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METAL-OLEFIN COMPLEXES: SYNTHESIS AND MOLECULAR STRUCTURE OF *trans*-CHLORO(ETHYLENE)BIS(TRIPHENYLPHOSPHINE)-IRIDIUM(I), $IrCl(C_2H_4)(PPh_3)_2$

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Summary

The complex, *trans*-$IrCl(C_2H_4)(PPh_3)_2$ has been isolated and its structure in the solid state determined by single-crystal X-ray diffraction. The crystals are monoclinic $P2_1/c$, with $a = 12.334(2)$, $b = 22.957(4)$, $c = 14.039(2)$ Å, $\beta = 125.54(1)°$, $Z = 4$. The structure was solved by the heavy-atom method and refined by least-squares techniques to an R value of 0.032 for 4006 reflections. The molecule has a *trans*-square planar configuration. The coordinated ethylene is π-bonded to the iridium atom and is essentially perpendicular to the P_2IrCl plane with a very short C=C distance of 1.375(10) Å. The olefin exerts a negligible *trans*-influence on the Ir—Cl bond. Principal bond lengths are: Ir—Cl, 2.371(2); Ir—P, 2.318(3), 2.312(3); Ir—C(1), 2.123(8); Ir—C(2), 2.112(8) Å.

Introduction

We have initiated studies of the *trans*-influence of carbon donor ligands in mononuclear iridium(I) complexes. Structural data for the related square-planar Rh^I complexes [1], $RhCl(PPh_3)_3$ (I) and $RhCl(C_2F_4)(PPh_3)_2$ (II) suggest a *cis*-influence of tetrafluoroethylene relative to triphenylphosphine. Thus, there is a lengthening of the Rh—P bonds (2.372(8)* Å (avg.), in II, as compared to 2.321(8) Å (avg.) in I), whereas the Rh—Cl distances (2.375(8) Å in II and 2.373(8) Å in I) are essentially identical. The disordered complex, *trans*-$RhCl(CO)(PPh_3)_2$ [2] possesses a longer Rh—Cl bond, 2.40(2) Å, as well as Rh—P bonds, 2.33(1) Å, similar to those observed in I, implying that there is a slight *trans*-influence of the carbonyl ligand relative to triphenylphosphine in

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* Numbers in parentheses here and in succeeding discussions are estimated standard deviations in the least significant digit.

trans-RhCl(CO)(PPh_3)$_2$ [2]. Structural data for the related mononuclear platinum(II) complex, *trans*-[PtCl(CO)(PEt_3)$_2$]$^+$ indicate that longer than usual Pt—P distances exist in this complex (2.34 and 2.35 Å) [3]; however, no inference with regard to the *trans*-influence of the CO ligand in this complex can be made without additional structural data.

Recently, we have reported [4] that IrCl(PPh_3)$_3$ [5] will react with a number of arenethiols, HSAr (Ar = 4-$CH_3OC_6H_4$, 4-$CH_3C_6H_4$, C_6H_5, 4-FC_6H_4 or 4-BrC_6H_4) to form [IrHCl(SAr)(PPh_3)$_2$]$_2$. We now report that these complexes can also be obtained by allowing IrCl(C_2H_4)(PPh_3)$_2$ · 0.5C_6H_6 (III) to react with excess arenethiol in benzene at room temperature and that during the course of isolating III, following the procedure of Van der Ent and Onderdelinden [6], we obtained orange crystals whose composition we have determined to be IrCl(C_2H_4)(PPh_3)$_2$ (IV) by single-crystal X-ray analysis. The crystals were obtained under dinitrogen from the mother liquor after III was collected by filtration from the benzene—pentane solution. The unsolvated complex, IV, is significantly more stable in the solid state when exposed to air than is III but rapidly decomposes in solution in the presence of dioxygen. The presence of the benzene of solvation in III appears to promote its instability in the solid state [6]. The infrared spectrum of IV is essentially identical to that of III, except for the presence of a sharp band of moderate intensity at 1971 cm^{-1} (Nujol) which is absent in the spectrum of III, and this prompted us to determine the structure of IV by X-ray analysis. Also, as far as we can ascertain, the only structural data available for a monomeric, four-coordinate iridium(I) complex are those which have been reported for the disordered structure of *trans*-IrCl(CO)(PAr_3)$_2$ (Ar = 2-$CH_3C_6H_4$) [7].

Experimental

Crystal data

The compound IrCl(C_2H_4)(PPh_3)$_2$, M = 780, gives orange monoclinic crystals m.p. 172-174°C. The theoretical composition of the compound is C, 58.48; H, 4.36; Cl, 4.55% and an elemental analysis yielded C, 58.32; H, 4.39; Cl, 4.39%. The systematic absences ($0k0$), $k = 2n + 1$; $h0l$, $l = 2n + 1$) which were obtained from precession and Weissenberg photographs uniquely determined the space group as $P2_1/c$(C_{2h}^5, No. 14). The lattice constants were carefully measured by diffractometry and found to be a = 12.334(2), b = 22.957(4), c = 14.039(2) Å, β = 125.54(1)°. With four molecules in the unit cell the calculated density of 1.602 g cm^{-3} agrees with the measured value of 1.60(1) g cm^{-3} (identical density to that of carbon tetrachloride).

Intensity measurements were made on an automatic Hilger and Watts Y290 four-circle diffractometer equipped with a highly-oriented graphite single-crystal monochromater. Mo-K_α radiation (λ = 0.71069 Å) was used. The crystal was aligned on the diffractometer such that no symmetry axis was coincident with the ϕ axis. The data were measured by the θ—2θ scan techniques at a rate of 60 steps of 0.01° with a 1-second count at each step. Stationary-crystal/stationary-counter background counts (b_1, b_2) of 15 sec were taken at the beginning and end of each symmetric scan. No significant variation in the intensities of two standard reflections, which were monitored every 100 reflections, was noticed. Data were collected out to $2\theta = 50°$ and 5691 unique reflections were obtained. The intensity data were reduced to a set of observed amplitudes on an arbitrary scale and the 4005 reflections that had intensities greater than three times their own standard deviations, where $\sigma(I)$ = [scan count + $4(b_1 + b_2)]^{1/2}$ were considered to be observed. Only these reflections were used in the refinement of the structure. No absorption correction was made (μ = 45.9 cm^{-1}). (The crystal used, a parallelepiped of ca. 0.11 × 0.09 mm^2 in cross section and 0.33 mm in length, with the longest dimension along the a* axis, would lead to transmission factors of 63.9-67.4% for the data measured.) All calculations were carried out on the University IBM 370/55 computer with locally-modified programs for data-handling and the X-RAY-72 system [8a]*.

Solution and refinement

The heavy atom positions were found from an analysis of the three dimensional Patterson function and the carbon atoms were located in a heavy-atom-phased Fourier summation. The structure was then refined by the block-diagonal least-squares method to a final R value of 0.032 for the 4006 reflections considered to be observed. The iridium, chlorine and phosphorus atoms were refined anisotropically while the carbon atoms were refined with isotropic thermal parameters and scattering factors from ref. 8. In the refinement, the block-diagonal approximation to the normal matrix was used with the anisotropically-refined atoms in 9 × 9 blocks, the isotropically-refined atoms in 4 × 4 blocks and the scale factor and overall temperature factor in a separate 2 × 2 block. The real and imaginary parts of the anomalous dispersion correction were included for the iridium atom [9]. The final difference synthesis revealed only peaks 0.4-0.6 e/Å^2 associated with hydrogen positions. Phenyl hydrogen atoms (in calculated positions) as well as ethylene hydrogen atoms (in positions obtained from the difference synthesis), with an overall isotropic thermal parameter of U = 0.063 Å^2, were included in the structure-factor calculation but excluded from the refinement. The weighting scheme adopted had the form $\sqrt{\omega} = 1/[\sigma^2(F) + pF^2]^{1/2}$ where the final p parameter was 5×10^{-4}. The relative validity of the weighting scheme, as judged by the variation of the average of $\Sigma\omega\Delta^2$ with $\sin\theta/\lambda$ and $|F_0|$, was satisfactory. The weighted $R' = \sqrt{\{\Sigma\omega(|F_0|-|F_c|)^2/\Sigma\omega|F_0|^2\}}$ = 0.039. The maximum ratio of shift to estimated standard deviation on the final cycle was 0.4 and the standard deviation of an observation of unit weight is 0.5. A list of the observed and calculated structure amplitudes has been deposited as NAPS Document No. 02543, with ASIS/NAPS**.

Discussion

The molecular structure and atomic numbering of $IrCl(C_2H_4)(PPh_3)_2$ (IV) are illustrated in Fig. 1 which is an ORTEP [10] view of the molecule. The

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* The scattering functions for the non-hydrogen atoms were obtained from ref. 8b. The hydrogen scattering functions were obtained from ref. 8c.

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(continued on p 106)

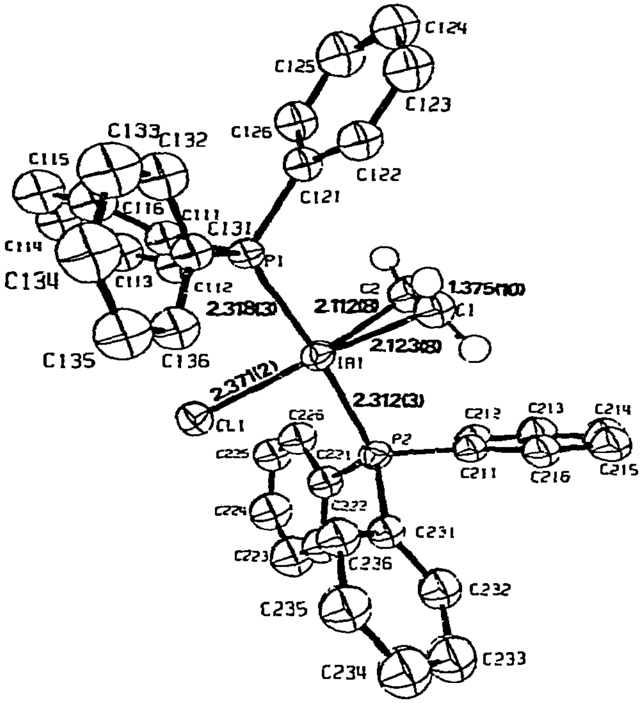

Fig. 1. A perspective view of the $IrCl(C_2H_4)(PPh_3)_2$ molecule. The thermal vibration ellipsoids enclose 50% probability.

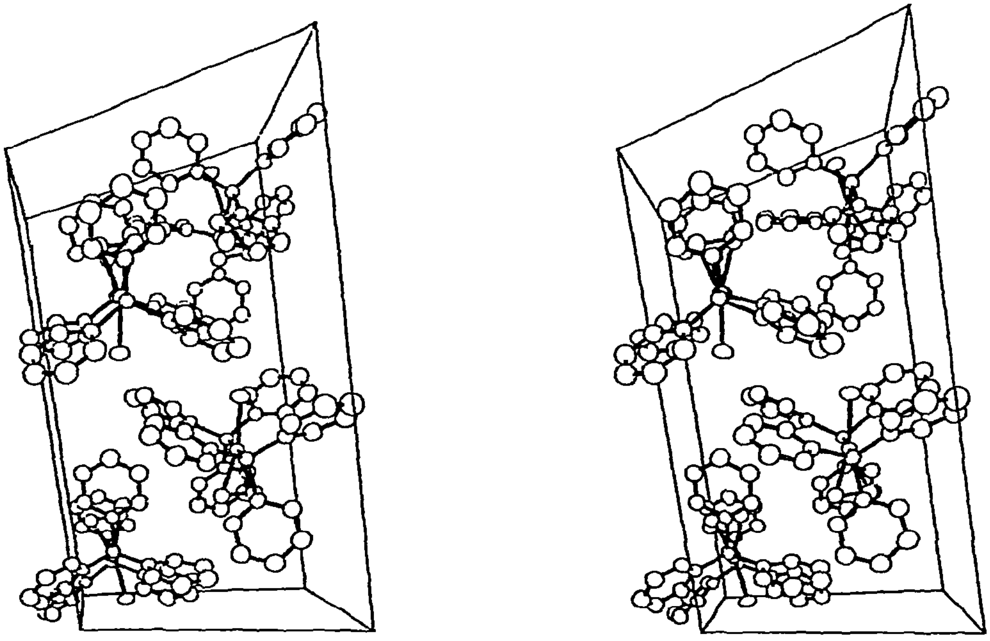

Fig. 2. A stereoview of the molecular packing diagram of $IrCl(C_2H_4)(PPh_3)_2$.

TABLE 1

POSITIONAL AND THERMAL (× 10^2) PARAMETERS FOR THE NON-HYDROGEN ATOMS IN $IrCl(C_2H_4)(PPh_3)_2$

Atom	x	y	z	U (Å^2)
Ir	0.18036(2)	0.15406(1)	0.17530(2)	[a]
P(1)	0.3566(2)	0.1279(1)	0.1675(1)	[a]
P(2)	−0.0028(2)	0.1713(1)	0.1776(2)	[a]
Cl(1)	0.1581(2)	0.0542(1)	0.2037(2)	[a]
C(1)	0.1656(7)	0.2382(3)	0.1057(6)	4.8(2)
C(2)	0.2505(7)	0.2403(3)	0.2259(6)	5.1(2)
C(111)	0.4805(7)	0.0847(3)	0.2946(6)	4.1(2)
C(112)	0.4933(8)	0.0916(3)	0.3988(7)	5.5(2)
C(113)	0.5880(8)	0.0586(4)	0.4978(7)	6.5(2)
C(114)	0.6654(9)	0.0203(4)	0.4920(7)	6.5(2)
C(115)	0.6569(10)	0.0133(4)	0.3919(8)	7.4(3)
C(116)	0.5634(8)	0.0450(4)	0.2929(7)	6.5(2)
C(121)	0.4542(6)	0.1867(3)	0.1626(6)	3.9(2)
C(122)	0.4037(7)	0.2153(3)	0.0579(6)	4.8(2)
C(123)	0.4738(8)	0.2607(4)	0.0513(7)	5.8(2)
C(124)	0.5958(8)	0.2774(4)	0.1490(7)	6.1(2)
C(125)	0.6466(9)	0.2497(4)	0.2528(7)	6.7(2)
C(126)	0.5761(8)	0.2038(3)	0.2601(7)	5.3(2)
C(131)	0.3133(6)	0.0842(3)	0.0407(8)	3.8(2)
C(132)	0.3989(8)	0.0803(4)	0.0056(7)	5.7(2)
C(133)	0.3630(9)	0.0486(4)	−0.0927(8)	6.8(2)
C(134)	0.2430(9)	0.0191(4)	−0.1557(8)	6.5(2)
C(135)	0.1602(8)	0.0209(4)	−0.1211(7)	6.0(2)
C(136)	0.1932(7)	0.0538(3)	−0.0251(6)	4.9(2)
C(211)	−0.0422(6)	0.2469(3)	0.1911(6)	3.9(2)
C(212)	0.0000(7)	0.2690(3)	0.2997(6)	5.0(2)
C(213)	−0.0254(8)	0.3265(4)	0.3120(7)	6.1(2)
C(214)	−0.0944(8)	0.3626(4)	0.2150(7)	6.3(2)
C(215)	−0.1358(8)	0.3413(3)	0.1079(7)	5.6(2)
C(216)	−0.1098(7)	0.2843(3)	0.0954(6)	4.8(2)
C(221)	0.0156(7)	0.1381(3)	0.3043(6)	4.3(2)
C(222)	−0.0920(8)	0.1177(4)	0.3030(7)	5.8(2)
C(223)	−0.0702(10)	0.0977(4)	0.4071(9)	8.0(3)
C(224)	0.0546(10)	0.0991(4)	0.5081(8)	7.5(3)
C(225)	0.1611(9)	0.1197(4)	0.5128(7)	6.5(2)
C(226)	0.1423(8)	0.1375(3)	0.4089(7)	5.5(2)
C(231)	−0.1613(6)	0.1458(3)	0.0477(6)	3.9(1)
C(232)	−0.2832(7)	0.1664(3)	0.0189(7)	5.0(2)
C(233)	−0.4026(8)	0.1471(4)	−0.0828(7)	6.0(2)
C(234)	−0.3992(8)	0.1072(4)	−0.1547(7)	6.4(2)
C(235)	−0.2790(8)	0.0866(4)	−0.1272(7)	5.8(2)
C(236)	−0.1604(7)	0.1058(3)	−0.0268(7)	4.8(2)

[a] The iridium, phosphorus, and chlorine atoms were assigned anisotropic thermal parameters U_{ij}, such that the form of the ellipsoid is:

$$\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)]$$

The values of U (Å^2 × 10^2) in that order are:

Ir	3.41(1)	3.45(1)	3.64(1)	0.19(1)	2.22(1)	0.17(1)
P(1)	3.43(9)	3.61(9)	3.76(9)	0.06(8)	2.33(8)	0.03(8)
P(2)	3.54(9)	3.68(9)	3.73(9)	0.30(7)	2.31(8)	−0.01(7)
Cl	5.13(10)	3.63(9)	6.70(12)	0.18(8)	4.05(10)	0.53(8)

final values of the positional and thermal parameters are listed in Tables 1 and 2. Table 3 gives the bond lengths and selected bond angles for the $IrCl(C_2H_4)(PPh_3)_2$ molecule. The appropriate estimated standard deviations, σ, derived from the inverse of the least-squares normal-equation matrix are also included in Tables 1, 2 and 3. The block-diagonal method used in the refinement of this structure takes into account only correlation effects which might exist between parameters of the same atom. An independent assessment of the accuracy of the bond length e.s.d.'s is obtained from the data on the 36 C—C bond lengths in the phenyl rings. The mean phenyl C—C bond distance is 1.384 Å and the standard deviation derived from the 36 phenyl C—C distances is 0.016 Å. The mean of the individual phenyl C—C bond length e.s.d.'s (Table 3) is 0.013 Å; this would indicate that the bond length e.s.d.'s given in Table 3 may be underestimated by ca. 20%. The results of the least-squares best plane calculations are included in Table 4.

The principal structural features are a square-planar geometry about the iridium atom with the coordinated ethylene molecule approximately perpendicular to the P_2IrCl plane and *trans* to chlorine. Thus, the C=C bond remains nearly perpendicular to and symmetrical about the iridium coordination plane. As is usually observed in square-planar olefin complexes (cf. compounds quoted in ref. 11), the structure departs slightly from ideal symmetry; the ethylene plane is inclined at 92.3° (Table 4) to the coordination plane and its centre is 0.22 Å below the plane. Also, the hydrogen atoms appear to be bent out of the ethylene plane away from the iridium atom (Table 4).

The *trans*-arrangement of ethylene and chlorine proposed by Van der Ent et al. [12] has been confirmed. The Ir—Cl bond lengths in IV (2.371(2) Å) and in the *o*-tolyl derivative, $IrCl(CO)(PAr_3)_2$ [7] (2.43(1) Å) suggest that the ethylene group exerts a significantly smaller *trans*-influence than CO. The Ir—P bonds are quite similar 2.315(3) Å (avg.) in IV compared to 2.338(5) Å in $IrCl(CO)(PAr_3)_2$ [7] and 2.327(6) Å in *trans*-$[Ir(C_6F_5)(CO)(PPh_3)_2]$ [13].

TABLE 2

POSITIONAL PARAMETERS FOR THE HYDROGEN ATOMS IN $IrCl(C_2H_4)(PPh_3)_2$

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
H(11)	0.181	0.230	0.048	H(135)	0.071	—0.002	—0.168
H(12)	0.067	0.249	0.050	H(136)	0.127	0.056	—0.002
H(21)	0.251	0.261	0.282	H(212)	0.052	0.242	0.373
H(22)	0.348	0.241	0.293	H(213)	0.007	0.343	0.394
H(112)	0.434	0.121	0.404	H(214)	—0.114	0.406	0.224
H(113)	0.598	0.064	0.576	H(215)	—0.189	0.368	0.034
H(114)	0.734	—0.005	0.566	H(216)	—0.141	0.269	0.013
H(115)	0.719	—0.016	0.390	H(222)	—0.188	0.117	0.225
H(116)	0.556	0.039	0.216	H(223)	—0.149	0.081	0.407
H(122)	0.312	0.203	—0.017	H(224)	0.071	0.084	0.586
H(123)	0.434	0.282	—0.028	H(225)	0.251	0.128	0.574
H(124)	0.649	0.311	0.144	H(226)	0.224	0.151	0.411
H(125)	0.737	0.263	0.327	H(232)	—0.286	0.197	0.073
H(126)	0.617	0.183	0.340	H(233)	—0.494	0.163	—0.104
H(132)	0.490	0.102	0.053	H(234)	—0.488	0.093	—0.231
H(133)	0.427	0.046	—0.118	H(235)	—0.279	0.056	—0.182
H(134)	0.215	—0.005	—0.230	H(236)	—0.070	0.090	—0.007

TABLE 3

BOND LENGTHS AND RELEVANT BOND ANGLES [a] FOR THE NON-HYDROGEN ATOMS IN $IrCl(C_2H_4)(PPh_3)_2$

Bond distances (Å)			
Ir—P(1)	2.318(3)	P(1)—C(121)	1.837(8)
Ir—P(2)	2.312(3)	P(1)—C(131)	1.832(8)
Ir—Cl	2.371(2)	P(2)—C(221)	1.824(9)
Ir—C(1)	2.123(8)	P(2)—C(211)	1.841(7)
Ir—C(2)	2.112(8)	P(2)—C(231)	1.829(6)
P(1)—C(111)	1.825(6)	C(1)—C(2)	1.375(10)
C(111)—C(112)	1.386(14)	C(211)—C(212)	1.390(12)
C(111)—C(116)	1.381(14)	C(211)—C(216)	1.392(10)
C(112)—C(113)	1.408(10)	C(212)—C(213)	1.388(12)
C(113)—C(114)	1.336(15)	C(213)—C(214)	1.386(12)
C(114)—C(115)	1.357(18)	C(214)—C(215)	1.367(14)
C(115)—C(116)	1.389(11)	C(215)—C(216)	1.383(12)
C(121)—C(122)	1.384(11)	C(221)—C(222)	1.398(15)
C(121)—C(126)	1.377(8)	C(221)—C(226)	1.390(8)
C(122)—C(123)	1.391(13)	C(222)—C(223)	1.401(16)
C(123)—C(124)	1.376(9)	C(223)—C(224)	1.358(11)
C(124)—C(125)	1.364(13)	C(224)—C(225)	1.362(17)
C(125)—C(126)	1.406(14)	C(225)—C(226)	1.398(15)
C(131)—C(132)	1.404(15)	C(231)—C(232)	1.393(12)
C(131)—C(136)	1.395(9)	C(231)—C(236)	1.397(12)
C(132)—C(133)	1.386(14)	C(232)—C(233)	1.399(9)
C(133)—C(134)	1.381(12)	C(233)—C(234)	1.383(15)
C(134)—C(135)	1.363(18)	C(234)—C(235)	1.380(14)
C(135)—C(136)	1.383(13)	C(235)—C(236)	1.387(9)
Bond angles (°)			
P(1)—Ir—P(2)	174.6(2)	P(2)—Ir—Cl	87.3(7)
P(1)—Ir—Cl	87.7(8)	Ir—P(1)—C(111)	111.7(3)
P(1)—Ir—Cl	92.6(3)	Ir—P(1)—C(121)	117.8(3)
P(1)—Ir—C(2)	92.7(3)	Ir—P(1)—C(131)	115.7(3)
P(2)—Ir—C(1)	91.6(3)	Ir—P(2)—C(221)	111.9(3)
P(2)—Ir—C(2)	92.7(3)	Ir—P(2)—C(211)	118.7(3)
Cl—Ir—C(1)	165.8(2)	Ir—P(2)—C(231)	114.7(3)
Cl—Ir—C(2)	156.2(2)		
C(116)—C(111)—C(112)	117.5(7)	C(216)—C(211)—C(212)	117.7(7)
C(111)—C(112)—C(113)	120.1(9)	C(211)—C(212)—C(213)	121.1(7)
C(112)—C(113)—C(114)	120.4(10)	C(212)—C(213)—C(214)	120.0(9)
C(113)—C(114)—C(115)	120.9(8)	C(213)—C(214)—C(215)	119.3(8)
C(114)—C(115)—C(116)	119.5(11)	C(214)—C(215)—C(216)	120.9(7)
C(115)—C(116)—C(111)	121.5(11)	C(215)—C(216)—C(211)	120.9(8)
C(126)—C(121)—C(122)	118.5(7)	C(226)—C(221)—C(222)	119.1(9)
C(121)—C(122)—C(123)	120.8(6)	C(221)—C(222)—C(223)	119.5(7)
C(122)—C(123)—C(124)	120.3(8)	C(222)—C(223)—C(224)	119.7(12)
C(123)—C(124)—C(125)	119.4(9)	C(223)—C(224)—C(225)	122.4(12)
C(124)—C(125)—C(126)	120.5(7)	C(224)—C(225)—C(226)	118.7(7)
C(125)—C(126)—C(121)	120.4(7)	C(225)—C(226)—C(221)	120.6(10)
C(136)—C(131)—C(132)	117.5(7)	C(236)—C(231)—C(232)	118.9(6)
C(131)—C(132)—C(133)	120.9(8)	C(231)—C(232)—C(233)	120.4(8)
C(132)—C(133)—C(134)	119.8(12)	C(232)—C(233)—C(234)	119.6(9)
C(133)—C(134)—C(135)	120.2(9)	C(223)—C(234)—C(235)	120.4(7)
C(134)—C(135)—C(136)	120.4(8)	C(234)—C(235)—C(236)	120.2(9)
C(135)—C(136)—C(131)	121.1(10)	C(235)—C(236)—C(231)	120.4(8)

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[a] Errors in the lattice parameters are included in the estimated standard deviations.

TABLE 4

LEAST-SQUARES PLANES FOR $IrCl(C_2H_4)(PPh_3)_2$

Plane	Atoms in plane	Equation of plane [a,b]
1	Ir, Cl, P(1), P(2)	$0.0561X + 0.1404Y + 0.9885Z - 2.4899 = 0$
2	Ir, C(1), C(2)	$0.9766X - 0.2115Y - 0.0393Z + 0.0513 = 0$
3	C(1), C(2), H(11), H(12), H(21), H(22)	$0.3398X + 0.9340Y - 0.1109Z - 5.4230 = 0$

DEVIATION OF ATOMS FROM PLANES (Å)

Atom	Plane 1	Plane 2	Plane 3
Ir	−0.0308(2)	0.0	−2.0722(2)
Cl	−0.001(2)		
P(1)	0.016(2)		
P(2)	0.016(2)		
C(1)	0.463(7)	0.0	−0.050(8)
C(2)	−0.905(7)	0.0	−0.133(8)
H(11)			0.07
H(12)			0.005
H(21)			0.09
H(22)			0.02

[a] The orthogonal vectors X, Y, Z are related to the unit cell vectors a, b, c as follows: X is parallel to a, Y perpendicular to a in the plane of a and b, and Z is perpendicular to the plane of a and b. [b] Dihedral angle between planes 1 and 2 is 89.2°; between planes 1 and 3 is 92.3°.

The observed C=C distance of 1.375(10) Å in IV is one of the shortest C=C distances reported for coordinated ethylene and is comparable to that reported for Zeise's salt, $K[Pt(C_2H_4)Cl_3]\cdot H_2O$ [14,15] (1.37(3) Å). The C=C distance is significantly shorter than that reported for the five-coordinate Ir^I complexes, $Ir(C_2H_4)_2(PPh_2C_6H_4)(PPh_3)$ [16] (1.45 Å avg.) and $Ir(C_2H_4)_2$-$(P\text{-}i\text{-}Pr_2C_3H_6)(P\text{-}i\text{-}Pr_3)$ [16] (1.43 Å avg.) which contain an internal metallated phosphine ligand. This short C=C distance would appear to be consistent with a fairly labile coordinated C_2H_4 group in solution since presence of the free C_2H_4 is required to isolate adducts such as $IrO_2Cl(C_2H_4)(PPh_3)_2$ [6] and $Ir(SO_2)Cl(C_2H_4)(PPh_3)_2$ [6] from solution.

With the hydrogen atoms left out of consideration, all intermolecular distances are greater than 3.4 Å; these correspond to normal Van der Waals contacts.

Further studies are in progress on related iridium(I) complexes with substituted phosphine and acetylene ligands.

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