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Crystal structure of *catena*-poly[bis(μ_2 -1,3-di(4*H*-1,2,4-triazol-4-yl)benzene- $\kappa^2N:N'$)-bis(thiocyanato- κ^1N)cobalt(II), $C_{22}H_{16}CoN_{14}S_2$

Table 1: Data collection and handling.

Crystal:	Clear light pink block
Size:	0.29 × 0.21 × 0.19 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.93 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	25°, >97%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	11227, 2076, 0.039
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1924
$N(\text{param})_{\text{refined}}$:	178
Programs:	CrysAlis ^{PRO} [1], SHELX [2]

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Abstract

$C_{22}H_{16}CoN_{14}S_2$, triclinic, $P\bar{1}$ (no. 2), $a = 7.2634(4)$ Å, $b = 9.5067(4)$ Å, $c = 9.7384(4)$ Å, $\alpha = 89.971(3)^\circ$, $\beta = 76.844(4)^\circ$, $\gamma = 67.575(4)^\circ$, $V = 602.49(5)$ Å³, $R_{\text{gt}}(F) = 0.0295$, $wR_{\text{ref}}(F^2) = 0.0658$, $Z = 1$, $T = 289.04(10)$ K.

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The crystal structure is shown in the figure. The symmetry operations for A–C are $2-x, 2-y, -z$; $1-x, 2-y, 1-z$; and $1+x, y, -1+z$. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared by hydrothermal method. A mixture of $CoCl_2 \cdot 6H_2O$ (0.048 g, 0.2 mmol), 1,3-di-(1,2,4-triazole-4-yl)benzene (0.0212 g, 0.1 mmol), NaSCN (0.005 g, 0.1 mmol), and H_2O (10 mL) was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 100 °C for 3 days. The reaction mixture was slowly cooled to room temperature at a rate of 5 °C/h, and the red block crystals were collected, washed with water, and dried in air.

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	1.0000	1.0000	0.0000	0.02193(13)
S1	0.66887(10)	1.03203(7)	−0.38717(7)	0.04282(19)
N1	0.8390(3)	0.66047(19)	0.23423(17)	0.0263(4)
N2	0.8982(3)	0.82826(19)	0.09709(17)	0.0278(4)
N3	0.8435(4)	0.7351(2)	0.02014(19)	0.0479(6)
N4	0.5368(3)	0.65156(18)	0.73118(16)	0.0234(4)
N5	0.2855(3)	0.81598(19)	0.89332(17)	0.0265(4)
N6	0.3802(3)	0.6870(2)	0.95734(18)	0.0376(5)
N7	0.8852(3)	0.9941(2)	−0.17728(18)	0.0325(4)
C1	0.8087(3)	0.5754(2)	0.3533(2)	0.0227(4)
C2	0.7019(3)	0.6543(2)	0.4850(2)	0.0229(4)
H2	0.6596	0.7598	0.4985	0.027*
C3	0.6600(3)	0.5720(2)	0.59568(19)	0.0210(4)
C4	0.7253(3)	0.4146(2)	0.5777(2)	0.0252(5)
H4	0.6932	0.3608	0.6530	0.030*
C5	0.8390(3)	0.3386(2)	0.4462(2)	0.0274(5)
H5	0.8878	0.2325	0.4340	0.033*
C6	0.8812(3)	0.4178(2)	0.3326(2)	0.0276(5)
H6	0.9568	0.3663	0.2440	0.033*
C7	0.8926(3)	0.7822(2)	0.2238(2)	0.0259(5)
H7	0.9215	0.8269	0.2967	0.031*
C8	0.8087(5)	0.6381(3)	0.1051(2)	0.0476(7)
H8	0.7678	0.5621	0.0804	0.057*
C9	0.3814(3)	0.7922(2)	0.7598(2)	0.0253(5)
H9	0.3481	0.8618	0.6932	0.030*
C10	0.5278(4)	0.5925(3)	0.8580(2)	0.0349(5)
H10	0.6164	0.4960	0.8722	0.042*
C11	0.7937(3)	1.0096(2)	−0.2629(2)	0.0258(5)

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C, aromatic ring})$. The final refinement by using geometrical restraints, with $\text{C} - \text{H} = 0.93 \text{ \AA}$ (aromatic ring).

Discussion

Coordination polymers (CPs) constructed by inorganic secondary building units and organic bridging ligands have taken wide attention [3–6]. It is well known that the structures and properties of the CPs are strongly dependent on the organic ligands and the metal ions. As a double-triazolate ligand, 1,3-di-(1,2,4-triazole-4-yl)benzene (L) has been demonstrated to be a powerful ligand for its various coordination modes [7–9]. Herein, we reported a new coordination polymer constructed from L and thiocyanate as co-ligand.

The asymmetric unit of the title compound consists of half a Co(II) ion, one 1,3-di-(1,2,4-triazole-4-yl)benzene ligand, and one thiocyanate anion (Figure). The Co(II) center is six-coordinated with an octahedral coordination geometry. The geometry is completed by four nitrogen atoms from four L ligands, and two nitrogen atoms from two thiocyanato ligands. The Co–N bond lengths are in the range of 2.0904(18)–2.1696(17) Å. In the title compound, each L ligand is coordinated with two center Co(II) ions by two nitrogen atoms from two triazole rings. So adjacent Co(II) ions are connected to each other to give a 1D chain. Bond lengths and angles are in the expected ranges. Surprisingly only one nitrogen atom of each triazolyl moiety coordinates, as it is known, that such triazolyl-based ligands can coordinate by two nitrogen atoms [10].

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