

Poly[[(μ -1*H*-benzimidazole-5,6-dicarboxylato)zinc(II)] monohydrate]

Zhao-yang Li, Jing-wei Dai and Shan-tang Yue*

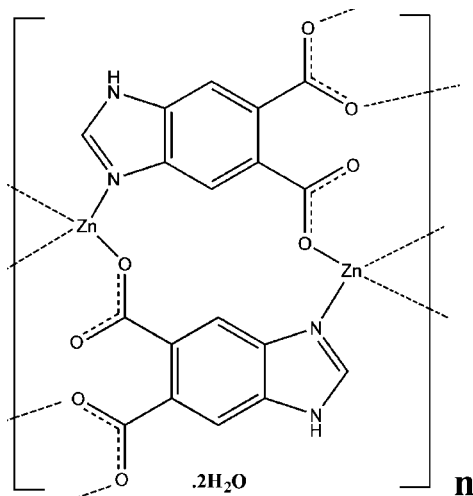
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Received 17 May 2009; accepted 10 June 2009

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.026; wR factor = 0.072; data-to-parameter ratio = 10.8.

The three-dimensional polymeric title compound, $\{[\text{Zn}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)]\cdot\text{H}_2\text{O}\}_n$, contains one crystallographically independent Zn^{II} atom, one fully deprotonated 1*H*-benzimidazole-5,6-dicarboxylate (bdc) ligand and one uncoordinated water molecule. The Zn^{II} atom is four-coordinated by three O atoms and one N atom from the bdc ligands, giving a distorted tetrahedral coordination geometry. The uncoordinated water molecule is bound to the main structure through a strong bdc-water $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond, and two much weaker water-bdc $\text{O}-\text{H}\cdots\text{O}$ interactions.

Related literature

 For structures of other bdc complexes, see: Gao *et al.* (2008); Lo *et al.* (2007); Wei *et al.* (2008); Yao *et al.* (2008).


Experimental

Crystal data

 $[\text{Zn}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)]\cdot\text{H}_2\text{O}$
 $M_r = 287.55$
 Monoclinic, $P2_1/c$
 $a = 6.4735$ (5) Å
 $b = 8.1836$ (6) Å
 $c = 18.4407$ (12) Å
 $\beta = 104.397$ (2)°

 $V = 946.25$ (12) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.61$ mm⁻¹
 $T = 298$ K
 $0.35 \times 0.26 \times 0.18$ mm

Data collection

 Bruker APEXII area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2004)
 $T_{\text{min}} = 0.444$, $T_{\text{max}} = 0.625$

 4613 measured reflections
 1665 independent reflections
 1513 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.072$
 $S = 1.06$
 1665 reflections

 154 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.54$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2}\cdots\text{O1W}$	0.86	2.02	2.809 (3)	152
$\text{O1W}-\text{H1W}\cdots\text{O1}^{\text{i}}$	0.93	2.45	3.211 (5)	139
$\text{O1W}-\text{H2W}\cdots\text{O4}^{\text{ii}}$	0.91	2.29	3.095 (3)	146

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: XP in SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXL97.

This work was supported financially by the Nature and Science Foundation of Guangdong Province (grant No. 7005808), Guangdong Provincial Science and Technology Bureau (grant 2008B010600009) and the NSFC (grant No. U0734005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2261).

References

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 Sheldrick, G. M. (2004). SADABS. University of Göttingen, Germany.
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 Yao, Y.-L., Che, Y.-X. & Zheng, J.-M. (2008). *Cryst. Growth Des.* 8, 2299–2306.

supplementary materials

Acta Cryst. (2009). E65, m775 [doi:10.1107/S1600536809022107]

Poly[[$(\mu$ -1*H*-benzimidazole-5,6-dicarboxylato)zinc(II)] monohydrate]

Z. Li, J. Dai and S. Yue

Comment

N-Heterocyclic carboxylic acids have attracted attention not only because their versatile coordination modes but also owing to their forming high-dimensional polymers through H-bonding interactions. 1*H*-benzimidazole-5,6-dicarboxylic acid (bdc), having six coordination points, is a good candidate for the generation of three-dimensional coordination polymers. However, up to now the complexes based on the bdc ligand are rare (Lo *et al.*, 2007; Gao *et al.*, 2008; Wei *et al.*, 2008; Yao *et al.*, 2008). Here we report the first three-dimensional Zn coordination polymer connected by bdc ligands, $[\text{Zn}(\text{C}_9\text{H}_4\text{N}_2\text{O}_2)]\cdot\text{H}_2\text{O}$.

As is shown in Figure 1, the asymmetric unit consists of one Zn^{2+} cation, a fully deprotonated bdc^{2-} ligand, and a free water molecule. The cation has a tetrahedral coordination environment, and is surrounded by three oxygen and one nitrogen atoms from the bdc ligands. A packing diagram showing the 3D structure coming out from the tetradentate character of the bdc ligand is shown in Figure 2. To the best of our knowledge, the title compound is the first 3D transition metal coordination polymer based on the 1*H*-benzimidazole-5,6-dicarboxylic acid ligand.

Experimental

A mixture of bdc (0.0415 g, 0.20 mmol), $\text{Zn}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ (0.0594 g, 0.20 mmol) and water (10 ml) was heated up to 430 K for 72 h in a 23 ml Teflon-lined stainless-steel autoclave and then cooled down to room temperature in a 278 K/hour rate. Colourless prismatic crystals were collected and dried in air.

Refinement

H atoms attached to carbon and nitrogen were placed at calculated positions and treated as riding on their parent atoms with $\text{C}-\text{H} = 0.93\text{\AA}$, $\text{C}-\text{N} = 0.86\text{\AA}$. Those attached to oxygen were found from the Fourier maps, and allowed to ride without further refinement. In all cases $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C}, \text{O})$.

Figures

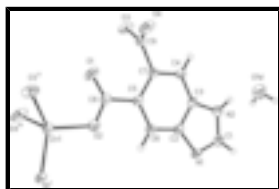


Fig. 1. Displacement ellipsoid plot (50% probability level) of the title compound, with atom numbering. Symmetry codes: (i) $-x, -y+2, -z+2$; (ii) $-x, y+1/2, -z+3/2$; (iii) $x-1, y, z$.

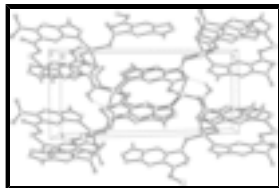


Fig. 2. The packing diagram of the title compound, with H atoms omitted for clarity. Hydrogen bonds are shown as dashed lines.

Poly[[$(\mu$ -1*H*-benzimidazole-5,6-dicarboxylato)zinc(II)] monohydrate]

Crystal data

[Zn(C₉H₄N₂O₄)]·H₂O

$M_r = 287.55$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 6.4735$ (5) Å

$b = 8.1836$ (6) Å

$c = 18.4407$ (12) Å

$\beta = 104.397$ (2)°

$V = 946.25$ (12) Å³

$Z = 4$

$F_{000} = 576$

$D_x = 2.018$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2639 reflections

$\theta = 2.3$ – 27.6 °

$\mu = 2.61$ mm⁻¹

$T = 298$ K

Block, colorless

$0.35 \times 0.26 \times 0.18$ mm

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ K

φ and ω scans

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

$T_{\min} = 0.444$, $T_{\max} = 0.625$

4613 measured reflections

1665 independent reflections

1513 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 25.0$ °

$\theta_{\min} = 2.3$ °

$h = -7 \rightarrow 7$

$k = -9 \rightarrow 8$

$l = -21 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

$wR(F^2) = 0.072$

$S = 1.06$

1665 reflections

154 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.8076P]$$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.54$ e Å⁻³

$\Delta\rho_{\min} = -0.32$ e Å⁻³

Primary atom site location: structure-invariant direct methods 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6805 (4)	0.7618 (3)	1.14674 (15)	0.0244 (6)
H1	0.7562	0.7565	1.1967	0.029*
C2	0.4362 (4)	0.8133 (3)	1.04587 (14)	0.0210 (6)
C3	0.5993 (4)	0.7274 (3)	1.02485 (14)	0.0209 (6)
C4	0.5896 (4)	0.6922 (3)	0.95017 (14)	0.0232 (6)
H4	0.6986	0.6358	0.9364	0.028*
C5	0.2433 (4)	0.8286 (3)	0.91858 (14)	0.0210 (6)
C6	0.2567 (4)	0.8630 (3)	0.99290 (14)	0.0225 (6)
H6	0.1474	0.9184	1.0070	0.027*
C7	0.4108 (4)	0.7447 (3)	0.89738 (14)	0.0198 (5)
C8	0.0478 (4)	0.8790 (3)	0.85989 (15)	0.0244 (6)
C9	0.4056 (4)	0.7163 (3)	0.81632 (14)	0.0200 (6)
N1	0.4937 (3)	0.8337 (3)	1.12397 (12)	0.0223 (5)
N2	0.7500 (3)	0.6973 (3)	1.09061 (12)	0.0255 (5)
H2	0.8682	0.6459	1.0948	0.031*
O1	0.0221 (4)	0.8307 (4)	0.79625 (13)	0.0700 (10)
O2	-0.0815 (3)	0.9719 (3)	0.88154 (11)	0.0371 (5)
O3	0.3461 (3)	0.5800 (3)	0.78853 (10)	0.0317 (5)
O4	0.4720 (4)	0.8254 (3)	0.78041 (11)	0.0360 (5)
Zn1	-0.35253 (5)	1.02462 (4)	0.814219 (16)	0.02108 (13)
O1W	1.1216 (4)	0.5187 (3)	1.15400 (15)	0.0533 (7)
H1W	1.0604	0.4556	1.1853	0.080*
H2W	1.1968	0.6024	1.1810	0.080*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0238 (14)	0.0330 (16)	0.0141 (13)	0.0009 (12)	0.0004 (11)	0.0029 (11)
C2	0.0226 (13)	0.0263 (14)	0.0138 (13)	0.0008 (11)	0.0037 (11)	-0.0001 (10)
C3	0.0189 (13)	0.0270 (15)	0.0153 (13)	0.0023 (11)	0.0013 (11)	0.0010 (11)
C4	0.0215 (13)	0.0306 (15)	0.0177 (14)	0.0056 (11)	0.0053 (11)	-0.0025 (11)

supplementary materials

C5	0.0212 (13)	0.0264 (15)	0.0146 (13)	0.0006 (11)	0.0029 (11)	-0.0019 (10)
C6	0.0206 (13)	0.0310 (15)	0.0159 (13)	0.0052 (11)	0.0046 (11)	-0.0016 (11)
C7	0.0222 (13)	0.0220 (14)	0.0151 (13)	-0.0006 (11)	0.0043 (10)	-0.0015 (10)
C8	0.0230 (14)	0.0329 (16)	0.0160 (14)	0.0016 (12)	0.0025 (11)	-0.0013 (11)
C9	0.0174 (12)	0.0266 (15)	0.0152 (12)	0.0018 (10)	0.0025 (10)	-0.0009 (11)
N1	0.0239 (12)	0.0313 (13)	0.0107 (11)	0.0047 (10)	0.0026 (9)	0.0001 (9)
N2	0.0208 (12)	0.0352 (14)	0.0189 (12)	0.0083 (10)	0.0017 (9)	0.0002 (10)
O1	0.0496 (15)	0.125 (3)	0.0230 (13)	0.0460 (16)	-0.0143 (11)	-0.0294 (14)
O2	0.0285 (11)	0.0578 (15)	0.0209 (11)	0.0200 (10)	-0.0012 (9)	-0.0072 (9)
O3	0.0511 (13)	0.0269 (11)	0.0190 (10)	-0.0077 (10)	0.0125 (9)	-0.0057 (8)
O4	0.0532 (14)	0.0376 (13)	0.0185 (10)	-0.0200 (10)	0.0117 (10)	-0.0050 (9)
Zn1	0.0221 (2)	0.0270 (2)	0.01325 (19)	0.00140 (12)	0.00268 (13)	-0.00017 (12)
O1W	0.0410 (14)	0.0652 (18)	0.0468 (16)	0.0148 (12)	-0.0022 (12)	-0.0085 (12)

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

C1—N1	1.316 (3)	C6—H6	0.9300
C1—N2	1.336 (3)	C7—C9	1.505 (4)
C1—H1	0.9300	C8—O1	1.210 (3)
C2—C6	1.380 (4)	C8—O2	1.266 (3)
C2—C3	1.401 (4)	C9—O3	1.247 (3)
C2—N1	1.405 (3)	C9—O4	1.250 (3)
C3—N2	1.376 (3)	N2—H2	0.8600
C3—C4	1.393 (4)	Zn1—O2	1.929 (2)
C4—C7	1.383 (4)	Zn1—N1 ⁱ	1.999 (2)
C4—H4	0.9300	Zn1—O3 ⁱⁱ	1.9587 (19)
C5—C6	1.381 (4)	Zn1—O4 ⁱⁱⁱ	1.996 (2)
C5—C7	1.418 (4)	O1W—H1W	0.9333
C5—C8	1.504 (4)	O1W—H2W	0.9127
N1—C1—N2	112.9 (2)	O1—C8—C5	119.8 (3)
N1—C1—H1	123.6	O2—C8—C5	116.2 (2)
N2—C1—H1	123.6	O3—C9—O4	122.2 (2)
C6—C2—C3	120.8 (2)	O3—C9—C7	118.3 (2)
C6—C2—N1	130.8 (2)	O4—C9—C7	119.3 (2)
C3—C2—N1	108.5 (2)	C1—N1—C2	105.2 (2)
N2—C3—C4	133.0 (2)	C1—N1—Zn1 ⁱ	126.26 (18)
N2—C3—C2	105.3 (2)	C2—N1—Zn1 ⁱ	127.64 (17)
C4—C3—C2	121.7 (2)	C1—N2—C3	108.1 (2)
C7—C4—C3	117.1 (2)	C1—N2—H2	125.9
C7—C4—H4	121.4	C3—N2—H2	125.9
C3—C4—H4	121.4	C8—O2—Zn1	119.85 (18)
C6—C5—C7	120.6 (2)	C9—O3—Zn1 ^{iv}	121.73 (18)
C6—C5—C8	119.5 (2)	C9—O4—Zn1 ^v	131.46 (18)
C7—C5—C8	119.9 (2)	O2—Zn1—O3 ⁱⁱ	116.08 (9)
C2—C6—C5	118.5 (2)	O2—Zn1—O4 ⁱⁱⁱ	111.99 (10)
C2—C6—H6	120.8	O3 ⁱⁱ —Zn1—O4 ⁱⁱⁱ	91.96 (9)
C5—C6—H6	120.8	O2—Zn1—N1 ⁱ	103.56 (9)

C4—C7—C5	121.3 (2)	O3 ⁱⁱ —Zn1—N1 ⁱ	122.67 (9)
C4—C7—C9	117.4 (2)	O4 ⁱⁱⁱ —Zn1—N1 ⁱ	110.27 (9)
C5—C7—C9	121.3 (2)	H1W—O1W—H2W	109.2
O1—C8—O2	124.0 (3)		
C6—C2—C3—N2	-179.7 (3)	C5—C7—C9—O3	-99.2 (3)
N1—C2—C3—N2	0.4 (3)	C4—C7—C9—O4	-92.4 (3)
C6—C2—C3—C4	1.5 (4)	C5—C7—C9—O4	84.8 (3)
N1—C2—C3—C4	-178.4 (3)	N2—C1—N1—C2	0.3 (3)
N2—C3—C4—C7	-178.8 (3)	N2—C1—N1—Zn1 ⁱ	-169.63 (19)
C2—C3—C4—C7	-0.5 (4)	C6—C2—N1—C1	179.7 (3)
C3—C2—C6—C5	-1.1 (4)	C3—C2—N1—C1	-0.4 (3)
N1—C2—C6—C5	178.8 (3)	C6—C2—N1—Zn1 ⁱ	-10.6 (4)
C7—C5—C6—C2	-0.2 (4)	C3—C2—N1—Zn1 ⁱ	169.32 (18)
C8—C5—C6—C2	179.0 (3)	N1—C1—N2—C3	0.0 (3)
C3—C4—C7—C5	-0.9 (4)	C4—C3—N2—C1	178.4 (3)
C3—C4—C7—C9	176.3 (2)	C2—C3—N2—C1	-0.2 (3)
C6—C5—C7—C4	1.3 (4)	O1—C8—O2—Zn1	7.0 (5)
C8—C5—C7—C4	-178.0 (3)	C5—C8—O2—Zn1	-173.02 (19)
C6—C5—C7—C9	-175.8 (3)	O4—C9—O3—Zn1 ^{iv}	0.2 (4)
C8—C5—C7—C9	4.9 (4)	C7—C9—O3—Zn1 ^{iv}	-175.59 (17)
C6—C5—C8—O1	-170.2 (3)	O3—C9—O4—Zn1 ^v	-160.8 (2)
C7—C5—C8—O1	9.1 (5)	C7—C9—O4—Zn1 ^v	14.9 (4)
C6—C5—C8—O2	9.8 (4)	C8—O2—Zn1—O3 ⁱⁱ	-44.1 (3)
C7—C5—C8—O2	-170.9 (3)	C8—O2—Zn1—O4 ⁱⁱⁱ	59.7 (2)
C4—C7—C9—O3	83.6 (3)	C8—O2—Zn1—N1 ⁱ	178.5 (2)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2 \cdots O1W	0.86	2.02	2.809 (3)	152
O1W—H1W \cdots O1 ^{vi}	0.93	2.45	3.211 (5)	139
O1W—H2W \cdots O4 ^{vii}	0.91	2.29	3.095 (3)	146

Symmetry codes: (vi) $-x+1, -y+1, -z+2$; (vii) $x+1, -y+3/2, z+1/2$.

Fig. 1

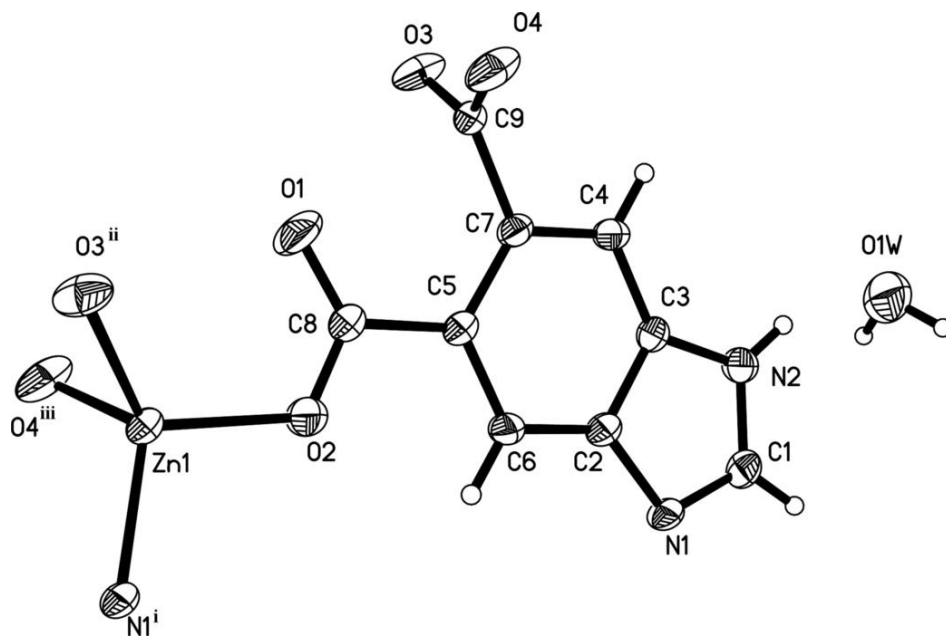


Fig. 2

