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Crystal structure of poly[μ_2 -1,4-bis((1*H*-imidazol-1-yl)methyl)benzene- $\kappa^2N:N'$)-(μ_2 -4-sulfidobenzoate- $\kappa^2O:S$)cobalt(II)] dihydrate, **$C_{42}H_{44}Co_2N_8O_7S_2$** **Table 1:** Data collection and handling.

Crystal:	Block, pink
Size:	0.25 × 0.22 × 0.13 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.92 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω -scans
$\theta_{\max}$, completeness:	27.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12109, 4902, 0.028
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4510
$N(\text{param})_{\text{refined}}$:	293
Programs:	CrysAlis ^{PRO} [1], SHELX [2], OLEX2 [3]

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.40973(6)	0.26321(4)	0.51084(4)	0.03170(13)
S1	0.15938(12)	0.26256(12)	0.61956(7)	0.0483(2)
O1	0.2776(3)	0.24359(17)	1.3156(2)	0.0378(7)
O1B	0.9095(5)	0.3303(4)	0.2675(5)	0.0887(14)
H1BA	1.009(6)	0.302(5)	0.270(9)	0.133*
H1BB	0.829(8)	0.294(4)	0.280(8)	0.133*
O2	0.5713(3)	0.2552(3)	1.3062(2)	0.0443(7)
O4 ^a	0.7901(15)	0.4929(6)	0.1918(13)	0.090(3)
H4A	0.829(12)	0.446(3)	0.236(6)	0.135*
H4B	0.764(12)	0.501(5)	0.104(3)	0.135*
N1	0.5383(5)	0.3794(2)	0.5554(3)	0.0330(8)
N2	0.7451(5)	0.4835(2)	0.6030(3)	0.0372(8)
N3	1.3485(5)	0.5445(2)	1.2823(4)	0.0465(9)
N4	1.4356(5)	0.6614(2)	1.4064(3)	0.0372(9)
C1	0.4073(5)	0.2466(2)	1.2456(3)	0.0327(9)
C2	0.3547(5)	0.2437(2)	1.0913(3)	0.0323(9)
C3	0.4751(5)	0.2725(4)	1.0090(3)	0.0387(9)
H3	0.594587	0.288633	1.050258	0.046*
C4	0.4188(5)	0.2776(3)	0.8654(3)	0.0416(11)
H4	0.500865	0.297706	0.811652	0.050*
C5	0.2412(5)	0.2530(3)	0.8003(3)	0.0385(9)
C6	0.1238(6)	0.2202(3)	0.8838(4)	0.0455(10)
H6	0.006833	0.200482	0.842597	0.055*
C7	0.1797(6)	0.2169(3)	1.0268(4)	0.0445(10)
H7	0.098503	0.196287	1.080928	0.053*
C8	0.7059(6)	0.4049(3)	0.5468(4)	0.0381(10)
H8	0.787135	0.371909	0.506338	0.046*
C9	0.5945(6)	0.5104(3)	0.6520(5)	0.0477(11)
H9	0.581294	0.563028	0.696574	0.057*

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Abstract

$C_{42}H_{44}Co_2N_8O_7S_2$, monoclinic, $P2_1$ (no. 4), $a = 7.3941(6)$ Å, $b = 15.3043(14)$ Å, $c = 9.7831(7)$ Å, $\beta = 101.315(7)^\circ$, $V = 1085.56(15)$ Å³, $Z = 1$, $R_{\text{gt}}(F) = 0.0392$, $wR_{\text{ref}}(F^2) = 0.0749$, $T = 293(2)$ K.

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The crystal 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.

Source of material

A mixture of 1,4-bis((1*H*-imidazol-1-yl)methyl)benzene (3.30 mg), $Co(NO_3)_2 \cdot 6H_2O$ (0.26 mg) and distilled H_2O (4.0 mL) were introduced and sealed in a Teflon-lined stainless steel vessel (25 mL), which was heated to 120 °C for 72 h

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Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C10	0.4687(6)	0.4465(3)	0.6237(5)	0.0431(10)
H10	0.352467	0.447395	0.646525	0.052*
C11	0.9251(6)	0.5271(3)	0.6275(5)	0.0493(11)
H11A	0.907062	0.589127	0.608931	0.059*
H11B	0.997458	0.504134	0.562965	0.059*
C12	1.0302(6)	0.5148(3)	0.7743(4)	0.0400(9)
C13	1.1818(7)	0.5665(3)	0.8258(5)	0.0484(12)
H13	1.214998	0.610958	0.770808	0.058*
C14	1.2843(7)	0.5527(3)	0.9579(5)	0.0581(13)
H14	1.387227	0.587293	0.989879	0.070*
C15	1.2370(7)	0.4889(3)	1.0427(4)	0.0486(11)
C16	1.0881(8)	0.4384(3)	0.9930(5)	0.0629(13)
H16	1.054081	0.395047	1.049569	0.075*
C17	0.9858(7)	0.4499(3)	0.8601(5)	0.0599(13)
H17	0.885687	0.413550	0.828078	0.072*
C18	1.3526(8)	0.4707(3)	1.1863(5)	0.0641(14)
H18A	1.306309	0.418741	1.224566	0.077*
H18B	1.479077	0.459606	1.177843	0.077*
C19	1.4856(6)	0.6006(3)	1.3251(4)	0.0426(10)
H19	1.601040	0.597507	1.300962	0.051*
C20	1.2026(7)	0.5703(4)	1.3384(5)	0.0551(13)
H20	1.087245	0.543865	1.325628	0.066*
C21	1.2581(7)	0.6416(3)	1.4160(5)	0.0471(12)
H21	1.186899	0.672503	1.467981	0.057*

^aOccupancy: 0.5.

and then cooled to room temperature at a rate of 3 °C/h. Red block crystals of the title structure in 31% yield (based on Co(NO₃)₂ · 6H₂O) were obtained by filtration and dried in the air.

Experimental details

H atoms bonded to C atoms from organic ligands were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, with $U_{iso}(H) = 1.2$ times $U_{eq}(C)$.

Discussion

N-containing ligands and O-containing ligands had been widely applied in the formation of many kinds of metal coordination complexes [4]. Some coordination complexes have been shown to be capable of binding with DNA, which might be potentially used for ablation of human ependymoma cells [5]. In this study two types of organic ligands C₁₄N₄H₁₄ and C₇H₅SO₂ were used to prepare a new Co²⁺ coordination polymer.

Single-crystal X-ray diffraction analysis reveals that the title structure exhibits the space group $P2_1$. The asymmetric unit of the title structure consists of one crystallographically independent Co(II) cation, one C₁₄N₄H₁₄, one C₇H₅SO₂ ligand and two isolated water molecules. In the structure, the Co(II) cation is tetra-coordinated by two N atoms from two different C₁₄N₄H₁₄ ligands, one O atom and one S atom from two adjacent thiolato ligands (see the figure). The bond distances of Co(II)—O and Co(II)—S are 1.990 Å and 2.301 Å, the bond lengths of Co—N are in the narrow range of 2.008 to 2.022 Å. These neighboring molecular structural units are further extended into a two-dimensional layered structure. The coordination modes of the C₁₄N₄H₁₄ ligand are similar with those in compounds [6–9].

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