

Poly[di- μ -thiocyanato- κ^2 N:S; κ^2 S:N-bis[2-(1*H*-1,2,3-triazol-1-yl)- κ N³]pyrazine]cadmium(II)]

 Cheng Qi Liu,^a Long Miao Xie^b and Ming Gen Zhao^{a*}

^aDepartment of Chemistry, Xinzhou Teachers' University, Shanxi, Xinzhou 034000, People's Republic of China, and ^bDepartment of Chemistry, Shandong Normal University, Jinan 250014, People's Republic of China
Correspondence e-mail: zhaomingen1957@yahoo.com.cn

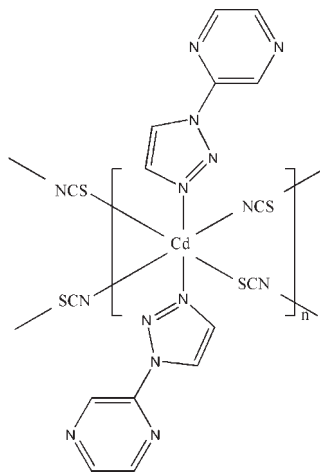
Received 14 July 2009; accepted 8 September 2009

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.026; wR factor = 0.064; data-to-parameter ratio = 14.5.

In the title two-dimensional coordination polymer, $[\text{Cd}(\text{NCS})_2(\text{C}_6\text{H}_5\text{N}_5)_2]_n$, the Cd^{II} ion (site symmetry $\bar{1}$) is coordinated by two N atoms from two 2-(1*H*-1,2,3-triazol-1-yl)pyrazine ligands and two N and two S atoms from four thiocyanate anions. The N—Cd bond lengths range from 2.323 (2) to 2.3655 (19) Å and the S—Cd bond length is 2.7117 (7) Å. The associated *cisoid* angles vary from 84.99 (7) to 95.01 (7)°, indicating that the Cd^{II} ion assumes a distorted octahedral geometry. In the complex, each thiocyanate anion functions as a bridging ligand, linking adjacent Cd^{II} ions with a separation of 6.4919 (6) Å, resulting in the formation of a two-dimensional sheet structure in the *bc* plane.

Related literature

For a related crystal structure, see: Yang & Shi (2008). For the synthesis of Cd^{II} complexes with thiocyanate anions and pyrazine derivatives as mixed bridging ligands, see: Li *et al.* (2008); Shi *et al.* (2007).



Experimental

Crystal data

$[\text{Cd}(\text{NCS})_2(\text{C}_6\text{H}_5\text{N}_5)_2]$
 $M_r = 522.86$
Monoclinic, $P2_1/c$
 $a = 12.5038$ (15) Å
 $b = 10.7240$ (13) Å
 $c = 7.3196$ (9) Å
 $\beta = 106.476$ (2)°

$V = 941.2$ (2) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 1.41$ mm⁻¹
 $T = 298$ K
 $0.24 \times 0.18 \times 0.16$ mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.728$, $T_{\text{max}} = 0.806$

5139 measured reflections
1923 independent reflections
1735 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.064$
 $S = 1.03$
1923 reflections

133 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.34$ e Å⁻³

Table 1

Selected bond angles (°).

N6 ⁱ —Cd1—N1	84.99 (7)	N1—Cd1—S1 ⁱⁱⁱ	94.56 (5)
N6 ⁱⁱ —Cd1—N1	95.01 (7)	N6 ⁱⁱ —Cd1—S1	88.93 (6)
N6 ⁱⁱ —Cd1—S1 ⁱⁱⁱ	91.07 (6)	N1—Cd1—S1	85.44 (5)

Symmetry codes: (i) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $-x, -y + 2, -z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2122).

References

- Bruker (1997). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, H., Xu, H. Y., Zhang, S. G. & Shi, J. M. (2008). *J. Coord. Chem.* **61**, 2807–2813.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Shi, J. M., Zhang, X., Xu, H. Y., Wu, C. J. & Liu, L. D. (2007). *J. Coord. Chem.* **60**, 647–654.
Yang, L. Y. & Shi, J. M. (2008). *Acta Cryst.* **E64**, m1387.

supplementary materials

Acta Cryst. (2009). E65, m1211 [doi:10.1107/S1600536809036332]

Poly[di- μ -thiocyanato- $\kappa^2N:S;\kappa^2S:N$ -bis[2-(1*H*-1,2,3-triazol-1-yl- κN^3)pyrazine]cadmium(II)]

C. Q. Liu, L. M. Xie and M. G. Zhao

Comment

2-(1*H*-1,2,3-triazol-1-yl)pyrazine is similar to 2-(pyrazol-1-yl)pyrazine (Yang & Shi 2008) in structure and therefore it should act as a bridging ligand. Our interest in synthesizing Cd^{II} complexes (Shi *et al.*, 2007; Li *et al.*, 2008) with thiocyanate anions and derivatives of pyrazine as mixed bridging ligands resulted in us selecting thiocyanato and 2-(1*H*-1,2,3-triazol-1-yl)pyrazine as ligands, but only the title complex was obtained, in which 2-(1*H*-1,2,3-triazol-1-yl)pyrazine only functions as a terminal ligand. Herein we report the crystal structure of the title complex.

The asymmetric unit and symmetry-related fragments of (I) are shown in Fig. 1, and Fig.1 and Table 1 reveal that Cd1 atom is in a distorted octahedral CdN₄S₂ coordination geometry. In the crystal each Cd^{II} ion is surrounded by four other symmetry-related Cd^{II} ions with separation with 6.4919 (6) Å and the adjacent Cd^{II} ions were bridged by one thiocyanato anions and it forms a two-dimensional sheet on *bc* plane as shown in Fig. 2. 2-(1*H*-1,2,3-triazol-1-yl)pyrazine only acts as a monodentate ligand.

Experimental

An 8 ml methanol solution of 2-(1*H*-1,2,3-triazol-1-yl)pyrazine (0.0401 g, 0.272 mmol), 5 ml water solution of Cd(ClO₄)₂·6H₂O (0.1120 g, 0.267 mmol) and 5 ml water solution of NaSCN (0.0435 g, 0.537 mmol) were mixed together and stirred for a few minutes. The colorless single crystals were obtained after the filtrate had been allowed to stand at room temperature for ten days.

Refinement

All H atoms were placed in calculated positions and refined as riding with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

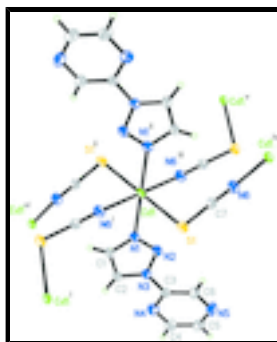


Fig. 1. The coordination structure of (I) showing the atom numbering scheme with thermal ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) $-x, y - 1/2, -z + 1/2$ (ii) $-x, -y + 2, -z$ (iii) $x, -y + 5/2, z - 1/2$ (iv) $-x, y + 1/2, -z - 1/2$ (v) $-x, y - 1/2, -z - 1/2$ (vi) $-x, y + 1/2, -z + 1/2$]

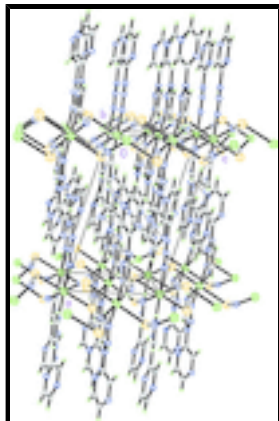


Fig. 2. Unit cell and the part of the two-dimensional sheet on *bc* plane.

Poly[di- μ -thiocyanato- κ^2 N:S; κ^2 S:N-\backslash bis[2-(1H-1,2,3-triazol-1-yl- κ N³)pyrazine]cadmium(II)]

Crystal data

[Cd(NCS)₂(C₆H₅N₅)₂]

$M_r = 522.86$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.5038$ (15) Å

$b = 10.7240$ (13) Å

$c = 7.3196$ (9) Å

$\beta = 106.476$ (2)°

$V = 941.2$ (2) Å³

$Z = 2$

$F_{000} = 516$

$D_x = 1.845$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3160 reflections

$\theta = 2.6$ – 28.0°

$\mu = 1.41$ mm⁻¹

$T = 298$ K

Block, colorless

$0.24 \times 0.18 \times 0.16$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.728$, $T_{\max} = 0.806$

5139 measured reflections

1923 independent reflections

1735 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\text{max}} = 26.4^\circ$

$\theta_{\text{min}} = 1.7^\circ$

$h = -15 \rightarrow 15$

$k = -13 \rightarrow 12$

$l = -6 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 0.6077P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
1923 reflections	$(\Delta/\sigma)_{\max} = 0.001$
133 parameters	$\Delta\rho_{\max} = 0.55 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1593 (2)	0.7435 (2)	0.0075 (4)	0.0390 (6)
H1	0.0980	0.6904	-0.0225	0.047*
C2	0.2671 (2)	0.7082 (2)	0.0439 (4)	0.0405 (6)
H2	0.2951	0.6278	0.0441	0.049*
C3	0.44202 (19)	0.8353 (2)	0.1282 (3)	0.0348 (5)
C4	0.6101 (2)	0.7616 (3)	0.1322 (4)	0.0521 (7)
H4	0.6555	0.6987	0.1083	0.063*
C5	0.6582 (2)	0.8710 (3)	0.2116 (4)	0.0530 (7)
H5	0.7347	0.8817	0.2350	0.064*
C6	0.4896 (2)	0.9434 (3)	0.2156 (5)	0.0506 (7)
H6	0.4446	1.0041	0.2468	0.061*
C7	0.08801 (19)	1.2249 (2)	0.3671 (3)	0.0331 (5)
Cd1	0.0000	1.0000	0.0000	0.03129 (10)
N1	0.15559 (16)	0.86932 (18)	0.0222 (3)	0.0370 (5)
N2	0.25664 (17)	0.91457 (18)	0.0669 (3)	0.0393 (5)
N3	0.32500 (16)	0.81662 (17)	0.0798 (3)	0.0336 (4)
N4	0.50015 (18)	0.7423 (2)	0.0879 (4)	0.0464 (5)
N5	0.5982 (2)	0.9623 (3)	0.2560 (5)	0.0615 (7)
N6	0.07295 (19)	1.32994 (19)	0.3793 (3)	0.0452 (5)
S1	0.11190 (7)	1.07527 (6)	0.35667 (11)	0.0530 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0328 (13)	0.0276 (11)	0.0548 (16)	0.0003 (9)	0.0097 (11)	-0.0064 (11)

supplementary materials

C2	0.0363 (13)	0.0268 (11)	0.0566 (16)	0.0025 (10)	0.0104 (12)	-0.0060 (11)
C3	0.0333 (12)	0.0363 (12)	0.0350 (12)	0.0027 (10)	0.0098 (10)	-0.0011 (10)
C4	0.0379 (15)	0.0618 (18)	0.0593 (19)	0.0058 (13)	0.0181 (13)	-0.0065 (15)
C5	0.0335 (14)	0.0681 (19)	0.0564 (18)	-0.0022 (13)	0.0113 (13)	0.0008 (15)
C6	0.0370 (14)	0.0413 (15)	0.070 (2)	0.0015 (12)	0.0094 (13)	-0.0099 (14)
C7	0.0310 (12)	0.0315 (12)	0.0370 (13)	-0.0020 (9)	0.0097 (10)	-0.0056 (10)
Cd1	0.02776 (14)	0.01935 (13)	0.04655 (17)	0.00164 (8)	0.01019 (11)	0.00206 (9)
N1	0.0321 (10)	0.0283 (10)	0.0496 (13)	0.0032 (8)	0.0098 (9)	-0.0009 (9)
N2	0.0340 (11)	0.0265 (10)	0.0578 (14)	0.0039 (8)	0.0134 (10)	-0.0011 (9)
N3	0.0311 (10)	0.0274 (9)	0.0415 (11)	0.0041 (8)	0.0087 (8)	-0.0024 (8)
N4	0.0379 (12)	0.0450 (12)	0.0575 (15)	0.0042 (10)	0.0157 (10)	-0.0089 (11)
N5	0.0397 (14)	0.0541 (14)	0.085 (2)	-0.0095 (12)	0.0082 (13)	-0.0145 (15)
N6	0.0462 (13)	0.0323 (11)	0.0571 (14)	0.0036 (9)	0.0145 (11)	-0.0081 (10)
S1	0.0712 (5)	0.0266 (3)	0.0485 (4)	0.0086 (3)	-0.0037 (3)	-0.0046 (3)

Geometric parameters (\AA , $^\circ$)

C1—C2	1.352 (3)	C6—N5	1.322 (4)
C1—N1	1.355 (3)	C6—H6	0.9300
C1—H1	0.9300	C7—N6	1.150 (3)
C2—N3	1.356 (3)	C7—S1	1.638 (2)
C2—H2	0.9300	Cd1—N6 ⁱ	2.323 (2)
C3—N4	1.316 (3)	Cd1—N6 ⁱⁱ	2.323 (2)
C3—C6	1.375 (4)	Cd1—N1	2.3655 (19)
C3—N3	1.419 (3)	Cd1—N1 ⁱⁱⁱ	2.3655 (19)
C4—N4	1.336 (4)	Cd1—S1 ⁱⁱⁱ	2.7117 (7)
C4—C5	1.370 (4)	Cd1—S1	2.7117 (7)
C4—H4	0.9300	N1—N2	1.306 (3)
C5—N5	1.328 (4)	N2—N3	1.341 (3)
C5—H5	0.9300	N6—Cd1 ^{iv}	2.323 (2)
C2—C1—N1	108.6 (2)	N6 ⁱⁱ —Cd1—N1 ⁱⁱⁱ	84.99 (7)
C2—C1—H1	125.7	N1—Cd1—N1 ⁱⁱⁱ	180.0
N1—C1—H1	125.7	N6 ⁱ —Cd1—S1 ⁱⁱⁱ	88.93 (6)
C1—C2—N3	104.2 (2)	N6 ⁱⁱ —Cd1—S1 ⁱⁱⁱ	91.07 (6)
C1—C2—H2	127.9	N1—Cd1—S1 ⁱⁱⁱ	94.56 (5)
N3—C2—H2	127.9	N1 ⁱⁱⁱ —Cd1—S1 ⁱⁱⁱ	85.44 (5)
N4—C3—C6	123.3 (2)	N6 ⁱ —Cd1—S1	91.07 (6)
N4—C3—N3	115.7 (2)	N6 ⁱⁱ —Cd1—S1	88.93 (6)
C6—C3—N3	121.0 (2)	N1—Cd1—S1	85.44 (5)
N4—C4—C5	122.2 (3)	N1 ⁱⁱⁱ —Cd1—S1	94.56 (5)
N4—C4—H4	118.9	S1 ⁱⁱⁱ —Cd1—S1	180.0
C5—C4—H4	118.9	N2—N1—C1	109.69 (19)
N5—C5—C4	121.6 (3)	N2—N1—Cd1	121.04 (14)
N5—C5—H5	119.2	C1—N1—Cd1	129.10 (16)
C4—C5—H5	119.2	N1—N2—N3	106.19 (18)
N5—C6—C3	121.0 (3)	N2—N3—C2	111.33 (19)

N5—C6—H6	119.5	N2—N3—C3	119.93 (19)
C3—C6—H6	119.5	C2—N3—C3	128.7 (2)
N6—C7—S1	178.2 (3)	C3—N4—C4	115.1 (2)
N6 ⁱ —Cd1—N6 ⁱⁱ	180.0	C6—N5—C5	116.6 (3)
N6 ⁱ —Cd1—N1	84.99 (7)	C7—N6—Cd1 ^{iv}	152.8 (2)
N6 ⁱⁱ —Cd1—N1	95.01 (7)	C7—S1—Cd1	106.59 (9)
N6 ⁱ —Cd1—N1 ⁱⁱⁱ	95.01 (7)		

Symmetry codes: (i) $-x, y-1/2, -z+1/2$; (ii) $x, -y+5/2, z-1/2$; (iii) $-x, -y+2, -z$; (iv) $-x, y+1/2, -z+1/2$.

Fig. 1

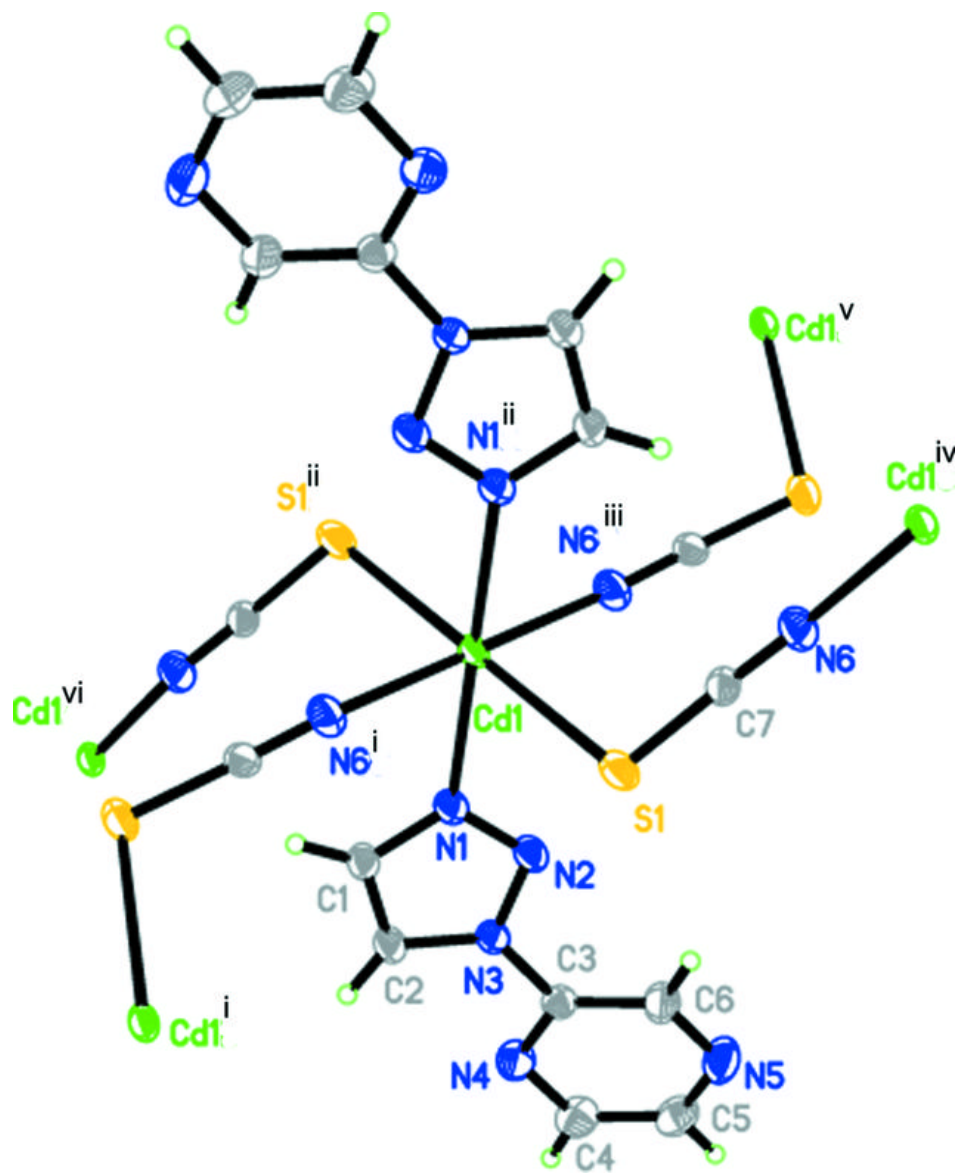


Fig. 2

