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N-INDOLYLTRIARYLPHOSPHINEGOLD(I) DERIVATIVES AS η^6-ARENE LIGANDS IN PENTAMETHYLCYCLOPENTADIENYLRHODIUM(III) COMPLEXES. X-RAY STRUCTURE OF $[(C_5Me_5)Rh(\mu\text{-In})AuP(C_6H_5)_3](ClO_4)_2 \cdot CH_2Cl_2$

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Summary

Cationic η^6-arene rhodium(III) complexes of the general formula $[(C_5Me_5)Rh(\mu\text{-In})AuPR_3](ClO_4)_2$ ($R = C_6H_5$, 2-MeC_6H_4, 4-MeC_6H_4) have been synthesised from the acetone-containing complex $[Rh(C_5Me_5)(Me_2CO)_3](ClO_4)_2$ by reaction with $Au(In)PR_3$. The structure of the complex $[(C_5Me_5)Rh(\mu\text{-In})AuP(C_6H_5)_3](ClO_4)_2 \cdot CH_2Cl_2$ has been determined by X-ray diffraction methods; it crystallizes in the triclinic space group $P\bar{1}$ with $Z = 2$ in a unit cell of dimensions a 13.289(9), b 16.388(11), c 10.794(6) Å, α 72.35(5), β 109.19(6), γ 106.32(6)°. The structure was solved from diffractometer data by Patterson and Fourier methods and refined by full-matrix least squares to $R = 0.072$ for 3314 independent observed reflections. In the cation the Rh atom is η^5-coordinated by a pentamethylcyclopentadienyl ligand and η^6-coordinated by the hexaatomic ring of an indolyl ligand, which is also σ-bonded, through the N atom, to a Au atom of a $AuPPh_3$ group.

Introduction

Recently we reported the synthesis of novel rhodium(I)-gold(I) heterometallic complexes containing the anionic forms derived from pyrazole [1], imidazole [2] and 2,2′-bibenzimidazole [3] as bridging ligands. In a recent preliminary communication [4] we described several mononuclear or heteronuclear complexes of the types $[(\text{diolefin})Rh(HIn)]ClO_4$ or $[(\text{diolefin})Rh(\mu\text{-In})AuPR_3]ClO_4$, where the indole or indolyl ligands are η^6-bonded to the rhodium atom. We now report some related rhodium(III)-gold(I) complexes of formula $[(C_5Me_5)Rh(\mu\text{-In})AuPR_3](ClO_4)_2$ along with the X-ray structure determination of $[(C_5Me_5)Rh(\mu\text{-In})AuP(C_6H_5)_3](ClO_4)_2 \cdot$

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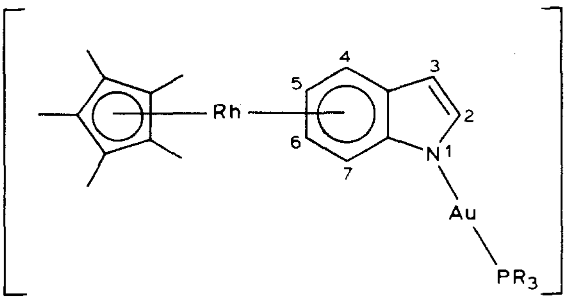
CH_2Cl_2. The ability of the indole group to act as η^5- or η^6-arene ligand through its five- or six-membered ring with rhodium(III) or iridium(III) has been shown by Maitlis et al. [5]. Some crystal structures of mononuclear arene-rhodium complexes have been previously reported [6].

Results and discussion

The complexes of the general formula $AuClPR_3$ ($R = C_6H_5$, 2-MeC_6H_4, 4-MeC_6H_4), prepared by addition of triarylphosphine to a dichloromethane solution of AuCl(tht) (tht = tetrahydrothiophen) [7], react with indole and potassium hydroxide yielding $Au(In)PR_3$. These *N*-indolyltriarylphosphinegold(I) derivatives are white air-stable solids but their solutions turn pink if water is present or when exposed for a long time to air. Their IR spectra show the absorptions corresponding to the coordinated indolyl group along with those of the triarylphosphines; they are not electrolytes in acetone.

The acetone-solvated complex $[Rh(C_5Me_5)(Me_2CO)_3](ClO_4)_2$ (prepared in situ * by treating $[Rh(C_5Me_5)Cl_2]_2$ [8] with $AgClO_4$ in acetone) has demonstrated to be an excellent starting material for the synthesis of arene complexes [5,10]. Thus, it reacts quantitatively with $Au(In)PR_3$ to give the corresponding rhodium(III)-gold(I) complexes (eq. 1), which are air-stable deep yellow solids and also stable in solution, and behave as 2/1 electrolytes in acetone (Table 1) [11].

$$[Rh(C_5Me_5)(Me_2CO)_3](ClO_4)_2 + Au(In)PR_3 \longrightarrow$$



$$(ClO_4)_2 + 3\ Me_2CO \qquad (1)$$

When the derivative with $R = C_6H_5$ is obtained by slow diffusion of n-pentane vapour through a saturated dichloromethane solution of the complex, it crystallizes with one molecule of solvent.

The proposed bonding for these complexes is supported by their analytical (Table 1), spectroscopic and X-ray diffraction data. Their IR spectra show a downwards shift [12] of the indolyl ring stretching vibration relative to $Au(In)PR_3$ (I: 1608 cm^{-1}, II: 1602 cm^{-1}, III: 1603 cm^{-1}, IV: 1553 cm^{-1}; V: 1552 cm^{-1}, VI: 1553 cm^{-1}), along with the corresponding absorptions of the other ligands and the perchlorate anion (Td) (ca. 1097 and 624 cm^{-1}) [13]. The ^1H NMR spectra of these rhodium(III)-gold(I) complexes (Table 2) show no significant displacement of the six-membered ring proton resonances of the indolyl group relative to $Au(In)PR_3$ **,

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* Attempts to isolate these materials failed since a series of complicated rearrangements occurred, these have been elucidated when the anion is PF_6^- [9].

** A significant upfield shift for these protons is observed when $Au(In)P(C_6H_5)_3$ is bonded through the six-membered ring of the indolyl group in the rhodium(I)-gold(I) complexes $[(diolefin)Rh(\mu\text{-}In)AuP(C_6H_5)_3]ClO_4$ [4].

TABLE 1

ANALYSES, CONDUCTANCES AND YIELDS OF THE COMPLEXES I–VI

Compound	Analysis (Found(calcd.)(%))			Λ_M [a] (ohm^{-1} cm^2 mol^{-1})	Yield (%)
	C	H	N		
$Au(In)P(C_6H_5)_3$ (I)	53.80 (54.28)	3.87 (3.85)	2.66 (2.43)	3.1	94
$Au(In)P(2\text{-}MeC_6H_4)_3$ (II)	55.96 (56.42)	4.24 (4.41)	2.37 (2.27)	2.5	96
$Au(In)P(4\text{-}MeC_6H_4)_3$ (III)	56.08 (56.42)	4.29 (4.41)	2.23 (2.27)	2.7	95
$[(C_5Me_5)Rh(\mu\text{-}In)AuP(C_6H_5)_3](ClO_4)_2$ (IV)	42.46 (42.71)	3.66 (3.58)	1.41 (1.38)	212	94
$[(C_5Me_5)Rh(\mu\text{-}In)AuP(2\text{-}MeC_6H_4)_3](ClO_4)_2$ (V)	44.58 (44.42)	4.20 (4.01)	1.20 (1.33)	205	97
$[(C_5Me_5)Rh(\mu\text{-}In)AuP(4\text{-}MeC_6H_4)_3](ClO_4)_2$ (VI)	43.76 (44.42)	4.32 (4.01)	1.22 (1.33)	218	94

[a] ca. 4×10^{-4} *M* acetone solutions.

but a notable shift to lower field occurs for the H(2) proton resonance, which changes from 7.6–7.8 ppm ($J_{2,3} \approx 3.5$ Hz) for $Au(In)PR_3$ compounds to 8.3–8.6 ppm ($J_{2,3} \approx 2.7$ Hz) for $[(C_5Me_5)Rh(\mu\text{-}In)AuPR_3](ClO_4)_2$ complexes.

The structure of $[(C_5Me_5)Rh(\mu\text{-}In)AuP(C_6H_5)_3](ClO_4)_2 \cdot CH_2Cl_2$

The crystal structure of the compound $[(C_5Me_5)Rh(\mu\text{-}In)AuP(C_6H_5)_3](ClO_4)_2 \cdot CH_2Cl_2$ consists of heterodinuclear rhodium(III)-gold(I) cationic complexes, perchlorate counter ions, and dichloromethane molecules of crystallization; selected bond distances and angles in them are given in Table 3. A view of the rhodium-gold cationic complex with the atomic numbering scheme is shown in Figure 1. The Rh atom is coordinated in a "sandwich" fashion by the pentamethylcyclopentadienyl and indolyl ligands, interacting η^5 with the cyclopentadienyl and η^6 with the arene ring from the indolyl ligand, which also is σ-bonded to the Au atom through the N

TABLE 2

^1H NMR DATA [a] FOR THE COMPLEXES I–VI

Compound	C_5Me_5	Indolyl group [b]				Phosphine	
		H(2)	H(3)	H(4,6)	H(5,7)	Ph	Me
I	–	7.77(d)	6.72(dd)	7.19(m)	7.84(m)	7.62(m)	–
II	–	7.69(d)	6.58(dd)	6.99(m)	7.77(m)	7.41(m)	2.86(s)
III	–	7.65(br)	6.60(br)	7.10(m)	7.80(m)	7.38(m)	2.47(s)
IV	1.83(s)	8.52(d)	6.86(br)	7.10(m)	7.95(m)	7.55(m)	–
V	1.81(s)	8.33(d)	6.83(dd)	7.04(m)	7.87(m)	7.48(m)	2.75(s)
VI	1.84(s)	8.35(d)	6.76(br)	7.07(m)	7.66(m)	7.34(m)	2.42(s)

[a] Chemical shifts δ in ppm, s, singlet; d, doublet; dd, double doublet; m, multiplet; br, broad unresolved signal. [b] The assignment of these protons has been made according to ref. 5.

TABLE 3

SELECTED BOND DISTANCES (Å) AND ANGLES (°)

(a) around the metal atoms			
Au–P	2.249(5)	Rh–C(3)	2.33(2)
Au–N	2.04(1)	Rh–C(4)	2.34(2)
Rh–C(9)	2.18(2)	Rh–C(5)	2.24(2)
Rh–C(10)	2.14(2)	Rh–C(6)	2.21(2)
Rh–C(11)	2.11(2)	Rh–C(7)	2.22(2)
Rh–C(12)	2.11(2)	Rh–C(8)	2.29(2)
Rh–C(13)	2.09(2)		
P–Au–N	175.1(4)		
(b) in the ligands			
C(9)–C(10)	1.43(3)	C(3)–C(8)	1.43(2)
C(10)–C(11)	1.45(4)	C(3)–C(4)	1.43(2)
C(11)–C(12)	1.41(4)	C(4)–C(5)	1.40(2)
C(12)–C(13)	1.28(4)	C(5)–C(6)	1.41(2)
C(9)–C(13)	1.38(3)	C(6)–C(7)	1.46(3)
N–C(1)	1.33(2)	C(7)–C(8)	1.39(3)
N–C(4)	1.41(2)	P–C(19)	1.81(1)
C(1)–C(2)	1.39(3)	P–C(25)	1.80(1)
C(2)–C(3)	1.46(3)	P–C(31)	1.79(1)
C(13)–C(19)–C(10)	106(2)	C(4)–C(3)–C(2)	106(2)
C(9)–C(10)–C(11)	105(2)	C(8)–C(3)–C(2)	133(2)
C(10)–C(11)–C(12)	107(2)	C(8)–C(3)–C(4)	121(2)
C(11)–C(12)–C(13)	108(2)	C(3)–C(4)–C(5)	121(2)
C(12)–C(13)–C(9)	114(3)	N–C(4)–C(3)	109(2)
C(1)–N–C(4)	106(2)	C(5)–C(4)–N	130(2)
C(1)–N–Au	132(1)	C(4)–C(5)–C(6)	120(2)
C(4)–N–Au	122(1)	C(5)–C(6)–C(7)	118(2)
C(2)–C(1)–N	116(2)	C(6)–C(7)–C(8)	124(2)
C(3)–C(2)–C(1)	103(2)	C(7)–C(8)–C(3)	116(2)
(c) in the perchlorate anions and in the dichloromethane molecule			
Cl–O(1)	1.30(3)	Cl–O(5)	1.53(3)
Cl–O(2)	1.45(3)	Cl–O(6)	1.30(3)
Cl–O(3)	1.36(4)	Cl–O(7)	1.31(4)
Cl–O(4)	1.35(4)	Cl–O(8)	1.40(3)
C(37)–Cl(3)	1.77(2)	C(37)–Cl(4)	1.68(2)
O(1)–Cl(1)–O(2)	111(2)	O(5)–Cl(2)–O(6)	108(2)
O(1)–Cl(1)–O(3)	111(2)	O(5)–Cl(2)–O(7)	104(2)
O(1)–Cl(1)–O(4)	101(2)	O(5)–Cl(2)–O(8)	107(2)
O(2)–Cl(1)–O(3)	121(2)	O(6)–Cl(2)–O(7)	109(2)
O(2)–Cl(1)–O(4)	102(2)	O(6)–Cl(2)–O(8)	114(2)
O(3)–Cl(1)–O(4)	109(2)	O(7)–Cl(2)–O(8)	114(2)
Cl(3)–C(37)–Cl(4)	113(2)		

atom of the pentaatomic ring. In this way the indolyl ligand acts as a σ,η bridge through the N atom of the pentaatomic ring and the aromatic hexaatomic ring, respectively. The coordination around Rh is shown in Fig. 2 as a view along the barycentres of the two rings. The Rh–C distances to the cyclopentadienyl ring carbons are in the range 2.09–2.18 Å (the distance with the barycentre being 1.767 Å); those to the arene are in the range 2.21–2.34 Å (the distance with the barycentre

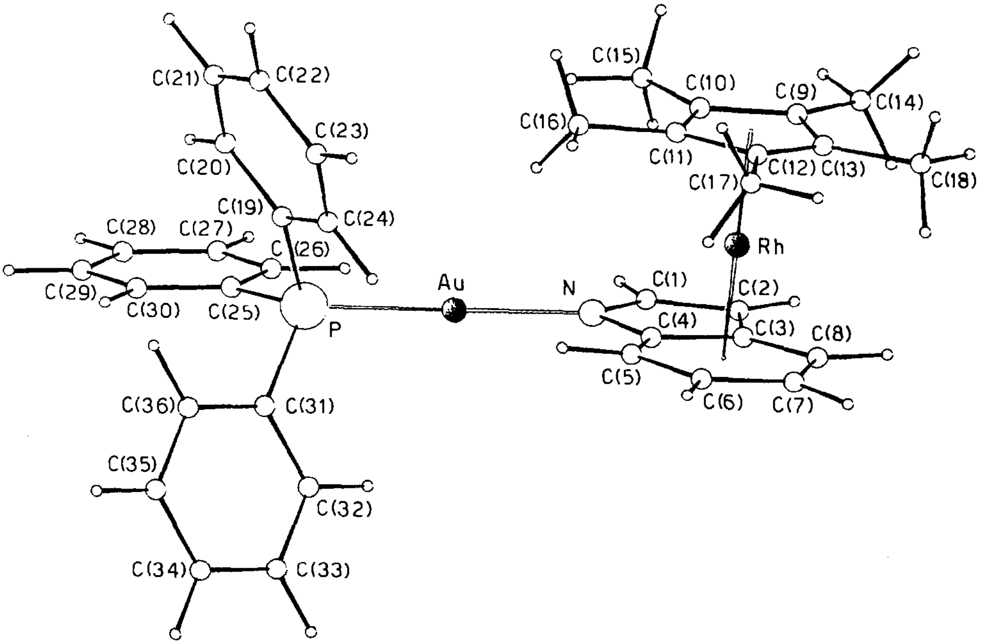

Fig. 1. View of the cationic complex $[(C_5Me_5)Rh(\mu\text{-}In)AuP(C_6H_5)_3]^{2+}$ showing the labeling scheme.

being 1.770 Å). The two rings are practically parallel, the dihedral angle between the mean planes through them being 3.3° only. The cyclopentadienyl ring is planar within experimental errors, atomic averaged deviations from the mean plane through it being 0.01 Å. The analysis of the planarity of the indolyl ring shows some interesting features. If the pentaatomic ring can be considered planar (deviations of N, C(1), C(2), C(3) and C(4) atoms from the mean plane being −0.003, 0.009, −0.007, 0.003 and 0.001 Å, respectively), the hexaatomic ring is slightly puckered (deviations of C(3), C(4), C(5), C(6), C(7) and C(8) atoms being −0.01, 0.03, −0.03, 0.01, 0.03 and −0.03 Å, respectively, with e.s.d.'s of 0.01 Å). The slight puckering of the ring is indicated also by the torsion angles: C(3)C(4)C(5)C(6) −5.8°; C(4)C(5)C(6)C(7) 2.8°; C(5)C(6)C(7)C(8) 3.2°; C(6)C(7)C(8)C(3) −5.8°;

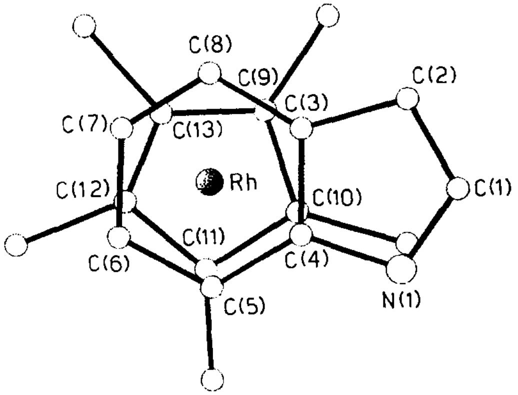

Fig. 2. Projection of the pentamethylcyclopentadienyl and indolyl ligands along the line through the barycentres of the cyclopentadienyl and arene rings.

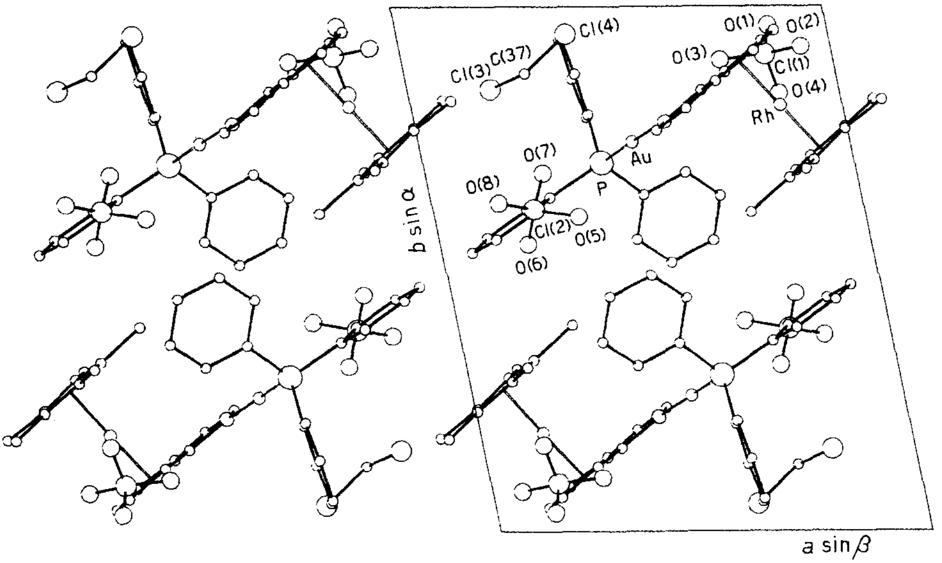

Fig. 3. Projection of the structure along the *c* axis, showing the packing of the cationic complexes, of the perchlorate anions and of the dichloromethane molecules.

C(7)C(8)C(3)C(4) 2.7°; C(8)C(3)C(4)C(5) 3.0° with averaged e.s.d.'s of 1.5°. Both atomic deviations from the planarity and torsion angles in the ring are consistent with a skew conformation of the hexaatomic ring, but the low values of the deviations and the rather large e.s.d.'s preclude certain assignment of the conformation. A deviation from the planarity of the η^6-coordinated arene has been observed in the other arene-rhodium complexes whose structures have been determined [6], and sometimes skew or boat conformations were assigned to the ring. Such distortions of the bonded arenes have been attributed to packing forces in the solid state or to a slight localization of the bonding MO's of the ring on some carbon atoms.

The N atom from the pentaatomic ring of the indolyl ligand is σ-bonded to the Au atom (Au–N 2.04(1) Å). The coordination at the Au atom, involving also a P atom from the $P(C_6H_5)_3$ ligand (Au–P 2.249(5) Å), is essentially linear (P–Au–N = 175.1(4)°). The bonding of the Au atom is comparable with that found in the heteronuclear cationic complex $[(Ph_3P)_2Au_2(\mu\text{-BiBzIm})Rh(COD)]^+$ [3], though the Au–N bonds in it, involving the 2,2′-bibenzimidazolate ligand, were much shorter (1.94 and 1.96 Å).

The packing in the crystals of the heteronuclear cations, of the perchlorate anions and of the dichloromethane molecules is presented in Fig. 3.

Experimental

The C, H, and N analyses were carried out with a Perkin–Elmer 240-B microanalyzer. IR spectra were recorded on a Perkin–Elmer 599 spectrophotometer using Nujol mulls between polyethylene sheets. ^1H NMR spectra were recorded in $CDCl_3$ with $SiMe_4$ as internal standard on a 80 MHz Varian FT-80A instrument. Conductivities were measured with a Philips 9501/01 conductimeter. Since the methods used to prepare the compounds were very similar, only some typical procedures are given; the only variation was that in some cases n-hexane or diethyl ether was used to precipitate the product. Solvents were dried and distilled before use.

Preparation of $Au(In)P(C_6H_5)_3$

A solution of potassium hydroxide (4.16 ml, 0.079 *M* in methanol, 0.404 mmol) and indole (47.4 mg, 0.404 mmol) in methanol (10 ml) was stirred for 30 min, then $AuClP(C_6H_5)_3$ (200 mg, 0.404 mmol) in dichloromethane (10 ml) was added. After 2 h of stirring the solvent was removed in vacuo and the oily residue was extracted with dichloromethane. The dichloromethane solution was filtered through kiesselguhr to remove potassium chloride. n-Hexane was added, and the colourless solution was evaporated in vacuo to ca. 1 ml to give a white solid. The solid was filtered off, washed with diethyl ether and hexane, and vacuum dried.

Preparation of $[(C_5Me_5)Rh(\mu\text{-}In)AuP(C_6H_5)_3](ClO_4)_2$

A solution of $[Rh(C_5Me_5)Cl_2]_2$ (99.4 mg, 0.161 mmol) and silver perchlorate (133 mg, 0.644 mmol) in acetone (15 ml) was stirred for 30 min. Silver chloride was filtered off and $Au(In)P(C_6H_5)_3$ (185 mg, 0.322 mmol) was added to the filtrate. After 15 min of stirring the solvent was removed in vacuo and the residue extracted with dichloromethane. The filtered solution was evaporated to dryness to give a yellow-orange oil, which was kept under vacuum (0.1 mmHg) for 15 min. Diethyl ether was then added and the solid was filtered off, washed with diethyl ether and vacuum-dried.

X-Ray data collection and structure refinement for $[(C_5Me_5)Rh(\mu\text{-}In)AuP(C_6H_5)_3](ClO_4)_2 \cdot CH_2Cl_2$

An irregularly shaped red-orange crystal of the compound, having approximate dimensions of 0.15 × 0.25 × 0.30 mm, was used for the data collection. The cell parameters were obtained from a least-squares refinement of the θ values of 29 reflections accurately measured on a Siemens AED single-crystal diffractometer. The crystal data were as follows: $C_{37}H_{38}AuCl_4NO_8PRh$, $M = 1097.37$, triclinic, a 13.289(9), b 16.388(11), c 10.794(6) Å, α 72.35(5), β 109.19(6), γ 106.32(6)°; V 2072(3) Å^3, $Z = 2$, D_c 1.759 g cm^{-3}, Mo-K_α radiation ($\bar{\lambda}$ 0.710688 Å), μ(Mo-K_α) 42.67 cm^{-1}, space group $P\bar{1}$ from structure determination.

A complete set of intensity data was collected, with θ in the range 3–25°, on the same Siemens diffractometer using the Nb-filtered Mo-K_α radiation and the $\theta/2\theta$ scan technique. Of a total of 6952 independent reflections, 3314 having $I \geqslant 2\sigma(I)$ were considered observed and used in the analysis. One reflection was remeasured after 20 reflections as a check on crystal and instrument stability; no significant change in the measured intensity of this reflection was observed during the data collection.

The structure amplitudes were obtained after the usual Lorentz and polarization reduction and the absolute scale was established by Wilson's method. No correction for absorption effects was applied.

The structure was solved by the heavy-atom method starting from a three-dimensional Patterson map. The positions of all non-hydrogen atoms were revealed by the subsequent Fourier synthesis phased on the contribution of the Au and Rh atoms. The refinement was carried out by least-squares full-matrix cycles using the SHELX system of computer programs [14] with first isotropic thermal parameters, then anisotropic thermal parameters were assigned to all the atoms except the carbon atoms of the methyl and phenyl groups, the oxygen atoms of the perchlorate anions, and the atoms of the dichloromethane molecule. The phosphine phenyl rings were constrained into the D_{6h} geometry (C–C 1.395 Å). A difference Fourier map did not reveal clearly the positions of all the hydrogen atoms, so they were placed in their geometrically calculated positions and included in the final structure factor calculations. The function minimized in the least-squares calculations was $\Sigma w|\Delta F|^2$; unit weights were used in the first cycles of refinement, the weight calculated as $w = K/[\sigma^2(F_0) + gF_0^2]$ with $K = 0.5541$ and $g = 0.01366$ was chosen in the final cycles. The atomic scattering factors (corrected for anomalous dispersion of Au, Rh, Cl and P) were taken from the International Tables [15]. The final R value was 0.072 (observed reflections only).

The atomic fractional coordinates for the non-hydrogen atoms and hydrogen atoms are listed in Tables 4 and 5 respectively; Lists of thermal parameters and of observed and calculated structure factors are available from the authors on request.

TABLE 4

FRACTIONAL ATOMIC COORDINATES ($\times 10^4$) WITH e.s.d.'s IN PARENTHESES FOR THE NON HYDROGEN ATOMS

	x/a	y/b	z/c		x/a	y/b	z/c
Au	4937(1)	7425(1)	5421(1)	C(22)	6350(12)	5539(10)	2898(16)
Rh	8556(1)	8120(1)	8260(2)	C(23)	6726(12)	6398(10)	3045(16)
Cl(1)	8443(6)	9085(5)	2973(7)	C(24)	6031(12)	6840(10)	3192(16)
Cl(2)	2345(6)	6146(5)	8306(8)	C(25)	2777(10)	6377(10)	3272(15)
P	4132(4)	7032(4)	3444(6)	C(26)	2359(10)	6095(10)	4393(15)
N	5791(14)	7812(12)	7170(17)	C(27)	1325(10)	5565(10)	4315(15)
C(1)	5570(18)	7647(17)	8345(26)	C(28)	710(10)	5318(10)	3115(15)
C(2)	6352(18)	8060(16)	9305(21)	C(29)	1128(10)	5599(10)	1994(15)
C(3)	7179(15)	8580(13)	8599(20)	C(30)	2162(10)	6129(10)	2073(15)
C(4)	6802(16)	8405(13)	7286(21)	C(31)	4047(13)	7951(8)	2034(12)
C(5)	7441(16)	8754(12)	6374(22)	C(32)	3943(13)	8722(8)	2233(12)
C(6)	8429(17)	9351(14)	6699(22)	C(33)	3794(13)	9443(8)	1148(12)
C(7)	8767(18)	9548(13)	8025(28)	C(34)	3748(13)	9392(8)	−137(12)
C(8)	8201(17)	9152(15)	8999(22)	C(35)	3852(13)	8621(8)	−336(12)
C(9)	9083(23)	7066(16)	9952(27)	C(36)	4001(13)	7900(8)	749(12)
C(10)	8420(23)	6735(16)	8795(38)	C(37)	2795(23)	8734(22)	5750(30)
C(11)	9017(34)	7143(22)	7781(27)	Cl(3)	1927(11)	8436(8)	4243(13)
C(12)	9956(33)	7708(22)	8351(50)	Cl(4)	3915(11)	9487(9)	5520(14)
C(13)	9948(22)	7664(17)	9552(35)	O(1)	8645(27)	9644(22)	1895(35)
C(14)	8848(33)	6906(26)	11308(33)	O(2)	9320(34)	9237(26)	4155(43)
C(15)	7349(26)	6076(22)	8770(38)	O(3)	7385(39)	8979(28)	2957(44)
C(16)	8601(35)	6875(28)	6458(35)	O(4)	8598(39)	8347(34)	2816(49)
C(17)	10760(32)	8227(26)	7467(40)	O(5)	3338(26)	6005(19)	9501(31)
C(18)	10949(29)	8215(24)	10394(38)	O(6)	2038(26)	5476(21)	7764(31)
C(19)	4960(12)	6423(10)	3192(16)	O(7)	2721(38)	6836(30)	7456(45)
C(20)	4584(12)	5564(10)	3045(16)	O(8)	1557(30)	6268(23)	8797(36)
C(21)	5279(12)	5122(10)	2897(16)				

TABLE 5

CALCULATED FRACTIONAL COORDINATES ($\times 10^4$) FOR THE HYDROGEN ATOMS

	x/a	y/b	z/c
H(1)	4829	7219	8543
H(2)	6350	8009	10325
H(5)	7179	8567	5422
H(6)	8918	9652	5992
H(7)	9501	10030	8262
H(8)	8513	9268	10002
H(141)	8124	6405	11357
H(142)	8726	7503	11413
H(143)	9528	6697	12113
H(151)	7007	5931	7786
H(152)	6788	6347	8983
H(153)	7493	5483	9524
H(161)	9138	7240	5826
H(162)	7795	7008	5961
H(163)	8571	6185	6638
H(171)	11437	8630	8031
H(172)	10342	8636	6563
H(173)	11057	7773	7196
H(181)	10843	8122	11381
H(182)	11016	8898	9887
H(183)	11680	8006	10496
H(20)	3755	5241	3046
H(21)	4988	4457	2782
H(22)	6888	5196	2785
H(23)	7555	6721	3045
H(24)	6322	7505	3306
H(26)	2836	6287	5322
H(27)	1001	5346	5183
H(28)	-91	4909	3054
H(29)	652	5407	1066
H(30)	2486	6347	1205
H(32)	3978	8761	3228
H(33)	3714	10040	1303
H(34)	3632	9950	-977
H(35)	3817	8582	-1331
H(36)	4081	7303	594
H(371)	3044	8155	6461
H(372)	2345	8995	6158

Calculations were performed on the CYBER 7600 computer of the Centro di Calcolo Interuniversitario dell'Italia Nord-Orientale, Bologna, with financial support from the University of Parma.

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