catena-Poly[bis[aqua(1,10-phenanthroline)-zinc(II)]-μ_4-benzene-1,2,4,5-tetracarboxylato]

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The pyromellitate tetraanion in the title polymeric complex, [Zn$_2$(C$_{10}$H$_2$O$_8$)(C$_{12}$H$_8$N$_2$)$_2$(H$_2$O)$_2$]$_n$, uses only one O atom from each carboxylate group to bind to one Zn atom, which is also chelated by the heterocycle; the fifth coordination site of the trigonal bipyramid around the Zn atom is occupied by a water molecule. The ribbons are linked by hydrogen bonds into sheets. The pyromellitate tetranion lies on an inversion center.

Comment

Benzene-1,2,4,5-tetracarboxylic acid forms a large number of complexes with transition metals; for zinc(II), in particular, the authenticated examples include dizinc pyromellitate heptahydrate (Robl, 1987), diammonium pyromellitatozinc octahydrate (Sun *et al.*, 2002), piperazinium tetraaqua-pyromellitatozincate tetrahydrate (Murugavel *et al.*, 2002), dizinc pyromellitate 4,4′-bipyridine dihydrate (Wu *et al.*, 2001; Yang *et al.*, 2002) and dizinc pyromellitate tetrakisimidazole (Wu *et al.*, 2001).


(I)
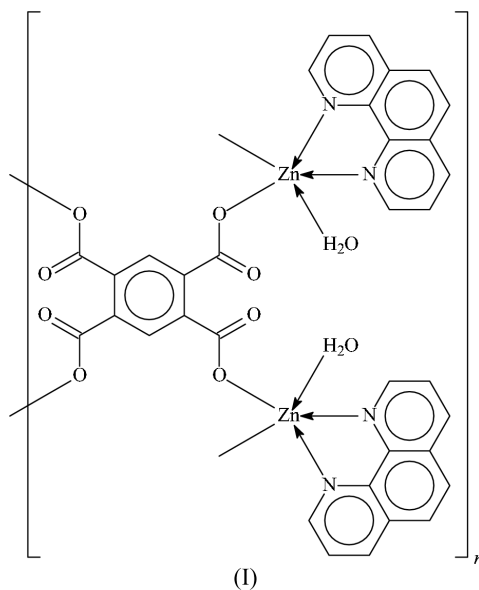
In the adducts with bipyridine and imidazole, the dizinc pyromellitate unit displays a chain motif as the tetra-carboxylate entity binds to four metal atoms. The present 1,10-phenanthroline adduct, (I) (Fig. 1), adopts a linear ribbon structure in which the pyromellitate tetraanion uses only one O atom from each carboxylate group to bind to one Zn atom; each Zn atom is also chelated by the heterocycle and its fifth coordination site is occupied by a water molecule. The pyro-mellitate tetraanion lies on an inversion center. The geometry
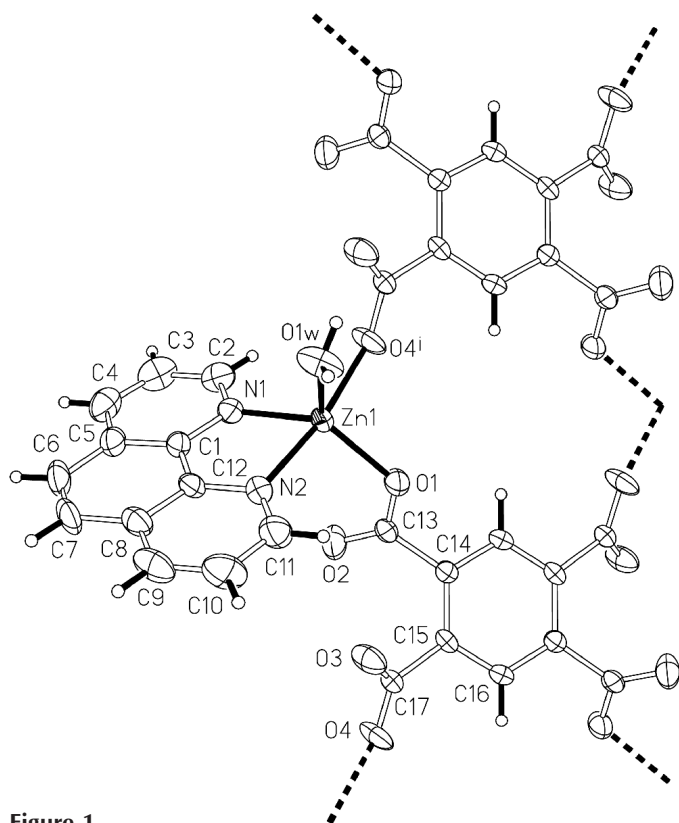
Figure 1
ORTEPII plot (Johnson, 1976) illustrating a portion of the chain of (I). Displacement ellipsoids are drawn at the 70% probability level and H atoms are drawn as spheres of arbitrary radii.
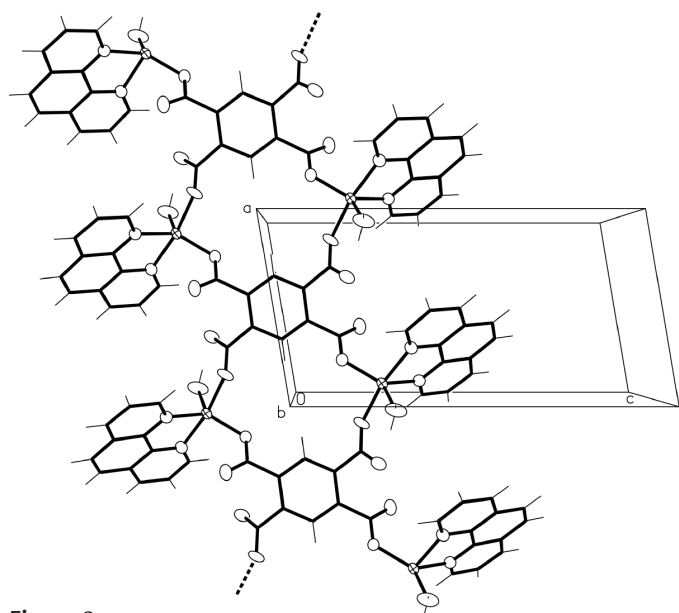
Figure 2
Schematic representation of the chain structure.

around the metal atom is trigonal bipyramidal in which the heterocycle spans the axial-equatorial sites. The copper(II) analog having a similar formulation is a tetrahedral compound (Zhang *et al.*, 2003), whereas the cobalt(II) analog is an octahedral compound (Fu *et al.*, 2004). Hydrogen bonds in (I) link the ribbons (Fig. 2) into layers (Table 2).

Experimental

A mixture of zinc nitrate hexahydrate (180 mg, 0.6 mmol), benzene-1,2,4,5-tetracarboxylic acid (78 mg, 0.3 mmol) and 1,10-phenanthroline (128 mg, 0.7 mmol) in water (15 ml) was placed in a Teflon-lined stainless-steel Parr bomb that was heated to 413 K for 72 h. The bomb was then cooled to room temperature over a period of 24 h. Colorless crystals were isolated in 20% yield.

Crystal data

$C_{34}H_{22}N_4O_{10}Zn_2$	$D_x = 1.810$ Mg m^{-3}
$M_r = 777.30$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 10 914
$a = 7.9612 (2)$ Å	reflections
$b = 11.8020 (3)$ Å	$\theta = 2.6–27.5°$
$c = 15.3935 (4)$ Å	$\mu = 1.76$ mm^{-1}
$\beta = 99.614 (1)°$	$T = 295 (2)$ K
$V = 1426.03 (6)$ Å^3	Block, colorless
$Z = 2$	$0.3 \times 0.2 \times 0.1$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	3276 independent reflections
ω scans	2830 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.066$
	$\theta_{max} = 27.5°$
$T_{min} = 0.490$, $T_{max} = 0.844$	$h = -10 \rightarrow 10$
6341 measured reflections	$k = -15 \rightarrow 15$
	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$+ 0.7927P]$
$wR(F^2) = 0.105$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3276 reflections	$\Delta\rho_{max} = 0.67$ e Å^{-3}
234 parameters	$\Delta\rho_{min} = -0.62$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.973 (2)	Zn1—N1	2.094 (2)
Zn1—O4^i	2.066 (2)	Zn1—N2	2.142 (2)
Zn1—O1w	2.080 (2)		
O1—Zn1—O4^i	93.1 (1)	O4^i—Zn1—N1	97.3 (1)
O1—Zn1—O1w	120.1 (1)	O4^i—Zn1—N2	169.0 (1)
O1—Zn1—N1	128.9 (1)	O1w—Zn1—N1	110.0 (1)
O1—Zn1—N2	97.3 (1)	O1w—Zn1—N2	82.5 (1)
O4^i—Zn1—O1w	89.3 (1)	N1—Zn1—N2	78.9 (1)

Symmetry code: (i) $x - 1, y, z$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1w—H1w1$\cdots$O2^{ii}	0.85 (1)	1.94 (1)	2.781 (3)	171 (4)
O1w—H1w2$\cdots$O3^i	0.84 (1)	1.86 (2)	2.638 (3)	153 (4)

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

The data collection software found 10 914 reflections that it used to calculate the unit cell; it then partially averaged them to 6341 measured reflections. Carbon-bound H atoms were positioned geometrically and were allowed to ride on their parent atoms [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The water H atoms were located and refined with a distance restraint of 0.85 (1) Å.

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