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Key indicators

Single-crystal X-ray study  
 T = 292 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
 R factor = 0.022  
 wR factor = 0.065  
 Data-to-parameter ratio = 10.4

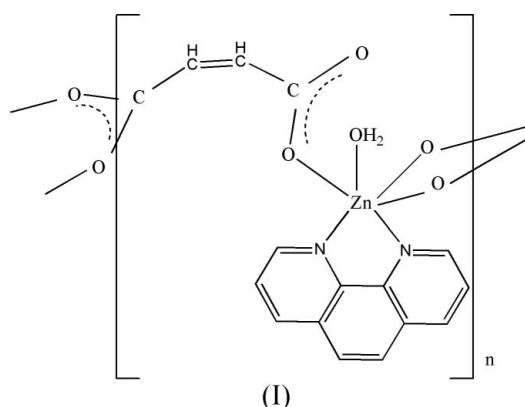
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

catena-Poly[[aqua(1,10-phenanthroline)zinc(II)]- $\mu$ -maleato- $\kappa^3\text{O},\text{O}:\text{O}'$ ]

In the title compound,  $[\text{Zn}(\text{C}_4\text{H}_2\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]_n$ , the octahedrally coordinated Zn atom is bonded to two N atoms from phenanthroline, three carboxyl O atoms and one water O atom.

Comment

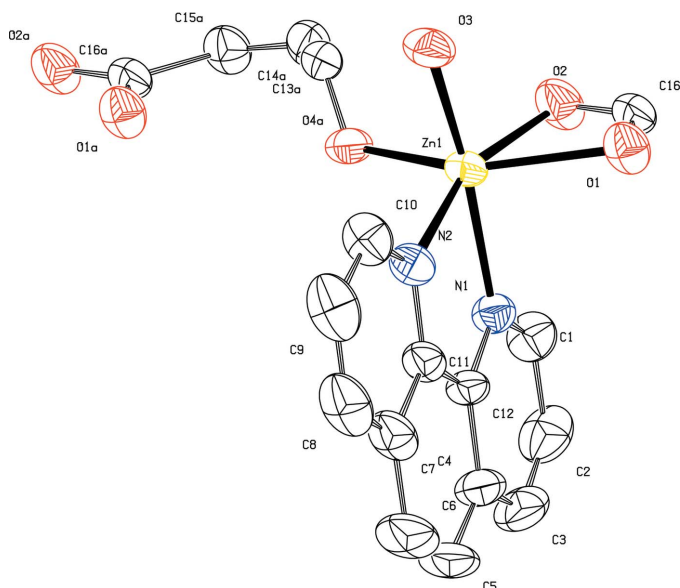
Metal-organic coordination polymers containing the maleate ligand have been extensively studied, due to their wide range of applications (Zheng *et al.*, 2003; Liu *et al.*, 2004). Here, we report the crystal structure of a new such  $\text{Zn}^{\text{II}}$  compound, the title compound, (I),  $[\text{Zn}(\text{mal})(\text{H}_2\text{O})(\text{phen})]_n$  (mal = maleate and phen = 1,10-phenanthroline).



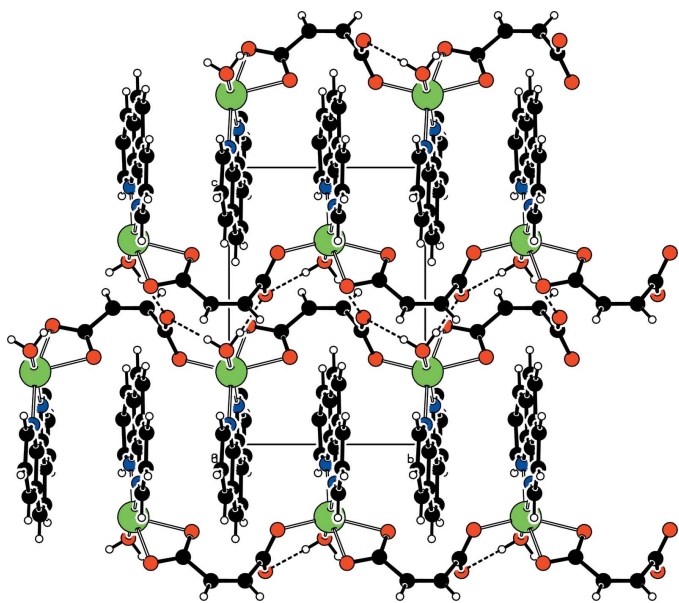
In the structure of (I), the  $\text{Zn}^{\text{II}}$  atom has a distorted octahedral coordination geometry, defined by two N atoms from one phen, three carboxyl O atoms belonging to two different maleate dianions, and one O atom of the water molecule (Fig. 1). The Zn1–N1 and Zn1–N2 distances are 2.1741 (19) and 2.1295 (17) Å, respectively (Table 1). The average Zn1–O bond length is 2.133 Å. The shortest distance is 2.042 (2) Å for Zn1–O4, where the O atom is from the monodentate carboxylate group. The other two Zn–O distances [Zn1–O1 2.242 (3) Å and Zn1–O2 2.153 (2) Å] involving the bidentate carboxylate group are slightly longer than the Zn1–O3 distance [2.0951 (18) Å]. The Zn–O3 distance in (I) is slightly longer than the Zn1–O1W [1.98 (1) Å] and Zn2–O2W [2.01 (1) Å] distances in *catena*-poly[[aqua(imidazole)zinc(II)]- $\mu$ -maleate- $\kappa^3\text{O},\text{O}:\text{O}'$ ],  $[\text{Zn}(\mu\text{-O}_2\text{CCH}=\text{CHCO}_2)(\text{C}_3\text{H}_4\text{N}_2)(\text{H}_2\text{O})]_n$  (Liu *et al.*, 2004).

The maleate dianions of (I) bridge the Zn atoms into one-dimensional polymeric chains extending along the [010] direction, with the chelating phen ligands parallel to one another. Each phen ligand of one chain enters the void space between two phen ligands from an adjacent chain, resulting in the formation of supramolecular double chains. The zipper-

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**Figure 1**  
A view of (I), showing the labelling of the non-H atoms and 50% probability ellipsoids. H atoms have been omitted. [Symmetry code: (a)  $x$ ,  $y - 1$ ,  $z$ .]



**Figure 2**  
A packing diagram for (I), viewed along the  $a$  axis. Intermolecular O—H...O hydrogen bonds are shown by dashed lines.

like double chains form two-dimensional layers *via* hydrogen bonds (Table 2 and Fig. 2).

## Experimental

Maleic acid (0.232 g, 2.00 mmol) and phenanthroline monohydrate (0.399 g, 2.00 mmol) were dissolved in a water–methanol mixture (50 ml, 1:1) and solid ZnO (0.163 g, 2.00 mmol) was added to the solution. The mixture was stirred at 333 K for 2 h. After filtration, the colourless solution was allowed to stand at room temperature, and

colourless block-shaped crystals of (I) were obtained by slow evaporation over two months.

### Crystal data

[Zn(C<sub>4</sub>H<sub>2</sub>O<sub>4</sub>)(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)(H<sub>2</sub>O)]  
 $M_r = 377.65$   
 Monoclinic,  $P2_1$   
 $a = 9.9906$  (8) Å  
 $b = 7.2954$  (6) Å  
 $c = 10.2946$  (9) Å  
 $\beta = 91.8930$  (10)°  
 $V = 749.92$  (11) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.672$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 3990 reflections  
 $\theta = 2.8$ – $28.3$ °  
 $\mu = 1.67$  mm<sup>-1</sup>  
 $T = 292$  (2) K  
 Block, colourless  
 $0.44 \times 0.42 \times 0.20$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.516$ ,  $T_{\max} = 0.717$   
 4505 measured reflections

2355 independent reflections  
 2303 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.019$   
 $\theta_{\max} = 27.5$ °  
 $h = -12 \rightarrow 12$   
 $k = -9 \rightarrow 4$   
 $l = -13 \rightarrow 13$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.065$   
 $S = 1.10$   
 2355 reflections  
 226 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 0.0065P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.004$   
 $\Delta\rho_{\max} = 0.23$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.33$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), with 498 Friedel pairs  
 Flack parameter: 0.283 (16)

**Table 1**

Selected geometric parameters (Å, °).

Zn1—O1	2.242 (3)	Zn1—O4	2.042 (2)
Zn1—O2	2.153 (2)	Zn1—N1	2.1741 (19)
Zn1—O3	2.0951 (18)	Zn1—N2	2.1295 (17)
O1—Zn1—O2	59.48 (8)	O2—Zn1—N1	90.08 (8)
O1—Zn1—O3	92.11 (11)	O2—Zn1—N2	161.42 (10)
O1—Zn1—O4	148.31 (7)	O3—Zn1—N1	166.59 (8)
O2—Zn1—O3	102.62 (9)	O3—Zn1—N2	89.60 (7)
O2—Zn1—O4	88.96 (10)	O4—Zn1—N1	92.38 (9)
O3—Zn1—O4	92.16 (11)	O4—Zn1—N2	104.70 (12)
O1—Zn1—N1	90.65 (9)	N1—Zn1—N2	77.04 (7)
O1—Zn1—N2	106.72 (11)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3A $\cdots$ O5	0.84 (4)	1.83 (4)	2.666 (4)	171 (5)
O3—H3B $\cdots$ O5 <sup>i</sup>	0.85 (3)	1.84 (4)	2.687 (3)	171 (4)

Symmetry code: (i)  $-x + 1, y + \frac{1}{2}, -z + 1$ .

All H atoms were initially located in a difference Fourier map. The water H atoms were then restrained to an ideal geometry, with O—H distances of 0.85 (3) and 0.84 (4) Å, and their  $U_{\text{iso}}(\text{H})$  values were refined freely. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The structure was refined as an inversion twin. The twinning ratio refined to 0.283 (16).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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