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catena-Poly[[[(dipyrido[3,2-*a*:2′,3′-*c*]phenazine)-zinc(II)]-μ-benzene-1,4-dicarboxylato] dipyrido-[3,2-*a*:2′,3′-*c*]phenazine 0.67-solvate]

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In the title compound, $[Zn(C_8H_4O_4)(C_{18}H_{10}N_4)]_{3n}\cdot 2nC_{18}H_{10}N_4$, the three distinct Zn^{II} atoms each exhibit a distorted *cis*-ZnN_2O_4 octahedral coordination geometry arising from an *N*,*N*-bidentate dipyrido[3,2-*a*:2,3′-*c*]-phenazine ($C_{18}H_{10}N_4$; DPPZ) molecule and two *O*,*O*-bidentate 1,4-benzenedicarboxylate ($C_8H_4O_4$; BDC) dianions. The three crystallographically independent $[Zn(C_8H_4O_4)(C_{18}H_{10}N_4)]_n$ polymeric strands propagate in the [001] direction. Two uncoordinated DPPZ molecules complete the asymmetric unit. The structure is stabilized by C—H···O, C—H···N and π–π interactions.

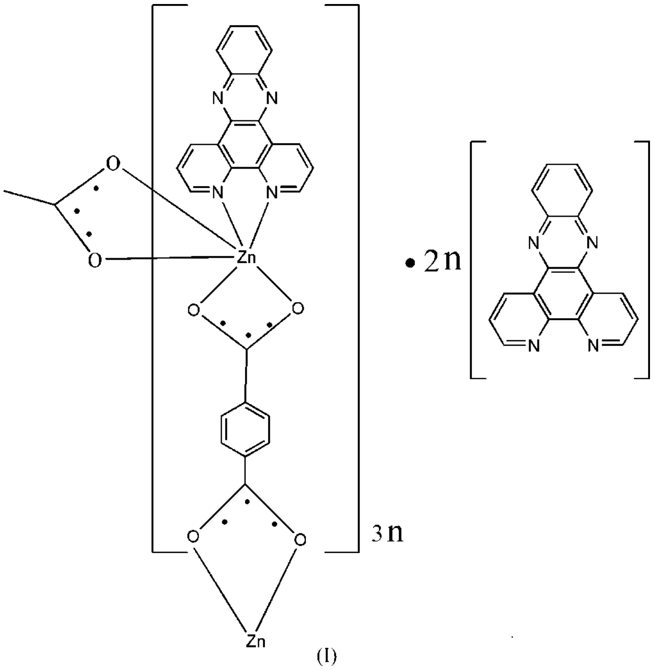
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.045
wR factor = 0.088
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.

Comment

Recently, polycyclic aromatic bidentate ligands such as 2,2-bipyridyl (2,2-bipy) and 1,10-phenanthroline (1,10-phen) have been used in combination with polycarboxylates, leading to novel supramolecular architectures which are stabilized through π–π stacking interactions (Chen & Liu, 2002; Liu *et al.*, 2002). Based on the above synthesis strategy, we obtained the title compound, (I), using 1,4-benzenedicarboxylic acid ($C_8H_6O_4$; H_2BDC), the bidentate chelating ligand dipyrido[3,2-*a*:2,3′-*c*]phenazine ($C_{18}H_{10}N_4$; DPPZ), and Zn^{II} ion as starting materials.



(I)

Compound (I) (Fig. 1) is a one-dimensional metal–organic coordination polymer. There are three crystallographically

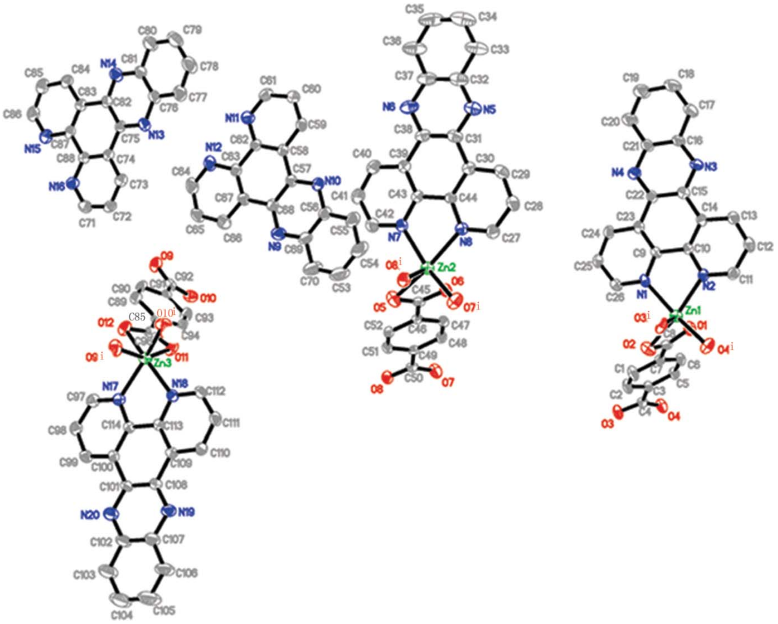


Figure 1

The asymmetric unit of (I), together with additional atoms to complete the Zn coordination, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $x, \frac{3}{2} - y, \frac{1}{2} + z$.]

distinct Zn^{II} ions, each of them showing the same coordination with a distorted octahedral geometry, arising from two N atoms of a DPPZ molecule and four O atoms from two bidentate BDC dianions. In addition, there are two uncoordinated DPPZ molecules in the asymmetric unit.

Each BDC ligand acts in a bidentate mode and bridges two Zn^{II} ions, resulting in $[Zn(BDC)(DPPZ)]_n$ chains, with the additional DPPZ molecules interleaved between them (Fig. 2). The average Zn···Zn···Zn angle formed by three adjacent Zn^{II} ions is 126° for the three chains.

Various C—H···O and C—H···N interactions (Table 2) provide cohesion between adajcent polymeric chains. Close offset π–π stacking contacts are also apparent between free and coordinated DPPZ molecules, with face-to-face separations of 3.33 and 3.36 Å. In turn, these non-covalent interactions generate undulating layers and then a three-dimensional supramolecular structure.

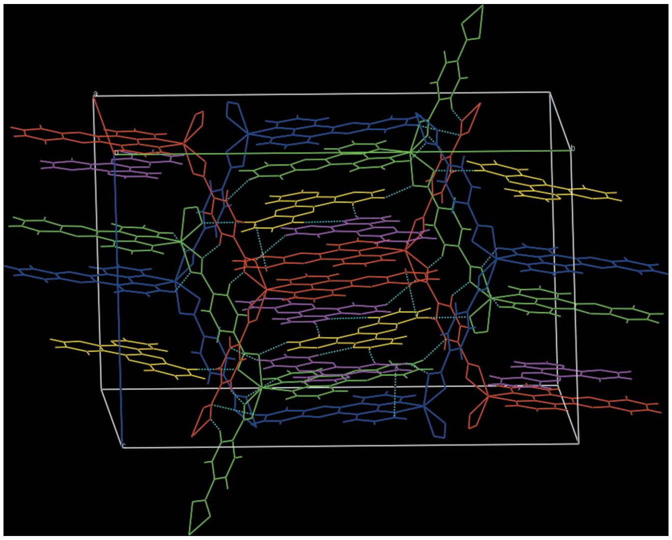


Figure 2

A packing diagram for (I), showing the three polymeric chains (red, green and blue) and the uncoordinated DPPZ molecules (yellow and purple).

Experimental

The title compound was prepared from a mixture of $Zn(CH_3COO)_2 \cdot 2H_2O$ (0.1095 g), 1,4-benzenedicarboxylic acid (0.0517 g), dipyrido[3,2-*a*:2′,3′-*c*]phenazine (0.0831 g) and H_2O (30 ml) in a 40 ml Teflon-lined autoclave under autogenous pressure at 443 K for 4 d. The pH was adjusted to 7.5 with NaOH. Upon cooling, yellow crystals of (I) were obtained.

Crystal data

$[Zn(C_8H_4O_4)(C_{18}H_{10}N_4)]_3 \cdot 2C_{18}H_{10}N_4$
$M_r = 2099.95$
Monoclinic, $P2_1/c$
$a = 18.474$ (2) Å
$b = 28.718$ (4) Å
$c = 19.019$ (2) Å
$\beta = 116.092$ (2)°
$V = 9062$ (2) Å^3
$Z = 4$
$D_x = 1.539$ Mg m$^{-3$}
Mo $K\alpha$ radiation
$\mu = 0.87$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.20 × 0.14 × 0.11 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.861$, $T_{max} = 0.910$
50984 measured reflections
17865 independent reflections
6083 reflections with $I > 2\sigma(I)$
$R_{int} = 0.090$
$\theta_{max} = 26.1$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.088$
$S = 0.71$
17865 reflections
1342 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0159P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

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Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.121 (4)	Zn2—O5	2.294 (3)
Zn1—N2	2.130 (4)	Zn2—O8^{i}	2.024 (3)
Zn1—O1	2.098 (3)	Zn2—O7^{i}	2.304 (3)
Zn1—O2	2.176 (3)	Zn3—N18	2.123 (4)
Zn1—O3^{i}	2.044 (3)	Zn3—N17	2.118 (4)
Zn1—O4^{i}	2.260 (3)	Zn3—O11	2.049 (3)
Zn2—N8	2.125 (4)	Zn3—O12	2.225 (3)
Zn2—N7	2.121 (4)	Zn3—O10^{i}	2.114 (3)
Zn2—O6	2.037 (3)	Zn3—O9^{i}	2.164 (3)
O8^{i}—Zn2—O6	140.77 (11)	O10^{i}—Zn3—O9^{i}	61.63 (12)
O8^{i}—Zn2—N7	103.00 (12)	N17—Zn3—O9^{i}	93.89 (13)
O6—Zn2—N7	106.86 (12)	N18—Zn3—O9^{i}	95.29 (12)
O8^{i}—Zn2—N8	106.44 (12)	O11—Zn3—O12	61.15 (10)
O6—Zn2—N8	104.53 (12)	O10^{i}—Zn3—O12	103.70 (12)
N7—Zn2—N8	77.21 (13)	N17—Zn3—O12	95.26 (13)
O8^{i}—Zn2—O5	96.08 (11)	N18—Zn3—O12	159.91 (12)
O6—Zn2—O5	60.38 (10)	O9^{i}—Zn3—O12	103.96 (12)
N7—Zn2—O5	88.50 (14)	O3^{i}—Zn1—O1	152.83 (14)
N8—Zn2—O5	155.46 (12)	O3^{i}—Zn1—N1	100.52 (12)
O8^{i}—Zn2—O7^{i}	60.10 (11)	O1—Zn1—N1	98.78 (12)
O6—Zn2—O7^{i}	97.67 (11)	O3^{i}—Zn1—N2	102.06 (12)
N7—Zn2—O7^{i}	153.93 (13)	O1—Zn1—N2	100.73 (12)
N8—Zn2—O7^{i}	88.38 (14)	N1—Zn1—N2	77.18 (15)
O5—Zn2—O7^{i}	111.72 (11)	O3^{i}—Zn1—O2	98.85 (13)
C45—Zn2—C50^{i}	119.23 (13)	O1—Zn1—O2	61.95 (11)
O11—Zn3—O10^{i}	102.46 (13)	N1—Zn1—O2	90.52 (13)
O11—Zn3—N17	104.90 (13)	N2—Zn1—O2	157.32 (13)
O10^{i}—Zn3—N17	151.84 (13)	O3^{i}—Zn1—O4^{i}	60.91 (10)
O11—Zn3—N18	102.19 (12)	O1—Zn1—O4^{i}	102.94 (11)
O10^{i}—Zn3—N18	90.35 (13)	N1—Zn1—O4^{i}	157.77 (11)
N17—Zn3—N18	77.54 (15)	N2—Zn1—O4^{i}	94.07 (13)
O11—Zn3—O9^{i}	156.60 (14)	O2—Zn1—O4^{i}	103.76 (13)

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*B*···O5^{ii}	0.93	2.42	3.238 (6)	147
C112—H11*B*···O3^{iii}	0.93	2.31	2.993 (6)	130
C26—H26*A*···O11^{iv}	0.93	2.42	3.003 (6)	120
C48—H48*A*···O12^{iv}	0.93	2.51	3.340 (6)	149
C52—H52*A*···O4^{iii}	0.93	2.52	3.345 (6)	147
C55—H55*A*···N15^{v}	0.93	2.60	3.525 (8)	171
C60—H60*A*···O1^{vi}	0.93	2.56	3.388 (6)	149
C72—H72*A*···O9	0.93	2.57	3.455 (6)	158
C80—H80*A*···O10^{vii}	0.93	2.58	3.433 (7)	152
C89—H89*A*···O7^{viii}	0.93	2.41	3.219 (7)	145

Symmetry codes: (ii) $x-1, y, z-1$; (iii) $x+1, y, z+1$; (iv) $x-1, -y+\frac{3}{2}, z-\frac{1}{2}$; (v) $x-1, y, z$; (vi) $-x+1, -y+1, -z$; (vii) $-x+3, y-\frac{1}{2}, -z+\frac{1}{2}$; (viii) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.

H atoms were positioned geometrically, with C—H = 0.93 Å, and refined with a riding model, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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