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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$
 R factor = 0.020
 wR factor = 0.047
Data-to-parameter ratio = 20.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Dibromobis[pyridine-2(1*H*)-thione- κ S]cadmium(II)

In the title compound, $[\text{CdBr}_2(\text{C}_5\text{H}_5\text{NS})_2]$, the Cd^{II} cation (site symmetry 2) is coordinated by the S atoms of two pyridine-2-thione ligands and two Br^- ions in a distorted tetrahedral geometry [$\text{Cd}-\text{S} = 2.5171(10)\text{ \AA}$ and $\text{Cd}-\text{Br} = 2.5911(6)\text{ \AA}$]. The molecules are linked *via* $\text{N}-\text{H}\cdots\text{Br}$, $\text{C}-\text{H}\cdots\text{Br}$ and $\text{C}-\text{H}\cdots\text{S}$ interactions into an extended network.

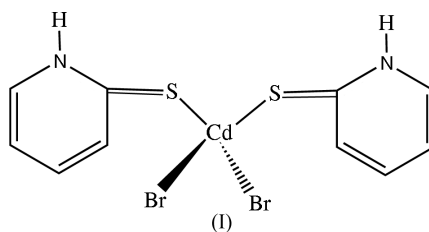
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Comment

Pyridine-2-thione (HPyS) is a versatile sulfur-containing ligand with differing coordination modes to metal cations (Su *et al.*, 2000, 2002; Hao *et al.*, 2000). In a further exploration of the coordination chemistry of HPyS, we report the synthesis and structure of the title compound, dibromobis(pyridine-2(1*H*)-thione- κ S)cadmium(II), (I) (Fig. 1), in which the HPyS acts as a terminal S-bonded species.



Compound (I) is isostructural with dichlorobis(pyridinium-2-thiolato)cadmium, (II) (Wang *et al.*, 2004). The asymmetric unit of (I) consist of an HPyS molecule, a Br^- ion and a Cd^{II} cation, the latter occupying a special position with twofold symmetry. The Cd^{II} atom is thus coordinated by two S atoms of two HPyS ligands and two bromide ions in a distorted tetrahedral geometry (Table 1). The largest angle, $\text{S}-\text{Cd}-\text{S}^i$

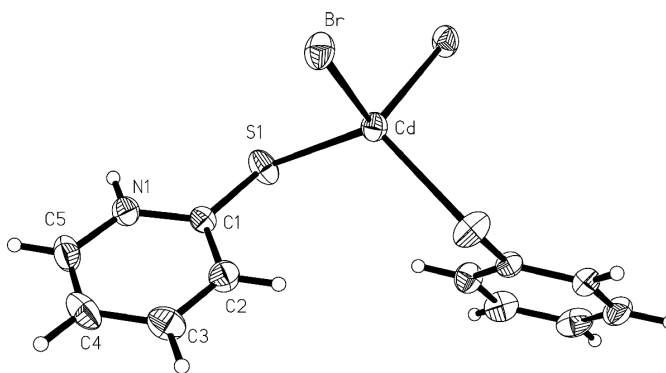


Figure 1

View of (I), with displacement ellipsoids drawn at the 30% probability level and H atoms shown as small spheres of arbitrary radii. The unlabelled atoms are generated by the symmetry code $(\frac{1}{2} - x, \frac{1}{2} - y, z)$.

(see Table 1 for symmetry code), is $121.16(6)^\circ$, while the smallest angle, $\text{Br}-\text{Cd}-\text{S}^{\text{i}}$, is $101.73(2)^\circ$. The dihedral angle between $\text{S}-\text{Cd}-\text{S}^{\text{i}}$ and $\text{Br}-\text{Cd}-\text{Br}^{\text{i}}$, which can be considered as an indication of the degree of distortion of a tetrahedral complex, is $85.2(2)^\circ$.

The $\text{Cd}-\text{S}$ bond length in (I) is $2.5171(10) \text{ \AA}$, which is similar to that in (II) (Wang *et al.*, 2004), but longer than that in $[\text{Cd}(\text{S}-2\text{-PhCONHC}_6\text{H}_4)_2(1\text{-MeIm})_2]$ (1-MeIm is 1-methylimidazole; Sun *et al.*, 1999). The $\text{Cd}-\text{Br}$ bond length in (I) is $2.5911(6) \text{ \AA}$, which is within the sum of the covalent radii for cadmium and bromine (2.63 \AA).

There are $\text{N}-\text{H}\cdots\text{Br}$ hydrogen bonds and weak $\text{C}-\text{H}\cdots\text{Br}$ and $\text{C}-\text{H}\cdots\text{S}$ interactions (Venkataramanan *et al.*, 2004; Nishio, 2004) in (I) (Table 2). These result in a three-dimensional network (Fig. 2).

Experimental

A solution of $\text{Cd}(\text{NO}_3)_2\cdot 4\text{H}_2\text{O}$ (0.238 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 and stirred at room temperature for 3 h. Bu_4NBr (0.322 g, 1 mmol) was then added to the mixture and stirring was continued for 3 h. About three weeks later, light-yellow crystals of (I) were obtained as the solvent slowly evaporated.

Crystal data

$[\text{CdBr}_2(\text{C}_5\text{H}_5\text{NS})_2]$	Mo $K\alpha$ radiation
$M_r = 494.54$	Cell parameters from 2990 reflections
Orthorhombic, <i>Fdd2</i>	$\theta = 2.9\text{--}27.0^\circ$
$a = 13.050(3) \text{ \AA}$	$\mu = 7.04 \text{ mm}^{-1}$
$b = 28.521(6) \text{ \AA}$	$T = 293(2) \text{ K}$
$c = 8.065(2) \text{ \AA}$	Rod, light yellow
$V = 3001.8(12) \text{ \AA}^3$	$0.18 \times 0.07 \times 0.06 \text{ mm}$
$Z = 8$	
$D_x = 2.189 \text{ Mg m}^{-3}$	

Data collection

Bruker SMART CCD diffractometer	1622 independent reflections
ω scans	1535 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$R_{\text{int}} = 0.027$
$T_{\text{min}} = 0.559$, $T_{\text{max}} = 0.656$	$\theta_{\text{max}} = 27.0^\circ$
4357 measured reflections	$h = -16 \rightarrow 7$
	$k = -36 \rightarrow 35$
	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0271P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.020$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.047$	$(\Delta/\sigma)_{\text{max}} = 0.026$
$S = 0.99$	$\Delta\rho_{\text{max}} = 0.43 \text{ e \AA}^{-3}$
1622 reflections	$\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$
78 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	745 Friedel pairs
	Flack parameter = 0.060 (8)

Table 1

Selected geometric parameters (\AA , $^\circ$).

$\text{Cd}-\text{S1}$	$2.5171(10)$	$\text{Cd}-\text{Br}$	$2.5911(6)$
$\text{S1}^{\text{i}}-\text{Cd}-\text{S1}$	$121.16(6)$	$\text{S1}-\text{Cd}-\text{Br}$	$109.04(3)$
$\text{S1}^{\text{i}}-\text{Cd}-\text{Br}$	$101.73(2)$	$\text{Br}-\text{Cd}-\text{Br}^{\text{i}}$	$114.77(3)$

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

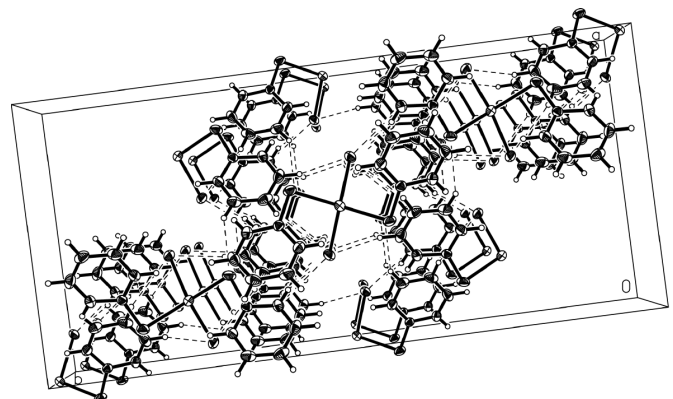


Figure 2

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

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C5}-\text{H5A}\cdots\text{Br}^{\text{ii}}$	0.93	3.00	$3.776(4)$	142
$\text{C3}-\text{H3A}\cdots\text{S1}^{\text{iii}}$	0.93	2.90	$3.715(4)$	147
$\text{N1}-\text{H1A}\cdots\text{Br}^{\text{iv}}$	0.86	2.55	$3.382(3)$	163

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

All H atoms were apparent in a difference map. They were repositioned in idealized positions and refined as riding on their carrier atoms [$\text{C}-\text{H} = 0.93 \text{ \AA}$ 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, 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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