

Dichlorobis(pyridinium-2-thiolato)cadmium(II)

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Key indicators

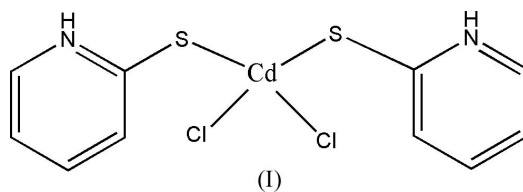
Single-crystal X-ray study
 $T = 130$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.019
 wR factor = 0.046
Data-to-parameter ratio = 21.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $[\text{Cd}(\text{C}_5\text{H}_5\text{NS})_2\text{Cl}_2]$, was prepared by the self-assembly reaction of isophthalic acid, $\text{CdCl}_2 \cdot 5\text{H}_2\text{O}$ and pyridine-2-thiol in methanol/ H_2O . The Cd^{II} atom lies on a twofold axis and is tetrahedrally coordinated by two S atoms from two pyridinium-2-thiolate ligands and two Cl atoms. Molecules are linked by $\text{N}-\text{H} \cdots \text{Cl}$ hydrogen bonds to form sheets parallel to the bc plane.

Received 7 March 2005
Accepted 24 March 2005
Online 31 March 2005

Comment

The coordination chemistry of the pyridine-2-thiol ligand with transition metals has undergone extensive development in recent years owing to its abundant coordination ability. The pyridine-2-thiol ligand can coordinate both in the 'thiolate' and the tautomeric 'thione' forms and it has several binding modes, for instance, monodentate, bidentate chelating, bidentate bridging and doubly bridging. Recently, some coordination polymers constructed from pyridine-2-thione (or pyridinium-2-thiolate) have been reported (Lobana *et al.*, 2000; Hong *et al.*, 1999; Berardini *et al.*, 1997). We report here the synthesis and crystal structure of the title mononuclear cadmium(II) compound, (I).



As shown in Fig. 1, the Cd atom in (I) lies on a twofold axis and is coordinated by two S atoms from two pyridinium-2-thiolate ligands and two Cl atoms in a distorted tetrahedral geometry, with Cd—S and Cd—Cl distances of 2.5172 (9) and 2.4730 (9) Å, respectively. The title compound is isostructural with the Co analog, $[\text{Co}(\text{C}_5\text{H}_5\text{NS})_2\text{Cl}_2]$ (Binamira-Soriaga *et al.*, 1979).

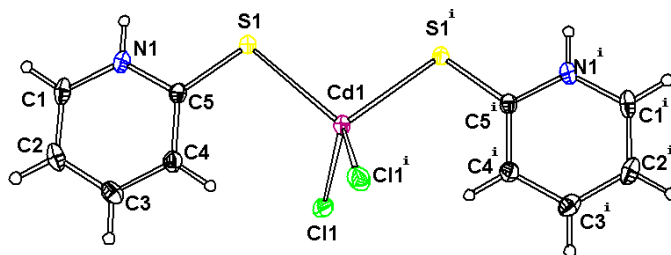


Figure 1

A view of the structure of (I), showing 50% probability displacement ellipsoids [symmetry code: (i) $-x, y, \frac{1}{2} - z$].

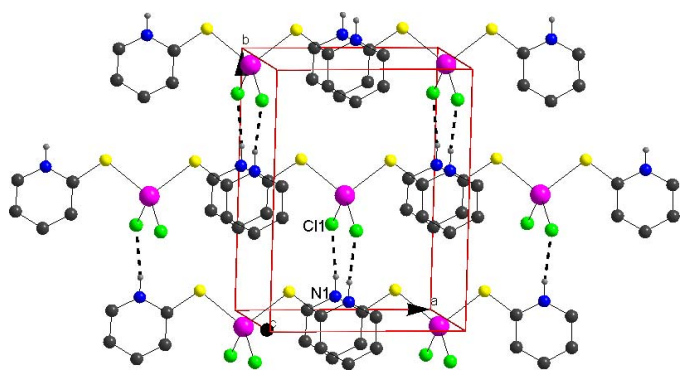


Figure 2
Packing diagram of (I), showing the two-dimensional hydrogen-bonded structure. H atoms not involved in hydrogen bonding have been omitted and the hydrogen bonds are shown as dashed lines.

In the crystal structure, there are N—H···Cl hydrogen bonds involving the protonated N atoms and the Cl atoms from symmetry-related molecules (see Table 2). As shown in Fig. 2, molecules are linked by these interactions to form two-dimensional sheets parallel to the *bc* plane.

Experimental

The title compound was prepared by mixing a 1:1 molar ratio of isophthalic acid (0.083 g, 0.5 mmol) and CdCl₂·5H₂O (0.114 g, 0.5 mmol) in a solution of MeOH/H₂O (3:2 v/v, 25 ml). The solution was stirred at 333 K for 30 min, pyridine-2-thiol (0.056 g, 0.5 mmol) was added and the resulting mixture stirred for a further 1 h. The reaction mixture was filtered and colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent.

Crystal data

[Cd(C ₅ H ₅ NS) ₂ Cl ₂]	<i>D</i> _x = 1.949 Mg m ⁻³
<i>M</i> _r = 405.62	Mo Kα radiation
Monoclinic, <i>C</i> 2/ <i>c</i>	Cell parameters from 2053 reflections
<i>a</i> = 9.364 (4) Å	<i>θ</i> = 2.9–28.3°
<i>b</i> = 11.445 (4) Å	<i>μ</i> = 2.25 mm ⁻¹
<i>c</i> = 13.597 (6) Å	<i>T</i> = 130 (2) K
<i>β</i> = 108.46 (2)°	Prism, colorless
<i>V</i> = 1382.1 (10) Å ³	0.50 × 0.25 × 0.08 mm
<i>Z</i> = 4	

Data collection

Bruker SMART CCD diffractometer	1709 independent reflections
<i>ω</i> scans	1659 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R</i> _{int} = 0.020
<i>T</i> _{min} = 0.515, <i>T</i> _{max} = 0.836	<i>θ</i> _{max} = 28.3°
5486 measured reflections	<i>h</i> = -12 → 6
	<i>k</i> = -15 → 15
	<i>l</i> = -16 → 18

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0221P)^2 + 1.6413P]$
$R[F^2 > 2\sigma(F^2)] = 0.019$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.046$	(Δ/σ) _{max} = 0.002
<i>S</i> = 1.09	$\Delta\rho_{max} = 0.67 \text{ e \AA}^{-3}$
1709 reflections	$\Delta\rho_{min} = -0.65 \text{ e \AA}^{-3}$
78 parameters	

Table 1

Selected geometric parameters (Å, °).

Cd1—Cl1	2.4730 (9)	Cd1—S1	2.5172 (9)
Cl1 ⁱ —Cd1—Cl1	110.87 (4)	Cl1—Cd1—S1	108.11 (3)
Cl1 ⁱ —Cd1—S1	112.83 (2)	S1—Cd1—S1 ⁱ	103.97 (4)

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

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1B···Cl1 ⁱⁱ	0.86	2.30	3.1487 (18)	171

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

All H atoms were included in calculated positions and refined using the riding-model approximation [C—H = 0.93 Å, N—H = 0.86 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C,N)].

Data collection: SMART (Siemens, 1996); cell refinement: SMART and SAINT (Siemens, 1994); data reduction: SAINT and XPREP in SHELXTL (Siemens, 1994); program(s) used to solve structure: SHELXTL; program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

This project (No. 20030710) was supported by the Education Department of Zhejiang Province.

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