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Di-μ-adipato-$\kappa^6O,O':O'';O:O',O''$-bis[aqua-(1,10-phenanthroline-κ^2N,N)zinc(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.024
wR factor = 0.065
Data-to-parameter ratio = 13.3

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

In the title compound, $[Zn_2(C_6H_8O_4)_2(C_{12}H_8N_2)_2(H_2O)_2]$, each Zn atom is six-coordinated in the ZnO_4N_2 form in a distorted tetragonal–bipyramidal geometry. The water molecules act as donors in O—H···O hydrogen bonds, connecting the molecules into chains. The packing is further stabilized by intermolecular C—H···O interactions.

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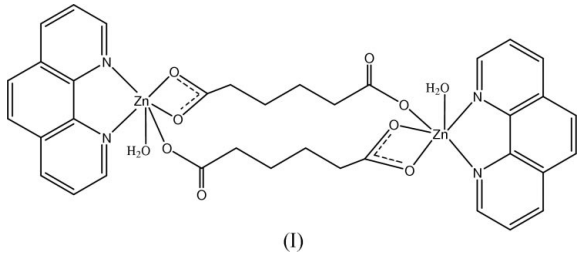
Comment

Increasing interest in inorganic–organic hybrid framework assemblies has resulted in a great amount of research effort focused on the development of new functional materials with various potential applications in catalysis, electrical conductivity and magnetism (Wang *et al.*, 1995; Hagrman *et al.*, 1999). In recent years, rigid ligands with *N*-donor 1,10-phenanthroline and its derivatives have been extensively investigated in both analytical and preparative coordination chemistry (Olenyuk *et al.*, 1998). Adipate, a ligand with flexible stereochemistry, exhibits a variety of modes of binding to metal ions. Its complexes have been extensively studied, due to their unique ability to form stable chelates in diverse coordination modes (Zheng *et al.*, 2003). We present here the crystal structure of the title binuclear complex, (I).



(I)

The asymmetric unit of (I) contains one half of the dimeric complex (Fig. 1), the other half being related by an inversion centre. The Zn^{II} atom is six-coordinated by two N atoms from

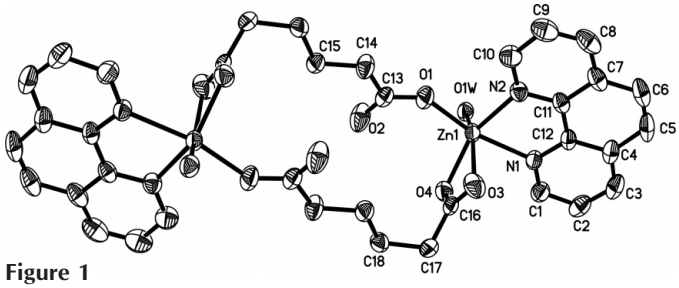


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. Unlabelled atoms are related to labelled atoms by $-x$, $-y$, $-z$.

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one *o*-phenanthroline ligand and four O atoms from two adipate anions, and one water molecule. This ZnO_4N_2 coordination forms a distorted tetragonal–bipyramidal geometry. One axial position is occupied by atom O1 from one adipate ligand, with a Zn—O distance of 2.016 (1) Å. The other axial position is occupied by atom N1 from the *o*-phenanthroline ligand. The Zn1—N1 distance is 2.216 (1) Å, longer than that of the Zn1—N2 bond [2.125 (1) Å].

The short O1···C10 distance of 3.029 (3) Å indicates a possible intramolecular C—H···O hydrogen bond. The mean planes of the two *o*-phenanthroline groups are parallel to each other. Atoms Zn1/N1/C12/C11/N2 form a five-membered planar ring, with a maximum deviation from the mean plane of 0.062 (4) Å for atom Zn1. This plane is coplanar with the *o*-phenanthroline ring and perpendicular to the Zn1/O1/C16/O4 plane, with dihedral angles of 0.74 (6) and 85.81 (8)°, respectively.

In the crystal structure, the water molecule acts as a donor to form O1*W*—H1*WB*···O4 and O1*W*—H2*WA*···O2 hydrogen bonds (Table 2). These hydrogen bonds link the molecules into chains along the *b* direction (Fig. 2). The packing is further stabilized by intermolecular C—H···O interactions (Table 2).

Experimental

To a solution of 1,10-phenanthroline (1.80 g, 1 mmol) and adipic acid (1.46 g, 1 mmol) in ethanol (10 ml) was added zinc acetate (1.24 g, 1 mmol) in distilled water (10 ml). The mixture was stirred and refluxed for 3 h. The hot solution was then filtered into another flask containing ethanol (10 ml). Pink crystals of (I) appeared over a period of 20 d by slow evaporation at room temperature.

Crystal data

$[Zn_2(C_6H_8O_4)_2(C_{12}H_8N_2)_2(H_2O)_2]$
M_r = 407.71
Triclinic, $P\overline{1}$
a = 8.1984 (4) Å
b = 9.7549 (5) Å
c = 11.8636 (6) Å
α = 70.971 (1)°
β = 75.508 (1)°
γ = 72.077 (1)°
V = 841.48 (7) Å^3
Z = 1
D_x = 1.609 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3889 reflections
θ = 2.3–26.0°
μ = 1.49 mm^{-1}
T = 293 (2) K
Plate, pink
0.54 × 0.15 × 0.08 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.500, T_{max} = 0.890
4743 measured reflections
3228 independent reflections
3094 reflections with $I > 2\sigma(I)$
R_{int} = 0.009
θ_{max} = 26.0°
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 12$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.08
3228 reflections
243 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 0.2537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

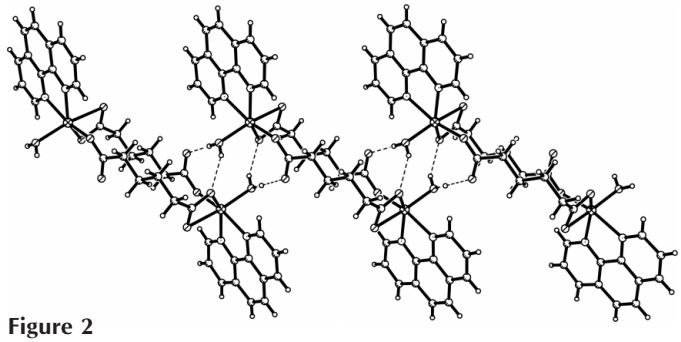

Figure 2
A packing diagram for (I), showing the hydrogen-bonded (dashed lines) chains.

Table 1
Selected bond lengths (Å).

Zn1—O1	2.0161 (13)	Zn1—N2	2.1249 (14)
Zn1—O1*W*	2.0361 (13)	Zn1—N1	2.2162 (14)
Zn1—O4	2.0663 (12)	Zn1—O3	2.4441 (15)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O1^{i}	0.93	2.49	3.030 (3)	117
O1*W*—H1*WB*···O4^{i}	0.77 (2)	2.06 (2)	2.750 (2)	148 (3)
O1*W*—H1*WA*···O2^{i}	0.85 (3)	1.74 (3)	2.588 (2)	173 (3)
C3—H3···O3^{ii}	0.93	2.52	3.402 (3)	158
C9—H9···O3^{iii}	0.93	2.50	3.142 (3)	126

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

All H atoms were located in difference Fourier maps. The water H atoms were freely refined, while the remaining H atoms were refined using a riding model, with C—H distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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