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Poly[bis(μ_2-*O*,*O*′-dimethyl dithiophosphato)-mercury(II)]

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In the title compound, $[Hg(C_2H_6O_2PS_2)_2]_n$, the Hg atom is coordinated by four S atoms in a distorted tetrahedral arrangement. The Hg—S bond distances are in the range 2.508 (2)–2.662 (2) Å, and the six S—Hg—S angles are in the range 99.14 (7)–118.77 (8)°. In the crystal structure, a two-dimensional network of 16-membered rings of $[-Hg-S-P-S-]_4$ is formed parallel to the (100) plane.

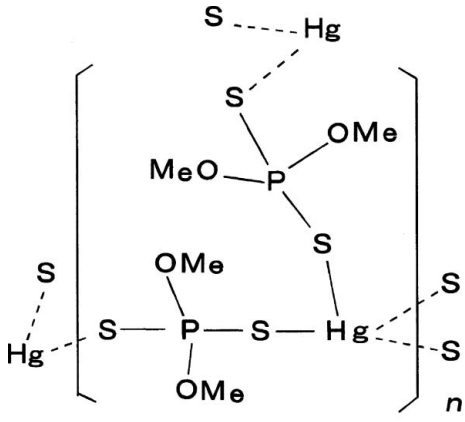
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(O–C) = 0.011 Å
R factor = 0.031
wR factor = 0.033
Data-to-parameter ratio = 16.0

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

Comment

As part of a study of metal xanthates and dialkyldithiophosphates (Ito, 2003; Ito & Maeda, 2004), the crystal structure of the title compound, (I), has been determined. A displacement ellipsoid plot of (I) is shown in Fig. 1. The S—P—S parts of the two ligands bridge adjacent Hg atoms, forming one half of a 16-membered ring, the other half being generated by a center of symmetry at the center of the ring.



(I)

The two-dimensional network structure of (I) is similar to that in mercury ethylxanthate, (II) (Watanabe, 1977). The distortion of the HgS_4 arrangement from a regular tetrahedron is much less in (I) than in (II). In (II), the four Hg—S distances are in the range 2.313 (8)–2.943 (10) Å, and the six S—Hg—S angles are in the range 81.8 (3)–148.8 (3)°.

Experimental

Potassium dimethyldithiophosphate (2.0 g) and mercury nitrate (1.8 g) were each dissolved in pure water (8.0 ml). A powder of (I) was precipitated by combining the two solutions. Recrystallization from an acetone solution of (I) at room temperature gave colorless plate-shaped crystals.

Crystal data

$[Hg(C_2H_6O_2PS_2)_2]$
M_r = 514.91
Monoclinic, $P2_1/c$
a = 9.930 (5) Å
b = 12.043 (2) Å
c = 11.885 (1) Å
β = 96.56 (2)°
V = 1412.0 (8) Å^3
Z = 4
D_x = 2.422 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 11.74 mm^{-1}
T = 296.1 K
Plate, colorless
0.16 × 0.16 × 0.09 mm

Data collection

Rigaku AFC-5S diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.182, T_{max} = 0.348
3580 measured reflections
3224 independent reflections
2372 reflections with $I > 3\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.5°
3 standard reflections
every 150 reflections
intensity decay: 0.5%

Refinement

Refinement on F
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.033
S = 1.46
2372 reflections
148 parameters
H-atom parameters constrained
$w = 1/\sigma^2(F_o)$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −1.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg—S1	2.662 (2)	P1—O1	1.581 (5)
Hg—S2^{i}	2.545 (2)	P1—O2	1.580 (6)
Hg—S3	2.547 (2)	P2—O3	1.563 (5)
Hg—S4^{ii}	2.508 (2)	P2—O4	1.579 (5)
S1—P1	1.965 (3)	O1—C1	1.422 (9)
S2—P1	2.003 (3)	O2—C2	1.42 (1)
S3—P2	1.983 (3)	O3—C3	1.449 (9)
S4—P2	2.000 (2)	O4—C4	1.43 (1)
S1—Hg—S2^{i}	100.51 (7)	S2^{i}—Hg—S3	109.53 (8)
S1—Hg—S3	99.14 (7)	S2^{i}—Hg—S4^{ii}	118.77 (8)
S1—Hg—S4^{ii}	107.34 (7)	S3—Hg—S4^{ii}	117.97 (6)

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

H atoms were placed in geometrically calculated positions (C—H = 0.95 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent atom). The deepest hole is located 0.83 Å from atom Hg.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CrystalStructure*; molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

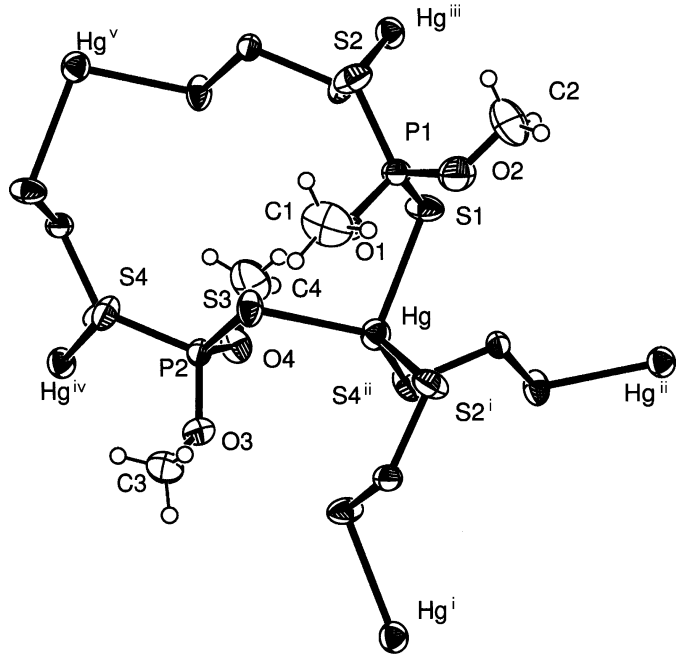


Figure 1
A view of part of the crystal structure of (I), showing 50% probability displacement ellipsoids. Atoms Hg^{i} and Hg^{iii}, and Hg^{ii} and Hg^{iv} are related by a unit translation along the c and b axes, respectively. [Symmetry codes: (i) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (ii) $1-x, y+\frac{1}{2}, \frac{1}{2}-z$; (iii) $x, \frac{3}{2}-y, z+\frac{1}{2}$; (iv) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (v) $1-x, 1-y, 1-z$.]

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