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Diisothiocyanato[3,6,14,17-tetraoxa-23,24-diazatricyclo[17.3.1.1^{8,12}]tetracosa-1(23),8,10,12 (24),19,21-hexaene]cadmium(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.014 Å
R factor = 0.045
wR factor = 0.136
Data-to-parameter ratio = 14.6

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

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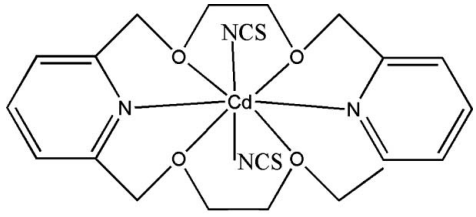
In the title complex, [Cd(NCS)$_2$(C$_{18}$H$_{22}$N$_2$O$_4$)], the Cd^{II} ion is coordinated by two NCS$^-$ anions and one bis-pyridino-18-crown-6 ligand in a distorted hexagonal–bipyramidal geometry.

Comment

Since the initial work of Pederson (1967), crown ethers have attracted much attention; those containing the pyridine unit have been studied extensively owing to their special coordination capability with transition metal ions (Lamb *et al.*, 1980). We report here the crystal structure of the title Cd^{II} complex, (I), with a pyridine-containing crown ether ligand.



(I)

The molecular structure of (I) is shown in Fig. 1. The Cd^{II} ion is coordinated by one bis-pyridino-18-crown-6 (L) ligand and two NCS$^-$ anions. The Cd1 atom and the six donor atoms of L are in an approximately planar array, while the two NCS$^-$ anions occupy the axial sites, forming a distorted hexagonal–bipyramidal coordination geometry. The average bond lengths of Cd—O(L) and Cd—N(pyridine) are 2.678 (5) and 2.578 (6) Å, respectively; these are longer than corresponding

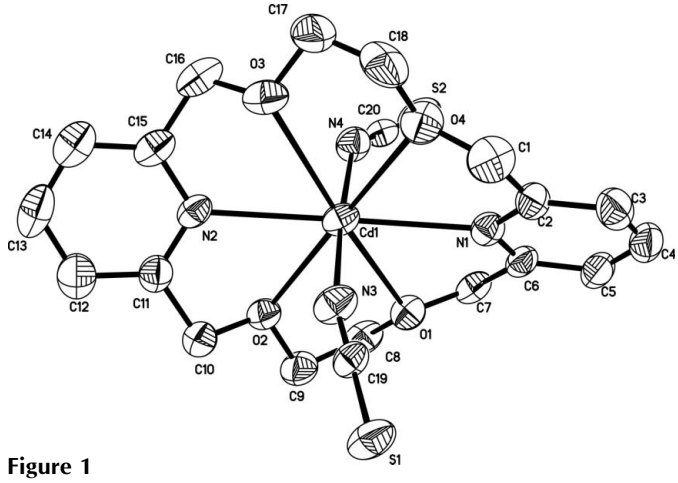


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

values of 2.613 (2) and 2.398 (3) Å in [2,6-bis(2-aminophenoxymethyl)pyridine]bis(nitrato-O)cadmium(II) (Adam *et al.*, 1990). The average Cd—N(NCS) bond length of 2.189 (7) Å is much shorter than 2.732 (7) Å in [(18-crown-6)K][Cd(SCN)$_3$] (Zhong *et al.*, 1996).

Experimental

To a solution of *L* (0.165 g, 0.5 mmol) in 5 ml 1,2-dichloroethane was added 5 ml of an aqueous solution of $CdCl_2{\cdot}2.5H_2O$ (0.228 g, 0.1 mmol) and NaSCN (0.80 g, 1 mmol). The mixture was stirred for 2 h at room temperature and then filtered. The residue was dissolved in a mixed solvent of CH_3CN and CH_3COCH_3 (1:1 *v*/*v*). Single crystals of (I) were obtained by slow evaporation.

Crystal data

$[Cd(NCS)_2(C_{18}H_{22}N_2O_4)]$	$Z = 8$
$M_r = 558.94$	$D_x = 1.612$ Mg m^{-3}
Orthorhombic, *Pbcn*	Mo $K\alpha$ radiation
$a = 16.178$ (3) Å	$\mu = 1.16$ mm^{-1}
$b = 8.9156$ (17) Å	$T = 298$ (2) K
$c = 31.928$ (6) Å	Block, colorless
$V = 4605.1$ (15) Å^3	0.28 × 0.16 × 0.13 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	22921 measured reflections 4075 independent reflections
φ and ω scans	2167 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.058$
$T_{min} = 0.737$, $T_{max} = 0.864$	$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 14.4849P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.136$	$\Delta\rho_{max} = 0.46$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -0.51$ e Å^{-3}
4075 reflections	
280 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Cd1—O1	2.674 (5)	Cd1—N1	2.584 (6)
Cd1—O2	2.624 (5)	Cd1—N2	2.572 (6)
Cd1—O3	2.763 (5)	Cd1—N3	2.183 (6)
Cd1—O4	2.650 (5)	Cd1—N4	2.194 (7)

All H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H = 0.93 (aromatic) or 0.97 Å (methylene) and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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