

Poly[μ_2 -acetato- μ_2 -benzimidazolato-zinc(II)]

Xiu-Mei Li

Department of Chemistry, Tonghua Teachers' College, Tonghua 134002, People's Republic of China

Correspondence e-mail: lixm20032008@yahoo.com.cn

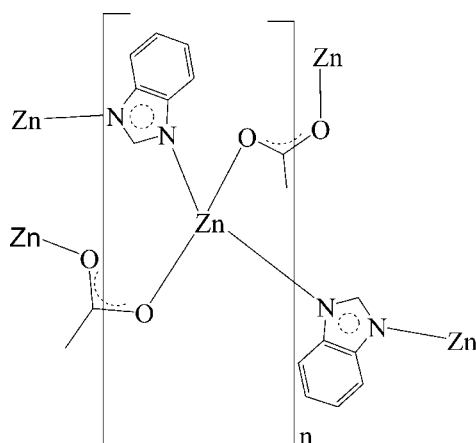
Received 19 June 2007; accepted 21 June 2007

 Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.023; wR factor = 0.063; data-to-parameter ratio = 14.4.

The title compound, $[\text{Zn}(\text{C}_7\text{H}_5\text{N}_2)(\text{C}_2\text{H}_3\text{O}_2)]_n$, was obtained unintentionally as the product of an attempted synthesis of a polycarboxylate-bridged network complex of zinc(II) using naphthalene-1,4,5,8-tetracarboxylic acid as the organic acid. The Zn atom is four-coordinated by two O atoms from two acetate (OAc) ligands and two N atoms from two different benzimidazole (bzim) ligands, resulting in a ZnN_2O_2 tetrahedron. The OAc and bzim ligands bridge the Zn atoms to form an infinite three-dimensional network.

Related literature

For a related structure, see: Huang *et al.* (2003). For background, see: Eddaoudi *et al.* (2002); Orpen *et al.* (1989).



Experimental

Crystal data

 $[\text{Zn}(\text{C}_7\text{H}_5\text{N}_2)(\text{C}_2\text{H}_3\text{O}_2)]$
 $M_r = 241.54$

 Monoclinic, $P2_1/c$
 $a = 10.8177$ (8) Å

 $b = 9.8371$ (7) Å

 $c = 8.8206$ (6) Å

 $\beta = 98.938$ (1)°

 $V = 927.24$ (11) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 2.62$ mm⁻¹
 $T = 292$ (2) K

 $0.47 \times 0.35 \times 0.12$ mm

Data collection

 Bruker SMART CCD
 diffractometer

 Absorption correction: multi-scan
 (SADABS; Bruker, 2001)

 $T_{\min} = 0.344$, $T_{\max} = 0.728$

7653 measured reflections

1825 independent reflections

 1646 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.063$
 $S = 1.03$

1825 reflections

127 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.35$ e Å⁻³
Table 1

Selected bond lengths (Å).

Zn1—N1	1.9735 (17)	Zn1—O2	1.9880 (15)
Zn1—N2 ⁱ	1.9802 (17)	Zn1—O1 ⁱⁱ	2.0046 (14)

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXL97.

The author thanks Miss Ling-Jie OuYang and Mr Jia-Jun Wang of Jilin Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2445).

References

- Orpen, G., Brammer, L., Allen, F. H., Kennard, O., Watson, D. G. & Taylor, R. (1989). *J. Chem. Soc. Dalton Trans.* pp. S1–83.
- Bruker (2001). SMART, SAINT, SADABS and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
- Eddaoudi, M., Kim, J., O'Keeffe, M. & Yaghi, O. M. (2002). *J. Am. Chem. Soc.* **124**, 376–377.
- Huang, X.-C., Zhang, J.-P. & Chen, X.-M. (2003). *Chin. Sci. Bull.* **48**, 1491–1494.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E63, m1984 [doi:10.1107/S1600536807030309]

Poly[μ_2 -acetato- μ_2 -benzimidazolato-zinc(II)]

X.-M. Li

Comment

Coordination polymers with a variety of supramolecular structures have been studied extensively because of their novel topologies and potential applications as functional materials (Eddaoudi *et al.*, 2002). However, such compounds containing deprotonated benzimidazole ($C_7H_5N_2^-$, bzim) ligands have been rarely studied (Huang *et al.*, 2003). We now report the title compound, (I), which is a new coordination polymer containing Zn^{2+} cations, bzim anions, and acetate ($C_2H_3O_2^-$) anions. These species combine in a 1:1:1 ratio, to ensure charge balance.

In compound (I), the Zn atom is coordinated by two N atoms of two different bzim ligands and two O atoms from two different acetate anions, in a slightly distorted tetrahedral geometry (Fig. 1). The bond lengths (Table 1) are normal (Orpen *et al.*, 1989). The C—O bond lengths of the acetate ion imply charge delocalization.

The acetic acid anion serves to link two Zn^{2+} ions together and the bzim species also acts as a bridge between two zinc ions. This connectivity results the coordination polymer in a three-dimensional network framework structure (Fig. 2).

Experimental

Naphthalene-1,4,5,8-tetracarboxylic acid, benzimidazole and zinc acetate dihydrate were reacted in a molar ratio of 1:2:2. The mixture was stirred for 30 min, then the pH was adjusted to 8.0 with an aqueous solution of KOH (0.1 M). The mixture with a total volume of 21 ml was heated at 393 K for 5 d in a sealed 24 ml Teflon-lined stainless steel vessel under autogenous pressure. After the reaction mixture was slowly cooled to room temperature at a rate of 3 K h^{-1} , pale yellow crystals of (I) were obtained.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(\text{methyl C})$.

Figures

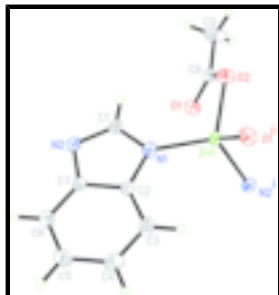


Fig. 1. The asymmetric unit of (I) expanded to show the Zn coordination sphere. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). Symmetry codes: (i) $1 - x, -1/2 + y, 3/2 - z$, (ii) $x, -1/2 - y, -1/2 + z$.

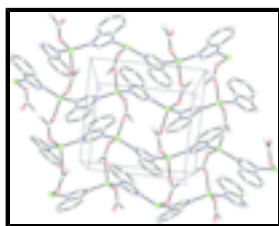


Fig. 2. The packing diagram for (I), showing the three-dimensional network structure.

Poly[μ_2 -acetato- μ_2 -benzimidolato-zinc(II)]

Crystal data

[Zn(C₇H₅N₂)(C₂H₃O₂)]

$M_r = 241.54$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.8177$ (8) Å

$b = 9.8371$ (7) Å

$c = 8.8206$ (6) Å

$\beta = 98.938$ (1)°

$V = 927.24$ (11) Å³

$Z = 4$

$F_{000} = 488$

$D_x = 1.730$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 1655 reflections

$\theta = 6.0$ – 26.1 °

$\mu = 2.62$ mm⁻¹

$T = 292$ (2) K

Block, pale yellow

$0.47 \times 0.35 \times 0.12$ mm

Data collection

Bruker SMART CCD
diffractometer

1825 independent reflections

Radiation source: fine-focus sealed tube

1646 reflections with $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.020$

$T = 293$ (2) K

$\theta_{\text{max}} = 26.0$ °

ω scans

$\theta_{\text{min}} = 2.8$ °

Absorption correction: multi-scan
(SADABS; Bruker, 2001)

$h = -13 \rightarrow 13$

$T_{\text{min}} = 0.344$, $T_{\text{max}} = 0.728$

$k = -12 \rightarrow 12$

7653 measured reflections

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.023$	H-atom parameters constrained
$wR(F^2) = 0.063$	$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 0.3915P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
1825 reflections	$(\Delta/\sigma)_{\max} = 0.001$
127 parameters	$\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > \sigma(F^2)$ 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.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.35482 (2)	-0.27314 (2)	0.65710 (2)	0.02707 (10)
O2	0.19757 (15)	-0.19050 (17)	0.70465 (16)	0.0377 (4)
O1	0.31062 (14)	-0.18521 (17)	0.93276 (16)	0.0343 (3)
N2	0.60329 (16)	0.04848 (17)	0.74407 (19)	0.0291 (4)
N1	0.48884 (16)	-0.13627 (18)	0.66275 (19)	0.0305 (4)
C1	0.49555 (19)	-0.0187 (2)	0.7378 (2)	0.0306 (5)
H1A	0.4295	0.0145	0.7830	0.037*
C3	0.6497 (2)	-0.2471 (2)	0.5230 (3)	0.0402 (5)
H3A	0.6023	-0.3231	0.4889	0.048*
C7	0.67473 (19)	-0.0327 (2)	0.6622 (2)	0.0285 (4)
C6	0.7953 (2)	-0.0167 (2)	0.6286 (3)	0.0401 (5)
H6A	0.8439	0.0581	0.6642	0.048*
C4	0.7678 (3)	-0.2287 (3)	0.4880 (3)	0.0506 (7)
H4A	0.8006	-0.2930	0.4279	0.061*
C2	0.60357 (19)	-0.1473 (2)	0.6118 (2)	0.0284 (4)
C5	0.8401 (3)	-0.1151 (3)	0.5410 (3)	0.0533 (7)
H5A	0.9202	-0.1062	0.5163	0.064*
C8	0.2094 (2)	-0.1628 (2)	0.8459 (2)	0.0316 (5)

supplementary materials

C9	0.1003 (3)	-0.1018 (3)	0.9057 (3)	0.0608 (8)
H9A	0.0316	-0.0923	0.8233	0.091*
H9B	0.1231	-0.0141	0.9489	0.091*
H9C	0.0760	-0.1598	0.9835	0.091*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02846 (16)	0.02436 (15)	0.02842 (15)	-0.00019 (9)	0.00446 (10)	0.00056 (9)
O2	0.0378 (9)	0.0475 (9)	0.0278 (8)	0.0105 (7)	0.0052 (6)	-0.0014 (7)
O1	0.0332 (8)	0.0444 (9)	0.0260 (7)	0.0030 (7)	0.0062 (6)	0.0027 (6)
N2	0.0327 (9)	0.0243 (9)	0.0302 (9)	-0.0011 (7)	0.0050 (7)	-0.0005 (7)
N1	0.0335 (10)	0.0267 (9)	0.0312 (9)	-0.0039 (7)	0.0049 (7)	-0.0004 (7)
C1	0.0327 (11)	0.0271 (11)	0.0332 (11)	0.0002 (9)	0.0092 (9)	0.0017 (8)
C3	0.0477 (15)	0.0337 (12)	0.0391 (13)	-0.0036 (10)	0.0069 (11)	-0.0115 (9)
C7	0.0336 (11)	0.0256 (10)	0.0259 (10)	0.0018 (8)	0.0032 (8)	0.0020 (8)
C6	0.0337 (12)	0.0346 (12)	0.0529 (14)	-0.0047 (10)	0.0095 (10)	-0.0047 (10)
C4	0.0529 (16)	0.0459 (15)	0.0563 (16)	0.0036 (12)	0.0191 (13)	-0.0173 (12)
C2	0.0308 (11)	0.0294 (11)	0.0243 (10)	-0.0003 (8)	0.0020 (8)	0.0010 (8)
C5	0.0417 (14)	0.0524 (17)	0.0708 (18)	-0.0015 (12)	0.0243 (13)	-0.0114 (14)
C8	0.0337 (12)	0.0308 (11)	0.0317 (11)	0.0052 (9)	0.0091 (9)	0.0023 (9)
C9	0.0490 (16)	0.089 (2)	0.0461 (15)	0.0285 (15)	0.0146 (13)	-0.0058 (14)

Geometric parameters (\AA , $^\circ$)

Zn1—N1	1.9735 (17)	C3—C2	1.396 (3)
Zn1—N2 ⁱ	1.9802 (17)	C3—H3A	0.9300
Zn1—O2	1.9880 (15)	C7—C6	1.390 (3)
Zn1—O1 ⁱⁱ	2.0046 (14)	C7—C2	1.398 (3)
C8—O2	1.262 (3)	C6—C5	1.373 (3)
C8—O1	1.254 (3)	C6—H6A	0.9300
O1—Zn1 ⁱⁱⁱ	2.0046 (14)	C4—C5	1.402 (4)
N2—C1	1.334 (3)	C4—H4A	0.9300
N2—C7	1.389 (3)	C5—H5A	0.9300
N2—Zn1 ^{iv}	1.9802 (17)	C8—C9	1.492 (3)
N1—C1	1.329 (3)	C9—H9A	0.9600
N1—C2	1.388 (3)	C9—H9B	0.9600
C1—H1A	0.9300	C9—H9C	0.9600
C3—C4	1.372 (4)		
N1—Zn1—N2 ⁱ	118.46 (7)	C6—C7—C2	120.78 (19)
N1—Zn1—O2	111.41 (7)	C5—C6—C7	117.7 (2)
N2 ⁱ —Zn1—O2	114.47 (7)	C5—C6—H6A	121.2
N1—Zn1—O1 ⁱⁱ	103.06 (7)	C7—C6—H6A	121.2
N2 ⁱ —Zn1—O1 ⁱⁱ	104.87 (7)	C3—C4—C5	121.3 (2)
O2—Zn1—O1 ⁱⁱ	102.19 (6)	C3—C4—H4A	119.3
C8—O2—Zn1	109.73 (13)	C5—C4—H4A	119.3
C8—O1—Zn1 ⁱⁱⁱ	133.67 (14)	N1—C2—C3	130.7 (2)

C1—N2—C7	104.28 (17)	N1—C2—C7	108.05 (18)
C1—N2—Zn1 ^{iv}	126.61 (14)	C3—C2—C7	121.2 (2)
C7—N2—Zn1 ^{iv}	129.08 (14)	C6—C5—C4	121.5 (2)
C1—N1—C2	104.28 (17)	C6—C5—H5A	119.2
C1—N1—Zn1	126.11 (15)	C4—C5—H5A	119.2
C2—N1—Zn1	128.97 (14)	O1—C8—O2	120.65 (19)
N1—C1—N2	115.59 (18)	O1—C8—C9	121.22 (19)
N1—C1—H1A	122.2	O2—C8—C9	118.1 (2)
N2—C1—H1A	122.2	C8—C9—H9A	109.5
C4—C3—C2	117.4 (2)	C8—C9—H9B	109.5
C4—C3—H3A	121.3	H9A—C9—H9B	109.5
C2—C3—H3A	121.3	C8—C9—H9C	109.5
N2—C7—C6	131.4 (2)	H9A—C9—H9C	109.5
N2—C7—C2	107.79 (18)	H9B—C9—H9C	109.5

Symmetry codes: (i) $-x+1, y-1/2, -z+3/2$; (ii) $x, -y-1/2, z-1/2$; (iii) $x, -y-1/2, z+1/2$; (iv) $-x+1, y+1/2, -z+3/2$.

Fig. 1

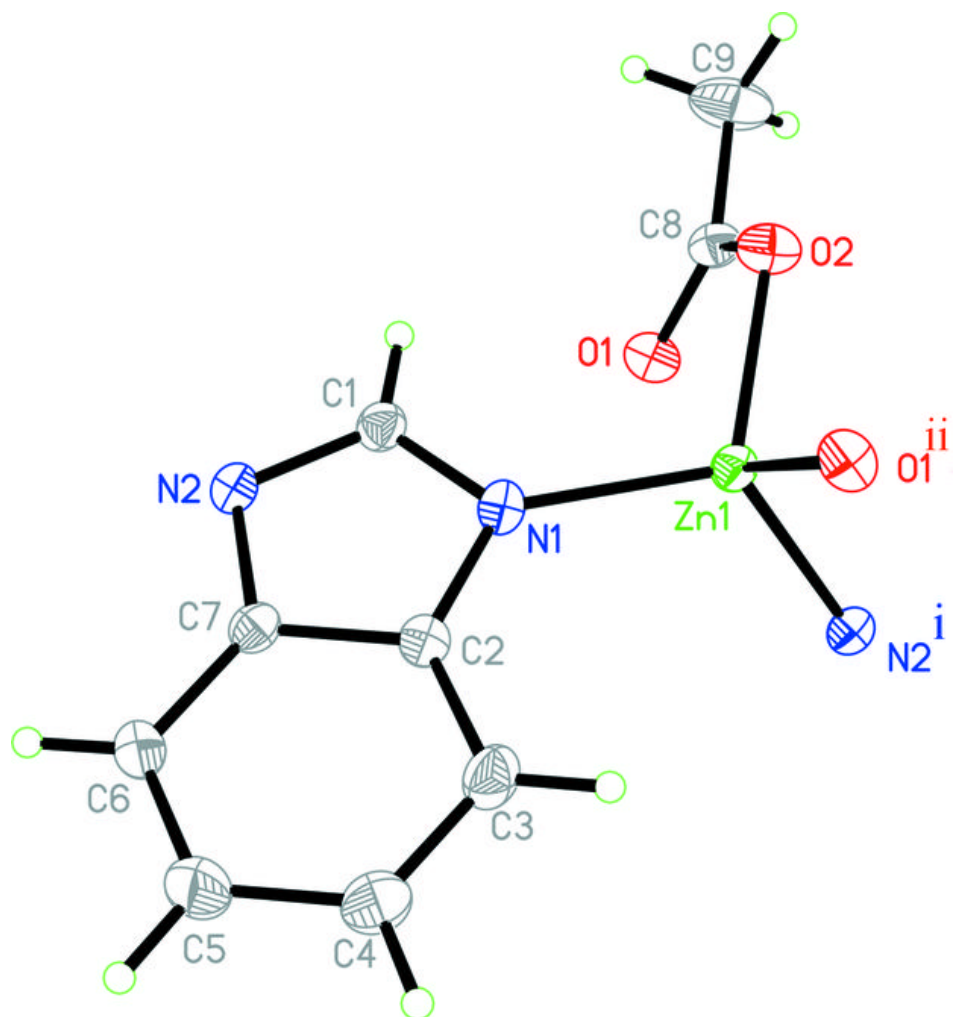


Fig. 2

