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Crystal structure of *catena*-poly[(μ_2 -2,5-di(pyridin-3-yl)-1,3,4-thiadiazole- $\kappa^2N:N'$)-bis(2,5-di(pyridin-3-yl)-1,3,4-thiadiazole- κ^1N)-bis(thiocyanato- κ^1N)cobalt(II)], $C_{38}H_{24}CoN_{14}S_5$

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Abstract

$C_{38}H_{24}CoN_{14}S_5$, triclinic, $P\bar{1}$, $a = 10.6306(6)$ Å, $b = 13.1604(5)$ Å, $c = 15.1858(7)$ Å, $\alpha = 81.039(4)^\circ$, $\beta = 82.393(4)^\circ$, $\gamma = 66.803(4)^\circ$, $V = 1923.04(17)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0420$, $wR_{\text{ref}}(F^2) = 0.0882$, $T = 291.6(7)$ K.

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The crystal structure is shown in the figure. 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

A mixture of $CoCl_2 \cdot 6H_2O$ (0.048 g, 0.2 mmol), 2,5-di(pyridin-3-yl)-1,3,4-thiadiazole (0.024 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.

Experimental details

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

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Table 1: Data collection and handling.

Crystal:	Clear light pink block
Size:	$0.26 \times 0.24 \times 0.23$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.77 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	25.5° , 98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	35727, 6923, 0.039
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5886
$N(\text{param})_{\text{refined}}$:	523
Programs:	CrysAlis ^{PRO} [1], SHELX [2]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co01	0.28177(3)	0.50159(3)	0.72551(2)	0.03077(10)
S1	0.26781(8)	1.03980(5)	0.76445(4)	0.04038(18)
S2	0.20884(8)	0.90011(6)	0.45241(5)	0.0478(2)
S3	0.27016(8)	0.15005(6)	1.01157(5)	0.04650(19)
S4	0.73618(8)	0.46526(8)	0.64012(7)	0.0694(3)
S5	−0.10519(13)	0.45421(12)	0.90213(8)	0.1106(5)
N1	0.2319(2)	0.65142(16)	0.79162(13)	0.0328(5)
N2	0.3226(2)	0.90967(17)	0.64541(14)	0.0387(5)
N3	0.3529(2)	0.99823(17)	0.60450(14)	0.0402(5)
N4	0.3403(2)	1.35600(16)	0.64963(14)	0.0343(5)
N5	0.1495(2)	0.59967(17)	0.61499(14)	0.0357(5)
N6	−0.0019(2)	0.9102(2)	0.38544(17)	0.0519(6)
N7	0.0270(2)	0.9991(2)	0.34230(16)	0.0516(6)
N8	0.3506(3)	1.1756(2)	0.3320(2)	0.0727(8)
N9	0.4019(2)	0.40963(17)	0.84363(14)	0.0364(5)
N10	0.4910(2)	0.1099(2)	1.08280(16)	0.0504(6)
N11	0.4458(3)	0.02706(19)	1.12059(16)	0.0502(6)
N12	0.0901(3)	−0.1086(2)	1.1016(2)	0.0658(8)
N13	0.4536(2)	0.52716(18)	0.66144(14)	0.0398(5)
N14	0.1207(2)	0.46721(18)	0.79437(15)	0.0406(5)
C1	0.1623(3)	0.6665(2)	0.87198(17)	0.0368(6)
H1	0.1354	0.6101	0.9018	0.044*
C2	0.1288(3)	0.7612(2)	0.91238(17)	0.0392(6)
H2	0.0826	0.7678	0.9690	0.047*
C3	0.1652(3)	0.8471(2)	0.86716(17)	0.0368(6)
H3	0.1421	0.9127	0.8926	0.044*
C4	0.2362(2)	0.83395(19)	0.78410(15)	0.0286(5)
C5	0.2693(3)	0.7336(2)	0.75033(17)	0.0341(6)
H5	0.3206	0.7230	0.6956	0.041*
C6	0.2768(2)	0.91952(19)	0.72882(16)	0.0288(5)
C7	0.3302(2)	1.07283(19)	0.65873(16)	0.0305(6)

Table 2 (continued)

Atom	x	y	z	U _{iso} */U _{eq}
C8	0.3184(2)	1.26261(19)	0.67805(16)	0.0328(6)
H8	0.2749	1.2563	0.7348	0.039*
C9	0.3575(2)	1.17429(19)	0.62715(16)	0.0293(5)
C10	0.4216(3)	1.1853(2)	0.54249(17)	0.0355(6)
H10	0.4509	1.1275	0.5069	0.043*
C11	0.4415(3)	1.2815(2)	0.51168(18)	0.0393(6)
H11	0.4819	1.2909	0.4544	0.047*
C12	0.4007(3)	1.3639(2)	0.56690(17)	0.0377(6)
H12	0.4158	1.4287	0.5458	0.045*
C13	0.0419(3)	0.5750(2)	0.60436(18)	0.0420(7)
H13	0.0315	0.5139	0.6396	0.050*
C14	−0.0534(3)	0.6349(2)	0.5443(2)	0.0493(7)
H14	−0.1260	0.6143	0.5389	0.059*
C15	−0.0406(3)	0.7259(2)	0.49212(19)	0.0464(7)
H15	−0.1052	0.7682	0.4516	0.056*
C16	0.0692(3)	0.7540(2)	0.50047(16)	0.0345(6)
C17	0.1620(3)	0.6875(2)	0.56224(16)	0.0348(6)
H17	0.2373	0.7049	0.5673	0.042*
C18	0.0840(3)	0.8513(2)	0.44493(17)	0.0354(6)
C19	0.1344(3)	1.0045(2)	0.36960(16)	0.0361(6)
C20	0.2994(3)	1.0977(3)	0.3629(2)	0.0556(8)
H20	0.3433	1.0438	0.4081	0.067*
C21	0.1867(3)	1.0916(2)	0.33276(17)	0.0363(6)
C22	0.1216(3)	1.1723(2)	0.26512(19)	0.0467(7)
H22	0.0450	1.1715	0.2424	0.056*
C23	0.1720(3)	1.2535(2)	0.2322(2)	0.0564(8)
H23	0.1300	1.3086	0.1871	0.068*
C24	0.2853(4)	1.2513(3)	0.2673(2)	0.0635(9)
H24	0.3188	1.3064	0.2445	0.076*
C25	0.5007(3)	0.4368(2)	0.86725(18)	0.0430(7)
H25	0.5225	0.4927	0.8314	0.052*
C26	0.5715(3)	0.3862(2)	0.94183(19)	0.0483(7)
H26	0.6392	0.4077	0.9558	0.058*
C27	0.5412(3)	0.3035(2)	0.99550(19)	0.0488(7)
H27	0.5874	0.2690	1.0466	0.059*
C28	0.4407(3)	0.2723(2)	0.97233(17)	0.0372(6)
C29	0.3742(3)	0.3282(2)	0.89655(17)	0.0372(6)
H29	0.3060	0.3081	0.8813	0.045*
C30	0.4100(3)	0.1799(2)	1.02462(17)	0.0397(6)
C31	0.3334(3)	0.0360(2)	1.09028(17)	0.0407(7)
C32	0.1561(3)	−0.0394(2)	1.0784(2)	0.0521(8)
H32	0.1254	0.0157	1.0309	0.062*
C33	0.2661(3)	−0.0434(2)	1.11958(18)	0.0436(7)
C34	0.3135(3)	−0.1262(2)	1.19068(19)	0.0535(8)
H34	0.3874	−0.1320	1.2206	0.064*
C35	0.2476(4)	−0.1987(2)	1.2151(2)	0.0620(9)
H35	0.2768	−0.2552	1.2619	0.074*
C36	0.1382(4)	−0.1870(3)	1.1699(3)	0.0689(10)
H36	0.0947	−0.2368	1.1878	0.083*
C37	0.5722(3)	0.5014(2)	0.65217(16)	0.0361(6)
C38	0.0276(3)	0.4600(2)	0.83936(18)	0.0435(7)

Comment

Coordination polymers (CPs) constructed by inorganic building units and organic bridging ligands have taken wide attention owing to their intriguing structural as well as distinctive properties such as catalytic, luminescence, gas adsorption, and magnetism [3–5]. It is well known that the structures and properties of the CPs are strongly dependent on the ligands and the metal [6, 7]. *N*-heterocyclic ligands have received much interesting in the construction of CPs. Herein, we reported a new coordination polymer constructed from 3-(5-(pyridin-3-yl)-1,3,4-thiadiazol-2-yl)pyridine (*L*), and thiocyanate as co-ligand.

The asymmetric unit of the title compound consists of a Co(II) ion, three 3-(5-(pyridin-3-yl)-1,3,4-thiadiazol-2-yl)pyridine ligands, and two anions (Figure). The Co(II) center is six-coordinated with a slightly distorted octahedral geometry. The geometry is completed by four nitrogen atoms from four *L* ligands, and two nitrogen atoms from two anions. The Co–N bond lengths are in the range of 2.054(2)–2.242(2) Å. In the title compound, one bridging *L* ligand is coordinated with two Co(II) ions by two nitrogen atoms from two pyridine rings. Adjacent Co(II) ions are connected to give a one-dimensional chain. Two *L* ligands and the two thiocyanate anions as terminal ligands to occupy remaining coordination positions.

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