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catena-Poly[[triazazinc(II)]- μ -1*H*-1,2,4-triazole-3,5-dicarboxylato]

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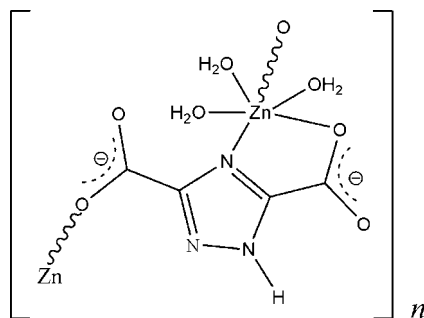
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 12.1.

In the title compound, $[\text{Zn}(\text{C}_4\text{HN}_3\text{O}_4)(\text{H}_2\text{O})_3]_n$, each Zn^{II} atom adopts a distorted octahedral coordination geometry, being surrounded by one chelating and one monodentate 1*H*-1,2,4-triazole-3,5-dicarboxylate ligand and three water molecules. Adjacent Zn^{II} cations are linked by a 1*H*-1,2,4-triazole-3,5-dicarboxylate ligand in a μ_2, κ^3 fashion to form a chain running along the c axis. The crystal packing is stabilized by $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

 For related literature, see: Yang *et al.* (2004); Yin *et al.* (2001); Tian *et al.* (2003).


Experimental

Crystal data

 $[\text{Zn}(\text{C}_4\text{HN}_3\text{O}_4)(\text{H}_2\text{O})_3]$
 $M_r = 274.50$

 Monoclinic, $P2_1/c$
 $a = 10.7388$ (11) Å
 $b = 6.6608$ (7) Å
 $c = 13.7789$ (10) Å
 $\beta = 120.384$ (6)°
 $V = 850.22$ (14) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.92$ mm⁻¹
 $T = 293$ (2) K
 $0.13 \times 0.12 \times 0.12$ mm

Data collection

 Bruker APEX CCD diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Sheldrick, 2000)
 $T_{\text{min}} = 0.703$, $T_{\text{max}} = 0.721$

 4297 measured reflections
 1652 independent reflections
 1501 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.090$
 $S = 1.06$
 1652 reflections

 136 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.53$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2A}\cdots\text{O1}^{\text{i}}$	0.81	1.95	2.723 (3)	161
$\text{O1W}-\text{H1WA}\cdots\text{O2}^{\text{ii}}$	0.85	1.85	2.697 (3)	176
$\text{O1W}-\text{H1WB}\cdots\text{O3W}^{\text{iii}}$	0.85	2.16	2.946 (3)	154
$\text{O2W}-\text{H2WA}\cdots\text{N1}^{\text{iv}}$	0.85	2.08	2.925 (4)	172
$\text{O2W}-\text{H2WB}\cdots\text{O3}^{\text{v}}$	0.85	2.01	2.848 (3)	170
$\text{O3W}-\text{H3WA}\cdots\text{O3}$	0.85	1.86	2.708 (3)	174
$\text{O3W}-\text{H3WB}\cdots\text{O4}^{\text{v}}$	0.85	1.91	2.753 (3)	174

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: BT2754).

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supplementary materials

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catena-Poly[[triaquazinc(II)]- μ -1*H*-1,2,4-triazole-3,5-dicarboxylato]

Y.-Y. Sun, Y.-W. Zhang, G. Zhang and L. Cheng

Comment

Synthesis and characterization of coordination polymers is of great interest due to the formation of fascinating structures with interesting applications (Yin *et al.* 2001; Yang *et al.* 2004). Among these coordination polymers, one-dimensional chain complexes as important precursors of molecular magnets have attracted wide interest of experimental and theoretical chemists (Tian *et al.* 2003). Herein, we report a new one-dimensional compound [Zn(Htda)(H₂O)₃]*n* (H₃tda = 1*H*-1,2,4-triazole-3,5-dicarboxylic acid).

The asymmetric unit of the title compound, [Zn(Htda)(H₂O)₃]*n* (H₃tda = 1*H*-1,2,4-triazole-3,5-dicarboxylic acid), contains a Zn^{II} cation, a Htda anion and three coordinated water molecules. In the compound, the Zn^{II} ion displays a slightly distorted octahedral geometry, being surrounded by one chelating and one monodentate Htda ligands, and three H₂O molecules. Meanwhile, the adjacent Zn^{II} cations are linked by a μ^3 -Htda ligand to form a one-dimensional chain. The shortest intrachain Zn \cdots Zn distance is 6.936 (4) Å. The chains are further stabilized by N—H \cdots O and O—H \cdots O hydrogen bonds.

Experimental

A mixture of H₃tda (0.0157 g, 0.1 mmol), Zn(NO₃)₂·6H₂O (0.0297 g, 0.1 mmol), and water (10 ml) was stirred for 1 h at room temperature, and then filtered. The filtrate was allowed to evaporate slowly at room temperature. After 3 weeks, colorless block crystals were obtained in 30% yield (0.0082 g) based on Zn^{II}.

Refinement

H atoms were located in a difference map but refined as riding with N—H = 0.80 Å and O—H = 0.85 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{iso}}(\text{N}, \text{O})$.

Figures

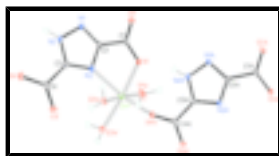


Fig. 1. Local coordination environment of the title compound with 30% thermal ellipsoids. Symmetry code: a: $x, -1/2 - y, -1/2 + z$.

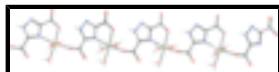


Fig. 2. The one-dimensional chain of the title compound.

catena-Poly[[triaquazinc(II)]- μ -1H-1,2,4-triazole-3,5-dicarboxylato]

Crystal data

[Zn(C₄HN₃O₄)(H₂O)₃]

$M_r = 274.50$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.7388$ (11) Å

$b = 6.6608$ (7) Å

$c = 13.7789$ (10) Å

$\beta = 120.384$ (6)°

$V = 850.22$ (14) Å³

$Z = 4$

$F_{000} = 552$

$D_x = 2.144$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 805 reflections

$\theta = 2.5$ – 28.0 °

$\mu = 2.92$ mm⁻¹

$T = 293$ (2) K

Block, colourless

$0.13 \times 0.12 \times 0.12$ mm

Data collection

Bruker APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2000)

$T_{\min} = 0.703$, $T_{\max} = 0.721$

4297 measured reflections

1652 independent reflections

1501 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\text{max}} = 26.0$ °

$\theta_{\text{min}} = 2.2$ °

$h = -12 \rightarrow 13$

$k = -8 \rightarrow 7$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.090$

$S = 1.06$

1652 reflections

136 parameters

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

$$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 1.155P]$$

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

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

$\Delta\rho_{\text{max}} = 0.53$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.31$ e Å⁻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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	-0.21910 (4)	-0.31001 (6)	-0.54678 (3)	0.01968 (16)
C1	-0.5300 (4)	-0.3318 (5)	-0.6300 (2)	0.0150 (6)
C2	-0.4615 (3)	-0.2580 (5)	-0.5104 (2)	0.0138 (6)
C3	-0.2985 (3)	-0.1691 (5)	-0.3493 (3)	0.0158 (6)
C4	-0.1588 (4)	-0.1138 (5)	-0.2453 (3)	0.0188 (7)
N1	-0.5320 (3)	-0.2264 (4)	-0.4566 (2)	0.0164 (6)
N2	-0.4261 (3)	-0.1687 (4)	-0.3544 (2)	0.0166 (6)
H2A	-0.4471	-0.1452	-0.3071	0.020*
N3	-0.3183 (3)	-0.2244 (4)	-0.4487 (2)	0.0155 (5)
O1	-0.4393 (2)	-0.3607 (4)	-0.66272 (18)	0.0200 (5)
O2	-0.6604 (3)	-0.3595 (4)	-0.68401 (19)	0.0258 (6)
O3	-0.0468 (3)	-0.1174 (5)	-0.2503 (2)	0.0327 (6)
O4	-0.1676 (2)	-0.0634 (4)	-0.16134 (18)	0.0227 (5)
O1W	-0.2327 (3)	-0.0209 (4)	-0.60933 (19)	0.0305 (6)
H1WA	-0.2626	0.0338	-0.6731	0.037*
H1WB	-0.1556	0.0484	-0.5776	0.037*
O2W	-0.1842 (2)	-0.6059 (4)	-0.47695 (19)	0.0231 (5)
H2WA	-0.2630	-0.6585	-0.4892	0.028*
H2WB	-0.1227	-0.6151	-0.4072	0.028*
O3W	-0.0099 (2)	-0.2331 (4)	-0.42261 (18)	0.0199 (5)
H3WA	-0.0169	-0.1900	-0.3675	0.024*
H3WB	0.0497	-0.3301	-0.3975	0.024*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0174 (2)	0.0265 (2)	0.0153 (2)	-0.00014 (16)	0.00829 (18)	0.00025 (15)
C1	0.0181 (16)	0.0154 (15)	0.0108 (15)	-0.0001 (12)	0.0069 (13)	0.0002 (12)
C2	0.0149 (16)	0.0154 (14)	0.0108 (14)	0.0004 (12)	0.0062 (13)	0.0004 (12)
C3	0.0148 (16)	0.0180 (15)	0.0142 (15)	-0.0001 (12)	0.0070 (13)	0.0000 (12)
C4	0.0200 (17)	0.0205 (16)	0.0114 (15)	-0.0017 (14)	0.0047 (14)	-0.0023 (12)
N1	0.0147 (14)	0.0214 (14)	0.0127 (13)	-0.0021 (11)	0.0066 (11)	-0.0020 (10)

supplementary materials

N2	0.0192 (14)	0.0234 (14)	0.0097 (13)	0.0000 (11)	0.0090 (12)	-0.0015 (10)
N3	0.0149 (14)	0.0185 (13)	0.0117 (13)	-0.0020 (11)	0.0058 (11)	-0.0016 (10)
O1	0.0192 (12)	0.0314 (13)	0.0105 (11)	-0.0023 (10)	0.0083 (10)	-0.0029 (9)
O2	0.0139 (12)	0.0414 (15)	0.0172 (12)	-0.0040 (11)	0.0042 (10)	-0.0087 (11)
O3	0.0151 (13)	0.0615 (18)	0.0201 (13)	-0.0055 (12)	0.0079 (11)	-0.0142 (12)
O4	0.0230 (13)	0.0337 (13)	0.0122 (11)	-0.0086 (11)	0.0095 (10)	-0.0049 (10)
O1W	0.0323 (15)	0.0272 (13)	0.0200 (12)	-0.0081 (11)	0.0045 (11)	0.0055 (10)
O2W	0.0187 (12)	0.0288 (13)	0.0187 (12)	-0.0025 (10)	0.0072 (10)	0.0037 (10)
O3W	0.0187 (12)	0.0252 (12)	0.0170 (11)	0.0015 (10)	0.0098 (10)	-0.0006 (10)

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

Zn1—O1W	2.085 (2)	C3—C4	1.505 (5)
Zn1—O3W	2.085 (2)	C4—O3	1.241 (4)
Zn1—O4 ⁱ	2.096 (2)	C4—O4	1.252 (4)
Zn1—O1	2.106 (2)	N1—N2	1.342 (4)
Zn1—O2W	2.141 (2)	N2—H2A	0.8053
Zn1—N3	2.177 (3)	O4—Zn1 ⁱⁱ	2.096 (2)
C1—O2	1.223 (4)	O1W—H1WA	0.8499
C1—O1	1.278 (4)	O1W—H1WB	0.8500
C1—C2	1.508 (4)	O2W—H2WA	0.8500
C2—N1	1.316 (4)	O2W—H2WB	0.8500
C2—N3	1.348 (4)	O3W—H3WA	0.8500
C3—N3	1.328 (4)	O3W—H3WB	0.8500
C3—N2	1.336 (4)		
O1W—Zn1—O3W	86.17 (10)	N2—C3—C4	123.4 (3)
O1W—Zn1—O4 ⁱ	92.88 (10)	O3—C4—O4	125.8 (3)
O3W—Zn1—O4 ⁱ	97.55 (9)	O3—C4—C3	118.0 (3)
O1W—Zn1—O1	91.02 (10)	O4—C4—C3	116.2 (3)
O3W—Zn1—O1	172.75 (9)	C2—N1—N2	102.3 (3)
O4 ⁱ —Zn1—O1	89.25 (9)	C3—N2—N1	110.9 (3)
O1W—Zn1—O2W	174.71 (10)	C3—N2—H2A	131.1
O3W—Zn1—O2W	89.22 (9)	N1—N2—H2A	118.0
O4 ⁱ —Zn1—O2W	85.14 (9)	C3—N3—C2	103.4 (3)
O1—Zn1—O2W	93.86 (9)	C3—N3—Zn1	147.1 (2)
O1W—Zn1—N3	93.49 (10)	C2—N3—Zn1	109.04 (19)
O3W—Zn1—N3	95.09 (9)	C1—O1—Zn1	118.15 (19)
O4 ⁱ —Zn1—N3	166.20 (10)	C4—O4—Zn1 ⁱⁱ	139.4 (2)
O1—Zn1—N3	78.40 (9)	Zn1—O1W—H1WA	137.2
O2W—Zn1—N3	89.51 (9)	Zn1—O1W—H1WB	116.3
O2—C1—O1	127.2 (3)	H1WA—O1W—H1WB	93.4
O2—C1—C2	119.3 (3)	Zn1—O2W—H2WA	111.1
O1—C1—C2	113.4 (3)	Zn1—O2W—H2WB	115.7
N1—C2—N3	114.6 (3)	H2WA—O2W—H2WB	108.8
N1—C2—C1	124.5 (3)	Zn1—O3W—H3WA	105.7
N3—C2—C1	120.9 (3)	Zn1—O3W—H3WB	115.1
N3—C3—N2	108.8 (3)	H3WA—O3W—H3WB	106.3

N3—C3—C4 127.8 (3)
 Symmetry codes: (i) $x, -y-1/2, z-1/2$; (ii) $x, -y-1/2, z+1/2$.

Hydrogen-bond geometry (Å, °)

<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—H2A \cdots O1 ⁱⁱ	0.81	1.95	2.723 (3)	161
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Fig. 1

