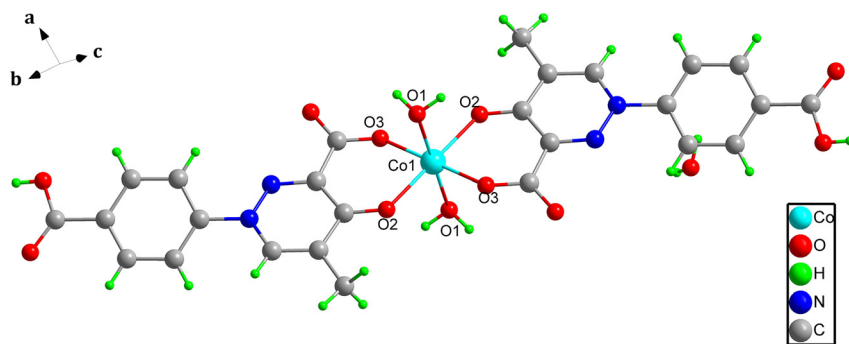


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Crystal structure of diaqua-bis(1-(3-carboxyphenyl)-5-methyl-4-oxo-1,4-dihydropyridazine3-carboxylato-*O,O'*)-cobalt(ii) dihydrate, $C_{26}H_{36}N_4O_{14}Co$



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Abstract

$C_{26}H_{36}N_4O_{14}Co$, triclinic, $P\bar{1}$ (no. 2), $a = 7.1895(7) \text{ \AA}$, $b = 8.7773(9) \text{ \AA}$, $c = 10.9067(11) \text{ \AA}$, $\alpha = 98.180(2)^\circ$, $\beta = 104.0480(10)^\circ$, $\gamma = 90.180(2)^\circ$, $V = 660.37(11) \text{ \AA}^3$, $Z = 1$, $R_{gt}(F) = 0.0287$, $wR_{ref}(F^2) = 0.0751$, $T = 296.15 \text{ K}$.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

The mixture of cobalt nitrate hexahydrate 18.3 mg (0.1 mmol), 1-(3-carboxyphenyl)-5-methyl-4-oxo-1,4-dihydropyridazine3-

Table 1: Data collection and handling.

Crystal:	Pink block
Size:	$0.13 \times 0.12 \times 0.11 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation (0.71073 $\text{\AA}$)
μ :	0.74 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	27.6° , 98 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3947, 2873, 0.009
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2616
$N(\text{param})_{\text{refined}}$:	211
Programs:	Bruker, ¹ Olex2, ² SHELX ^{3,4}

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 95°C for 72 h, then cooled to room temperature over 24 h. Pink block crystals were collected after cooling to room temperature.

2 Experimental details

Using Olex2,² the structure was solved with the ShelXT³ structure solution program and refined with the ShelXL⁴ refinement package.

3 Comment

In recent years, metal coordination polymers have provoked great interest for their promising applications such as laser

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
C1	0.8177 (2)	0.53203 (19)	0.08521 (16)	0.0267 (3)
H1C	0.782836	0.540667	−0.004184	0.040*
H1D	0.854625	0.428824	0.095956	0.040*
H1E	0.923150	0.602843	0.127879	0.040*
C2	0.6498 (2)	0.56906 (17)	0.14128 (14)	0.0206 (3)
C3	0.5538 (2)	0.70841 (17)	0.11989 (14)	0.0195 (3)
C4	0.3993 (2)	0.73897 (17)	0.18441 (14)	0.0202 (3)
C5	0.2862 (2)	0.88570 (18)	0.18060 (15)	0.0229 (3)
C6	0.5831 (2)	0.47216 (18)	0.20949 (15)	0.0223 (3)
H6A	0.640663	0.378536	0.219733	0.027*
C7	0.3628 (2)	0.41100 (17)	0.33875 (14)	0.0222 (3)
C8	0.4745 (2)	0.29861 (19)	0.39282 (16)	0.0292 (4)
H8	0.595210	0.281488	0.377920	0.035*
C9	0.4040 (3)	0.21099 (19)	0.47010 (16)	0.0295 (4)
H9	0.478315	0.135057	0.506894	0.035*
C10	0.1809 (2)	0.4350 (2)	0.35769 (17)	0.0329 (4)
H10	0.105574	0.509559	0.319643	0.039*
C11	0.1128 (2)	0.3465 (2)	0.43395 (18)	0.0338 (4)
H11	−0.009881	0.361267	0.446192	0.041*
C12	0.2246 (2)	0.23622 (18)	0.49236 (15)	0.0252 (3)
C13	0.1552 (3)	0.15222 (19)	0.58426 (15)	0.0284 (4)
Co1	0.500000	1.000000	0.000000	0.02143 (10)
N1	0.43392 (18)	0.50986 (14)	0.26283 (12)	0.0216 (3)
N2	0.34452 (18)	0.64200 (15)	0.25161 (12)	0.0217 (3)
O1	0.72855 (17)	1.11327 (14)	0.15262 (11)	0.0303 (3)
H1A	0.830417	1.118667	0.126338	0.045*
H1B	0.757445	1.057518	0.211917	0.045*
O2	0.60237 (16)	0.79293 (13)	0.04835 (11)	0.0269 (3)
O3	0.34324 (16)	0.99251 (13)	0.13130 (11)	0.0271 (3)
O4	0.14187 (19)	0.89420 (16)	0.22336 (15)	0.0447 (4)
O5	0.2408 (2)	0.05043 (16)	0.63433 (14)	0.0437 (3)
O6	−0.0050 (2)	0.20786 (18)	0.60669 (14)	0.0470 (4)
H6	−0.034971	0.164695	0.661406	0.070*
O7	0.04654 (19)	0.19259 (16)	0.07818 (14)	0.0400 (3)
H7A	0.145620	0.147736	0.113485	0.060*
H7B	0.040145	0.172332	−0.001339	0.060*

sensor,⁵ photosensitive material,⁶ fluorescent probe⁷ and so on. 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 construct 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 the figure, the asymmetric unit of the title complex consists of half Co²⁺ ions, one unidentate coordinated water molecule, one 1-(3-carboxyphenyl)-5-methyl-4-oxo-1,4-dihydropyridazine-3-carboxylic acid ligand and one free water molecule. The carboxyl group on the benzene ring is not dehydrogenated. Each Co ion connects six O atoms to form an octahedral coordination model, which is completed by four oxygen atoms from two symmetric 1-(3-carboxyphenyl)-5-methyl-4-oxo-1,4-dihydropyridazine-3-carboxylic acid and two water molecule ligands. The hydrogen bonds are formed between the free water molecule (O7), and coordinated water molecules (O1), carboxyl group on the benzene ring and pyridazine rings (O2, O3, O4), and coordination carboxyl oxygen atom. Finally, those hydrogen bonds connect the title complexes to form a 3D supramolecular network.

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

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