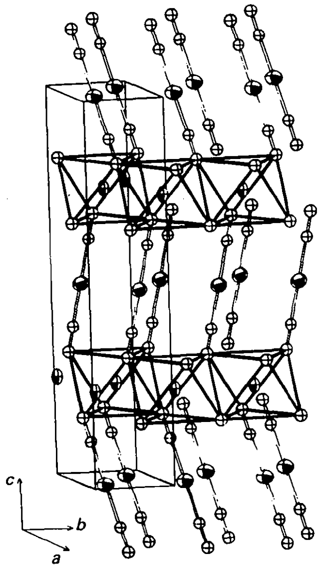

Fig. 1. *ORTEP* diagram (Johnson, 1976) of the crystal structure of $Na[Ag(CN)_2]$.

The structure (Fig. 1) comprises layers of linear NC—Ag—CN groups. These groups are canted by about 21° with respect to the *c* axis. In this way, pseudohexagonal layers of N atoms are formed with the sequence *ABAB*.... The Na ions occupy octahedral holes between the nitrogen layers.

Related literature. Surprisingly little is known about the crystal structures of dicyanoargentates. The few examples are $K_2Na[Ag(CN)_2]_3$ (Zabel, Kühnel & Range, 1989), $Ca[Ag(CN)_2]_2.2H_2O$, $Sr[Ag(CN)_2]_2.23H_2O$ (Range, Zabel, Meyer & Fischer, 1985) and, with complex cations, $[M(en)_3][Ag(CN)_2]_2$ and $[M(en)_2][Ag(CN)_2]_2$ (Kappenstein, Ouali, Guerin, Cernak & Chomic, 1988). The crystal structure of $K[Ag(CN)_2]$, proposed more than fifty years ago (Hoard, 1933), is at variance with spectroscopic evidence (Bottger, 1968) and still needs to be confirmed by modern techniques. A close relation exists between the structures of $Na[Ag(CN)_2]$ and $K[I(CN)_2]$ (Tebbe & Krauss, 1988).

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Acta Cryst. (1989). C45, 1420–1422

Structure of (2-Benzoxazolethiolato)(triphenylphosphine)gold(I)

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Abstract. $[Au(C_7H_4NOS)(C_{18}H_{15}P)]$, $M_r = 609{\cdot}7$, monoclinic, $P2_1/n$, $a = 12{\cdot}709\ (3)$, $b = 12{\cdot}871\ (4)$, $c = 13{\cdot}462\ (6)$ Å, $\beta = 94{\cdot}64\ (3)°$, $V = 2195\ (2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}84$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 68{\cdot}7$ cm^{-1}, $F(000) = 1176$, $T = 296$ K, final $R = 0{\cdot}033$ for 2823 unique observed reflections. The 2-benzoxazolethiolate ligand (Sboz), which contains three potential coordination sites (N, O and S), forms a linear complex with a P—Au—S angle of 176·43 (8)°. The Au—P and Au—S distances are 2·258 (2) and 2·299 (2) Å, respectively. This angle and these bond distances are similar to those of other phosphorous–gold–sulfur complexes such as the antiarthritic drug auranofin.

Experimental. Ph_3PAuCl (0·21 mmol) (De Stefano & Burmeister, 1971) was placed in a beaker containing 20 ml ethanol. NaOH (0·25 mmol) and then HSboz (0·26 mmol) (Fluka) were added and the solution stirred and heated. A powder formed, which was

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isolated by vacuum filtration and recrystallized from CH_2Cl_2 to yield light-yellow crystals with an elemental analysis consistent with the formula $C_{25}H_{19}AuNOPS$. Analysis: Calculated: C, 49·12; H, 3·11%. Found: C, 48·25; H, 3·24%.

Rectangular plate, D_m not determined, 0·50 × 0·30 × 0·30 mm, Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, ω–2θ scan, scan width $(0{\cdot}9 + 0{\cdot}34\tan\theta)^\circ$, $2\theta_{\max} = 53^\circ$, lattice parameters from least-squares refinement of 24 reflections in the range of $10 < \theta < 12^\circ$. Systematic absences $0k0$ $(k = 2n + 1)$, $h0l$ $(h + l = 2n + 1)$; $+h+k\pm l$ with $h \leq 15$, $k \leq 16$, $|l| \leq 16$; three standard reflections, intensities constant within experimental error; total unique reflections measured 4751, 2823 with $F^2 > 2\sigma^2(F_o)$, $\sigma(F_o) = \{[\sigma^2(I_{\text{raw}}) + (0{\cdot}04F_o^2)^2]^{1/2}/2F_o\}$. Absorption corrections from ψ scans, relative transmission factors 0·831–0·995. Structure was solved with the Enraf–Nonius *Structure Determination Package* (Frenz, 1986), heavy-atom and difference Fourier methods; isotropic then anisotropic refinement on F of all non-H atoms, H atoms at calculated positions [C—H 0·95 Å, $U(\text{H}) = 1{\cdot}3U(\text{C})$]; 271 parameters refined, $R = 0{\cdot}033$, $wR = 0{\cdot}039$, $w = 1/[\sigma^2(F_o)]$, $S = 1{\cdot}0$; difference syntheses showed no densities above 0·47 e Å^{-3} (min. −0·33 e Å^{-3}); max $\Delta/\sigma = 0{\cdot}01$. Neutral-atom scattering factors were used (*International Tables for X-ray Crystallography,* 1974), and were corrected for anomalous dispersion (Cromer & Liberman, 1970). No correction for secondary extinction. The possibility of disordered N and O atoms in this molecule was suggested by their thermal parameters and the similarity in related bond lengths and angles. All disordered models, however, resulted in higher R values and chemically improbable distances and angles.

The atomic coordinates and equivalent isotropic temperature factors are listed in Table 1, and selected bond lengths and angles in Table 2.* An *ORTEP* plot (Johnson, 1976) of the title compound with the atom numbering is shown in Fig. 1, and the packing of molecules (Motherwell, 1976) in Fig. 2. The benzoxazole rings are stacked in parallel planes in the crystal, but they are not close enough to permit any interaction.

Related literature. The coordination of the benzoxazolethiolate ligand through the S, rather than through the N or O, is consistent with the known facile binding of Au$^{\text{I}}$ to thiols. The complex

Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å^2) *for* [(Ph$_3$P)Au(Sboz)]

	x	y	z	B (Å^2)
Au	0·31279 (2)	0·39706 (2)	0·41710 (2)	3·703 (6)
S	0·3439 (2)	0·3219 (2)	0·2673 (2)	5·97 (6)
P	0·2916 (2)	0·4662 (2)	0·5683 (1)	3·24 (4)
O	0·3752 (5)	0·4398 (6)	0·1070 (5)	6·6 (2)
N	0·2291 (5)	0·4765 (5)	0·1819 (4)	3·6 (1)
C1	0·3755 (6)	0·4050 (6)	0·6672 (5)	3·4 (1)
C2	0·4809 (6)	0·3883 (7)	0·6523 (6)	4·7 (2)
C3	0·5473 (7)	0·3411 (8)	0·7245 (7)	5·6 (2)
C4	0·5081 (7)	0·3094 (7)	0·8130 (6)	5·2 (2)
C5	0·4036 (8)	0·3277 (8)	0·8291 (7)	6·0 (2)
C6	0·3368 (7)	0·3739 (7)	0·7563 (6)	5·1 (2)
C7	0·3266 (5)	0·6039 (6)	0·5747 (5)	3·2 (1)
C8	0·3011 (6)	0·6626 (6)	0·4906 (6)	4·1 (2)
C9	0·3228 (7)	0·7675 (7)	0·4933 (7)	5·5 (2)
C10	0·3694 (7)	0·8126 (7)	0·5784 (7)	5·3 (2)
C11	0·3967 (7)	0·7538 (7)	0·6594 (7)	5·2 (2)
C12	0·3747 (7)	0·6477 (7)	0·6577 (6)	4·4 (2)
C13	0·1586 (6)	0·4570 (6)	0·6038 (5)	3·5 (2)
C14	0·1191 (6)	0·5277 (7)	0·6724 (6)	4·4 (2)
C15	0·0160 (6)	0·5173 (7)	0·6985 (6)	4·6 (2)
C16	−0·0465 (6)	0·4381 (8)	0·6600 (6)	5·1 (2)
C17	−0·0095 (7)	0·3693 (8)	0·5935 (7)	5·3 (2)
C18	0·0926 (6)	0·3785 (6)	0·5655 (6)	3·9 (2)
C19	0·3172 (7)	0·4199 (7)	0·1840 (6)	4·8 (2)
C20	0·2284 (7)	0·5369 (7)	0·0962 (6)	4·5 (2)
C21	0·1517 (9)	0·6048 (8)	0·0561 (9)	7·3 (3)
C22	0·173 (1)	0·6513 (8)	−0·0329 (8)	7·9 (3)
C23	0·266 (1)	0·6302 (8)	−0·0777 (8)	7·4 (3)
C24	0·3419 (8)	0·5621 (8)	−0·0373 (7)	6·3 (2)
C25	0·3187 (7)	0·5165 (7)	0·0502 (6)	4·7 (2)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $(4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

Table 2. *Selected bond lengths* (Å) *and angles* (°) *in* [(Ph$_3$P)Au(Sboz)]

Au—S	2·299 (2)	P—C13	1·797 (8)
Au—P	2·258 (2)	O—C19	1·34 (1)
S—C19	1·704 (9)	O—C25	1·41 (1)
P—C1	1·816 (7)	N—C19	1·33 (1)
P—C7	1·827 (8)	N—C20	1·39 (1)
C—C(phosphine phenyl, av.)	1·37 (1)	C—C(benzoxazole, av.)	1·38 (1)

S—Au—P	176·43 (8)	P—C7—C12	122·3 (5)
Au—S—C19	103·1 (3)	P—C13—C14	121·4 (6)
Au—P—C1	112·6 (2)	P—C13—C18	120·3 (6)
Au—P—C7	112·2 (2)	S—C19—O	123·8 (7)
Au—P—C13	113·4 (2)	S—C19—N	122·7 (6)
C1—P—C7	105·1 (3)	O—C19—N	113·0 (7)
C1—P—C13	106·6 (3)	N—C20—C21	129·3 (8)
C7—P—C13	106·4 (3)	N—C20—C25	108·5 (7)
C19—O—C25	105·4 (7)	O—C25—C20	107·2 (7)
C19—N—C20	105·8 (6)	O—C25—C24	129·1 (8)
P—C1—C2	118·6 (6)	C—C—C(phosphine Ph, av.)	120·0 (8)
P—C1—C6	122·0 (6)	C—C—C(benzoxazole, av.)	119·9 (9)
P—C7—C8	116·9 (5)		

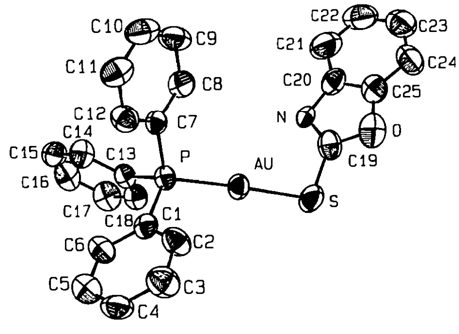

Fig. 1. Labeling of atoms in [(Ph$_3$P)Au(Sboz)] (50% probability ellipsoids).

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* Lists of structure factors, anisotropic thermal factors, H-atom parameters and least-square planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51854 (54 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

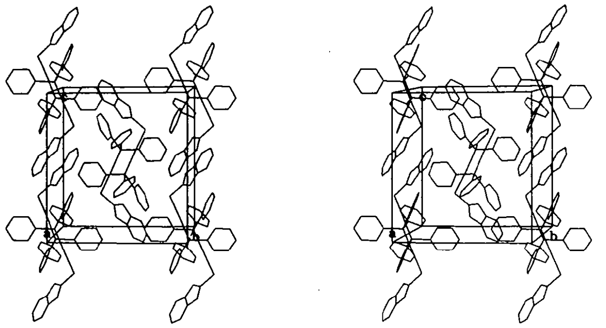

Fig. 2. Packing diagram of [$(Ph_3P)Au(Sboz)$] in the unit cell.

[$(Ph_3P)Au(Sboz)$] 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. [$HgCl_2(C_9H_8N_2)$], $M_r = 415{\cdot}7$, monoclinic, $P2_1/n$, $a = 3{\cdot}9110\,(3)$, $b = 26{\cdot}645\,(3)$, $c = 10{\cdot}6753\,(12)$ Å, $\beta = 98{\cdot}234\,(9)°$, $V = 1101{\cdot}0$ Å^3, $Z = 4$, $D_x = 2{\cdot}507$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 14{\cdot}43$ mm^{-1}, $F(000) = 760$, $T = 295$ K, $R = 0{\cdot}0497$ 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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