

Poly[cadmium(II)- μ -4,4'-oxydianiline- $N:N'$ -di- μ -thiocyanato- $N:S$]Hong-Ji Chen,^{a*} Wen-Juan Yu,^a Xiao-Ming Chen^b and Wen-Jie Zheng^a^aDepartment of Chemistry, Jinan University, Guangzhou 510632, People's Republic of China, and ^bSchool of Chemistry and Chemical Engineering, Zhongshan University, Guangzhou 510275, People's Republic of China
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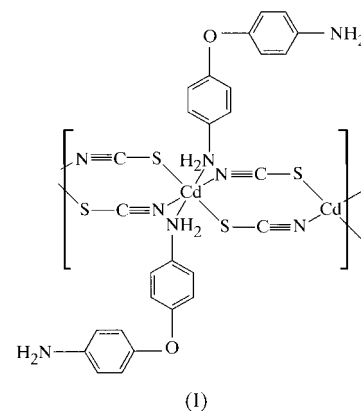
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The title polymeric complex, $[\text{Cd}(\text{SCN})_2(\text{C}_{12}\text{H}_{12}\text{N}_2\text{O})]_n$, exhibits a three-dimensional framework in which each Cd^{II} atom is bridged by two η -1,3-(SCN)⁻ groups, forming a double-stranded chain. The unique Cd^{II} atom lies on an inversion centre and the coordination sphere is completed by two terminal N atoms from two different 4,4'-Oda ligands, furnishing a CdS_2N_4 octahedral geometry. Adjacent polymeric double-stranded chains are linked *via* the 4,4'-Oda ligands, which lie across twofold rotation axes.

Comment

In the past two decades, polymeric Lewis base adducts of cadmium(II) thiocyanate, $[\text{Cd}(\text{SCN})_2(L)_2]_n$ (where L is 2-, 3-

or 4-methylpyridine, benzylamine, dibenzylamine, tri-*m*-tolylphosphine or 1*H*-1,2,4-triazole), exhibiting one-dimensional double-stranded chain structures comprising eight-membered $(-\text{N}-\text{C}-\text{S}-\text{Cd})_2$ rings in a chair conformation, have been documented (Ram *et al.*, 1981; Taniguchi *et al.*, 1987; Taniguchi & Ouchi, 1987). Recently, these one-dimensional chains have been linked into two-dimensional hydrogen-bonded networks by means of the bifunctional ligands imidazole and nicotinic acid (Chen *et al.*, 1999; Yang *et al.*, 2001). We report here the title covalent polymeric complex, $[\text{Cd}(\text{SCN})_2(4,4'\text{-Oda})]_n$, (I), where the organic 4,4'-Oda (4,4'-oxydianiline) ligand links the one-dimensional chains into a three-dimensional framework.



In compound (I), the Cd^{II} ion is located at an inversion centre, and is octahedrally coordinated by a pair of S atoms from two SCN^- groups, a pair of N atoms from another two SCN^- groups and a pair of N atoms from two 4,4'-Oda organic ligands. Each pair of adjacent metal atoms is bridged by a pair of SCN^- groups through opposite ends, resulting in a double-

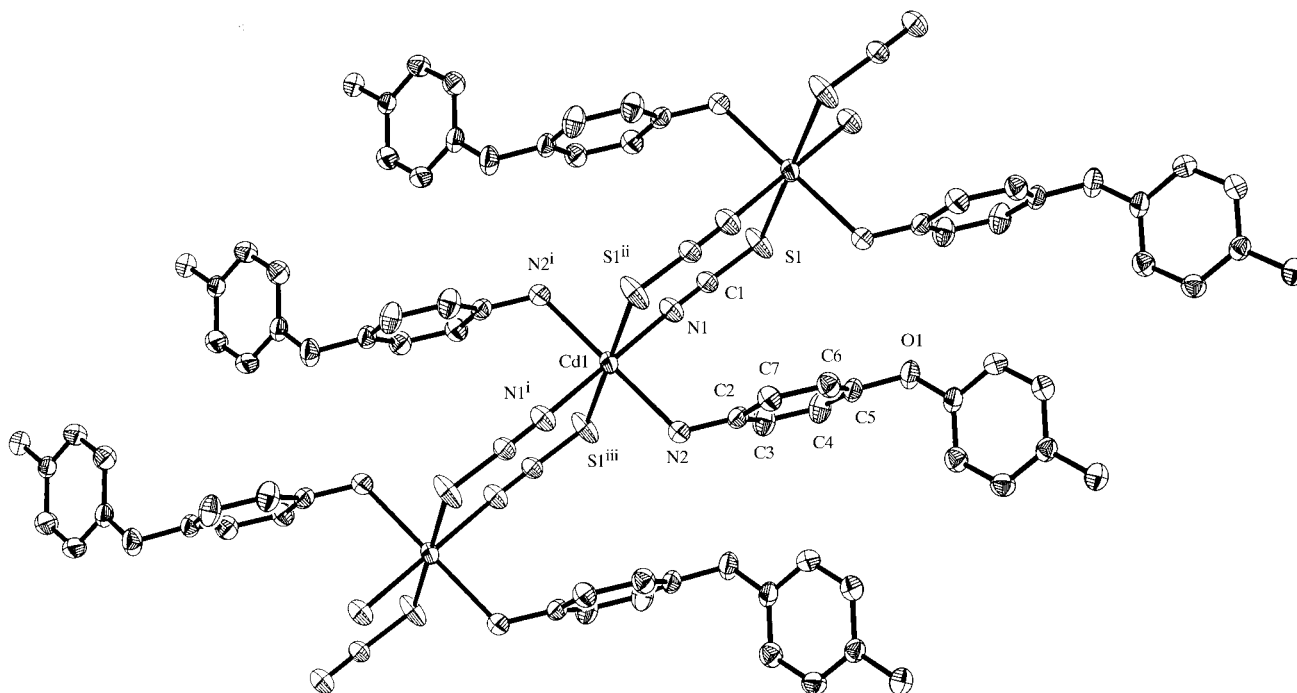


Figure 1

A view of the coordination environment in (I), with 30% probability displacement ellipsoids [symmetry codes: (i) $-x, -y, 1-z$; (ii) $\frac{1}{2}-x, -\frac{1}{2}-y, 1-z$; (iii) $x-\frac{1}{2}, \frac{1}{2}+y, z$].

stranded chain comprising eight-membered $(-N-C-S-Cd)_2$ rings in a chair conformation, with a $Cd \cdots Cd$ separation of 6.215 Å (Fig. 1). Within each unit cell, two such chains, related by the C -centring operation, run parallel to $[1\bar{1}0]$ at $z = \frac{1}{2}$, and a further pair of chains, generated from the first pair by the twofold rotation axes, runs parallel to $[100]$ at $z = 0$.

As expected, adjacent double-stranded chains are linked by the 4,4'-Oda ligands, which lie across the twofold rotation axes with a dihedral angle between the two aryl rings of 85.3 (3)°. This results in a three-dimensional framework, in which a row of parallel double-stranded chains runs in one direction and

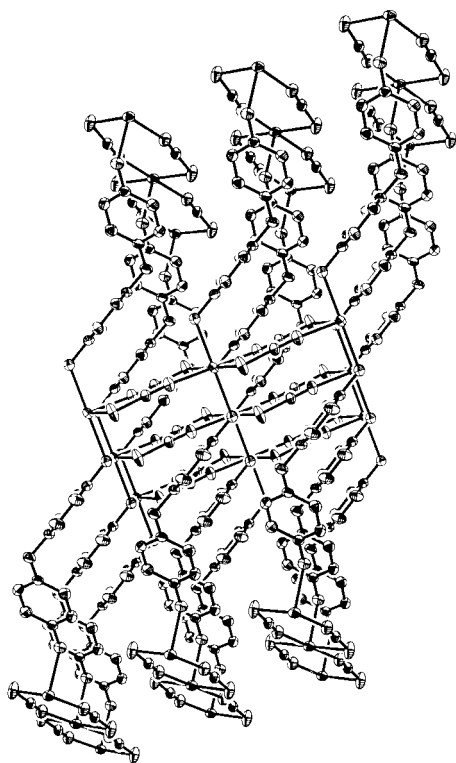


Figure 2
A view of the three-dimensional framework of (I).

the adjacent rows of parallel double-stranded chains run vertical to the first row, with a $Cd \cdots Cd$ separation of 13.566 Å, as shown in Fig. 2. Each 4,4'-Oda ligand links one $[110]$ chain to one $[1\bar{1}0]$ chain.

Experimental

A hot ethanol-water (1:1 v/v) solution (5 ml) of 4,4'-oxydianiline (0.50 g, 2.5 mmol) was added to an aqueous solution (5 ml) of $Cd(SCN)_2$ (0.57 g, 2.5 mmol). After vigorous stirring, the solution was adjusted to pH 5 by addition of dilute HNO_3 and the resulting solution was allowed to evaporate at room temperature for 6 d, resulting in the formation of colourless crystals of (I) (yield 56%). IR data (ν , cm^{-1}): 3329 (*m*), 3237 (*s*), 3149 (*m*), 3017 (*w*), 2869 (*w*), 2115 (*vs*), 1876 (*w*), 1590 (*m*), 1499 (*s*), 1211 (*s*), 1094 (*w*), 991 (*s*),

925 (*w*), 828 (*w*), 785 (*m*), 573 (*m*), 523 (*m*), 439 (*w*). Elemental analysis, found: C 39.5, H 2.9, N 12.9, S 14.9%; calculated for $C_{14}H_{12}CdN_4OS_2$: C 39.2, H 2.8, N 13.1, S 15.0%.

Crystal data

$[Cd(SCN)_2(C_{12}H_{12}N_2O)]$	$D_x = 1.809 \text{ Mg m}^{-3}$
$M_r = 428.80$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 25 reflections
$a = 9.441 (4) \text{ \AA}$	$\theta = 7-14^\circ$
$b = 8.085 (3) \text{ \AA}$	$\mu = 1.66 \text{ mm}^{-1}$
$c = 20.666 (11) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 93.490 (1)^\circ$	Block, colourless
$V = 1574.5 (12) \text{ \AA}^3$	$0.38 \times 0.35 \times 0.29 \text{ mm}$
$Z = 4$	

Data collection

Siemens $R3m$ diffractometer	$R_{int} = 0.021$
ω scans	$\theta_{max} = 27^\circ$
Absorption correction: semi-empirical based on ψ scan (Kopfmann & Huber, 1968)	$h = 0 \rightarrow 12$
$T_{min} = 0.555$, $T_{max} = 0.618$	$k = 0 \rightarrow 10$
1833 measured reflections	$l = -27 \rightarrow 26$
1717 independent reflections	2 standard reflections every 200 reflections
1433 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.4572P]$
$R[F^2 > 2\sigma(F^2)] = 0.030$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.083$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.49 \text{ e \AA}^{-3}$
1717 reflections	$\Delta\rho_{min} = -0.36 \text{ e \AA}^{-3}$
103 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Cd1—N1	2.338 (3)	C1—S1	1.660 (3)
Cd1—N2	2.352 (3)	C2—N2	1.435 (4)
Cd1—S1 ⁱ	2.7544 (13)	C5—O1	1.402 (3)
C1—N1	1.149 (4)		
N1—Cd1—N2 ⁱⁱ	88.66 (10)	N1—C1—S1	177.6 (3)
N1—Cd1—N2	91.34 (10)	C1—N1—Cd1	161.7 (3)
N1—Cd1—S1 ⁱ	87.83 (8)	C2—N2—Cd1	119.76 (19)
N2—Cd1—S1 ⁱ	95.76 (7)	H2B—N2—H2A	112
N1—Cd1—S1 ⁱⁱⁱ	92.17 (8)	C5 ^{iv} —O1—C5	115.4 (3)
N2—Cd1—S1 ⁱⁱⁱ	84.24 (7)	C1—S1—Cd1 ^v	106.59 (11)

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

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H2B \cdots S1 ⁱ	0.90	2.91	3.438 (3)	119
N2—H2A \cdots S1 ⁱⁱ	0.90	2.55	3.431 (3)	167

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

All H atoms were treated as riding, with a C—H distance of 0.96 Å.

Data collection: *SHELXTL-Plus* (Siemens, 1990); cell refinement: *SHELXTL-Plus*; data reduction: *SHELXTL-Plus*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD1168). Services for accessing these data are described at the back of the journal.

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