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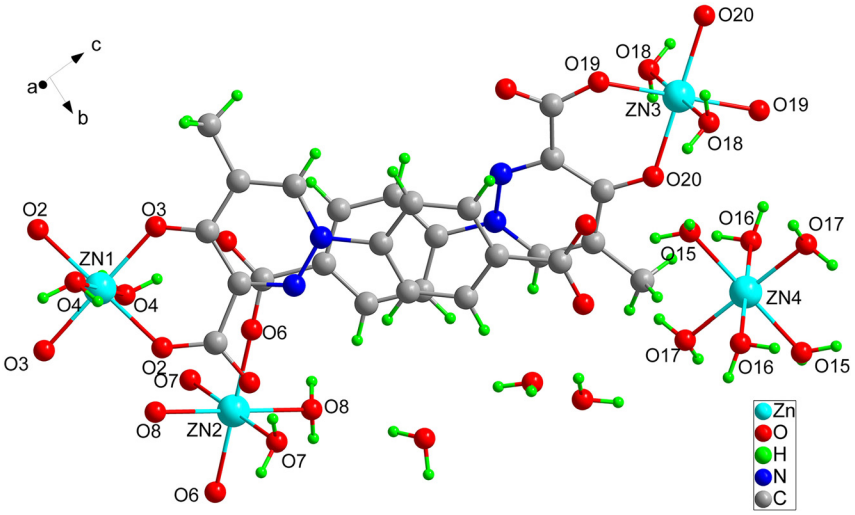
Crystal structure of hexaaquazinc(II) *catena*-poly [bis(1-(3-carboxyphenyl)-5-methyl-4-oxo-1,4-dihydropyridazine-3-carboxylato-κ^2O,O′)-bis(μ_2-1-(3-carboxyphenyl)-5-methyl-4-oxo-1,4-dihydropyridazine-3-carboxylato-κ^2O:O′) trizinc(II)] hexahydrate $C_{26}H_{36}N_4O_{20}Zn_2$



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Abstract

$C_{26}H_{36}N_4O_{20}Zn_2$, triclinic, $P\bar{1}$ (no. 2), a = 6.9872(4) Å, b = 8.9052(5) Å, c = 8.9052(5) Å, α = 94.441(4)°, β = 93.552(4)°, γ = 90.045(5)°, V = 1651.61(16) Å^3, Z = 2, $R_{gt}(F)$ = 0.0748, $wR_{ref}(F^2)$ = 0.2021, T = 293 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.14 × 0.12 × 0.11 mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ:	2.63 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max}, completeness:	71.1°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	10,909, 6228, 0.050
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4370
$N(param)_{refined}$:	495
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	1.0119 (8)	0.2031 (7)	0.6119 (2)	0.0263 (12)
C2	1.0320 (8)	0.2934 (7)	0.5660 (2)	0.0280 (13)
C3	0.9556 (16)	−0.1848 (9)	0.6609 (3)	0.065 (3)
H3A	0.854564	−0.221880	0.637086	0.098*
H3B	0.924189	−0.204988	0.694259	0.098*
H3C	1.073325	−0.234286	0.653093	0.098*
C4	0.9783 (10)	−0.0195 (7)	0.6581 (2)	0.0358 (15)
C5	0.9899 (8)	0.0410 (7)	0.6106 (2)	0.0263 (12)
C6	0.9878 (10)	0.0766 (8)	0.7003 (2)	0.0374 (15)
H6	0.981352	0.038462	0.731628	0.045*
C7	1.0074 (9)	0.3336 (7)	0.7411 (2)	0.0312 (13)
C8	1.0548 (10)	0.2895 (8)	0.7887 (2)	0.0383 (15)
H8	1.092386	0.190805	0.792758	0.046*
C9	1.0467 (10)	0.3907 (8)	0.8301 (2)	0.0356 (14)
H9	1.077748	0.360372	0.862148	0.043*
C10	0.9919 (9)	0.5390 (8)	0.8238 (2)	0.0327 (14)
C11	0.9552 (10)	0.5846 (8)	0.7761 (2)	0.0371 (15)
H11	0.925560	0.684727	0.771694	0.045*
C12	0.9622 (10)	0.4823 (8)	0.7347 (2)	0.0387 (15)
H12	0.936503	0.513270	0.702433	0.046*
C13	0.9805 (9)	0.6498 (8)	0.8689 (2)	0.0356 (15)
C14	0.5169 (8)	0.2577 (7)	0.5882 (2)	0.0279 (13)
C15	0.5050 (8)	0.3189 (7)	0.6428 (2)	0.0266 (12)
C16	0.5090 (10)	0.2245 (7)	0.6812 (2)	0.0354 (15)
H16	0.518242	0.121115	0.673580	0.043*
C17	0.4995 (10)	0.2798 (8)	0.7309 (2)	0.0376 (15)
H17	0.498654	0.214045	0.756298	0.045*
C18	0.4912 (8)	0.4323 (7)	0.7424 (2)	0.0277 (12)
C19	0.4872 (12)	0.5292 (8)	0.7044 (2)	0.0453 (18)
H19	0.481737	0.632686	0.712118	0.054*
C20	0.4913 (11)	0.4719 (7)	0.6550 (2)	0.0399 (16)
H20	0.484826	0.537441	0.629420	0.048*
C21	0.4473 (8)	0.6357 (7)	0.8090 (2)	0.0283 (12)
H21	0.408268	0.699938	0.784530	0.034*
C22	0.4587 (8)	0.6882 (7)	0.8584 (2)	0.0287 (13)
C23	0.5134 (8)	0.5885 (7)	0.8958 (2)	0.0284 (13)
C24	0.5610 (8)	0.4383 (7)	0.8765 (2)	0.0284 (13)
C25	0.6399 (9)	0.3162 (7)	0.9089 (2)	0.0329 (14)
C26	0.4113 (11)	0.8501 (7)	0.8737 (2)	0.0400 (16)
H26A	0.318502	0.853308	0.898822	0.060*
H26B	0.359499	0.897682	0.844754	0.060*
H26C	0.525602	0.902359	0.887149	0.060*
N1	1.0193 (7)	0.2905 (6)	0.65411 (18)	0.0288 (11)
N2	1.0068 (7)	0.2283 (6)	0.69750 (18)	0.0295 (11)
N3	0.4922 (7)	0.4902 (6)	0.79509 (17)	0.0288 (11)
N4	0.5520 (7)	0.3931 (6)	0.82839 (18)	0.0287 (11)
O1	1.0239 (6)	0.4328 (5)	0.57219 (16)	0.0341 (10)
O2	1.0645 (7)	0.2200 (5)	0.52502 (15)	0.0369 (11)
O3	0.9739 (7)	−0.0475 (5)	0.57148 (15)	0.0345 (10)
O4	0.7075 (6)	0.0690 (5)	0.49053 (16)	0.0354 (10)
H4A	0.662279	0.086290	0.519261	0.053*
H4B	0.640249	−0.003892	0.476482	0.053*
O5	0.5215 (7)	0.1186 (5)	0.57924 (15)	0.0367 (10)
O6	0.5224 (7)	0.3501 (5)	0.55586 (15)	0.0393 (11)
O7	0.7252 (6)	0.6207 (5)	0.53825 (16)	0.0336 (10)
H7A	0.793104	0.659563	0.517213	0.050*
H7B	0.800542	0.560534	0.552854	0.050*
O8	0.3021 (6)	0.6287 (5)	0.54402 (16)	0.0355 (10)
H8A	0.207575	0.573179	0.549529	0.053*
H8B	0.252466	0.697177	0.526837	0.053*
O9	0.4554 (14)	0.8567 (7)	0.6310 (2)	0.087 (2)
H9A	0.469899	0.939677	0.617878	0.130*
H9B	0.413120	0.796137	0.606577	0.130*
O10	0.4045 (12)	0.9032 (8)	0.7377 (2)	0.081 (2)
H10A	0.390658	0.860792	0.708047	0.122*
H10B	0.524996	0.913817	0.743248	0.122*
O11	0.7490 (10)	0.9971 (7)	0.79863 (19)	0.0600 (15)
H11A	0.829903	0.940588	0.812976	0.090*
H11B	0.716410	1.060142	0.822116	0.090*
O12	0.9234 (8)	0.7816 (6)	0.86119 (18)	0.0518 (13)
O13	1.0262 (8)	0.6066 (6)	0.91103 (17)	0.0520 (14)
O14	0.7128 (8)	0.2063 (6)	0.88784 (17)	0.0527 (14)
O15	1.0668 (10)	0.7790 (7)	0.99203 (19)	0.0658 (19)
H15A	1.064927	0.739957	0.961889	0.099*
H15B	1.176150	0.756227	1.004939	0.099*
O16	0.6670 (10)	0.9161 (7)	0.9999 (3)	0.082 (2)
H16A	0.653036	0.860892	1.024848	0.124*
H16B	0.639296	0.854753	0.973478	0.124*
O17	1.0331 (10)	0.9869 (7)	1.0734 (2)	0.073 (2)
H17A	1.080131	1.069431	1.087382	0.109*
H17B	1.117883	0.921191	1.080032	0.109*
O18	0.7718 (8)	0.5877 (6)	1.0344 (2)	0.0568 (14)
H18A	0.829785	0.519230	1.049752	0.085*
H18B	0.845304	0.607262	1.011453	0.085*
O19	0.3679 (7)	0.6620 (5)	1.04379 (15)	0.0440 (12)
O20	0.5212 (7)	0.6344 (5)	0.94260 (16)	0.0394 (11)
Zn1	1.000000	0.000000	0.500000	0.0263 (3)
Zn2	0.500000	0.500000	0.500000	0.0270 (3)
Zn3	0.500000	0.500000	1.000000	0.0387 (3)
Zn4	1.000000	1.000000	1.000000	0.0823 (7)

1 Source of material

The mixture of zinc nitrate hexahydrate 29.7 mg (0.1 mmol), 1-(3-carboxyphenyl)-5-methyl-4-oxo-1,4-dihydropyridazine-3-carboxylic acid 27.4 mg (0.1 mmol), NaOH 8 mg (0.2 mmol) and ethyl alcohol (10 mL) were placed in the autoclave lined with PTFE and heated at 110 °C for 48 h, then cooled to room temperature over 24 h. Colourless block crystals were collected after cooling to room temperature.

2 Experimental details

Using Olex2 [2], the structure was solved with the ShelXT [3] structure solution program and refined with the ShelXL [4] refinement package.

3 Comment

In recent years, metal coordination polymers have provoked great interest for their promising applications [5–7]. However, the diversity in the framework architectures of such coordination polymers counts on many factors, such as the metal atom species, the coordination geometry of metal centers, the coordination ability of organic ligands and the reaction conditions (pH, temperature, solvent and so on) [8–11], So that the selection of organic ligands and metal ions is the key to constructing fluorescent coordination polymers. The coordination polymers constructed by rigid N-donor and carboxyl groups mixed ligands were a widely effective adopted strategy in this field. For example, the incorporation of functional groups including pyridyl, imidazole and carboxyl group into the internal of coordination polymers could enhance the fluorescence sensing capability through various host–guest interactions, for synthesis of coordination polymers with appropriate luminous performance and are vital [12].

As shown in Figure, each Zn(II) ion exhibits a different coordination geometry, where Zn1 is six-coordinated with two oxygen atoms from two coordinated water molecules and four oxygen atoms from two organic ligands. Meanwhile, Zn2 is six-coordinated with four oxygen atoms from four coordinated water molecules, two carbonyl oxygen atoms and two carboxyl oxygen atoms from two organic ligands. Zn4 is six-coordinated with six oxygen atoms from six organic ligands as a bidentate ligand bridging adjacent above-mentioned two crystallographically independent Zn(II) ions to form a 1D zigzag chain. The chains and hydrated zinc ions are linked by intermolecular hydrogen bonding to form a 3D supermolecular structure. All bonding parameters are in the expected ranges [13].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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