Discussion. Two alanine groups and two Ag^+ ions form a centrosymmetric dimer. Within this dimer the Ag–Ag separation of 2·855 (4) Å is comparable to the smallest distance of 2·88 Å found in metallic silver (Griffith, 1943). The nitrate groups are in a *trans* configuration. The Ag—O bond distances are 2·210 (19) and 2·198 (19) Å, which are comparable to those reported, respectively, for silver perfluorobutyrate and silver oxalate (Blakeslee & Hoard, 1956; Griffith, 1943). The O–Ag–O angle is 161·6 (8)°, which is comparable to the usual value of 160–163° (Blakeslee & Hoard, 1956; Rao & Viswamitra, 1972). Two independent Ag—O distances to the nitro groups are 2·58 (3) and 2·57 (3) Å. There are hydrogen bonds of type N—H···O between the alanine and the nitro groups which stabilize the crystal packing.

One of us (MEK) is deeply indebted and wishes to express his gratitude to Dr J.-P. Declercq and Professor G. S. D. King for their invaluable advice given to him during his short stay at Louvain-la-Neuve, Belgium.

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Acetato(triphenylphosphine)gold(I), $[Au(C_2H_3O_2)(C_{18}H_{15}P)]$*

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Abstract. $M_r = 518{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 11{\cdot}088$ (3), $b = 12{\cdot}050$ (4), $c = 13{\cdot}839$ (5) Å, $V = 1849$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}862$ (1) Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 8·0 mm^{-1}, $F(000) = 992$, $R = 0{\cdot}028$, 3055 reflections. Isostructural with Ph_3PAuCl and $Ph_3AsAuBr$. The Au—O bond length is 2·063 (6) Å, with a short Au—P bond of 2·207 (3) Å. The second acetate O is not involved in bonding at the metal [Au···O 2·93 (1) Å], which thus shows a linear coordination geometry [P—Au—O 177·3 (2)°].

Introduction. We have begun a systematic study of gold carboxylate complexes and here report the structure of $Ph_3PAuOCOCH_3$, (1). This is one of the few gold carboxylate complexes to have been chemically characterized (Nichols & Charleston, 1969). Colourless prisms were obtained by diffusion of petroleum ether (40°–60° C) into a dichloromethane solution of (1).

Experimental. D_m not determined. Crystal 0·6 × 0·25 × 0·1 mm, elongated along **b**. 3247 profile-fitted intensities (Clegg, 1981) recorded on a Stoe–Siemens four-circle diffractometer. Monochromated Mo $K\alpha$ radiation, $2\theta_{\max}$ 50°, octants hkl and $\bar{h}\bar{k}\bar{l}$ (no equivalents). Three standard reflections, no intensity change. Lp and empirical absorption corrections (ψ scans; transmissions 0·61–0·96). 3055 reflections with $F > 4\sigma(F)$ used for all calculations (program system *SHELXTL*, Sheldrick, 1978). Cell constants refined from 2θ values of 48 reflections in the range 20–24°. Structure solution by heavy-atom method. Refinement on F to R 0·028, R_w 0·028 [all non-H atoms anisotropic; phenyl H atoms using riding model with C—H 0·96 Å, H on external bisector of appropriate C—C—C angle; methyl H not included; 217

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* Carboxylate and Related Complexes of Gold. 2. Part 1: Jones (1984).

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parameters, weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}0002F^2$, $S = 1{\cdot}28$, slope of normal probability plot 1·18]. Max. Δ/σ 0·01. Max. and min. heights in final $\Delta\rho$ map +1·4 (near Au), −0·9 e Å^{-3}. Rogers's (1981) η refinement gave $\eta = 1{\cdot}04\,(2)$, thus showing that the correct enantiomorph had been chosen [although (1) itself is achiral].

Discussion. Final atomic coordinates and derived parameters are given in Tables 1 and 2.* Fig. 1 shows the atom numbering.

The similarity of cell constants to those of Ph_3PAuCl (Baenziger, Bennett & Soboroff, 1976) and $Ph_3AsAuBr$ (Einstein & Restivo, 1975) suggested that (1) might be isostructural; this indeed proves to be the case, presumably because the crystal packing is determined by the bulky Ph_3E ligands.

The Au atom shows the expected linear coordination, with P—Au—O(1) 177·3 (2)°; the Au···O(2) contact of 2·93 (1) Å may be regarded as non-bonding [consistent with the high thermal motion of O(2)], although it is not always clear where to draw the line between two- and three-coordination for Au^I (Jones, 1981). The Au—O(1) bond length is 2·063 (6) Å, which is the first accurate Au^I—O bond length to be determined; in $[(Ph_3PAu)_3O]^+BF_4^-$ (Nesmeyanov, Perevalova, Struchkov, Antipin, Grandberg & Dyadchenko, 1980) the average Au—O distance is 1·97 Å, but the structure is of low accuracy (e.s.d.'s 0·07–0·08 Å for Au—O). Au^I has little affinity for O ligands (Puddephatt, 1978); this is reflected in the shortness of the Au—P bond [2·207 (3) Å], compared with the usual range of 2·235–2·29 Å for Ph_3PAuX complexes (Jones, 1981).

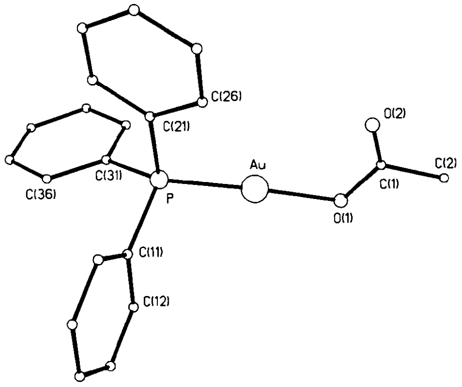

Fig. 1. A molecule of (1), showing the atom-numbering scheme.

Table 1. *Atom coordinates* (×10^4) *and isotropic temperature factors* (Å^2 ×10^3)

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

	x	y	z	U_{eq}
Au	6322 (1)	641 (1)	2057 (1)	52 (1)
P	4605 (1)	1256 (1)	2660 (1)	44 (1)
O(1)	7910 (4)	−6 (4)	1523 (4)	65 (2)
O(2)	8839 (6)	933 (6)	2643 (6)	130 (3)
C(1)	8847 (6)	310 (5)	1971 (6)	62 (2)
C(2)	10010 (7)	−253 (9)	1626 (9)	110 (4)
C(11)	3618 (5)	130 (4)	3055 (4)	46 (2)
C(12)	3350 (6)	−699 (5)	2397 (5)	56 (2)
C(13)	2613 (6)	−1557 (5)	2650 (6)	63 (3)
C(14)	2158 (7)	−1614 (6)	3565 (6)	75 (3)
C(15)	2419 (7)	−831 (7)	4234 (6)	82 (3)
C(16)	3173 (7)	64 (6)	3995 (5)	62 (3)
C(21)	4847 (5)	2113 (5)	3712 (4)	46 (2)
C(22)	4078 (6)	2956 (5)	3974 (4)	50 (2)
C(23)	4251 (6)	3554 (6)	4803 (5)	61 (2)
C(24)	5209 (7)	3336 (7)	5406 (6)	76 (3)
C(25)	6011 (7)	2516 (9)	5123 (7)	88 (3)
C(26)	5829 (7)	1900 (7)	4292 (6)	75 (3)
C(31)	3686 (7)	2091 (5)	1868 (4)	53 (2)
C(32)	4259 (9)	2766 (6)	1197 (5)	76 (3)
C(33)	3532 (11)	3493 (6)	638 (6)	106 (4)
C(34)	2281 (11)	3466 (7)	714 (8)	112 (5)
C(35)	1742 (9)	2821 (7)	1367 (7)	105 (4)
C(36)	2443 (7)	2099 (6)	1946 (6)	69 (3)

Table 2. *Selected bond lengths* (Å) *and angles* (°)

Au—P	2·207 (3)	Au—O(1)	2·063 (6)
C(1)—O(1)	1·268 (9)	C(1)—O(2)	1·195 (12)
C(1)—C(2)	1·533 (12)	C(11)—P	1·827 (7)
C(11)—C(12)	1·385 (10)	C(11)—C(16)	1·392 (10)
C(12)—C(13)	1·363 (10)	C(13)—C(14)	1·365 (13)
C(14)—C(15)	1·353 (13)	C(15)—C(16)	1·405 (12)
C(21)—P	1·805 (7)	C(21)—C(22)	1·375 (9)
C(21)—C(26)	1·377 (11)	C(22)—C(23)	1·369 (10)
C(23)—C(24)	1·376 (12)	C(24)—C(25)	1·385 (13)
C(25)—C(26)	1·384 (14)	C(31)—P	1·803 (7)
C(31)—C(32)	1·388 (11)	C(31)—C(36)	1·382 (12)
C(32)—C(33)	1·419 (13)	C(33)—C(34)	1·391 (18)
C(34)—C(35)	1·333 (15)	C(35)—C(36)	1·416 (13)
P—Au—O(1)	177·3 (2)	Au—P—C(11)	112·3 (3)
Au—P—C(21)	111·6 (3)	C(11)—P—C(21)	105·8 (4)
Au—P—C(31)	116·4 (3)	C(11)—P—C(31)	105·0 (4)
C(21)—P—C(31)	104·8 (4)	Au—O(1)—C(1)	114·3 (5)
O(1)—C(1)—O(2)	124·2 (8)	O(1)—C(1)—C(2)	113·8 (8)
O(2)—C(1)—C(2)	121·8 (8)		

In the Au^{III} acetate complex $SrAu_2(OCOCH_3)_8$ the Au—O bonds are, as expected from the increased charge, shorter than in (1); indeed, most Au^{III}—O bond lengths lie in the range 1·97–2·02 Å (Jones, 1981, 1984). In both complexes the acetate ligands show a marked asymmetry of C—O bond lengths, since the main bonding interactions involve only one O atom.

(1) shows no unusually short intermolecular contacts and, in particular, no Au···Au interactions of the kind often observed in Au^I complexes (Jones, 1981).

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond distances and angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39392 (24 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 Bis(L-histidinato-*O*,*N*,*N'*)chromium(III) Nitrate, $[Cr(C_6H_8N_3O_2)_2]NO_3$

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Abstract. $M_r = 422{\cdot}3$, monoclinic, $P2_1$, $a = 7{\cdot}404$ (2), $b = 7{\cdot}209$ (3), $c = 15{\cdot}663$ (5) Å, $\beta = 100{\cdot}68$ (2)°, $V = 821{\cdot}5$ (9) Å^3, $Z = 2$, $D_x = 1{\cdot}707$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 7{\cdot}32$ cm^{-1}, $F(000) = 434$, $T = 294$ K, final $R = 0{\cdot}036$ for 1812 observed reflections. The L-histidinate anions function as tridentate ligands, with the two imidazole rings in the *trans* orientation. The imidazole rings are planar with the Cr atom out of these planes. Hydrogen bonding occurs between amine groups and nitrate oxygen atoms and also between amine and carboxylate groups.

Introduction. Histidine is frequently found to be a metal-binding site in metalloproteins (Ibers & Holm, 1980) and metal complexes of the histidine anion are important for metal-ion transport in blood plasma (Lau & Sarkar, 1971). The L-histidine anion generally functions as either a bidentate or a tridentate ligand (Martin, 1979); several isomers have been reported for octahedral complexes involving two tridentate histidine ligands around Co^{III} (Bagger, Gibson & Sorensen, 1972) and Cr^{III} (Hoggard, 1981). We report here the structure of the bis(L-histidinato)chromium(III) isomer with *trans* imidazole rings, which was determined in order to verify the spectroscopic structural assignment for this most dominant product of the Cr^{III}–histidine reaction and also to provide structural data for comparisons with future structural work on binuclear chromium complexes with histidine.

Experimental. Title compound prepared by general method reported by Hoggard (1981); orange-red crystal used for data collection, dimensions $0{\cdot}2 \times 0{\cdot}2 \times 0{\cdot}3$ mm, mounted with epoxy on a glass fiber; all data collected using Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation; 25 reflections with 2θ between 17 and 32° used for least-squares determination of cell constants. 2753 reflections measured, ω–2θ scans, 2θ from 4 to 60° ($h = 0$ to 10, $k = \overline{10}$ to 0, $l = \overline{22}$ to 22). $R_{\rm int} = 0{\cdot}028$. Scan range $(1{\cdot}00 + 0{\cdot}35\tan\theta)°$, scan speeds 4–20° min^{-1}. Intensities of three reflections ($\bar{1}\bar{3}\bar{2}$, $0\bar{3}\bar{6}$ and $\bar{1}1\bar{6}$) measured periodically during 30·0 h of data collection varied by 1·9%, indicating crystal and electronic stability; 801 reflections with $I \leq 3\sigma(I)$ considered unobserved; systematic absences of $0k0$ for k odd indicate space group $P2_1$ or $P2_1/m$; however, statistical tests of intensity distribution of data set and chemical composition of the cation which precludes crystallographically imposed symmetry (a necessary condition for $P2_1/m$, $Z = 2$) confirmed space group $P2_1$. Structure solved by Patterson methods and refined by full-matrix least squares based on $(|F_o| - |F_c|)^2$. H atoms constrained to idealized positions (C—H = 0·95 Å, N—H = 0·90 Å). Anisotropic refinement of non-hydrogen atoms gave 243 parameters for parameter/reflection ratio 1:7·5. No absorption or secondary-extinction corrections; $1\bar{1}\bar{2}$ and 103 reflections given zero weight due to evidence of extinction problems. Final $R = 0{\cdot}036$, $R_w = 0{\cdot}044$, $S = 0{\cdot}98$; weighting scheme based on counting statistics $\{\sigma(F^2)$

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