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trans-Bis(isothiocyanato-κN)tetrapyridine-cadmium(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.037
wR factor = 0.093
Data-to-parameter ratio = 18.1

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

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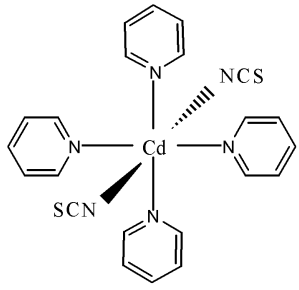
In the title complex, $[Cd(NCS)_2(C_5H_5N)_4]$, the Cd^{II} atom lies on a center of inversion. It is coordinated by four N atoms from four pyridines and two N atoms from two isothiocyanate ions and has a slightly distorted octahedral geometry.

Comment

Coordination complex synthesis as an important design element for generating new materials has been providing substances with unusual structural characteristics as well as extraordinary physical properties (Eddaoudi *et al.*, 2002).



(I)

We report here the structure of a new cadmium complex, (I), where the Cd^{II} atom lies on an inversion center and is hexacoordinated by the two N atoms of isothiocyanate ions and four pyridine N atoms, as shown in Fig. 1. The coordination environment of the Cd^{II} atom adopts a distorted octahedral geometry in which two N atoms of isothiocyanate ions occupy apical sites, in *trans* positions. The axial Cd—N bond distance of 2.374 (3) Å is slightly shorter than the average Cd—N bond of 2.392 (3) Å in the equatorial plane. The Cd—N(NCS) bond distance of 2.328 (3) Å is a little longer than the mean value of 2.283 (2) Å found by Moon & Lee (2000) in a similar complex. The average value for the Cd—N(pyridine) bond distance, 2.383 (2) Å, is longer than the average value reported for seven- and eight-coordinate cadmium complexes (Odoko *et al.*, 2002). The *cis* angles around the Cd^{II} atom deviate slightly from the ideal angle of 90° [87.57 (9)–92.43 (9)°]; thus, the Cd^{II} coordination center has slightly distorted octahedral geometry.

Experimental

All reagents and solvents were used as obtained without further purification. To 30 ml of aqueous ethanol (1:1 *v*/*v*) were added $CdCl_2{\cdot}H_2O$ (0.4 g, 2 mmol), KSCN (0.39 g, 4 mmol) and pyridine (2.0 ml, 20 mmol). The mixture was stirred for *ca* 30 min, whereupon a clear solution was obtained. After allowing the resulting solution to stand in air for one month, large yellow single crystals formed. They

were isolated, washed with aqueous alcohol solution twice and dried in a vacuum desiccator using $CaCl_2$ (yield 48%). Elemental analysis found: C 48.36, H 3.6, N 15.03, Cd 20.74%; calculated for $C_{22}H_{20}CdN_6S_2$: C 48.49, H 3.70, N 15.42, Cd 20.63%.

Crystal data

$[Cd(NCS)_2(C_5H_5N)_4]$	D_x = 1.497 Mg m^{-3}
M_r = 544.96	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 2576 reflections
a = 12.580 (3) Å	θ = 2.5–24.4°
b = 13.247 (3) Å	μ = 1.10 mm^{-1}
c = 15.216 (3) Å	T = 293 (2) K
β = 107.48 (3)°	Platee, colorless
V = 2418.6 (9) Å^3	0.42 × 0.26 × 0.07 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2576 independent reflections
	2337 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.017
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 27.0°
	$h = -14 \rightarrow 16$
T_{min} = 0.626, T_{max} = 0.926	$k = -15 \rightarrow 16$
6707 measured reflections	$l = -19 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 4.4917P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	
$wR(F^2)$ = 0.093	
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
2576 reflections	$\Delta\rho_{max}$ = 0.42 e Å^{-3}
142 parameters	$\Delta\rho_{min}$ = −0.42 e Å^{-3}
H-atom parameters constrained	

H atoms were placed in calculated positions and treated as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}$(parent C atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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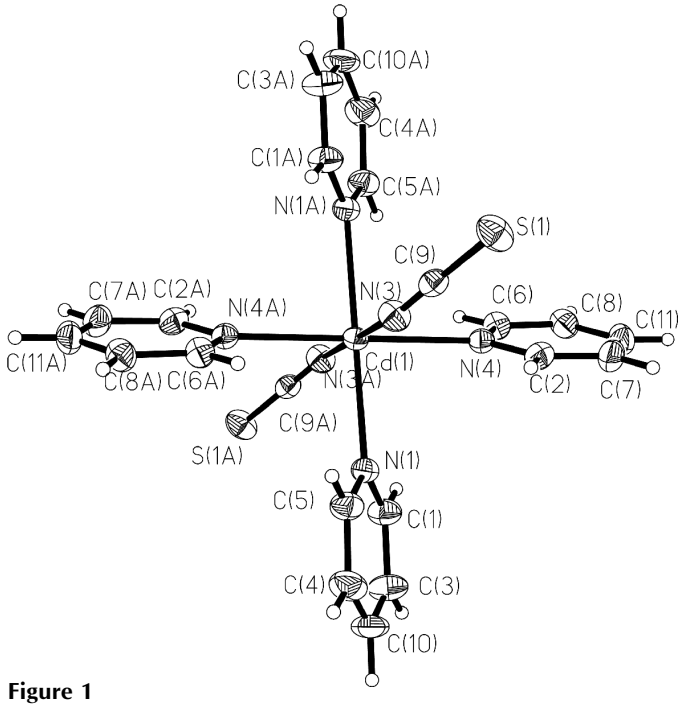

Figure 1
The structure of the title compound, (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Symmetry code: (*A*) $\frac{1}{2} - x, \frac{1}{2} - y, -z$.

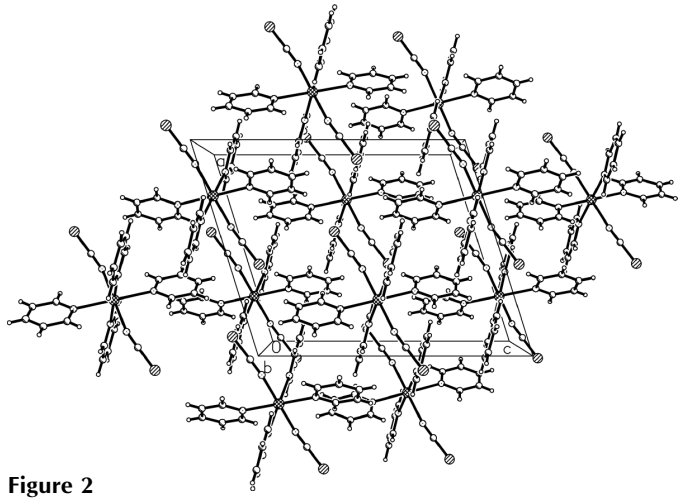

Figure 2
The crystal packing of (I), viewed along the *b* axis.

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