Elemental analyses

[IrCl(C_2H_4)(P*i*Pr$_3$)(Sb*i*Pr$_3$)] (2)

$C_{20}H_{46}ClIrPSb$ (667.0)	Ber.	C 36.02	H 6.95		
	Gef.	C 35.77	H 6.70		

[IrCl(=CPh$_2$)(P*i*Pr$_3$)(Sb*i*Pr$_3$)] (3a)

$C_{31}H_{52}ClIrPSb$ (805.2)	Ber.	C 46.24	H 6.51		
	Gef.	C 46.49	H 6.43		

[IrCl(=C{*p*-Tol}$_2$)(P*i*Pr$_3$)(Sb*i*Pr$_3$)] (3b)

$C_{33}H_{56}ClIrPSb$ (833.2)	Ber.	C 47.57	H 6.77	Sb 14.61	Ir 23.07
	Gef.	C 47.33	H 6.74	Sb 14.50	Ir 22.75

***trans*-[IrCl(=CPh$_2$)(P*i*Pr$_3$)$_2$] (4a)**

$C_{31}H_{52}ClIrP_2$ (714.4)	Ber.	C 52.12	H 7.34	Ir 26.91
	Gef.	C 51.92	H 7.35	Ir 27.10

***trans*-[IrCl{=C(*p*-Tol)$_2$}(P*i*Pr$_3$)$_2$] (4b)**

$C_{33}H_{56}ClIrP_2$ (742.4)	Ber.	C 53.39	H 7.60	P 8.34	Ir 25.89
	Gef.	C 53.32	H 7.72	P 8.20	Ir 26.20

[Ir(η^5-C_5H_5)(=CPh_2)(P*i*Pr_3)] (5)

$C_{27}H_{36}IrP$ (583.8)

Ber. C 55.55 H 6.22
Gef. C 55.34 H 6.09

[Ir(η^5-C_5H_5)($CHPh_2$)(Cl)(P*i*Pr_3)] (6)

$C_{27}H_{37}ClIrP$ (620.2)

Ber. C 52.29 H 6.01
Gef. C 52.54 H 5.90

[Ir(η^5-$C_5H_4CHPh_2$)(Cl)(H)(P*i*Pr_3)] (7)

$C_{27}H_{37}ClIrP$ (620.2)

Ber. C 52.29 H 6.01
Gef. C 51.98 H 5.78

[Ir(H)(Cl)(=CPh_2)(P*i*Pr_3)$_2$][BF_4] (9)

$C_{31}H_{53}BClF_4IrP_2$ (802.2)

Ber. C 46.42 H 6.66
Gef. C 46.79 H 6.98

Table 1. Crystal data and structure refinement for **5**.

formula	$C_{27}\ H_{36}\ Ir\ P$
fw	583.73
crystal size, mm^3	0.22 x 0.16 x 0.13
crystal system	Monoclinic
space group	$P2_1/n$ (No. 14)
cell dimensions determn	25 reflcns, $10 < \Theta < 15$
a, Å	11.017(2)
b, Å	14.709(2)
c, Å	15.374(3)
β, deg	96.006(9)
V, $Å^3$	2477.7(7)
Z	4
dcalc, gcm^{-3}	1.565
diffractometer	CAD4 (Enraf-Nonius)
radiation	Mo-K_α (0.71073 Å), graphite monochromator, Zr filter (factor 15.4)
temp, K	293(2)
μ, mm^{-1}	0.138
scan method	Ω/Θ-scan
2Θ (max), deg	49.90
tot. no. of reflcns scanned	4496
no. of unique rflcns	4328 [R(int) = 0.0206]
no. of data	4327
no. of obsd rflcns [$I>2\sigma(I)$]	3565
correct. appl.	LP- and empirical abs.-corr. (Ψ-scans, min. transm. 83.92 %)
structure solution	SHELXS-86
param	269 (full-matrix least-squares on F^2 (SHELXL-93))
reflex/param ratio	16.08
final R indices [$I>2\sigma(I)$]	R_1 = 0.0287, wR_2 = 0.0612 *)
R indices (all data)	R_1 = 0.0407, wR_2 = 0.0696 *)
resid electron density, $eÅ^{-3}$	0.697 / -0.568

*) $w = 1/[\sigma^2(F_o^2) + (0.0267P)^2 + 4.9566P]$, $P = [F_o^2 + 2F_c^2]/3$

remarks: Die Atome C14 -C18 (Cp-Ring) wurden mit restraints auf die anisotropen Auslenkungsparameter in Richtung der Bindungen verfeinert.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ir	241(1)	2908(1)	3273(1)	41(1)
P	711(1)	4265(1)	2701(1)	45(1)
C(1)	1610(5)	2759(3)	4125(3)	39(1)
C(2)	1447(5)	2115(4)	4860(3)	43(1)
C(3)	692(6)	2337(5)	5495(4)	61(2)
C(4)	524(7)	1733(6)	6166(5)	81(2)
C(5)	1064(8)	898(6)	6204(6)	91(3)
C(6)	1820(8)	674(5)	5587(6)	83(2)
C(7)	2027(6)	1277(4)	4924(4)	59(2)
C(8)	2895(5)	3096(3)	4215(3)	40(1)
C(9)	3397(5)	3529(4)	4969(4)	50(1)
C(10)	4595(6)	3825(5)	5056(4)	66(2)
C(11)	5325(6)	3658(5)	4393(5)	72(2)
C(12)	4858(6)	3199(5)	3661(5)	70(2)
C(13)	3654(5)	2930(4)	3567(4)	52(1)
C(14)	-1858(6)	2820(6)	3022(6)	85(2)
C(15)	-1477(8)	2294(8)	3717(6)	96(3)
C(16)	-739(8)	1623(6)	3456(7)	97(3)
C(17)	-669(7)	1745(6)	2526(7)	91(2)
C(18)	-1400(7)	2501(6)	2285(6)	79(2)
C(20)	-726(5)	4933(4)	2461(4)	57(2)
C(21)	1841(6)	4990(4)	3351(5)	63(2)
C(22)	1274(6)	4253(5)	1593(4)	69(2)
C(23)	-1383(6)	5136(6)	3265(5)	88(3)
C(24)	-667(7)	5806(5)	1910(6)	96(3)
C(25)	2264(8)	5862(6)	2922(7)	130(4)
C(26)	1453(7)	5206(5)	4258(5)	84(2)
C(27)	2544(8)	3851(8)	1602(6)	122(4)
C(28)	397(8)	3776(7)	917(5)	102(3)

Table 3. Bond lengths [Å] for **5**.

Ir-C(1)	1.904(5)

Ir-C(16)	2.210(7)
Ir-C(17)	2.239(7)
Ir-P	2.262(2)
Ir-C(15)	2.266(7)
Ir-C(14)	2.308(7)
Ir-C(18)	2.316(6)
P-C(21)	1.851(6)
P-C(20)	1.867(6)
P-C(22)	1.872(6)
C(1)-C(8)	1.492(7)
C(1)-C(2)	1.499(7)
C(2)-C(3)	1.386(8)
C(2)-C(7)	1.387(8)
C(3)-C(4)	1.388(9)
C(4)-C(5)	1.363(12)
C(5)-C(6)	1.366(12)
C(6)-C(7)	1.388(10)
C(8)-C(13)	1.387(8)
C(8)-C(9)	1.387(7)
C(9)-C(10)	1.383(8)
C(10)-C(11)	1.385(9)
C(11)-C(12)	1.366(9)
C(12)-C(13)	1.378(8)
C(14)-C(15)	1.349(12)
C(14)-C(18)	1.370(11)
C(15)-C(16)	1.365(12)
C(16)-C(17)	1.451(12)
C(17)-C(18)	1.399(11)
C(20)-C(23)	1.526(9)
C(20)-C(24)	1.542(9)
C(21)-C(26)	1.534(10)
C(21)-C(25)	1.536(9)
C(22)-C(28)	1.516(10)
C(22)-C(27)	1.518(10)

Table 4. Bond angles [deg] for **5**.

C(1)-Ir-C(16)	100.2(3)
C(1)-Ir-C(17)	123.0(3)
C(16)-Ir-C(17)	38.1(3)
C(1)-Ir-P	99.9(2)
C(16)-Ir-P	159.8(2)
C(17)-Ir-P	125.6(3)

C(1)-Ir-C(15)	111.9(3)
C(16)-Ir-C(15)	35.5(3)
C(17)-Ir-C(15)	60.4(3)
P-Ir-C(15)	134.5(3)
C(1)-Ir-C(14)	144.7(3)
C(16)-Ir-C(14)	58.6(3)
C(17)-Ir-C(14)	58.9(3)
P-Ir-C(14)	104.5(2)
C(15)-Ir-C(14)	34.3(3)
C(1)-Ir-C(18)	158.3(3)
C(16)-Ir-C(18)	60.2(3)
C(17)-Ir-C(18)	35.7(3)
P-Ir-C(18)	99.7(2)
C(15)-Ir-C(18)	58.3(3)
C(14)-Ir-C(18)	34.5(3)
C(21)-P-C(20)	108.1(3)
C(21)-P-C(22)	103.2(3)
C(20)-P-C(22)	100.4(3)
C(21)-P-Ir	117.8(2)
C(20)-P-Ir	108.5(2)
C(22)-P-Ir	117.2(3)
C(8)-C(1)-C(2)	109.2(4)
C(8)-C(1)-Ir	134.5(4)
C(2)-C(1)-Ir	116.2(4)
C(3)-C(2)-C(7)	117.7(6)
C(3)-C(2)-C(1)	120.7(5)
C(7)-C(2)-C(1)	121.6(5)
C(2)-C(3)-C(4)	120.6(7)
C(5)-C(4)-C(3)	121.2(8)
C(4)-C(5)-C(6)	118.8(7)
C(5)-C(6)-C(7)	121.0(7)
C(2)-C(7)-C(6)	120.7(7)
C(13)-C(8)-C(9)	117.6(5)
C(13)-C(8)-C(1)	120.8(5)
C(9)-C(8)-C(1)	121.4(5)
C(10)-C(9)-C(8)	121.2(6)
C(9)-C(10)-C(11)	119.7(6)
C(12)-C(11)-C(10)	119.8(6)
C(11)-C(12)-C(13)	120.3(6)
C(12)-C(13)-C(8)	121.3(6)
C(15)-C(14)-C(18)	110.4(9)
C(15)-C(14)-Ir	71.1(4)
C(18)-C(14)-Ir	73.1(4)
C(14)-C(15)-C(16)	109.1(9)
C(14)-C(15)-Ir	74.6(4)

C(16)-C(15)-Ir	70.0(4)
C(15)-C(16)-C(17)	107.1(8)
C(15)-C(16)-Ir	74.5(5)
C(17)-C(16)-Ir	72.0(4)
C(18)-C(17)-C(16)	105.7(8)
C(18)-C(17)-Ir	75.1(4)
C(16)-C(17)-Ir	69.9(4)
C(14)-C(18)-C(17)	107.7(8)
C(14)-C(18)-Ir	72.4(4)
C(17)-C(18)-Ir	69.1(4)
C(23)-C(20)-C(24)	109.4(6)
C(23)-C(20)-P	114.0(5)
C(24)-C(20)-P	117.6(5)
C(26)-C(21)-C(25)	110.1(7)
C(26)-C(21)-P	112.0(4)
C(25)-C(21)-P	117.8(5)
C(28)-C(22)-C(27)	110.3(7)
C(28)-C(22)-P	112.3(5)
C(27)-C(22)-P	112.8(5)

Table 5. Anisotropic displacement parameters (Å^2 x 10^3) for **5**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ir	35(1)	41(1)	46(1)	2(1)	-3(1)	-6(1)
P	37(1)	43(1)	52(1)	7(1)	-1(1)	0(1)
C(1)	38(3)	34(3)	46(3)	-3(2)	6(2)	1(2)
C(2)	38(3)	44(3)	46(3)	0(3)	-4(2)	-8(2)
C(3)	61(4)	63(4)	60(4)	1(3)	9(3)	-8(3)
C(4)	83(5)	110(7)	52(4)	8(4)	21(4)	-31(5)
C(5)	96(6)	90(6)	79(6)	34(5)	-23(5)	-46(5)
C(6)	91(6)	54(4)	97(6)	20(4)	-25(5)	-3(4)
C(7)	60(4)	51(4)	65(4)	10(3)	-6(3)	6(3)
C(8)	38(3)	37(3)	43(3)	5(2)	-2(2)	0(2)
C(9)	47(3)	57(4)	45(3)	0(3)	-3(3)	-9(3)
C(10)	61(4)	75(5)	59(4)	-7(4)	-10(3)	-21(4)
C(11)	38(3)	90(5)	87(5)	-4(4)	-2(3)	-22(4)
C(12)	43(4)	92(5)	77(5)	-11(4)	9(3)	-8(3)

C(13)	42(3)	59(4)	54(3)	-9(3)	4(3)	-3(3)
C(14)	45(4)	101(6)	106(6)	5(6)	-11(4)	-21(4)
C(15)	64(5)	141(8)	83(5)	6(6)	7(4)	-57(5)
C(16)	86(6)	66(5)	128(6)	31(5)	-46(6)	-43(5)
C(17)	72(5)	71(5)	126(6)	-48(5)	-7(5)	-21(4)
C(18)	63(5)	93(5)	76(4)	5(4)	-25(4)	-30(4)
C(20)	44(3)	54(4)	70(4)	4(3)	-3(3)	6(3)
C(21)	49(4)	49(4)	86(5)	16(3)	-13(3)	-10(3)
C(22)	58(4)	95(5)	56(4)	24(4)	13(3)	7(4)
C(23)	55(4)	101(6)	106(6)	-26(5)	-3(4)	30(4)
C(24)	74(5)	67(5)	141(8)	38(5)	-12(5)	16(4)
C(25)	113(7)	85(6)	176(10)	66(7)	-52(7)	-54(6)
C(26)	71(5)	67(5)	108(6)	-31(4)	-17(4)	0(4)
C(27)	88(6)	202(11)	84(6)	41(7)	44(5)	42(7)
C(28)	118(7)	138(8)	53(4)	-1(5)	18(5)	-3(6)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **5**.

	x	y	z	U(eq)
H(3)	294(6)	2896(5)	5471(4)	73
H(4)	35(7)	1902(6)	6596(5)	97
H(5)	920(8)	489(6)	6642(6)	109
H(6)	2201(8)	110(5)	5612(6)	100
H(7)	2561(6)	1118(4)	4519(4)	71
H(9)	2919(5)	3623(4)	5425(4)	60
H(10)	4908(6)	4135(5)	5557(4)	79
H(11)	6130(6)	3858(5)	4446(5)	87
H(12)	5356(6)	3068(5)	3225(5)	84
H(13)	3344(5)	2630(4)	3059(4)	62
H(14)	-2359(6)	3326(6)	3040(6)	102
H(15)	-1684(8)	2377(8)	4283(6)	116
H(16)	-354(8)	1172(6)	3809(7)	117
H(17)	-230(7)	1394(6)	2165(7)	109
H(18)	-1549(7)	2743(6)	1725(6)	95
H(20)	-1279(5)	4528(4)	2101(4)	68
H(21)	2574(6)	4614(4)	3461(5)	75
H(22)	1325(6)	4888(5)	1406(4)	83
H(23A)	-1290(45)	4630(17)	3660(18)	132

H(23B)	-2235(11)	5235(40)	3088(7)	132
H(23C)	-1039(36)	5670(23)	3551(22)	132
H(24A)	-362(52)	5661(8)	1365(17)	143
H(24B)	-134(44)	6237(16)	2224(18)	143
H(24C)	-1470(12)	6062(23)	1800(34)	143
H(25A)	2542(69)	5715(9)	2368(25)	195
H(25B)	2919(52)	6133(31)	3295(26)	195
H(25C)	1595(23)	6282(22)	2836(49)	195
H(26A)	2160(9)	5357(37)	4650(11)	126
H(26B)	1058(45)	4684(13)	4477(16)	126
H(26C)	897(40)	5711(24)	4215(8)	126
H(27A)	3097(16)	4175(35)	2016(38)	183
H(27B)	2812(31)	3901(50)	1030(14)	183
H(27C)	2526(16)	3222(15)	1767(50)	183
H(28A)	-392(18)	4058(30)	895(31)	153
H(28B)	332(47)	3147(12)	1073(24)	153
H(28C)	695(33)	3821(40)	354(9)	153