | 0.87 (2) | 2.07 (2) | 2.940 (2) | 171.9 (2) |
| C4—H4 \cdots O14 ^x | 0.93 | 2.45 | 3.331 (2) | 158 |
| C19—H19 \cdots O4 ⁱⁱ | 0.93 | 2.36 | 3.175 (2) | 146 |
| C25—H25 \cdots O17 ⁱⁱⁱ | 0.93 | 2.41 | 3.284 (2) | 157 |
| C27—H27 \cdots O7 ^{xi} | 0.93 | 2.47 | 3.214 (2) | 138 |
| C34—H34 \cdots O22 ^{xii} | 0.93 | 2.51 | 3.329 (2) | 148 |
| C35—H35 \cdots O15 ^{xiii} | 0.93 | 2.45 | 3.304 (2) | 152 |
| C47—H47 \cdots O10 ^{vii} | 0.93 | 2.27 | 3.146 (2) | 156 |
| C53—H53 \cdots O20 ^{viii} | 0.93 | 2.31 | 3.172 (2) | 154 |
| C59—H59 \cdots O8 ^{xi} | 0.93 | 2.58 | 3.390 (2) | 146 |
| C60—H60 \cdots O6 | 0.93 | 2.42 | 3.282 (2) | 153 |
| C75—H75 \cdots O12 ^{ix} | 0.93 | 2.39 | 3.212 (2) | 147 |

supplementary materials

C81—H81...O1ⁱⁱⁱ

0.93

2.44

3.306 (2)

156

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y+1, -z+1$; (iii) $-x+2, -y+1, -z+1$; (iv) $-x+1, -y, -z+2$; (v) $x, y-1, z$; (vi) $-x+1, -y+2, -z+1$; (vii) $-x, -y+1, -z+2$; (viii) $x, y-1, z+1$; (ix) $x, y+1, z-1$; (x) $-x, -y, -z+2$; (xi) $-x+1, -y+1, -z+1$; (xii) $-x+2, -y+2, -z+1$; (xiii) $-x+1, -y+1, -z+2$.

Fig. 1

