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catena-Poly[[aqua(pyrazine-2-carboxylato-κ^2N^1,O)zinc(II)]-μ-pyrazine-2-carboxylato-$\kappa^2N^1,O:N^4$]

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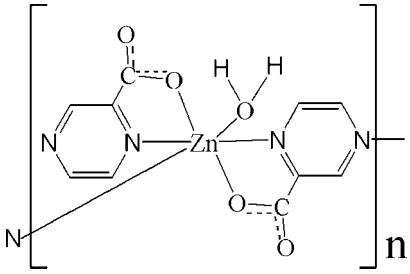
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.034; wR factor = 0.096; data-to-parameter ratio = 12.5.

The title compound, $[Zn(C_5H_3N_2O_2)_2(H_2O)]_n$, prepared by hydrothermal synthesis, is isostructural with its Fe^{II}, Co^{II}, Ni^{II} and Cu^{II} analogues. The asymmetric unit contains two bidentate pyrazine-2-carboxylate anions bonded to Zn^{II} in the equatorial plane through one N and one O atom each. The Zn^{II} atoms are linked into a chain by the second N atom of the anion bonding to an axial site of a neighbouring Zn^{II} atom. The slightly distorted octahedral coordination around Zn^{II} is completed by a water molecule, which forms hydrogen bonds to link the chains into a three-dimensional structure. The crystal studied was an inversion twin.

Related literature

For the isostructural Fe^{II}, Co^{II}, Ni^{II} and Cu^{II} analogues, see: Hao & Liu (2007); Hao *et al.* (2007); Gao *et al.* (2007*a*,*b*).



Experimental

Crystal data

$[Zn(C_5H_3N_2O_2)_2(H_2O)]$
M_r = 329.57
Orthorhombic, $P2_12_12_1$
a = 7.8932 (6) Å
b = 9.7615 (10) Å
c = 14.8921 (15) Å
V = 1147.43 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.17 mm^{-1}
T = 298 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.812, T_{max} = 0.812
6232 measured reflections
2353 independent reflections
2200 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.00
2353 reflections
188 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), with 974 Friedel pairs
Flack parameter: 0.469 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O3^{i}	0.82 (4)	2.08 (4)	2.781 (4)	144 (7)
O5—H2W···O1^{ii}	0.82 (4)	1.89 (2)	2.695 (4)	166 (8)

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

Data collection: *APEX2* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2188).

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supplementary materials

Acta Cryst. (2007). E**63**, m2143 [**doi:10.1107/S1600536807033041**]

catena-Poly[[aqua(pyrazine-2-carboxylato-κ^2N^1,O)zinc(II)]-μ-pyrazine-2-carboxylato-$\kappa^2N^1,O:N^4$]

Y.-X. Gao, L.-B. Wang, Y.-L. Niu and L.-J. Hao

Comment

The title compound, (I), $[Zn(C_5H_3N_2O_2)_2(H_2O)]_n$, is isostructural with its Fe^{II}, Co^{II}, Ni^{II}, and Cu^{II} analogues (Hao & Liu, 2007; Hao *et al.*, 2007; Gao *et al.*, 2007*a*,b). The Zn^{II} atoms is coordinated in a bidentate fashion by two O and two N atoms from two independent pyrazine-2-carboxylate anions. The distorted octhedral coordiantion is completed by another N atom from a third pyrazine-2-carboxylate ligand, and by the O atom of a water molecule (Fig. 1). The Zn—N and Zn—O bond lengths are in the range of 2.058 (3)–2.105 (3) and 2.042 (3)–2.073 (3) Å, respectively. One pyrazine-2-carboxylate ligand coordinates to a neighboring Zn^{II} atom *via* its second N atom, leading to polymeric structure with zigzag chains extending parallel to the *b* axis (Fig. 2). Hydrogen bonds between the water molecule and the carboxylate groups stabilize the structure. The refined Flack parameter of 0.469 (18) indicates inversion twinning.

Experimental

All chemicals used were purchased from Jinan Henghua Sci & Tec Co. Ltd. A mixture of Zinc(II) acetate dihydrate (0.5 mmol), potassium hydroxide (0.5 mmol), 2-pyrazine caboxylic acid (0.5 mmol), EtOH (8 ml) and H_2O (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was kept at 413 K for 2 d, and then cooled to room temperature. Colorless crystals of (I) were obtained in a yield of 36%. Anal. Calc. for $C_{10}H_8ZnN_4O_5$: C 36.62, H 2.44, N 17.09%; Found: C 36.59, H 2.47, N 17.01%.

Refinement

C-bound H atoms were generated geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of the water molecule were located in a difference density map and were refined with distance restraints of O—H = 0.82 (1) and H—H = 1.38 (2) Å.

Figures

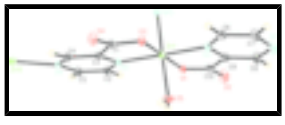

Fig. 1. A fragment of the structure of the title compound, showing 30% probability displacement ellipsoids. Atoms labeled with I at the symmetry positions (−*x* + 1, *y* − 1/2, −*z* + 3/2).

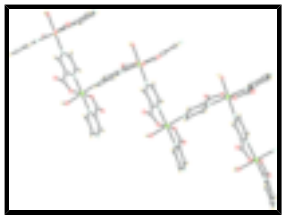

Fig. 2. A part of polymeric structure of the title compound.

catena-Poly[aquabis(pyrazine-2-carboxylato-κ^2N^1,O)zinc(II)]- μ-pyrazine-2-carboxylato-$\kappa^3N^1,O:N^4$]

Crystal data

$[Zn(C_5H_3N_2O_2)_2(H_2O)]$	F_{000} = 664
M_r = 329.57	D_x = 1.908 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2347 reflections
a = 7.8932 (6) Å	θ = 2.5–26.7º
b = 9.7615 (10) Å	μ = 2.17 mm^{-1}
c = 14.8921 (15) Å	T = 298 (2) K
V = 1147.43 (19) Å^3	Cube, colorless
Z = 4	0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEX II CCD area-detector diffractometer	2353 independent reflections
Radiation source: fine-focus sealed tube	2200 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 298(2) K	θ_{max} = 26.5º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	h = −8→9
T_{min} = 0.812, T_{max} = 0.812	k = −12→11
6232 measured reflections	l = −18→9

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.072P)^2 + 0.4177P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.096	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.98 e Å^{-3}
2353 reflections	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
188 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), 974 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.469 (18)
Secondary atom site location: difference Fourier map	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.92678 (6)	0.86587 (4)	0.90927 (3)	0.02030 (14)
C1	0.6936 (5)	0.6911 (4)	0.8171 (2)	0.0175 (7)
C2	1.1621 (5)	0.6694 (4)	0.7997 (3)	0.0207 (8)
H2	1.2562	0.7111	0.8254	0.025*
C3	0.8722 (4)	0.6460 (4)	0.7893 (2)	0.0155 (7)
C4	1.1047 (5)	1.0415 (4)	0.7732 (2)	0.0182 (8)
H4	1.1989	0.9959	0.7960	0.022*
C5	0.8158 (5)	1.0668 (4)	0.7636 (3)	0.0230 (8)
H5	0.7069	1.0406	0.7801	0.028*
C6	0.6757 (5)	1.0566 (4)	1.0101 (3)	0.0241 (8)
H6	0.5873	1.0211	0.9760	0.029*
C7	0.6414 (5)	1.1488 (4)	1.0786 (3)	0.0278 (8)
H7	0.5299	1.1738	1.0901	0.033*
C8	0.9257 (6)	1.1651 (4)	1.1088 (3)	0.0307 (9)
H8	1.0146	1.2021	1.1418	0.037*
C9	0.9613 (5)	1.0733 (4)	1.0410 (3)	0.0218 (8)
C10	1.1434 (5)	1.0288 (4)	1.0192 (3)	0.0214 (8)
H1W	1.011 (4)	0.703 (6)	1.031 (5)	0.080*
H2W	0.839 (5)	0.680 (5)	1.015 (5)	0.080*
N1	0.7664 (5)	1.2023 (4)	1.1284 (3)	0.0361 (9)
N2	0.8349 (4)	1.0186 (3)	0.9928 (2)	0.0183 (6)
N3	1.0061 (4)	0.7089 (3)	0.8242 (2)	0.0171 (6)
N4	0.9497 (4)	1.0051 (3)	0.80119 (19)	0.0189 (6)
O1	1.1531 (3)	0.9352 (3)	0.95911 (17)	0.0196 (5)
O2	1.2633 (4)	1.0798 (4)	1.0587 (2)	0.0402 (8)
O3	0.6936 (3)	0.7969 (3)	0.86870 (17)	0.0191 (5)
O4	0.5686 (3)	0.6308 (3)	0.79110 (18)	0.0275 (6)
O5	0.9181 (4)	0.7349 (3)	1.01674 (18)	0.0253 (6)

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Zn1	0.0199 (2)	0.0205 (2)	0.0205 (2)	0.00011 (17)	0.00053 (17)	−0.00065 (17)
C1	0.0161 (17)	0.0199 (17)	0.0166 (17)	0.0015 (14)	0.0025 (14)	0.0033 (14)
C2	0.0168 (18)	0.022 (2)	0.0236 (18)	0.0008 (15)	−0.0016 (15)	−0.0049 (15)
C3	0.0178 (17)	0.0162 (16)	0.0124 (14)	0.0000 (13)	0.0005 (12)	0.0004 (14)
C4	0.0180 (19)	0.0184 (17)	0.0182 (16)	−0.0013 (14)	−0.0005 (14)	0.0040 (14)
C5	0.0190 (19)	0.0247 (19)	0.025 (2)	−0.0006 (16)	−0.0003 (15)	0.0044 (16)
C6	0.0194 (19)	0.0221 (19)	0.031 (2)	−0.0023 (15)	−0.0030 (16)	−0.0006 (16)
C7	0.0216 (18)	0.028 (2)	0.034 (2)	0.0025 (16)	0.0026 (17)	−0.0086 (19)
C8	0.027 (2)	0.032 (2)	0.033 (2)	−0.002 (2)	−0.0027 (19)	−0.0137 (16)
C9	0.021 (2)	0.0233 (19)	0.0217 (18)	−0.0011 (15)	−0.0001 (14)	0.0029 (15)
C10	0.0188 (19)	0.0220 (19)	0.0233 (18)	0.0022 (15)	0.0001 (15)	0.0042 (15)
N1	0.032 (2)	0.037 (2)	0.039 (2)	0.0051 (17)	0.0042 (17)	−0.0166 (17)
N2	0.0179 (15)	0.0165 (15)	0.0205 (15)	0.0002 (12)	0.0003 (13)	−0.0005 (12)
N3	0.0175 (14)	0.0179 (15)	0.0160 (15)	−0.0017 (12)	0.0005 (12)	0.0019 (12)
N4	0.0208 (16)	0.0175 (14)	0.0182 (14)	0.0007 (13)	−0.0019 (13)	0.0012 (12)
O1	0.0165 (12)	0.0192 (13)	0.0230 (13)	0.0023 (10)	−0.0012 (11)	−0.0033 (11)
O2	0.0228 (15)	0.047 (2)	0.051 (2)	−0.0052 (14)	−0.0092 (14)	−0.0173 (16)
O3	0.0145 (12)	0.0234 (14)	0.0195 (13)	0.0001 (11)	0.0021 (10)	−0.0048 (11)
O4	0.0161 (12)	0.0330 (14)	0.0333 (14)	−0.0063 (15)	0.0019 (12)	−0.0075 (12)
O5	0.0220 (13)	0.0283 (14)	0.0255 (13)	−0.0088 (13)	−0.0038 (13)	0.0119 (11)

Geometric parameters (Å, °)

Zn1—O5	2.049 (2)	C5—N4	1.339 (5)
Zn1—O1	2.050 (3)	C5—C2^{ii}	1.386 (5)
Zn1—O3	2.051 (3)	C5—H5	0.9300
Zn1—N2	2.073 (3)	C6—N2	1.335 (5)
Zn1—N3	2.085 (3)	C6—C7	1.386 (6)
Zn1—N4	2.114 (3)	C6—H6	0.9300
C1—O4	1.213 (5)	C7—N1	1.340 (6)
C1—O3	1.287 (5)	C7—H7	0.9300
C1—C3	1.534 (5)	C8—N1	1.341 (6)
C2—N3	1.341 (5)	C8—C9	1.379 (6)
C2—C5^{i}	1.386 (5)	C8—H8	0.9300
C2—H2	0.9300	C9—N2	1.339 (5)
C3—N3	1.328 (5)	C9—C10	1.537 (5)
C3—C4^{i}	1.392 (5)	C10—O2	1.220 (5)
C4—N4	1.341 (5)	C10—O1	1.281 (5)
C4—C3^{ii}	1.392 (5)	O5—H1W	0.82 (4)
C4—H4	0.9300	O5—H2W	0.82 (4)
O5—Zn1—O1	87.28 (11)	N2—C6—C7	120.4 (4)
O5—Zn1—O3	89.72 (11)	N2—C6—H6	119.8
O1—Zn1—O3	175.86 (11)	C7—C6—H6	119.8
O5—Zn1—N2	88.17 (12)	N1—C7—C6	121.1 (4)
O1—Zn1—N2	81.37 (12)	N1—C7—H7	119.5
O3—Zn1—N2	95.68 (12)	C6—C7—H7	119.5
O5—Zn1—N3	91.51 (12)	N1—C8—C9	121.8 (4)
O1—Zn1—N3	101.61 (12)	N1—C8—H8	119.1

O3—Zn1—N3	81.32 (11)	C9—C8—H8	119.1
N2—Zn1—N3	176.98 (13)	N2—C9—C8	120.0 (4)
O5—Zn1—N4	176.63 (14)	N2—C9—C10	118.1 (3)
O1—Zn1—N4	89.35 (12)	C8—C9—C10	121.9 (4)
O3—Zn1—N4	93.64 (11)	O2—C10—O1	125.5 (4)
N2—Zn1—N4	91.41 (12)	O2—C10—C9	120.6 (4)
N3—Zn1—N4	89.09 (11)	O1—C10—C9	113.9 (3)
O4—C1—O3	125.4 (3)	C7—N1—C8	117.6 (4)
O4—C1—C3	121.5 (3)	C6—N2—C9	119.1 (3)
O3—C1—C3	113.1 (3)	C6—N2—Zn1	130.2 (3)
N3—C2—C5^{i}	120.5 (4)	C9—N2—Zn1	110.3 (3)
N3—C2—H2	119.7	C3—N3—C2	119.5 (3)
C5^{i}—C2—H2	119.7	C3—N3—Zn1	109.8 (2)
N3—C3—C4^{i}	119.7 (3)	C2—N3—Zn1	130.7 (3)
N3—C3—C1	119.5 (3)	C5—N4—C4	118.1 (3)
C4^{i}—C3—C1	120.7 (3)	C5—N4—Zn1	122.7 (3)
N4—C4—C3^{ii}	121.4 (3)	C4—N4—Zn1	119.0 (2)
N4—C4—H4	119.3	C10—O1—Zn1	115.9 (2)
C3^{ii}—C4—H4	119.3	C1—O3—Zn1	116.0 (2)
N4—C5—C2^{ii}	120.7 (4)	Zn1—O5—H1W	114 (5)
N4—C5—H5	119.7	Zn1—O5—H2W	114 (5)
C2^{ii}—C5—H5	119.7	H1W—O5—H2W	116 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1W···O3^{iii}	0.82 (4)	2.08 (4)	2.781 (4)	144 (7)
O5—H2W···O1^{iv}	0.82 (4)	1.89 (2)	2.695 (4)	166 (8)

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

Fig. 1

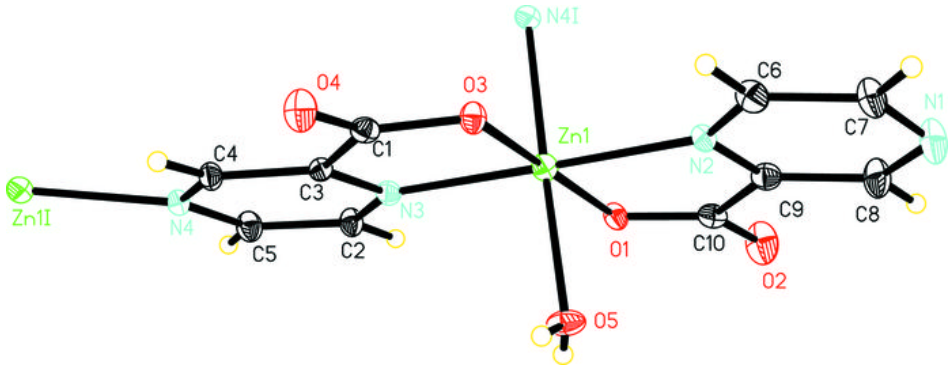

Fig. 2