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catena-Poly[[[aqua(5-amino-1*H*-1,2,4-triazole-κN^4)zinc(II)]-μ-5-carboxybenzene-1,3-dicarboxylato] dihydrate]

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Key indicators

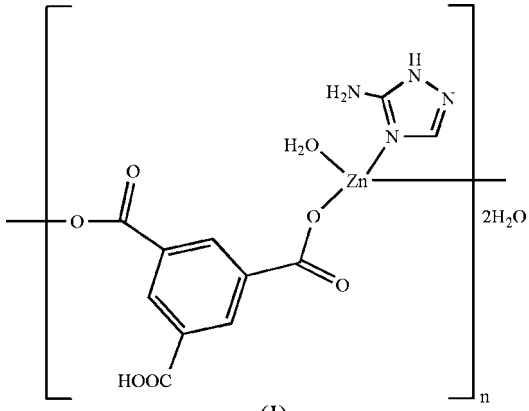
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.008 Å
R factor = 0.055
wR factor = 0.152
Data-to-parameter ratio = 11.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title complex, $\{[Zn(C_9H_4O_6)(C_2H_4N_4)(H_2O)]\cdot 2H_2O\}_n$, contains extended one-dimensional chains with 5-carboxybenzene-1,3-dicarboxylate anions bridging Zn^{II} atoms. The unique Zn^{II} atom is in a distorted tetrahedral coordination environment. In the crystal structure, intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds link the chains and solvent water molecules into a three-dimensional network.

Comment

In recent years, considerable interest has been focused on using multicarboxylic acids of benzene, especially benzene-1,3,5-tricarboxylic acid (H_3btc), as building blocks to construct metal–organic frameworks (Chen *et al.*, 2004; Dai *et al.*, 2003; Li *et al.*, 2003; Lin *et al.*, 2004; Wang *et al.*, 2003). The extent of the deprotonation of H_3btc affects the self-assembly of metal cations into novel structures having attractive properties (Zheng *et al.*, 2004). We have introduced 3-amino-1*H*-1,2,4-triazole (AT) into our system, as this molecule has extensive biological significance, showing antibacterial and herbicidal properties (Palmer & Christen, 2004). Here, we present the structure of the product, (I), of the reaction of $Zn(ClO_4)_2$ with AT and H_3btc.



(I)

The asymmetric unit of (I) (and a symmetry-related Hbtc ligand) is shown in Fig. 1 and selected bond lengths and angles are listed in Table 1. The Zn^{II} atom is in a distorted tetrahedral coordination environment involving one N atom from an AT ligand, two O atoms from two Hbtc ligands and one O atom from a coordinated water molecule. The Hbtc ligand acts in a bis-monodentate mode, bridging symmetry-related Zn^{II} atoms (Fig. 2), thus forming an extended one-dimensional structure along [10$\bar{1}$].

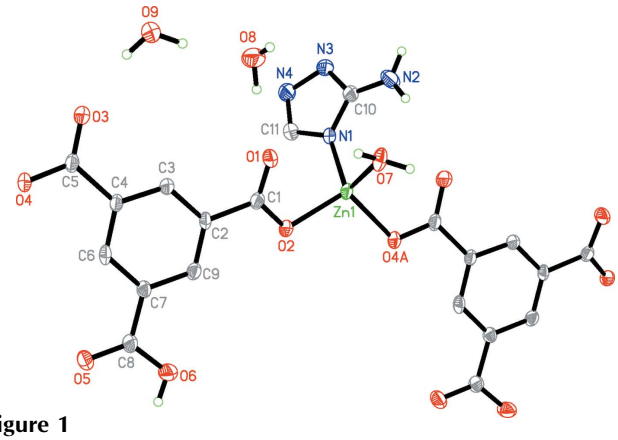


Figure 1
A portion of the one-dimensional title complex, with atom labelling of the asymmetric unit, showing ligands coordinated to Zn1. [Symmetry code: (A) $1+x, -1+y, z$.]

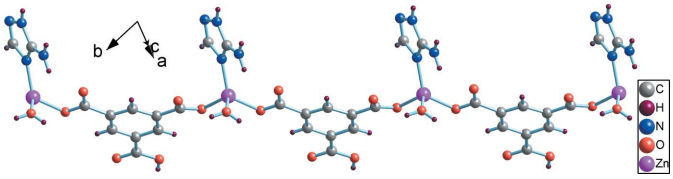


Figure 2
Part of the one-dimensional chain of (I).

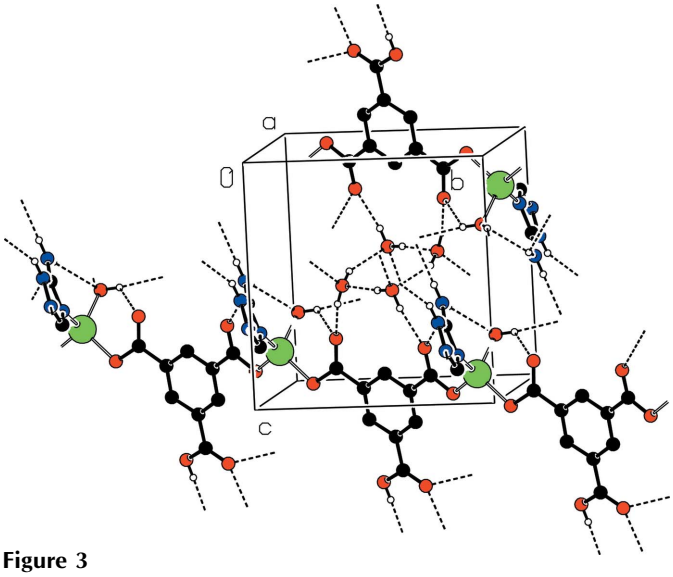


Figure 3
Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines.

In the crystal structure of (I), intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds (Table 2) link the one-dimensional chains and solvent water molecules into a three-dimensional network (Fig. 3).

Experimental

3-Amino-1*H*-1,2,4-triazole (16.8 mg, 0.2 mmol) was dissolved in a C_2H_5OH–H_2O mixture (1:1, 10 ml) and an aqueous NaOH solution (0.1 *M*, 2 ml) was added. An ethanol solution (10 ml) of benzene-1,3,5-tricarboxylic acid (21 mg, 0.1 mmol) was then added and the mixture was stirred for 30 min, after which a dilute aqueous solution (5 ml) of $Zn(ClO_4)_2$ (20.1 mg, 0.2 mmol) was added. The resulting solution was filtered and left to stand at room temperature after a further 30 min of stirring. Colourless block crystals of (I) suitable for X-ray diffraction were obtained within 2 weeks in 61% yield (12.1 mg, based on H_3btc). Analysis, calculated for $C_{22}H_{28}N_8O_{18}Zn_2$: C 60.73, H 3.71, N 9.66%; found: C 60.50, H 3.65, N 9.76%.

Crystal data

$[Zn(C_9H_4O_6)(C_2H_4N_4)(H_2O)]\cdot 2H_2O$	$\gamma = 69.562\ (7)^\circ$
$M_r = 411.65$	$V = 792.0\ (8)$ Å^3
Triclinic, $P\overline{1}$	$Z = 2$
$a = 7.730\ (4)$ Å	$D_x = 1.726$ Mg m^{-3}
$b = 10.000\ (6)$ Å	Mo $K\alpha$ radiation
$c = 11.533\ (6)$ Å	$\mu = 1.61$ mm^{-1}
$\alpha = 85.672\ (7)^\circ$	$T = 294\ (2)$ K
$\beta = 71.590\ (7)^\circ$	Block, colourless
	0.20 × 0.19 × 0.15 mm

Data collection

Bruker APEXII diffractometer	4222 measured reflections
φ and ω scans	2712 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	1917 reflections with $I > 2\sigma(I)$
$T_{min} = 0.719$, $T_{max} = 0.786$	$R_{int} = 0.035$
	$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 1.0815P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.055$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.152$	$\Delta\rho_{max} = 0.85$ e Å^{-3}
$S = 1.05$	$\Delta\rho_{min} = -0.68$ e Å^{-3}
2712 reflections	
227 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O4^{i}	1.959 (4)	Zn1—N1	1.990 (5)
Zn1—O2	1.989 (4)	Zn1—O7	2.018 (4)
O4^{i}—Zn1—O2	105.53 (16)	O4^{i}—Zn1—O7	100.41 (17)
O4^{i}—Zn1—N1	125.53 (19)	O2—Zn1—O7	112.91 (18)
O2—Zn1—N1	108.81 (17)	N1—Zn1—O7	103.43 (19)

Symmetry code: (i) $x+1, y-1, z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O3^{i}	0.86	2.58	3.173 (8)	127
N2—H2*A*···O7	0.86	2.51	3.173 (8)	135
N2—H2*B*···O5^{ii}	0.86	2.08	2.908 (7)	160
N3—H3′···O8^{iii}	0.86	1.99	2.795 (8)	155
O6—H6···O9^{iv}	0.82	1.90	2.710 (7)	167
O7—H7*A*···O1	0.82	2.42	2.897 (7)	118
O7—H7*A*···O5^{v}	0.82	2.16	2.885 (6)	148
O7—H7*B*···N4^{vi}	0.85	1.90	2.738 (8)	166
O8—H8*A*···O1	0.85	1.84	2.664 (7)	161
O8—H8*B*···O9^{vii}	0.85	2.07	2.842 (8)	150
O9—H9*A*···O3	0.85	1.94	2.748 (6)	158
O9—H9*B*···O8	0.85	1.91	2.751 (8)	172

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

H atoms were initially located in difference maps, but were subsequently introduced in calculated positions and treated as riding, with C—H = 0.93, O—H = 0.85 and N—H = 0.86 Å. Water H atoms were refined using restraints [O—H = 0.85 (1) Å and H···H = 1.39 (2) Å]. All H atoms were allocated displacement parameters related to those of their parent atoms [U_{iso}(H) = 1.2U_{eq}(C,N), or 1.5U_{eq}(O).

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2003) and *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXTL*.

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