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Crystal structure of *catena*-poly[bis(μ_2 -thiocyanato- $\kappa^2 N:S$)-(2-(5-methyl-1*H*-pyrazol-3-yl)pyridine- $\kappa^2 N,N'$)cadmium(II)]–dioxane (1/1), $C_{15}H_{17}CdN_5O_2S_2$

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Abstract

$C_{15}H_{17}CdN_5O_2S_2$, triclinic, $P\bar{1}$ (no. 2), $a = 9.6685(4)$ Å, $b = 10.4511(4)$ Å, $c = 11.2840(5)$ Å, $\alpha = 100.763(2)^\circ$, $\beta = 114.948(2)^\circ$, $\gamma = 96.816(2)^\circ$, $V = 990.36(7)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0316$, $wR_{ref}(F^2) = 0.1169$, $T = 296(2)$ 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:	Colorless block
Size:	0.10 × 0.05 × 0.05 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.33 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART APEX II, φ and ω
θ_{max} , completeness:	27.8°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	16640, 4605, 0.028
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3901
$N(param)_{refined}$:	226
Programs:	Bruker [1], SHELX [2, 3], Diamond [4]

Source of material

First, 3-(4-pyridyl)pyrazole was prepared by using 4-acetyl pyridine, *N,N*-dimethylacetamide dimethyl acetal (CAS:18871-66-4) and hydrazine under certain conditions according to the described method [5, 6]. Then, the 1 mL aqueous solution of CdCl₂ (0.1 mol/L) and KSCN (0.2 mol/L) was slowly dropped into the 10 mL acetonitrile solution of 2-(5-methyl-1*H*-pyrazol-3-yl)pyridine (15.9 mg, 0.1 mmol)

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Cd1	0.15298 (2)	0.28051 (2)	0.55214 (2)	0.04682 (11)
S1	0.26784 (11)	0.12944 (9)	0.73965 (9)	0.0574 (2)
S2	−0.03993 (11)	0.61617 (10)	0.28509 (10)	0.0561 (2)
N1	0.3343 (3)	0.2180 (3)	0.4753 (3)	0.0541 (7)
N2	0.3921 (3)	0.4388 (3)	0.6743 (3)	0.0476 (6)
N3	0.4514 (3)	0.5544 (3)	0.7716 (3)	0.0509 (6)
H3	0.400700	0.590000	0.811101	0.061*
N4	0.0388 (4)	−0.1037 (3)	0.5982 (3)	0.0707 (10)
N5	0.0613 (4)	0.4092 (3)	0.4000 (3)	0.0583 (7)
C1	0.3082 (5)	0.1052 (4)	0.3823 (4)	0.0704 (11)
H1	0.207900	0.049600	0.339600	0.085*
C2	0.4176 (7)	0.0676 (5)	0.3471 (5)	0.0906 (15)
H2	0.394100	−0.012100	0.282700	0.109*
C3	0.5607 (7)	0.1477 (6)	0.4079 (6)	0.0979 (18)
H3A	0.638801	0.125901	0.385100	0.118*
C4	0.5920 (5)	0.2649 (5)	0.5033 (4)	0.0732 (11)
H4	0.691001	0.321901	0.546399	0.088*
C5	0.4772 (4)	0.2971 (4)	0.5352 (3)	0.0513 (8)
C6	0.5035 (4)	0.4192 (3)	0.6386 (3)	0.0456 (7)
C7	0.6365 (4)	0.5235 (4)	0.7160 (4)	0.0564 (8)
H7	0.730900	0.533100	0.711201	0.068*
C8	0.5985 (4)	0.6074 (4)	0.7993 (4)	0.0568 (8)
C9	0.6895 (6)	0.7345 (5)	0.9058 (5)	0.0841 (13)
H9A	0.626600	0.767600	0.945499	0.127*
H9B	0.720100	0.798800	0.865801	0.127*
H9C	0.781700	0.718101	0.974399	0.127*
C10	0.1318 (4)	−0.0065 (3)	0.6552 (3)	0.0439 (7)
C11	0.0178 (4)	0.4938 (3)	0.3535 (3)	0.0460 (7)
C12	0.6930 (6)	0.3342 (5)	−0.0362 (4)	0.0774 (12)
H12A	0.691801	0.428201	−0.028700	0.094*
H12B	0.604400	0.282399	−0.119699	0.094*
C13	0.8395 (7)	0.3095 (6)	−0.0391 (5)	0.0855 (14)
H13A	0.844300	0.331700	−0.117200	0.103*
H13B	0.929200	0.368401	0.041600	0.103*
C14	0.8431 (6)	0.1414 (5)	0.0699 (5)	0.0832 (13)
H14A	0.932599	0.196600	0.153101	0.100*
H14B	0.849000	0.049100	0.065500	0.100*
C15	0.6954 (6)	0.1638 (5)	0.0712 (5)	0.0799 (12)
H15A	0.608400	0.105301	−0.008900	0.097*
H15B	0.692201	0.142100	0.149900	0.097*
O1	0.6821 (4)	0.2983 (3)	0.0757 (3)	0.0698 (7)
O2	0.8531 (5)	0.1753 (4)	−0.0434 (3)	0.0909 (10)

and triethylamine (16 mL, 0.1 mmol). The mixture solution was stirred at room temperature for 30 min. After filtration, it was stood to evaporate for one week to form colorless block crystals of the title compound.

Experimental details

H atoms were added geometrically. Their *U*_{iso} values were set to 1.2*U*_{eq} of the parent atoms.

Comment

2-(5-Methyl-1*H*-pyrazol-3-yl)pyridine have been widely studied as important ligands [7], which has the similar bidentate coordination sites as the magnetism-active ligands [8, 9]. These ligands usually transmit antiferromagnetic coupling.

In the title compound, all the bond lengths are within normal ranges, similar to its mononuclear analogue [5, 10]. The Cd is chelated by one 2-(5-methyl-pyrazolate-3-yl)pyridine, and bridged by two SCN[−] to form a 1D chain. The chains of the title compound are interlinked to form 3D supramolecular networks by one classical intermolecular H-bond N3–H3A⋯O1 (−*x* + 1, −*y* + 1, −*z* + 1) (length 2.890(2) Å).

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