metal-organic compounds

catena-Poly[[bis[2-(1H-1,2,4-triazol-1-yl-κN⁴)pyrazine]cadmium(II)]-di-μ-thiocyanato-κ²S:N;κ²N:S]

Hong Li[a]* and Long Miao Xie[b]

[a]Department of Chemistry and Chemical Engineering, Institute of Materials Chemistry, Binzhou University, Binzhou 256603, People's Republic of China, and [b]Department of Chemistry, Shandong Normal University, Jinan 250014, People's Republic of China

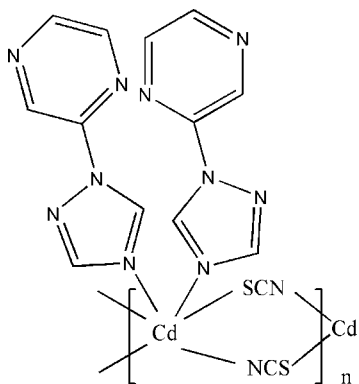Correspondence e-mail: honglizhang1968@yahoo.cn

The title compound, $[Cd(NCS)_2(C_6H_5N_5)_2]_n$, is a coordination polymer with the Cd^{II} centre located on a twofold rotation axis. The Cd^{II} centre assumes a distorted octahedral geometry. The thiocyanate anions function as bridging ligands between the Cd^{II} centres, leading to a chain-like arrangement expanding along [001].

Related literature

For a related structure, see: Yang & Shi (2008).

Experimental

Crystal data

$[Cd(NCS)_2(C_6H_5N_5)_2]$	V = 1929.1 (5) Å^3
M_r = 522.86	Z = 4
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 25.818 (4) Å	μ = 1.38 mm^{-1}
b = 7.4077 (10) Å	T = 298 K
c = 11.0276 (15) Å	0.41 × 0.21 × 0.20 mm
β = 113.843 (2)°	

Data collection

Bruker SMART APEX CCD diffractometer	5381 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	2085 independent reflections
	2005 reflections with $I > 2\sigma(I)$
T_{min} = 0.602, T_{max} = 0.770	R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022	133 parameters
$wR(F^2)$ = 0.058	H-atom parameters constrained
S = 1.10	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
2085 reflections	$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SMART, SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, L. Y. & Shi, J. M. (2008). *Acta Cryst.* E**64**, m1387.

supporting information

catena-Poly[[bis[2-(1*H*-1,2,4-triazol-1-yl-*κN*⁴)pyrazine]cadmium(II)]-di-*µ*-thio-cyanato-*κ²S:N;κ²N:S*]

Hong Li and Long Miao Xie

S1. Comment

2-(1*H*-1,2,4-triazol-1-yl)pyrazine is similar to 2-(pyrazol-1-yl)pyrazine (Yang & Shi, 2008) and therefore it should act as a brdiging ligand. We are interested in synthesizing complexes with mixed bridging ligands and selected thiocyanato and 2-(1*H*-1,2,4-triazol-1-yl)pyrazine as ligands. However, 2-(1*H*-1,2,4-triazol-1-yl)pyrazine only functions as a terminal ligand.

The coordination geometry of the Cd centres is shown in Fig. 1. The Cd atom is in a distorted octahedral CdN_4S_2 coordination geometry. In the crystal each Cd^{II} ion is surrounded by two other symmetry-related Cd^{II} ions with separation with 5.7105 (7) Å and the adjacent Cd^{II} ions were bridged by two thiocyanato anions and it forms a one-dimensional chain along the *c* axis. 2-(1*H*-1,2,4-triazol-1-yl)pyrazine only acts as a monodentate ligand.

S2. Experimental

6 ml methanol solution of 2-(1*H*-1,2,4-triazol-1-yl)pyrazine (0.0345 g, 0.191 mmol), 5 ml C d(ClO₄)₂.6H₂O (0.0809 g, 0.193 mmol) H₂O solution and 5 ml NaSCN (0.0315 g, 0.389 mmol) H₂O solution 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 two weeks.

S3. Refinement

All H atoms were placed in calculated positions and refined as riding with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.
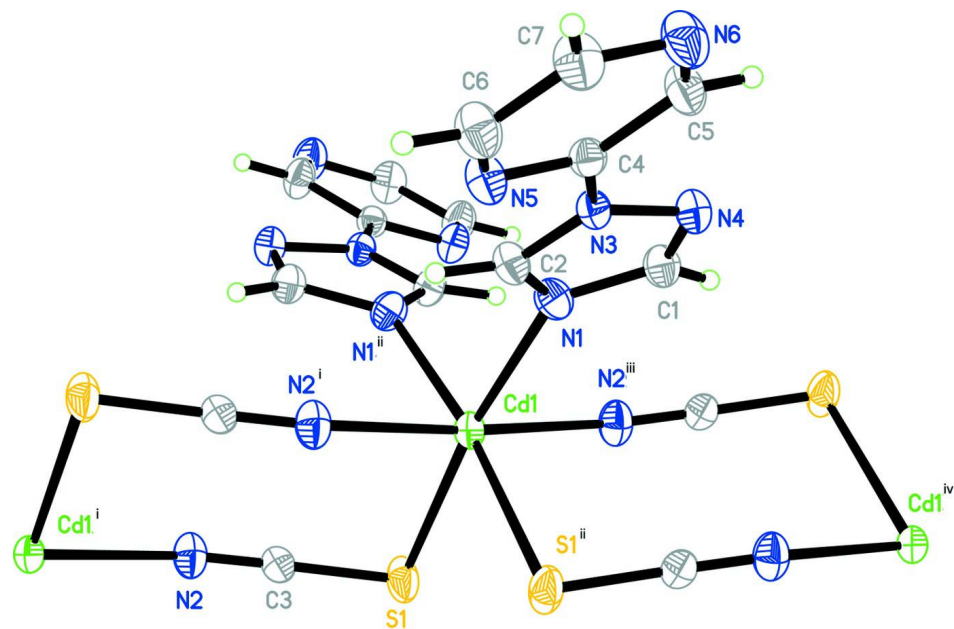
Figure 1

Coordination around the Cd atom with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) -*x* + 1, -*y*, -*z* + 1 (ii) -*x* + 1, *y*, -*z* + 3/2 (iii) *x*, -*y*, *z* + 1/2 (iv) -*x* + 1, -*y*, -*z* + 2]
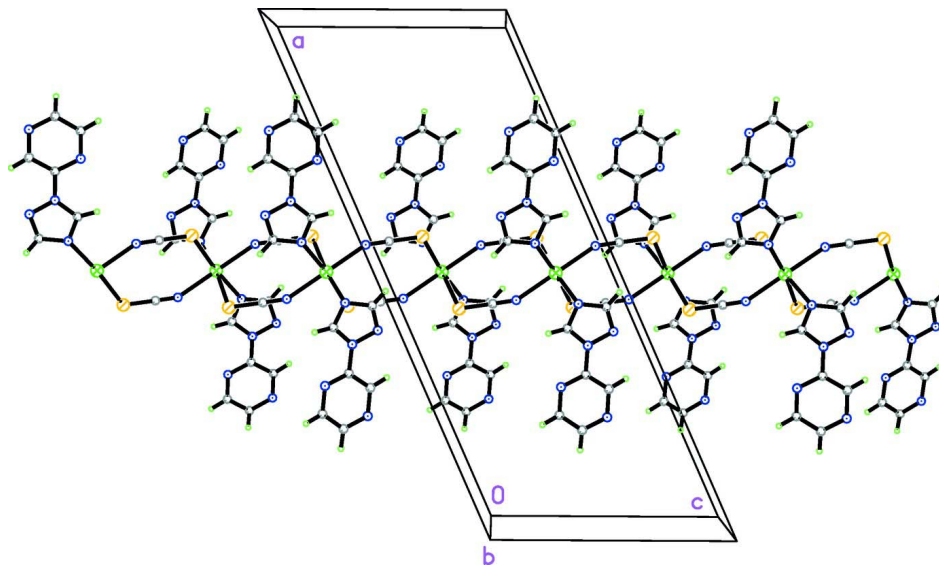
Figure 2

Packing diagram of the title compound.

***catena*-Poly[[bis[2-(1*H*-1,2,4-triazol-1-yl- *κN*⁴)pyrazine]cadmium(II)]-di-*µ*-thiocyanato- *κ*²*S*:*N*;*κ*²*N*:*S*]**

Crystal data

[Cd(NCS)₂(C₆H₅N₅)₂]
$M_r = 522.86$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 25.818 (4) Å

b = 7.4077 (10) Å
c = 11.0276 (15) Å
β = 113.843 (2)°
V = 1929.1 (5) Å³
Z = 4

$F(000) = 1032$

$D_x = 1.800$ Mg m^{-3}

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

Cell parameters from 4306 reflections

$\theta = 2.9–28.3°$

$\mu = 1.38$ mm^{-1}

$T = 298$ K

Block, colourless

$0.41 \times 0.21 \times 0.20$ mm

Data collection

Bruker SMART APEX CCD
   diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
   (*SADABS*; Bruker, 1997)

$T_{min} = 0.602$, $T_{max} = 0.770$

5381 measured reflections

2085 independent reflections

2005 reflections with $I > 2\sigma(I)$

$R_{int} = 0.022$

$\theta_{max} = 27.0°$, $\theta_{min} = 1.7°$

$h = -32\rightarrow23$

$k = -7\rightarrow9$

$l = -10\rightarrow13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.058$

$S = 1.10$

2085 reflections

133 parameters

0 restraints

Primary atom site location: structure-invariant
   direct methods

Secondary atom site location: difference Fourier
   map

Hydrogen site location: inferred from
   neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 1.3229P]$
   where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.35$ e Å^{-3}

$\Delta\rho_{min} = -0.47$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick,
   2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$

Extinction coefficient: 0.0082 (3)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.43493 (9)	0.3626 (3)	0.9002 (2)	0.0392 (5)
H1	0.4636	0.3440	0.9838	0.047*
C2	0.39121 (9)	0.3614 (3)	0.6932 (2)	0.0382 (4)
H2	0.3808	0.3457	0.6027	0.046*
C3	0.56274 (8)	−0.1295 (3)	0.5829 (2)	0.0334 (4)
C4	0.30256 (8)	0.5013 (3)	0.68395 (18)	0.0322 (4)
C5	0.27688 (11)	0.5921 (3)	0.7544 (2)	0.0455 (5)
H5	0.2974	0.6177	0.8437	0.055*
C6	0.22301 (10)	0.5174 (4)	0.4984 (2)	0.0493 (5)
H6	0.2029	0.4949	0.4084	0.059*

C7	0.19638 (11)	0.6044 (3)	0.5671 (3)	0.0505 (6)
H7	0.1586	0.6371	0.5226	0.061*
Cd1	0.5000	0.10030 (3)	0.7500	0.03107 (10)
N1	0.43983 (7)	0.3119 (2)	0.78646 (17)	0.0391 (4)
N2	0.55550 (9)	−0.1113 (3)	0.47410 (19)	0.0455 (5)
N3	0.35900 (7)	0.4377 (2)	0.74783 (16)	0.0317 (3)
N4	0.38687 (8)	0.4394 (2)	0.88241 (17)	0.0377 (4)
N5	0.27701 (8)	0.4642 (3)	0.55708 (17)	0.0422 (4)
N6	0.22297 (9)	0.6433 (3)	0.6954 (2)	0.0535 (5)
S1	0.57240 (3)	−0.15916 (10)	0.73782 (5)	0.05367 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0367 (11)	0.0455 (11)	0.0340 (10)	−0.0001 (9)	0.0129 (9)	−0.0018 (9)
C2	0.0371 (11)	0.0444 (11)	0.0356 (10)	0.0028 (9)	0.0172 (9)	−0.0052 (8)
C3	0.0287 (9)	0.0379 (10)	0.0307 (10)	0.0051 (7)	0.0089 (8)	−0.0017 (7)
C4	0.0329 (9)	0.0331 (9)	0.0335 (10)	0.0004 (7)	0.0162 (8)	0.0008 (7)
C5	0.0460 (13)	0.0563 (14)	0.0358 (11)	0.0117 (10)	0.0181 (10)	−0.0034 (9)
C6	0.0409 (12)	0.0649 (15)	0.0373 (11)	0.0040 (11)	0.0106 (9)	−0.0060 (10)
C7	0.0370 (12)	0.0666 (16)	0.0452 (14)	0.0126 (10)	0.0138 (11)	0.0007 (10)
Cd1	0.03018 (13)	0.03752 (14)	0.02687 (13)	0.000	0.01294 (9)	0.000
N1	0.0349 (9)	0.0439 (10)	0.0404 (9)	0.0014 (7)	0.0171 (7)	−0.0046 (8)
N2	0.0428 (10)	0.0607 (12)	0.0319 (10)	0.0058 (8)	0.0141 (8)	0.0017 (8)
N3	0.0321 (8)	0.0356 (8)	0.0300 (8)	−0.0009 (6)	0.0153 (7)	−0.0026 (6)
N4	0.0367 (9)	0.0465 (9)	0.0302 (9)	0.0006 (7)	0.0138 (7)	−0.0024 (7)
N5	0.0369 (9)	0.0549 (10)	0.0349 (9)	0.0035 (8)	0.0146 (7)	−0.0061 (8)
N6	0.0476 (11)	0.0696 (13)	0.0450 (11)	0.0190 (10)	0.0204 (9)	−0.0017 (10)
S1	0.0699 (4)	0.0614 (4)	0.0296 (3)	0.0323 (3)	0.0201 (3)	0.0093 (2)

Geometric parameters (Å, º)

C1—N4	1.306 (3)	C6—N5	1.337 (3)
C1—N1	1.363 (3)	C6—C7	1.372 (3)
C1—H1	0.9300	C6—H6	0.9300
C2—N1	1.313 (3)	C7—N6	1.331 (3)
C2—N3	1.334 (3)	C7—H7	0.9300
C2—H2	0.9300	Cd1—N2^i	2.3031 (19)
C3—N2	1.145 (3)	Cd1—N2^{ii}	2.3031 (19)
C3—S1	1.639 (2)	Cd1—N1^{iii}	2.3528 (18)
C4—N5	1.312 (3)	Cd1—N1	2.3528 (17)
C4—C5	1.383 (3)	Cd1—S1^{iii}	2.7220 (6)
C4—N3	1.418 (2)	Cd1—S1	2.7220 (6)
C5—N6	1.331 (3)	N2—Cd1^{ii}	2.3031 (19)
C5—H5	0.9300	N3—N4	1.363 (2)
N4—C1—N1	114.71 (19)	N2^{ii}—Cd1—N1	89.56 (7)
N4—C1—H1	122.6	N1^{iii}—Cd1—N1	96.47 (9)

N1—C1—H1	122.6	N2^i—Cd1—S1^iii	96.54 (5)
N1—C2—N3	109.75 (19)	N2^ii—Cd1—S1^iii	86.34 (5)
N1—C2—H2	125.1	N1^iii—Cd1—S1^iii	173.10 (5)
N3—C2—H2	125.1	N1—Cd1—S1^iii	87.01 (5)
N2—C3—S1	178.9 (2)	N2^i—Cd1—S1	86.34 (5)
N5—C4—C5	123.5 (2)	N2^ii—Cd1—S1	96.54 (5)
N5—C4—N3	115.64 (17)	N1^iii—Cd1—S1	87.01 (5)
C5—C4—N3	120.82 (18)	N1—Cd1—S1	173.10 (5)
N6—C5—C4	120.5 (2)	S1^iii—Cd1—S1	90.16 (4)
N6—C5—H5	119.7	C2—N1—C1	103.22 (18)
C4—C5—H5	119.7	C2—N1—Cd1	122.72 (14)
N5—C6—C7	121.9 (2)	C1—N1—Cd1	130.85 (14)
N5—C6—H6	119.1	C3—N2—Cd1^ii	153.59 (19)
C7—C6—H6	119.1	C2—N3—N4	110.16 (17)
N6—C7—C6	122.0 (2)	C2—N3—C4	128.28 (17)
N6—C7—H7	119.0	N4—N3—C4	121.46 (16)
C6—C7—H7	119.0	C1—N4—N3	102.16 (16)
N2^i—Cd1—N2^ii	175.94 (10)	C4—N5—C6	115.50 (19)
N2^i—Cd1—N1^iii	89.56 (7)	C7—N6—C5	116.5 (2)
N2^ii—Cd1—N1^iii	87.73 (7)	C3—S1—Cd1	97.98 (7)
N2^i—Cd1—N1	87.73 (7)		

Symmetry codes: (i) *x*, −*y*, *z*+1/2; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+1, *y*, −*z*+3/2.