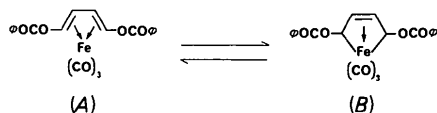


As Fig. 1 shows, this structure contains the diphenyl-ester-vinyl ligand complexed to the tricarbonyl unit as a four-electron ligand and can be represented by a resonance hybrid between the diene (*A*) and the $2\sigma-\pi$ structure (*B*). Thus, the whole molecular arrangement bears a very close similarity to the structures of butadieneiron tricarbonyl (Mills & Robinson, 1963), tricarbonyl(dimethyl 4-methyl-1-oxo-1,3-pentadiene-2,3-dicarboxylate)iron (Fischer & Ricard, 1982) and tricarbonyl(η^4 -*syn*-1,4-diacetoxy-1,3-butadiene)iron(0) (Soriano-García, Alvarez, Toscano & Cano, 1987).



The molecule has approximate *m* symmetry: the mirror plane passes through the O(1)–C(1)–Fe atoms and bisects the C(5)–C(6) bond, while the other carbonyl groups [C(2)–O(2) and C(3)–O(3)] lie over the C(4)–C(5) and C(6)–C(7) bonds, respectively. A similar situation occurs in butadieneiron tricarbonyl and tricarbonyl(η^4 -*syn*-1,4-diacetoxy-1,3-butadiene)iron(0) structures.

The arrangement of ligands about Fe can be described as approximately square pyramidal, the base of the pyramid being formed by the carbonyl atoms C(2) and C(3) and by C(4) and C(7) of the butadiene system. The dihedral angle between planes formed by O(1)–C(1)–Fe and C(4)–C(5)–C(6)–C(7) is $47.8(6)^\circ$, whereas in butadieneiron tricarbonyl and tricarbonyl(η^4 -*syn*-1,4-diacetoxy-1,3-butadiene)iron(0) this angle is 61 and $75.4(6)^\circ$, respectively.

The Fe–C bond distances vary over a small range [$2.055(4)$ to $2.091(3)$ Å], reflecting the fact that the metal–ligand bonding is nearly the same for the four C atoms of the η^4 -system in spite of the presence of the two phenyl rings.

The two φ -COO-ester groups are synclinal to each other about the C(5)–C(6) bond. Both φ -COO-ester

groups at C(4) and C(7) are planar within the limits of experimental error; maximum deviations are -0.105 , 0.113 and -0.116 Å for C(7), O(4) and C(4) respectively. The dihedral angle between the two φ -COO-esters is $40.6(6)^\circ$. Both phenyl rings show normal geometry and the C=O groups are *syn* to the C(4)–H, C(7)–H bonds, respectively (Mathieson, 1965; Chothia & Pauling, 1970).

The butadiene system is planar within $\pm 0.002(6)$ Å. The pairs of atoms [H(4), H(7)] and [H(5), H(6)] are displaced out of this plane away from and towards the Fe atom respectively, at distances of -0.521 , -0.574 and 0.085 , 0.065 Å from the plane. The dihedral angles between the butadiene system and the φ -COO-ester group at C(4) and C(7) are $18.6(6)$ and $22.4(6)^\circ$, respectively.

The molecular packing is shown in Fig. 2. There is only one intermolecular approach of non-hydrogen atoms < 3.3 Å, C(18)···O(2) ($-1+x, 0.5-y, -0.5+z$) = $3.297(6)$ Å. The molecules are, therefore, held in the crystal by van der Waals forces.

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Acta Cryst. (1988). **C44**, 53–56

Ethyltriphenylphosphonium Dibromobis(succinimido)aurate(III)

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Abstract. $(C_6H_5)_3P^+C_2H_5.[AuBr_2(C_4H_4NO_2)_2]^-$, $M_r = 2955(3)$ Å³, $Z = 4$, $D_x = 1.90$ g cm⁻³, Mo *K*α radiation, $\lambda = 0.71073$ Å, $\mu(Mo K\alpha) = 77.3$ cm⁻¹, $F(000) = 1624$. For 2313 observed reflections, $R =$

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0.028, $wR = 0.030$. There are two independent anions with essentially identical *trans* geometry lying about independent inversion centres. Principal dimensions include: Au—Br 2.394 (1), 2.404 (1), Au—N 1.990 (7), 2.000 (6) Å, Br—Au—N 89.3 (2), 89.8 (2)°. The two independent five-membered rings are rotated 80.2 and 87.0° out of the coordination plane.

Introduction. Only a small amount of work has been reported on haloimidogold(III) complexes. With succinimide, it was claimed (Kharasch & Isbell, 1931; Pope, 1929, 1931) that two, three or even four imido groups could coordinate to the gold. Later, it was suggested that coordination of four imide moieties is not possible (Tyabji & Gibson, 1952; Malik, Sadler, Neidle & Taylor, 1978), that complexes of succinimide itself are not very stable (Malik *et al.*, 1978) and that reaction of an alkali tetrahaloaurate with succinimide gives a complex containing three imido groups (Tyabji & Gibson, 1952), 'whatever proportions of the reactants were chosen'. We have now prepared substantially pure (thin-layer chromatography, ¹H NMR) samples of $[\text{AuBr}_n(\text{C}_4\text{H}_4\text{NO}_2)_{4-n}]^-$, $n = 1, 2, 3$ with counterions Ph_3EtP^+ and Ph_4As^+ , either by reaction of gold leaf with *N*-bromosuccinimide, or of potassium tetrabromoaurate with succinimide and base, and then treatment with the appropriate arsonium or phosphonium bromide. Although the ¹H NMR and UV and visible spectral data are consonant with the gross structures assigned, the stereochemistry of the $[\text{AuBr}_2(\text{C}_4\text{H}_4\text{NO}_2)_2]^-$ complex was unknown. We report here the crystal structure analysis of $\text{Ph}_3\text{EtP}^+[\text{AuBr}_2(\text{C}_4\text{H}_4\text{NO}_2)_2]^-$ which reveals that the anion has *trans* stereochemistry. In a recent study (Price, DiMartino, Hill, Kuroda, Mazid & Sadler, 1985), reaction of $\text{AuBr}_3(\text{PET}_3)$ with two molar equivalents of potassium phthalimide was reported to give *cis*- $[\text{Et}_3\text{PAuBr}(\text{C}_8\text{H}_4\text{NO}_2)_2]$.

Experimental. Pale yellow multifaceted prisms grown from dichloromethane–toluene. Accurate cell dimensions and crystal-orientation matrix determined on a CAD-4 diffractometer by a least-squares treatment of the setting angles of 25 reflections in the range $6 < \theta < 14^\circ$. Crystal dimensions $0.16 \times 0.24 \times 0.32$ mm; intensities of reflections with indices h 0 to 12, k 0 to 17, l -30 to 30, with $2 < 2\theta < 54^\circ$ measured; ω - 2θ scans; ω -scan width $(0.60 + 0.35 \tan \theta)^\circ$, graphite-monochromatized $\text{Mo } K\alpha$ radiation; intensities of three reflections measured every 2 h showed no evidence of crystal decay. 5261 reflections measured, 4589 unique, 2313 with $I > 3\sigma(I)$ labelled observed and used in structure solution and refinement; $R_{\text{int}} = 0.013$. Data corrected for Lorentz, polarization and absorption effects (max. and min. transmission factors 0.391, 0.287), Gaussian integration, grid $12 \times 8 \times 14$. Space group $P2_1/n$ uniquely from systematic absences $h0l$,

Table 1. Positional parameters and their estimated standard deviations

	x	y	z	$B_{\text{eq}}(\text{Å}^2)$
Au1	0.0	0.0	0.0	3.264 (9)
Br1	0.21505 (9)	0.02351 (7)	-0.03154 (4)	5.55 (3)
N11	0.0008 (7)	0.1455 (5)	0.0197 (2)	3.9 (2)
C12	-0.0400 (8)	0.2200 (7)	-0.0208 (3)	4.5 (2)
O12	-0.0989 (7)	0.2057 (5)	-0.0713 (2)	6.6 (2)
C13	-0.0032 (11)	0.3200 (7)	0.0080 (4)	6.4 (3)
C14	0.0531 (10)	0.2975 (7)	0.0716 (4)	5.4 (3)
C15	0.0580 (8)	0.1843 (6)	0.0748 (4)	4.1 (2)
O15	0.1013 (7)	0.1349 (4)	0.1176 (2)	5.7 (2)
Au2	0.0	0.0	0.5	3.664 (9)
Br2	-0.1831 (1)	-0.00388 (8)	0.55211 (4)	6.14 (3)
N21	0.0422 (7)	0.1430 (5)	0.5246 (3)	3.8 (2)
C22	-0.0322 (10)	0.2220 (7)	0.4949 (4)	5.5 (3)
O22	-0.1280 (8)	0.2149 (4)	0.4516 (3)	7.6 (2)
C23	0.0224 (10)	0.3169 (7)	0.5264 (4)	6.2 (3)
C24	0.1412 (9)	0.2851 (6)	0.5765 (3)	4.6 (2)
C25	0.1444 (8)	0.1708 (6)	0.5737 (3)	3.9 (2)
O25	0.2189 (7)	0.1153 (4)	0.6072 (3)	6.1 (2)
P	0.6529 (2)	0.1646 (2)	0.27861 (9)	3.35 (5)
C31	0.5843 (7)	0.0849 (5)	0.2178 (3)	3.0 (2)
C32	0.6757 (8)	0.0222 (6)	0.1989 (3)	3.8 (2)
C33	0.6252 (9)	-0.0462 (7)	0.1545 (3)	4.5 (2)
C34	0.4793 (9)	-0.0516 (6)	0.1295 (3)	4.7 (2)
C35	0.3861 (9)	0.0110 (7)	0.1479 (4)	5.3 (2)
C36	0.4369 (9)	0.0779 (6)	0.1926 (3)	4.4 (2)
C41	0.5480 (8)	0.2779 (6)	0.2710 (3)	3.4 (2)
C42	0.5345 (8)	0.3278 (6)	0.3211 (3)	3.9 (2)
C43	0.4661 (9)	0.4191 (6)	0.3157 (4)	4.9 (2)
C44	0.4098 (8)	0.4625 (7)	0.2638 (4)	5.0 (2)
C45	0.4240 (10)	0.4144 (6)	0.2145 (4)	5.8 (3)
C46	0.4888 (10)	0.3245 (7)	0.2176 (4)	5.4 (3)
C51	0.8355 (8)	0.1965 (6)	0.2800 (3)	3.6 (2)
C52	0.9495 (9)	0.1698 (7)	0.3264 (4)	4.7 (2)
C53	1.0870 (9)	0.1992 (7)	0.3281 (4)	5.2 (3)
C54	1.1131 (10)	0.2543 (7)	0.2831 (4)	6.2 (3)
C55	1.0017 (9)	0.2817 (7)	0.2372 (4)	6.1 (3)
C56	0.8626 (9)	0.2544 (7)	0.2362 (4)	5.2 (3)
C61	0.6479 (9)	0.0993 (6)	0.3433 (3)	4.4 (2)
C62	0.4965 (9)	0.0679 (7)	0.3460 (4)	5.3 (3)

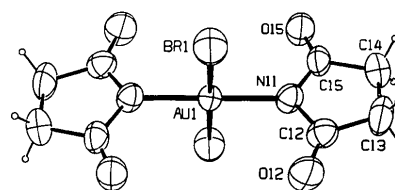
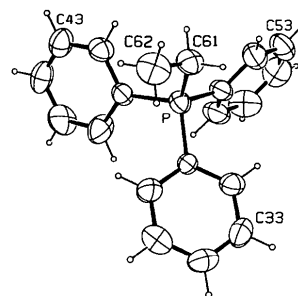
Anisotropically refined atoms are given in the form of the equivalent isotropic thermal parameter defined as:

$$\frac{1}{3}(a^2B_{11} + b^2B_{22} + c^2B_{33} + abc\cos\gamma B_{12} + accos\beta B_{13} + bccos\alpha B_{23}).$$

$h + l = 2n + 1$; $0k0$, $k = 2n + 1$. It became apparent from a detailed study of the three-dimensional Patterson function that the asymmetric unit had to have two Au atoms lying on independent inversion centres and the coordinates of the two independent Br atoms were also gleaned. The coordinates of the remaining non-hydrogen atoms were developed *via* the heavy-atom method which was complicated by dominant pseudo-mirror symmetry arising from the Au and Br atoms all having y coordinates close to zero. Refinement was by full-matrix least-squares calculations, initially with isotropic and then with anisotropic thermal parameters. At an intermediate stage in the refinement, difference maps showed maxima in positions consistent with the expected locations of the H atoms; in the final rounds of calculations the hydrogen atoms were positioned on geometrical grounds (C—H 0.95 Å) and included (as riding atoms) in the structure-factor calculations with an overall B_{iso} of 6.0 Å². The final cycle of refinement included 347 variable parameters, $R = 0.0278$, $wR = 0.0305$, goodness-of-fit 1.08, $w = 1/[\sigma^2(F_o) + 0.035(F_o)^2]$. Max. shift/e.s.d. = 0.005; density in final difference map $\pm 0.89 \text{ e \AA}^{-3}$; no chemically significant features. Scattering factors and anomalous

Table 2. Bond lengths (Å) and angles (°)

Au1-Br1	2.394 (1)	P-C61	1.788 (9)
Au1-N11	1.990 (7)	C31-C32	1.369 (11)
N11-C12	1.371 (10)	C31-C36	1.391 (10)
N11-C15	1.392 (10)	C32-C33	1.388 (11)
C12-O12	1.211 (9)	C33-C34	1.377 (11)
C12-C13	1.498 (12)	C34-C35	1.376 (13)
C13-C14	1.511 (13)	C35-C36	1.381 (11)
C14-C15	1.508 (12)	C41-C42	1.404 (11)
C15-O15	1.199 (10)	C41-C46	1.404 (11)
Au2-Br2	2.404 (1)	C42-C43	1.370 (12)
Au2-N21	2.000 (6)	C43-C44	1.352 (12)
N21-C22	1.363 (10)	C44-C45	1.380 (13)
N21-C25	1.375 (9)	C45-C46	1.341 (13)
C22-O22	1.201 (10)	C51-C52	1.391 (10)
C22-C23	1.494 (12)	C51-C56	1.378 (12)
C23-C24	1.489 (11)	C52-C53	1.368 (12)
C24-C25	1.521 (11)	C53-C54	1.378 (14)
C25-O25	1.186 (9)	C54-C55	1.371 (12)
P-C31	1.785 (7)	C55-C56	1.378 (13)
P-C41	1.796 (8)	C61-C62	1.530 (13)
P-C51	1.797 (8)		
Br1-Au1-N11	89.8 (2)	C41-P-C51	108.9 (4)
Au1-N11-C12	123.5 (5)	C41-P-C61	110.8 (4)
Au1-N11-C15	124.1 (5)	C51-P-C61	110.0 (4)
C12-N11-C15	112.0 (7)	P-C31-C32	119.8 (5)
N11-C12-O12	124.7 (8)	P-C31-C36	121.0 (6)
N11-C12-C13	108.9 (6)	C32-C31-C36	118.9 (7)
O12-C12-C13	126.4 (8)	C31-C32-C33	121.5 (7)
C12-C13-C14	105.7 (7)	C32-C33-C34	119.0 (8)
C13-C14-C15	104.2 (7)	C33-C34-C35	120.1 (8)
N11-C15-C14	108.9 (7)	C34-C35-C36	120.6 (7)
N11-C15-O15	125.1 (7)	C31-C36-C35	119.8 (8)
C14-C15-O15	126.1 (7)	P-C41-C42	118.8 (5)
Br2-Au2-N21	89.3 (2)	P-C41-C46	123.2 (7)
Au2-N21-C22	122.6 (5)	C42-C41-C46	117.8 (7)
Au2-N21-C25	123.6 (5)	C41-C42-C43	119.0 (7)
C22-N21-C25	113.7 (6)	C42-C43-C44	122.2 (9)
N21-C22-O22	125.0 (8)	C43-C44-C45	119.1 (8)
N21-C22-C23	108.6 (6)	C44-C45-C46	120.8 (8)
O22-C22-C23	126.4 (8)	C41-C46-C45	121.1 (9)
C22-C23-C24	105.3 (7)	P-C51-C52	121.2 (7)
C23-C24-C25	105.5 (6)	P-C51-C56	119.5 (6)
N21-C25-C24	106.8 (6)	C52-C51-C56	119.2 (8)
N21-C25-O25	125.8 (7)	C51-C52-C53	120.4 (8)
C24-C25-O25	127.4 (7)	C52-C53-C54	119.8 (8)
C31-P-C41	109.6 (3)	C53-C54-C55	120.4 (9)
C31-P-C51	108.0 (4)	C54-C55-C56	119.8 (9)
C31-P-C61	109.5 (4)	C51-C56-C55	120.3 (7)
		P-C61-C62	113.9 (5)

Fig. 1. A view of one of the $[\text{AuBr}_2(\text{C}_4\text{H}_4\text{NO}_2)_2]^-$ ions showing our numbering scheme.Fig. 2. A general view of the $(\text{Ph}_3\text{EtP})^+$ ion with an indication of our numbering scheme. The phenyl-ring carbon atoms are numbered C*i*1 to C*i*6, with *i* = 3, 4, 5.

lous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). All calculations were performed on a PDP11/73 computer using *SDP-Plus* (B. A. Frenz & Associates, 1983). Atomic coordinates, and details of molecular geometry are given in Tables 1 and 2.* Figs. 1 and 2 are views, prepared using *ORTEPII* (Johnson, 1976), of one of the anions and of the cation.

Discussion. The crystal structure contains discrete cations and anions, separated by normal van der Waals distances. The two independent anions lie on independent inversion centres; consequently, *trans*-planar coordination is required for each Au atom. Both anions have essentially identical dimensions (one anion is

shown in Fig. 1), with mean Au-Br 2.399 (1), mean Au-N 1.995 (7) Å and mean Br-Au-N 89.6 (2)°. In tribromo(triethylphosphine)gold(III) (Eggleston, Chodosh, Hill & Girard, 1984), the *trans* Au-Br distances are 2.407 (1) and 2.416 (1) Å. The succinimido rings have normal dimensions and are rotated 80.2 and 87.0° about the Au-N bonds from a planar conformation; these small conformational differences are presumably ascribable to packing effects.

The ethyltriphenylphosphonium cation (Fig. 2) has the expected tetrahedral geometry at P. The P-C(ethyl) distance, 1.788 (5) Å, is not significantly different from the mean P-C(phenyl) distance, 1.793 (8) Å, and the P-CH₂-CH₃ angle [113.9 (5)°] is just greater than tetrahedral. These dimensions are comparable with those reported previously, e.g. P-C(ethyl) 1.80 (1), P-C(phenyl) 1.80 (1) Å, P-CH₂-CH₃ 115.2 (5)° (Caira, de Wet, du Preez & Gellatly, 1978), P-C(ethyl) 1.807 (4), mean P-C(phenyl) 1.793 (3) Å, P-CH₂-CH₃ 113.7 (3)° (Fleming, Shaikh, Skelton & White, 1979) and P-C(ethyl) 1.88 (3), mean P-C(phenyl) 1.78 (3) Å, P-CH₂-CH₃ 120 (3)° (Al-Karaghoulis & Wood, 1973).

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* Lists of structure factors, thermal parameters, calculated H-atom coordinates and mean-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44388 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1988). C44, 56–58

Structure of *mer*-(Acetonitrile)trichloro[1-methyl-3-(2-pyridyl)-1,2,4-triazole]ruthenium(III)

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Abstract. [RuCl₃(C₂H₃N)(C₈H₈N₄)], $M_r = 408.63$, monoclinic, $P2_1/c$, $a = 11.929$ (1), $b = 7.472$ (1), $c = 16.486$ (3) Å, $\beta = 95.11$ (2)°, $V = 1463.7$ Å³, $Z = 4$, $D_x = 1.85$ (1), $D_m = 1.81$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.7145$ Å, $\mu = 1.586$ mm⁻¹, $F(000) = 804$, $T = 298$ K, $R = 0.018$ for 1337 unique reflections [$I > 2\sigma(I)$]. The planar pyridyltriazole ligand is coordinated to the central metal atom *via* N(1') and N(4). No water molecules leading to hydrogen bonding have been detected. The Ru–Cl distances of 2.33–2.34 Å are in the range expected for ruthenium(III) compounds.

Introduction. Ruthenium(II) compounds with 2,2'-bipyridine-like ligands have been studied in great detail because of their possible application in the photochemical decomposition of water (Seddon, 1982; Kalyanasandaram, 1982). However, less attention has been paid to ruthenium(III) compounds; no crystal structures have been reported for ruthenium(III) compounds with asymmetric chelating N-donor ligands. Recently it was predicted, on the basis of ¹H NMR data, that 1-methyl-3-(2-pyridyl)-1,2,4-triazole (1Mepytr) would coordinate *via* N(1') and N(4) to ruthenium(II) (Hage, Haasnoot, Reedijk & Vos, 1986). The ligand has two coordination modes [N(1') and N(2) or N(1') and N(4)]; see Fig. 1]. Until now no

crystal structures of compounds containing this ligand have been reported. The crystal structure of a ruthenium(III) compound containing both 1Mepytr and acetonitrile is described in this paper.

Experimental. Bright red crystals of the title compound were obtained after heating RuCl₃ and 1Mepytr in acetonitrile. A hexagonal single crystal of dimensions 0.12 × 0.09 × 0.06 mm was selected for crystal-structure determination. D_m was determined by flotation. Intensity data were collected at room temperature by using an Enraf-Nonius CAD-4 diffractometer. Graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71745$ Å) was used. Cell parameters were obtained by least-squares methods for 24 reflections; the

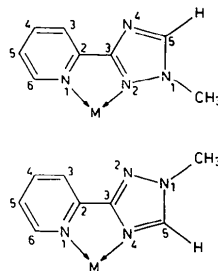


Fig. 1. Atomic numbering and coordination modes of 1-methyl-3-(2-pyridyl)-1,2,4-triazole.

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