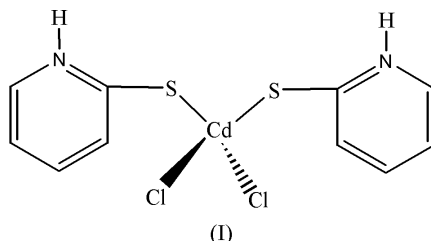


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wang1_xj@yahoo.com.cn**Key indicators**Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.018
 wR factor = 0.041
Data-to-parameter ratio = 20.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Dichlorobis(pyridinium-2-thiolato)cadmium(II)**

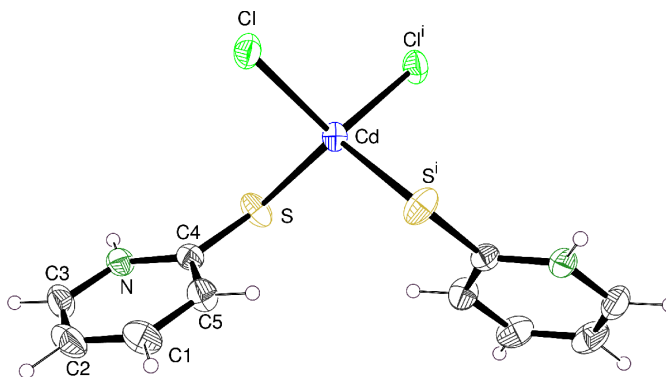
In the title compound, $[\text{CdCl}_2(\text{C}_5\text{H}_5\text{NS})_2]$, the Cd^{II} atom (site symmetry 2) is coordinated by the S atoms of two zwitterionic pyridine-2-thione ligands and two Cl atoms in distorted tetrahedral geometry [$\text{Cd}-\text{S} = 2.5068(8)\text{ \AA}$ and $\text{Cd}-\text{Cl} = 2.4684(8)\text{ \AA}$]. The molecules are linked *via* $\text{N}-\text{H}\cdots\text{Cl}$, $\text{C}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{S}$ interactions into an extended network.

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Online 20 November 2004**Comment**

Thiolate complexes are of considerable interest in terms of their structures and differing physical properties due to the versatile binding modes of the sulfur atoms (Dance *et al.*, 1987). Pyridine-2-thione (HPyS) is a versatile sulfur ligand, since it can behave either as a neutral (bonding through the S atom), monoanionic S-monodentate, N,S-bidentate, S-bridging or N,S-bridging species (Su *et al.*, 2002). In a further exploration of the coordination behaviour of HPyS, we report the synthesis and structure of the title compound, (I), in which the HPyS acts as a neutral S-bonded ligand.



The asymmetric unit of (I) consists of an HPyS molecule, a Cl ion and a Cd^{II} cation, the latter occupying a special position with twofold symmetry (Table 1 and Fig. 1). The complete

**Figure 1**

View of (I), with displacement ellipsoids drawn at the 30% probability level and H atoms shown as small spheres of arbitrary radii. The symmetry code is as given in Table 1.

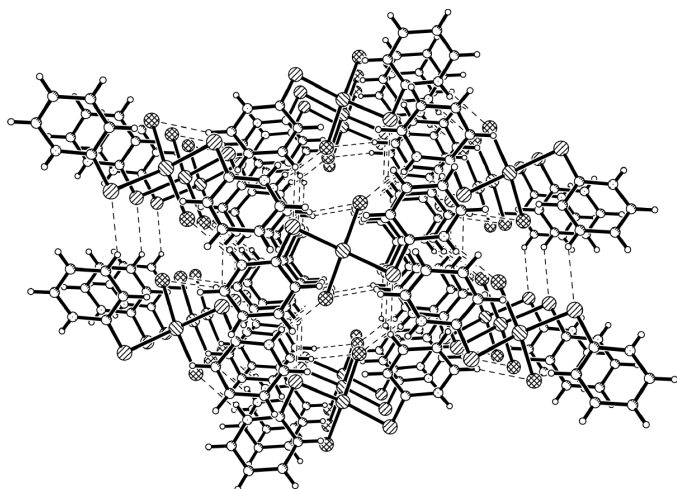


Figure 2
The crystal packing in (I), showing hydrogen bonds as dashed lines.

molecule is generated by twofold symmetry; the Cd atom is coordinated by two S atoms from two HPyS ligands and two chloride ions in a distorted tetrahedral geometry. The largest angle, S—Cd—Sⁱ (see Table 1 for symmetry code) is 121.33 (4)°, while the smallest, Cl—Cd—Sⁱ, is 101.08 (3)°. The dihedral angle between the S—Cd—Sⁱ and Cl—Cd—Clⁱ planes, which is usually considered as an indication of the degree of distortion of a complex with tetrahedral coordination geometry, is 84.4 (3)°. These data indicate a relatively large deviation from ideal *T_d* symmetry.

The Cd—S bond length in (I) is 2.5068 (8) Å, which is similar to the Cd—S (terminal) bond length in the complex [Cd(3-Me₃Sipy₂)₂] (3-Me₃Sipy₂ is 3-trimethylsilylpyridine-2-thionate; Castro *et al.*, 1993), but longer than that in [Cd(S-2-PhCONHC₆H₄)₂(1-MeIm)₂] (1-MeIm is 1-methylimidazole; Sun *et al.*, 1999). The Cd—Cl bond length in (I) is 2.4684 (8) Å, which is within the sum of the covalent radii of cadmium and chlorine (2.48 Å).

There are weak N—H···Cl, C—H···Cl and C—H···S interactions (Venkataramanan *et al.*, 2004; Nishio, 2004) in (I) (Table 2), giving rise to a three-dimensional network (Fig. 2).

Experimental

A solution of CdCl₂·4H₂O (0.191 g, 0.75 mmol) in methanol (10 ml) was added to a solution (10 ml) of pyridine-2-thiol (0.166 g, 1.5 mmol) in methanol, with stirring at room temperature for 3 h. The filtrate was allowed to slowly evaporate. Two weeks later, light-yellow crystals of (I) were obtained.

Crystal data

[CdCl₂(C₅H₅NS)₂]
M_r = 405.62
 Orthorhombic, *Fdd2*
a = 12.837 (3) Å
b = 27.526 (6) Å
c = 8.140 (2) Å
V = 2876.3 (12) Å³
Z = 8
D_x = 1.873 Mg m⁻³

Mo *K*α radiation
 Cell parameters from 2850 reflections
 θ = 1.9–27.0°
 μ = 2.16 mm⁻¹
T = 293 (2) K
 Rod, light yellow
 0.15 × 0.07 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
 T_{\min} = 0.834, T_{\max} = 0.879
 4192 measured reflections

1579 independent reflections
 1520 reflections with $I > 2\sigma(I)$
 R_{int} = 0.020
 θ_{max} = 27.0°
 h = -13 → 16
 k = -34 → 27
 l = -10 → 10

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)]$ = 0.018
 $wR(F^2)$ = 0.041
 S = 1.02
 1579 reflections
 78 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0224P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}}$ = 0.029
 $\Delta\rho_{\text{max}}$ = 0.30 e Å⁻³
 $\Delta\rho_{\text{min}}$ = -0.30 e Å⁻³
 Absolute structure: Flack (1983),
 729 Friedel pairs
 Flack parameter = 0.04 (2)

Table 1

Selected geometric parameters (Å, °).

Cd—S	2.5068 (8)	Cd—Cl	2.4684 (8)
S ⁱ —Cd—S	121.33 (4)	Cl ⁱ —Cd—S ⁱ	109.60 (3)
Cl ⁱ —Cd—Cl	114.83 (4)	Cl—Cd—S ⁱ	101.08 (3)

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

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>
Cl1—H1A···S ⁱⁱ	0.93	2.84	3.643 (3)	145
C3—H3A···Cl ⁱⁱⁱ	0.93	2.87	3.619 (3)	139
N—H0A···Cl ^{iv}	0.86	2.39	3.231 (2)	167

Symmetry codes: (ii) $\frac{1}{2} + x, y, \frac{1}{2} + z$; (iii) $\frac{3}{4} - x, \frac{1}{4} + y, \frac{3}{4} + z$; (iv) $x - \frac{1}{4}, \frac{3}{4} - y, \frac{1}{4} + z$.

All H atoms were apparent in a difference map. They were repositioned in idealized positions and refined as riding on their carrier atoms [C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$].

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* for Windows (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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References

- Bruker (1998). *SMART, SAINT, and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dance, I. G., Garbutt, R. G. & Craig, D. C. (1987). *Inorg. Chem.* **26**, 3732–3740.
- Castro, A., José, A., García-Vázquez, R. J. & Sousa, A. (1993). *Inorg. Chim. Acta*, **211**, 47–54.
- Farrugia, L. J. (1997). *J. App. Cryst.* **30**, 565.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Nishio, M. (2004). *CrystEngComm*, **6**, 130–158.
- Sheldrick, G. M. (1997). *SHELXS97 and SHELXL97*. University of Göttingen, Germany.
- Su, W., Hong, M., Weng, J., Liang, Y., Zhao, Y., Cao, R., Zhou, Z. & Chan, A. S. C. (2002). *Inorg. Chim. Acta*, **331**, 8–15.
- Sun, W. Y., Zhang, L. & Yu, K. B. (1999). *J. Chem. Soc. Dalton Trans.* pp. 795–798.
- Venkataramanan, B., Saifudin, M. A., Jagadese, J. V. & Suresh, V. (2004). *CrystEngComm*, **6**, 284–289.