Jian-Ge Wang*

Crystal structure of bis(2,5-di(pyridin-2-yl)-1,3,4-thiadiazole- $\kappa^2 N, N'$)-bis(thiocyanato- $\kappa^1 N$) cobalt(II), $C_{26}H_{16}CoN_{10}S_4$

Table 1: Data collection and handling.

Crystal:	Clear bluish red block
Size:	0.28 × 0.17 × 0.15 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.93 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	29.3°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	23914, 6859, 0.031
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5058
$N(\text{param})_{\text{refined}}$:	373
Programs:	CrysAlis ^{PRO} [1], SHELX [2], Olex2 [3]

<https://doi.org/10.1515/ncrs-2018-0119>

Received June 17, 2018; accepted August 23, 2018; available online September 13, 2018

Abstract

$C_{26}H_{16}CoN_{10}S_4$, monoclinic, $P2_1/n$ (no. 14), $a = 22.8034(10)$ Å, $b = 7.9953(2)$ Å, $c = 16.6238(7)$ Å, $\beta = 110.050(5)^\circ$, $V = 2847.2(2)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0490$, $wR_{\text{ref}}(F^2) = 0.0953$, $T = 290$ K.

CCDC no.: 1863559

One of the two crystallographically independent title complexes forming 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-2-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.

*Corresponding author: Jian-Ge Wang, College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P.R. China, e-mail: miaoshaobin@126.com

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	1.0000	0.5000	0.03894(13)
S1	0.35637(3)	0.59981(8)	0.48745(5)	0.04791(18)
S2	0.33857(4)	1.20785(11)	0.24809(5)	0.0684(2)
N1	0.49954(10)	0.7787(2)	0.42636(13)	0.0413(5)
N2	0.43180(10)	0.8441(2)	0.52556(13)	0.0412(5)
N3	0.39589(10)	0.8644(3)	0.57609(14)	0.0449(5)
N4	0.26885(10)	0.6039(3)	0.58019(14)	0.0480(6)
N5	0.42990(11)	1.0933(3)	0.39495(15)	0.0521(6)
C1	0.53568(13)	0.7448(3)	0.38029(17)	0.0498(7)
H1	0.5673	0.8198	0.3822	0.060*
C2	0.52866(15)	0.6043(4)	0.32997(19)	0.0574(8)
H2	0.5550	0.5847	0.2990	0.069*
C3	0.48186(16)	0.4942(4)	0.3266(2)	0.0651(9)
H3	0.4758	0.3985	0.2929	0.078*
C4	0.44386(15)	0.5266(3)	0.37363(19)	0.0567(8)
H4	0.4120	0.4530	0.3723	0.068*
C5	0.45368(12)	0.6688(3)	0.42240(16)	0.0404(6)
C6	0.41744(11)	0.7118(3)	0.47680(15)	0.0394(6)
C7	0.35462(12)	0.7454(3)	0.56341(16)	0.0409(6)
C8	0.30960(12)	0.7296(3)	0.60840(16)	0.0430(6)
C9	0.31031(14)	0.8373(4)	0.67306(19)	0.0589(8)
H9	0.3396	0.9228	0.6903	0.071*
C10	0.26586(16)	0.8144(5)	0.7119(2)	0.0686(9)
H10	0.2648	0.8842	0.7561	0.082*
C11	0.22371(15)	0.6872(5)	0.6837(2)	0.0666(9)
H11	0.1933	0.6696	0.7084	0.080*
C12	0.22672(14)	0.5860(4)	0.6189(2)	0.0582(8)

Table 2 (continued)

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
H12	0.1978	0.4999	0.6008	0.070*
C13	0.39187(12)	1.1383(3)	0.33356(18)	0.0411(6)
Co2	0.0000	0.5000	0.5000	0.03684(12)
S3	0.14310(3)	0.58653(9)	0.36984(4)	0.04542(17)
S4	0.16480(4)	0.17461(12)	0.69205(5)	0.0669(2)
N6	0.01182(9)	0.3083(3)	0.41545(13)	0.0400(5)
N7	0.07004(9)	0.6012(2)	0.45554(13)	0.0373(5)
N8	0.10173(9)	0.7499(2)	0.47195(13)	0.0393(5)
N9	0.21471(12)	0.8927(3)	0.38227(16)	0.0610(7)
N10	0.06890(11)	0.3842(3)	0.59927(15)	0.0520(6)
C14	−0.01806(13)	0.1620(3)	0.39708(18)	0.0503(7)
H14	−0.0489	0.1388	0.4203	0.060*
C15	−0.00504(14)	0.0435(4)	0.34505(19)	0.0541(7)
H15	−0.0266	−0.0574	0.3339	0.065*
C16	0.04010(13)	0.0767(4)	0.31001(17)	0.0506(7)
H16	0.0494	−0.0011	0.2746	0.061*
C17	0.07148(12)	0.2269(3)	0.32803(16)	0.0439(6)
H17	0.1024	0.2519	0.3052	0.053*
C18	0.05621(11)	0.3391(3)	0.38044(15)	0.0359(5)
C19	0.08611(11)	0.5030(3)	0.40396(15)	0.0359(5)
C20	0.14162(11)	0.7593(3)	0.43169(14)	0.0362(5)
C21	0.18390(12)	0.9006(3)	0.43728(16)	0.0403(6)
C22	0.19151(13)	1.0264(3)	0.49579(18)	0.0517(7)
H22	0.1692	1.0267	0.5333	0.062*
C23	0.23310(15)	1.1527(4)	0.4977(2)	0.0653(9)
H23	0.2396	1.2399	0.5368	0.078*
C24	0.26457(17)	1.1474(4)	0.4411(2)	0.0780(11)
H24	0.2928	1.2313	0.4409	0.094*
C25	0.25407(17)	1.0173(4)	0.3849(2)	0.0801(11)
H25	0.2755	1.0154	0.3464	0.096*
C26	0.10859(12)	0.2974(3)	0.63765(16)	0.0391(6)

Experimental details

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

Comment

Complexes constructed from inorganic metal ions and organic ligands have been widely studied in coordination chemistry and material chemistry. It is well known that the structures and properties of the complexes are strongly dependent on the nature of the organic ligands and the metal ions [4–6].

Among various organic ligands, dipyridine-heterocyclic compounds have been proven to be excellent ones for their diverse coordination modes [7, 8]. Herein, we reported a new complexes constructed from a N-heterocyclic ligand 2-(5-(pyridin-2-yl)-1,3,4-thiadiazol-2-yl)pyridine.

The structure of the title compound consists of two crystallographically independent (at inversion centers) Co(II) ions, each is coordinated by two 2-(5-(pyridin-2-yl)-1,3,4-thiadiazol-2-yl)pyridine ligands and two thiocyanate anions (figure). The Co(II) centers are both six-coordinated with slightly distorted octahedral geometry. The coordination polyhedron is formed in both cases by six nitrogen atoms from two chelating N-heterocyclic ligands and two terminal thiocyanate anions. The Co–N bond lengths are in the range of 2.061(2)–2.150(2) Å.

References

1. Agilent Technologies: CrysAlis^{PRO} Software system, version 1.171.38.41r, Agilent Technologies UK Ltd, Oxford, UK (2015).
2. Sheldrick, G. M.: A short history of *SHELX*. *Acta Crystallogr.* **A64** (2008) 112–122.
3. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H.: OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **42** (2009) 339–341.
4. Du, M.; Li, C.-P.; Liu, C.-S.; Fang, S.-M.: Design and construction of coordination polymers with mixed-ligand synthetic strategy. *Coord. Chem. Rev.* **257** (2013) 1282–1305.
5. Tian, A. X.; Ying, J.; Peng, J.; Sha, J. Q.; Pang, H. J.; Zhang, P. P.; Chen, Y.; Zhu, M.; Su, Z. M.: Tuning the dimensionality of the coordination polymer based on polyoxometalate by changing the spacer length of ligands. *Cryst. Growth Des.* **8** (2008) 3717–3724.
6. Miao, S. B.; Li, Z. H.; Xu, C. Y.; Ji, B. M.: Syntheses, characterization, and luminescence properties of three novel Ag(I) coordination polymers based on polycarboxylic acid ligands and 1,3-di-(1,2,4-triazole-4-yl)benzene. *CrystEngComm* **18** (2016) 4636–4642.
7. Zhu, D. R.; Song, Y.; Xu, Y.; Zhang, Y.; Raj, S. S. S.; Fun, H. K.; You, X. Z.: Syntheses, crystal structures and properties of the novel Co(II) and Ni(II) complexes with 4-(*p*-methylphenyl)-3,5-bis(pyridin-2-yl)-1,2,4-triazole. *Polyhedron* **19** (2000) 2019–2025.
8. Klingele, J.; Kaase, D.; Klingele, M. H.; Lach, J.; Demeshko, S.: Two-step spin crossover in the mononuclear iron(II) complex [Fe(L)₂(NCS)₂] (L = 2,5-di-(2-pyridyl)-1,3,4-thiadiazole). *Dalton Trans.* **39** (2010) 1689–1691.