

The Crystal and Molecular Structure of Bis(triphenylphosphine)-[2-3- η -(1,4-benzoquinone)]platinum(0)

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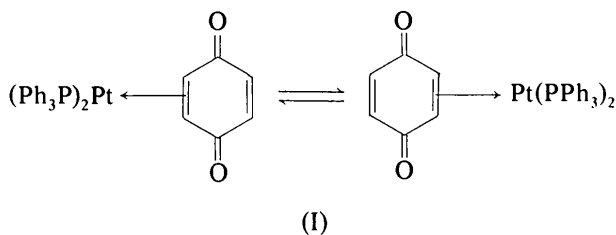
(Received 16 April 1977; accepted 21 May 1977)

$C_{42}H_{34}O_2P_2Pt$ is monoclinic, space group $P2_1/n$, with $a = 11.83$ (2), $b = 20.62$ (4), $c = 14.09$ (3) Å, $\beta = 92.7$ (1)°, $Z = 4$. The structure was refined to $R = 0.090$ for 2507 visually measured reflexions. The benzoquinone molecule acts as a mono-olefinic ligand to the Pt, which is bonded to the two P atoms [Pt–P 2.232 (8), 2.286 (9) Å] and two olefinic C atoms [Pt–C 2.11 (3) Å] of one side of the quinone molecule in a distorted square-planar arrangement. The coordinated olefinic bond length is 1.49 (4) Å [compared with the free olefinic value of 1.30 (5) Å] indicating that it is largely of single-bond character. The quinone ring adopts an irregular boat conformation with the carbonyl C atoms bent away from Pt by 16 and 11° and the C=O bonds bent back 6 and 4° towards Pt. The metal–olefin bond is at 92° to the plane containing the four olefinic C atoms; there is a small twist (11°) about this bond. There are no unusual intermolecular contacts, although small distortions in the triphenylphosphine groups due to crystal packing occur.

Introduction

Several examples of transition-metal complexes of 1,4-benzoquinones have been described and some have been structurally characterized. The quinone appears to act as a strong π acid of bidentate function, although the stabilities of the adducts are greatly dependent on the nature of any substituents in the ring (Fischer & Werner, 1966).

Cenini, Ugo & LaMonica (1971) isolated a series of bis(triphenylphosphine)platinum(0) complexes of substituted 1,2- and 1,4-benzoquinones. They noted several different bonding modes to the Pt atom with different ring substituents, although from NMR data a bidentate function was assigned to the unsubstituted quinone complex. In a separate study, Johnson, Nyholm & Vagg (1977) noticed that the temperature-dependent NMR spectrum of the title complex indicated the existence of the exchange process (I) in solution.



In the solid state, therefore, both fluxional isomers may be expected to exist. This structure determination was undertaken to confirm the monofunctional nature of benzoquinone in this complex.

Experimental

The complex was prepared by the reaction of tetrakis(triphenylphosphine)platinum(0) with 1,4-benzoquinone in a stoichiometric ratio in tetrahydrofuran under reflux for 3 h. After solvent removal the product was recrystallized from chloroform/benzene to yield thick golden-orange plates.

Crystal data

$C_{42}H_{34}O_2P_2Pt$, $M_r = 827.8$, monoclinic, $a = 11.83$ (2), $b = 20.62$ (4), $c = 14.09$ (3) Å, $\beta = 92.7$ (1)°, $U = 3433.2$ Å³, $D_m = 1.59$ (by flotation), $D_c = 1.602$ g cm⁻³, $Z = 4$, $F(000) = 1240$, $\mu(\text{Mo } K\alpha) = 4.43$ cm⁻¹. Systematic absences: $0k0$ when $k = 2n + 1$, $h0l$ when $h + l = 2n + 1$; space group $P2_1/n$.

Cell parameters were determined from precession photographs with Mo $K\alpha$ radiation. Intensities were measured visually from precession photographs for the layers 0–5 about [100], 0–4 about [010] and 0–6 about [001]. Data were corrected for Lorentz and polarization but not for absorption or extinction. 3680 non-zero reflexions were recorded which, after internal correlation, yielded 2507 unique reflexions.

Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). All calculations were carried out on a Univac 1106 computer with programs written by F. S. Stephens.

Structure determination

The structure was solved by the heavy-atom method and refined by full-matrix least squares in which the

Table 1. *Final atomic coordinates (fractional, $\times 10^4$ for nonhydrogen atoms, $\times 10^3$ for hydrogen atoms) and isotropic thermal parameters (\AA^2) with estimated standard deviations in parentheses*For all H atoms $B = 6.0 \text{\AA}^2$.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i>		<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i>
Pt	2121 (1)	574 (1)	1516 (1)		C(231)	1269 (23)	1549 (13)	3374 (21)	2.8 (5)
P(1)	2026 (6)	-498 (4)	1723 (6)		C(232)	761 (27)	1541 (15)	4279 (24)	3.9 (6)
P(2)	2313 (6)	962 (4)	3035 (6)		C(233)	-80 (32)	1966 (19)	4440 (28)	5.4 (8)
C(1)	2188 (26)	751 (15)	46 (23)	3.7 (6)	C(234)	-449 (28)	2408 (17)	3779 (26)	4.7 (7)
C(2)	2076 (25)	1369 (15)	576 (22)	3.5 (6)	C(235)	8 (33)	2439 (20)	2841 (29)	5.7 (9)
C(3)	3105 (25)	1728 (16)	725 (22)	3.6 (6)	C(236)	895 (31)	1985 (19)	2726 (28)	5.3 (8)
C(4)	4218 (31)	1403 (19)	555 (28)	5.3 (8)	H(1)	152	46	-7	
C(5)	4280 (25)	848 (16)	119 (23)	3.7 (6)	H(2)	133	154	81	
C(6)	3235 (26)	529 (16)	-312 (23)	3.8 (6)	H(4)	499	157	75	
O(3)	3142 (25)	2320 (15)	1076 (23)	7.9 (8)	H(5)	507	68	11	
O(6)	3337 (22)	87 (13)	-840 (20)	6.2 (6)	H(112)	-23	11	203	
C(111)	725 (25)	-812 (15)	2197 (23)	3.6 (6)	H(113)	-155	-17	254	
C(112)	-264 (24)	-413 (14)	2208 (22)	3.2 (6)	H(114)	-219	-132	296	
C(113)	-1174 (34)	-615 (20)	2565 (30)	5.8 (9)	H(115)	-59	-208	309	
C(114)	-1342 (30)	-1229 (18)	2845 (27)	5.0 (8)	H(116)	127	-174	238	
C(115)	-493 (27)	-1652 (16)	2807 (24)	4.2 (7)	H(122)	243	-134	348	
C(116)	597 (24)	-1439 (15)	2491 (22)	3.3 (6)	H(123)	390	-162	440	
C(121)	3200 (22)	-799 (13)	2436 (21)	2.7 (5)	H(124)	586	-129	400	
C(122)	3201 (28)	-1168 (17)	3288 (25)	4.4 (7)	H(125)	609	-65	242	
C(123)	4101 (33)	-1355 (20)	3764 (30)	5.7 (9)	H(126)	437	-23	166	
C(124)	5174 (30)	-1152 (18)	3493 (28)	5.1 (8)	H(132)	64	-52	5	
C(125)	5272 (28)	-776 (16)	2737 (25)	4.3 (7)	H(133)	64	-121	-156	
C(126)	4265 (28)	-608 (17)	2165 (25)	4.4 (7)	H(134)	187	-203	-159	
C(131)	2075 (23)	-977 (14)	682 (20)	2.9 (5)	H(135)	331	-227	-41	
C(132)	1192 (32)	-874 (19)	-82 (28)	5.4 (8)	H(136)	330	-157	112	
C(133)	1156 (31)	-1254 (19)	-973 (28)	5.5 (8)	H(212)	399	49	435	
C(134)	1940 (32)	-1752 (20)	-1018 (28)	5.6 (8)	H(213)	394	-26	577	
C(135)	2765 (28)	-1892 (16)	-286 (25)	4.4 (7)	H(214)	223	-82	609	
C(136)	2812 (22)	-1502 (13)	523 (20)	2.8 (5)	H(215)	65	-66	507	
C(211)	2317 (21)	401 (12)	4056 (19)	2.3 (5)	H(216)	67	9	368	
C(212)	3271 (22)	270 (14)	4613 (20)	2.8 (5)	H(222)	305	214	410	
C(213)	3287 (28)	-182 (17)	5347 (26)	4.4 (7)	H(223)	487	257	453	
C(214)	2286 (27)	-499 (15)	5555 (24)	4.0 (6)	H(224)	661	215	372	
C(215)	1342 (28)	-394 (17)	4941 (26)	4.5 (7)	H(225)	636	130	266	
C(216)	1400 (27)	36 (16)	4178 (25)	4.3 (7)	H(226)	450	70	242	
C(221)	3686 (25)	1345 (15)	3252 (23)	3.7 (6)	H(232)	106	122	477	
C(222)	3772 (33)	1926 (19)	3845 (30)	5.7 (9)	H(233)	-50	198	510	
C(223)	4786 (34)	2224 (21)	4055 (30)	6.4 (9)	H(234)	-112	274	391	
C(224)	5782 (33)	1968 (19)	3621 (30)	5.6 (9)	H(235)	-28	274	240	
C(225)	5662 (31)	1483 (18)	2996 (28)	5.2 (8)	H(236)	130	197	207	
C(226)	4604 (25)	1149 (15)	2801 (23)	3.7 (6)					

function minimized was $\Sigma w\Delta^2$. Weights $w = (1.00 + 0.03|F_o| + 0.0002|F_o|^2)^{-1}$ were used. Reflexions for which $|F_o| < 0.33|F_c|$ were omitted from the refinement.

Positions for all H atoms on the phenyl and quinone rings were calculated assuming trigonal C atoms. They were included in subsequent calculations with $B = 6.0 \text{\AA}^2$ but were not refined. Anisotropic thermal parameters for the Pt and P atoms were introduced and refinement terminated when the maximum shift in any parameter was $< 0.1\sigma$. The final R , based on all 2507 reflexions, was 0.090 and $R' [= (\Sigma w\Delta^2 / \Sigma w|F_o|^2)^{1/2}]$ was 0.122; 2505 reflexions were included in the final

cycle. A final difference synthesis showed no unusual features. Atomic parameters are given in Table 1.*

Discussion

Bond distances and angles are given in Table 2. Fig. 1 shows a drawing of the molecule and the labelling of the

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32791 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2. Bond lengths (\AA) and angles ($^\circ$) with estimated standard deviations in parentheses

Pt—P(1)	2.232 (8)	Pt—P(2)	2.286 (9)	C(1)—C(6)—C(5)	115 (3)	C(2)—C(3)—C(4)	119 (3)
Pt—C(1)	2.11 (3)	Pt—C(2)	2.11 (3)	C(4)—C(5)—C(6)	121 (3)	C(3)—C(4)—C(5)	122 (3)
O(3)—C(3)	1.32 (4)	O(6)—C(6)	1.19 (4)	O(3)—C(3)—C(2)	123 (3)	O(6)—C(6)—C(1)	126 (3)
C(1)—C(2)	1.49 (4)	C(4)—C(5)	1.30 (5)	O(3)—C(3)—C(4)	117 (3)	O(6)—C(6)—C(5)	119 (3)
C(2)—C(3)	1.43 (4)	C(6)—C(1)	1.43 (4)	Pt—P(1)—C(111)	117 (1)	Pt—P(2)—C(211)	120 (1)
C(3)—C(4)	1.51 (4)	C(5)—C(6)	1.50 (4)	Pt—P(1)—C(121)	112 (1)	Pt—P(2)—C(221)	111 (1)
P(1)—C(111)	1.82 (3)	P(2)—C(211)	1.85 (3)	Pt—P(1)—C(131)	116 (1)	Pt—P(2)—C(231)	116 (1)
P(1)—C(121)	1.79 (3)	P(2)—C(221)	1.82 (3)	C(111)—P(1)—C(121)	109 (1)	C(211)—P(2)—C(221)	100 (1)
P(1)—C(131)	1.77 (3)	P(2)—C(231)	1.81 (3)	C(111)—P(1)—C(131)	100 (1)	C(211)—P(2)—C(231)	111 (1)
C(111)—C(112)	1.43 (4)	C(211)—C(212)	1.37 (3)	C(121)—P(1)—C(131)	103 (1)	C(221)—P(2)—C(231)	106 (1)
C(112)—C(113)	1.28 (5)	C(212)—C(213)	1.39 (4)	P(1)—C(111)—C(112)	120 (2)	P(2)—C(211)—C(212)	123 (2)
C(113)—C(114)	1.34 (5)	C(213)—C(214)	1.40 (4)	P(1)—C(111)—C(116)	124 (2)	P(2)—C(211)—C(216)	119 (2)
C(114)—C(115)	1.33 (4)	C(214)—C(215)	1.40 (4)	P(1)—C(121)—C(122)	129 (2)	P(2)—C(221)—C(222)	119 (2)
C(115)—C(116)	1.45 (4)	C(215)—C(216)	1.40 (5)	P(1)—C(121)—C(126)	116 (2)	P(2)—C(221)—C(226)	122 (2)
C(116)—C(111)	1.37 (4)	C(216)—C(211)	1.34 (4)	P(1)—C(131)—C(132)	118 (2)	P(2)—C(231)—C(232)	123 (2)
C(121)—C(122)	1.42 (4)	C(221)—C(222)	1.46 (5)	P(1)—C(131)—C(136)	127 (2)	P(2)—C(231)—C(236)	118 (2)
C(122)—C(123)	1.29 (4)	C(222)—C(223)	1.37 (5)	C(116)—C(111)—C(112)	116 (3)	C(216)—C(211)—C(212)	118 (3)
C(123)—C(124)	1.41 (5)	C(223)—C(224)	1.45 (5)	C(111)—C(112)—C(113)	121 (3)	C(211)—C(212)—C(213)	123 (3)
C(124)—C(125)	1.33 (5)	C(224)—C(225)	1.34 (5)	C(112)—C(113)—C(114)	124 (4)	C(212)—C(213)—C(214)	119 (3)
C(125)—C(126)	1.45 (4)	C(225)—C(226)	1.44 (4)	C(113)—C(114)—C(115)	119 (4)	C(213)—C(214)—C(215)	117 (3)
C(126)—C(121)	1.39 (4)	C(226)—C(221)	1.35 (4)	C(114)—C(115)—C(116)	120 (3)	C(214)—C(215)—C(216)	121 (3)
C(131)—C(132)	1.48 (5)	C(231)—C(232)	1.44 (4)	C(115)—C(116)—C(111)	119 (3)	C(215)—C(216)—C(211)	122 (3)
C(132)—C(133)	1.48 (5)	C(232)—C(233)	1.35 (4)	C(126)—C(121)—C(122)	115 (3)	C(226)—C(221)—C(222)	119 (3)
C(133)—C(134)	1.39 (5)	C(233)—C(234)	1.36 (5)	C(121)—C(122)—C(123)	124 (3)	C(221)—C(222)—C(223)	122 (4)
C(134)—C(135)	1.42 (5)	C(234)—C(235)	1.45 (5)	C(122)—C(123)—C(124)	120 (4)	C(222)—C(223)—C(224)	118 (3)
C(135)—C(136)	1.39 (4)	C(235)—C(236)	1.42 (5)	C(123)—C(124)—C(125)	120 (3)	C(223)—C(224)—C(225)	119 (3)
C(136)—C(131)	1.41 (4)	C(236)—C(231)	1.34 (4)	C(124)—C(125)—C(126)	119 (3)	C(224)—C(225)—C(226)	123 (3)
				C(125)—C(126)—C(121)	121 (3)	C(225)—C(226)—C(221)	119 (3)
				C(136)—C(131)—C(132)	114 (3)	C(236)—C(231)—C(232)	118 (3)
				C(131)—C(132)—C(133)	122 (3)	C(231)—C(232)—C(233)	119 (3)
				C(132)—C(133)—C(134)	116 (3)	C(232)—C(233)—C(234)	122 (4)
				C(133)—C(134)—C(135)	124 (4)	C(233)—C(234)—C(235)	122 (3)
				C(134)—C(135)—C(136)	119 (3)	C(234)—C(235)—C(236)	113 (4)
				C(135)—C(136)—C(131)	125 (3)	C(235)—C(236)—C(231)	125 (4)
P(1)—Pt—P(2)	103.2 (3)	C(1)—Pt—C(2)	41.3 (12)				
P(1)—Pt—C(1)	107.7 (9)	P(2)—Pt—C(2)	108.3 (9)				
Pt—C(1)—C(2)	69 (2)	Pt—C(2)—C(1)	69 (2)				
Pt—C(1)—C(6)	111 (2)	Pt—C(2)—C(3)	108 (2)				
C(2)—C(1)—C(6)	123 (3)	C(1)—C(2)—C(3)	115 (3)				

atoms (Johnson, 1965). Fig. 2 shows the packing viewed down **a**.

The Pt atom is bonded to the two P atoms and two olefinic C atoms of one side of the quinone molecule in

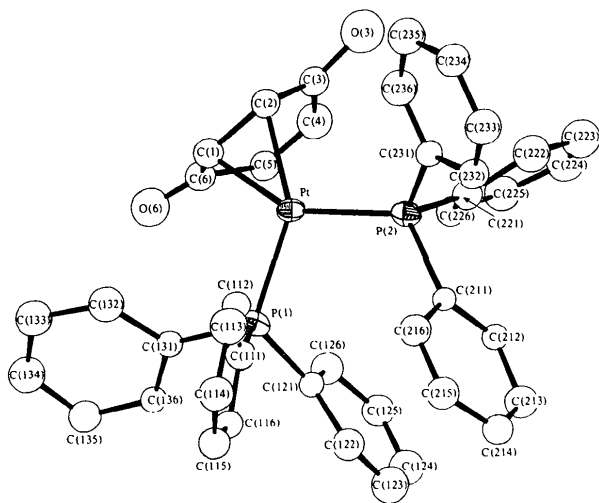


Fig. 1. Perspective drawing of the molecule showing the labelling of the atoms. Thermal ellipsoids are scaled to include 35% probability.

a distorted square-planar arrangement (Table 3, plane 1). The benzoquinone acts, therefore, as a mono-olefinic ligand, as was suggested by NMR data (Johnson, Nyholm & Vagg, 1977). There is a small but significant difference in the two Pt—P lengths [Pt—P(1) 2.232 (8), Pt—P(2) 2.286 (9) \AA] but the two Pt—C bonds are equivalent [Pt—C 2.11 (3) \AA]. These values are very similar to lengths in other bis(triphenylphosphine)platinum(0) compounds (Ittel & Ibers, 1976).

This is the first structural example of an unsubstituted 1,4-benzoquinone–metal complex, although substituted quinone complexes of Ni (Glick & Dahl, 1965; Aleksandrov & Struchkov, 1973), Co (Uchtmann & Dahl, 1972), Ir (Aleksandrov & Struchkov, 1971*b*) and Rh (Aleksandrov & Struchkov, 1969, 1970*a,b*, 1971*a*) have been characterized. In each of these latter structures the substituted quinone acts as a di-olefinic ligand, adopting a boat conformation. The carbonyl C(3) and C(6) atoms are bent back away from the plane containing the four olefinic C atoms (Table 3, planes 2, 3 and 4) by 16 and 11 $^\circ$, with C(3)—O(3) and C(6)—O(6) bent back 6 and 4 $^\circ$ respectively towards Pt. This form of angular distortion is

Table 3. *Least-squares planes*

Equations are given by $lX' + mY' + nZ' - p = 0$, where X' , Y' and Z' are orthogonal coordinates related to the atomic coordinates X , Y and Z by $X' = X \sin \beta$, $Y' = Y$, and $Z' = Z + X \cos \beta$. Deviations (Å) from the planes are given in square brackets.

	<i>l</i>	<i>m</i>	<i>n</i>	<i>p</i>
Plane 1: Pt, P(1), P(2), C(1), C(2) [Pt -0.03; P(1) -0.04; P(2) 0.06; C(1) 0.13; C(2) -0.12]	0.9976	-0.0500	-0.0470	2.3745
Plane 2: C(2), C(3), C(4) [O(3) -0.10]	-0.0623	0.3055	-0.9501	0.0534
Plane 3: C(1), C(5), C(6) [O(6) -0.12]	-0.0617	0.7060	-0.7055	0.9734
Plane 4: C(1), C(2), C(4), C(5) [O(3) 0.31; O(6) 0.41; C(3) 0.15; C(6) 0.21; C(1), C(4) 0.01; C(2), C(5) -0.01]	-0.0539	0.4883	-0.8710	0.6558
Plane 5: Pt, P(1), P(2) [C(1) 0.23; C(2) -0.06]	0.9946	-0.0617	-0.0829	2.2529
Plane 6: Pt, C(1), C(2) [P(1) -0.28; P(2) 0.40]	0.9951	0.0836	0.0520	2.6983
Plane 7: C(1)-C(3), C(6) [C(1) -0.009; C(2) 0.009; C(3) -0.004; C(6) 0.005; O(3) 0.161; O(6) 0.173]	-0.1956	0.4896	-0.8497	0.3100
Plane 8: C(111), C(131), C(121)	-0.0019	-0.9884	0.1517	2.1155
Plane 9: C(211), C(221), C(231)	0.1580	0.4221	0.8927	5.7669
Plane 10: C(111)-C(116) [C(111) 0.02; C(112) -0.04; C(113) 0.03; C(114) 0.004; C(115) -0.03; C(116) 0.01; P(1) -0.03]	0.2972	0.2695	0.9160	2.5844
Plane 11: C(121)-C(126) [C(121), C(124) -0.01; C(122), C(125) 0.03; C(123), C(126) -0.02; P(1) 0.08]	-0.0720	0.8275	0.5568	0.1846
Plane 12: C(131)-C(136) [C(131), C(133) -0.02; C(132) 0.03; C(134), C(136) -0.004; C(135) 0.02; P(1) 0.07]	-0.6278	-0.6296	0.4577	0.1346
Plane 13: C(211) C(216) [C(211) 0.05; C(212) -0.005; C(213) -0.04; C(214) 0.04; C(215) 0.003; C(216) -0.05; P(2) -0.009]	-0.2831	0.7262	0.6265	3.2733
Plane 14: C(221)-C(226) [C(221) 0.05; C(222), C(225) -0.04; C(223) -0.004; C(224) 0.04; C(226) -0.01; P(2) 0.05]	0.1953	-0.6189	0.7608	2.4162
Plane 15: C(231)-C(236) [C(231), C(232) -0.001; C(233) -0.005; C(234) 0.01; C(235) -0.01; C(236) 0.008; P(2) -0.14]	0.6767	0.6626	0.3210	4.6359

present in the quinone molecules of each of the previously reported structures.

Fig. 3 shows interatomic distances around Pt. The two planes defined by Pt, P(1) and P(2), and Pt, C(1) and C(2) (Table 3, planes 5 and 6) intersect at 11° , indicating a slight tetrahedral distortion and hence a corresponding twist around the metal-olefin bond. Again this phenomenon has been observed in d^{10} metal-olefin complexes (Ittel & Ibers, 1976; Hartley, 1972) and it has been suggested that such rotation may occur frequently, solely to lessen non-bonded contacts (Ittel & Ibers, 1976).

The long, coordinated 'olefinic' length of 1.49 (4) Å suggests that this bond is largely of single-bond

character. The remaining bond lengths and angles in the quinone differ little from those of the free molecule (Hagen & Hedberg, 1973). The plane of best fit of the four olefinic C atoms and the plane defined by Pt, C(1) and C(2) (Table 3, planes 4 and 6) intersect at 92° , indicating that the metal-olefin bond is approximately perpendicular to the quinone residue. However, the corresponding angle of intersection of this latter plane with the half of the ring defined by C(1), C(2), C(3) and C(6) (Table 3, plane 7) is 102° , a value similar to the torsion angles found in other d^{10} metal complexes of substituted mono-olefins (Ittel & Ibers, 1976).

A small 'pointing' effect (Ittel & Ibers, 1976) of the triphenylphosphine groups is evidenced by the 106.4°

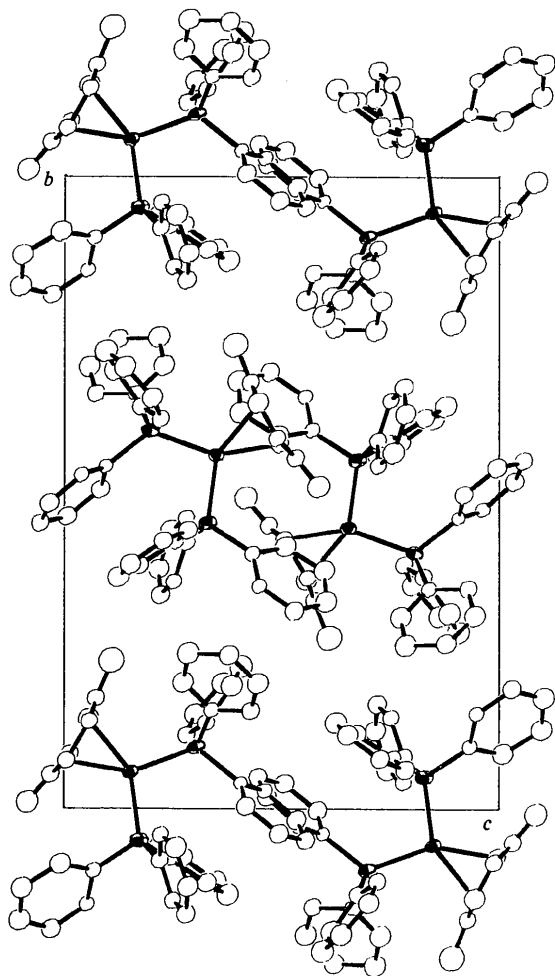


Fig. 2. Molecular packing in the crystal.

dihedral angle of the two α -carbon atom planes (Table 3, planes 8 and 9) compared with the P(1)—Pt—P(2) angle of 103.2 (3)°. This common effect most probably arises from non-bonded interactions between the triphenylphosphine groups. Indeed, although the six phenyl rings are planar (Table 3, planes 10–15) the respective P atoms sometimes show a marked deviation from the planes of these rings (Table 3, planes 11, 12 and 15). This effect would be attributable to crystal packing. There are no unusual intermolecular interactions; in particular, the benzoquinone molecule has no intermolecular contacts below 3.5 Å.

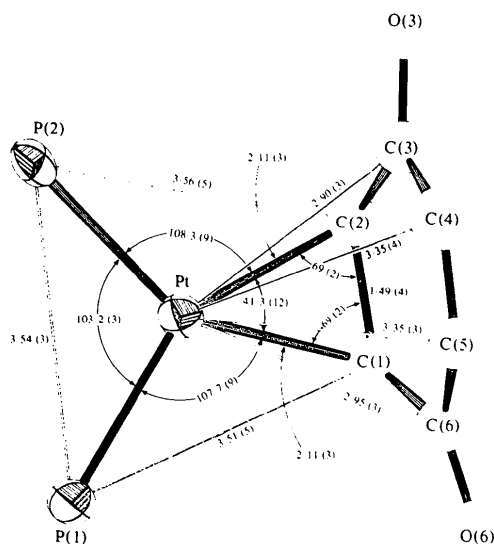


Fig. 3. Interatomic distances (Å) and angles (°) around the Pt atom.

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