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catena-Poly[[bis(*O*,*O*′-dimethyl dithiophosphato-κ^2S,S')cadmium(II)]-μ-4,4′-bipyridine-*N*:*N*′]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.042
wR factor = 0.109
Data-to-parameter ratio = 21.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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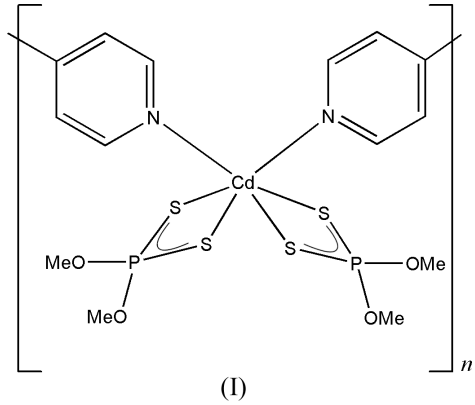
The title compound, $[Cd(C_2H_6O_2PS_2)_2(C_{10}H_8N_2)]_n$, contains zigzag chains linked through the 4,4′-bipyridine groups. The Cd atom exhibits a slightly distorted octahedral coordination environment, consisting of four S atoms of the chelating dimethyl dithiophosphate ligands and two N atoms of the centrosymmetric bridging 4,4′-bipyridine ligand.

Comment

The organodithio-derivatives of phosphorus are of interest because of their versatile coordination modes towards metals (Ito, 1972; Shety & Quintus, 1970; McCleverty *et al.*, 1982; Zheng *et al.*, 1999), and studies related to metal phosphorodithioates as lubrication oil and in the plastics industry (So *et al.*, 1993; Mikhailov *et al.*, 1970; Lawton *et al.*, 1972) have demonstrated extensive commercial applications. We have used 4,4′-bipyridine in this study because amines in lubrication oil have a great influence on its properties (Shiomi *et al.*, 1989). We report here the synthesis and crystal structure of a new compound, $[Cd(dtp)_2(bpy)]_n$ (dtp is dimethyl dithiophosphate and bpy is 4,4′-bipyridine), (I).



(I)

The title compound consists of alternating $Cd(dtp)_2$ and bpy units. A crystallographic center of inversion is present at the mid-point of the C—C bond of the bpy ligand; thus the pyridine rings in the bpy ligands are coplanar. A couple of dtp ligands are coordinated to the Cd atom by their two S atoms (Fig. 1). The average Cd—N bond length [2.378 (3) Å] is in good agreement with that for $[\{Cd(SC\{O\}Ph)_2\}_2(\mu\text{-bpy})_n]$ [2.333 (2) Å; Vittal *et al.*, 2003], while the the average Cd—S bond length [2.701 (1) Å] is consistent with those for other six-coordinate Cd complexes (Shimoi *et al.*, 1982; McCleverty *et al.*,1982). The S—P distances [1.965 (2)–1.986 (2) Å] are close to the typical double S═P bond length (1.94 Å). The S1—Cd1—S2 and S3—Cd1—S4 angles [76.37 (5) and 75.93 (4)°]

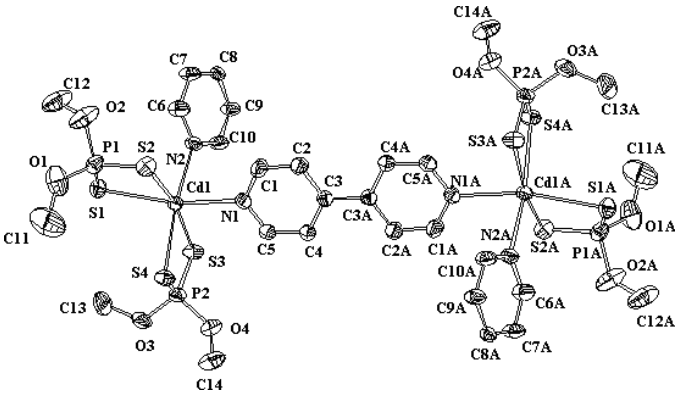


Figure 1
Section of the crystal structure of the title compound. Displacement ellipsoids are plotted at the 30% probability level. Hydrogen atoms are omitted for clarity. Atoms labeled with the suffix *A* are at $(-1-x, 1-y, 1-z)$.

are comparable with the value in the complex $[Cd(S_2P^iBu_2)_2]_2$ [78.82 (6)°; Byrom *et al.*, 2000]. Thus, the Cd atom exists in a slightly distorted octahedral configuration. The bpy ring and the metal lie almost in the same plane; the mean deviations of N1 and N2 from the mean plane are 0.0047 and 0.0338 Å, respectively. The four-membered ring formed by atoms Cd1, S1, S2 and P1 is also planar, as is the Cd1/S3/S4/P2 ring. These two planes make a dihedral angle of 84.4°. A perspective view of the polymer packing is presented in Fig. 2.

Experimental

$Cd(dtp)_2$ (0.227 g, 0.5 mmol) and bpy (0.078 g, 0.5 mmol) were dissolved in CH_2Cl_2 (10 ml). The mixture was stirred for 15 min and filtered. The filtrate was added to CH_3CN (10 ml) and left in air at room temperature. After a few days, colorless block-shaped crystals of (I) were obtained in 58% yield.

Crystal data

$[Cd(C_2H_6O_2PS_2)_2(C_{10}H_8N_2)]$
$M_r = 582.90$
Triclinic, $P\overline{1}$
$a = 10.281\ (3)$ Å
$b = 10.672\ (4)$ Å
$c = 12.945\ (5)$ Å
$\alpha = 79.209\ (15)°$
$\beta = 67.071\ (12)°$
$\gamma = 63.502\ (13)°$
$V = 1170.5\ (7)$ Å^3
$Z = 2$
$D_x = 1.654$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3009 reflections
$\theta = 3.4$–$27.5°$
$\mu = 1.45$ mm^{-1}
$T = 293\ (2)$ K
Prism, colorless
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku Mercury 70 diffractometer
ω scan
Absorption correction: multi-scan, (*CrystalClear*; Rigaku, 2000)
$T_{min} = 0.654$, $T_{max} = 0.744$
8921 measured reflections
5256 independent reflections
4625 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 27.5°$
$h = -13 \rightarrow 12$
$k = -12 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.109$
$S = 1.06$
5256 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 1.0677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.96$ e Å^{-3}
$\Delta\rho_{min} = -0.86$ e Å^{-3}

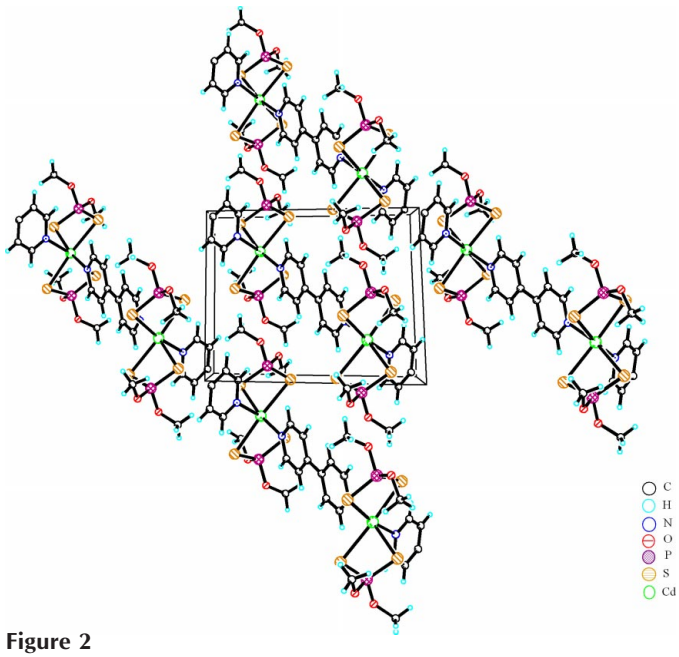


Figure 2
Packing diagram of (I).

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.377 (3)	Cd1—S4	2.691 (1)
Cd1—N2	2.378 (3)	P1—S1	1.984 (2)
Cd1—S1	2.696 (1)	P1—S2	1.965 (2)
Cd1—S2	2.706 (1)	P2—S3	1.986 (2)
Cd1—S3	2.711 (1)	P2—S4	1.967 (2)
N1—Cd1—N2	83.13 (14)	S1—P1—S2	115.51 (7)
S1—Cd1—S2	76.37 (5)	S3—P2—S4	114.43 (6)
S3—Cd1—S4	75.93 (4)		

All H atoms were placed at calculated positions (C–H = 0.93 and 0.96 Å), riding on their parent atoms [U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C)].

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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