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Crystal structure of *catena*-poly[[[tetraaquazinc(II)]-μ-1,4-bis[4-(1*H*-imidazol-1-yl)benzoyl]piperazine] dinitrate monohydrate]

Chen Hou, Hong-Mei Gan and Jia-Cheng Liu*

College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou 730070, People's Republic of China. *Correspondence e-mail: jcliuchem@163.com

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Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

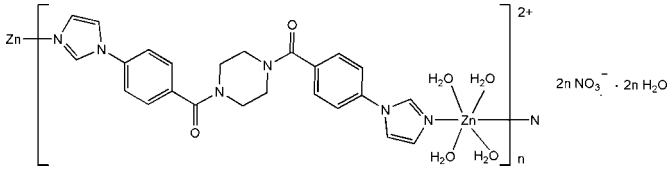
In the title polymeric complex, $\{[Zn(C_{24}H_{22}N_6O_2)(H_2O)_4](NO_3)_2\cdot 2H_2O\}_n$, the Zn^{II} cation, located about a twofold rotation axis, is coordinated by two imidazole groups and four water molecules in a distorted N_2O_4 octahedral geometry; among the four coordinate water molecules, two are located on the same twofold rotation axis. The 1,4-bis[4-(1*H*-imidazol-1-yl)benzoyl]piperazine] ligand is centro-symmetric, with the centroid of the piperazine ring located on an inversion center, and bridges the Zn^{II} cations, forming polymeric chains propagating along [201]. In the crystal, O—H···O and weak C—H···O hydrogen bonds link the polymeric chains, nitrate anions and solvent water molecules into a three-dimensional supramolecular architecture. A short O···O contact of 2.823 (13) Å is observed between neighboring nitrate anions.

Keywords: crystal structure; zinc complex; one-dimensional coordination polymer; piperazine.

CCDC reference: 1060401

1. Related literature

For related coordination polymers and their potential applications, see: Xu *et al.* (2004); Gandolfo & LaDuca (2011*a*,*b*); Wang *et al.* (2011, 2014).



2. Experimental

2.1. Crystal data

$[Zn(C_{24}H_{22}N_6O_2)(H_2O)_4](NO_3)_2\cdot 2H_2O$
M_r = 723.96
Monoclinic, $C2/c$
a = 22.051 (4) Å
b = 7.8861 (16) Å
c = 17.837 (4) Å
β = 102.65 (3)°
V = 3026.5 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 294 K
0.27 × 0.25 × 0.22 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.79, T_{max} = 0.83
5133 measured reflections
2720 independent reflections
2212 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.144
S = 1.05
2720 reflections
196 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O4^{i}	0.84	1.96	2.795 (6)	174
O2—H2A···O5^{ii}	0.84	2.16	2.956 (15)	159
O2—H2A···O6^{ii}	0.84	2.32	3.060 (10)	148
O2—H2B···O8	0.85	1.83	2.676 (7)	176
O3—H3A···O4^{iii}	0.84	1.99	2.804 (6)	163
O8—H8A···O7	0.85	2.14	2.914 (11)	151
O8—H8B···O7^{iv}	0.82	2.14	2.926 (11)	160
C1—H1···O6^{ii}	0.93	2.51	3.232 (11)	135
C5—H5···O6^{ii}	0.93	2.59	3.485 (12)	162

Symmetry codes: (i) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+2$; (ii) $x, y+1, z$; (iii) $-x+\frac{3}{2}, -y+\frac{5}{2}, -z+2$; (iv) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

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

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5847).

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supporting information

Acta Cryst. (2015). E**71**, m120–m121 [https://doi.org/10.1107/S2056989015007719]

Crystal structure of *catena*-poly[[[tetraaquazinc(II)]-μ-1,4-bis[4-(1*H*-imidazol-1-yl)benzoyl]piperazine] dinitrate monohydrate]

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S1. Structural commentary

Piperazine derivatives as N-containing ligands which have different combination of span, multi-coordination point and hydrogen-bonding points of contact, to conform coordination complexes has attracted great attention. (Wang *et al.*, 2011, 2014; Gandolfo & LaDuca *et al.*, 2011a,b; Xu *et al.*, 2004). Nevertheless, piperazine derivatives-containing the imidazole group as the coordinated point have been designed forming coordination compounds relatively few. As the imidazole has a similar properties with pyridine, so in this context, we design and successfully synthesized the compound $\{[Zn(C_{24}H_{22}N_6O_2)(H_2O)_4](NO_3)_2(H_2O)_2\}_n$ based on the piperazine-1,4-diylbis((4-(1H-imidazol-1-yl)phenyl)methanone) ligand, obtained under hydrothermal technique. An asymmetric unit of the title compound includes a half Zn^{II}, a half piperazine-1,4-diylbis((4-(1H-imidazol-1-yl)phenyl)methanone) ligands, two coordinated water molecules, an uncoordinated nitrate anion and one uncoordinated water molecule (Fig. 1). The Zn^{II} atom is coordinated and lies on an inversion centre of a slighter distorted octahedral, with two ligands [two imidazole N atoms, Zn—N = 2.122 (3) Å] and four coordinated water molecules [Zn—O bond lengths in the range of 2.112 (4) – 2.138 (3) Å]. Between the 1D chains formed by the ligand and Zn^{II} atoms are interconnected via water O—H···O hydrogen bonds to form a three dimension supramolecular architecture. In the crystal, in the nitrate anions and the uncoordinated water molecules forming the O—H···N hydrogen bonds to stabilize the three dimension skeleton (Fig. 2).

S2. Synthesis and crystallization

A mixture of L (0.1 mmol, 0.0462 g), $Zn(NO_3)_2.6H_2O$ (0.2 mmol, 0.059 g), distilled water (6.0 mL) sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 130 °C for 72 h under auto-pressure, after cooling to room temperature. Primrose yellow prismatic single crystals were removed (yield: 24%).

S3. Refinement details

Water H atoms were located in a difference Fourier map and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(O)$. Other H atoms were placed in calculated positions with C—H = 0.93–0.96 Å and refined using a riding model, $U_{iso}(H) = 1.2U_{eq}(C)$.

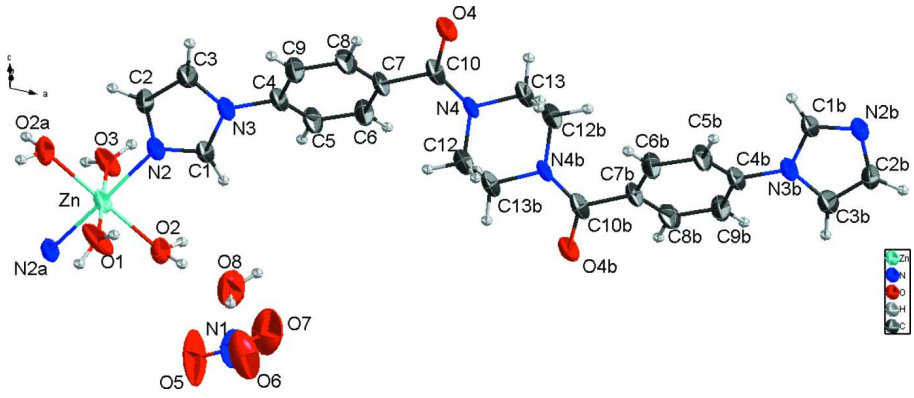

Figure 1

A part of the polymeric chain of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

catena-Poly[[[tetraaquazinc(II)]-μ-1,4-bis[4-(1*H*-imidazol-1-yl)benzoyl]piperazine] dinitrate monohydrate]

Crystal data

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V = 3026.5 (11) Å^3
Z = 4
F(000) = 1504
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Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 7728 reflections
θ = 2.7–28.6°
μ = 0.90 mm^{-1}
T = 294 K
Block, colorless
0.27 × 0.25 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.79, T_{max} = 0.83
5133 measured reflections
2720 independent reflections
2212 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.2°, θ_{min} = 3.3°
h = −26→26
k = −9→6
l = −21→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.144
S = 1.05
2720 reflections
196 parameters
6 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 8.9494P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.96013 (12)	0.7500	0.0363 (3)
N1	0.6774 (3)	0.2834 (11)	0.7201 (4)	0.078 (2)
N2	0.56556 (19)	0.9716 (6)	0.8564 (2)	0.0366 (10)
N3	0.6522 (2)	0.9960 (6)	0.9451 (3)	0.0380 (11)
O1	0.5000	0.6945 (7)	0.7500	0.0656 (19)
H1A	0.5215	0.6270	0.7813	0.079*
O2	0.57119 (17)	0.9622 (6)	0.6871 (2)	0.0541 (11)
H2A	0.5960	1.0433	0.6903	0.065*
H2B	0.5993	0.8872	0.6922	0.065*
O3	0.5000	1.2290 (7)	0.7500	0.0530 (15)
H3A	0.5283	1.2929	0.7738	0.064*
O4	0.92408 (18)	1.0374 (6)	1.1542 (2)	0.0508 (11)
O5	0.6282 (4)	0.3010 (19)	0.6852 (6)	0.224 (7)
O6	0.6930 (4)	0.1535 (12)	0.7462 (6)	0.164 (4)
O7	0.7160 (4)	0.3959 (12)	0.7332 (7)	0.167 (4)
O8	0.6636 (2)	0.7354 (8)	0.7064 (4)	0.104 (2)
H8A	0.6651	0.6280	0.7091	0.125*
H8B	0.6952	0.7741	0.7339	0.125*
C1	0.6268 (2)	0.9722 (8)	0.8698 (3)	0.0410 (13)
H1	0.6496	0.9579	0.8321	0.049*
C2	0.5516 (3)	0.9983 (8)	0.9263 (3)	0.0466 (15)
H2	0.5115	1.0051	0.9347	0.056*
C3	0.6038 (3)	1.0134 (9)	0.9812 (3)	0.0499 (16)
H3	0.6065	1.0320	1.0333	0.060*
C4	0.7176 (2)	1.0017 (7)	0.9795 (3)	0.0380 (13)
C5	0.7578 (2)	1.0726 (8)	0.9392 (3)	0.0426 (14)
H5	0.7429	1.1197	0.8909	0.051*
C6	0.8208 (2)	1.0726 (8)	0.9719 (3)	0.0440 (14)
H6	0.8484	1.1186	0.9447	0.053*
C7	0.8435 (2)	1.0051 (7)	1.0444 (3)	0.0381 (13)
C8	0.8017 (3)	0.9408 (8)	1.0846 (3)	0.0445 (14)
H8	0.8161	0.9001	1.1343	0.053*
C9	0.7385 (3)	0.9360 (8)	1.0522 (3)	0.0447 (14)
H9	0.7108	0.8893	1.0789	0.054*
C10	0.9109 (3)	1.0080 (7)	1.0844 (3)	0.042

N4	0.95517 (18)	0.9803 (6)	1.0449 (2)	0.036
C12	0.9476 (3)	0.8984 (9)	0.9696 (3)	0.050
H12A	0.9037	0.8881	0.9463	0.060*
H12B	0.9651	0.7851	0.9762	0.060*
C13	1.0212 (3)	1.0026 (9)	1.0821 (4)	0.0522 (16)
H13A	1.0410	0.8927	1.0926	0.063*
H13B	1.0248	1.0620	1.1305	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0232 (5)	0.0463 (6)	0.0345 (5)	0.000	−0.0042 (3)	0.000
N1	0.057 (4)	0.099 (6)	0.076 (4)	0.007 (4)	0.010 (4)	0.036 (4)
N2	0.024 (2)	0.047 (3)	0.034 (2)	0.0000 (19)	−0.0029 (18)	−0.001 (2)
N3	0.023 (2)	0.054 (3)	0.033 (2)	−0.0007 (19)	−0.0043 (18)	−0.001 (2)
O1	0.069 (4)	0.042 (3)	0.063 (4)	0.000	−0.035 (3)	0.000
O2	0.027 (2)	0.086 (3)	0.047 (2)	0.004 (2)	0.0023 (18)	−0.005 (2)
O3	0.047 (3)	0.044 (3)	0.054 (4)	0.000	−0.019 (3)	0.000
O4	0.033 (2)	0.076 (3)	0.037 (2)	−0.001 (2)	−0.0075 (17)	−0.008 (2)
O5	0.069 (5)	0.422 (19)	0.157 (8)	0.008 (7)	−0.027 (5)	0.171 (10)
O6	0.126 (7)	0.130 (7)	0.210 (10)	−0.035 (6)	−0.019 (6)	0.073 (7)
O7	0.127 (7)	0.104 (6)	0.276 (13)	−0.019 (6)	0.054 (8)	0.027 (7)
O8	0.055 (3)	0.113 (5)	0.137 (6)	0.025 (3)	0.004 (3)	−0.029 (4)
C1	0.025 (3)	0.063 (4)	0.031 (3)	0.003 (3)	−0.002 (2)	−0.006 (3)
C2	0.024 (3)	0.073 (4)	0.041 (3)	0.000 (3)	0.003 (2)	−0.004 (3)
C3	0.034 (3)	0.080 (5)	0.034 (3)	−0.005 (3)	0.004 (2)	−0.004 (3)
C4	0.025 (3)	0.050 (3)	0.033 (3)	−0.001 (2)	−0.006 (2)	−0.001 (2)
C5	0.031 (3)	0.057 (4)	0.033 (3)	−0.002 (3)	−0.005 (2)	0.009 (3)
C6	0.029 (3)	0.061 (4)	0.040 (3)	−0.006 (3)	0.002 (2)	0.007 (3)
C7	0.024 (3)	0.050 (3)	0.035 (3)	−0.001 (2)	−0.007 (2)	−0.003 (2)
C8	0.037 (3)	0.059 (4)	0.031 (3)	0.000 (3)	−0.007 (2)	0.005 (3)
C9	0.029 (3)	0.065 (4)	0.037 (3)	−0.005 (3)	0.002 (2)	0.006 (3)
C10	0.029	0.049	0.040	−0.001	−0.010	0.002
N4	0.018	0.055	0.029	−0.006	−0.006	−0.009
C12	0.030	0.063	0.050	−0.006	−0.004	−0.014
C13	0.027 (3)	0.079 (5)	0.043 (3)	−0.005 (3)	−0.009 (2)	−0.011 (3)

Geometric parameters (Å, º)

Zn1—O1	2.095 (6)	C2—H2	0.9300
Zn1—O2^{i}	2.120 (4)	C3—H3	0.9300
Zn1—O2	2.120 (4)	C4—C5	1.375 (8)
Zn1—O3	2.120 (6)	C4—C9	1.379 (8)
Zn1—N2	2.121 (4)	C5—C6	1.384 (7)
Zn1—N2^{i}	2.121 (4)	C5—H5	0.9300
N1—O5	1.136 (9)	C6—C7	1.387 (8)
N1—O6	1.146 (10)	C6—H6	0.9300
N1—O7	1.216 (10)	C7—C8	1.383 (8)

N2—C1	1.318 (7)	C7—C10	1.501 (7)
N2—C2	1.364 (7)	C8—C9	1.386 (8)
N3—C1	1.351 (7)	C8—H8	0.9300
N3—C3	1.369 (7)	C9—H9	0.9300
N3—C4	1.439 (6)	C10—N4	1.342 (7)
O1—H1A	0.8391	N4—C12	1.466 (7)
O2—H2A	0.8351	N4—C13	1.471 (6)
O2—H2B	0.8465	C12—C13^{ii}	1.489 (9)
O3—H3A	0.8409	C12—H12A	0.9700
O4—C10	1.235 (7)	C12—H12B	0.9700
O8—H8A	0.8490	C13—C12^{ii}	1.489 (9)
O8—H8B	0.8196	C13—H13A	0.9700
C1—H1	0.9300	C13—H13B	0.9700
C2—C3	1.344 (8)		

O1—Zn1—O2^{i}	90.45 (13)	N3—C3—H3	126.8
O1—Zn1—O2	90.45 (13)	C5—C4—C9	121.5 (5)
O2^{i}—Zn1—O2	179.1 (3)	C5—C4—N3	119.4 (5)
O1—Zn1—O3	180.000 (3)	C9—C4—N3	119.1 (5)
O2^{i}—Zn1—O3	89.55 (13)	C4—C5—C6	118.8 (5)
O2—Zn1—O3	89.55 (13)	C4—C5—H5	120.6
O1—Zn1—N2	92.45 (13)	C6—C5—H5	120.6
O2^{i}—Zn1—N2	87.99 (16)	C5—C6—C7	121.1 (5)
O2—Zn1—N2	91.97 (16)	C5—C6—H6	119.4
O3—Zn1—N2	87.55 (13)	C7—C6—H6	119.4
O1—Zn1—N2^{i}	92.45 (13)	C8—C7—C6	118.6 (5)
O2^{i}—Zn1—N2^{i}	91.97 (16)	C8—C7—C10	117.5 (5)
O2—Zn1—N2^{i}	87.99 (16)	C6—C7—C10	123.8 (5)
O3—Zn1—N2^{i}	87.55 (13)	C7—C8—C9	121.1 (5)
N2—Zn1—N2^{i}	175.1 (3)	C7—C8—H8	119.5
O5—N1—O6	119.8 (11)	C9—C8—H8	119.5
O5—N1—O7	124.1 (11)	C4—C9—C8	118.7 (5)
O6—N1—O7	116.1 (9)	C4—C9—H9	120.6
C1—N2—C2	105.2 (4)	C8—C9—H9	120.6
C1—N2—Zn1	129.2 (4)	O4—C10—N4	121.4 (5)
C2—N2—Zn1	125.3 (4)	O4—C10—C7	118.2 (5)
C1—N3—C3	106.5 (4)	N4—C10—C7	120.4 (5)
C1—N3—C4	125.9 (5)	C10—N4—C12	127.1 (4)
C3—N3—C4	127.5 (5)	C10—N4—C13	120.4 (4)
Zn1—O1—H1A	129.4	C12—N4—C13	111.6 (4)
Zn1—O2—H2A	121.3	N4—C12—C13^{ii}	111.2 (5)
Zn1—O2—H2B	123.2	N4—C12—H12A	109.4
H2A—O2—H2B	94.3	C13^{ii}—C12—H12A	109.4
Zn1—O3—H3A	126.8	N4—C12—H12B	109.4
H8A—O8—H8B	108.6	C13^{ii}—C12—H12B	109.4
N2—C1—N3	111.5 (5)	H12A—C12—H12B	108.0
N2—C1—H1	124.3	N4—C13—C12^{ii}	109.3 (5)
N3—C1—H1	124.3	N4—C13—H13A	109.8

C3—C2—N2	110.5 (5)	C12^{ii}—C13—H13A	109.8
C3—C2—H2	124.8	N4—C13—H13B	109.8
N2—C2—H2	124.8	C12^{ii}—C13—H13B	109.8
C2—C3—N3	106.3 (5)	H13A—C13—H13B	108.3
C2—C3—H3	126.8		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O4^{iii}	0.84	1.96	2.795 (6)	174
O2—H2*A*···O5^{iv}	0.84	2.16	2.956 (15)	159
O2—H2*A*···O6^{iv}	0.84	2.32	3.060 (10)	148
O2—H2*B*···O8	0.85	1.83	2.676 (7)	176
O3—H3*A*···O4^{v}	0.84	1.99	2.804 (6)	163
O8—H8*A*···O7	0.85	2.14	2.914 (11)	151
O8—H8*B*···O7^{vi}	0.82	2.14	2.926 (11)	160
C1—H1···O6^{iv}	0.93	2.51	3.232 (11)	135
C5—H5···O6^{iv}	0.93	2.59	3.485 (12)	162

Symmetry codes: (iii) −*x*+3/2, −*y*+3/2, −*z*+2; (iv) *x*, *y*+1, *z*; (v) −*x*+3/2, −*y*+5/2, −*z*+2; (vi) −*x*+3/2, *y*+1/2, −*z*+3/2.