

Xiu-Jian Wang,\* Liu-Chen Gui,  
Zhong-Su Shen, Qing-Ling Ni  
and Jian-Qiang ZengSchool of Chemistry and Chemical Engineering,  
Guangxi Normal University, Guilin 541004,  
People's Republic of ChinaCorrespondence e-mail:  
wang1\_xj@yahoo.com.cn

## Key indicators

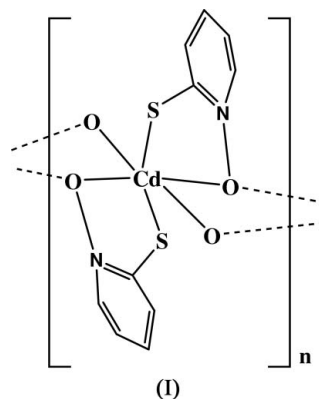
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.023  
 $wR$  factor = 0.060  
Data-to-parameter ratio = 15.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*catena*-Poly[cadmium(II)-di- $\mu$ -*N*-oxopyridine-  
2-thiolato]

In the title complex,  $[\text{Cd}(\text{C}_5\text{H}_4\text{NOS})_2]_n$ , (I), the Cd atom is located on an inversion center and is coordinated by two S [ $\text{Cd}-\text{S} = 2.5225(6)$  Å] and four O [ $\text{Cd}-\text{O} = 2.3931(16)$  and  $2.5543(17)$  Å] atoms in a distorted octahedral geometry. Two *N*-oxopyridine-2-thiolate (PySO) ligands chelate the Cd atom to occupy four sites of the equatorial plane, while two O atoms from another two PySO ligands occupy the axial sites. PySO acts as a bridging chelating ligand ( $S-\mu_2-O$ ), connecting adjacent Cd atoms to form a polymeric chain.

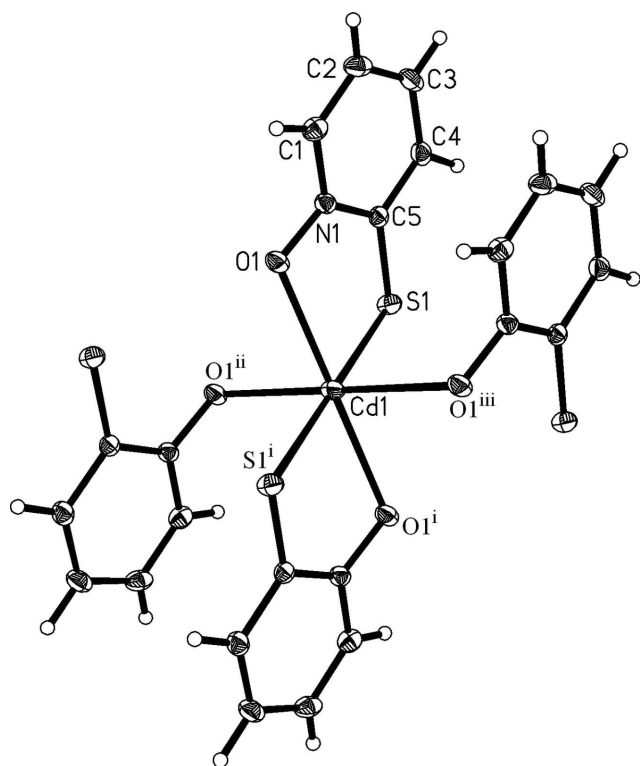
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## Comment

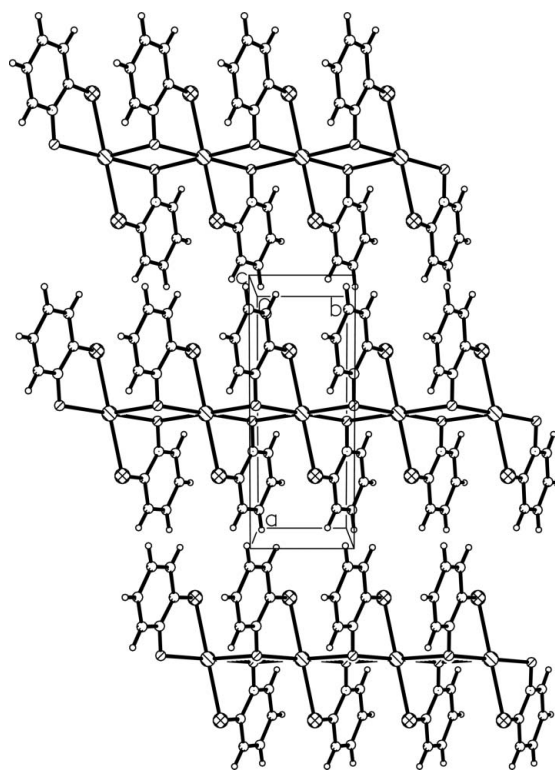
Significant research efforts in the syntheses and studies of coordination polymers have been made in the past decade, because of their potential applications in new materials, catalysis, nonlinear optics and separation (Janiak, 2003, and references therein). The construction of coordination polymers usually requires multidentate ligands with two or more chelating atoms. Studies have mainly been focused on ligands containing nitrogen and oxygen donors. We believe that many opportunities still remain for organosulfur ligands, because sulfur may exhibit versatile modes of coordination (terminal,  $S-\mu_2$ ,  $S-\mu_3$ ,  $S-\mu_4$ ). The *N*-oxopyridine-2-thiolate (PySO) ligand can behave as a bidentate chelating ( $\eta^2-O,S$ ) or tridentate chelating bridging  $\{\eta^3-(S-\mu-O)\}$  ligand (Barnett *et al.*, 1977; Manivannan *et al.*, 1993). Its complexes of Fe, Co, Ni and Cu have been found only as monomers or dimers (Chen *et al.*, 1991; Manivannan *et al.*, 1993). We report here the structure of the cadmium polymeric complex  $[\text{Cd}(\text{C}_5\text{H}_4\text{NOS})_2]_n$ , (I), which is to our knowledge the first example of a metal polymeric compound assembled by the PyOS ligand.



In (I) (Fig. 1), the Cd atom is located on an inversion center. The PySO ligand, behaving in a bridging chelating mode ( $S-\mu_2-O$ ), chelates one Cd and bridges another Cd atom through



**Figure 1**  
View of a segment of (I) with the atom-labeling scheme and displacement ellipsoids at the 30% probability level [symmetry codes: (i)  $1 - x, -y, -z$ ; (ii)  $x, 1 + y, z$ ; (iii)  $1 - x, -1 - y, -z$ ].



**Figure 2**  
The crystal packing showing one-dimensional polymeric chains in a perspective view along the  $c$  axis.

the O atom to form a polymeric chain (Fig. 2). This chain in (I) is similar to that observed in the polymeric structure  $[\text{Cd}(\text{PyS})_2]_n$ , (II), (PyS is pyridine-1-thiolate) (Hursthouse *et al.*, 1990), where sulfur acts as a bridging atom.

The octahedral coordination of Cd is  $[\text{S}_2\text{O}_4]$  with the equatorial plane defined by atoms O1, O1<sup>i</sup>, S1 and S1<sup>i</sup> and axial sites occupied by O1<sup>ii</sup> and O1<sup>iii</sup> [symmetry codes: (i)  $1 - x, -y, -z$ ; (ii)  $x, 1 + y, z$ ; (iii)  $1 - x, -1 - y, -z$ ]. The values of the coordinating angles (Table 1) indicate that the Cd atom has a slightly distorted octahedral configuration. The chelating angle O1–Cd1–S1 [ $74.55(5)^\circ$ ] is smaller than that found in a dimeric zinc(II) complex ( $82.4\text{--}85.4^\circ$ ; Barnett *et al.*, 1977).

The Cd–S bond length [ $2.5225(6) \text{ \AA}$ ] is close to that found previously between cadmium and terminal thiolate sulfur ( $2.549\text{--}2.588 \text{ \AA}$ ; Labisbal *et al.*, 2000). In the case where the ligand acts as a bridge, the two distances for the Cd–O bond [ $2.3931(16)$  and  $2.5543(17) \text{ \AA}$ ] are different, *i.e.* the bridge is not symmetrical and both distances are longer than those found in  $[\text{Cd}(\text{N-inoO})_2] \cdot (\text{H}_2\text{O})_2$  (N-inoO is 1-oxide-4-cyanopyridine; Zheng *et al.*, 2001). The N–O bond length of  $1.350(3) \text{ \AA}$  is shorter than that [ $1.388(2) \text{ \AA}$ ] found in  $\text{Me}_3\text{NO}$  where no  $\pi$  bonding can occur (Caron *et al.*, 1964). The C–S, N–O and N–C bond lengths (Table 1) suggest their double-bond character and delocalization of charge density in the S/C/N/O group (Raper, 1996; Lobana, *et al.*, 1999).

## Experimental

A solution of  $\text{CdCl}_2 \cdot 4\text{H}_2\text{O}$  (0.191 g, 0.75 mmol) in dimethylformamide (DMF, 10 ml) was added to a solution of DMF (10 ml) containing *N*-oxopyridine-2-thiol (0.166 g, 1.5 mmol) with stirring at room temperature for 3 h. The filtrate was allowed to evaporate slowly. Light-yellow plate crystals of the title compound suitable for X-ray diffraction study were obtained within two months.

### Crystal data

$[\text{Cd}(\text{C}_5\text{H}_4\text{NOS})_2]$   
 $M_r = 364.70$   
Monoclinic,  $P2_1/c$   
 $a = 10.0858(9) \text{ \AA}$   
 $b = 3.8057(4) \text{ \AA}$   
 $c = 14.5664(13) \text{ \AA}$   
 $\beta = 100.648(2)^\circ$   
 $V = 549.48(9) \text{ \AA}^3$   
 $Z = 2$

$D_x = 2.204 \text{ Mg m}^{-3}$   
Mo  $K\alpha$  radiation  
Cell parameters from 4354 reflections  
 $\theta = 2.2\text{--}27.0^\circ$   
 $\mu = 2.35 \text{ mm}^{-1}$   
 $T = 293(2) \text{ K}$   
Plate, light yellow  
 $0.35 \times 0.17 \times 0.03 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 1998)  
 $T_{\text{min}} = 0.682$ ,  $T_{\text{max}} = 0.932$   
5731 measured reflections

1195 independent reflections  
1077 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$   
 $\theta_{\text{max}} = 27.0^\circ$   
 $h = -12 \rightarrow 12$   
 $k = -4 \rightarrow 4$   
 $l = -18 \rightarrow 18$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.023$   
 $wR(F^2) = 0.060$   
 $S = 1.06$   
1195 reflections  
79 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0416P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.039$   
 $\Delta\rho_{\text{max}} = 1.13 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$

**Table 1**  
Selected geometric parameters (Å, °).

Cd1—O1	2.3931 (16)	S1—C5	1.719 (2)
Cd1—S1	2.5225 (6)	O1—N1	1.350 (3)
Cd1—O1 <sup>iii</sup>	2.5543 (17)	N1—C1	1.364 (3)
O1 <sup>i</sup> —Cd1—O1	180.0	S1 <sup>i</sup> —Cd1—O1 <sup>ii</sup>	86.85 (4)
O1—Cd1—S1 <sup>i</sup>	105.45 (5)	S1—Cd1—O1 <sup>ii</sup>	93.15 (4)
O1—Cd1—S1	74.55 (5)	C5—S1—Cd1	98.84 (7)
S1 <sup>i</sup> —Cd1—S1	180.0	N1—O1—Cd1	113.53 (12)
O1 <sup>i</sup> —Cd1—O1 <sup>ii</sup>	79.48 (7)	N1—O1—Cd1 <sup>iv</sup>	110.87 (11)
O1—Cd1—O1 <sup>ii</sup>	100.52 (7)		

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

H atoms were observed in a difference Fourier map, but were placed in idealized positions and refined as riding on their carrier atoms [ $C-H = 0.93 \text{ \AA}$  and  $U_{iso}(H) = 1.2U_{eq}(C)$ ]. The highest residual peak is located  $0.996 (11) \text{ \AA}$  from the Cd atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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