

Table 2. Selected geometric parameters (\AA , $^\circ$)

Ir(1)—C(1)	1.78 (2)	C(15)—C(16)	1.530 (9)
Ir(1)—P(1)	2.345 (2)	C(21)—C(22)	1.519 (9)
Ir(1)—P(1 ⁱ)	2.345 (2)	C(21)—C(26)	1.529 (9)
Ir(1)—Cl(1)	2.398 (7)	C(22)—C(23)	1.521 (10)
P(1)—C(11)	1.847 (6)	C(23)—C(24)	1.518 (10)
P(1)—C(31)	1.853 (6)	C(24)—C(25)	1.523 (10)
P(1)—C(21)	1.856 (6)	C(25)—C(26)	1.530 (10)
O(1)—C(1)	1.10 (2)	C(31)—C(36)	1.516 (9)
C(11)—C(12)	1.520 (9)	C(31)—C(32)	1.540 (8)
C(11)—C(16)	1.531 (8)	C(32)—C(33)	1.512 (9)
C(12)—C(13)	1.529 (9)	C(33)—C(34)	1.519 (11)
C(13)—C(14)	1.520 (10)	C(34)—C(35)	1.497 (11)
C(14)—C(15)	1.506 (11)	C(35)—C(36)	1.529 (9)
C(1)—Ir(1)—P(1)	89.0 (6)	C(14)—C(15)—C(16)	111.2 (6)
C(1)—Ir(1)—P(1 ⁱ)	91.0 (6)	C(15)—C(16)—C(11)	110.4 (6)
P(1)—Ir(1)—P(1 ⁱ)	180.0	C(22)—C(21)—C(26)	110.2 (6)
C(1)—Ir(1)—Cl(1)	176.1 (7)	C(22)—C(21)—P(1)	114.2 (5)
P(1)—Ir(1)—Cl(1)	91.24 (13)	C(26)—C(21)—P(1)	110.5 (4)
P(1 ⁱ)—Ir(1)—Cl(1)	88.76 (13)	C(21)—C(22)—C(23)	111.2 (6)
C(11)—P(1)—C(31)	109.6 (3)	C(24)—C(23)—C(22)	111.2 (6)
C(11)—P(1)—C(21)	103.8 (3)	C(23)—C(24)—C(25)	110.0 (6)
C(31)—P(1)—C(21)	103.0 (3)	C(24)—C(25)—C(26)	110.7 (6)
C(11)—P(1)—Ir(1)	112.6 (2)	C(21)—C(26)—C(25)	111.6 (6)
C(31)—P(1)—Ir(1)	114.5 (2)	C(36)—C(31)—C(32)	109.5 (6)
C(21)—P(1)—Ir(1)	112.4 (2)	C(36)—C(31)—P(1)	113.9 (5)
O(1)—C(1)—Ir(1)	178.3 (15)	C(32)—C(31)—P(1)	118.7 (5)
C(12)—C(11)—C(16)	110.3 (6)	C(33)—C(32)—C(31)	110.9 (6)
C(12)—C(11)—P(1)	114.9 (4)	C(32)—C(33)—C(34)	111.5 (7)
C(16)—C(11)—P(1)	116.7 (5)	C(35)—C(34)—C(33)	111.1 (7)
C(11)—C(12)—C(13)	111.0 (6)	C(34)—C(35)—C(36)	112.6 (7)
C(14)—C(13)—C(12)	111.7 (6)	C(31)—C(36)—C(35)	111.1 (6)
C(15)—C(14)—C(13)	111.7 (6)		

Symmetry code: (i) $-x, -y, -z$.

The results of a ψ scan indicated that no correction for absorption was required. The position of the Ir atom was input for a *SHELXS86* (Sheldrick, 1990) tangential expansion (*TEXP*) using 135 E values greater than 1.5. The resulting difference map revealed the atomic positions for the chloride and tricyclohexylphosphine ligands. These atoms, including occupancies of 50% for the Ir and Cl atoms, were input into *SHELXL93* (Sheldrick, 1994). The C- and O-atom positions of the carbonyl group were determined, and the carbonyl group was assigned an occupancy of 50%. The Cl and carbonyl-group atoms were refined isotropically. All other non-H atoms were refined anisotropically. Idealized methine ($\text{C}—\text{H} = 0.98 \text{ \AA}$) and methylene ($\text{C}—\text{H} = 0.97 \text{ \AA}$) H atoms of the cyclohexyl groups were geometrically located then refined with fixed isotropic displacement parameters ($U = 0.05 \text{ \AA}^2$) using a riding model. Geometrical calculations were performed using *SHELXL93*. Data collection: *P2₁ Assembler Language Data Collection Programs* (Syntex, 1975). Data reduction: local program (Tipton, 1977). Molecular graphics: *ORTEP* (Johnson, 1965). Software used to prepare material for publication: *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances and angles involving non-H atoms have been deposited with the IUCr (Reference: BK1025). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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[1,1'-Bis(diphenylphosphino)ferrocene]-tetracarbonylmolybdenum

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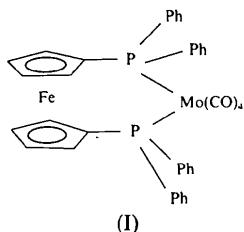
(Received 13 April 1992; accepted 15 December 1993)

Abstract

Two crystallographically independent but chemically similar molecules (*A* and *B*) form the asymmetric unit of tetracarbonyl-1 κ^4 C-bis[μ -1 κ P:2(η^5)-diphenylphosphinocyclopentadienyl]iron-molybdenum, [{(C₁₇H₁₄P)₂Fe}Mo(CO)₄]. The [bis(diphenylphosphino)ferrocene] ligand coordinates via the two P atoms, completing the *cis*-octahedral coordination of molybdenum. The carbonyl ligands *trans* to these phosphorus donors show the expected carbon–metal bond shortening. The ferrocene ligands have slightly non-parallel cyclopentadienyl rings, with staggered arrangements, and the P atoms are significantly elevated from the planes of the cyclopentadienyl rings.

Comment

The structure of the title complex (**I**) has been reported previously as its benzene solvate (Butler, Cullen, Kim, Rettig & Trotter, 1985). The title structure is of particular interest as the bond parameters



of the two independent molecules deviate significantly and in opposite directions from those of the benzene solvate structure. The angular displacement of the phosphino groups about the Cp(centroid)-metal-Cp(centroid) axis is 41.0° for the previous example; the two independent molecules in the title structure show variation: 50.3 (molecule *A*) and 35.2° (molecule *B*). The P···P distances are 3.880 (4) Å for *A* and 3.764 (4) Å for *B*, which may be compared to the value of 3.784 (3) Å in the previous report. Other

reported complexes involving 1,1'-disubstituted phosphinoferrocene ligands include nickel[1,1'-bis(diphenylphosphino)ferrocene](Cl)₂ and palladium[1,1'-bis(diphenylphosphino)ferrocene](Cl)₂ (Hor, Phang, Liu & Wen, 1990). The square-planar Pd complex and the Mo complexes contain staggered Cp rings in the ferrocene ligand, while the tetrahedral Ni complex has an eclipsed Cp ring orientation. All structures show non-parallel Cp rings with deviations from coplanarity of 6.2, 6.2 and 2.2° for the Ni, Pd and Mo (benzene solvate) complexes, respectively, and 2.8 (A) and 2.2° (B) for the title complex.

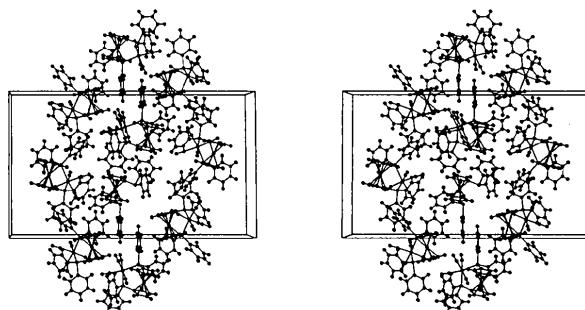


Fig. 2. Unit-cell packing diagram as viewed down the α axis.

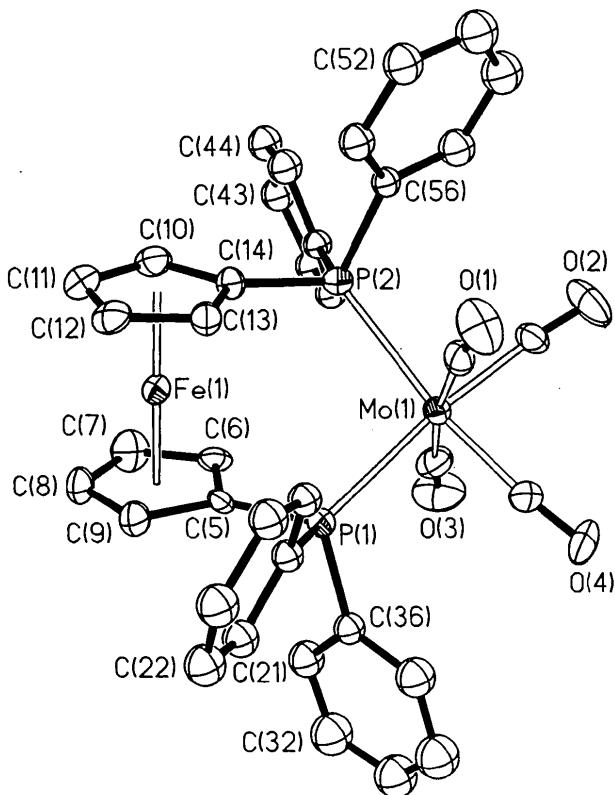


Fig. 1. The molecular structure of tetracarbonyl[bis(diphenylphosphino)ferrocene]molybdenum with the atom-labeling scheme.

Experimental

Crystals were obtained from the reaction of Mo(CO)₆ and bis(diphenylphosphino)ferrocene in dichloromethane/hexane (Hor & Phang, 1989).

Crystal data

[FeMo(C ₁₇ H ₁₄ P) ₂ (CO) ₄]	Mo $K\alpha$ radiation
$M_r = 762.3$	$\lambda = 0.71073 \text{ \AA}$
Monoclinic	Cell parameters from 25 reflections
$P2_1/n$	$\theta = 10-12.5^\circ$
$a = 9.373 (5) \text{ \AA}$	$\mu = 0.948 \text{ mm}^{-1}$
$b = 34.821 (18) \text{ \AA}$	$T = 295 \text{ K}$
$c = 20.434 (8) \text{ \AA}$	Block
$\beta = 92.60 (4)^\circ$	$0.42 \times 0.22 \times 0.18 \text{ mm}$
$V = 6662 (5) \text{ \AA}^3$	Yellow
$Z = 8$	
$D_x = 1.520 \text{ Mg m}^{-3}$	

Data collection

Siemens P4 diffractometer	$\theta_{\max} = 24^\circ$
Modified ω scans	$h = -10 \rightarrow 10$
Absorption correction:	$k = 0 \rightarrow 39$
empirical ellipsoidal	$l = 0 \rightarrow 23$
$T_{\min} = 0.854, T_{\max} = 0.999$	3 standard reflections monitored every 197 reflections
9907 measured reflections	intensity variation: <2%
9907 independent reflections	
5558 observed reflections	
$[F_o > 4\sigma(F_o)]$	

RefinementRefinement on F $R = 0.0567$ $wR = 0.0586$ $S = 1.15$

5558 reflections

589 parameters

H atoms

 $w = 1/(\sigma^2|F_o| + 0.0008F_o^2)$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.63 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

Atomic scattering factors
from *International Tables*
for X-ray Crystallography
(1974, Vol. IV)

C(4')	0.6859 (11)	0.2455 (3)	0.4233 (5)	0.043 (4)
C(5')	1.1516 (9)	0.1886 (3)	0.5014 (4)	0.028 (3)
C(6')	1.2871 (10)	0.2072 (3)	0.4922 (4)	0.034 (3)
C(7')	1.3967 (11)	0.1803 (3)	0.5048 (4)	0.041 (4)
C(8')	1.3314 (11)	0.1442 (3)	0.5206 (4)	0.038 (4)
C(9')	1.1843 (11)	0.1501 (3)	0.5195 (5)	0.040 (4)
C(10')	1.3464 (10)	0.1758 (3)	0.3420 (4)	0.039 (4)
C(11')	1.3745 (12)	0.1369 (3)	0.3581 (5)	0.046 (4)
C(12')	1.2404 (12)	0.1187 (3)	0.3635 (4)	0.044 (4)
C(13')	1.1301 (10)	0.1456 (2)	0.3535 (4)	0.031 (3)
C(14')	1.1978 (10)	0.1817 (2)	0.3392 (4)	0.027 (3)
C(21')	0.8706 (13)	0.2702 (3)	0.5676 (5)	0.060 (3)
C(22')	0.8697 (12)	0.2983 (3)	0.6170 (5)	0.055 (3)
C(23')	0.9876 (11)	0.3029 (3)	0.6554 (5)	0.053 (3)
C(24')	1.1049 (13)	0.2804 (3)	0.6498 (6)	0.066 (3)
C(25')	1.1033 (12)	0.2519 (3)	0.6009 (5)	0.055 (3)
C(26')	0.9870 (10)	0.2468 (3)	0.5583 (5)	0.037 (2)
C(31')	0.8296 (12)	0.1741 (3)	0.5915 (6)	0.061 (3)
C(32')	0.7529 (13)	0.1433 (4)	0.6171 (7)	0.077 (4)
C(33')	0.7115 (13)	0.1140 (4)	0.5793 (6)	0.072 (4)
C(34')	0.7436 (14)	0.1119 (4)	0.5157 (7)	0.086 (4)
C(35')	0.8226 (12)	0.1431 (3)	0.4883 (6)	0.061 (3)
C(36')	0.8670 (10)	0.1733 (3)	0.5277 (5)	0.038 (2)
C(41')	1.0260 (10)	0.1843 (3)	0.2077 (5)	0.042 (3)
C(42')	0.9885 (11)	0.1801 (3)	0.1405 (5)	0.056 (3)
C(43')	0.9776 (12)	0.2115 (3)	0.1003 (6)	0.059 (3)
C(44')	1.0058 (11)	0.2471 (3)	0.1262 (5)	0.054 (3)
C(45')	1.0444 (10)	0.2516 (3)	0.1921 (5)	0.043 (3)
C(46')	1.0554 (9)	0.2201 (2)	0.2333 (4)	0.029 (2)
C(51')	1.3329 (11)	0.2659 (3)	0.2735 (5)	0.046 (3)
C(52')	1.4374 (12)	0.2947 (3)	0.2763 (6)	0.064 (3)
C(53')	1.4465 (12)	0.3185 (3)	0.3286 (6)	0.061 (3)
C(54')	1.3558 (12)	0.3161 (3)	0.3793 (6)	0.060 (3)
C(55')	1.2508 (10)	0.2870 (3)	0.3763 (5)	0.040 (3)
C(56')	1.2397 (10)	0.2623 (3)	0.3239 (4)	0.034 (2)

Table 1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) U_{iso} for phenyl C atoms; $U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$ for others.

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}/U_{\text{eq}}$
Mo(1)	0.6939 (1)	0.0321 (1)	0.2506 (1)	0.030 (1)
Mo(1')	0.8752 (1)	0.2390 (1)	0.3837 (1)	0.032 (1)
Fe(1)	0.9996 (2)	-0.0538 (1)	0.1803 (1)	0.035 (1)
Fe(1')	1.2615 (1)	0.1630 (1)	0.4294 (1)	0.031 (1)
P(1)	0.7599 (3)	-0.0351 (1)	0.2930 (1)	0.030 (1)
P(2)	0.8527 (3)	0.0324 (1)	0.1499 (1)	0.030 (1)
P(1')	0.9761 (3)	0.2110 (1)	0.4927 (1)	0.031 (1)
P(2')	1.0981 (3)	0.2257 (1)	0.3215 (1)	0.029 (1)
O(1)	0.4320 (9)	0.0117 (2)	0.1529 (4)	0.069 (3)
O(2)	0.6051 (10)	0.1165 (2)	0.2224 (4)	0.081 (4)
O(3)	0.9083 (10)	0.0636 (2)	0.3622 (4)	0.081 (4)
O(4)	0.4572 (10)	0.0394 (3)	0.3519 (5)	0.100 (4)
O(1')	0.9303 (10)	0.3245 (2)	0.4307 (5)	0.090 (4)
O(2')	0.7587 (9)	0.2814 (3)	0.2578 (4)	0.086 (4)
O(3')	0.7391 (10)	0.1638 (3)	0.3233 (5)	0.104 (4)
O(4')	0.5773 (8)	0.2499 (2)	0.4440 (4)	0.069 (3)
C(1)	0.5309 (12)	0.0176 (3)	0.1869 (5)	0.041 (4)
C(2)	0.6416 (11)	0.0859 (3)	0.2302 (5)	0.042 (4)
C(3)	0.8369 (13)	0.0515 (3)	0.3205 (5)	0.049 (4)
C(4)	0.5480 (13)	0.0352 (3)	0.3163 (5)	0.053 (4)
C(5)	0.9356 (11)	-0.0515 (2)	0.2735 (4)	0.033 (3)
C(6)	1.0532 (10)	-0.0271 (3)	0.2661 (4)	0.038 (3)
C(7)	1.1694 (11)	-0.0501 (3)	0.2465 (5)	0.056 (4)
C(8)	1.1253 (11)	-0.0881 (3)	0.2417 (5)	0.045 (4)
C(9)	0.9807 (11)	-0.0898 (3)	0.2582 (5)	0.043 (4)
C(10)	1.0488 (11)	-0.0248 (3)	0.0979 (5)	0.047 (4)
C(11)	1.0448 (13)	-0.0646 (3)	0.0851 (5)	0.058 (5)
C(12)	0.9085 (12)	-0.0785 (3)	0.0971 (5)	0.047 (4)
C(13)	0.8257 (11)	-0.0472 (3)	0.1187 (4)	0.037 (3)
C(14)	0.9110 (10)	-0.0135 (3)	0.1194 (4)	0.032 (3)
C(21)	0.6641 (11)	-0.1107 (3)	0.3117 (5)	0.043 (3)
C(22)	0.5898 (11)	-0.1435 (3)	0.2948 (5)	0.053 (3)
C(23)	0.4990 (12)	-0.1436 (3)	0.2399 (5)	0.052 (3)
C(24)	0.4796 (11)	-0.1110 (3)	0.2022 (5)	0.046 (3)
C(25)	0.5535 (10)	-0.0776 (3)	0.2214 (4)	0.035 (2)
C(26)	0.6496 (10)	-0.0774 (3)	0.2739 (4)	0.033 (2)
C(31)	0.8980 (12)	-0.0412 (3)	0.4174 (5)	0.050 (3)
C(32)	0.9029 (14)	-0.0402 (3)	0.4871 (6)	0.071 (4)
C(33)	0.7806 (13)	-0.0357 (3)	0.5166 (6)	0.072 (4)
C(34)	0.6528 (14)	-0.0342 (3)	0.4857 (6)	0.071 (4)
C(35)	0.6455 (12)	-0.0338 (3)	0.4156 (5)	0.057 (3)
C(36)	0.7707 (10)	-0.0364 (3)	0.3823 (4)	0.036 (2)
C(41)	1.0912 (10)	0.0737 (3)	0.2014 (5)	0.038 (2)
C(42)	1.2209 (11)	0.0933 (3)	0.1965 (5)	0.048 (3)
C(43)	1.2783 (12)	0.0980 (3)	0.1360 (5)	0.049 (3)
C(44)	1.2043 (11)	0.0853 (3)	0.0804 (5)	0.049 (3)
C(45)	1.0739 (11)	0.0668 (3)	0.0849 (5)	0.046 (3)
C(46)	1.0172 (10)	0.0602 (3)	0.1456 (4)	0.032 (2)
C(51)	0.6842 (10)	0.0308 (3)	0.0316 (5)	0.043 (3)
C(52)	0.5951 (11)	0.0481 (3)	-0.0167 (5)	0.053 (3)
C(53)	0.5677 (12)	0.0867 (3)	-0.0160 (6)	0.061 (3)
C(54)	0.6323 (12)	0.1095 (3)	0.0306 (5)	0.062 (3)
C(55)	0.7213 (11)	0.0924 (3)	0.0795 (5)	0.048 (3)
C(56)	0.7469 (9)	0.0532 (3)	0.0802 (4)	0.030 (2)
C(1')	0.9214 (11)	0.2932 (3)	0.4151 (5)	0.044 (4)
C(2')	0.7998 (11)	0.2652 (3)	0.3036 (6)	0.054 (4)
C(3')	0.7940 (11)	0.1898 (3)	0.3465 (5)	0.051 (4)

Table 2. Selected geometric parameters (\AA , $^\circ$)*Cp* is the centroid of the cyclopentadienyl ring.

Mo(1)—P(1)	2.560 (3)	Mo(1')—P(1')	2.571 (3)
Mo(1)—P(2)	2.593 (3)	Mo(1')—P(2')	2.536 (3)
Mo(1)—C(1)	2.024 (11)	Mo(1')—C(1')	2.035 (11)
Mo(1)—C(2)	1.978 (10)	Mo(1')—C(2')	1.977 (11)
Mo(1)—C(3)	2.031 (11)	Mo(1')—C(3')	2.011 (11)
Mo(1)—C(4)	1.963 (11)	Mo(1')—C(4')	1.997 (10)
O(1)—C(1)	1.152 (13)	O(1')—C(1')	1.135 (13)
O(3)—C(3)	1.139 (14)	O(3')—C(3')	1.134 (15)
O(2)—C(2)	1.127 (12)	O(2')—C(2')	1.144 (14)
O(4)—C(4)	1.154 (15)	O(4')—C(4')	1.130 (13)
Fe(1)—Cp(1)	1.649 (9)	Fe(1')—Cp(1')	1.643 (9)
Fe(1)—Cp(2)	1.649 (9)	Fe(1')—Cp(2')	1.644 (9)
P(1)···P(2)	3.880 (4)	P(1')···P(2')	3.764 (4)
Cp(1)—Fe—Cp(2)	179.2 (4)	Cp(1')—Fe—Cp(2')	178.3 (4)
C(1)—Mo(1)—C(2)	85.9 (4)	C(1')—Mo(1')—C(2')	84.0 (5)
C(1)—Mo(1)—C(3)	171.8 (4)	C(1')—Mo(1')—C(3')	169.0 (4)
C(1)—Mo(1)—C(4)	85.7 (4)	C(1')—Mo(1')—C(4')	86.9 (4)
C(2)—Mo(1)—C(3)	88.8 (4)	C(2')—Mo(1')—C(3')	88.0 (5)
C(2)—Mo(1)—C(4)	85.3 (4)	C(2')—Mo(1')—C(4')	89.5 (4)
C(3)—Mo(1)—C(4)	87.6 (5)	C(3')—Mo(1')—C(4')	85.5 (4)
P(1)—Mo(1)—P(2)	97.7 (1)	P(1')—Mo(1')—P(2')	94.9 (1)
P(1)—Mo(1)—C(1)	98.9 (3)	P(1')—Mo(1')—C(1')	90.8 (3)
P(1)—Mo(1)—C(2)	172.3 (3)	P(1')—Mo(1')—C(2')	174.7 (4)
P(1)—Mo(1)—C(3)	85.7 (3)	P(1')—Mo(1')—C(3')	97.1 (3)
P(1)—Mo(1)—C(4)	89.1 (3)	P(1')—Mo(1')—C(4')	89.5 (3)
P(2)—Mo(1)—C(1)	86.3 (3)	P(2')—Mo(1')—C(1')	99.2 (3)
P(2)—Mo(1)—C(2)	88.6 (3)	P(2')—Mo(1')—C(2')	86.6 (3)
P(2)—Mo(1)—C(3)	99.9 (3)	P(2')—Mo(1')—C(3')	87.8 (3)
P(2)—Mo(1)—C(4)	170.2 (3)	P(2')—Mo(1')—C(4')	172.4 (3)

The structure was solved by direct methods (*TREF* in *SHELXTL-PC*; Sheldrick, 1990). All non-H atoms, except for the phenyl C atoms, were refined anisotropically. Phenyl rings were constrained as rigid planar groups. H atoms were included as idealized contributions ($\text{C}—\text{H} = 0.96 \text{ \AA}$).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HH1018). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Chloro[*o*-(diphenylphosphino)benzaldehyde]-{*N*-[*o*-(diphenylphosphino)benzylidene]ethylamine}(tetrachloro-*o*-catecholato)iridium(III)

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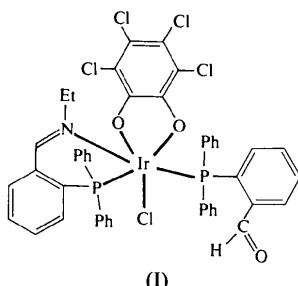
Abstract

The title structure, chloro{2-(diphenylphosphino)-benzaldehyde-*P*}[*N*-{2-(diphenylphosphino)benzylidene}ethylamine-*N,P*](3,4,5,6-tetrachloro-1,2-benzenediolato-*O,O'*)iridium butanol hemisolvate, [IrCl(C₆Cl₄O₂)(C₁₉H₁₅OP)(C₂₁H₂₀NP)]·0.5C₄H₁₀O, consists of two independent molecules in the asymmetric unit with an Ir^{III} metal atom pseudo octahedrally coordinated by the following donors: two catecholate O atoms, one Cl[−] anion, two phosphine groups and one imino group.

Comment

In the course of our studies on transition metal complexes with *o*-quinoid ligands (Bianchini, Masi, Mealli, Meli, Martini, Laschi & Zanello, 1987; Barbaro, Bianchini, Linn, Mealli, Meli, Laschi & Zanello, 1992; Bianchini, Frediani, Laschi, Meli, Vizza & Zanello, 1990), we have found that the square-planar complex [(NPet)₂Ir]Cl (Barbaro, Bianchini, Laschie, Midollini, Moneti, Scapacci &

Zanello, 1994) [NPet = {*o*-(diphenylphosphino)benzylidene}ethylamino] reacts in acetone with a stoichiometric amount of tetrachloro-*o*-quinone (TCIQ) to give the title compound [(NPet)(C₆H₄-PPh₂CHO)IrCl(TClCat)], (I) (TClCat = tetrachloro-*o*-catecholato). The product has been characterized by spectroscopic techniques and by an X-ray crystal structure determination.



The reaction of [(NPet)₂Ir]⁺ with TCIQ is not well understood since several products are generally obtained. However, a complex is selectively produced when the reaction mixture is exposed to air. In this case, [(NPet)(C₆H₄-PPh₂CHO)IrCl(TClCat)] forms as a result of the oxidative addition of TCIQ to iridium, followed by hydrolysis of one imino group to a formyl group (March, 1985).

A perspective view of one of the two molecules in the asymmetric unit is shown in Fig. 1. The compound has a distorted octahedral structure with the metal center coordinated by the N and P donor

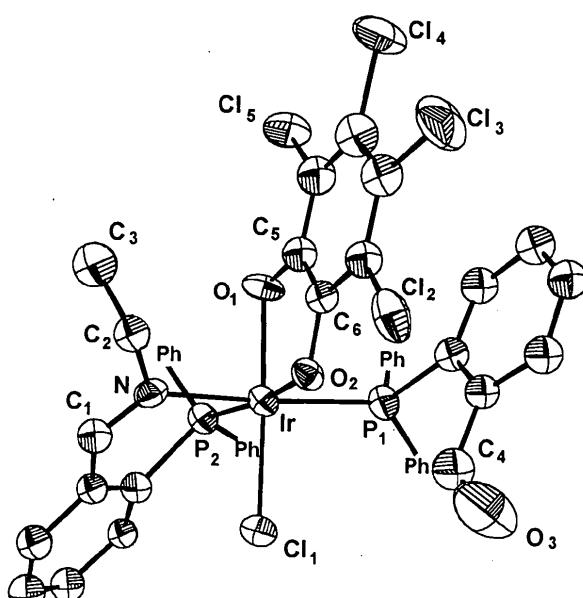


Fig. 1. ORTEP drawing of one of the molecules of the title complex showing the labeling scheme. The phenyl substituents on the P atoms are abbreviated for clarity.