Table 2. *Selected bond distances* (Å) *and angles* (°)

Al(1)—N(1)	2·073 (4)	Al(1)—N(2)	1·906 (4)
Al(1)—C(6)	1·967 (5)	Al(1)—C(8)	1·967 (6)
Al(2)—N(2)	2·025 (4)	Al(2)—C(10)	1·985 (5)
Al(2)—C(12)	1·995 (6)	Al(2)—C(14)	2·000 (5)
N(1)—C(1)	1·510 (7)	N(1)—C(2)	1·493 (6)
N(1)—C(3)	1·508 (6)	N(2)—C(5)	1·491 (6)
C(1)—C(2*A*)	1·520 (7)	C(3)—C(4)	1·526 (8)
C(4)—C(5)	1·517 (8)		

N(1)—Al(1)—N(2)	98·3 (2)	N(1)—Al(1)—C(6)	104·5 (2)
N(2)—Al(1)—C(6)	116·0 (2)	N(1)—Al(1)—C(8)	105·6 (2)
N(2)—Al(1)—C(8)	109·6 (2)	C(6)—Al(1)—C(8)	119·8 (2)
N(2)—Al(2)—C(10)	105·9 (2)	N(2)—Al(2)—C(12)	105·2 (2)
C(10)—Al(2)—C(12)	114·5 (3)	N(2)—Al(2)—C(14)	107·5 (2)
C(10)—Al(2)—C(14)	112·7 (2)	C(12)—Al(2)—C(14)	110·4 (2)
Al(1)—N(1)—C(1)	106·7 (3)	Al(1)—N(1)—C(2)	111·7 (3)
C(1)—N(1)—C(2)	106·3 (4)	Al(1)—N(1)—C(3)	109·3 (3)
C(1)—N(1)—C(3)	109·9 (4)	C(2)—N(1)—C(3)	112·7 (4)
Al(1)—N(2)—Al(2)	114·8 (2)	Al(1)—N(2)—C(5)	113·8 (4)
Al(2)—N(2)—C(5)	109·7 (3)	N(1)—C(1)—C(2*A*)	112·9 (4)
N(1)—C(2)—C(1*A*)	114·7 (4)	N(1)—C(3)—C(4)	113·5 (4)
C(3)—C(4)—C(5)	115·2 (4)	N(2)—C(5)—C(4)	114·5 (4)

difference map peaks ranged from -0.23 to 0.26 e Å^{-3}. Computer programs of Sheldrick (1986), scattering factors from Cromer & Waber (1974), and real and imaginary anomalous-dispersion corrections from Cromer (1974). Final atomic coordinates are given in Table 1,* selected distances and angles are reported in Table 2. The molecule is displayed in Fig. 1.

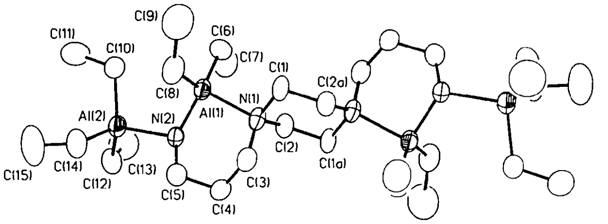

Fig. 1. Thermal ellipsoid plot (35% probability) and atomic numbering for $[Al(C_2H_5)_2]_2[C_{10}H_{22}N_4][Al(C_2H_5)_3]_2$.

Related literature. Synthesis and structure of the methyl derivative: Robinson, Moise, Pennington & Sangokoya (1988). For related structures of other multidentate open-chain amine/organoaluminium products see Sangokoya, Moise, Pennington, Self & Robinson (1989), Robinson, Moise, Pennington & Sangokoya (1989), Robinson, Sangokoya, Moise & Pennington (1988), Robinson, Moise, Pennington & Sangokoya (1988) and Robinson & Sangokoya (1987).

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* A summary of crystallographic details, tables of anisotropic thermal parameters, distances and angles, H-atom coordinates and observed and calculated structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52598 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of an Iridium Bis(phosphine) Diene Complex, a Catalyst for Homogeneous Hydrogenation

By M. S. Abbassioun, P. A. Chaloner* and P. B. Hitchcock

School of Chemistry and Molecular Sciences, University of Sussex, Falmer, Brighton BN1 9QJ, England

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Abstract. (η^4-1,5-Cyclooctadiene)bis{tris(4-methoxyphenyl)phosphine}iridium(I) hexafluorophosphate, $[Ir(C_8H_{12})(C_{21}H_{21}O_3P)_2][PF_6]$, $M_r = 1150{\cdot}1$, monoclinic, space group $P2_1/c$, $a = 11{\cdot}757\,(5)$, $b = 19{\cdot}759\,(7)$, $c = 20{\cdot}468\,(8)$ Å, $\beta = 93{\cdot}85\,(4)°$, $V = 4744{\cdot}0$ Å^3, $Z = 4$, $D_x = 1{\cdot}61$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 29{\cdot}7$ cm^{-1}, $F(000) = 2312$, $T = 295$ K; $R = 0{\cdot}039$, $wR = 0{\cdot}055$ for 3793 reflections with $|F^2| > 3\sigma(F^2)$. The geometry at iridium is approximately square planar, with the expected distortions due to the size of the phosphine ligands: Ir—P1 2·359 (3), Ir—P2 2·341 (3) Å, P1—Ir—P2

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* To whom correspondence should be addressed.

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Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($\times 10^3$)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq} (Å^2)
Ir	2083·2 (3)	2080·5 (2)	2626·8 (2)	29·3 (1)
P1	1758·9 (23)	1809·3 (15)	1507·5 (13)	30 (1)
P2	2462·8 (22)	969·8 (14)	2975·0 (13)	32 (1)
P3	2797·3 (31)	7581·5 (22)	7207·0 (18)	64 (2)
F1	2691 (10)	7020 (5)	6683 (4)	114 (7)
F2	2788 (11)	8126 (6)	6646 (5)	148 (8)
F3	4115 (8)	7547 (8)	7190 (7)	157 (10)
F4	2865 (12)	7052 (5)	7757 (5)	132 (8)
F5	2950 (11)	8155 (6)	7733 (6)	139 (8)
F6	1502 (8)	7683 (8)	7225 (6)	156 (9)
O1	6060 (7)	2372 (6)	237 (4)	78 (6)
O2	195 (7)	−909 (4)	528 (4)	55 (5)
O3	−1730 (6)	3644 (5)	176 (4)	64 (5)
O4	5484 (8)	−380 (5)	1148 (5)	84 (6)
O5	4610 (6)	867 (4)	5721 (4)	53 (5)
O6	−2001 (6)	−326 (4)	3372 (4)	57 (5)
C1	1160 (11)	3052 (5)	2532 (5)	47 (6)
C2	2214 (11)	3135 (5)	2273 (6)	48 (7)
C3	3217 (13)	3486 (7)	2681 (7)	72 (8)
C4	3493 (14)	3219 (7)	3361 (7)	83 (9)
C5	3102 (11)	2499 (6)	3462 (6)	58 (7)
C6	1985 (11)	2348 (7)	3666 (5)	56 (7)
C7	1017 (14)	2850 (8)	3753 (7)	98 (10)
C8	776 (12)	3325 (7)	3183 (6)	67 (8)
C9	3048 (9)	1956 (5)	1086 (5)	35 (6)
C10	3119 (10)	1790 (7)	433 (5)	46 (6)
C11	4157 (10)	1935 (7)	114 (5)	50 (7)
C12	5047 (9)	2226 (6)	487 (6)	53 (7)
C13	4987 (9)	2384 (7)	1136 (5)	50 (7)
C14	3993 (9)	2258 (5)	1439 (5)	39 (6)
C15	6240 (11)	2282 (9)	−437 (6)	77 (9)
C16	1302 (9)	964 (5)	1236 (5)	37 (6)
C17	2089 (10)	510 (6)	989 (6)	50 (7)
C18	1748 (9)	−134 (6)	764 (6)	48 (7)
C19	616 (10)	−312 (6)	770 (5)	44 (6)
C20	−167 (9)	122 (6)	1008 (6)	49 (7)
C21	171 (9)	758 (6)	1249 (6)	46 (7)
C22	993 (11)	−1394 (7)	316 (7)	67 (8)
C23	698 (8)	2367 (5)	1070 (5)	31 (5)
C24	997 (9)	2786 (5)	573 (5)	35 (6)
C25	202 (10)	3221 (6)	244 (5)	43 (6)
C26	−912 (9)	3227 (6)	452 (6)	41 (6)
C27	−1208 (9)	2818 (6)	955 (5)	41 (6)
C28	−431 (9)	2388 (6)	1265 (5)	43 (6)
C29	−1435 (13)	4100 (8)	−329 (7)	91 (9)
C30	3414 (9)	505 (6)	2476 (5)	33 (6)
C31	4303 (9)	883 (6)	2241 (5)	41 (6)
C32	5034 (10)	592 (6)	1799 (6)	50 (7)
C33	4886 (10)	−74 (6)	1608 (6)	56 (7)
C34	4026 (10)	−470 (6)	1869 (6)	56 (7)
C35	3290 (9)	−184 (6)	2296 (5)	42 (6)
C36	6324 (12)	18 (9)	839 (7)	116 (10)
C37	3159 (9)	879 (6)	3794 (5)	36 (6)
C38	4332 (9)	940 (6)	3906 (5)	42 (6)
C39	4860 (9)	936 (6)	4549 (5)	43 (6)
C40	4177 (9)	873 (6)	5091 (5)	43 (6)
C41	3010 (9)	807 (6)	4987 (5)	45 (7)
C42	2492 (9)	796 (6)	4346 (5)	39 (6)
C43	5830 (10)	912 (7)	5854 (6)	58 (7)
C44	1138 (9)	519 (5)	3037 (5)	36 (6)
C45	131 (9)	889 (6)	2891 (5)	41 (6)
C46	−930 (9)	620 (6)	2992 (5)	41 (6)
C47	−993 (9)	−34 (6)	3214 (5)	41 (6)
C48	−19 (9)	−414 (6)	3361 (6)	45 (6)
C49	1056 (10)	−143 (6)	3277 (6)	48 (7)
C50	−3055 (10)	55 (7)	3217 (7)	59 (8)

Table 2. *Selected intramolecular distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

Ir—P1	2·359 (3)	Ir—P2	2·341 (3)
Ir—C1	2·207 (11)	Ir—C2	2·214 (11)
Ir—C5	2·182 (12)	Ir—C6	2·203 (11)
Ir—*M*1	2·098	Ir—*M*2	2·072
*M*1—Ir—*M*2	86·0	*M*1—Ir—P1	89·2
*M*1—Ir—P2	174·6	*M*2—Ir—P1	171·4
*M*2—Ir—P2	89·5	P1—Ir—P2	95·6 (1)
Ir—P1—C9	109·8 (3)	Ir—P1—C16	121·8 (4)
Ir—P1—C23	113·3 (3)	C9—P1—C16	103·8 (5)
C9—P1—C23	103·4 (5)	C16—P1—C23	102·8 (5)
Ir—P2—C30	114·5 (4)	Ir—P2—C37	115·9 (4)
Ir—P2—C44	109·6 (4)	C30—P2—C37	102·3 (5)

*M*1 and *M*2 are the midpoints of the C1—C2 and C5—C6 bonds.

95·6 (1), *M*1—Ir—P1 89·2, *M*1—Ir—*M*2 86·0, *M*2—Ir—P2 89·5° (*M*1 and *M*2 are the midpoints of the C1—C2 and C5—C6 bonds).

Experimental. The complex was prepared by the addition of tris(4-methoxyphenyl)phosphine to $[Ir(cod)(py)_2][PF_6]$ (Crabtree & Moorehouse 1986) and well formed crystals obtained by diffusion of ether into a solution in dichloromethane (cod = 1,5-cyclooctadiene, py = pyridine). Data collected using a crystal *ca* 0·4 × 0·3 × 0·2 mm, coated in epoxy glue, on an Enraf–Nonius CAD-4 diffractometer, monochromated Mo $K\alpha$ radiation in the θ–2θ mode, with $\Delta\theta = (0{\cdot}8 + 0{\cdot}35\tan\theta)°$ and a maximum scan time of 1 min. Cell dimensions from setting angles for 25 reflections with $7{\cdot}5 < \theta < 10{\cdot}4°$. A total of 6010 unique reflections were measured for $2 < \theta < 22°$ and h $0\rightarrow12$, k $0\rightarrow20$, l $-21\rightarrow21$, and 3793 reflections with $|F^2| > 3\sigma(F^2)$, where $\sigma(F^2) = [\sigma^2(I) + (0{\cdot}04I)^2]^{1/2}/Lp$, were used in the refinement. Two reference reflections remeasured every 30 min showed no significant variation. An absorption correction was applied using *DIFABS* (Walker & Stuart, 1983), after isotropic refinement, and gave maximum and minimum corrections of 1·10 and 0·90. The structure was solved by routine heavy-atom methods and non-H atoms refined anisotropically by full-matrix least squares. H atoms were held fixed at calculated positions with $B_{iso} = 1{\cdot}3\ B_{eq}$ for the atoms to which they are bonded. With a weighting scheme of $w = 1/\sigma^2(F)$, the final residuals were $R = 0{\cdot}039$ and $wR = 0{\cdot}055$, 595 variables, $S = 1{\cdot}64$, $(\Delta/\sigma)_{max} = 0{\cdot}03$, $\Delta\rho_{max} = 0{\cdot}7$, $\Delta\rho_{min} = -0{\cdot}5$ e Å^{-3}. Programs from the Enraf–Nonius (1982) *SDP-Plus* package were run on a MicroVAX computer. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Atomic parameters are given in Table 1,* selected intramolecular bond distances and angles in Table 2. Fig. 1 shows the molecular structure and the numbering scheme.

Related literature. This complex has proved to be useful as a hydrogenation catalyst (Abbassioun &

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* Lists of structure factors, anisotropic temperature factors, H-atom parameters, complete intramolecular distances and angles, least-squares planes and a packing diagram have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52615 (34 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

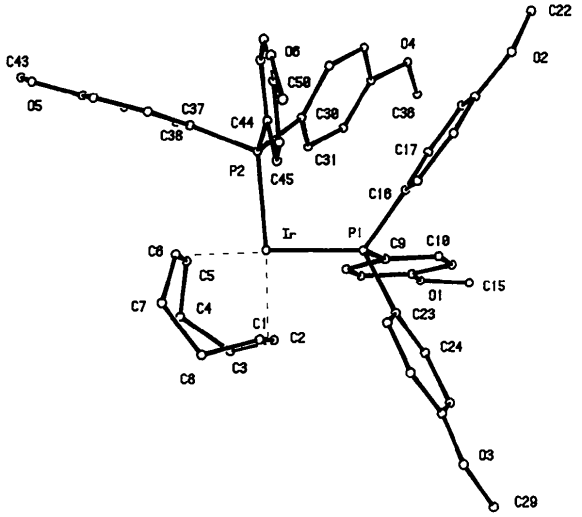

Fig. 1. Molecular structure and numbering scheme for $[Ir\{P(4\text{-}MeOC_6H_4)_3\}_2(cod)]^+$.

Chaloner, 1989), and is related to $[Ir(PCy_3)(py)(cod)][PF_6]$, which has been widely used as a catalyst for the reduction of hindered alkenes (Crabtree, 1979). The structures of $[Ir(PCy_3)(py)(cod)][PF_6]$ and $[Ir\{P(2\text{-}MeOC_6H_4)_3\}(py)][PF_6]$ have been determined, and show distortions due to the bulk of the phosphine ligands (Abbassioun, Hitchcock & Chaloner, 1989*a*). The conformation of the cod ligand is similar in these complexes. The structure of $[Ir(py)_2(cod)][BPh_4]$, containing the precursor cation, has also been established (Abbassioun, Hitchcock & Chaloner, 1989*b*)

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Structure of Difluorobis(trifluoromethyl)tellurium

By Hans Preut

Fachbereich Chemie, Universität Dortmund, Postfach 500500, *D*-4600 *Dortmund* 50,
Federal Republic of Germany

Bernd Wilkes

Kali-Chemie AG, Postfach 220, *D*-3000 *Hannover* 1, *Federal Republic of Germany*

and Dieter Naumann

Institut für Anorganische Chemie, Universität zu Köln, Greinstrasse 6, *D*-5000 *Köln* 41,
Federal Republic of Germany

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Abstract. $[TeF_2(CF_3)_2]$, $M_r = 303{\cdot}61$, monoclinic, $C2/c$, $a = 22{\cdot}065\ (4)$, $b = 9{\cdot}764\ (2)$, $c = 8{\cdot}981\ (3)$ Å, $\beta = 91{\cdot}66\ (2)^\circ$, $V = 1934{\cdot}1\ (8)$ Å^3, $Z = 12$, $D_x = 3{\cdot}128$ Mg m^{-3}, $F(000) = 1632$, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 4{\cdot}71$ mm^{-1}, $T = 291\ (1)$ K, final $R = 0{\cdot}039$ for 2474 unique observed $[F \geq 4{\cdot}0\sigma(F)]$ diffractometer data. The asymmetric unit of the crystal contains one and a half $(CF_3)_2TeF_2$ molecules. The surrounding of each of the two independent Te atoms can roughly be described as a trigonal bipyramid with two C atoms and the non-bonding electron pair in the equatorial plane. The crystal contains intermolecular Te···F and F···F distances which are significantly shorter than the sum of the corresponding van der Waals radii.

Experimental. The title compound was prepared from $Te(CF_3)_2$ with XeF_2 (Naumann & Herberg,

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