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catena-Poly[[bis(3-aminobenzoic acid-κN)-μ-thiocyanato-$\kappa^4 N{:}S;S{:}N$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.069
wR factor = 0.042
Data-to-parameter ratio = 13.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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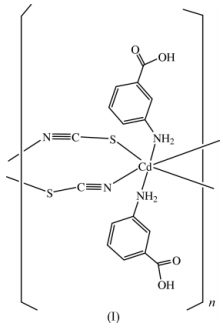
The title compound, $[Cd(\mu\text{-}SCN)_2(C_7H_7NO_2)_2]_n$, has been prepared from the reaction of 3-aminobenzoic acid, NH_4SCN and $Cd(NO_3)_2{\cdot}6H_2O$ in MeOH/H_2O. It consists of one-dimensional polymeric chains, which are extended into a two-dimensional layer structure by head-to-head hydrogen bonds involving carboxyl groups from adjacent chains.

Comment

Crystal engineering of inorganic/organic hybrid materials is currently of great interest, owing to their interesting structural topologies and potential application in materials science, such as ion-exchange, adsorption, molecular recognition, catalysis and magnetism (Aakeroy *et al.*, 1999; Hagrman *et al.*, 1999). Considerable effort has been devoted to supramolecular networks organized and held together by means of coordination covalent bonds, hydrogen bonds, and their combination, because of the strength, directionality and complementarity of coordination bonds and hydrogen bonds, as well as extensive applications of hydrogen-bonded complexes in crystal engineering (Carlucci *et al.*, 1997; Dong *et al.*, 2000; Moulton & Zaworotko, 2001). A number of promising supramolecular complexes have been designed and constructed from mononuclear (Kuehl *et al.*, 2001; Pan *et al.*, 2001) or polynuclear coordination complexes (Copp *et al.*, 1993; Liang *et al.*, 2001) and lower-dimensional coordination polymers (Chen & Chen, 2002; Dong *et al.*, 2000; Goher & Mautner, 2001; Prior & Rosseinsky, 2001) through using hydrogen bonds as linkers. Here we report a hydrogen-bonded two-dimensional complex, $[Cd(\mu\text{-SCN-N,S})_2(HL)_2]_n$ (HL = 3-aminobenzoic acid), constructed from one-dimensional polymeric chains *via* head-to-head carboxylic acid hydrogen bonds.



(I)

The single-crystal X-ray diffraction analysis reveals that the title compound contains HL ligands attached to polymeric cadmium-thiocyanate chains in a *trans* arrangement. As shown in Fig. 1, each Cd(II) is in a distorted octahedral environment and is coordinated by two N atoms from HL ligands, two independent thiocyanate S atoms and another two thiocyanate

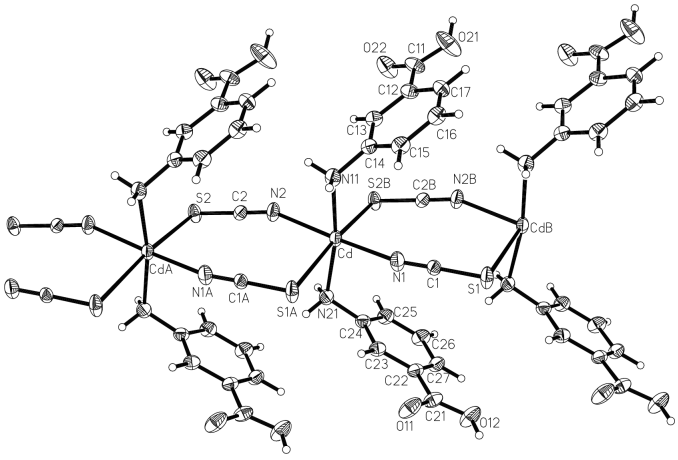


Figure 1
A section of the one-dimensional chain of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

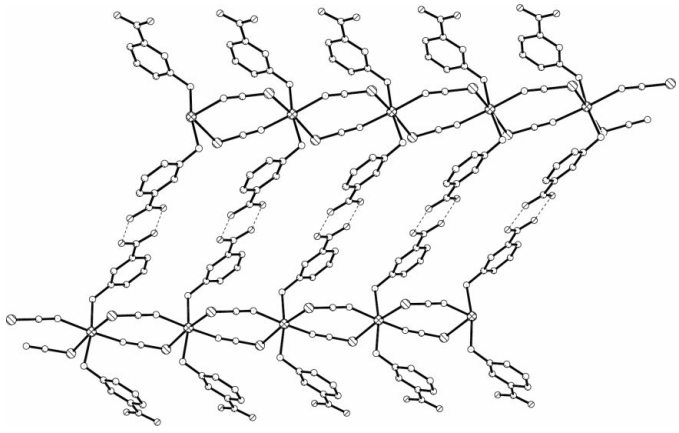


Figure 2
Hydrogen bonds between adjacent chains, forming a two-dimensional layer.

N atoms. Each pair of adjacent Cd(II) atoms is bridged by two independent SCN^- ligands to form a one-dimensional cadmium-thiocyanate chain consisting of eight-membered $(N-C-S-Cd)_2$ rings. The Cd···Cd separation in the eight-membered rings is 5.8547 (2) Å, which is close to those in cadmium-thiocyanate chains (Chen *et al.*, 1999; Chen & Chen, 2002; Taniguchi *et al.*, 1986; Taniguchi *et al.*, 1987). The bond distances of $Cd-N_{HL}$ [2.249 (5) and 2.296 (5) Å] are longer than that of $Cd-N_{SCN}$ [2.375 (4) and 2.386 (4) Å]. The bond distances of Cd—S are 2.7001 (14) and 2.8054 (14) Å, comparable with those in the above cadmium-thiocyanate complexes. The remaining two positions around the six-coordinate Cd(II) centers in the polymeric chain are occupied by N atoms of two independent H*L* ligands with a N11—Cd—N21 bond angle of 170.50 (2)°. The carboxylic acid groups in the H*L* ligands are connected *via* head-to-head O—H···O hydrogen bonds [$R_2^2(8)$ in graph set notation (Bernstein *et al.*, 1995)], connecting one-dimensional $[Cd(SCN)_2(HL)_2]_n$ chains into an infinite two-dimensional layer structure. There are no short contacts or noteworthy aryl–aryl interactions between adjacent chains or between neighboring layers.

Experimental

A solution of $Cd(NO_3)_2\cdot 6H_2O$ (0.15 g, 0.5 mmol) and NH_4SCN (0.08 g, 1 mmol) in H_2O (5 ml) was added slowly to a solution of H*L* (0.07 g, 0.5 mmol) in MeOH (10 ml). The reaction mixture was stirred for 30 min. and gave a colorless solution, which was filtered. Pale yellow crystals of the title compound were obtained by leaving the resulting solution in air for 2–3 weeks.

Crystal data

$[Cd(NCS)_2(C_7H_7NO_2)_2]$	D_x = 1.740 Mg m^{-3}
M_r = 502.83	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 82 reflections
a = 14.6733 (1) Å	θ = 1.7–25.0°
b = 5.8547 (2) Å	μ = 1.38 mm^{-1}
c = 22.3503 (5) Å	T = 293 (2) K
β = 90.730 (2)°	Plate, pale yellow
V = 1919.91 (8) Å^3	0.50 × 0.30 × 0.08 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3372 independent reflections
ω scans	2508 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.034
T_{min} = 0.614, T_{max} = 0.895	θ_{max} = 25.0°
6782 measured reflections	$h = -15 \rightarrow 17$
	$k = -4 \rightarrow 6$
	$l = -18 \rightarrow 26$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 4.0666P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.069	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.042	$\Delta\rho_{max}$ = 1.15 e Å^{-3}
S = 1.07	$\Delta\rho_{min}$ = −0.91 e Å^{-3}
3372 reflections	
244 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cd—N1	2.250 (5)	Cd—S1^{ii}	2.805 (1)
Cd—N2	2.297 (5)	O11—C11	1.258 (7)
Cd—N21	2.374 (4)	O12—C11	1.253 (7)
Cd—N11	2.386 (4)	O21—C21	1.268 (7)
Cd—S2^{i}	2.700 (1)	O22—C21	1.259 (7)
N1—Cd—N2	173.02 (18)	N11—Cd—S2^{i}	98.60 (10)
N1—Cd—N21	97.39 (17)	N1—Cd—S1^{ii}	84.35 (12)
N2—Cd—N21	88.53 (16)	N2—Cd—S1^{ii}	92.63 (12)
N1—Cd—N11	88.77 (17)	N21—Cd—S1^{ii}	84.13 (11)
N2—Cd—N11	84.90 (17)	N11—Cd—S1^{ii}	89.29 (10)
N21—Cd—N11	170.49 (16)	S2^{i}—Cd—S1^{ii}	172.10 (5)
N1—Cd—S2^{i}	95.41 (12)	O12—C11—O11	123.6 (5)
N2—Cd—S2^{i}	88.45 (12)	O22—C21—O21	123.7 (5)
N21—Cd—S2^{i}	88.07 (11)		

Symmetry codes: (i) $x, 1+y, z$; (ii) $x, y-1, z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O11—H11···O22^{iii}	0.82	1.82	2.618 (6)	166
O21—H21···O12^{iv}	0.82	1.81	2.622 (5)	169

Symmetry codes: (iii) $\frac{1}{2}+x, \frac{7}{2}-y, \frac{1}{2}+z$; (iv) $x-\frac{1}{2}, \frac{7}{2}-y, z-\frac{1}{2}$.

The positions of H atoms were generated geometrically (C—H = 0.93–0.96, N—H = 0.90, O—H = 0.82 Å), assigned isotropic displacement parameters and allowed to ride on their parent atoms. The maximum electron-density peak lies close to the Cd^{II} atom.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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