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Tetrakis(4-amino-3-methylpyridine)diisothiocyanatocadmium(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.021
wR factor = 0.059
Data-to-parameter ratio = 16.8

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

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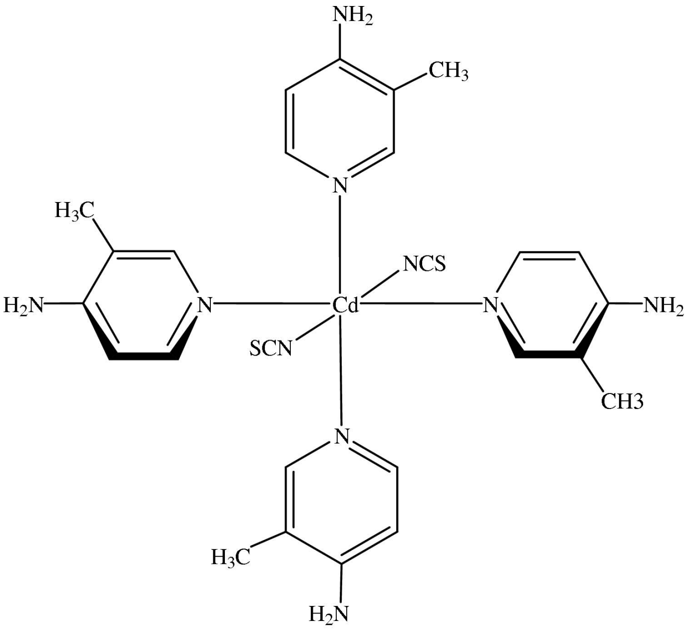
In the centrosymmetric title compound, $[Cd(NCS)_2(C_6H_8N_2)_4]$, the Cd^{II} atom is in a distorted octahedral environment. The crystal structure is stabilized by N—H$\cdots$S hydrogen bonds and weak N—H$\cdots\pi$ and C—H$\cdots\pi$ interactions.

Comment

Pyridine derivatives have been widely used in synthesizing optical materials and medical products (Miller *et al.*, 2002; Haginoya *et al.*, 2004; Tian *et al.*, 1999; Chantrapromma *et al.*, 2005). Asymmetric pyridine derivatives have nonlinear optical properties (Dong *et al.*, 1997), and a typical example is 3-methyl-4-nitropyridine-*N*-oxide. In general, the stability of optical materials made from metal complexes is superior to those of organic optical materials. It is expected that the design and synthesis of asymmetric metal pyridinyl compounds may be a possible way of obtaining potential non-linear optical materials (Tian *et al.*,1999). In this paper, the crystal structure of the title compound, (I), is reported.



(I)

Compound (I) consists of discrete neutral centrosymmetric $[Cd(NCS)_2L_4]$ molecules (Fig. 1), where L is 3-methyl-4-aminopyridine. The Cd atom lies on a crystallographic inversion centre and is in a distorted octahedral environment, with two isothiocyanate and four L ligands coordinated to the Cd^{II} atom through the N atoms. The three *trans* angles at the Cd^{II}

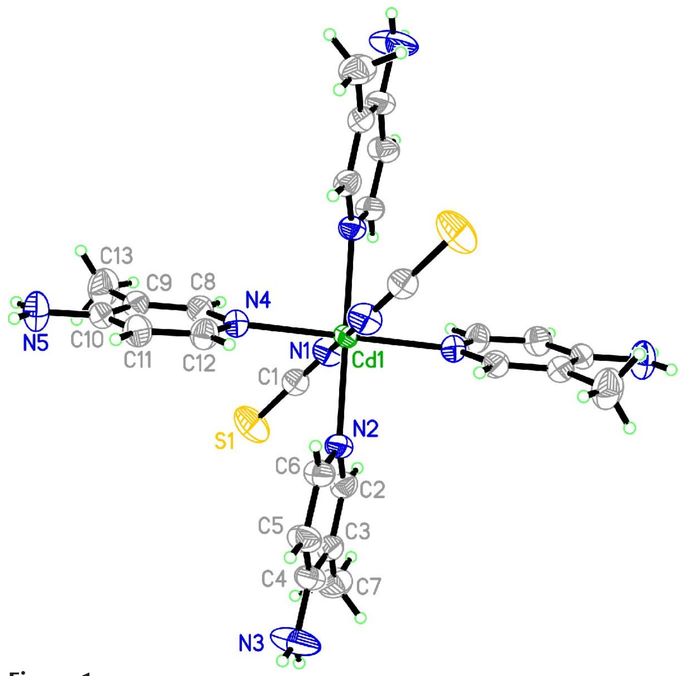


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The unlabelled atoms are related to the labelled atoms by ($\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$).

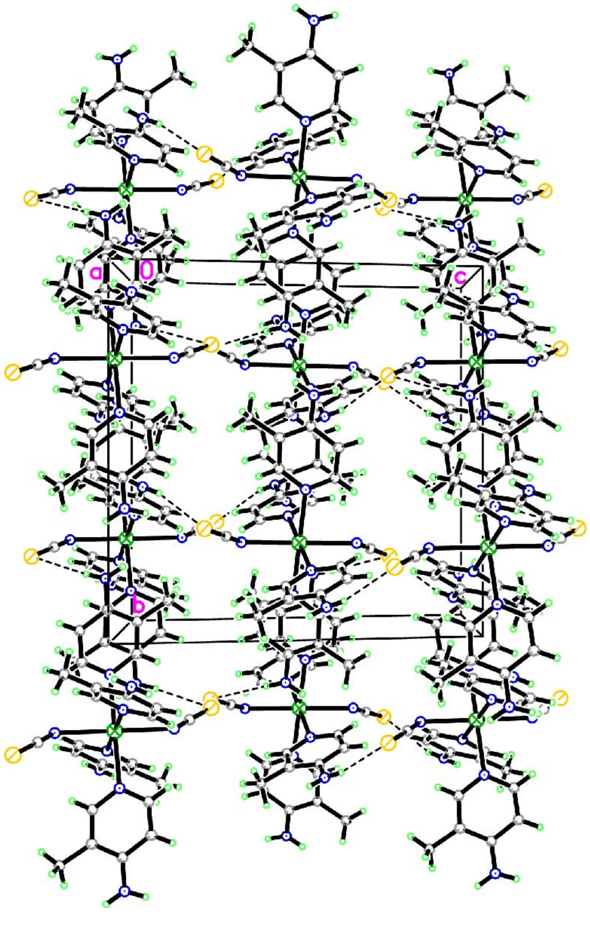


Figure 2
The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

atom are exactly 180° by virtue of crystallographic symmetry, and the other angles subtended at the Cd^{II} atom are close to 90°, ranging from 88.56 (5) to 91.44 (5)° (Table 1). The Cd—N distances are comparable to those observed in closely related structures (Banerjee *et al.*, 2005; Jiang *et al.*, 2002). The dihedral angle between the two independent pyridine rings is 87.91 (5)°.

In the crystal structure, the molecules are linked together through N—H$\cdots$S intermolecular interactions (Table 2). In addition, weak N—H$\cdots\pi$ and C—H$\cdots\pi$ interactions involving the N2/C2–C6 (centroid *Cg*1) and N4/C8–C12 (centroid *Cg*2) pyridine rings are also observed.

Experimental

3-Methyl-4-aminopyridine was synthesized according to the method of Zhang *et al.* (1999). Cadmium thiocyanate and 3-methyl-4-aminopyridine (1:2) were added to dry methanol. The mixture was stirred for 4 h at room temperature and then filtered. Colourless transparent single crystals were grown from the filtrate at ambient temperature over a period of a few days.

Crystal data

$[Cd(NCS)_2(C_6H_8N_2)_4]$
$M_r = 661.17$
Monoclinic, $C2/c$
$a = 14.4737 (5)$ Å
$b = 14.6771 (5)$ Å
$c = 15.1822 (6)$ Å
$\beta = 106.877 (1)°$
$V = 3086.28 (19)$ Å^3
$Z = 4$
$D_x = 1.423$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8164 reflections
$\theta = 2.7–26.0°$
$\mu = 0.88$ mm^{-1}
$T = 293 (2)$ K
Block, colourless
0.50 × 0.50 × 0.44 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.652$, $T_{max} = 0.680$
8164 measured reflections
3031 independent reflections
2763 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 26.0°$
$h = -17 \rightarrow 12$
$k = -18 \rightarrow 17$
$l = -17 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.059$
$S = 1.12$
3031 reflections
180 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0292P)^2 + 2.4296P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.70$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N4	2.3545 (14)	Cd1—N1	2.3681 (17)
Cd1—N2	2.3571 (14)		
N4—Cd1—N4^i	180	N2—Cd1—N1^i	89.13 (6)
N4—Cd1—N2^i	88.56 (5)	N4—Cd1—N1	90.61 (5)
N4—Cd1—N2	91.44 (5)	N2—Cd1—N1	90.87 (6)
N2^i—Cd1—N2	180	N1^i—Cd1—N1	180
N4—Cd1—N1^i	89.39 (5)		

Symmetry code: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N3—H3$A\cdots$S1^{ii}	0.86	2.74	3.520 (2)	152
N5—H5$A\cdots$S1^{iii}	0.86	2.77	3.624 (2)	171
N3—H3$B\cdots Cg2^{iv}$	0.86	2.69	3.328 (2)	132
N5—H5$B\cdots Cg1^{iii}$	0.86	2.64	3.324 (2)	137
C7—H7$C\cdots Cg1^{v}$	0.96	2.85	3.545 (2)	130

Symmetry codes: (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+1, -y, -z+1$; (iv) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (v) $-x+1, -y+1, -z+1$. $Cg1$ and $Cg2$ are the centroids of the N2/C2–C6 and N4/C8–C12 pyridine rings, respectively.

H atoms were positioned geometrically and were treated as riding on their parent atoms with C—H = 0.93 (aromatic) and 0.96 Å (methyl), N—H = 0.86 Å, and U_{iso}(H) = $1.5U_{eq}$(C) for the methyl H atoms and $1.2U_{eq}$(C,N) for other H atoms. A rotating group model was used for the methyl groups.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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* and *PLATON* (Spek, 2003).

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References

Banerjee, S., Wu, B., Lassahn, P. G., Janiak, C. & Ghosh, A. (2005). *Inorg. Chim. Acta*, **358**, 535–544.

Chantrapromma, S., Fun, H. K., Feng, X. J., Yang, J. X., Wu, J. Y. & Tian, Y. P. (2005). *Acta Cryst.* E**61**, m733–m735.

Dong, M. B., Li, S. X. & Li, W. S. (1997). *J. Syn. Cryst.* **26**, 78–81.

Haginoya, N., Kobayashi, S., Komoriya, S., Yoshino, T., Nagata, T., Hirokawa, Y. & Nagahara, T. (2004). *Bioorg. Med. Chem.* **12**, 5579–5586.

Jiang, X. H., Zhang, W. G., Zhong, Y. & Wang, S. L. (2002). *Molecules*, **7**, 549–553.

Miller, W. H., Seefeld, M. A., Newlander, K. A., Uzinskas, I. N., Burgess, W. J., Heerding, D. A., Yuan, C. C., Head, M. S., Payne, D. J., Rittenhouse, S. F., Moore, T. D., Pearson. S. C., Berry, V., Dewolf, W. E. Jr, Keller, P. M., Polizzi, B. J., Qiu, X., Janson, C. A. & Huffman, W. F. (2002). *J. Med. Chem.* **45**, 3246–3256.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Tian, Y. P., Yu, W. T., Fang, Q., Yuan, D. R. & Jiang, M. H. (1999). *Acta Cryst.* C**55**, 1639–1641.

Zhang, H., Wang, X. M. Zhang, K & Teo, B. K. (1999). *Coord. Chem. Rev.* **183**, 157–195.

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