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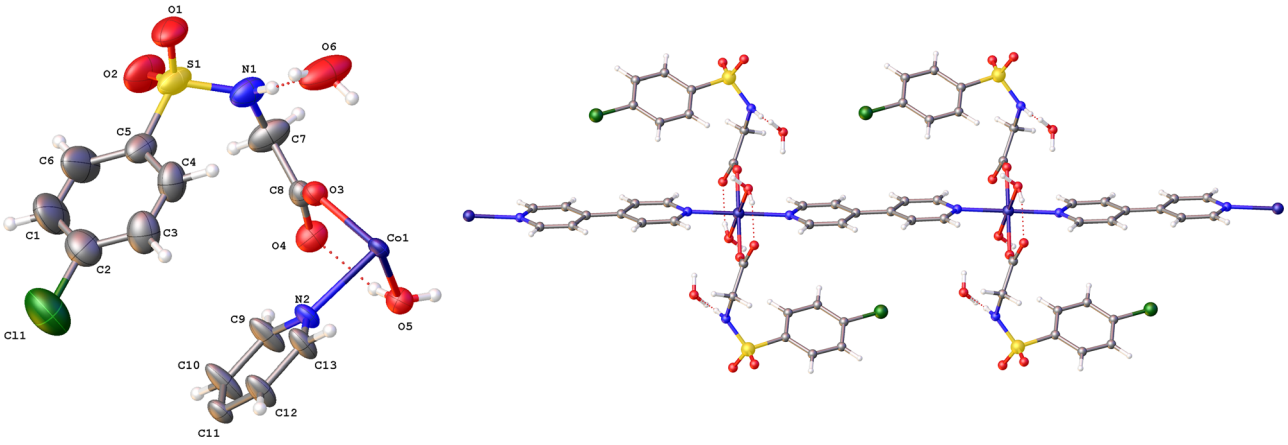
Crystal structure of catena-poly-{diaqua-bis [μ-(((4-chlorophenyl)sulfonyl)glycinato-κO)](μ_2-4, 4′-bipyridine-$\kappa^2 N:N'$)cobalt(II)} dihydrate, $C_{26}H_{30}Cl_2CoN_4O_{12}S_2$



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Abstract

$C_{26}H_{30}Cl_2CoN_4O_{12}S_2$, monoclinic, $P2_1/c$ (no. 14), a = 11.4094(5) Å, b = 14.2343(6) Å, c = 11.6775(4) Å, β = 114.3130(10)°, V = 1728.28(12) Å^3, Z = 2, $R_{gt}(F)$ = 0.0393, $wR_{ref}(F^2)$ = 0.1046, T = 293(2) 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.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.44 × 0.43 × 0.23 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.84 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	27.5°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	26,660, 3972, 0.025
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3446
$N(param)_{refined}$:	229
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

1 Source of material

Glycine (7.51 g, 100 mmol) and sodium hydroxide (8.00 g, 200 mmol) were dissolved in 100 mL water. Then, 4-chlorobenzenesulfonyl chloride (21.11 g, 0.5 mmol) was added to the mixture solution and stirred at room temperature for reaction. After 10 h of reaction, the pH of the reaction mixture was adjusted to 1 with 6 mol/L HCl solution to induce precipitation. The precipitate was filtered and washed with distilled water to obtain white solid ((4-chlorophenyl)sulfonyl)glycine.

A mixture of ((4-chlorophenyl)sulfonyl)glycine (249.7 mg, 1.0 mmol), $Co(CH_3COO)_2{\cdot}4H_2O$ (124.6 mg, 0.5 mmol) and 4,4′-bipyridine (4,4′-bipy) (78.1 mg, 0.5 mmol) was stirred

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Co1	1.000000	0.500000	1.000000	0.02278 (11)
Cl1	0.34243 (10)	0.68006 (9)	0.69096 (12)	0.1083 (4)
S1	0.76865 (7)	0.65006 (5)	0.48759 (5)	0.05214 (18)
O1	0.81337 (19)	0.74451 (14)	0.48920 (19)	0.0674 (6)
O2	0.7112 (2)	0.60208 (17)	0.37056 (16)	0.0772 (7)
O3	0.92586 (13)	0.51774 (10)	0.80691 (12)	0.0312 (3)
O4	0.86450 (16)	0.37442 (11)	0.72942 (14)	0.0438 (4)
O5	0.97593 (16)	0.35131 (11)	0.97907 (16)	0.0359 (3)
H5A	0.937 (3)	0.346 (2)	0.907 (3)	0.053 (8)*
H5B	1.042 (3)	0.317 (2)	0.998 (3)	0.057 (8)*
N1	0.8906 (2)	0.59102 (16)	0.58016 (19)	0.0527 (5)
H1	0.945 (3)	0.617 (2)	0.644 (3)	0.060 (8)*
N2	0.80841 (15)	0.50532 (12)	0.99410 (16)	0.0309 (4)
C1	0.4279 (3)	0.6641 (4)	0.5096 (3)	0.0999 (14)
H1A	0.341678	0.665565	0.453740	0.120*
C2	0.4620 (3)	0.6714 (2)	0.6353 (3)	0.0701 (8)
C3	0.5889 (3)	0.6723 (2)	0.7190 (3)	0.0657 (8)
H3	0.610864	0.677778	0.804748	0.079*
C4	0.6833 (3)	0.6650 (2)	0.6749 (2)	0.0585 (7)
H4	0.769527	0.666928	0.730652	0.070*
C5	0.6502 (2)	0.65486 (18)	0.5486 (2)	0.0509 (6)
C6	0.5221 (3)	0.6546 (3)	0.4663 (3)	0.0904 (13)
H6	0.499479	0.647819	0.380576	0.108*
C7	0.8822 (3)	0.49040 (18)	0.5928 (2)	0.0602 (8)
H7A	0.951181	0.460741	0.577862	0.072*
H7B	0.801497	0.468563	0.528361	0.072*
C8	0.89033 (18)	0.45854 (14)	0.72029 (18)	0.0314 (4)
C9	0.7102 (2)	0.4597 (2)	0.9075 (2)	0.0526 (7)
H9	0.723886	0.428823	0.843912	0.063*
C10	0.5894 (2)	0.4555 (2)	0.9067 (2)	0.0573 (8)
H10	0.524525	0.421791	0.844267	0.069*
C11	0.56436 (17)	0.50136 (14)	0.99863 (19)	0.0312 (4)
C12	0.66514 (19)	0.55045 (19)	1.0865 (2)	0.0449 (6)
H12	0.653359	0.583580	1.149583	0.054*
C13	0.78387 (18)	0.55059 (18)	1.0811 (2)	0.0416 (5)
H13	0.850284	0.584296	1.141846	0.050*
O6	1.0687 (3)	0.69088 (18)	0.7901 (2)	0.0978 (10)
H6A	1.095896	0.674030	0.866518	0.147*
H6B	1.015175	0.734563	0.782625	0.147*

into 50 mL of 50 % methanolic solution at room temperature. Then the pH was adjusted to 7 with 2 mol L^{-1} NaOH solution. The reaction mixture was heated for 12 h at 80 °C in a Teflon-lined reaction vessel and then filtered. Colourless block-crystals of the title compound were obtained by slow evaporation at room temperature within 2 weeks.

2 Experimental details

Hydrogen atoms were added using riding models. Their U_{iso} values were set to 1.2U_{eq} of the parent atoms. The structure was solved with the ShelXT [3] structure solution program and refined with the ShelXL [4].

3 Comment

The design and synthesis of metal-organic coordination polymers is one of the hot spots in current chemical research [5–9]. Amino acids have more coordination modes after being protected by sulfonyl group (Ar–SO_2–), and can form complexes with various structures through the coordination of carboxyl oxygen, amino nitrogen and even sulfonyl group oxygen [10–14]. Therefore, sulfonylated amino acids provide more possibilities for the design of metal-organic coordination polymers. This contribution is part of our ongoing interest in metal-organic coordination polymers.

In this paper, the synthesis and crystal structure of a new cobalt(II) complex with ((4-chlorophenyl)sulfonyl) glycine and 4,4′-bipyridine were reported. The asymmetric unit is composed of half an independent Co(II) ion, one ((4-chlorophenyl)sulfonyl)glycine ligand, half a 4,4′-bipyridine ligand, one coordinated water molecule and one lattice water molecule. The crystallographically unique Co(II) ion of the title complex is six-coordinated by two N atoms (N2, N2′) from 4,4′-bipyridine group, two O atoms (O3, O3′) from ((4-chlorophenyl)sulfonyl)glycine group and two O atoms (O5, O5′) from water group, giving rise to an octahedron geometry. Co–O bond lengths fall in the range 2.0719(13)–2.1353(15) Å [15], and Co–N bond lengths are 2.1598(15) Å. The bond lengths are in the expected ranges. Each 4,4′-bipyridine adopts a μ_2-coordination mode bridging Co atoms to form one one-dimensional chain along *a* direction. Furthermore, the extended three-dimensional supramolecular network is formed through O–H···O and N–H···O hydrogen bonds (O5···O1^a: 2.738(2) Å, O5–H5B···O1^a angle 170(3)°; N1···O6: 2.838(3) Å, N1–H1···O6 angle 174(3)°. $a = -x + 2, -y, -z + 1/2$).

Research ethics: Not applicable.

Author contributions: The authors have accepted responsibility for the entire content of this manuscript and approved its submission.

Competing interests: The authors state no conflict of interest.

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Data availability: The raw data can be obtained on request from the corresponding author.

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