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Poly[[bis(4,4′-bipyridine)bis(μ-oxalato)-trizinc(II)]-di-μ-4,4′-bipyridine-μ-oxalato]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.062
Data-to-parameter ratio = 13.6

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

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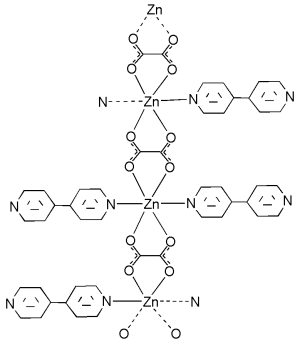
The hydrothermally prepared title compound, $[Zn_3(C_{10}H_8N_2)_4(C_2O_4)_3]$, isostructural with the Fe analog, consists of undulating chains of oxalate-bridged Zn centers linked into infinite two-dimensional layers by bridging 4,4′-bipyridine ligands. An additional 4,4′-bipyridine ligand is coordinated to two of the three inequivalent Zn centers as a terminal ligand.

Comment

The title compound, (I), is isostructural with a previously reported iron analog (Zheng *et al.*, 1999). Three crystallographically inequivalent octahedral Zn^{2+} centers are linked into undulating chains along [010] by three inequivalent bridging oxalate groups. The chain subunits are further linked into infinite two-dimensional layers by two of the four crystallographically independent 4,4′-bipyridine ligands. Two additional 4,4′-bipyridine ligands coordinate to Zn1 and Zn3 in a terminal mode (Fig. 1), creating a 'self-interdigitating' layered network. The layers stack along [101].



(I)

The Zn—O distances [range 2.060 (1)–2.091 (1) Å; Table 1] and Zn—N distances [range 2.150 (2)–2.337 (2) Å; Table 1] are consistent with the reported Fe—O distances, and in good agreement with those in the related zinc–oxalato–4,4′-bipyridine layered polymer [Zn(ox)(bipy)] (Lu *et al.*, 1999).

Experimental

The title compound was prepared by hydrothermal reaction of $Zn(NO_3)_2{\cdot}6H_2O$ (0.576 g, 0.2 mmol) with 4,4′-bipyridine (0.0160 g, 0.1 mmol) and oxalic acid (0.0124 g, 0.1 mmol) in water (0.80 ml) in an evacuated sealed Pyrex tube. The reaction was heated to 418 K at 10 K min^{-1} and held at that temperature for 48 h before cooling slowly (0.2 K min^{-1}) to 298 K. The reaction yielded a plentiful supply of yellow crystals.

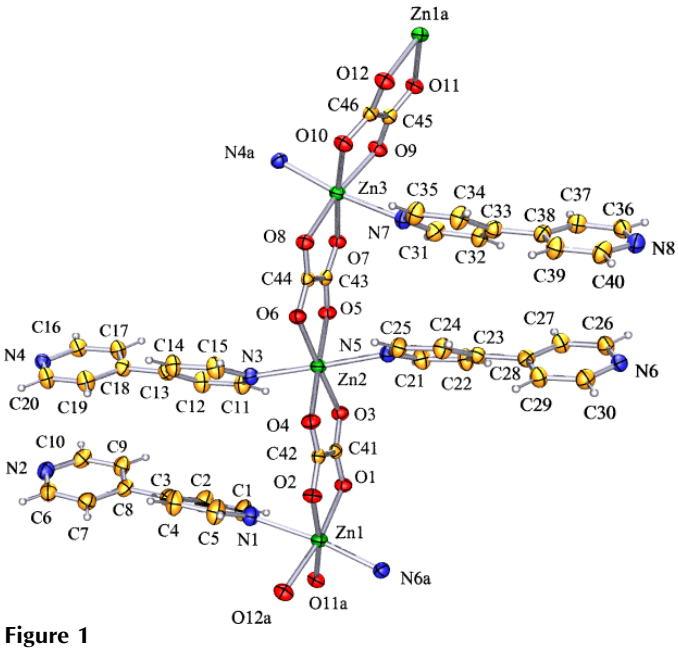


Figure 1
View of (I), with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms with suffix 'a' are symmetry generated; see Table 1 for details.

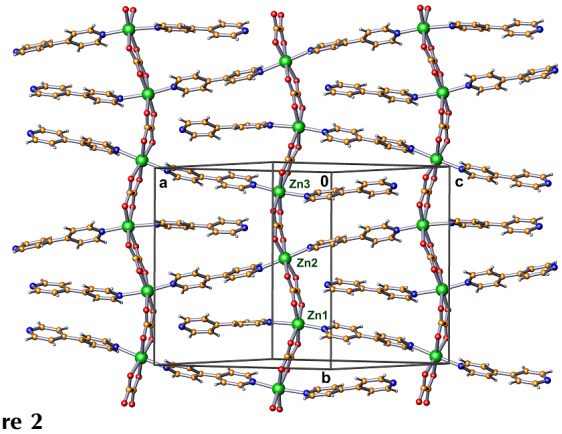


Figure 2
A single layer of (I), showing the undulating chains of oxalato-bridged Zn atoms and terminal and bridging 4,4′-bipyridine ligands.

Crystal data

$[Zn_3(C_{10}H_8N_2)_4(C_2O_4)_3]$
M_r = 1084.91
Monoclinic, $P2_1/c$
a = 16.2513 (9) Å
b = 15.5891 (9) Å
c = 16.376 (1) Å
β = 94.000 (1)°
V = 4138.6 (4) Å^3
Z = 4
D_x = 1.741 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9955 reflections
θ = 2.6–26.4°
μ = 1.81 mm^{-1}
T = 293 (2) K
Bar, yellow
0.42 × 0.40 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.415, T_{max} = 0.594
32100 measured reflections
8443 independent reflections
6454 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 26.4°
$h = -14 \rightarrow 20$
$k = -18 \rightarrow 19$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.062
S = 1.03
8443 reflections
622 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0256P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å).

Zn1—O2	2.0630 (13)	Zn2—O5	2.0880 (14)
Zn1—O1	2.0668 (13)	Zn2—N3	2.2152 (15)
Zn1—O12^{i}	2.0749 (14)	Zn2—N5	2.2419 (15)
Zn1—O11^{i}	2.0806 (14)	Zn3—O7	2.0601 (13)
Zn1—N6^{ii}	2.1601 (15)	Zn3—O8	2.0800 (13)
Zn1—N1	2.3370 (16)	Zn3—O10	2.0886 (14)
Zn2—O3	2.0733 (13)	Zn3—O9	2.0910 (14)
Zn2—O6	2.0782 (13)	Zn3—N4^{iii}	2.1497 (15)
Zn2—O4	2.0866 (14)	Zn3—N7	2.2669 (16)

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

H atoms were geometrically idealized, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{iso}(C).

Data collection: *SMART-NT* (Bruker, 1999); cell refinement: *SAINT-Plus-NT* (Bruker, 1999); data reduction: *SAINT-Plus-NT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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