

requirements of P_4 occupying four approximately planar positions.

The $\text{Ph}_2\text{P}-\text{Pt}-\text{PPh}_2$ angle in (1) [$109.5(2)^\circ$] is wide open compared with the $\text{PhP}-\text{Pt}-\text{PPh}_2$ angles and the $\text{PhP}-\text{Pt}-\text{PPh}$ angle (mean value 84.3 , $\Delta_{\text{max}} = 1.8^\circ$). The mean values of the $\text{PhP}-M-\text{PPh}_2$ angles and the $\text{PhP}-M-\text{PPh}$ angle in (2) [82.8 , $\Delta_{\text{max}} = 3.4^\circ$], (3) (84.6 , $\Delta_{\text{max}} = 3.5^\circ$), and (4) (83.2 , $\Delta_{\text{max}} = 2.4^\circ$) is comparable with the corresponding value in (1). The $\text{Ph}_2\text{P}-M-\text{PPh}_2$ angles in (2), (3) and (4) are also wide open: they are $97.2(2)$, $101.4(2)$ and $109.8(2)^\circ$, respectively. Obviously, replacing a $3d$ [in (2) and (3)] by a $4d$ central atom [in (4)] leads to a larger opening of the $\text{Ph}_2\text{P}-M-\text{PPh}_2$ angles, whereas the replacement by a $5d$ central atom in (1) results in no further opening of this angle. All intermolecular distances of the crystal structure of (1) are larger than the corresponding van der Waals radii and no packing effects are observed.

The cation of (1) is destabilized by the deviations from an idealized square-planar structure, which is electronically favoured in the case of d^8 complexes. The occurrence of sterically favoured tetrahedral complexes, which are common for some d^8 metals (Rappoli, Churchill, Janik, Rees & Atwood, 1987), is not possible for Pt^{II} , where this coordination is completely electronically destabilized (Atwood, 1985).

However, in the synthesis of (1) a five-coordinate intermediate occurs, which shows the tetrahedral arrangement of P_4 (Brüggeller, 1989).

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Structure of Iodo- $1\kappa I-\mu-(O\text{-isopropyl dithiocarbonato-}1\kappa^2 S, S':2\kappa S')$ -bis[($O\text{-isopropyl dithiocarbonato}$)cadmium] $\text{Cd}_2\text{I}(\text{S}_2\text{CO}^i\text{Pr})_3$

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Abstract. $[\text{Cd}_2\text{I}(\text{C}_4\text{H}_7\text{OS}_2)_3]$, $M_r = 757.4$, monoclinic, $P2_1/c$, $a = 12.028(2)$, $b = 19.261(4)$, $c = 10.864(2)$ Å, $\beta = 102.60(2)^\circ$, $V = 2456$ Å³, $Z = 4$, $D_m = 2.05$, $D_x = 2.048$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 3.440$ mm⁻¹, $F(000) = 1448$, $T = 295(2)$ K, $R = 0.028$ for 3511 observed reflections. The structure is polymeric with Cd atoms linked by xanthate (ROCS_2^-) bridges forming infinite chains in the c direction. The chains are interlinked by a series of $(\text{S}_2\text{CO}^i\text{Pr})_2\text{CdI}_2\text{Cd}(\text{S}_2\text{CO}^i\text{Pr})_2$ bridging units.

Introduction. Structural studies of metal halo xanthate complexes have shown a range of novel structures which are often a consequence of the halo atoms' ability to bridge metal centres (Gable, Hos-

kins, Steen & Winter, 1982; Gable, Hoskins, Steen, Tiekink & Winter, 1983). Further interest in these complexes has emerged from their usefulness in the preparation of mixed-ligand complexes (Hoskins, Tiekink & Winter, 1985). Recently we have reported (Abrahams, Corbett, Dakternieks, Gable, Hoskins, Tiekink & Winter, 1986) on the reaction of cadmium and mercury isopropyl xanthates $[\text{M}(\text{ipxan})_2]$ with the corresponding metal halides. Significant shifts in the characteristic IR absorptions of the xanthate ligands in the C—O and C—S region are consistent with the formation of metal halo xanthate complexes (Abrahams *et al.*, 1986). The poor solubility of the products, suggesting a polymeric structure, prevented examination by NMR spectroscopy. However, the

Table 1. Final fractional atomic coordinates and U_{eq} values (Å²)

	x	y	z	U_{eq}
$U_{eq} = (U_{11} + U_{22} + U_{33})/3.$				
Cd(1)	0.12886 (3)	0.22940 (2)	0.11412 (3)	0.0361 (2)
Cd(2)	0.37996 (3)	0.07222 (2)	0.45517 (4)	0.0453 (2)
I(1)	0.48501 (3)	0.00383 (2)	0.68566 (3)	0.0523 (2)
S(1)	0.2157 (1)	0.11762 (7)	0.2135 (1)	0.0447 (7)
S(2)	0.1767 (1)	0.02648 (7)	0.4172 (1)	0.0478 (7)
C(1)	0.1258 (4)	0.0797 (2)	0.2945 (4)	0.037 (2)
O(1)	0.0172 (2)	0.0926 (2)	0.2541 (3)	0.045 (2)
C(2)	-0.0688 (4)	0.0616 (3)	0.3171 (5)	0.054 (3)
C(3)	-0.1035 (6)	-0.0063 (3)	0.2543 (7)	0.085 (5)
C(4)	-0.1611 (5)	0.1152 (4)	0.3026 (7)	0.079 (5)
S(3)	0.2960 (1)	0.18361 (6)	0.6201 (1)	0.0464 (7)
S(4)	0.4667 (1)	0.19209 (7)	0.4596 (1)	0.0543 (7)
C(5)	0.3792 (3)	0.2296 (2)	0.5416 (4)	0.036 (2)
O(2)	0.3715 (3)	0.2978 (2)	0.5506 (3)	0.041 (2)
C(6)	0.4354 (4)	0.3457 (3)	0.4850 (5)	0.049 (3)
C(7)	0.3657 (5)	0.4105 (3)	0.4637 (6)	0.062 (3)
C(8)	0.5523 (5)	0.3558 (3)	0.5651 (7)	0.075 (4)
S(5)	-0.0569 (1)	0.28849 (9)	0.1332 (1)	0.0576 (8)
S(6)	0.1139 (1)	0.27359 (8)	0.3703 (1)	0.0532 (7)
C(9)	-0.0155 (4)	0.2989 (3)	0.2910 (4)	0.041 (2)
O(3)	-0.0791 (3)	0.3283 (2)	0.3606 (3)	0.058 (2)
C(10)	-0.1913 (5)	0.3600 (4)	0.3041 (6)	0.068 (4)
C(11)	-0.2002 (6)	0.4193 (3)	0.3923 (7)	0.085 (5)
C(12)	-0.2799 (6)	0.3060 (4)	0.2995 (9)	0.098 (6)

addition of tertiary phosphines solubilized the mercury products and a ¹⁹⁹Hg and ³¹P NMR analysis of the resulting solutions strongly suggested the formation of phosphine adducts of HgX(ipxan) (X = Cl, Br, I). Although the resulting cadmium complexes could also be solubilized by the addition of tertiary phosphine, the resulting ¹¹³Cd and ³¹P NMR spectra were more complicated and did not allow the identification of corresponding cadmium complexes.

Despite the poor solubility of the proposed cadmium halo xanthate complexes, a small number of crystals of a cadmium iodo xanthate complex were obtained by the slow evaporation of a dichloromethane solution. The IR spectrum of this complex was identical to that of the fine powder initially precipitated from the solution.

A crystal determination of this species has been undertaken in order to (i) determine the stoichiometry and (ii) establish the extent and type of bridging in the polymeric structure.

Experimental. Crystals of the title compound were obtained by the slow evaporation of a suspension of CdI₂ and Cd(ipxan)₂ in dichloromethane. Enraf-Nonius CAD-4F four-circle single-crystal automatic diffractometer, Mo K α (graphite-monochromatized) radiation, ω -2 θ scan method. Plate-like crystal used, 0.33 × 0.373 × 0.160 mm. Accurate cell dimensions from least-squares procedure on 20 reflections (13.5 ≤ θ ≤ 24.5°). Analytical absorption corrections applied (Sheldrick, 1976); max./min. transmission factors 0.5410 and 0.3451. Total of 5541 reflections (1 ≤ θ ≤ 25°) measured in the range -14 ≤ h ≤ 14,

Table 2. Interatomic distances (Å) and bond angles (°)

Cd(1)—S(1)	2.530 (1)	Cd(1)—S(3')	2.607 (1)
Cd(1)—S(5)	2.556 (1)	Cd(1)—S(6)	2.953 (1)
Cd(1)—S(6')	2.616 (1)	Cd(2)—S(1)	3.049 (1)
Cd(2)—S(2)	2.546 (1)	Cd(2)—S(3)	3.102 (1)
Cd(2)—S(4)	2.530 (1)	Cd(2)—I(1)	2.8673 (5)
Cd(2)—I(1 ⁱⁱ)	2.8650 (5)	S(1)—C(1)	1.701 (5)
S(2)—C(1)	1.687 (4)	C(1)—O(1)	1.308 (5)
O(1)—C(2)	1.485 (6)	C(2)—C(3)	1.492 (8)
C(2)—C(4)	1.499 (9)	S(3)—C(5)	1.699 (4)
S(4)—C(5)	1.683 (4)	C(5)—O(2)	1.322 (5)
O(2)—C(6)	1.480 (6)	C(6)—C(7)	1.493 (8)
C(6)—C(8)	1.496 (8)	S(5)—C(9)	1.690 (4)
S(6)—C(9)	1.679 (5)	C(9)—O(3)	1.315 (6)
O(3)—C(10)	1.486 (7)	C(10)—C(11)	1.51 (1)
C(10)—C(12)	1.48 (1)		
S(1)—Cd(1)—S(3')	106.98 (4)	S(1)—Cd(1)—S(6')	129.14 (4)
S(1)—Cd(1)—S(6)	86.99 (4)	S(1)—Cd(1)—S(6)	110.13 (4)
S(3')—Cd(1)—S(5)	113.25 (5)	S(3')—Cd(1)—S(6)	89.80 (4)
S(3')—Cd(1)—S(6)	85.51 (4)	S(5)—Cd(1)—S(6)	63.97 (3)
S(5)—Cd(1)—C(6)	102.92 (4)	S(6)—Cd(1)—S(6')	162.88 (5)
Cd(1)—S(6')—Cd(1')	160.56 (6)	Cd(1)—S(3')—Cd(2')	140.95 (4)
Cd(1)—S(1)—Cd(2)	137.83 (5)	Cd(1)—S(1)—C(1)	109.7 (2)
Cd(1)—S(3')—C(5')	100.8 (1)	Cd(1)—S(5)—C(9)	93.8 (2)
Cd(1)—S(6)—C(9)	80.8 (2)	Cd(1)—S(6')—C(9')	112.2 (2)
S(1)—Cd(2)—S(2)	62.67 (4)	S(1)—Cd(2)—S(3)	93.87 (3)
S(1)—Cd(2)—S(4)	86.66 (4)	S(1)—Cd(2)—I(1)	164.36 (3)
S(1)—Cd(2)—I(1 ⁱⁱ)	91.32 (3)	S(2)—Cd(2)—S(3)	84.88 (4)
S(2)—Cd(2)—S(4)	134.13 (4)	S(2)—Cd(2)—I(1)	101.96 (3)
S(2)—Cd(2)—I(1 ⁱⁱ)	111.88 (3)	S(3)—Cd(2)—S(4)	62.78 (3)
S(3)—Cd(2)—I(1)	87.15 (2)	S(3)—Cd(2)—I(1 ⁱⁱ)	162.93 (3)
S(4)—Cd(2)—I(1)	107.54 (3)	S(4)—Cd(2)—I(1 ⁱⁱ)	101.38 (3)
I(1)—Cd(2)—I(1 ⁱⁱ)	92.20 (1)	Cd(2)—I(1)—Cd(2 ⁱⁱ)	87.80 (1)
Cd(2)—S(1)—Cd(2 ⁱⁱ)	87.80 (1)	Cd(2)—S(1)—O(1)	78.3 (2)
Cd(2)—S(2)—C(1)	95.0 (2)	Cd(2)—S(3)—C(5)	76.6 (1)
Cd(2)—S(4)—C(5)	95.7 (1)	S(1)—C(1)—S(2)	120.5 (3)
S(1)—C(1)—O(1)	116.5 (3)	S(2)—C(1)—O(1)	123.0 (3)
C(1)—O(1)—C(2)	120.9 (4)	O(1)—C(2)—C(3)	107.2 (4)
O(1)—C(2)—C(4)	104.4 (5)	C(3)—C(2)—C(4)	115.4 (5)
S(3)—C(5)—S(4)	123.1 (2)	S(3)—C(5)—O(2)	115.0 (3)
S(4)—C(5)—O(2)	121.9 (3)	C(5)—O(2)—C(6)	122.1 (4)
O(2)—C(6)—C(7)	105.2 (4)	O(2)—C(6)—C(8)	108.8 (4)
C(7)—C(6)—C(8)	114.0 (5)	S(5)—C(9)—S(6)	121.4 (3)
S(5)—C(9)—O(3)	123.7 (4)	S(6)—C(9)—O(3)	114.9 (3)
C(9)—O(3)—C(10)	121.9 (4)	O(3)—C(10)—C(11)	103.4 (5)
O(3)—C(10)—C(12)	107.9 (6)	C(11)—C(10)—C(12)	113.7 (6)

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

-1 ≤ k ≤ 22 and -1 ≤ l ≤ 12 of which 4313 were unique, $R_{int} = 0.0321$, and 3511 satisfied $I \geq 2\sigma(I)$. The intensities of three reference reflections ($\bar{2}, \bar{1}, \bar{1}$, $\bar{7}, \bar{1}, \bar{4}$, $\bar{6}, \bar{2}, \bar{6}$) measured every 3600 s of X-ray exposure time showed no significant variation. Structure solved from interpretation of Patterson map (SHELX86; Sheldrick, 1985), full-matrix least-squares refinement of 226 parameters based on F^2 (Sheldrick, 1976). Anisotropic thermal parameters applied to all non-H atoms; H atoms included in the model at their geometrically estimated positions. At convergence $R = 0.0276$, $wR = 0.0280$, $w = [\sigma^2(F) + 0.0003F^2]^{-1}$, $S = 1.407$, $(\Delta/\sigma)_{max} = 0.002$, $\Delta\rho_{max} = 0.45$, $\Delta\rho_{min} = -1.16 \text{ e } \text{Å}^{-3}$; no extinction correction. Scattering factors for atomic C, H, O and S given in SHELX76 (Sheldrick, 1976) and those for neutral Cd and I corrected for f' and f'' were from International Tables for X-ray Crystallography (1974). All calcula-

tions on VAX11/780 and 11/8650 computer systems. Atomic parameters are given in Table 1,* interatomic distances and bond angles in Table 2, the numbering scheme used is shown in Fig. 1. The superscripted Roman numerals appearing in the text, diagrams and tables refer to the symmetry transformations listed in Table 2.

Discussion. The structure reveals that the compound has the stoichiometry $\text{Cd}_2\text{I}(\text{ipxan})_3$ and formally may be considered as $\text{Cd}(\text{ipxan})_2\cdot\text{Cd}(\text{ipxan})\text{I}$. The structure is complex possessing two non-equivalent Cd atoms and three independent xanthate moieties. The Cd(1) atoms are linked by xanthate bridges to form an almost linear chain. A similar combination of bridges connects the Cd(1) and Cd(2) atoms resulting in a six-membered $(\text{Cd}-\text{S})_3$ ring. A double iodo bridge connects the Cd(2) atoms resulting in a bridging unit [see Fig 1(b)] that connects the chains to form an infinite two-dimensional network (see Fig. 2).

A further interesting feature of this structure is the appearance of 16-membered rings comprising eight

* Lists of anisotropic thermal parameters, H-atom parameters, equations of mean planes and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52366 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

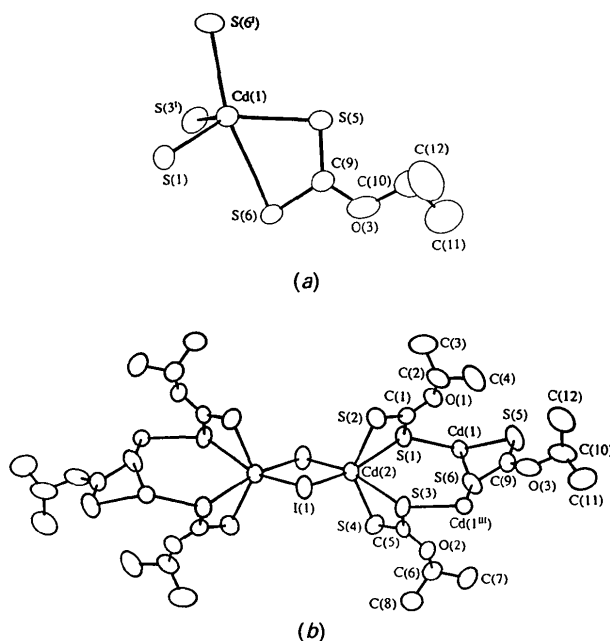


Fig. 1. The numbering scheme and coordination environment of (a) Cd(1) and (b) Cd(2); (b) also shows the interaction of the $(\text{ipxan})_2\text{CdI}_2\text{Cd}(\text{ipxan})_2$ bridging unit with the Cd(1) atoms resulting in the formation of $\text{Cd}-\text{S}$ six-membered rings. The Roman-numeral superscripts refer to the symmetry transformations given in Table 2.

Cd [4 Cd(1) and 4 Cd(2)], six S [2 S(6), 2 S(3) and 2 S(1)] and two I atoms formed between successive $(\text{ipxan})_2\text{CdI}_2\text{Cd}(\text{ipxan})_2$ bridges linking adjacent chains. This is highlighted in Fig. 2. 16-membered rings have been found frequently in polymeric alkyl xanthates of the zinc triad (Winter, 1980) although in these structures, four metal atoms are linked by $-\text{S}-\text{C}-\text{S}-$ bridges.

Cd(1) is coordinated by five S atoms in a distorted trigonal-bipyramidal arrangement. Atoms S(1), S(3') and S(5) form a trigonal plane, with the Cd atom lying 0.4809 Å out of the plane towards the direction of atom S(6') [see Fig. 1(a)]. In contrast Cd(2) is six coordinate in, what appears to be, a distorted octahedral environment arising from two asymmetrically chelating xanthate ligands and two bridging I atoms. The Cd—I bond lengths of 2.8650 (5) and 2.8673 (5) Å are similar to those observed for the bridging I atoms in $[\text{CdI}_2\text{PEt}_3]_2$ [2.878 (1) and 2.862 (1) Å] (Bell, Dee, Goldstein & Nowell, 1982).

The asymmetry in the chelation of the xanthate ligands to the Cd atoms is most likely due to the additional bond formed by one of the two S atoms. It is more pronounced in the chelation to the Cd(2) atom which is more highly coordinated than Cd(1). The short Cd—S bond lengths are in the range 2.530 (1) to 2.616 (1) Å and are comparable to the Cd—S bond lengths of 2.536 (3) and 2.586 (2) Å observed in polymeric $\text{Cd}(\text{ipxan})_2$ (Imura, 1973). The longer Cd—S bond lengths 2.953 (1) and 3.102 (1) Å are well within the sum of the van der Waals radii [3.40 Å (Bondi, 1964)] and are therefore indicative of a bonding interaction. The corresponding Cd—S distance in $\text{Cd}(\text{ipxan})_2$ is 3.291 Å and while this distance may not represent a significant

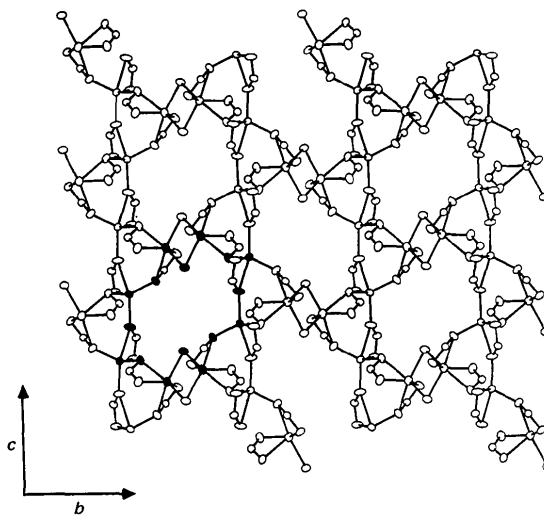


Fig. 2. The two-dimensional network which extends in the bc plane. A 16-membered $\text{Cd}_8\text{S}_6\text{I}_2$ ring is highlighted. The $-\text{O}-\text{Pr}$ groups have been omitted for clarity.

bonding interaction, the general arrangement of the bridge is similar.

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Structure of Mononuclear Bis{aqua[2,2'-(1,3,4-oxadiazole-2,5-diyl)dipyridine-N,N']}copper(II) Diperchlorate

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Abstract. [Cu(C₁₂H₈N₄O)₂(H₂O)₂](ClO₄)₂, *M_r* = 746.5, monoclinic, *P*₂₁/*n*, *a* = 13.579 (2), *b* = 10.904 (3), *c* = 10.329 (2) Å, β = 103.5°, *V* = 1487.1 Å³, *Z* = 2, *D_x* = 1.667, *D_m* = 1.67 g cm⁻³, λ(Mo *K*α) = 0.7107 Å, μ = 9.38 cm⁻¹, *F*(000) = 722, *R* = 0.053 for 769 reflexions. The structure consists of alternate layers of mononuclear centrosymmetric cations and ClO₄⁻ anions. Each ligand is bidentate, linked to the Cu atoms through one N atom of the oxadiazole and the N atom of one of the pyridines. The two water molecules complete a square-bipyramidal surrounding of the metal ion.

Introduction. Symmetrical 2,5-disubstituted-1,3,4-oxadiazoles are reported to show a broad spectrum of biological activities (Sharma & Tandon, 1984). No report on these kinds of molecules as ligands in metal compounds has appeared so far. In order to investigate the coordination mode in this type of compound, we selected 2,2'-(1,3,4-oxadiazole-2,5-diyl)dipyridine (odp).

Coordination compounds with 2,2'-(1,2,4-triazole-3,5-diyl)dipyridine have been identified (Keij, de Graff, Haasnoot & Reedijk, 1984); the crystal struc-

ture determination of an Ni compound showed the dinucleating properties of this ligand. Surprisingly, in spite of the similarity of the ligand structure, a mononuclear compound was obtained in our case.

Experimental. The odp ligand was synthesized according to Sharma & Tandon (1984). 0.18 g (8 × 10⁻⁴ mol) odp was added to a warm solution of 0.3 g (8 × 10⁻⁴ mol) Cu(ClO₄)₂·6H₂O in 40 ml of water. Green crystals appeared on standing for several days and were isolated by filtration.

Air stable tabular crystal mounted on glass rod. Unit-cell dimensions refined from 25 reflexions (4 < θ < 6°). Philips PW 1100 automated diffractometer. 1595 reflexions with 2 < θ < 20°, 0 < *h* < 13, 0 < *k* < 10, 0 < *l* < 10, 769 unique reflexions [*I* > 3σ(*I*)], *R_{int}* = 0.040; three standards (120, 211, 301) stable throughout data collection.

Observed reflexions limited by 0*k*0 (*k* = 2*n*) and *h*0*l* (*h* + *l* = 2*n*) leading to the non-standard space group *P*₂₁/*n*.

Crystal size: 0.155 × 0.3 × 0.02 mm with corresponding faces of the type (100), (010) and (001). Absorption correction applied, transmission factors: