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Poly[bis(μ_2-*trans*-di-4-pyridylethylene-κ^2N:N')bis(nitrato-κ^2O,O')bis(μ_4-succinato-κ^4O:O':O'':O''')(μ_4-succinato-κ^4O:O:O':O')-tetrazinc(**II**)]

Ji-Yang Xu,[a] Fatima Zapata,[b] Brandy H. Courtney,[c] Frank R. Fronczek[c] and Banglin Chen[b]*

[a]Department of Biochemistry, China Pharmaceutical University, Nanjing 210009, People's Republic of China, [b]Department of Chemistry, The University of Texas-Pan American, Edinburgh, TX 78541-2999, USA, and [c]Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803-1804, USA

Correspondence e-mail: banglin@utpa.edu

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In the title compound, $[Zn_4(C_4H_4O_4)_3(NO_3)_2(C_{12}H_{10}N_2)_2]$, the tetranuclear Zn_4(*gauche*-succinato)$_2$ building blocks are bridged by succinate and *trans*-di-4-pyridylethylene ligands to form a distorted two-dimensional (4,4)-square grid. Packing of these square grids leads to a condensed metal–organic framework. One of the two independent Zn atoms shows tetrahedral whereas the other shows octahedral coordination. They are bridged by three succinate ligands, with a Zn···Zn distance of 3.1505 (12) Å.

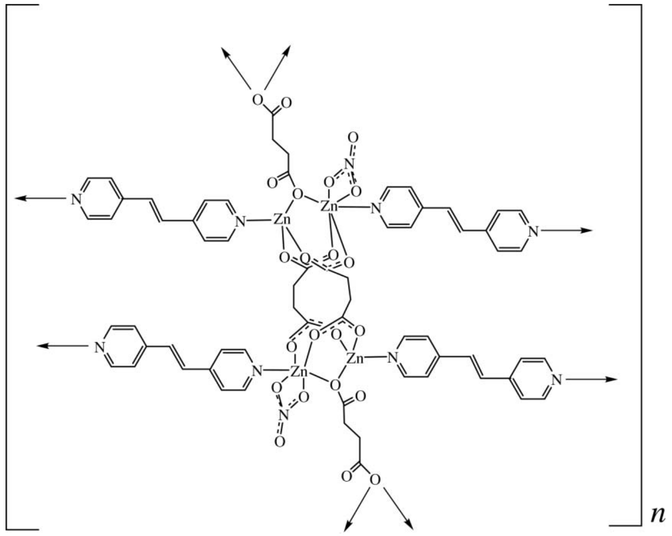
Key indicators

Single-crystal X-ray study
T = 110 K
Mean σ(C–C) = 0.005 Å
R factor = 0.050
wR factor = 0.086
Data-to-parameter ratio = 17.1

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

Comment

Porous metal–organic frameworks (MOFs) self-assembled by the coordination of suitable metal ions/clusters with organic building blocks are of interest owing to potential applications in gas storage, separation, molecular recognition, magnetism and catalysis (Eddaoudi *et al.*, 2001; Kitagawa *et al.*, 2004; Yaghi *et al.*, 2003; Janiak, 2003). Recently, we have been interested in the construction of porous MOFs by making use of mixed organic linkers (Rather & Zaworotko, 2003; Chun *et al.*, 2005; Ma *et al.*, 2005; Chen *et al.*, 2006). The title compound, (I), is one of the MOFs constructed from zinc(II) nitrate and organic linkers succinate and *trans*-di-4-pyridylethylene (4,4′-Bpe).


(I)

The asymmetric unit of (I) is shown in Fig. 1. There are two types of Zn atoms bridged by two μ_4-*gauche*-succinate and one μ_4-anti-succinate ligand, Zn1 being distorted octahedral and Zn2 distorted tetrahedral. Atom Zn1 is further coordinated by atom N1 from 4,4′-Bpe and is capped with nitrate,

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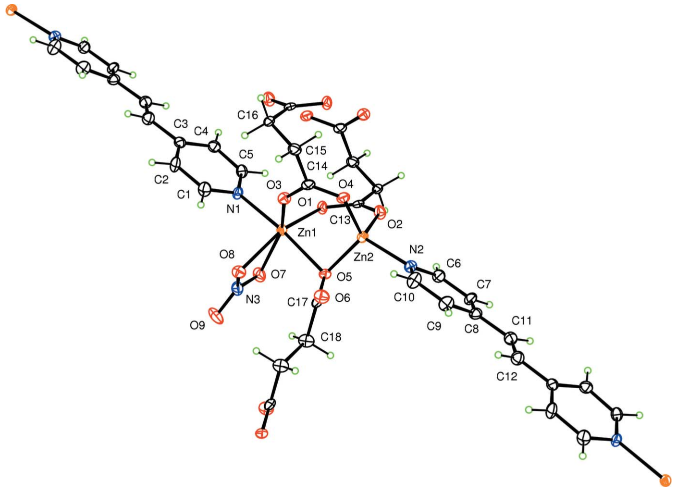

Figure 1
A portion of the structure, with the asymmetric unit labeled and displacement ellipsoids drawn at the 50% probability level.

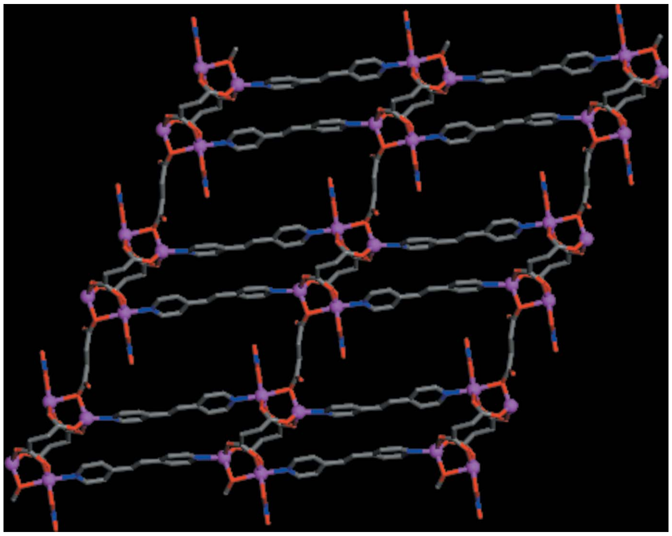

Figure 2
Distorted two-dimensional (4,4)-square grid sheet of the title compound (key: Zn purple, C gray, N blue and O red). H atoms have been omitted.

while Zn2 is coordinated by atom N2 from 4,4′-Bpe. Topologically, the structure can be viewed as a distorted two-dimensional (4,4)-square grid constructed by the tetranuclear Zn_4(*gauche*-succinato)$_2$ building blocks. These tetranuclear building blocks are further bridged by mixed organic linkers anti-succinato and 4,4′-Bpe to form a layer structure (Fig. 2). Crystal packing indicates that the title compound is a condensed MOF in which the layers are stacked (Fig. 3).

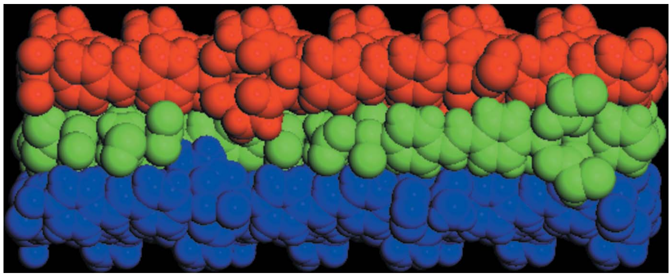

Figure 3
Crystal packing in the structure of (I), indicating successive sheets in red, green and blue forming a condensed MOF.

Experimental

The title compound was synthesized by hydrothermal reaction of $Zn(NO_3)_2\cdot 6H_2O$, succinic acid and *trans*-di-4-pyridylethylene (1:1:0.5 molar ratio) in DMF/ethanol/water (3:3:2 volume ratio) at 353 K. Small colorless crystals of the title compound formed and were collected in 54% yield.

Crystal data

$[Zn_4(C_4H_4O_4)_3(NO_3)_2(C_{12}H_{10}N_2)_2]$
$M_r = 1098.16$
Triclinic, $P\overline{1}$
$a = 9.615\ (4)$ Å
$b = 9.804\ (4)$ Å
$c = 11.729\ (4)$ Å
$\alpha = 82.58\ (2)^\circ$
$\beta = 80.87\ (2)^\circ$
$\gamma = 69.097\ (14)^\circ$
$V = 1016.6\ (7)$ Å^3
$Z = 1$
$D_x = 1.794$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4442 reflections
$\theta = 2.6$–28.3°
$\mu = 2.42$ mm^{-1}
$T = 110$ K
Irregular fragment, colorless
0.08 × 0.08 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer (with an Oxford Cryosystems Cryostream cooler)
ω scans with κ offsets
Absorption correction: multi-scan (*DENZO* and *SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.861$, $T_{max} = 0.930$
16627 measured reflections
4947 independent reflections
3320 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 28.3^\circ$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 12$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.086$
$S = 1.01$
4947 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 1.0067P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.002 (2)	Zn2—O5	1.977 (2)
Zn1—O3	2.023 (3)	Zn2—N2	2.001 (3)
Zn1—N1	2.102 (3)	C3—C12^{i}	1.458 (5)
Zn1—O8	2.182 (3)	C11—C12	1.336 (5)
Zn1—O7	2.210 (3)	C12—C3^{ii}	1.458 (5)
Zn1—O5	2.233 (2)	C13—C16^{iii}	1.504 (5)
Zn2—O4	1.940 (3)	C16—C13^{iii}	1.504 (5)
Zn2—O2	1.968 (2)	C18—C18^{iv}	1.515 (7)
C8—C11—C12—C3^{ii}	177.7 (3)	C14—C15—C16—C13^{iii}	−57.7 (4)

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

H atoms on C atoms were placed in idealized positions, with C—H distances of 0.95–0.99 Å, and thereafter treated as riding. Displacement parameters for H atoms were assigned as $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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