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Bis(1,10-phenanthroline-κ^2N,N')(2-phenethylmalonato-κ^2O,O')zinc(II) octahydrate

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The title compound, $[Zn(C_{11}H_{11}O_4)(C_{12}H_8N_2)]\cdot 8H_2O$, was synthesized by the reaction of 1,10-phenanthroline (phen) and 2-phenethylmalonic acid (H_2pmal) with $Zn(NO_3)_2$. Two molecules of phen and one H_2pmal are chelated to the Zn^{II} ion in a bidentate manner in a distorted octahedral geometry. The structure is stabilized by extensive C—H···O intra- and intermolecular interactions, forming a three-dimensional network. In addition, π–π and C—H···π interactions are also present in the crystal structure.

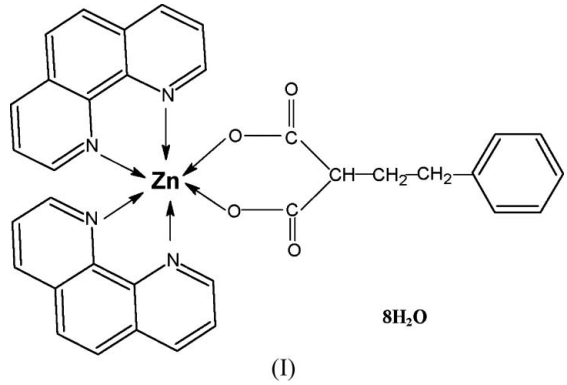
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.090
Data-to-parameter ratio = 12.3

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

Comment

Recently, the rational design of novel metal coordination compounds of d^{10} with aromatic di-, tri- or tetracarboxylic acids based on covalent or weaker intermolecular forces has become an appealing field to many researchers. A series of Zn^{II} and Cd^{II} metal–organic frameworks have been studied, not only because of their intriguing structures but also due to their potential applications in the field of photoluminesence (Tong *et al.*, 1999; Wang *et al.*, 2004).



(I)

The title compound, (I), is a zinc complex containing two molecules of 1,10-phenanthroline and one phenethylmalonate ligand, each chelating in bidentate manner through their N or O atoms, and eight water molecules of crystallization (Fig. 1). The geometry about the Zn atom is distorted octahedral, with O1 and N3 occupying the axial positions with an angle of 172.67 (8)° about the Zn atom. Atoms O3, N1, N2 and N4 occupy the equatorial positions, with *cis* angles at the Zn atom between 76.77 (8) and 98.64 (8)°. The average Zn—O and Zn—N bond lengths of 2.065 (6) and 2.180 (5) Å, respectively, are comparable to those in zinc complexes such as $\{[Zn(C_8H_4O_5)(C_{12}H_8N_3)]\cdot H_2O\}_n$ (Cao *et al.*, 2004).

The crystal structure of (I) is stabilized by an extensive intra- and intermolecular interactions involving O atoms of the carboxylate groups and the water molecules (Table 2),

forming a three-dimensional network. In addition, there are π–π interactions between the (C15–C23)^{vi} [symmetry code: (vi) $1-x, 2-y, 1-z$] rings, the distance between the centroids being 3.636 Å, and C—H$\cdots\pi$ interactions between (C27–C35)^{viii} [symmetry code: (viii) $2-x, 2-y, 1-z$] and C19/H19, with an angle about the H atom of 166° and the closest distance being 2.88 Å.

Experimental

A mixture of $Zn(NO_3)_2$ (0.0189 g. 0.1 mmol), phenethylmalonic acid (0.0208 g, 0.1 mmol), Na_2CO_3 (0.0212 g, 0.2 mmol) and phen (0.0358 g, 0.2 mmol) in 40 ml distilled water was refluxed for 0.5 h. After cooling to room temperature, the solution was filtered and left to slowly evaporate. Single crystals of (I) were obtained from the filtrate after 2 d [yield 54% (0.0419 g); m.p. 405–407 K].

Crystal data

$[Zn(C_{11}H_{11}O_4)(C_{12}H_8N_2)]\cdot 8H_2O$
$M_r = 776.10$
Triclinic, $P\overline{1}$
$a = 10.493$ (2) Å
$b = 13.144$ (3) Å
$c = 14.214$ (3) Å
$\alpha = 76.395$ (4)°
$\beta = 83.852$ (4)°
$\gamma = 71.694$ (4)°
$V = 1807.8$ (7) Å^3
$Z = 2$
$D_x = 1.426$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.75$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.831$, $T_{max} = 0.877$
9290 measured reflections
6343 independent reflections
4663 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.090$
$S = 1.05$
6343 reflections
517 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 0.4083P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.0639 (18)	Zn1—N3	2.196 (2)
Zn1—O3	2.0654 (19)	O1—C1	1.280 (3)
Zn1—N4	2.165 (2)	O2—C1	1.229 (3)
Zn1—N1	2.173 (2)	O3—C3	1.276 (3)
Zn1—N2	2.185 (2)	O4—C3	1.227 (3)
O1—Zn1—O3	91.19 (7)	N4—Zn1—N2	94.36 (8)
O1—Zn1—N4	96.33 (8)	N1—Zn1—N2	76.77 (8)
O3—Zn1—N4	98.65 (8)	O1—Zn1—N3	172.67 (8)
O1—Zn1—N1	94.45 (8)	O3—Zn1—N3	88.51 (8)
O3—Zn1—N1	90.08 (8)	N4—Zn1—N3	76.49 (9)
N4—Zn1—N1	165.96 (8)	N1—Zn1—N3	92.88 (9)
O1—Zn1—N2	89.32 (8)	N2—Zn1—N3	92.64 (8)
O3—Zn1—N2	166.85 (8)		

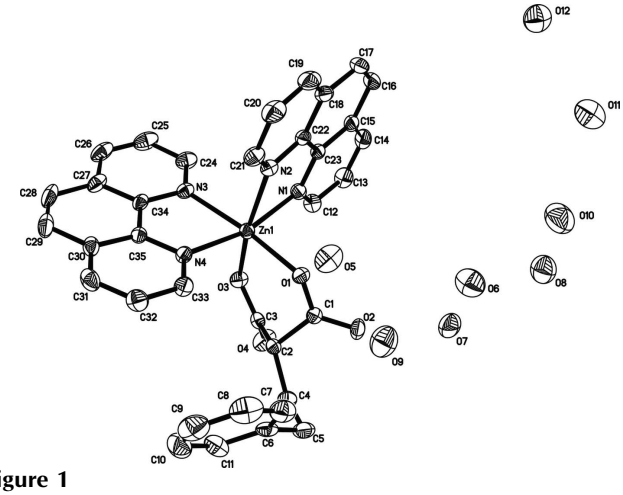


Figure 1
The asymmetric unit of the title structure with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been ommited for clarity.

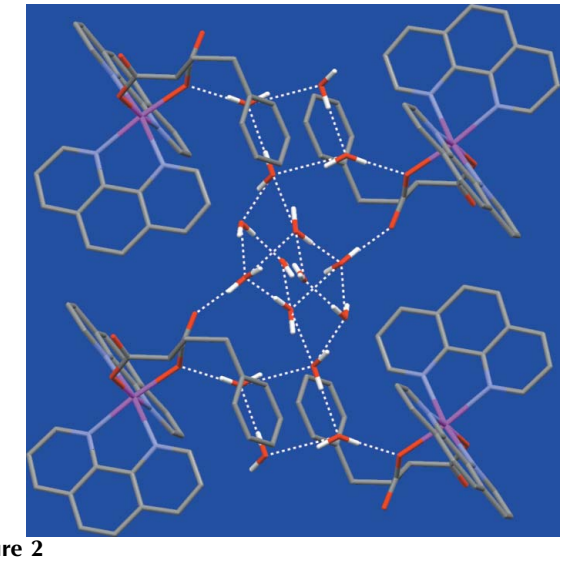


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O12—H12$B\cdots$O11	0.88 (2)	2.03 (3)	2.869 (4)	160 (3)
O12—H12$A\cdots$O3^{i}	0.88 (2)	2.03 (3)	2.885 (3)	163 (3)
O11—H11$B\cdots$O12^{ii}	0.84 (2)	2.05 (3)	2.871 (4)	165 (5)
O11—H11$A\cdots$O4^{i}	0.87 (2)	1.81 (2)	2.671 (3)	173 (4)
O10—H10$B\cdots$O11	0.90 (3)	1.92 (3)	2.798 (4)	166 (5)
O10—H10$A\cdots$O6	0.92 (3)	1.97 (3)	2.798 (4)	149 (5)
O9—H9$B\cdots$O8^{iii}	0.91 (2)	1.89 (2)	2.774 (4)	162 (4)
O9—H9$A\cdots$O5^{iv}	0.90 (2)	1.89 (2)	2.787 (4)	178 (4)
O8—H8$B\cdots$O7	0.85 (2)	2.10 (3)	2.933 (4)	167 (4)
O8—H8$A\cdots$O10	0.88 (2)	1.91 (3)	2.780 (4)	169 (4)
O7—H7$B\cdots$O6^{iii}	0.88 (2)	2.06 (3)	2.875 (4)	153 (4)
O7—H7$A\cdots$O2	0.89 (2)	1.84 (2)	2.730 (3)	176 (4)
O6—H6$B\cdots$O7	0.91 (3)	1.88 (3)	2.787 (4)	172 (4)
O6—H6$A\cdots$O9	0.93 (2)	2.00 (3)	2.814 (4)	145 (4)
O5—H5$D\cdots$O9	0.84 (2)	2.11 (2)	2.907 (4)	160 (4)
O5—H5$C\cdots$O1	0.89 (2)	1.91 (2)	2.794 (3)	174 (4)

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

Water H atoms were located in a difference Fourier map and refined with a restrained O—H distance of 0.85 (3) Å and $U_{iso}(H) = 1.5U_{eq}(O)$. Other H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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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