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# [2-(2-Carboxyphenyl)benzoato]bis(1,10-phenanthroline)zinc(II) 2-(2-carboxyphenyl)benzoate monohydrate

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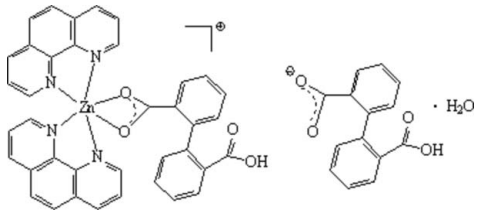
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.064; $wR$ factor = 0.145; data-to-parameter ratio = 15.6.

In the title compound, $[Zn(C_{14}H_9O_4)(C_{12}H_8N_2)_2](C_{14}H_9O_4)\cdot H_2O$, the $Zn^{II}$ atom of the complex cation is six-coordinated in an octahedral geometry by four N atoms from two 1,10-phenanthroline ligands and two O atoms of a carboxylate group from a singly deprotonated diphenic acid. The phenanthroline and carboxylate ligands act as chelating ligands. The dihedral angles between the two benzene rings in the deprotonated diphenic acid groups are 81.05 (2) (ligand) and 89.10 (2)° (anion). O—H···O and C—H···O hydrogen bonds link the components into a three-dimensional network.

## Related literature

For related structures containing the diphenic acid anion, see: Wan & Zhang (2003); Vodak *et al.* (2001); Chui *et al.* (2001); Fernandes *et al.* (2001); Trombe *et al.* (2002); Xu *et al.* (2003); Nie *et al.* (2001); Sun *et al.* (2001).



## Experimental

### Crystal data

$[Zn(C_{14}H_9O_4)(C_{12}H_8N_2)_2]\cdot(C_{14}H_9O_4)\cdot H_2O$
$M_r$ = 926.24
Triclinic, $P\overline{1}$
$a$ = 10.8208 (11) Å
$b$ = 13.7475 (14) Å
$c$ = 14.9231 (16) Å
$\alpha$ = 77.824 (2)°
$\beta$ = 77.294 (2)°
$\gamma$ = 85.052 (2)°
$V$ = 2115.0 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.65 mm$^{-1}$
$T$ = 298 (2) K
0.46 × 0.28 × 0.07 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min}$ = 0.800, $T_{max}$ = 0.960
13020 measured reflections
9403 independent reflections
4505 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.103

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.144
$S$ = 0.82
9403 reflections
603 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.89 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.48 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—O2 | 2.078 (3) | Zn1—N3 | 2.145 (4) |
| Zn1—N1 | 2.128 (3) | Zn1—N2 | 2.145 (3) |
| Zn1—N4 | 2.130 (3) | Zn1—O1 | 2.334 (3) |
| | | | |
| O2—Zn1—N1 | 102.73 (12) | N4—Zn1—N2 | 167.99 (13) |
| O2—Zn1—N4 | 97.11 (12) | N3—Zn1—N2 | 90.84 (13) |
| N1—Zn1—N4 | 100.12 (12) | O2—Zn1—O1 | 59.17 (10) |
| O2—Zn1—N3 | 155.43 (11) | N1—Zn1—O1 | 155.22 (11) |
| N1—Zn1—N3 | 101.83 (13) | N4—Zn1—O1 | 98.98 (11) |
| N4—Zn1—N3 | 77.99 (14) | N3—Zn1—O1 | 97.46 (11) |
| O2—Zn1—N2 | 94.88 (12) | N2—Zn1—O1 | 86.71 (11) |
| N1—Zn1—N2 | 77.67 (12) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O9—H9$B$···O7$^{i}$ | 0.84 (4) | 2.10 (5) | 2.936 (6) | 171 (6) |
| O4—H4$B$···O5$^{ii}$ | 0.82 | 1.86 | 2.633 (5) | 158 |
| O9—H9$A$···O5 | 0.87 (5) | 1.96 (6) | 2.817 (6) | 171 (7) |
| O8—H8$B$···O6 | 0.82 | 1.69 | 2.500 (5) | 171 |
| C3—H3···O1 | 0.93 | 2.55 | 3.130 (5) | 121 |
| C4—H4$A$···O6$^{ii}$ | 0.93 | 2.42 | 3.221 (5) | 144 |
| C12—H12···O9 | 0.93 | 2.42 | 3.273 (6) | 152 |
| C16—H16···O7$^{i}$ | 0.93 | 2.43 | 3.199 (7) | 139 |
| C19—H19···O6$^{iii}$ | 0.93 | 2.56 | 3.377 (5) | 146 |
| C22—H22···O1$^{iv}$ | 0.93 | 2.43 | 3.249 (6) | 147 |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: CI2560).

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# supplementary materials

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# [2-(2-Carboxyphenyl)benzoato]bis(1,10-phenanthroline)zinc(II) 2-(2-carboxyphenyl)benzoate monohydrate

**W.-W. Huang and S.-P. Yang**

## Comment

In all types of carboxylic acids, diphenic acid is widely used in the construction of coordination polymers due to their capability of acting as bridging and chelating ligand in various coordination modes (Wan & Zhang, 2003). Much interest has been paid to the preparation of metal aromatic carboxylates under hydrothermal conditions (Vodak *et al.*, 2001; Chui *et al.*, 2001; Nie *et al.*, 2001; Sun *et al.*, 2001; Fernandes *et al.*, 2001; Trombe *et al.* 2002; Xu *et al.* 2003). Recently, we have prepared the title compound and report here its crystal structure.

The asymmetric unit of the title compound consists of a $[Zn(C_{12}H_8N_2)_2(C_{14}H_9O_4)]^+$ complex cation, one singly deprotonated diphenic acid anion ($C_{14}H_9O_4^-$) and one water molecule (Fig. 1). In the complex cation, the $Zn^{II}$ atom is six-coordinated in an octahedral geometry by four N atoms from two 1,10-phenanthroline ligands and two O atoms of a carboxylate group from a diphenic acid, with Zn—N distances of 2.128 (3)–2.145 (4) Å and Zn—O distances of 2.078 (3) and 2.334 (3) Å. The N—Zn—N, N—Zn—O and O—Zn—O bond angles are in the ranges 77.99 (14)–167.99 (13)°, 86.71 (11)–155.23 (11)° and 59.17 (10)°, respectively (Table 1). The phenanthroline and diphenic acid act as chelating ligands (Table 1 and Fig.1). The dihedral angle between the two benzene rings in diphenic acid is *ca* 81.05 (2)° (cation) and 89.10 (2)° (anion).

Intermolecular O—H···O and C—H···O hydrogen bonds (Table 2) link complex cations, anions and water molecules to form a three-dimensional network (Fig. 2).

## Experimental

A mixture of diphenic acid (0.0484 g, 0.2 mmol), phenanthroline (0.04 g, 0.2 mmol), $Zn(NO_3)_2{\cdot}6H_2O$ (0.1 mmol) and NaOH (0.012 g, 0.3 mmol) with a molar ratio of 2/2/1/3 in $H_2O$—$CH_3CH_2OH$ (*v*/*v* 4/1) (15 ml) was sealed in a Teflon-lined stainless steel Parr bomb. The bomb was heated to 433 K for 72 h and then cooled to room temperature at 5 K $h^{-1}$. A large amount of yellow crystals formed, which were collected by filtration, washed with water, and dried in air.

## Refinement

The water H atoms were located in a difference map and their positional parameters were refined with O—H distances restrained to 0.85 (3) Å. The remaining H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å, O—H = 0.82 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.2$U_{eq}$(O). The components of the displacement parameters in the direction of the C31—C32 bond were restrained to be equal.

**Figures**

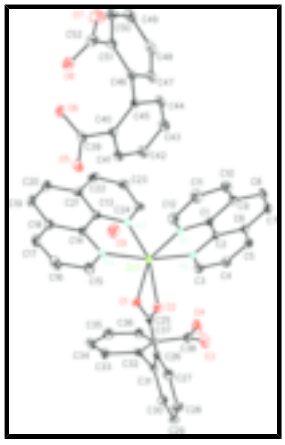

Fig. 1. The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

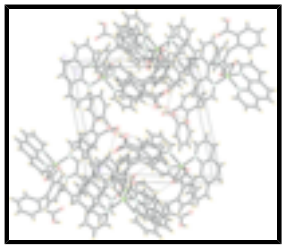

Fig. 2. The crystal packing of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

**[2-(2-Carboxyphenyl)benzoato]bis(1,10-phenanthroline)zinc(II) 2-(2-carboxyphenyl)benzoate monohydrate**

*Crystal data*

| | |
|---|---|
| $[Zn(C_{14}H_9O_4)(C_{12}H_8N_2)_2](C_{14}H_9O_4)\cdot H_2O$ | $Z = 2$ |
| $M_r = 926.24$ | $F_{000} = 956$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.454$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 10.8208$ (11) Å | Cell parameters from 1630 reflections |
| $b = 13.7475$ (14) Å | $\theta = 4.8$–$40.2^\circ$ |
| $c = 14.9231$ (16) Å | $\mu = 0.65$ mm$^{-1}$ |
| $\alpha = 77.824$ (2)° | $T = 298$ (2) K |
| $\beta = 77.294$ (2)° | Block, yellow |
| $\gamma = 85.052$ (2)° | 0.46 × 0.28 × 0.07 mm |
| $V = 2115.0$ (4) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 9403 independent reflections |
| Radiation source: fine-focus sealed tube | 4505 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.103$ |
| $T = 298$(2) K | $\theta_{max} = 28.3^\circ$ |
| φ and ω scans | $\theta_{min} = 1.5^\circ$ |

Absorption correction: multi-scan (SADABS; Bruker, 1998)
$T_{min}$ = 0.800, $T_{max}$ = 0.960
13020 measured reflections

$h$ = −11→14
$k$ = −17→17
$l$ = −16→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.144
$S$ = 0.82
9403 reflections
603 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.89 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.48 e Å$^{-3}$
Extinction correction: none

*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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.64423 (5) | 0.88673 (4) | 0.74002 (3) | 0.03550 (16) |
| O1 | 0.7838 (3) | 1.0069 (2) | 0.64852 (19) | 0.0426 (8) |
| O2 | 0.8139 (3) | 0.9051 (2) | 0.77676 (18) | 0.0405 (7) |
| O3 | 0.7914 (4) | 1.2521 (3) | 0.7375 (3) | 0.0767 (12) |
| O4 | 0.7058 (4) | 1.3718 (3) | 0.6419 (3) | 0.0865 (13) |
| H4B | 0.6644 | 1.3840 | 0.6916 | 0.130* |
| N1 | 0.5364 (3) | 0.8073 (2) | 0.8672 (2) | 0.0368 (9) |
| N2 | 0.5425 (3) | 1.0045 (2) | 0.8031 (2) | 0.0355 (8) |
| N3 | 0.5155 (3) | 0.9006 (2) | 0.6470 (2) | 0.0366 (9) |
| N4 | 0.7090 (3) | 0.7673 (2) | 0.6686 (2) | 0.0369 (9) |
| C1 | 0.4516 (4) | 0.8671 (3) | 0.9161 (3) | 0.0350 (10) |
| C2 | 0.4569 (4) | 0.9721 (3) | 0.8828 (3) | 0.0339 (10) |

| | | | | |
|---|---|---|---|---|
| C3 | 0.5528 (4) | 1.1024 (3) | 0.7720 (3) | 0.0469 (12) |
| H3 | 0.6133 | 1.1252 | 0.7185 | 0.056* |
| C4 | 0.4759 (4) | 1.1718 (3) | 0.8172 (3) | 0.0491 (12) |
| H4A | 0.4836 | 1.2396 | 0.7930 | 0.059* |
| C5 | 0.3890 (4) | 1.1393 (3) | 0.8973 (3) | 0.0483 (12) |
| H5 | 0.3376 | 1.1850 | 0.9281 | 0.058* |
| C6 | 0.3773 (4) | 1.0374 (3) | 0.9329 (3) | 0.0384 (11) |
| C7 | 0.2920 (4) | 0.9964 (4) | 1.0161 (3) | 0.0522 (13) |
| H7 | 0.2391 | 1.0390 | 1.0499 | 0.063* |
| C8 | 0.2853 (4) | 0.8969 (4) | 1.0478 (3) | 0.0514 (13) |
| H8A | 0.2276 | 0.8727 | 1.1025 | 0.062* |
| C9 | 0.3653 (4) | 0.8282 (3) | 0.9989 (3) | 0.0428 (11) |
| C10 | 0.3674 (5) | 0.7248 (4) | 1.0305 (3) | 0.0557 (14) |
| H10 | 0.3105 | 0.6964 | 1.0841 | 0.067* |
| C11 | 0.4531 (5) | 0.6656 (4) | 0.9822 (3) | 0.0609 (15) |
| H11 | 0.4568 | 0.5970 | 1.0035 | 0.073* |
| C12 | 0.5357 (5) | 0.7098 (3) | 0.9000 (3) | 0.0501 (13) |
| H12 | 0.5927 | 0.6688 | 0.8670 | 0.060* |
| C13 | 0.5415 (4) | 0.8322 (3) | 0.5895 (3) | 0.0365 (10) |
| C14 | 0.6448 (4) | 0.7631 (3) | 0.6003 (3) | 0.0374 (11) |
| C15 | 0.8014 (5) | 0.6997 (3) | 0.6810 (3) | 0.0495 (12) |
| H15 | 0.8443 | 0.7003 | 0.7285 | 0.059* |
| C16 | 0.8374 (5) | 0.6272 (3) | 0.6259 (4) | 0.0617 (15) |
| H16 | 0.9042 | 0.5817 | 0.6360 | 0.074* |
| C17 | 0.7750 (5) | 0.6236 (4) | 0.5582 (4) | 0.0600 (15) |
| H17 | 0.7984 | 0.5757 | 0.5213 | 0.072* |
| C18 | 0.6766 (5) | 0.6907 (3) | 0.5438 (3) | 0.0482 (13) |
| C19 | 0.6023 (5) | 0.6905 (4) | 0.4744 (3) | 0.0641 (16) |
| H19 | 0.6232 | 0.6450 | 0.4348 | 0.077* |
| C20 | 0.5024 (6) | 0.7560 (4) | 0.4665 (3) | 0.0661 (16) |
| H20 | 0.4551 | 0.7532 | 0.4221 | 0.079* |
| C21 | 0.4670 (5) | 0.8289 (4) | 0.5235 (3) | 0.0464 (12) |
| C22 | 0.3630 (5) | 0.8974 (4) | 0.5197 (3) | 0.0579 (14) |
| H22 | 0.3120 | 0.8971 | 0.4771 | 0.070* |
| C23 | 0.3367 (5) | 0.9635 (4) | 0.5774 (3) | 0.0518 (13) |
| H23 | 0.2673 | 1.0082 | 0.5757 | 0.062* |
| C24 | 0.4157 (4) | 0.9631 (3) | 0.6391 (3) | 0.0451 (12) |
| H24 | 0.3976 | 1.0097 | 0.6777 | 0.054* |
| C25 | 0.8448 (4) | 0.9804 (3) | 0.7112 (3) | 0.0355 (10) |
| C26 | 0.9559 (4) | 1.0368 (3) | 0.7160 (3) | 0.0335 (10) |
| C27 | 1.0267 (5) | 0.9982 (4) | 0.7824 (3) | 0.0525 (13) |
| H27 | 1.0055 | 0.9369 | 0.8210 | 0.063* |
| C28 | 1.1267 (5) | 1.0449 (4) | 0.7949 (4) | 0.0639 (15) |
| H28 | 1.1724 | 1.0155 | 0.8403 | 0.077* |
| C29 | 1.1583 (5) | 1.1361 (4) | 0.7392 (4) | 0.0597 (15) |
| H29 | 1.2254 | 1.1696 | 0.7464 | 0.072* |
| C30 | 1.0889 (5) | 1.1765 (4) | 0.6728 (3) | 0.0545 (14) |
| H30 | 1.1105 | 1.2383 | 0.6355 | 0.065* |
| C31 | 0.9879 (4) | 1.1300 (3) | 0.6582 (3) | 0.0382 (11) |

| | | | | |
|---|---|---|---|---|
| C32 | 0.9304 (4) | 1.1779 (3) | 0.5740 (3) | 0.0467 (12) |
| C33 | 0.9827 (5) | 1.1414 (3) | 0.4889 (3) | 0.0505 (13) |
| H33 | 1.0407 | 1.0874 | 0.4896 | 0.061* |
| C34 | 0.9473 (5) | 1.1854 (4) | 0.4096 (4) | 0.0703 (17) |
| H34 | 0.9760 | 1.1592 | 0.3558 | 0.084* |
| C35 | 0.8636 (5) | 1.2748 (4) | 0.4069 (4) | 0.0711 (17) |
| H35 | 0.8431 | 1.3082 | 0.3507 | 0.085* |
| C36 | 0.8155 (5) | 1.3089 (4) | 0.4883 (3) | 0.0525 (13) |
| H36 | 0.7614 | 1.3653 | 0.4875 | 0.063* |
| C37 | 0.8477 (5) | 1.2592 (4) | 0.5721 (3) | 0.0515 (13) |
| C38 | 0.7835 (5) | 1.2933 (4) | 0.6589 (4) | 0.0517 (13) |
| O5 | 0.5364 (3) | 0.4416 (3) | 0.7713 (2) | 0.0637 (10) |
| O6 | 0.3732 (3) | 0.3897 (2) | 0.7279 (2) | 0.0534 (9) |
| O7 | −0.0451 (4) | 0.4415 (3) | 0.7539 (3) | 0.0927 (13) |
| O8 | 0.1589 (4) | 0.4398 (3) | 0.6921 (2) | 0.0643 (10) |
| H8B | 0.2255 | 0.4224 | 0.7097 | 0.096* |
| C39 | 0.4238 (5) | 0.4485 (3) | 0.7635 (3) | 0.0440 (12) |
| C40 | 0.3400 (4) | 0.5330 (3) | 0.7956 (3) | 0.0378 (11) |
| C41 | 0.3802 (4) | 0.6285 (3) | 0.7610 (3) | 0.0513 (13) |
| H41 | 0.4601 | 0.6381 | 0.7225 | 0.062* |
| C42 | 0.3053 (5) | 0.7102 (3) | 0.7819 (3) | 0.0567 (14) |
| H42 | 0.3323 | 0.7743 | 0.7553 | 0.068* |
| C43 | 0.1916 (5) | 0.6958 (3) | 0.8416 (3) | 0.0568 (14) |
| H43 | 0.1407 | 0.7501 | 0.8577 | 0.068* |
| C44 | 0.1511 (4) | 0.5996 (3) | 0.8790 (3) | 0.0496 (13) |
| H44 | 0.0737 | 0.5904 | 0.9211 | 0.059* |
| C45 | 0.2223 (4) | 0.5183 (3) | 0.8554 (3) | 0.0352 (10) |
| C46 | 0.1725 (4) | 0.4179 (3) | 0.8974 (3) | 0.0373 (11) |
| C47 | 0.1929 (4) | 0.3696 (3) | 0.9849 (3) | 0.0471 (12) |
| H47 | 0.2418 | 0.3994 | 1.0149 | 0.057* |
| C48 | 0.1422 (5) | 0.2782 (4) | 1.0288 (3) | 0.0571 (14) |
| H48 | 0.1603 | 0.2451 | 1.0859 | 0.069* |
| C49 | 0.0635 (5) | 0.2368 (4) | 0.9855 (4) | 0.0640 (16) |
| H49 | 0.0285 | 0.1757 | 1.0142 | 0.077* |
| C50 | 0.0370 (4) | 0.2852 (3) | 0.9012 (4) | 0.0541 (14) |
| H50 | −0.0188 | 0.2583 | 0.8746 | 0.065* |
| C51 | 0.0930 (4) | 0.3744 (3) | 0.8553 (3) | 0.0431 (11) |
| C52 | 0.0630 (6) | 0.4223 (4) | 0.7638 (4) | 0.0559 (13) |
| O9 | 0.7109 (4) | 0.5128 (3) | 0.8546 (3) | 0.0742 (11) |
| H9A | 0.652 (4) | 0.497 (5) | 0.830 (4) | 0.111* |
| H9B | 0.785 (3) | 0.495 (5) | 0.830 (4) | 0.111* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0397 (3) | 0.0354 (3) | 0.0325 (3) | −0.0046 (2) | −0.0036 (2) | −0.0120 (2) |
| O1 | 0.043 (2) | 0.0487 (19) | 0.0378 (18) | −0.0073 (15) | −0.0123 (15) | −0.0061 (15) |
| O2 | 0.0471 (19) | 0.0346 (17) | 0.0341 (17) | −0.0083 (14) | −0.0023 (14) | 0.0018 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O3 | 0.098 (3) | 0.065 (2) | 0.056 (2) | 0.011 (2) | 0.004 (2) | −0.014 (2) |
| O4 | 0.099 (3) | 0.088 (3) | 0.070 (3) | 0.031 (3) | −0.016 (2) | −0.026 (2) |
| N1 | 0.049 (2) | 0.030 (2) | 0.033 (2) | −0.0050 (17) | −0.0075 (17) | −0.0103 (16) |
| N2 | 0.039 (2) | 0.033 (2) | 0.036 (2) | −0.0035 (17) | −0.0071 (17) | −0.0091 (16) |
| N3 | 0.040 (2) | 0.035 (2) | 0.033 (2) | −0.0099 (18) | −0.0012 (17) | −0.0070 (16) |
| N4 | 0.041 (2) | 0.034 (2) | 0.032 (2) | −0.0026 (18) | −0.0001 (17) | −0.0033 (16) |
| C1 | 0.037 (3) | 0.038 (3) | 0.033 (2) | −0.005 (2) | −0.012 (2) | −0.006 (2) |
| C2 | 0.034 (3) | 0.042 (3) | 0.030 (2) | −0.004 (2) | −0.0107 (19) | −0.011 (2) |
| C3 | 0.057 (3) | 0.037 (3) | 0.044 (3) | −0.005 (2) | −0.007 (2) | −0.007 (2) |
| C4 | 0.055 (3) | 0.031 (2) | 0.064 (3) | 0.004 (2) | −0.014 (3) | −0.015 (2) |
| C5 | 0.046 (3) | 0.048 (3) | 0.058 (3) | 0.010 (2) | −0.013 (2) | −0.027 (3) |
| C6 | 0.036 (3) | 0.046 (3) | 0.036 (3) | 0.000 (2) | −0.008 (2) | −0.016 (2) |
| C7 | 0.045 (3) | 0.068 (4) | 0.046 (3) | 0.004 (3) | −0.002 (2) | −0.027 (3) |
| C8 | 0.048 (3) | 0.072 (4) | 0.029 (2) | 0.003 (3) | 0.005 (2) | −0.013 (2) |
| C9 | 0.043 (3) | 0.052 (3) | 0.033 (2) | −0.011 (2) | −0.002 (2) | −0.009 (2) |
| C10 | 0.066 (4) | 0.053 (3) | 0.039 (3) | −0.014 (3) | 0.004 (2) | 0.000 (2) |
| C11 | 0.082 (4) | 0.040 (3) | 0.050 (3) | −0.011 (3) | 0.000 (3) | 0.002 (2) |
| C12 | 0.060 (3) | 0.042 (3) | 0.046 (3) | −0.005 (3) | −0.009 (2) | −0.006 (2) |
| C13 | 0.043 (3) | 0.035 (2) | 0.029 (2) | −0.013 (2) | −0.002 (2) | −0.0024 (19) |
| C14 | 0.042 (3) | 0.040 (3) | 0.028 (2) | −0.013 (2) | 0.003 (2) | −0.008 (2) |
| C15 | 0.057 (3) | 0.048 (3) | 0.037 (3) | 0.004 (3) | −0.003 (2) | −0.003 (2) |
| C16 | 0.065 (4) | 0.037 (3) | 0.065 (4) | 0.012 (3) | 0.010 (3) | −0.003 (3) |
| C17 | 0.076 (4) | 0.045 (3) | 0.054 (3) | −0.009 (3) | 0.014 (3) | −0.024 (3) |
| C18 | 0.056 (3) | 0.046 (3) | 0.041 (3) | −0.014 (3) | 0.008 (2) | −0.019 (2) |
| C19 | 0.080 (4) | 0.077 (4) | 0.041 (3) | −0.026 (3) | 0.003 (3) | −0.031 (3) |
| C20 | 0.074 (4) | 0.095 (5) | 0.038 (3) | −0.028 (4) | −0.009 (3) | −0.026 (3) |
| C21 | 0.053 (3) | 0.055 (3) | 0.031 (3) | −0.024 (3) | −0.009 (2) | 0.001 (2) |
| C22 | 0.060 (4) | 0.072 (4) | 0.043 (3) | −0.030 (3) | −0.022 (3) | 0.008 (3) |
| C23 | 0.049 (3) | 0.053 (3) | 0.052 (3) | −0.010 (3) | −0.016 (3) | 0.002 (3) |
| C24 | 0.041 (3) | 0.043 (3) | 0.051 (3) | −0.007 (2) | −0.008 (2) | −0.007 (2) |
| C25 | 0.031 (3) | 0.039 (3) | 0.039 (3) | 0.006 (2) | −0.004 (2) | −0.020 (2) |
| C26 | 0.031 (3) | 0.037 (2) | 0.033 (2) | 0.004 (2) | −0.0042 (19) | −0.012 (2) |
| C27 | 0.054 (3) | 0.055 (3) | 0.047 (3) | −0.005 (3) | −0.012 (3) | −0.006 (2) |
| C28 | 0.055 (4) | 0.080 (4) | 0.064 (4) | −0.013 (3) | −0.026 (3) | −0.015 (3) |
| C29 | 0.038 (3) | 0.084 (4) | 0.067 (4) | −0.015 (3) | −0.006 (3) | −0.035 (3) |
| C30 | 0.050 (3) | 0.058 (3) | 0.059 (3) | −0.016 (3) | −0.003 (3) | −0.021 (3) |
| C31 | 0.032 (3) | 0.046 (3) | 0.038 (2) | −0.004 (2) | −0.002 (2) | −0.017 (2) |
| C32 | 0.034 (3) | 0.035 (3) | 0.067 (3) | −0.013 (2) | 0.003 (2) | −0.012 (2) |
| C33 | 0.064 (4) | 0.049 (3) | 0.034 (3) | −0.013 (3) | 0.005 (2) | −0.008 (2) |
| C34 | 0.056 (4) | 0.098 (5) | 0.051 (4) | −0.003 (3) | 0.008 (3) | −0.022 (3) |
| C35 | 0.074 (4) | 0.090 (5) | 0.050 (3) | −0.019 (4) | −0.013 (3) | −0.007 (3) |
| C36 | 0.057 (3) | 0.063 (3) | 0.037 (3) | −0.014 (3) | −0.009 (2) | −0.003 (2) |
| C37 | 0.049 (3) | 0.053 (3) | 0.051 (3) | −0.018 (3) | 0.007 (2) | −0.019 (3) |
| C38 | 0.063 (4) | 0.052 (3) | 0.042 (3) | −0.013 (3) | 0.000 (3) | −0.019 (3) |
| O5 | 0.039 (2) | 0.078 (3) | 0.076 (2) | 0.0133 (19) | −0.0019 (18) | −0.038 (2) |
| O6 | 0.065 (2) | 0.0467 (19) | 0.050 (2) | 0.0005 (17) | −0.0018 (17) | −0.0241 (16) |
| O7 | 0.067 (3) | 0.101 (3) | 0.114 (4) | 0.006 (3) | −0.042 (3) | −0.009 (3) |
| O8 | 0.076 (3) | 0.073 (3) | 0.048 (2) | −0.005 (2) | −0.021 (2) | −0.0099 (18) |
| C39 | 0.046 (3) | 0.044 (3) | 0.036 (3) | 0.002 (2) | 0.005 (2) | −0.009 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C40 | 0.042 (3) | 0.034 (2) | 0.035 (2) | −0.003 (2) | 0.001 (2) | −0.010 (2) |
| C41 | 0.047 (3) | 0.048 (3) | 0.052 (3) | −0.009 (3) | 0.009 (2) | −0.011 (2) |
| C42 | 0.064 (4) | 0.034 (3) | 0.062 (3) | −0.010 (3) | 0.008 (3) | −0.007 (2) |
| C43 | 0.058 (4) | 0.034 (3) | 0.072 (4) | 0.005 (2) | 0.006 (3) | −0.018 (2) |
| C44 | 0.045 (3) | 0.039 (3) | 0.053 (3) | 0.001 (2) | 0.015 (2) | −0.010 (2) |
| C45 | 0.033 (3) | 0.034 (2) | 0.038 (2) | −0.001 (2) | −0.002 (2) | −0.0104 (19) |
| C46 | 0.036 (3) | 0.034 (2) | 0.037 (3) | 0.001 (2) | 0.004 (2) | −0.008 (2) |
| C47 | 0.046 (3) | 0.048 (3) | 0.040 (3) | 0.004 (2) | 0.005 (2) | −0.009 (2) |
| C48 | 0.058 (4) | 0.054 (3) | 0.044 (3) | 0.012 (3) | 0.012 (3) | −0.004 (3) |
| C49 | 0.071 (4) | 0.035 (3) | 0.065 (4) | −0.001 (3) | 0.025 (3) | −0.002 (3) |
| C50 | 0.048 (3) | 0.039 (3) | 0.073 (4) | −0.010 (2) | 0.002 (3) | −0.018 (3) |
| C51 | 0.044 (3) | 0.032 (2) | 0.049 (3) | −0.002 (2) | 0.000 (2) | −0.009 (2) |
| C52 | 0.060 (4) | 0.045 (3) | 0.066 (4) | 0.002 (3) | −0.023 (3) | −0.010 (3) |
| O9 | 0.089 (3) | 0.065 (3) | 0.071 (3) | −0.009 (3) | −0.008 (2) | −0.024 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Zn1—O2 | 2.078 (3) | C23—C24 | 1.387 (6) |
| Zn1—N1 | 2.128 (3) | C23—H23 | 0.93 |
| Zn1—N4 | 2.130 (3) | C24—H24 | 0.93 |
| Zn1—N3 | 2.145 (4) | C25—C26 | 1.507 (5) |
| Zn1—N2 | 2.145 (3) | C26—C27 | 1.375 (6) |
| Zn1—O1 | 2.334 (3) | C26—C31 | 1.409 (6) |
| Zn1—C25 | 2.528 (4) | C27—C28 | 1.371 (6) |
| O1—C25 | 1.237 (5) | C27—H27 | 0.93 |
| O2—C25 | 1.276 (5) | C28—C29 | 1.374 (7) |
| O3—C38 | 1.207 (5) | C28—H28 | 0.93 |
| O4—C38 | 1.326 (6) | C29—C30 | 1.370 (6) |
| O4—H4B | 0.82 | C29—H29 | 0.93 |
| N1—C12 | 1.327 (5) | C30—C31 | 1.391 (6) |
| N1—C1 | 1.370 (5) | C30—H30 | 0.93 |
| N2—C3 | 1.333 (5) | C31—C32 | 1.525 (6) |
| N2—C2 | 1.355 (5) | C32—C37 | 1.369 (6) |
| N3—C24 | 1.331 (5) | C32—C33 | 1.446 (6) |
| N3—C13 | 1.373 (5) | C33—C34 | 1.331 (6) |
| N4—C15 | 1.321 (5) | C33—H33 | 0.93 |
| N4—C14 | 1.366 (5) | C34—C35 | 1.462 (7) |
| C1—C9 | 1.409 (5) | C34—H34 | 0.93 |
| C1—C2 | 1.426 (5) | C35—C36 | 1.374 (6) |
| C2—C6 | 1.405 (5) | C35—H35 | 0.93 |
| C3—C4 | 1.394 (6) | C36—C37 | 1.394 (6) |
| C3—H3 | 0.93 | C36—H36 | 0.93 |
| C4—C5 | 1.366 (6) | C37—C38 | 1.478 (6) |
| C4—H4A | 0.93 | O5—C39 | 1.243 (5) |
| C5—C6 | 1.394 (6) | O6—C39 | 1.274 (5) |
| C5—H5 | 0.93 | O7—C52 | 1.211 (6) |
| C6—C7 | 1.415 (5) | O8—C52 | 1.314 (6) |
| C7—C8 | 1.353 (6) | O8—H8B | 0.82 |
| C7—H7 | 0.93 | C39—C40 | 1.503 (6) |

| | | | |
|---|---|---|---|
| C8—C9 | 1.430 (6) | C40—C41 | 1.376 (6) |
| C8—H8A | 0.93 | C40—C45 | 1.389 (5) |
| C9—C10 | 1.400 (6) | C41—C42 | 1.377 (6) |
| C10—C11 | 1.365 (6) | C41—H41 | 0.93 |
| C10—H10 | 0.93 | C42—C43 | 1.353 (6) |
| C11—C12 | 1.403 (6) | C42—H42 | 0.93 |
| C11—H11 | 0.93 | C43—C44 | 1.390 (6) |
| C12—H12 | 0.93 | C43—H43 | 0.93 |
| C13—C21 | 1.414 (6) | C44—C45 | 1.365 (5) |
| C13—C14 | 1.418 (6) | C44—H44 | 0.93 |
| C14—C18 | 1.410 (6) | C45—C46 | 1.484 (5) |
| C15—C16 | 1.401 (6) | C46—C47 | 1.390 (6) |
| C15—H15 | 0.93 | C46—C51 | 1.407 (6) |
| C16—C17 | 1.343 (7) | C47—C48 | 1.387 (6) |
| C16—H16 | 0.93 | C47—H47 | 0.93 |
| C17—C18 | 1.370 (7) | C48—C49 | 1.395 (7) |
| C17—H17 | 0.93 | C48—H48 | 0.93 |
| C18—C19 | 1.444 (7) | C49—C50 | 1.371 (7) |
| C19—C20 | 1.356 (7) | C49—H49 | 0.93 |
| C19—H19 | 0.93 | C50—C51 | 1.389 (6) |
| C20—C21 | 1.423 (6) | C50—H50 | 0.93 |
| C20—H20 | 0.93 | C51—C52 | 1.477 (6) |
| C21—C22 | 1.406 (7) | O9—H9A | 0.87 (5) |
| C22—C23 | 1.351 (6) | O9—H9B | 0.84 (2) |
| C22—H22 | 0.93 | | |
| O2—Zn1—N1 | 102.73 (12) | C23—C22—C21 | 120.6 (5) |
| O2—Zn1—N4 | 97.11 (12) | C23—C22—H22 | 119.7 |
| N1—Zn1—N4 | 100.12 (12) | C21—C22—H22 | 119.7 |
| O2—Zn1—N3 | 155.43 (11) | C22—C23—C24 | 118.4 (5) |
| N1—Zn1—N3 | 101.83 (13) | C22—C23—H23 | 120.8 |
| N4—Zn1—N3 | 77.99 (14) | C24—C23—H23 | 120.8 |
| O2—Zn1—N2 | 94.88 (12) | N3—C24—C23 | 124.5 (4) |
| N1—Zn1—N2 | 77.67 (12) | N3—C24—H24 | 117.8 |
| N4—Zn1—N2 | 167.99 (13) | C23—C24—H24 | 117.8 |
| N3—Zn1—N2 | 90.84 (13) | O1—C25—O2 | 121.2 (4) |
| O2—Zn1—O1 | 59.17 (10) | O1—C25—C26 | 122.0 (4) |
| N1—Zn1—O1 | 155.22 (11) | O2—C25—C26 | 116.7 (4) |
| N4—Zn1—O1 | 98.98 (11) | O1—C25—Zn1 | 66.7 (2) |
| N3—Zn1—O1 | 97.46 (11) | O2—C25—Zn1 | 55.0 (2) |
| N2—Zn1—O1 | 86.71 (11) | C26—C25—Zn1 | 167.7 (3) |
| O2—Zn1—C25 | 30.21 (12) | C27—C26—C31 | 117.9 (4) |
| N1—Zn1—C25 | 129.98 (14) | C27—C26—C25 | 119.0 (4) |
| N4—Zn1—C25 | 101.56 (13) | C31—C26—C25 | 123.1 (4) |
| N3—Zn1—C25 | 126.52 (13) | C28—C27—C26 | 123.7 (5) |
| N2—Zn1—C25 | 88.57 (12) | C28—C27—H27 | 118.1 |
| O1—Zn1—C25 | 29.12 (11) | C26—C27—H27 | 118.1 |
| C25—O1—Zn1 | 84.2 (2) | C27—C28—C29 | 118.9 (5) |
| C25—O2—Zn1 | 94.8 (3) | C27—C28—H28 | 120.6 |
| C38—O4—H4B | 109.5 | C29—C28—H28 | 120.6 |

| | | | |
|---|---|---|---|
| C12—N1—C1 | 118.0 (4) | C30—C29—C28 | 118.6 (5) |
| C12—N1—Zn1 | 128.5 (3) | C30—C29—H29 | 120.7 |
| C1—N1—Zn1 | 113.3 (3) | C28—C29—H29 | 120.7 |
| C3—N2—C2 | 118.5 (4) | C29—C30—C31 | 123.6 (5) |
| C3—N2—Zn1 | 127.8 (3) | C29—C30—H30 | 118.2 |
| C2—N2—Zn1 | 113.7 (3) | C31—C30—H30 | 118.2 |
| C24—N3—C13 | 117.3 (4) | C30—C31—C26 | 117.4 (4) |
| C24—N3—Zn1 | 129.6 (3) | C30—C31—C32 | 117.4 (4) |
| C13—N3—Zn1 | 113.1 (3) | C26—C31—C32 | 124.8 (4) |
| C15—N4—C14 | 117.6 (4) | C37—C32—C33 | 120.0 (5) |
| C15—N4—Zn1 | 129.0 (3) | C37—C32—C31 | 124.1 (4) |
| C14—N4—Zn1 | 113.5 (3) | C33—C32—C31 | 115.4 (4) |
| N1—C1—C9 | 122.2 (4) | C34—C33—C32 | 119.6 (5) |
| N1—C1—C2 | 117.6 (4) | C34—C33—H33 | 120.2 |
| C9—C1—C2 | 120.1 (4) | C32—C33—H33 | 120.2 |
| N2—C2—C6 | 122.6 (4) | C33—C34—C35 | 120.2 (5) |
| N2—C2—C1 | 117.1 (4) | C33—C34—H34 | 119.9 |
| C6—C2—C1 | 120.3 (4) | C35—C34—H34 | 119.9 |
| N2—C3—C4 | 122.2 (4) | C36—C35—C34 | 119.2 (5) |
| N2—C3—H3 | 118.9 | C36—C35—H35 | 120.4 |
| C4—C3—H3 | 118.9 | C34—C35—H35 | 120.4 |
| C5—C4—C3 | 119.4 (4) | C35—C36—C37 | 120.2 (5) |
| C5—C4—H4A | 120.3 | C35—C36—H36 | 119.9 |
| C3—C4—H4A | 120.3 | C37—C36—H36 | 119.9 |
| C4—C5—C6 | 120.0 (4) | C32—C37—C36 | 120.7 (4) |
| C4—C5—H5 | 120.0 | C32—C37—C38 | 121.5 (5) |
| C6—C5—H5 | 120.0 | C36—C37—C38 | 117.7 (5) |
| C5—C6—C2 | 117.3 (4) | O3—C38—O4 | 122.4 (5) |
| C5—C6—C7 | 124.3 (4) | O3—C38—C37 | 125.5 (5) |
| C2—C6—C7 | 118.4 (4) | O4—C38—C37 | 111.9 (5) |
| C8—C7—C6 | 121.8 (4) | C52—O8—H8B | 109.5 |
| C8—C7—H7 | 119.1 | O5—C39—O6 | 124.5 (4) |
| C6—C7—H7 | 119.1 | O5—C39—C40 | 119.0 (4) |
| C7—C8—C9 | 121.3 (4) | O6—C39—C40 | 116.4 (4) |
| C7—C8—H8A | 119.3 | C41—C40—C45 | 119.1 (4) |
| C9—C8—H8A | 119.3 | C41—C40—C39 | 118.3 (4) |
| C10—C9—C1 | 117.8 (4) | C45—C40—C39 | 122.5 (4) |
| C10—C9—C8 | 124.1 (4) | C40—C41—C42 | 121.8 (4) |
| C1—C9—C8 | 118.0 (4) | C40—C41—H41 | 119.1 |
| C11—C10—C9 | 119.8 (4) | C42—C41—H41 | 119.1 |
| C11—C10—H10 | 120.1 | C43—C42—C41 | 118.9 (4) |
| C9—C10—H10 | 120.1 | C43—C42—H42 | 120.5 |
| C10—C11—C12 | 119.1 (5) | C41—C42—H42 | 120.5 |
| C10—C11—H11 | 120.5 | C42—C43—C44 | 119.9 (4) |
| C12—C11—H11 | 120.5 | C42—C43—H43 | 120.0 |
| N1—C12—C11 | 123.1 (4) | C44—C43—H43 | 120.0 |
| N1—C12—H12 | 118.5 | C45—C44—C43 | 121.5 (4) |
| C11—C12—H12 | 118.5 | C45—C44—H44 | 119.2 |
| N3—C13—C21 | 121.7 (4) | C43—C44—H44 | 119.2 |

| | | | |
|---|---|---|---|
| N3—C13—C14 | 117.4 (4) | C44—C45—C40 | 118.6 (4) |
| C21—C13—C14 | 120.9 (4) | C44—C45—C46 | 118.6 (4) |
| N4—C14—C18 | 121.7 (4) | C40—C45—C46 | 122.8 (4) |
| N4—C14—C13 | 117.9 (4) | C47—C46—C51 | 118.4 (4) |
| C18—C14—C13 | 120.4 (4) | C47—C46—C45 | 119.9 (4) |
| N4—C15—C16 | 122.8 (5) | C51—C46—C45 | 121.3 (4) |
| N4—C15—H15 | 118.6 | C48—C47—C46 | 121.7 (5) |
| C16—C15—H15 | 118.6 | C48—C47—H47 | 119.2 |
| C17—C16—C15 | 119.6 (5) | C46—C47—H47 | 119.2 |
| C17—C16—H16 | 120.2 | C47—C48—C49 | 118.6 (5) |
| C15—C16—H16 | 120.2 | C47—C48—H48 | 120.7 |
| C16—C17—C18 | 119.9 (5) | C49—C48—H48 | 120.7 |
| C16—C17—H17 | 120.1 | C50—C49—C48 | 120.8 (5) |
| C18—C17—H17 | 120.1 | C50—C49—H49 | 119.6 |
| C17—C18—C14 | 118.5 (5) | C48—C49—H49 | 119.6 |
| C17—C18—C19 | 123.5 (5) | C49—C50—C51 | 120.3 (5) |
| C14—C18—C19 | 118.0 (5) | C49—C50—H50 | 119.8 |
| C20—C19—C18 | 120.6 (5) | C51—C50—H50 | 119.8 |
| C20—C19—H19 | 119.7 | C50—C51—C46 | 120.0 (5) |
| C18—C19—H19 | 119.7 | C50—C51—C52 | 118.0 (5) |
| C19—C20—C21 | 122.5 (5) | C46—C51—C52 | 121.9 (4) |
| C19—C20—H20 | 118.7 | O7—C52—O8 | 121.0 (5) |
| C21—C20—H20 | 118.7 | O7—C52—C51 | 121.9 (5) |
| C22—C21—C13 | 117.5 (4) | O8—C52—C51 | 117.0 (5) |
| C22—C21—C20 | 125.0 (5) | H9A—O9—H9B | 115 (6) |
| C13—C21—C20 | 117.5 (5) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O9—H9B···O7$^{i}$ | 0.84 (4) | 2.10 (5) | 2.936 (6) | 171 (6) |
| O4—H4B···O5$^{ii}$ | 0.82 | 1.86 | 2.633 (5) | 158 |
| O9—H9A···O5 | 0.87 (5) | 1.96 (6) | 2.817 (6) | 171 (7) |
| O8—H8B···O6 | 0.82 | 1.69 | 2.500 (5) | 171 |
| C3—H3···O1 | 0.93 | 2.55 | 3.130 (5) | 121 |
| C4—H4A···O6$^{ii}$ | 0.93 | 2.42 | 3.221 (5) | 144 |
| C12—H12···O9 | 0.93 | 2.42 | 3.273 (6) | 152 |
| C16—H16···O7$^{i}$ | 0.93 | 2.43 | 3.199 (7) | 139 |
| C19—H19···O6$^{iii}$ | 0.93 | 2.56 | 3.377 (5) | 146 |
| C22—H22···O1$^{iv}$ | 0.93 | 2.43 | 3.249 (6) | 147 |

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

**Fig. 1**

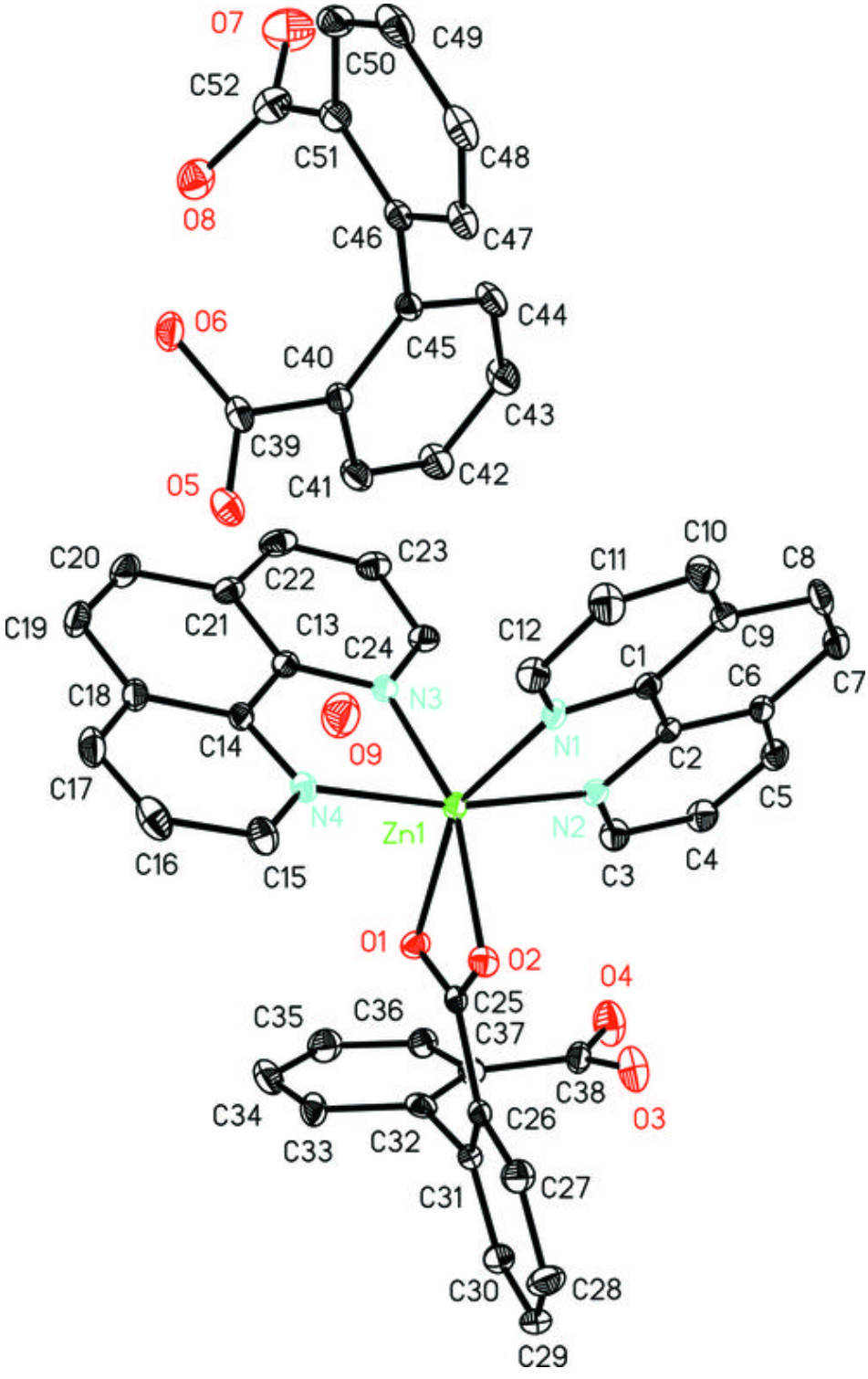
O7
C49
C50
C52
C51
C48
O8
C46
C47
O6
C44
C40
C45
C43
C39
C41
C42
O5
C20
C23
C22
C10
C11
C8
C19
C21
C13
C24
C12
C9
C1
C6
C7
C18
N3
N1
C14
O9
C2
C17
N4
Zn1
N2
C5
C16
C15
C3
C4
O1
O2
O4
C25
C35
C36
C37
C38
O3
C34
C26
C33
C32
C27
C31
C30
C28
C29

**Fig. 2**