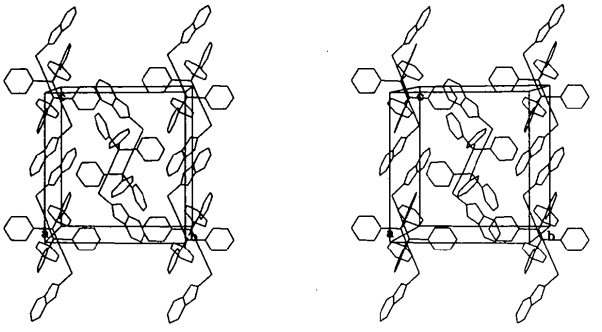

Fig. 2. Packing diagram of [(Ph_3P)Au(Sboz)] in the unit cell.

[(Ph_3P)Au(Sboz)] is linear with a P—Au—S angle of 176·48 (8)°. The Au—P and Au—S distances are 2·258 (2) and 2·299 (2) Å, respectively. The chrysotherapeutic drug auranofin (Hill & Sutton, 1980) is similar with P—Au—S 173·6 (1)°, Au—P 2·259 (3) and Au—S 2·293 (3) Å. Also, the complex [(Ph_3P)-Au(S_2CNEt_2)] (Wijnhoven, Bosman & Beurskens, 1972) has a similar structure with P—Au—S 175·7 (1)°, Au—P 2·251 (3) and Au—S 2·338 (3) Å. In the dimer [$AuSC_2CH_2PEt_2]_2$ (Crane & Beall, 1978), the P—Au—S angle is somewhat smaller (173·5°) as a result of Au—Au interaction.

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Structure of Dichloro(2-methylquinoxaline-N^4)mercury(II)

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Abstract. [$HgCl_2(C_9H_8N_2)$], $M_r = 415·7$, monoclinic, $P2_1/n$, $a = 3·9110$ (3), $b = 26·645$ (3), $c = 10·6753$ (12) Å, $\beta = 98·234$ (9)°, $V = 1101·0$ Å^3, $Z = 4$, $D_x = 2·507$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 14·43$ mm^{-1}, $F(000) = 760$, $T = 295$ K, $R = 0·0497$ for 810 unique observed reflections. The structure consists of infinite, polymeric chains running parallel to the a axis: these are formed by chloride bridging between parallel dimeric units which are themselves chloride bridged. The closest Hg—Hg distances of 3·911 Å occur between dimers, rather than within them where the Hg–Hg separation is 4·328 Å. The coordination around the mercury(II) cation is distorted octahedral.

Experimental. Compound prepared by dropwise addition of 2-methylquinoxaline (0·05 mol) to $HgCl_2$ (0·025 mol) in boiling ethanol (70 cm^3) followed by

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Table 1. *Atomic coordinates and isotropic thermal parameters with e.s.d.'s*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}/U_{iso}(Å^2)
Hg	0·6116 (3)	0·57196 (5)	0·42110 (10)	0·0468 (6)
Cl(1)	0·2112 (16)	0·5099 (3)	0·3429 (6)	0·045 (4)
Cl(2)	1·0247 (17)	0·6236 (3)	0·5346 (6)	0·051 (4)
N(1)	0·226 (7)	0·6963 (12)	0·0416 (20)	0·086 (22)
N(4)	0·492 (6)	0·6322 (14)	0·2266 (20)	0·087 (21)
C(2)	0·214 (11)	0·7072 (18)	0·149 (4)	0·109 (14)
C(2*M*)	0·110 (9)	0·7613 (15)	0·185 (3)	0·085 (11)
C(3)	0·356 (8)	0·6783 (15)	0·257 (3)	0·076 (10)
C(5)	0·495 (8)	0·6149 (14)	0·109 (3)	0·072 (10)
C(6)	0·619 (8)	0·5759 (15)	0·078 (3)	0·072 (9)
C(7)	0·628 (10)	0·5588 (16)	−0·051 (4)	0·100 (13)
C(8)	0·485 (8)	0·5888 (13)	−0·143 (3)	0·071 (10)
C(9)	0·349 (10)	0·6338 (17)	−0·116 (4)	0·095 (12)
C(10)	0·354 (7)	0·6521 (12)	−0·002 (3)	0·049 (7)

Table 2. *Bond lengths* (Å) *and bond angles* (°) *with e.s.d.'s*

Hg—Cl(1)	2·348 (7)	C(2)—C(3)	1·43 (6)
Hg—Cl(1′)	3·081 (7)	C(3)—N(4)	1·39 (5)
Hg—Cl(1″)	3·328 (7)	N(4)—C(5)	1·33 (5)
Hg—Cl(2)	2·326 (7)	C(5)—C(6)	1·22 (5)
Hg—Cl(2‴)	3·070 (7)	C(5)—C(10)	1·58 (4)
Hg—N(4)	2·61 (3)	C(6)—C(7)	1·45 (5)
N(1)—C(2)	1·19 (5)	C(7)—C(8)	1·33 (5)
N(1)—C(10)	1·39 (4)	C(8)—C(9)	1·36 (5)
C(2)—C(2*M*)	1·56 (6)	C(9)—C(10)	1·31 (5)

Cl(1)—Hg—Cl(2)	168·56 (24)	C(2)—N(1)—C(10)	126·5 (33)
Cl(1)—Hg—Cl(1′)	91·16 (20)	N(1)—C(2)—C(2*M*)	121·0 (39)
Cl(1′)—Hg—Cl(1″)	76·65 (17)	N(1)—C(2)—C(3)	125·5 (41)
Cl(1′)—Hg—Cl(2)	87·69 (22)	C(2*M*)—C(2)—C(3)	112·2 (35)
Cl(1′)—Hg—Cl(2‴)	171·31 (18)	C(2)—C(3)—N(4)	113·8 (33)
Cl(1)—Hg—Cl(1″)	82·14 (20)	Hg—N(4)—C(3)	112·8 (21)
Cl(1)—Hg—Cl(2‴)	87·57 (21)	Hg—N(4)—C(5)	120·5 (22)
Cl(2)—Hg—Cl(1″)	86·53 (21)	C(3)—N(4)—C(5)	125·3 (30)
Cl(2‴)—Hg—Cl(1″)	96·66 (18)	N(4)—C(5)—C(6)	127·8 (35)
Cl(2)—Hg—Cl(2‴)	91·85 (22)	N(4)—C(5)—C(10)	115·9 (28)
Cl(1″)—Hg—N(4)	176·3 (6)	C(6)—C(5)—C(10)	116·1 (31)
Cl(1′)—Hg—N(4)	99·9 (7)	C(5)—C(6)—C(7)	126·3 (35)
Cl(2‴)—Hg—N(4)	88·8 (6)	C(6)—C(7)—C(8)	116·7 (34)
Cl(1)—Hg—N(4)	96·6 (7)	C(7)—C(8)—C(9)	120·6 (35)
Cl(2)—Hg—N(4)	94·8 (7)	C(8)—C(9)—C(10)	124·8 (36)
Hg—Cl(1)—Hg‴	91·16 (20)	N(1)—C(10)—C(5)	112·7 (25)
Hg—Cl(1)—Hg″	97·86 (21)	N(1)—C(10)—C(9)	131·9 (30)
Hg‴—Cl(1)—Hg″	103·35 (19)	C(5)—C(10)—C(9)	115·0 (29)
Hg—Cl(2)—Hg′	91·85 (23)		

Atoms denoted by the following primes are related to those without such primes as shown: (′) $1+x, y, z$; (″) $1-x, 1-y, 1-z$; (‴) $-1+x, y, z$.

allowing the solution to stand overnight. Crystals isolated by filtration and washed with ethanol. Colourless lath, 0·54 × 0·054 × 0·008 mm, STADI-4 four-circle diffractometer, graphite-monochromated Mo $K\alpha$ X-radiation, cell parameters from 2θ values of 30 reflections measured at $\pm\omega$ ($10 < \theta < 11°$). For data collection, ω–2θ scans with ω-scan width $(1{\cdot}20 + 0{\cdot}35\tan\theta)°$, $2\theta_{max} = 45°$, h −4→4, k 0→28, l 0→11, slight crystal decay (*ca* 6%) corrected for during processing, absorption correction using 144 ψ scans (min. and max. transmission factors 0·0375 and 0·5383 respectively), 1488 unique reflections, of which 810 with $F > 6\sigma(F)$ were used for structure solution [from a Patterson synthesis (Hg) followed by iterative cycles of least-squares refinement and difference Fourier synthesis] and refinement [using full-matrix least squares on F (Sheldrick, 1976)]. Anisotropic thermal parameters for Hg, Cl and N, isotropic for C; H atoms in fixed, calculated positions. At final convergence, $R = 0{\cdot}0497$, $wR = 0{\cdot}0582$, $S = 0{\cdot}954$ for 85 parameters, $(\Delta/\sigma)_{max}$ in final cycle 0·013, max. and min. residues in final ΔF synthesis 1·71, −1·29 e Å^{-3} respectively. The weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}000777F^2$ gave satisfactory agreement analyses. Scattering factors were inlaid (Sheldrick, 1976) except for Hg (Cromer & Mann, 1968). Atomic coordinates and equivalent isotropic thermal parameters are given in Table 1, while selected bond lengths and angles appear in

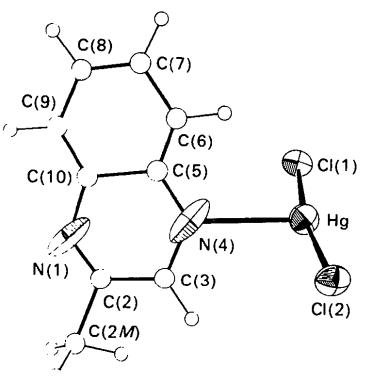

Fig. 1. A general view of one asymmetric unit showing the atom-numbering scheme employed: thermal ellipsoids are drawn at the 30% probability level, excepting those of C and H which have artificial radii of 0·15 and 0·10 Å, respectively, for clarity.

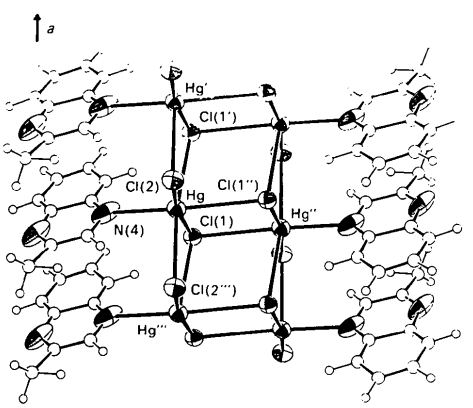

Fig. 2. A view of part of the polymeric structure formed by stacking of dimers along the crystallographic a axis. The symmetry operations indicated by the primes (′, ″, ‴) are defined in Table 2.

Table 2.* The atom-numbering scheme for the molecule is shown in Fig. 1 and Fig. 2 shows part of one infinite column of dimers: both were generated using *ORTEP* (Mallinson & Muir, 1985). Molecular-geometry calculations were performed using *CALC* (Gould & Taylor, 1985).

Related literature. The mean Hg—Cl bond in $HgCl_2$ is 2·283 (9) Å and the Cl—Hg—Cl angle is 178·6 (4)° (Subramanian & Seff, 1980). The closest non-bonded interactions occur at 3·33 Å (Cl···Cl) and at 3·37 and 3·44 Å (Hg···Cl). The closest Hg···Hg contact is at 4·33 Å.

We thank the SERC for funding towards the purchase of a diffractometer.

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51907 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 1,3-μ_2-Acetato-2-(pyridine)-μ_3-sulfido-tris[(diethyl dithiophosphato-*S*,*S*')-μ_2-sulfido-tungsten(IV)](3 *W*–*W*)

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(*Received* 17 *March* 1989; *accepted* 4 *April* 1989)

Abstract. $[W_3S_4(C_2H_3O_2)(C_4H_{10}O_2PS_2)_3(C_5H_5N)]$, M_r = 1374, triclinic, $P\bar{1}$, a = 13·939 (2), b = 16·018 (3), c = 9·627 (2) Å, α = 101·08 (2), β = 105·69 (2), γ = 77·64 (3)°, V = 2000·6 Å^3, Z = 2, D_x = 2·28 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 94·5 cm^{-1}, $F(000)$ = 1302, R = 0·050 for 3896 unique observed reflections $I \geq 8\sigma(I)$. The W atoms are all octahedrally coordinated by two μ_2-S atoms (W—μ_2S av. 2·298 Å), a μ_3-S atom (W—μ_3S av. 2·343 Å) and a chelating $S_2P(OC_2H_5)_2$ terminal ligand [W—S_t (dtp) 2·538 Å]; in addition, W(1) and W(3) are coordinated by a bridging CH_3COO ligand (W—O_b 2·174 Å), while W(2) is coordinated by a C_5H_5N molecule (W—N 2·390 Å). There are three W—W bonds [W(1)—W(2) 2·739, W(1)—W(3) 2·673, W(2)—W(3) 2·750 Å] in the cluster core $[W_3S_4]^{4+}$, which has an incomplete cubane-like structure.

Experimental. Crystals of the title compound were prepared by the method described by Zhan (1989). Crystal dimensions 0·30 × 0·25 × 0·35 mm. Data were collected on a CAD-4 κ-geometry diffractometer using Mo $K\alpha$ radiation at ~296 K. $\omega/2\theta$ scan, scan speed varied from 3 to 5° min^{-1} (in ω), the scan width was $(0{\cdot}60 + 0{\cdot}35\tan\theta)°$. Cell constants were obtained by least-squares analysis of 25 diffraction maxima ($26 \leq 2\theta \leq 27°$). The intensities were corrected for absorption using empirical scan data (maximum and minimum transmission factors 1·07 and, 0·95 respectively) and Lorentz and polarization factors to give a total of 6605 intensities, up to a

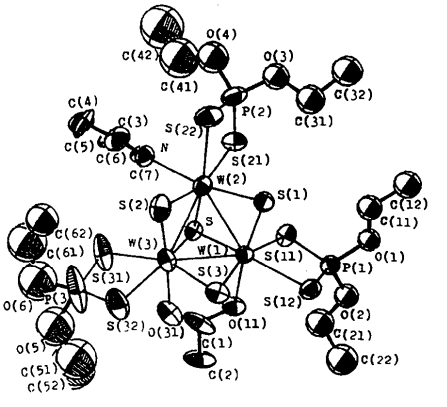

Fig. 1. Drawing of the title compound with thermal ellipsoids.

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