Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[(acetonitrile-κN)-μ_3-thiocyanato-$\kappa^3 N$:S:S-μ_2-thiocyanato-$\kappa^2 N$:S-cadmium]

Thorben Reinert,* Inke Jess and Christian Näther

Institut für Anorganische Chemie, Christian-Albrechts-Universität Kiel, Max-Eyth Strasse 2, D-24098 Kiel, Germany
Correspondence e-mail: treinert@ac.uni-kiel.de

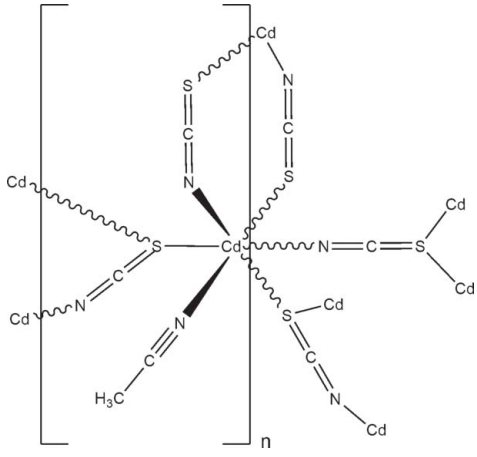
Received 5 June 2013; accepted 7 June 2013

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.090; data-to-parameter ratio = 21.7.

The asymmetric unit of the title compound, $[Cd(NCS)_2(CH_3CN)]_n$, consists of one Cd^{II} cation, two thiocyanate anions and one acetonitrile ligand, all in general positions. The Cd^{II} cation is coordinated by three N atoms of two thiocyanate anions and one acetonitrile ligand, as well as three S atoms of symmetry-related thiocyanate anions within a slightly distorted octahedral coordination environment. The Cd^{II} cations are linked by μ-1,3(*N*,*S*) and μ-1,1,3(*S*,*S*,*N*) thiocyanate anions into layers that are located in the *ab* plane.

Related literature

For related structures, see: Wöhlert *et al.* (2011). For background to transition metal thiocyanate coordination polymers and their magnetic properties, see: Boeckmann *et al.* (2010, 2011).



Experimental

Crystal data

$[Cd(NCS)_2(C_2H_3N)]$
M_r = 269.61
Orthorhombic, *Pbca*
a = 13.0939 (7) Å
b = 8.9752 (5) Å
c = 14.2986 (11) Å
V = 1680.38 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.02 mm^{-1}
T = 200 K
0.10 × 0.09 × 0.05 mm

Data collection

STOE IPDS-1 diffractometer
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2008)
T_{min} = 0.447, T_{max} = 0.799
22741 measured reflections
2022 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.17
2022 reflections
93 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N2	2.254 (3)	Cd1—S2^{i}	2.6253 (9)
Cd1—N1	2.287 (4)	Cd1—S1^{ii}	2.7522 (8)
Cd1—N11	2.340 (3)	Cd1—S1^{iii}	2.8780 (8)

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

Data collection: *X-AREA* (Stoe & Cie, 2008); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS92* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL92* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2011); software used to prepare material for publication: *SHELXTL* and *publCIF* (Westrip, 2010).

We gratefully acknowledge financial support by the DFG (project No. NA 720/5–1) and the State of Schleswig–Holstein. We thank Professor Dr Wolfgang Bensch for the opportunity to use his experimental facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2553).

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supporting information

Acta Cryst. (2013). E**69**, m398 [https://doi.org/10.1107/S1600536813015870]

Poly[(acetonitrile-κN)-μ_3-thiocyanato-$\kappa^3 N$:S:S-μ_2-thiocyanato-$\kappa^2 N$:S-cadmium]

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S1. Comment

The structure determination of the title compound was performed as part of a project on the synthesis of new coordination polymers based on transition metal thiocyanates and the investigations on their magnetic properties (Boeckmann *et al.* (2010, 2011)). Within this project, we have reacted cadmium(II)thiocyanate with 4-*tert*-butylpyridine in acetonitrile, which resulted in the formation of crystals of the title compound by accident. In the crystal structure the Cd cations are surrounded by three N atoms of two *N*-bonded μ-1,3-briding thiocyanato anions and one acetonitril ligand as well as three S atoms of three *S*-bonded μ-1,1,3-bridging thiocyanato anions in a slightly distorted octahedral geometry (Fig. 1 and Tab. 1). The Cd···N distances range from 2.2544 (28) Å to 2.3396 (28) Å, the Cd···S distances from 2.6254 (9) Å to 2.8781 (8) Å (Table 1). The Cd cations are linked into dimeric units by pairs of μ-1,3-briding thiocyanato anions that are further connected into chains by single μ-1,3-briding anionic ligands. These chains are further connected by pairs of μ-1,1,3-bridging thiocyanato anions into layers which are parallel to the crystallographic *a*-*b*-plane.

S2. Experimental

The title compound was obtained accidently during the reaction of 68.6 mg $Cd(NCS)_2$ (0.30 mmol) with 11.1 μL 4-*tert*-butylpyridine (0.08 mmol) in 1.0 ml acetonitrile at RT in a closed 3 ml snap cap vial. After several months colourless blocks of the title compound were obtained.

S3. Refinement

The H atoms were positioned with idealized geometry, allowed to rotate but not to tip and were refined isotropic with U_{iso}(H) = 1.5 U_{eq}(C) of the parent atom using a riding model with C—H = 0.98 Å.

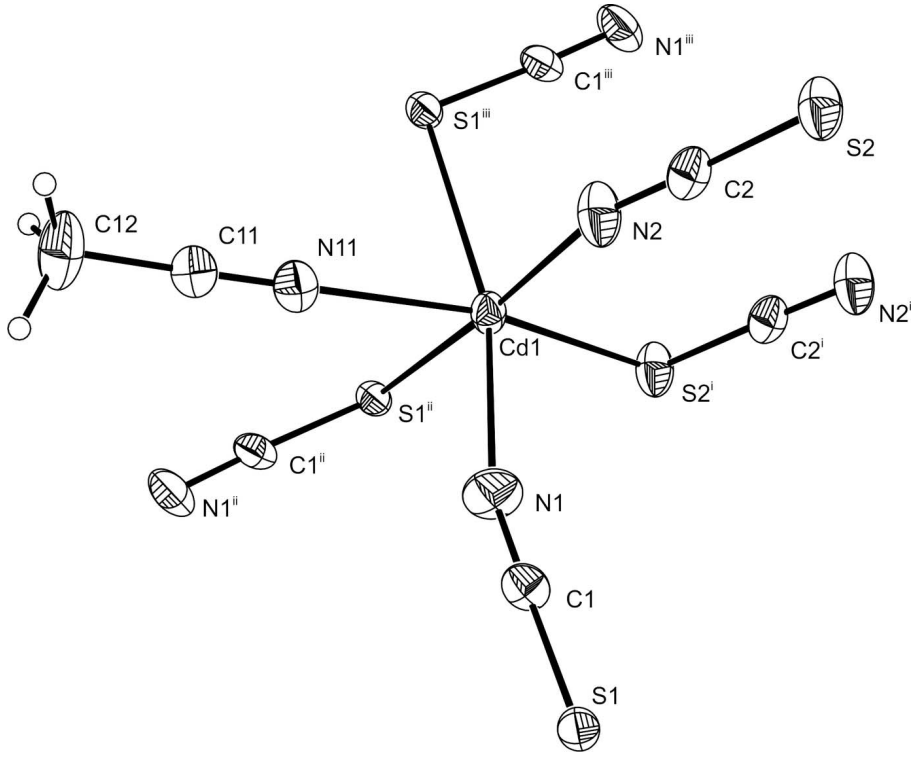

Figure 1

Crystal structure of the title compound with labelling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: i = -*x* + 1, -*y* + 2, -*z* + 1; ii = *x* - 1/2, -*y* + 3/2, -*z* + 1; iii = -*x* + 3/2, *y* - 1/2, *z*; iv = *x* + 1/2, -*y* + 3/2, -*z* + 1; v = -*x* + 3/2, *y* + 1/2, *z*.

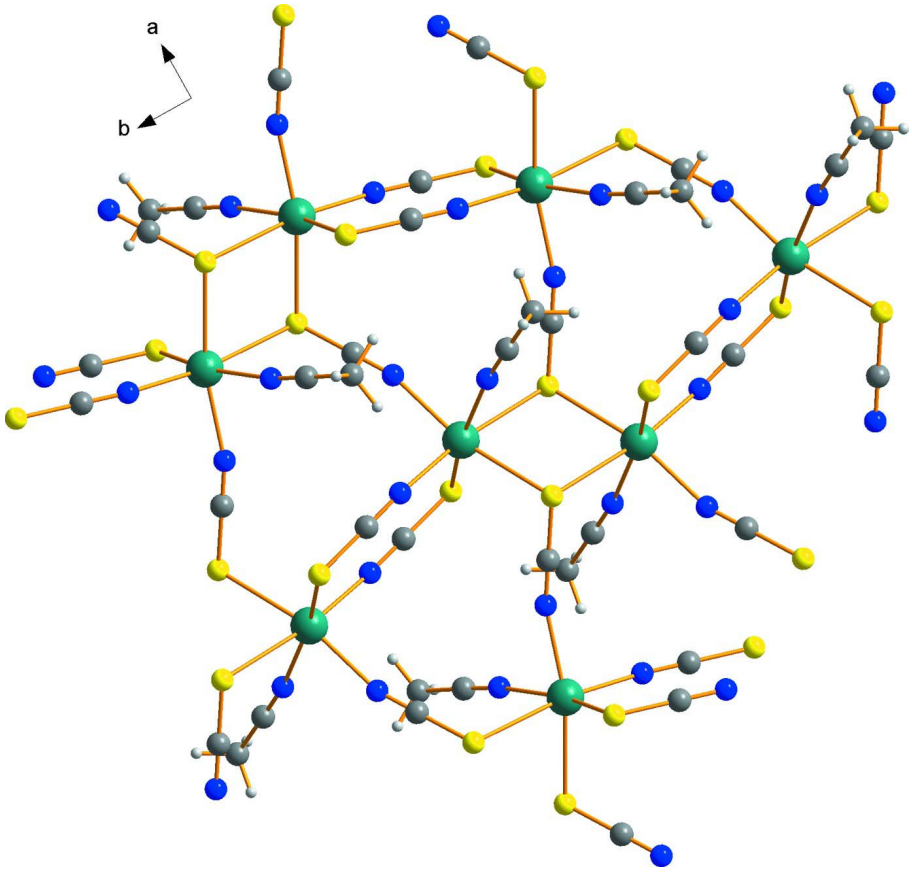

Figure 2

Crystal structure of the title compound with view along the crystallographic *c*-axis.

Poly[(acetonitrile-κN)-μ_3-thiocyanato-$\kappa^3 N$:*S*:*S*-μ_2-thiocyanato-$\kappa^2 N$:*S*-cadmium]

Crystal data

$[Cd(NCS)_2(C_2H_3N)]$
$M_r = 269.61$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 13.0939\ (7)$ Å
$b = 8.9752\ (5)$ Å
$c = 14.2986\ (11)$ Å
$V = 1680.38\ (18)$ Å^3
$Z = 8$
$F(000) = 1024$
$D_x = 2.131$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 22741 reflections
$\theta = 1.9$–$28.2°$
$\mu = 3.02$ mm^{-1}
$T = 200$ K
Block, colourless
0.10 × 0.09 × 0.05 mm

Data collection

STOE IPDS-1 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Phi scans
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2008)
$T_{min} = 0.447$, $T_{max} = 0.799$
22741 measured reflections
2022 independent reflections
1943 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 28.1°$, $\theta_{min} = 3.1°$
$h = -17 \rightarrow 17$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.090$
$S = 1.17$
2022 reflections
93 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
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 2.768P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.09$ e Å^{-3}
$\Delta\rho_{min} = -0.89$ e Å^{-3}
Extinction correction: *SHELXL92* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0100 (7)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.580143 (17)	0.70475 (2)	0.516796 (17)	0.02222 (14)
N1	0.7434 (3)	0.7780 (4)	0.4831 (2)	0.0369 (8)
C1	0.8127 (2)	0.8423 (4)	0.4550 (2)	0.0248 (6)
S1	0.91085 (5)	0.93385 (8)	0.40941 (5)	0.02174 (19)
N2	0.5499 (3)	0.9136 (3)	0.5999 (2)	0.0360 (7)
C2	0.5257 (2)	1.0352 (3)	0.6171 (2)	0.0264 (6)
S2	0.49199 (8)	1.20580 (8)	0.64506 (6)	0.0318 (2)
N11	0.6540 (2)	0.5645 (3)	0.6370 (2)	0.0298 (6)
C11	0.6836 (2)	0.4805 (4)	0.6898 (2)	0.0271 (6)
C12	0.7197 (4)	0.3726 (5)	0.7579 (3)	0.0470 (10)
H12A	0.6824	0.2789	0.7500	0.070*
H12B	0.7083	0.4113	0.8211	0.070*
H12C	0.7929	0.3550	0.7484	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01867 (18)	0.01728 (18)	0.03070 (19)	−0.00145 (7)	−0.00221 (7)	0.00423 (7)
N1	0.0250 (16)	0.0377 (19)	0.048 (2)	−0.0124 (13)	0.0000 (13)	−0.0006 (13)
C1	0.0195 (13)	0.0244 (14)	0.0305 (14)	−0.0026 (12)	−0.0042 (11)	−0.0042 (12)
S1	0.0181 (3)	0.0197 (4)	0.0274 (4)	−0.0017 (2)	−0.0021 (2)	0.0012 (3)
N2	0.0481 (18)	0.0210 (13)	0.0388 (15)	0.0052 (12)	−0.0079 (14)	−0.0011 (12)
C2	0.0282 (14)	0.0249 (14)	0.0260 (13)	−0.0030 (12)	−0.0053 (11)	0.0051 (11)

S2	0.0458 (5)	0.0209 (4)	0.0285 (4)	0.0052 (3)	−0.0061 (3)	−0.0017 (3)
N11	0.0296 (13)	0.0277 (13)	0.0322 (13)	0.0014 (11)	−0.0037 (11)	0.0020 (11)
C11	0.0276 (14)	0.0254 (14)	0.0283 (14)	−0.0016 (12)	−0.0055 (12)	−0.0017 (12)
C12	0.053 (2)	0.039 (2)	0.049 (2)	−0.0052 (17)	−0.0246 (19)	0.0138 (17)

Geometric parameters (Å, º)

Cd1—N2	2.254 (3)	S1—Cd1^{v}	2.8780 (8)
Cd1—N1	2.287 (4)	N2—C2	1.163 (4)
Cd1—N11	2.340 (3)	C2—S2	1.643 (3)
Cd1—S2^{i}	2.6253 (9)	S2—Cd1^{i}	2.6253 (9)
Cd1—S1^{ii}	2.7522 (8)	N11—C11	1.135 (4)
Cd1—S1^{iii}	2.8780 (8)	C11—C12	1.452 (5)
N1—C1	1.148 (5)	C12—H12A	0.9800
C1—S1	1.659 (3)	C12—H12B	0.9800
S1—Cd1^{iv}	2.7523 (8)	C12—H12C	0.9800
N2—Cd1—N1	92.08 (13)	N1—C1—S1	177.3 (3)
N2—Cd1—N11	97.64 (11)	C1—S1—Cd1^{iv}	104.43 (11)
N1—Cd1—N11	85.58 (11)	C1—S1—Cd1^{v}	103.92 (11)
N2—Cd1—S2^{i}	98.45 (8)	Cd1^{iv}—S1—Cd1^{v}	98.29 (2)
N1—Cd1—S2^{i}	93.60 (9)	C2—N2—Cd1	160.0 (3)
N11—Cd1—S2^{i}	163.90 (7)	N2—C2—S2	178.1 (3)
N2—Cd1—S1^{ii}	91.84 (9)	C2—S2—Cd1^{i}	99.62 (11)
N1—Cd1—S1^{ii}	164.41 (9)	C11—N11—Cd1	170.7 (3)
N11—Cd1—S1^{ii}	78.95 (7)	N11—C11—C12	179.1 (4)
S2^{i}—Cd1—S1^{ii}	100.74 (3)	C11—C12—H12A	109.5
N2—Cd1—S1^{iii}	172.22 (9)	C11—C12—H12B	109.5
N1—Cd1—S1^{iii}	95.29 (9)	H12A—C12—H12B	109.5
N11—Cd1—S1^{iii}	85.43 (7)	C11—C12—H12C	109.5
S2^{i}—Cd1—S1^{iii}	78.63 (2)	H12A—C12—H12C	109.5
S1^{ii}—Cd1—S1^{iii}	81.71 (2)	H12B—C12—H12C	109.5
C1—N1—Cd1	163.1 (3)		

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