Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[diaquazinc(II)]-μ-*trans*-4,4′-diazenediyldibenzoato-$\kappa^4O,O':O'',O'''$]

Bo Liu and Qiang Xu*

National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, Japan, and Graduate School of Science and Technology, Kobe University, Nada Ku, Kobe, Hyogo 657-8501, Japan
Correspondence e-mail: q.xu@aist.go.jp

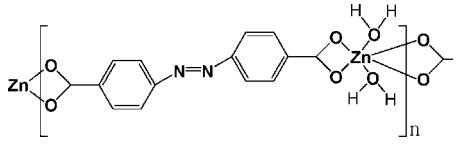
Received 27 February 2009; accepted 3 April 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.044; wR factor = 0.109; data-to-parameter ratio = 13.9.

The title compound, $[Zn(C_{14}H_8N_2O_4)(H_2O)_2]_n$, consists of zigzag chains of Zn atoms bridged by azobenzene-4,4′-dicarboxylate ligands. The Zn^{II} atom, lying on a twofold rotation axis, is coordinated by four O atoms from the carboxylate groups and two water molecules, giving rise to a considerably distorted octahedral coordination envionment. The ligand lies on an inversion center. In the crystal structure, π–π interactions between the ligands [interplanar distance = 3.527 (3) Å] assemble the chains into a sheet-like structure. O—H···O hydrogen bonds between the coordinated water molecules and carboxylate O atoms connect the sheets into a three-dimensional network.

Related literature

For related structures, see: Chen *et al.* (2008); Bai *et al.* (2008); Mukherjee *et al.* (2004); Reineke *et al.* (2000).



Experimental

Crystal data

$[Zn(C_{14}H_8N_2O_4)(H_2O)_2]$
M_r = 369.63
Monoclinic, $C2/c$
a = 22.392 (5) Å
b = 4.9308 (10) Å
c = 12.185 (2) Å
β = 90.30 (3)°
V = 1345.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.86 mm^{-1}
T = 293 K
0.14 × 0.09 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.781, T_{max} = 0.865
6205 measured reflections
1532 independent reflections
1194 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.04
1532 reflections
110 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O3	1.985 (3)	Zn1—O1	1.995 (2)
Zn1—O2	2.572 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O1^{i}	0.82	1.92	2.735 (4)	171
O3—H3B···O2^{ii}	0.81 (6)	1.91 (6)	2.712 (4)	173 (6)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank AIST and Kobe University for financial support. BL thanks MEXT for a Japanese Government Scholarship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2186).

References

Bai, J.-W., Wang, J., Hou, Y., Zhao, B.-Z. & Fu, Q. (2008). *Acta Cryst.* E**64**, m3–m4.
Chen, Z.-F., Zhang, Z.-L., Tan, Y.-H., Tang, Y.-Z., Fun, H.-K., Zhou, Z.-Y., Abrahams, B. F. & Liang, H. (2008). *CrystEngComm*, **10**, 217–231.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Mukherjee, P. S., Das, N., Kryschenko, Y. K., Arif, A. M. & Stang, P. L. (2004). *J. Am. Chem. Soc.* **126**, 2464–2473.
Reineke, T. M., Eddaoudi, M., Moler, D., O'Keeffe, M. & Yaghi, O. M. (2000). *J. Am. Chem. Soc.* **122**, 4843–4844.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

Acta Cryst. (2009). E**65**, m509 [doi:10.1107/S1600536809012604]

catena-Poly[[diaquazinc(II)]-*μ*-*trans*-4,4′-diazenediyldibenzoato-$\kappa^4O,O':O'',O'''$]

Bo Liu and Qiang Xu

S1. Comment

Metal-organic frameworks, in which metal ions are bridged by organic ligands, have a rapid development in the past decade due to the various topologies and wide applications. Azodibenzoate-based ligands are a kind of typical aromatic carboxylate ligand employed in the generation of coordination networks, including azobenzene-4,4′-dicarboxylate and azobenzene-3,3′-dicarboxylate and so on. A series of coordination polymers have been reported by employing these ligands as linkers (Chen *et al.*, 2008; Bai *et al.*, 2008; Mukherjee *et al.*, 2004; Reineke *et al.*, 2000). The title compound (Fig. 1 and Table 1) is an analogue to the reported compound $[Cd(C_{14}H_8N_2O_4)(H_2O)_2]_n$ (Chen *et al.*, 2008). The space group of the reported Cd complex is $P2_1/m$, while that of the title compound is determined to be $C2/c$. The seperation between the bridged Zn atoms is 17.211 (1) Å and the angle for the three neighboring Zn atoms is 95.84 (8)°. In comparison, the $O_{aq}\cdots O_{carboxylate}$ distances for hydrogen bonds are 2.712 (4) and 2.735 (4) Å in the title compound (Table 2), while they are greater than 3.19 Å in the Cd complex. Face-to-face π–π interaction between the ligands exists in the title compound [interplane distance = 3.527 (3) Å], which assembles the Zn–ligand chains into a sheet. O—H···O hydrogen bonds between the coordinated water molecules and carboxylate O atoms connect the sheets into a three-dimensional network (Fig. 2).

S2. Experimental

The single crystals of the title compound were obtained by solvothermal reaction of $Zn(NO_3)_2.6H_2O$ (0.013 g) and azobenzene-4,4′-dicarboxylic acid (0.007 g) in a mixed solvent of DMSO and H_2O (20 ml, volume ratio 1:1) at 393 K for 72 h.

S3. Refinement

Aromatic H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). H atoms of water molecule were located on a difference Fourier map. One (H3A) of the two water H atoms was fixed with O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O). The other H atom (H3B) was refined isotropically, with a distance restraint O—H = 0.82 (1) Å. In the final difference map, the highest peak and deepest hole were found to be 0.81 and 0.60 Å from N1 atom, respectively.

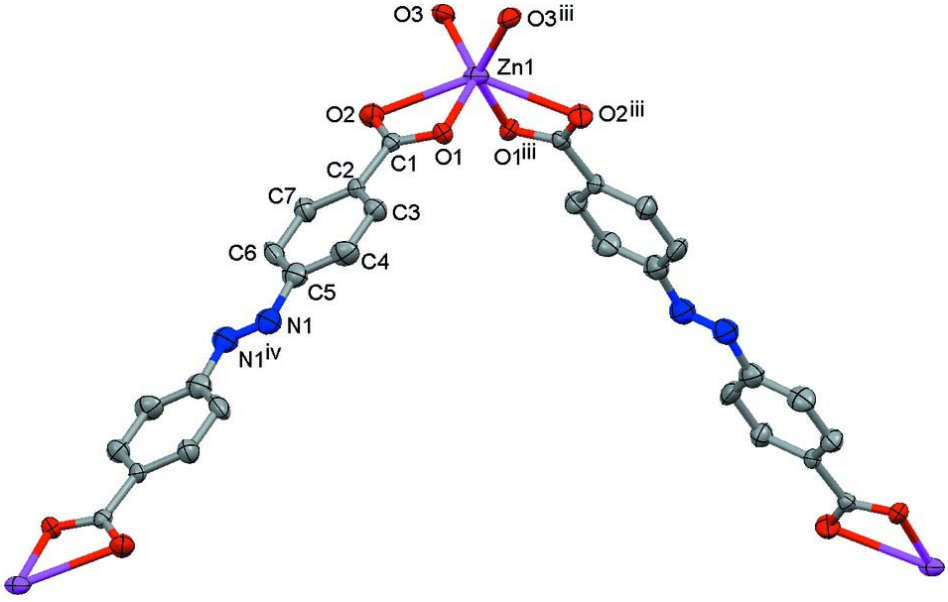


Figure 1

Part of the chain in the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (iii) -*x*, *y*, 3/2 - *z*; (iv) 1/2 - *x*, 5/2 - *y*, 1 - *z*.]

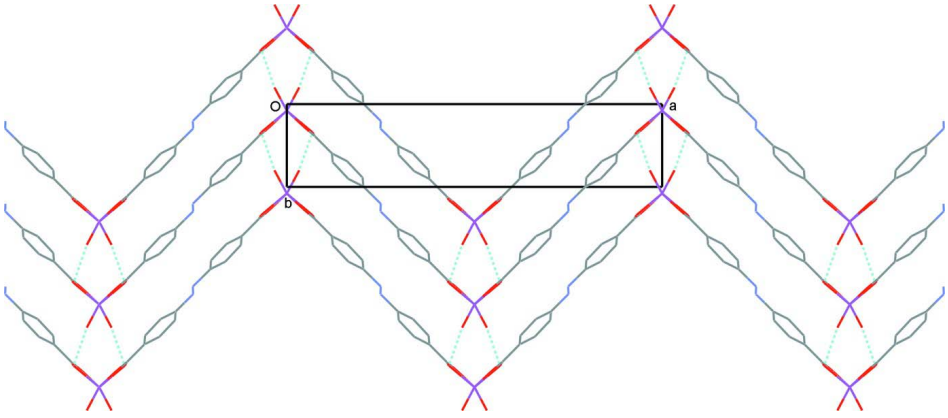


Figure 2

The crystal packing diagram showing hydrogen bonds (dashed lines).

***catena*-Poly[[diaquazinc(II)]-*μ*-*trans*-4,4′- diazenediyldibenzoato-$\kappa^4O,O':O'',O'''$]**

Crystal data

$[Zn(C_{14}H_8N_2O_4)(H_2O)_2]$
M_r = 369.63
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 22.392 (5) Å
b = 4.9308 (10) Å
c = 12.185 (2) Å
β = 90.30 (3)°
V = 1345.3 (5) Å^3
Z = 4
F(000) = 752
D_x = 1.825 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1194 reflections
θ = 3.3–27.5°
μ = 1.86 mm^{-1}
T = 293 K
Needle, orange
0.14 × 0.09 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotating anode
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.781, T_{max} = 0.865
6205 measured reflections
1532 independent reflections
1194 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −28→28
k = −6→6
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.04
1532 reflections
110 parameters
8 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 7.8756P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.0000	0.08046 (11)	0.7500	0.0287 (2)
O1	0.06809 (11)	0.3407 (5)	0.7428 (2)	0.0270 (6)
O2	0.04382 (12)	0.2669 (5)	0.5705 (2)	0.0343 (6)
C1	0.07463 (15)	0.3874 (7)	0.6402 (3)	0.0233 (7)
O3	−0.03292 (14)	−0.2000 (5)	0.6496 (2)	0.0364 (7)
H3A	−0.0458	−0.3274	0.6857	0.055*
C2	0.12028 (14)	0.5963 (7)	0.6090 (3)	0.0229 (7)
C6	0.16404 (19)	0.9039 (8)	0.4779 (4)	0.0401 (10)
H6	0.1651	0.9768	0.4075	0.048*
C5	0.20375 (18)	0.9943 (8)	0.5579 (4)	0.0399 (7)
C7	0.12236 (18)	0.7023 (8)	0.5038 (3)	0.0332 (8)
H7	0.0960	0.6394	0.4503	0.040*
C3	0.16064 (17)	0.6897 (8)	0.6873 (3)	0.0323 (8)
H3	0.1599	0.6179	0.7578	0.039*
C4	0.20196 (18)	0.8879 (8)	0.6617 (4)	0.0399 (10)
H4	0.2286	0.9492	0.7150	0.048*
H3B	−0.037 (2)	−0.207 (12)	0.584 (5)	0.068 (18)*
N1	0.25044 (16)	1.2046 (7)	0.5460 (3)	0.0415 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0257 (3)	0.0176 (3)	0.0429 (4)	0.000	0.0010 (2)	0.000
O1	0.0319 (14)	0.0247 (12)	0.0244 (13)	−0.0017 (10)	0.0061 (10)	0.0034 (10)
O2	0.0348 (15)	0.0331 (14)	0.0351 (15)	−0.0108 (12)	0.0020 (12)	−0.0059 (12)

C1	0.0230 (16)	0.0196 (16)	0.0274 (18)	0.0033 (13)	0.0045 (13)	−0.0015 (14)
O3	0.059 (2)	0.0231 (13)	0.0273 (16)	−0.0099 (13)	0.0025 (14)	0.0009 (11)
C2	0.0223 (16)	0.0206 (15)	0.0258 (17)	−0.0011 (13)	0.0080 (13)	−0.0001 (14)
C6	0.045 (2)	0.035 (2)	0.041 (2)	0.0047 (19)	0.0167 (19)	0.0171 (19)
C5	0.0342 (15)	0.0342 (15)	0.0513 (18)	0.0033 (13)	0.0110 (14)	0.0006 (14)
C7	0.038 (2)	0.034 (2)	0.028 (2)	−0.0023 (17)	0.0022 (16)	0.0028 (16)
C3	0.0288 (19)	0.0323 (19)	0.036 (2)	−0.0057 (15)	0.0039 (16)	−0.0006 (17)
C4	0.0274 (19)	0.037 (2)	0.056 (3)	−0.0095 (17)	0.0043 (18)	−0.0082 (19)
N1	0.0368 (15)	0.0375 (15)	0.0505 (17)	0.0050 (13)	0.0094 (14)	0.0012 (13)

Geometric parameters (Å, º)

Zn1—O3	1.985 (3)	C2—C3	1.389 (5)
Zn1—O3^{i}	1.985 (3)	C6—C5	1.389 (6)
Zn1—O2	2.572 (2)	C6—C7	1.401 (5)
Zn1—O1	1.995 (2)	C6—H6	0.9300
Zn1—O1^{i}	1.995 (2)	C5—C4	1.371 (6)
O1—C1	1.280 (4)	C5—N1	1.480 (5)
O2—C1	1.243 (4)	C7—H7	0.9300
C1—C2	1.501 (5)	C3—C4	1.383 (5)
O3—H3A	0.8200	C3—H3	0.9300
O3—H3B	0.81 (6)	C4—H4	0.9300
C2—C7	1.385 (5)	N1—N1^{ii}	1.207 (7)
O3—Zn1—O3^{i}	91.71 (17)	C5—C6—C7	119.6 (4)
O3—Zn1—O1	134.60 (11)	C5—C6—H6	120.2
O3^{i}—Zn1—O1	101.17 (12)	C7—C6—H6	120.2
O3—Zn1—O1^{i}	101.17 (12)	C4—C5—C6	120.2 (4)
O3^{i}—Zn1—O1^{i}	134.60 (11)	C4—C5—N1	112.5 (4)
O1—Zn1—O1^{i}	99.95 (15)	C6—C5—N1	127.3 (4)
C1—O1—Zn1	104.5 (2)	C2—C7—C6	120.2 (4)
C1—O2—Zn1	78.6 (2)	C2—C7—H7	119.9
O2—C1—O1	121.0 (3)	C6—C7—H7	119.9
O2—C1—C2	122.1 (3)	C4—C3—C2	120.9 (4)
O1—C1—C2	116.9 (3)	C4—C3—H3	119.6
Zn1—O3—H3A	109.5	C2—C3—H3	119.6
Zn1—O3—H3B	133 (4)	C5—C4—C3	120.1 (4)
H3A—O3—H3B	117.4	C5—C4—H4	120.0
C7—C2—C3	119.0 (3)	C3—C4—H4	120.0
C7—C2—C1	121.3 (3)	N1^{ii}—N1—C5	110.0 (5)
C3—C2—C1	119.7 (3)		
O3—Zn1—O1—C1	28.2 (3)	C3—C2—C7—C6	−1.1 (6)
O3^{i}—Zn1—O1—C1	131.9 (2)	C1—C2—C7—C6	177.8 (3)
O1^{i}—Zn1—O1—C1	−88.5 (2)	C5—C6—C7—C2	0.8 (6)
Zn1—O1—C1—O2	−3.7 (4)	C7—C2—C3—C4	0.8 (6)
Zn1—O1—C1—C2	175.3 (2)	C1—C2—C3—C4	−178.0 (3)
O2—C1—C2—C7	12.6 (5)	C6—C5—C4—C3	0.1 (6)

O1—C1—C2—C7	−166.5 (3)	N1—C5—C4—C3	179.6 (4)
O2—C1—C2—C3	−168.6 (3)	C2—C3—C4—C5	−0.4 (6)
O1—C1—C2—C3	12.3 (5)	C4—C5—N1—N1^{ii}	−178.8 (4)
C7—C6—C5—C4	−0.3 (6)	C6—C5—N1—N1^{ii}	0.7 (7)
C7—C6—C5—N1	−179.8 (4)		

Symmetry codes: (i) −*x*, *y*, −*z*+3/2; (ii) −*x*+1/2, −*y*+5/2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O1^{iii}	0.82	1.92	2.735 (4)	171
O3—H3*B*···O2^{iv}	0.81 (6)	1.91 (6)	2.712 (4)	173 (6)

Symmetry codes: (iii) −*x*, *y*−1, −*z*+3/2; (iv) −*x*, −*y*, −*z*+1.