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catena-Poly[[[diaquacadmium(II)]-di-μ-thiocyanato] bis(2-amino-4,6-dimethylpyrimidine)]

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Key indicators

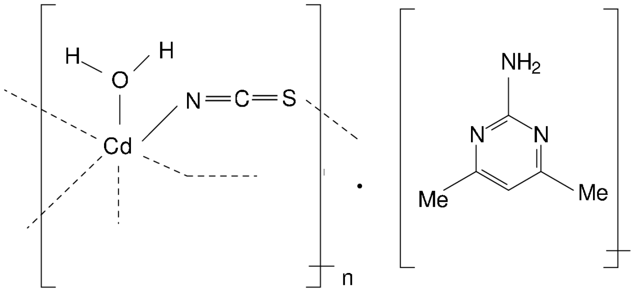
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.033
wR factor = 0.086
Data-to-parameter ratio = 20.0

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

The title complex, $\{[Cd(NCS)_2(H_2O)_2]\cdot 2C_6H_9N_3\}_n$, crystalizes in the triclinic space group $P\overline{1}$. The asymmetric unit contains one 2-amino-4,6-dimethylpyrimidine molecule, a thiocyanate ion, a water molecule and a cadmium ion (site symmetry $\overline{1}$). The cadmium ions are symmetrically doubly bridged by thiocyanate ions, leading to a polymeric chain motif. The octahedral coordination geometry of cadmium is completed by a pair of inversion-related water molecules. The 2-aminopyrimidine molecules are not coordinated to cadmium but are hydrogen-bonded to the coordinated water molecules and thiocyanate ions. There is also a pyrimidine–pyrimidine interaction *via* an N—H$\cdots$N hydrogen bond.

Comment

Thiocyanate is an ambidentate ion which can coordinate to a metal *via* its S or N atoms. Thiocyanate ions can also bridge metal ions by employing both the N and S atoms for coordination. The crystal structures of doubly bridged Cu^{II} (Julve *et al.*, 1993; Liu *et al.*, 2003), Mn^{II} (Barandika *et al.*, 2000), Ag^{I} (Ren *et al.*, 2001) and Cd^{II} (Cavalca *et al.*, 1960) complexes are known. The thiocyanate ion can also act as an acceptor in hydrogen-bond interactions. Studies of hydrogen-bonding interactions between pyrimidines and coordinated ligands are of current interest (Suksangpanya *et al.*, 2004). The present study is aimed at increasing our understanding of the interplay of coordination and hydrogen bonding in determining supramolecular organization.



(I)

The title compound, poly[aquabis(μ-thiocyanato)-cadmium(II): (2-amino-4,6-dimethylpyrimidine)], $[Cd(NCS)_2(H_2O)_2]_n\cdot 2(C_6H_9N_3)_n$, (I) is shown in Fig. 1. The asymmetric unit contains one 2-amino-4,6-dimethylpyrimidine molecule, a thiocyanate ion, a water molecule, and a cadmium ion, the last of these occupying an inversion centre. The cadmium ions are symmetrically doubly bridged by thiocyanate ions, leading to a polymeric chain motif. A similar

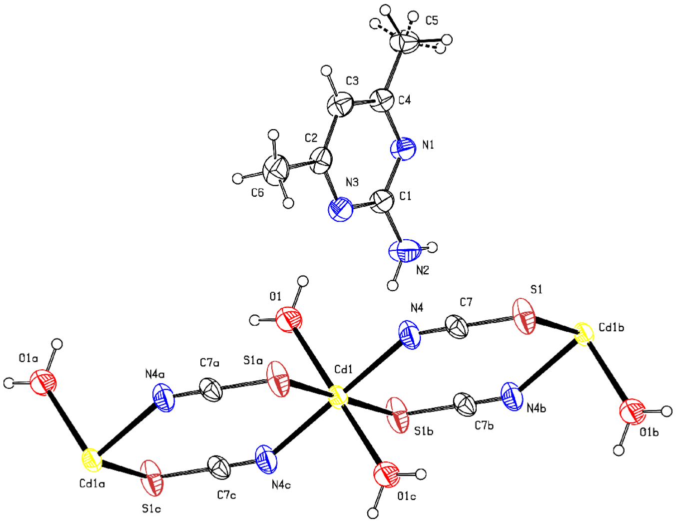


Figure 1
Fragment of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms). [Symmetry codes: (*a*) $1 - x$, $-y$, $-z$, (*b*) $1 + x$, y, z (*c*) $2 - x$, $-y$, $-z$.]

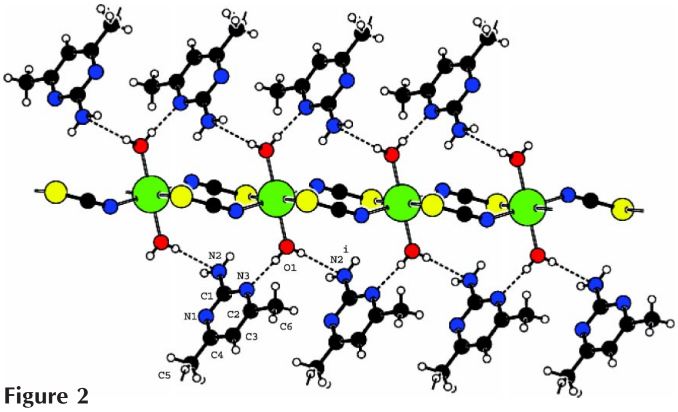


Figure 2
Hydrogen bonding in (I). Colour key: Cd green, O red, N blue, C black, H white. [Symmetry code: (i) $1 + x$, y, z.]

structural motif was observed in bis-ethylenethiourea cadmium(II)thiocyanate (Cavalca *et al.*, 1960). In (I), the octahedral coordination geometry of cadmium is completed by a pair of inversion-related water molecules. The bond distances [Cd—N = 2.284 (2) Å, Cd—S = 2.695 (8) Å; Cd—O1*W* = 2.289 (2) Å] agree with those reported in the literature for related materials (Mostafa *et al.*, 2000). The thiocyanate ligands are almost linear [(N—C—S) = 178.7 (3)°]. The 2-aminopyrimidine molecules are not coordinated to cadmium but are hydrogen-bonded to the coordinated water molecules and thiocyanate ions as shown in Fig. 2. There is also a pyrimidine–pyrimidine interaction *via* N—H···N hydrogen bonds (Table 2). The geometrical parameters of the 2-aminopyrimidine species are normal (Aoki & Yamazaki, 1989).

Experimental

An aqueous solution of cadmium nitrate [$Cd(NO_3)_2 \cdot 4H_2O$; 77.10 mg] in water (5 ml) was added to a solution of NH_4NCS (76.1 mg in 5 ml water). The mixture was stirred for 20 min. The ligand 2-amino-4,6-dimethylpyrimidine (63.25 mg dissolved in 10 ml methanol) was added slowly to this mixture. The resultant solution was stirred for 20 min and then filtered. After a few days, colourless crystals of (I) were obtained from the filtrate upon slow evaporation of the solvent.

Crystal data

$[Cd(NCS)_2(H_2O)_2] \cdot 2C_6H_9N_3$
$M_r = 510.92$
Triclinic, $P\overline{1}$
$a = 5.7221$ (4) Å
$b = 10.3906$ (8) Å
$c = 10.4865$ (8) Å
$\alpha = 117.4420$ (10)°
$\beta = 101.6770$ (8)°
$\gamma = 92.9510$ (10)°
$V = 534.31$ (7) Å^3
$Z = 1$
$D_x = 1.588$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4215 reflections
$\theta = 2.3$–28.3°
$\mu = 1.24$ mm^{-1}
$T = 293$ (2) K
Plate, colourless
0.48 × 0.48 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.447$, $T_{max} = 0.830$
4215 measured reflections
2560 independent reflections
2460 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 28.3°$
$h = -7 \rightarrow 7$
$k = -12 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.086$
$S = 1.06$
2560 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 0.1483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.90$ e Å^{-3}
$\Delta\rho_{min} = -1.01$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.018 (5)

Table 1
Selected bond lengths (Å).

Cd1—N4	2.284 (2)	Cd1—S1^i	2.6954 (8)
Cd1—O1	2.289 (2)		

Symmetry code: (i) $1 + x$, y, z.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H11···N3	0.92	1.83	2.742 (3)	171
O1—H12···N2^i	0.91	2.27	3.166 (4)	165
N2—H2*A*···N1^{ii}	0.86	2.19	3.052 (4)	177
N2—H2*B*···S1^{iii}	0.86	2.92	3.719 (3)	156

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

The H atoms of the water molecules were located in a difference Fourier map and refined as riding in their as-found relative positions. The other H atoms were placed in idealized locations (C—H = 0.96 Å and N—H = 0.86 Å). The constraint $U_{iso}(H) = 1.2U_{eq}$(carrier) or $1.5U_{eq}$(methyl carrier) was applied as appropriate. The H atoms attached to the methyl atom C5 appeared to be disordered over two sites. Two sets of H-atom positions were defined for this group and constrained refinement of the site-occupation factors led to a value of 0.62 (8) for the major component and 0.38 (8) for the minor component.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SHELXTL* (Bruker, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997);

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program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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