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Poly[(μ_2-*trans*-di-4-pyridylethylene-κ^2N:N')(μ_2-fumarato-κ^2O:O')zinc(II)]

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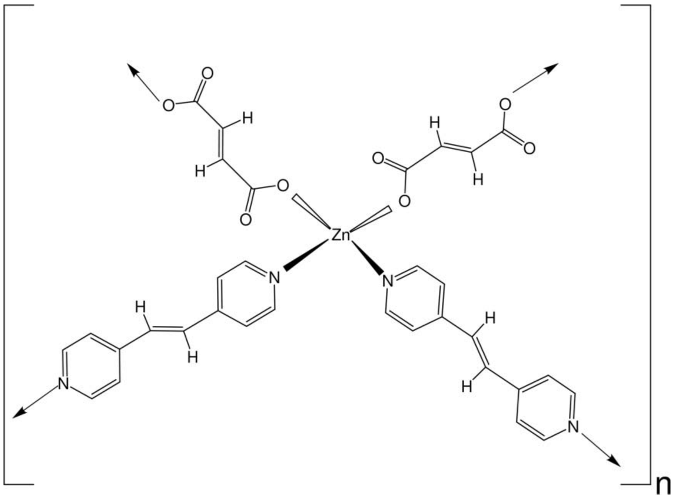
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.001 Å; R factor = 0.024; wR factor = 0.073; data-to-parameter ratio = 48.8.

In the title compound, [Zn($C_4H_2O_4$)($C_{12}H_{10}N_2$)], the Zn^{II} atom lies on a crystallographic twofold rotation axis in a distorted tetrahedral geometry. The Zn^{II} ions are bridged by fumarate and *trans*-di-4-pyridylethylene to form a porous triply interpenetrated diamond-like metal–organic framework.

Related literature

For related literature, see: Chen *et al.* (2006); Chun *et al.* (2005); Eddaoudi *et al.* (2001); Janiak (2003); Kitagawa *et al.* (2004); Ma *et al.* (2005); Rather & Zaworotko (2003); Yaghi *et al.* (2003). For the SQUEEZE procedure used to treat highly disordered solvent, see van der Sluis & Spek (1990).



Experimental

Crystal data

[Zn($C_4H_2O_4$)($C_{12}H_{10}N_2$)]
M_r = 361.67
Monoclinic, $C2/c$
a = 8.8488 (8) Å
b = 21.5285 (19) Å
c = 13.5042 (11) Å
β = 97.144 (4)°
V = 2552.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 173 (2) K
0.30 × 0.15 × 0.10 mm

Data collection

Bruker X8 APEX II diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.759, T_{max} = 0.909
25652 measured reflections
5175 independent reflections
4435 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.073
S = 1.09
5175 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997) and *PLATON* (Spek, 2003); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2035).

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supplementary materials

Acta Cryst. (2007). E**63**, m2205 [**doi:10.1107/S1600536807035209**]

Poly[(μ_2-*trans*-di-4-pyridylethylene-κ^2N:N')(μ_2-fumarato-κ^2O:O')zinc(II)]

J.-Y. Xu, E. J. Hurtado, E. B. Lobkovsky and B. Chen

Comment

Porous metal-organic frameworks (MOFs) self-assembled by the coordination of suitable metal ions/clusters with organic building blocks are of great interest for their 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 is one such MOF constructed from Zn^{II} and the organic linkers fumarato and *trans*-di-4-pyridylethylene.

A small portion of the extended framework of (I) is shown in Fig. 1. Atom Zn1 is in a distorted tetrahedral geometry. These Zn^{II} ions are bridged by fumarato and *trans*-di-4-pyridylethylene to form a porous triply-interpenetrated metal-organic framework with a diamond-like structure (Fig. 2).

Experimental

The title compound was synthesized by a hydrothermal reaction of $Zn(NO_3)_2{\cdot}6H_2O$, fumaric acid and *trans*-di-4-pyridylethylene (1:1:1 mole ratio) in DMF at 100 °C. Small, colorless crystals of the title compound formed and were collected in 38% yield.

Refinement

All the hydrogen atoms were found in a difference Fourier map and refined isotropically.

Figures

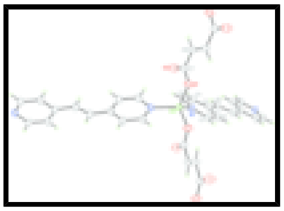

Fig. 1. A portion of the structure showing the labelling scheme of the asymmetric unit. Displacement ellipsoids are at the 50% probability level.

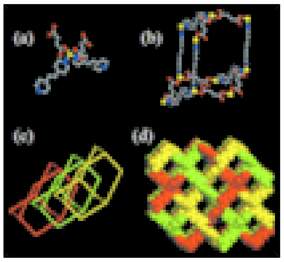

Fig. 2. (*a*) Coordination geometry around Zn; (*b*) one 'diamond' unit; (*c*) schematic illustration of the triply-interpenetrated metal-organic framework; (*d*) packing of the metal-organic framework indicating its porous structure (Zn yellow; C gray; N blue; O red).

Poly[(μ$_2$-*trans*-di-4-pyridylethylene-κ^2*N*:*N*')(μ$_2$-fumarato-\ κ^2*O*:*O*')zinc(II)]

Crystal data

$[Zn(C_4H_2O_4)(C_{12}H_{10}N_2)]$

$M_r = 361.67$

Monoclinic, $C2/c$

Hall symbol: -C 2yc

$a = 8.8488$ (8) Å

$b = 21.5285$ (19) Å

$c = 13.5042$ (11) Å

$\beta = 97.144$ (4)º

$V = 2552.6$ (4) Å^3

$Z = 4$

$F_{000} = 736$

$D_x = 0.941$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 8809 reflections

$\theta = 2.4$–32.0º

$\mu = 0.98$ mm^{-1}

$T = 173$ (2) K

Block, colourless

0.30 × 0.15 × 0.10 mm

Data collection

Bruker X8 APEX II
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 18 pixels mm^{-1}

$T = 173(2)$ K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2004)

$T_{min} = 0.759$, $T_{max} = 0.909$

25652 measured reflections

5175 independent reflections

4435 reflections with $I > 2\sigma(I)$

$R_{int} = 0.031$

$\theta_{max} = 34.2$º

$\theta_{min} = 1.9$º

$h = -13 \rightarrow 13$

$k = -33 \rightarrow 33$

$l = -18 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.073$

$S = 1.09$

5175 reflections

106 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.1113P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.31$ e Å^{-3}

$\Delta\rho_{min} = -0.53$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Due to a complete solvent area disorder data were treated with the SQUEEZE routine of the *PLATON* software package (van der Sluis & Spek, 1990). The calculated density is for the MOF only and does not include the solvent.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Zn1	0.0000	0.147618 (6)	0.2500	0.01800 (5)
O1	−0.10470 (8)	0.20659 (3)	0.15521 (5)	0.02760 (14)
O2	−0.21011 (10)	0.12225 (4)	0.07903 (6)	0.03675 (18)
N1	0.14390 (8)	0.09472 (4)	0.18136 (6)	0.02206 (14)
C1	0.28693 (11)	0.11406 (5)	0.17539 (8)	0.02768 (19)
H1A	0.3217	0.1509	0.2096	0.033*
C2	0.38538 (11)	0.08249 (5)	0.12157 (8)	0.0313 (2)
H2A	0.4852	0.0980	0.1184	0.038*
C3	0.33737 (10)	0.02748 (5)	0.07150 (7)	0.02544 (18)
C4	0.19073 (11)	0.00652 (5)	0.08083 (8)	0.0301 (2)
H4A	0.1550	−0.0314	0.0504	0.036*
C5	0.09708 (11)	0.04145 (5)	0.13489 (8)	0.02801 (19)
H5A	−0.0035	0.0272	0.1392	0.034*
C6	0.43108 (11)	−0.00836 (5)	0.00942 (8)	0.0300 (2)
H6A	0.3902	−0.0460	−0.0191	0.036*
C7	−0.18907 (11)	0.17920 (4)	0.08416 (7)	0.02391 (17)
C8	−0.26287 (11)	0.22001 (5)	0.00310 (7)	0.02724 (18)
H8A	−0.3330	0.2015	−0.0474	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01940 (7)	0.01775 (7)	0.01692 (7)	0.000	0.00252 (5)	0.000
O1	0.0334 (3)	0.0235 (3)	0.0233 (3)	0.0000 (3)	−0.0070 (3)	0.0022 (2)
O2	0.0468 (5)	0.0218 (4)	0.0378 (4)	−0.0040 (3)	−0.0099 (3)	0.0017 (3)
N1	0.0205 (3)	0.0232 (4)	0.0229 (3)	−0.0019 (3)	0.0045 (3)	−0.0043 (3)
C1	0.0230 (4)	0.0275 (5)	0.0334 (5)	−0.0056 (3)	0.0071 (3)	−0.0111 (4)
C2	0.0229 (4)	0.0340 (5)	0.0383 (5)	−0.0071 (4)	0.0094 (4)	−0.0129 (4)
C3	0.0214 (4)	0.0253 (4)	0.0304 (4)	−0.0030 (3)	0.0064 (3)	−0.0071 (3)
C4	0.0263 (4)	0.0266 (5)	0.0391 (5)	−0.0059 (4)	0.0112 (4)	−0.0122 (4)

C5	0.0225 (4)	0.0271 (5)	0.0357 (5)	−0.0049 (3)	0.0089 (4)	−0.0085 (4)
C6	0.0255 (4)	0.0291 (5)	0.0365 (5)	−0.0036 (4)	0.0079 (4)	−0.0130 (4)
C7	0.0260 (4)	0.0232 (4)	0.0215 (4)	0.0001 (3)	−0.0009 (3)	0.0022 (3)
C8	0.0302 (4)	0.0272 (5)	0.0218 (4)	−0.0003 (4)	−0.0068 (3)	0.0002 (3)

Geometric parameters (Å, °)

Zn1—O1^{i}	1.9529 (7)	C2—H2A	0.9500
Zn1—O1	1.9529 (7)	C3—C4	1.3941 (13)
Zn1—N1^{i}	2.0177 (8)	C3—C6	1.4693 (13)
Zn1—N1	2.0177 (8)	C4—C5	1.3913 (13)
O1—C7	1.2837 (11)	C4—H4A	0.9500
O2—C7	1.2406 (13)	C5—H5A	0.9500
N1—C1	1.3444 (11)	C6—C6^{ii}	1.3264 (19)
N1—C5	1.3475 (12)	C6—H6A	0.9500
C1—C2	1.3808 (13)	C7—C8	1.4895 (13)
C1—H1A	0.9500	C8—C8^{iii}	1.316 (2)
C2—C3	1.4031 (14)	C8—H8A	0.9500
O1^{i}—Zn1—O1	98.89 (4)	C4—C3—C6	118.63 (8)
O1^{i}—Zn1—N1^{i}	109.93 (3)	C2—C3—C6	124.04 (8)
O1—Zn1—N1^{i}	113.14 (3)	C5—C4—C3	119.62 (9)
O1^{i}—Zn1—N1	113.14 (3)	C5—C4—H4A	120.2
O1—Zn1—N1	109.93 (3)	C3—C4—H4A	120.2
N1^{i}—Zn1—N1	111.27 (5)	N1—C5—C4	122.39 (8)
C7—O1—Zn1	112.06 (6)	N1—C5—H5A	118.8
C1—N1—C5	118.22 (8)	C4—C5—H5A	118.8
C1—N1—Zn1	120.35 (6)	C6^{ii}—C6—C3	124.37 (12)
C5—N1—Zn1	121.28 (6)	C6^{ii}—C6—H6A	117.8
N1—C1—C2	122.64 (9)	C3—C6—H6A	117.8
N1—C1—H1A	118.7	O2—C7—O1	124.40 (8)
C2—C1—H1A	118.7	O2—C7—C8	119.53 (8)
C1—C2—C3	119.74 (9)	O1—C7—C8	116.06 (8)
C1—C2—H2A	120.1	C8^{iii}—C8—C7	124.20 (11)
C3—C2—H2A	120.1	C8^{iii}—C8—H8A	117.9
C4—C3—C2	117.33 (8)	C7—C8—H8A	117.9

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

Fig. 1

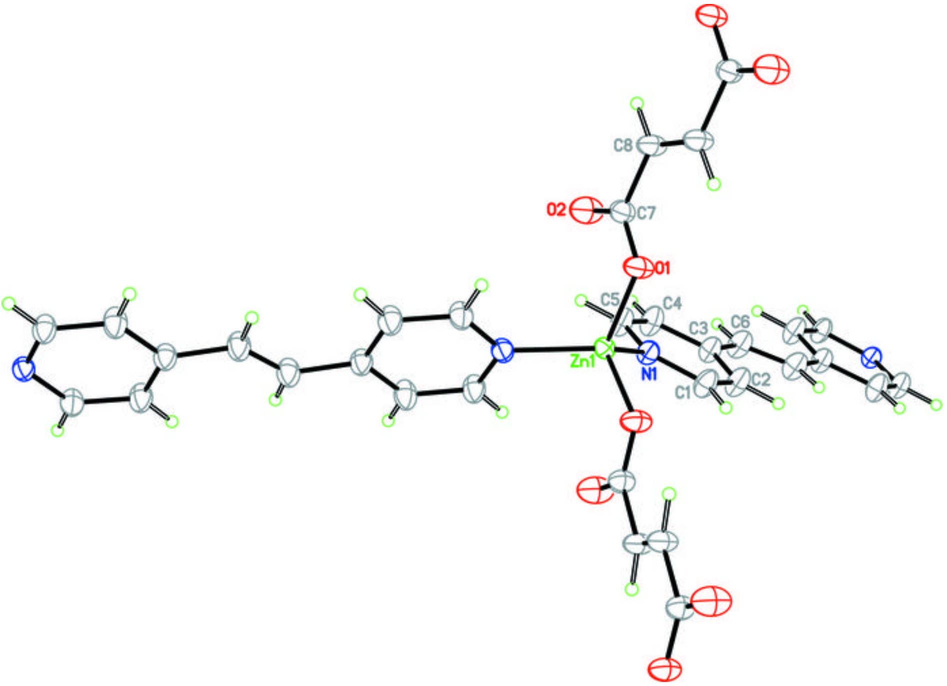

Fig. 2