CHARACTERISTIC STRUCTURAL FEATURES OF CYCLOPENTADIENYL DERIVATIVES OF POST-TRANSITION METALS

II *. SYNTHESIS AND STRUCTURE OF TRIS(TRIPHENYLPHOSPHINEGOLD)TETRAPHENYLCYCLOPENTADIENE TETRAFLUOROBORATE

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Summary

The trinuclear cationic complex $[Ph_4C_5(AuPPh_3)_3]^+[BF_4]^-$ (I) obtained by interaction of $C_5HPh_4AuPPh_3$ or $Ph_4C_5(AuPPh_3)_2$ with $[AuPPh_3]^+[BF_4]^-$ in THF was studied by X-ray diffraction. In the presence of benzene, triclinic crystals of the solvate $[Ph_4C_5(AuPPh_3)_3]^+[BF_4]^- \cdot 2\ C_6H_6$ are formed, $a = 12.845(6)$, $b = 16.042(8)$, $c = 22.642(11)$ Å, $\alpha = 86.62(4)$, $\beta = 77.51(4)$, $\gamma = 76.05(4)°$, space group $P\bar{1}$, $Z = 2$, 9494 reflections with $I > 2\sigma$ ($\lambda(Mo\text{-}K_\alpha)$, $\theta/2\theta$ scan, $2\theta \leqslant 46°$), with absorption correction $R = 0.054$. The complex represents a diaurated cation of tetraphenylcyclopentadienyl(triphenylphosphine)gold, containing a triangular Au_2C fragment (Au—Au 2.820(1) Å) which is bonded to the third Au atom (Au—Au 3.021(1) Å), coordinated to the cyclopentadienyl ligand by a bond intermediate between $\eta^1(\sigma)$ and η^3 (Au—C 2.21(2), 2.60(2) and 2.71(2) Å).

Introduction

Studies of organogold complexes, including X-ray structure investigations, have intensified during the last decade and have resulted in the preparation of a number of compounds with unusual structures, primarily polynuclear and cluster ones, revealing interesting chemical properties [1]. Most of the structurally studied organogold derivatives are σ-complexes; however, compounds with novel, formely unknown, types of metal—ligand bond have been found recently. In continuation of our investigations of organogold derivatives we

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* For part I see ref. 5.

have obtained a cationic trinuclear complex of tris(triphenylphosphinegold)-tetraphenylcyclopentadiene and established its structure by an X-ray analysis.

Results and discussion

The cationic complex $[Ph_4C_5(AuPPh_3)_3]^+[BF_4]^-$ (I) was obtained by us by interaction of both mono- ($C_5HPh_4AuPPh_3$, II) and di-gold(1+) (C_5Ph_4-$(AuPPh_3)_2$, III) derivatives of tetraphenylcyclopentadiene with the tetrafluoroborate salt of the cation $[Ph_3PAu]^+$, generated in situ [2]. In the presence of moisture complex I decomposes slowly with the formation of $[(Ph_3PAu)_3O]^+$-$[BF_4]^-$ and tetraphenylcyclopentadiene. With benzene complex I forms a dia-magnetic solvate, $[Ph_4C_5(AuPPh_3)_3]^+[BF_4]^- \cdot 2\,C_6H_6$ (Ia), of a constant composition.

The trinuclear complex Ia reacts with nucleophiles similarly to the binuclear cationic gold complexes studied by us earlier [3,4]. In all cases the binuclear compound III and a complex of the nucleophile with the eliminated cation $[Ph_3PAu]^+$ are formed. The action of hydrogen chloride on Ia causes elimination of all the three $AuPPh_3$ groups and formation of tetraphenylcyclopentadiene:

$$[Ph_4C_5(AuPPh_3)_3]^+[BF_4]^- \cdot 2\,C_6H_6 \xrightarrow[\text{THF ether}]{\text{HCl}} C_5H_2Ph_4 + ClAuPPh_3 + C_6H_6$$
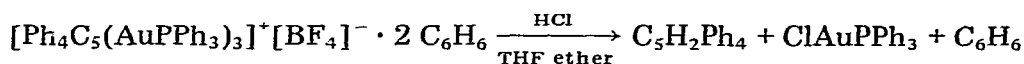
To elucidate the coordination of the gold atoms in I and details of the molecular geometry, an X-ray study was carried out of its solvate Ia.

Compound I is a tetrafluoroborate salt of a complex cation, viz. tetraphenyl-cyclopentadiene, into which three Ph_3PAu groups are introduced. Each of these groups forms a covalent Au—C bond with a carbon atom of the five-membered cycle. The cation 1 is shown in Fig. 1, the relevant bond lengths are presented in Fig. 2, and bond angles and characteristic planar fragments of the cation are listed in Tables 1 and 2, respectively. All three Ph_3P—Au—C fragments have a similar geometry with a small but significant deviation of the Au atom coordination from linearity (Table 3). The Au—P bond lengths are unexceptional for phosphine Au complexes, and the Au—C distances can be compared with those in the structures of tetraphenylcyclopentadienyltriphenylphosphinegold, $Ph_3PAuC_5Ph_4H$ (II), 2.15(1) Å [5], the tetrafluoroborate of the cation $[(Ph_3PAu)_2C_5H_4FeC_5H_5]^+$ (IV) (see Fig. 2) [4] and the diaurated malonic acid dinitrile $(Ph_3PAu)_2C(CN)_2$ (V), 2.107(9) and 2.095(9) Å [6]. The positions of all the three Au atoms with respect to the five-membered cyclic ligand * are quite different.

The Au(1) atom forms a covalent Au(1)—C(1) bond with the tetraphenyl-cyclopentadienyl ligand, almost perpendicular to the least-squares plane of the five-membered C(1)—C(5) cycle (the bond angles Au(1)—C(1)—C(2) and Au(1)—C(1)—C(5) are 91(1) and 88(1)°, respectively). The Au···C(2) and Au···C(5) distances, 2.71(2) and 2.60(2) Å, respectively, indicate a weak "secondary" Au···C interaction, similar to the Ag···C interaction in some Ag com-

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* We shall refer to this ligand as "cyclopentadienyl" in spite of a certain ambiguity of this term as applied to the cation I.
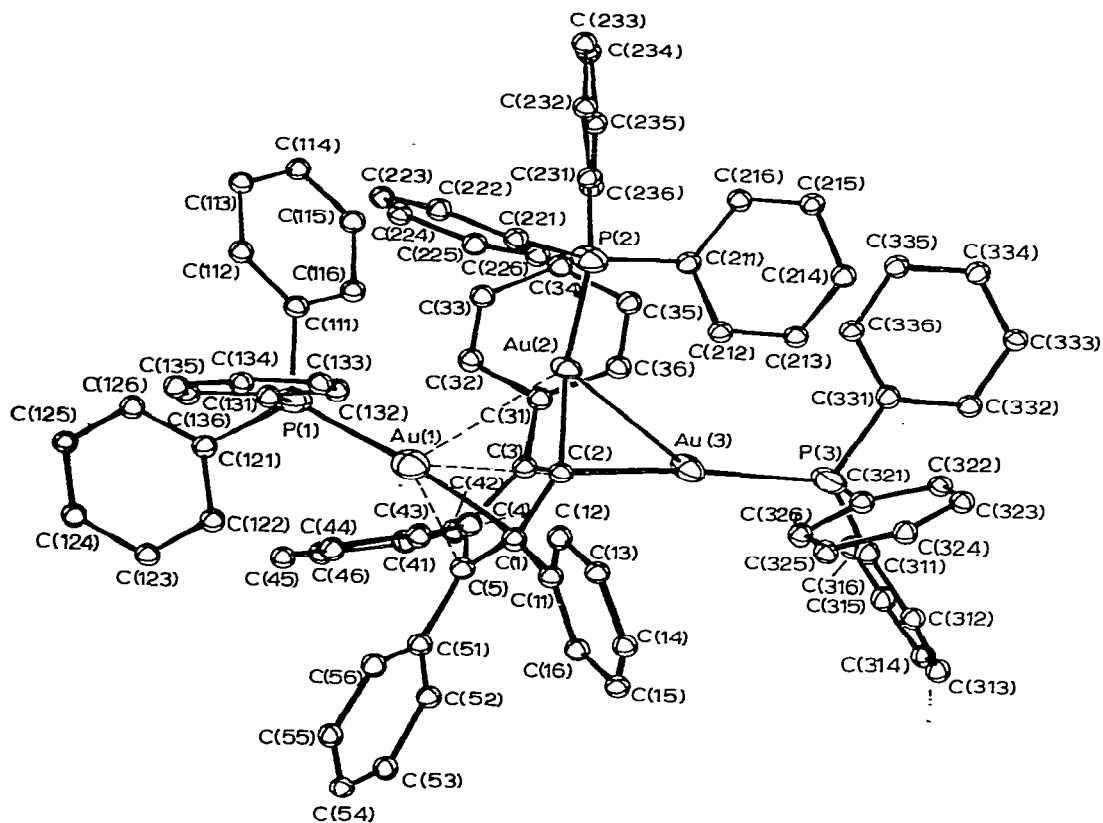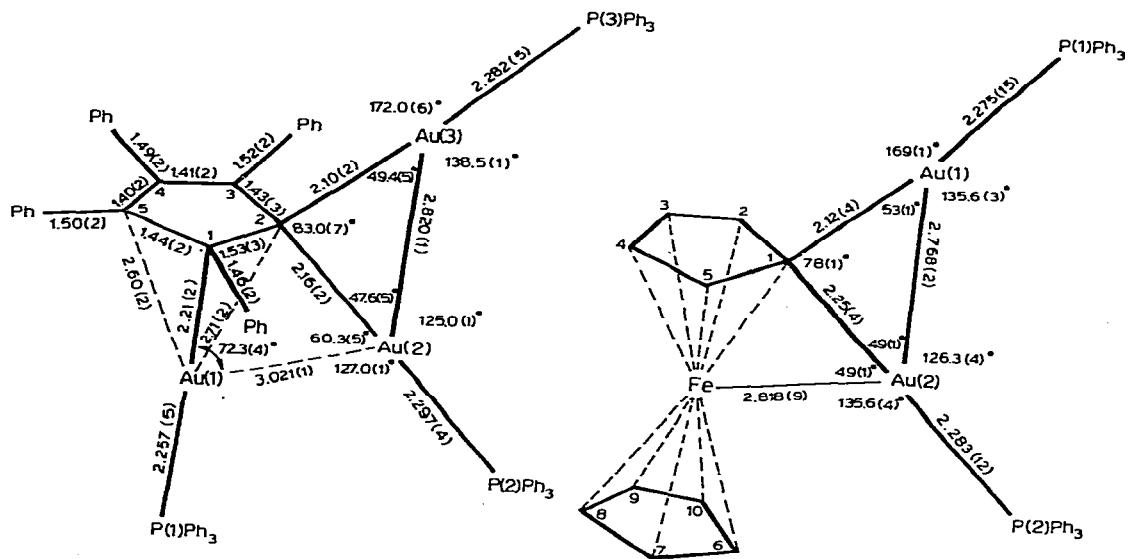
Fig. 1. Cation I.

Fig. 2. The most important geometrical parameters of cation I (this work) and cation IV (ref. 4).

TABLE 1

SELECTED BOND ANGLES ω (°) IN THE CATION I

Angle	ω	Angle	ω
C(1)Au(1)P(1)	172.8(4)	C(5)C(1)C(11)	129(1)
C(1)Au(1)Au(2)	72.3(4)	Au(2)C(2)Au(3)	83.0(7)
P(1)Au(1)Au(2)	114.9(1)	Au(2)C(2)C(1)	116(1)
C(2)Au(2)P(2)	172.4(5)	Au(2)C(2)C(3)	114(1)
C(2)Au(2)Au(1)	60.3(5)	Au(3)C(2)C(1)	116(1)
C(2)Au(2)Au(3)	47.6(5)	Au(3)C(2)C(3)	120(1)
P(2)Au(2)Au(1)	127.0(1)	C(1)C(2)C(3)	106(1)
P(2)Au(2)Au(3)	125.0(1)	C(2)C(3)C(4)	109(1)
Au(1)Au(2)Au(3)	103.93(3)	C(2)C(3)C(31)	124(1)
C(2)Au(3)P(3)	172.0(6)	C(4)C(3)C(31)	126(1)
Au(2)Au(3)P(3)	138.5(1)	C(3)C(4)C(5)	109(1)
C(2)Au(3)Au(2)	49.4(5)	C(3)C(4)C(41)	125(1)
Au(1)C(1)C(2)	91(1)	C(5)C(4)C(41)	126(1)
Au(1)C(1)C(5)	88(1)	C(4)C(5)C(1)	111(1)
Au(1)C(1)C(11)	113(1)	C(4)C(5)C(51)	126(1)
C(2)C(1)C(5)	104(1)	C(1)C(5)C(51)	123(1)
C(2)C(1)C(11)	121(1)		

pounds [1]. The bonding mode of the Au(1) atom to the cyclopentadienyl ligand is similar to the "slipped" coordination of the Be atom by one of the cyclopentadienyl rings in the crystal structure of beryllocene at —120°C [7] and represents a case of Cp—metal coordination intermediate between $\eta^1(\sigma)$ and $\eta^3(\pi$-allyl). Similar Au coordination to a C_5Ph_4H ligand was found by us in the structure of the monoaurated tetraphenylcyclopentadiene II [5]. In contrast to II, where the C(1) atom which is nearest to the Au atom bears also an H atom, detected in the PMR spectrum, in the structure of I the C(1) atom is bonded to the Ph-substituent C(11)—C(16). The bond angles C(11)—C(1)—C(2) and C(11)—C(1)—C(5), 121(1) and 129(1)°, respectively, exceed significantly the tetrahedral value, the sum of the C—C—C bond angles at the C(1) atom is 354°, i.e. close to 360°, and the C(1)—C(11) bond makes an angle of 18.2° with the least-squares plane of the C(1)—C(5) cycle. Thus the coordination of the C(1) atom in the Ph_4C_5 ligand is close to planar-trigonal, typical of metal π-complexes, which substantiates a significant contribution from the π-allyl form to the coordination of Au(1) to the cyclopentadienyl ligand.

The Au(2), Au(3) and C(2) atoms form a triangular fragment which is nearly normal to the least-squares plane of the C(1)—C(5) cycle (the dihedral angle is 87.5°). The P(2) and P(3) atoms deviate slightly from the Au(2)Au(3)C(2) plane, by 0.066 and 0.057 Å, respectively, and the Au(2)—Au(3) distance, 2.820(1) Å, is somewhat shorter than the interatomic distance, 2.884 Å, in gold metal [4]. A fragment with a similar configuration was found previously in the structures of the diaurated ferrocene cation IV (Fig. 2, Au—Au 2.768(2) Å [4]) and the neutral molecule V (Au—Au 2.912(1) Å [6]. In spite of the same general configuration of the Au_2C fragment in I, IV and V, the Au—Au distances in these compounds differ significantly, which is not suprising in view of the wide range of metal—metal distances in polynuclear Au complexes [1,8]. In cation I the Au(1) and Au(2) atoms are also brought rather

TABLE 2

LEAST-SQAURES PLANES IN THE CATION III

Plane	Coefficients of plane equations $Ax + By + Cz + D = 0$				Deviation of atoms from mean planes							
	A	B	C	D								
I	−0.3437	−0.8197	−0.4581	18.95	Au(1) 0	Au(2) 0	Au(3) 0	P(1)[a] 0.175	P(2)[a] −0.686	P(3)[a] −0.653	C(1)[a] −0.13	C(2)[a] 0.63
II	−0.6519	−0.7286	−0.2104	15.45	Au(2) 0	Au(3) 0	C(2) 0	P(2)[a] 0.066	P(3)[a] −0.057			
III	−0.4575	0.5498	−0.6988	7.0274	C(51)[a] 0.26	Au(1)[a] −2.233	Au(2)[a] −1.358	Au(3)[a] 1.458	C(5) 0.02	C(11)[a] 0.42	C(31)[a] −0.30	C(41)[a] −0.08
					C(1) −0.04	C(2) 0.04	C(3) −0.03	C(4) 0.00				
IV	−0.477	0.5611	−0.6762	6.7413	C(1) −0.01	C(3) 0.01	C(4) −0.01	C(5) 0.01	C(2)[a] 0.10			
V	−0.9825	0.1858	−0.0076	5.3194	C(11) 0.01	C(12) −0.01	C(13) 0.00	C(14) 0.00	C(15) 0.00	C(16) −0.01	C(1)[a] 0.07	
VI	−0.1903	−0.1841	−0.9643	16.58	C(31) 0.00	C(32) 0.00	C(33) 0.00	C(34) 0.00	C(35) 0.00	C(36) 0.00	C(3)[a] −0.14	
VII	0.3249	0.6147	−0.7187	1.1066	C(41) 0.00	C(42) −0.01	C(43) 0.01	C(44) −0.01	C(45) 0.00	C(46) 0.00	C(4)[a] −0.02	
VIII	0.2933	0.9547	−0.0509	7.5999	C(51) −0.01	C(52) 0.00	C(53) 0.00	C(54) 0.01	C(55) −0.02	C(56) 0.02	C(5)[a] −0.02	

[a] Atoms not included in the least-squares calculations. Dihedral angles between planes are: I/II 23.4°, I/III 88.5°, II/III 87.4°, III/IV 56.2°, III/VI 48.7°, III/VII 46.2°, III/VIII 46.0°

TABLE 3

COMPARISON OF THE GEOMETRIC PARAMETERS OF THE $Ph_3P-Au-C$ FRAGMENTS IN THE CATION I

Fragment	Au—P (Å)	Au—C (Å)	P—Au—C (°)
P(1)—Au(1)—C(1)	2.257(5)	2.21(2)	172.8(4)
P(2)—Au(2)—C(2)	2.297(4)	2.16(2)	172.4(5)
P(3)—Au(3)—C(2)	2.282(5)	2.10(2)	172.0(6)

close together, as the corresponding distance, 3.021(1) Å, although somewhat exceeding those in the metal, is still within the range of the Au—Au bond lengths, 2.932—3.091 Å, in the octahedral cluster dication $[(p-CH_3C_6H_4)_3PAu]_6^{2+}$ involving no bridging ligands [8]. The plane of the triangular Au(1)—Au(2)—Au(3) fragment makes a dihedral angle of 88.5° with the least-squares plane of the five-membered ring, and the Au(1)—Au(2)—Au(3) angle is 103.93(3)°. The Au(1)···Au(3) distance, 4.603(1) Å, does not correspond to a metal—metal interaction.

The tetraphenylcyclopentadienyl ligand has a "paddle wheel" configuration with similar values of the dihedral angles between the Ph—ring planes and the least-squares plane of the five-membered C(1)—C(5) cycle. The planarity of the C(1)—C(5) cycle in I is somewhat distorted (plane III, Table 2), viz., the C(2) atom deviates from the mean plane of the remaining four atoms away from the Au(1) atom by 0.10 Å (plane IV, Table 2), the *ipso*-carbons of the Ph substituents also have significant deviations from the C(1)—C(5) least-squares plane (Table 2). The bond lengths in the five-membered C(1)—C(5) cycle differ significantly from the diene system found in the structure of the monoaurated tetraphenylcyclopentadiene II [5], viz., this cycle involves one "long" C(1)—C(2) bond, 1.53(3) Å, two "short" C(3)—C(4) and C(4)—C(5) bonds, 1.41(2) and 1.40(2) Å, respectively, and two C(2)—C(3) and C(1)—C(5) bonds, 1.43(3) and 1.44(2) Å, respectively, of an intermediate length (Fig. 2). Comparison of the structures of I and II indicates that introduction of the Ph_3PAu groups into II with a formal transformation to the structure of the cation I is accompanied by a significant distortion of the Ph_4C_5 fragment and a redistribution of the bond lengths in the five-membered ring (the cyclopentadienyl ligand in II is planar and the *ipso*-carbons in the Ph substituents lie in its least-squares plane within the error limits [5]).

Considering I as a cation of diaurated tetraphenylcyclopentadienyltriphenylphosphinegold, one can readily establish a similarity of I and the diaurated ferrocene cation IV. Both cations I and IV are formed by the replacement of the H atom by the $(Ph_3PAu)_2$ fragment in a molecule of a monometallated cyclopentadienyl derivative LMC_5X_4H where M = Fe, L = C_5H_5, X = H in the ferrocene and M = Au, L = Ph_3P, X = Ph in II *. In addition, I and IV possess some common stereochemical features, viz., despite their different stoichiomet-

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* Coordination of the Au(1) atom by the tetraphenylcyclopentadienyl ligand in I differs from that of the Au atom in II by a formal 1,2-shift of the Ph_3PAu group in the five-membered ring.

ric composition and different types of coordination of the Fe atom in IV and the Au(1) atom in I by the cyclopentadienyl ligand, both cations have the $(Ph_3PAu)_2C$ fragment normal to the least-squares plane of the "spiro-" five-membered cycle and bonded by one of its Au atoms to the Fe atom in IV or the Au(1) atom in I (Fig. 2). The additional Au(2)—Fe coordination in IV or Au(2)—Au(1) coordination in I leads to an elongation of the Au(2)—C bond as compared with the other bond of this type in the Au_2C fragment (in contrast to V where both Au—C bond lengths coincide within the accuracy limit). The P(2), P(3) and C(2) atoms in I, as well as in IV, deviate from the plane of the three metal atoms in opposite directions (Table 2 and ref. 4). Both structures exhibit a similar distortion from planarity of the aurated cyclopentadienyl ligand, viz. a deviation of the C atom involved in the Au_2C triangle from the least-squares plane of the remaining four atoms of the five-membered cycle away from the Fe atom in IV, 0.28 Å, or the Au(1) atom in I, 0.10 Å.

The Au(1) and Au(3) atoms have a unsymmetrical planar three-fold coordination (P, C, Au), the sums of the bond angles at Au(1) and Au(3) are 360.0° and 359.0°, respectively. Contrary to IV where the Au(2) atom has a planar four-fold coordination, the four-fold coordination of the Au(2) atom in I is distinctly nonplanar. In fact, although the sum of the four angles, i.e. Au(1)—Au(2)—P(2), P(2)—Au(2)—Au(3), Au(3)—Au(2)—C(2) and C(2)—Au(2)—Au(1), is 359.8°, the P(2) and C(2) atoms are displaced from the Au(1)Au(2)Au(3) plane in opposite directions (Table 3), so that the sum of the three angles, Au(1)—Au(2)—P(2), Au(3)—Au(2)—P(2) and Au(1)—Au(2)—Au(3), is only 344.9°.

The triphenylphosphine ligands in I have a usual structure, viz. the P—C(Ph) bond lengths vary in the range 1.78 to 1.84(2) Å, and the bond angles Au—P—C(Ph) within 109.3—114.8(6)°. All the Ph cycles are planar, the maximum deviation of the carbon atoms from the least-squares plane of the corresponding ring does not exceed 0.02 Å and the C(Ph)—C(Ph) bond lengths vary within 1.33—1.45(3) Å. The BF_4^- anion has the usual tetrahedral configuration with B—F bond lengths of 1.36—1.38(3) Å. The crystals of I are built up of discrete $[Ph_3PAu)_3C_5Ph_4]^+$ and $[BF_4]^-$ ions and solvating benzene molecules. The interionic and intermolecular contacts correspond to normal Van der Waals interactions.

Experimental

The crystals of I are triclinic, at —120°C a = 12.845(6), b = 16.042(8), c = 22.642(11) Å, α = 86.02(4), β = 77.51(4), γ = 76.05(4)°, V = 4429(4) Å^3, M = 1988, Z = 2, $d_{calcd.}$ = 1.499 g/cm^3, space group $P\bar{1}$. The lattice parameters and intensities of 12 799 independent reflections (of which 9494 with $I > 2\sigma$ were used in calculations) were measured with a four-circle automatic Syntex P2$_1$ diffractometer at —120°C (λ(Mo-K_α, graphite monochromator, $\theta/2\theta$ scan, $2\theta \leqslant$ 46°). Absorption corrections, taking into account the form of the crystal, were applied according to the method given in ref. 9. The structure was solved by the heavy-atom method and refined by a block-diagonal least-squares technique in an anisotropic approximation. The difference Fourier map revealed two solvating benzene molecules, one of which was disordered over two positions. The

TABLE 4

ATOMIC COORDINATES MULTIPLIED BY 10^3 (for Au by 10^5, for P by 10^4)

Atom	x	y	z
Au(1)	18324(5)	66138(5)	72607(3)
Au(2)	−6156(5)	69799(4)	77268(3)
Au(3)	−14762(5)	80346(4)	68150(3)
P(1)	2828(3)	5683(3)	7836(2)
P(2)	−1522(3)	6901(3)	8714(2)
P(3)	−3013(3)	9058(3)	6724(2)
C(1)	105(1)	751(1)	661(1)
C(11) [a]	99(1)	841(1)	672(1)
C(12)	75(1)	870(1)	733(1)
C(13)	64(1)	956(1)	743(1)
C(14)	78(1)	1016(1)	696(1)
C(15)	103(1)	987(1)	637(1)
C(16)	115(1)	899(1)	625(1)
C(2)	3(1)	715(2)	678(1)
C(3)	27(1)	638(1)	643(1)
C(31)	−41(1)	571(1)	656(1)
C(32)	8(1)	486(1)	664(1)
C(33)	−54(1)	425(1)	681(1)
C(34)	−167(2)	449(1)	689(1)
C(35)	−218(2)	535(1)	681(1)
C(36)	−155(1)	597(1)	664(1)
C(4)	129(1)	630(1)	604(1)
C(41)	183(1)	557(1)	562(1)
C(42)	127(1)	527(1)	524(1)
C(43)	180(2)	459(1)	485(1)
C(44)	288(1)	416(1)	486(1)
C(45)	343(1)	444(1)	524(1)
C(46)	292(1)	513(1)	561(1)
C(5)	176(1)	697(1)	613(1)
C(51)	276(1)	719(1)	574(1)
C(52)	290(2)	713(1)	510(1)
C(53)	385(1)	733(1)	473(1)
C(54)	459(1)	758(1)	497(1)
C(55)	449(2)	763(1)	560(1)
C(56)	351(1)	745(1)	597(1)
C(111)	211(1)	488(1)	820(1)
C(112)	242(2)	437(1)	868(1)
C(113)	191(2)	371(1)	891(1)
C(114)	106(2)	359(1)	867(1)
C(115)	72(2)	410(1)	820(1)
C(116)	125(1)	477(1)	797(1)
C(121)	407(1)	508(1)	737(1)
C(122)	443(1)	542(1)	679(1)
C(123)	536(1)	495(1)	640(1)
C(124)	591(2)	415(2)	658(1)
C(125)	556(2)	380(1)	716(1)
C(126)	463(1)	428(1)	754(1)
C(131)	323(1)	618(1)	842(1)
C(132)	251(1)	691(1)	870(1)
C(133)	276(2)	730(1)	916(1)
C(134)	373(2)	699(1)	935(1)
C(135)	444(2)	625(1)	909(1)
C(136)	420(2)	584(1)	862(1)
C(211)	−258(1)	784(1)	888(1)
C(212)	−244(2)	863(1)	859(1)
C(213)	−320(2)	940(1)	873(1)
C(214)	−417(2)	943(2)	916(1)
C(215)	−431(2)	864(1)	946(1)

TABLE 4 (continued)

Atom	x	y	z
C(216)	−356(2)	789(1)	932(1)
C(221)	−65(1)	681(1)	927(1)
C(222)	−1(1)	602(1)	936(1)
C(223)	69(1)	596(1)	978(1)
C(224)	70(1)	668(1)	1007(1)
C(225)	6(2)	747(1)	997(1)
C(226)	−68(2)	756(1)	956(1)
C(231)	−216(1)	598(1)	888(1)
C(232)	−253(1)	575(1)	948(1)
C(232)	−304(1)	505(1)	960(1)
C(234)	−315(2)	460(1)	913(1)
C(235)	−278(2)	483(1)	853(1)
C(236)	−226(1)	554(1)	840(1)
C(311)	−307(1)	933(1)	595(1)
C(312)	−308(2)	865(1)	559(1)
C(313)	−318(2)	880(2)	497(1)
C(314)	−324(2)	961(2)	474(1)
C(315)	−319(2)	1027(2)	508(1)
C(316)	−312(2)	1014(1)	569(1)
C(321)	−309(1)	1004(1)	709(1)
C(322)	−407(2)	1060(2)	731(1)
C(323)	−408(2)	1136(1)	761(1)
C(324)	−314(1)	1151(1)	772(1)
C(325)	−215(1)	1092(1)	749(1)
C(326)	−209(1)	1019(1)	720(1)
C(331)	−428(1)	874(1)	703(1)
C(332) ·	−522(1)	911(1)	681(1)
C(333)	−622(1)	884(1)	704(1)
C(334)	−623(2)	823(1)	750(1)
C(335)	−529(1)	786(2)	773(1)
C(336)	−431(2)	814(1)	750(1)
B	494(2)	711(2)	96(1)
F(1)	425(1)	678(1)	141(1)
F(2)	435(1)	773(1)	65(1)
F(3)	558(1)	740(1)	127(1)
F(4)	553(1)	646(1)	58(1)
C(1')	106(2)	842(2)	412(1)
C(2')	58(2)	878(1)	469(1)
C(3')	−8(2)	835(2)	511(1)
C(4')	27(2)	240(2)	504(1)
C(5')	22(2)	723(2)	439(1)
C(6')	89(2)	766(2)	397(1)
C(7') [a]	294(3)	320(2)	674(2)
C(8') [a]	236(2)	290(2)	637(1)
C(9') [a]	222(2)	204(3)	650(1)
C(10') [a]	255(2)	160(2)	696(2)
C(11') [a]	307(3)	194(3)	735(2)
C(12') [a]	319(3)	279(2)	723(2)
C(13') [a]	268(3)	49(3)	961(2)
C(14') [a]	290(3)	107(3)	931(2)
C(15') [a]	327(3)	93(3)	874(2)
C(16') [a]	332(3)	18(3)	849(2)
C(17') [a]	295(4)	952(3)	881(2)
C(18') [a]	273(6)	965(3)	941(2)

[a] The first figure of the phenyl carbon atom number is the number of the P or C(Cp) atom bonded to the corresponding Ph group. Primed number correspond to C atoms of benzene molecules. Atoms C(7)—C(12) and C(13)—C(18) represent two positions of the disordered benzene molecule and were included in the refinement with a half weight (see Experimental).

H atoms were placed in the calculated positions and included in the refinement with fixed positional and isotropic thermal parameters ($B_{iso} = 5.0$ Å^2). Finally, $R = 0.054$, $R_w = 0.070$. All calculations were performed with an Eclipse S/200 computer using the modified EXTL programs *. The atomic coordinates are listed in Table 4 **.

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* Modifications were made in our laboratory by A.I. Yanovsky and R.G. Gerr.
** Table of anisotropic temperature parameters and the structure factors file can be obtained from the authors.