

Supporting Material

Silapentadienyl-Iridium-Phosphine Chemistry

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- a) X-ray crystallographic data for $(\eta^2\text{-cyclooctene})(\text{Me})\text{Ir}(\text{PMe}_3)_3$ (15 pages)
- b) X-ray crystallographic data for compound ***fac-5-acetone*** (15 pages)
- c) X-ray crystallographic data for compound ***fac-6*** (18 pages)
- d) X-ray crystallographic data for compound ***fac-7E*** (14 pages)

Table 1. Crystal data and structure refinement for jb7907 [(cyclooctene)(Me)Ir(PMe₃)₃]

Identification code	b7907/lt	
Empirical formula	C ₁₈ H ₄₄ Ir P ₃	
Formula weight	545.64	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 15.2176(6) Å	α = 90°.
	b = 9.3278(4) Å	β = 114.744(2)°.
	c = 17.7508(7) Å	γ = 90°.
Volume	2288.33(16) Å ³	
Z	4	
Density (calculated)	1.584 Mg/m ³	
Absorption coefficient	6.042 mm ⁻¹	
F(000)	1096	
Crystal size	0.26 x 0.21 x 0.16 mm ³	
Theta range for data collection	2.31 to 36.49°.	
Index ranges	-25 ≤ h ≤ 23, -15 ≤ k ≤ 15, -28 ≤ l ≤ 29	
Reflections collected	119939	
Independent reflections	11202 [R(int) = 0.054]	
Completeness to theta = 36.49°	99.7 %	
Absorption correction	Numerical	
Max. and min. transmission	0.4448 and 0.3026	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11202 / 0 / 375	
Goodness-of-fit on F ²	1.031	
Final R indices [I > 2σ(I)]	R1 = 0.0198, wR2 = 0.0344	
R indices (all data)	R1 = 0.0283, wR2 = 0.0360	
Largest diff. peak and hole	1.068 and -0.826 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb7907. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ir(1)	2705(1)	1819(1)	388(1)	10(1)
P(1)	3961(1)	2751(1)	1527(1)	12(1)
P(2)	3207(1)	-510(1)	710(1)	13(1)
P(3)	1520(1)	2284(1)	826(1)	13(1)
C(1)	2618(1)	3750(2)	-300(1)	13(1)
C(2)	3361(1)	2819(2)	-353(1)	13(1)
C(3)	3293(1)	2208(2)	-1163(1)	16(1)
C(4)	3651(1)	3228(2)	-1653(1)	19(1)
C(5)	2983(1)	4473(2)	-2102(1)	20(1)
C(6)	2863(1)	5656(2)	-1555(1)	19(1)
C(7)	1928(1)	5607(2)	-1430(1)	19(1)
C(8)	1749(1)	4200(2)	-1073(1)	16(1)
C(9)	1622(1)	848(2)	-718(1)	17(1)
C(11)	4020(1)	2410(2)	2561(1)	18(1)
C(12)	5178(1)	2229(2)	1669(1)	20(1)
C(13)	4138(1)	4695(2)	1601(1)	19(1)
C(21)	3863(1)	-1247(2)	142(1)	24(1)
C(22)	2279(1)	-1887(2)	491(1)	22(1)
C(23)	3984(1)	-1111(2)	1759(1)	24(1)
C(31)	1374(1)	1252(2)	1644(1)	22(1)
C(32)	1525(1)	4105(2)	1212(1)	20(1)
C(33)	272(1)	2256(2)	46(1)	22(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for *jb7907*.

Ir(1)-C(1)	2.1494(14)
Ir(1)-C(9)	2.1637(14)
Ir(1)-C(2)	2.1664(13)
Ir(1)-P(3)	2.2838(4)
Ir(1)-P(1)	2.2938(4)
Ir(1)-P(2)	2.2946(4)
P(1)-C(11)	1.8274(16)
P(1)-C(12)	1.8280(16)
P(1)-C(13)	1.8297(16)
P(2)-C(21)	1.8243(16)
P(2)-C(22)	1.8263(16)
P(2)-C(23)	1.8269(17)
P(3)-C(33)	1.8237(16)
P(3)-C(32)	1.8302(16)
P(3)-C(31)	1.8316(16)
C(1)-C(2)	1.459(2)
C(1)-C(8)	1.512(2)
C(1)-H(1)	0.939(16)
C(2)-C(3)	1.510(2)
C(2)-H(2)	0.956(18)
C(3)-C(4)	1.534(2)
C(3)-H(3A)	0.970(18)
C(3)-H(3B)	0.96(2)
C(4)-C(5)	1.529(2)
C(4)-H(4A)	0.981(16)
C(4)-H(4B)	0.960(19)
C(5)-C(6)	1.531(2)
C(5)-H(5A)	0.999(18)
C(5)-H(5B)	1.040(18)
C(6)-C(7)	1.530(2)
C(6)-H(6A)	0.980(17)
C(6)-H(6B)	0.974(19)
C(7)-C(8)	1.531(2)
C(7)-H(7A)	0.992(18)

C(7)-H(7B)	0.99(2)
C(8)-H(8A)	0.983(19)
C(8)-H(8B)	0.944(18)
C(9)-H(9A)	0.972(17)
C(9)-H(9B)	0.958(19)
C(9)-H(9C)	0.955(19)
C(11)-H(11A)	0.98(2)
C(11)-H(11B)	0.96(2)
C(11)-H(11C)	0.929(18)
C(12)-H(12A)	0.94(2)
C(12)-H(12B)	0.96(2)
C(12)-H(12C)	0.94(2)
C(13)-H(13A)	0.96(2)
C(13)-H(13B)	0.995(18)
C(13)-H(13C)	0.971(18)
C(21)-H(21A)	0.95(2)
C(21)-H(21B)	0.96(2)
C(21)-H(21C)	1.01(2)
C(22)-H(22A)	1.00(2)
C(22)-H(22B)	0.93(2)
C(22)-H(22C)	0.93(2)
C(23)-H(23A)	1.01(2)
C(23)-H(23B)	0.92(2)
C(23)-H(23C)	0.954(19)
C(31)-H(31A)	0.96(2)
C(31)-H(31B)	0.99(2)
C(31)-H(31C)	0.95(2)
C(32)-H(32A)	0.956(19)
C(32)-H(32B)	0.970(19)
C(32)-H(32C)	0.970(19)
C(33)-H(33A)	0.977(19)
C(33)-H(33B)	0.95(2)
C(33)-H(33C)	0.90(2)
C(1)-Ir(1)-C(9)	89.61(6)
C(1)-Ir(1)-C(2)	39.51(5)

C(9)-Ir(1)-C(2)	89.94(6)
C(1)-Ir(1)-P(3)	99.50(4)
C(9)-Ir(1)-P(3)	88.76(4)
C(2)-Ir(1)-P(3)	139.00(4)
C(1)-Ir(1)-P(1)	90.78(4)
C(9)-Ir(1)-P(1)	174.58(4)
C(2)-Ir(1)-P(1)	86.92(4)
P(3)-Ir(1)-P(1)	96.505(14)
C(1)-Ir(1)-P(2)	150.45(4)
C(9)-Ir(1)-P(2)	82.95(4)
C(2)-Ir(1)-P(2)	111.64(4)
P(3)-Ir(1)-P(2)	108.847(13)
P(1)-Ir(1)-P(2)	94.091(13)
C(11)-P(1)-C(12)	101.21(8)
C(11)-P(1)-C(13)	98.99(8)
C(12)-P(1)-C(13)	98.29(8)
C(11)-P(1)-Ir(1)	119.46(5)
C(12)-P(1)-Ir(1)	116.29(6)
C(13)-P(1)-Ir(1)	118.82(5)
C(21)-P(2)-C(22)	99.81(9)
C(21)-P(2)-C(23)	100.24(9)
C(22)-P(2)-C(23)	96.52(9)
C(21)-P(2)-Ir(1)	114.90(6)
C(22)-P(2)-Ir(1)	117.76(6)
C(23)-P(2)-Ir(1)	123.42(6)
C(33)-P(3)-C(32)	97.89(8)
C(33)-P(3)-C(31)	99.23(8)
C(32)-P(3)-C(31)	100.03(8)
C(33)-P(3)-Ir(1)	117.31(6)
C(32)-P(3)-Ir(1)	115.06(5)
C(31)-P(3)-Ir(1)	123.03(6)
C(2)-C(1)-C(8)	120.93(12)
C(2)-C(1)-Ir(1)	70.87(8)
C(8)-C(1)-Ir(1)	124.75(10)
C(2)-C(1)-H(1)	115.6(10)
C(8)-C(1)-H(1)	106.8(10)

Ir(1)-C(1)-H(1)	114.6(10)
C(1)-C(2)-C(3)	122.70(13)
C(1)-C(2)-Ir(1)	69.62(7)
C(3)-C(2)-Ir(1)	123.41(10)
C(1)-C(2)-H(2)	116.0(10)
C(3)-C(2)-H(2)	108.3(11)
Ir(1)-C(2)-H(2)	112.5(11)
C(2)-C(3)-C(4)	113.98(13)
C(2)-C(3)-H(3A)	111.8(11)
C(4)-C(3)-H(3A)	108.8(10)
C(2)-C(3)-H(3B)	107.7(12)
C(4)-C(3)-H(3B)	109.7(12)
H(3A)-C(3)-H(3B)	104.5(15)
C(5)-C(4)-C(3)	116.77(12)
C(5)-C(4)-H(4A)	106.6(10)
C(3)-C(4)-H(4A)	109.8(10)
C(5)-C(4)-H(4B)	110.0(11)
C(3)-C(4)-H(4B)	106.5(11)
H(4A)-C(4)-H(4B)	106.7(14)
C(4)-C(5)-C(6)	116.50(13)
C(4)-C(5)-H(5A)	109.5(10)
C(6)-C(5)-H(5A)	108.8(10)
C(4)-C(5)-H(5B)	108.0(10)
C(6)-C(5)-H(5B)	107.6(10)
H(5A)-C(5)-H(5B)	105.8(14)
C(7)-C(6)-C(5)	115.81(13)
C(7)-C(6)-H(6A)	110.1(10)
C(5)-C(6)-H(6A)	107.8(10)
C(7)-C(6)-H(6B)	108.4(11)
C(5)-C(6)-H(6B)	109.8(12)
H(6A)-C(6)-H(6B)	104.3(15)
C(6)-C(7)-C(8)	115.04(13)
C(6)-C(7)-H(7A)	108.9(11)
C(8)-C(7)-H(7A)	108.3(11)
C(6)-C(7)-H(7B)	110.0(11)
C(8)-C(7)-H(7B)	109.8(11)

H(7A)-C(7)-H(7B)	104.1(15)
C(1)-C(8)-C(7)	111.94(12)
C(1)-C(8)-H(8A)	111.7(11)
C(7)-C(8)-H(8A)	107.5(11)
C(1)-C(8)-H(8B)	111.4(10)
C(7)-C(8)-H(8B)	107.5(10)
H(8A)-C(8)-H(8B)	106.5(15)
Ir(1)-C(9)-H(9A)	113.2(10)
Ir(1)-C(9)-H(9B)	113.4(11)
H(9A)-C(9)-H(9B)	105.3(15)
Ir(1)-C(9)-H(9C)	111.4(11)
H(9A)-C(9)-H(9C)	106.5(15)
H(9B)-C(9)-H(9C)	106.3(16)
P(1)-C(11)-H(11A)	111.9(12)
P(1)-C(11)-H(11B)	112.8(12)
H(11A)-C(11)-H(11B)	106.7(17)
P(1)-C(11)-H(11C)	110.0(11)
H(11A)-C(11)-H(11C)	109.1(16)
H(11B)-C(11)-H(11C)	106.2(16)
P(1)-C(12)-H(12A)	111.0(12)
P(1)-C(12)-H(12B)	108.3(12)
H(12A)-C(12)-H(12B)	109.9(17)
P(1)-C(12)-H(12C)	109.9(12)
H(12A)-C(12)-H(12C)	108.2(17)
H(12B)-C(12)-H(12C)	109.5(18)
P(1)-C(13)-H(13A)	109.7(12)
P(1)-C(13)-H(13B)	109.2(10)
H(13A)-C(13)-H(13B)	108.1(15)
P(1)-C(13)-H(13C)	109.3(11)
H(13A)-C(13)-H(13C)	109.6(16)
H(13B)-C(13)-H(13C)	110.9(14)
P(2)-C(21)-H(21A)	109.7(13)
P(2)-C(21)-H(21B)	109.2(13)
H(21A)-C(21)-H(21B)	108.0(18)
P(2)-C(21)-H(21C)	112.7(12)
H(21A)-C(21)-H(21C)	106.4(17)

H(21B)-C(21)-H(21C)	110.8(18)
P(2)-C(22)-H(22A)	111.9(13)
P(2)-C(22)-H(22B)	107.7(13)
H(22A)-C(22)-H(22B)	112.2(18)
P(2)-C(22)-H(22C)	110.2(13)
H(22A)-C(22)-H(22C)	106.9(18)
H(22B)-C(22)-H(22C)	107.8(19)
P(2)-C(23)-H(23A)	109.4(12)
P(2)-C(23)-H(23B)	110.8(14)
H(23A)-C(23)-H(23B)	109.6(18)
P(2)-C(23)-H(23C)	112.8(11)
H(23A)-C(23)-H(23C)	108.6(16)
H(23B)-C(23)-H(23C)	105.6(18)
P(3)-C(31)-H(31A)	112.8(13)
P(3)-C(31)-H(31B)	109.6(12)
H(31A)-C(31)-H(31B)	111.1(18)
P(3)-C(31)-H(31C)	106.7(12)
H(31A)-C(31)-H(31C)	107.6(17)
H(31B)-C(31)-H(31C)	108.8(16)
P(3)-C(32)-H(32A)	109.6(11)
P(3)-C(32)-H(32B)	110.4(11)
H(32A)-C(32)-H(32B)	109.5(15)
P(3)-C(32)-H(32C)	113.0(11)
H(32A)-C(32)-H(32C)	106.2(15)
H(32B)-C(32)-H(32C)	108.0(16)
P(3)-C(33)-H(33A)	110.7(11)
P(3)-C(33)-H(33B)	109.6(13)
H(33A)-C(33)-H(33B)	109.7(17)
P(3)-C(33)-H(33C)	109.5(14)
H(33A)-C(33)-H(33C)	108.7(18)
H(33B)-C(33)-H(33C)	109(2)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb7907. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ir(1)	9(1)	11(1)	9(1)	0(1)	3(1)	-1(1)
P(1)	11(1)	13(1)	11(1)	0(1)	3(1)	-2(1)
P(2)	13(1)	12(1)	15(1)	0(1)	6(1)	0(1)
P(3)	12(1)	14(1)	13(1)	0(1)	6(1)	-1(1)
C(1)	16(1)	13(1)	11(1)	1(1)	6(1)	-2(1)
C(2)	12(1)	14(1)	13(1)	1(1)	5(1)	-2(1)
C(3)	17(1)	18(1)	15(1)	-1(1)	8(1)	-1(1)
C(4)	21(1)	24(1)	18(1)	-1(1)	12(1)	-2(1)
C(5)	22(1)	24(1)	14(1)	2(1)	8(1)	-3(1)
C(6)	19(1)	19(1)	17(1)	4(1)	6(1)	-4(1)
C(7)	19(1)	19(1)	18(1)	6(1)	6(1)	2(1)
C(8)	14(1)	18(1)	14(1)	3(1)	4(1)	-1(1)
C(9)	15(1)	18(1)	14(1)	-3(1)	4(1)	-4(1)
C(11)	20(1)	20(1)	13(1)	1(1)	5(1)	-3(1)
C(12)	12(1)	25(1)	19(1)	3(1)	3(1)	-2(1)
C(13)	20(1)	16(1)	17(1)	0(1)	4(1)	-5(1)
C(21)	26(1)	22(1)	29(1)	1(1)	16(1)	5(1)
C(22)	19(1)	14(1)	33(1)	0(1)	11(1)	-4(1)
C(23)	28(1)	17(1)	21(1)	5(1)	4(1)	1(1)
C(31)	27(1)	23(1)	23(1)	4(1)	16(1)	-1(1)
C(32)	22(1)	17(1)	25(1)	-3(1)	14(1)	1(1)
C(33)	12(1)	31(1)	22(1)	-2(1)	7(1)	-1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for jb7907.

	x	y	z	U(eq)
H(1)	2846(11)	4575(18)	27(10)	10(4)
H(2)	4016(13)	3100(18)	-29(11)	18(5)
H(3A)	2640(13)	1906(17)	-1519(11)	16(4)
H(3B)	3666(14)	1340(20)	-1040(12)	26(5)
H(4A)	4271(12)	3654(18)	-1281(10)	10(4)
H(4B)	3777(12)	2650(20)	-2043(11)	20(5)
H(5A)	2330(13)	4093(19)	-2471(11)	21(5)
H(5B)	3251(12)	4945(19)	-2494(11)	19(4)
H(6A)	3426(12)	5618(18)	-1017(11)	17(4)
H(6B)	2909(14)	6590(20)	-1779(12)	26(5)
H(7A)	1372(13)	5780(20)	-1970(12)	23(5)
H(7B)	1908(13)	6420(20)	-1079(12)	24(5)
H(8A)	1173(13)	4330(20)	-962(12)	29(5)
H(8B)	1586(12)	3498(19)	-1492(11)	13(4)
H(9A)	1170(12)	241(19)	-606(10)	15(4)
H(9B)	1889(13)	250(20)	-1007(12)	27(5)
H(9C)	1243(14)	1560(20)	-1106(12)	23(5)
H(11A)	4608(15)	2810(20)	2996(13)	30(5)
H(11B)	4012(14)	1400(20)	2678(13)	33(6)
H(11C)	3485(13)	2808(19)	2606(11)	17(4)
H(12A)	5648(14)	2660(20)	2140(13)	29(5)
H(12B)	5265(14)	2510(20)	1187(13)	29(5)
H(12C)	5252(14)	1230(20)	1735(12)	34(6)
H(13A)	3570(14)	5150(20)	1589(12)	32(5)
H(13B)	4245(12)	5038(18)	1115(11)	16(4)
H(13C)	4687(13)	4930(20)	2117(12)	23(5)
H(21A)	4454(15)	-750(20)	291(13)	39(6)
H(21B)	3486(15)	-1110(20)	-440(14)	38(6)
H(21C)	4036(15)	-2290(20)	273(13)	38(6)
H(22A)	2567(16)	-2870(30)	638(14)	43(6)

H(22B)	1854(16)	-1810(20)	-68(15)	36(6)
H(22C)	1927(16)	-1720(20)	804(14)	39(6)
H(23A)	4139(14)	-2160(20)	1746(13)	32(6)
H(23B)	3685(16)	-980(20)	2110(14)	44(6)
H(23C)	4577(14)	-590(20)	2000(12)	25(5)
H(31A)	842(16)	1580(20)	1754(14)	42(6)
H(31B)	1988(15)	1270(20)	2155(13)	31(5)
H(31C)	1241(13)	290(20)	1450(12)	29(5)
H(32A)	1515(12)	4780(20)	804(12)	22(5)
H(32B)	2097(14)	4260(20)	1724(12)	27(5)
H(32C)	962(14)	4310(20)	1317(12)	28(5)
H(33A)	-170(13)	2570(20)	285(11)	22(5)
H(33B)	107(15)	1310(30)	-169(14)	41(6)
H(33C)	210(16)	2850(20)	-372(14)	37(6)

Table 6. Torsion angles [$^{\circ}$] for jb7907.

C(1)-Ir(1)-P(1)-C(11)	140.88(7)
C(9)-Ir(1)-P(1)-C(11)	-125.0(5)
C(2)-Ir(1)-P(1)-C(11)	-179.78(7)
P(3)-Ir(1)-P(1)-C(11)	41.23(7)
P(2)-Ir(1)-P(1)-C(11)	-68.29(6)
C(1)-Ir(1)-P(1)-C(12)	-97.24(7)
C(9)-Ir(1)-P(1)-C(12)	-3.2(5)
C(2)-Ir(1)-P(1)-C(12)	-57.91(7)
P(3)-Ir(1)-P(1)-C(12)	163.10(6)
P(2)-Ir(1)-P(1)-C(12)	53.59(6)
C(1)-Ir(1)-P(1)-C(13)	19.85(7)
C(9)-Ir(1)-P(1)-C(13)	113.9(5)
C(2)-Ir(1)-P(1)-C(13)	59.19(7)
P(3)-Ir(1)-P(1)-C(13)	-79.80(6)
P(2)-Ir(1)-P(1)-C(13)	170.68(6)
C(1)-Ir(1)-P(2)-C(21)	-0.90(11)
C(9)-Ir(1)-P(2)-C(21)	75.68(8)
C(2)-Ir(1)-P(2)-C(21)	-11.45(8)
P(3)-Ir(1)-P(2)-C(21)	161.94(7)
P(1)-Ir(1)-P(2)-C(21)	-99.76(7)
C(1)-Ir(1)-P(2)-C(22)	-118.07(11)
C(9)-Ir(1)-P(2)-C(22)	-41.49(8)
C(2)-Ir(1)-P(2)-C(22)	-128.61(8)
P(3)-Ir(1)-P(2)-C(22)	44.77(7)
P(1)-Ir(1)-P(2)-C(22)	143.08(7)
C(1)-Ir(1)-P(2)-C(23)	121.86(11)
C(9)-Ir(1)-P(2)-C(23)	-161.55(8)
C(2)-Ir(1)-P(2)-C(23)	111.32(8)
P(3)-Ir(1)-P(2)-C(23)	-75.29(8)
P(1)-Ir(1)-P(2)-C(23)	23.01(8)
C(1)-Ir(1)-P(3)-C(33)	70.57(8)
C(9)-Ir(1)-P(3)-C(33)	-18.83(8)
C(2)-Ir(1)-P(3)-C(33)	69.66(9)
P(1)-Ir(1)-P(3)-C(33)	162.46(7)

P(2)-Ir(1)-P(3)-C(33)	-100.95(7)
C(1)-Ir(1)-P(3)-C(32)	-43.76(8)
C(9)-Ir(1)-P(3)-C(32)	-133.15(8)
C(2)-Ir(1)-P(3)-C(32)	-44.67(9)
P(1)-Ir(1)-P(3)-C(32)	48.13(7)
P(2)-Ir(1)-P(3)-C(32)	144.72(7)
C(1)-Ir(1)-P(3)-C(31)	-165.99(8)
C(9)-Ir(1)-P(3)-C(31)	104.61(8)
C(2)-Ir(1)-P(3)-C(31)	-166.90(9)
P(1)-Ir(1)-P(3)-C(31)	-74.10(7)
P(2)-Ir(1)-P(3)-C(31)	22.49(7)
C(9)-Ir(1)-C(1)-C(2)	-90.39(9)
P(3)-Ir(1)-C(1)-C(2)	-179.06(7)
P(1)-Ir(1)-C(1)-C(2)	84.21(8)
P(2)-Ir(1)-C(1)-C(2)	-15.51(13)
C(9)-Ir(1)-C(1)-C(8)	24.55(12)
C(2)-Ir(1)-C(1)-C(8)	114.94(15)
P(3)-Ir(1)-C(1)-C(8)	-64.13(12)
P(1)-Ir(1)-C(1)-C(8)	-160.86(11)
P(2)-Ir(1)-C(1)-C(8)	99.43(12)
C(8)-C(1)-C(2)-C(3)	-2.3(2)
Ir(1)-C(1)-C(2)-C(3)	117.36(13)
C(8)-C(1)-C(2)-Ir(1)	-119.70(13)
C(9)-Ir(1)-C(2)-C(1)	89.45(9)
P(3)-Ir(1)-C(2)-C(1)	1.41(11)
P(1)-Ir(1)-C(2)-C(1)	-94.97(8)
P(2)-Ir(1)-C(2)-C(1)	171.84(7)
C(1)-Ir(1)-C(2)-C(3)	-116.44(15)
C(9)-Ir(1)-C(2)-C(3)	-26.99(12)
P(3)-Ir(1)-C(2)-C(3)	-115.03(11)
P(1)-Ir(1)-C(2)-C(3)	148.59(12)
P(2)-Ir(1)-C(2)-C(3)	55.41(12)
C(1)-C(2)-C(3)-C(4)	83.67(17)
Ir(1)-C(2)-C(3)-C(4)	169.52(10)
C(2)-C(3)-C(4)-C(5)	-75.24(18)
C(3)-C(4)-C(5)-C(6)	69.64(18)

C(4)-C(5)-C(6)-C(7)	-101.68(16)
C(5)-C(6)-C(7)-C(8)	56.51(19)
C(2)-C(1)-C(8)-C(7)	-91.08(17)
Ir(1)-C(1)-C(8)-C(7)	-178.26(10)
C(6)-C(7)-C(8)-C(1)	50.68(18)

Projection view of the molecule with 50% thermal ellipsoids:

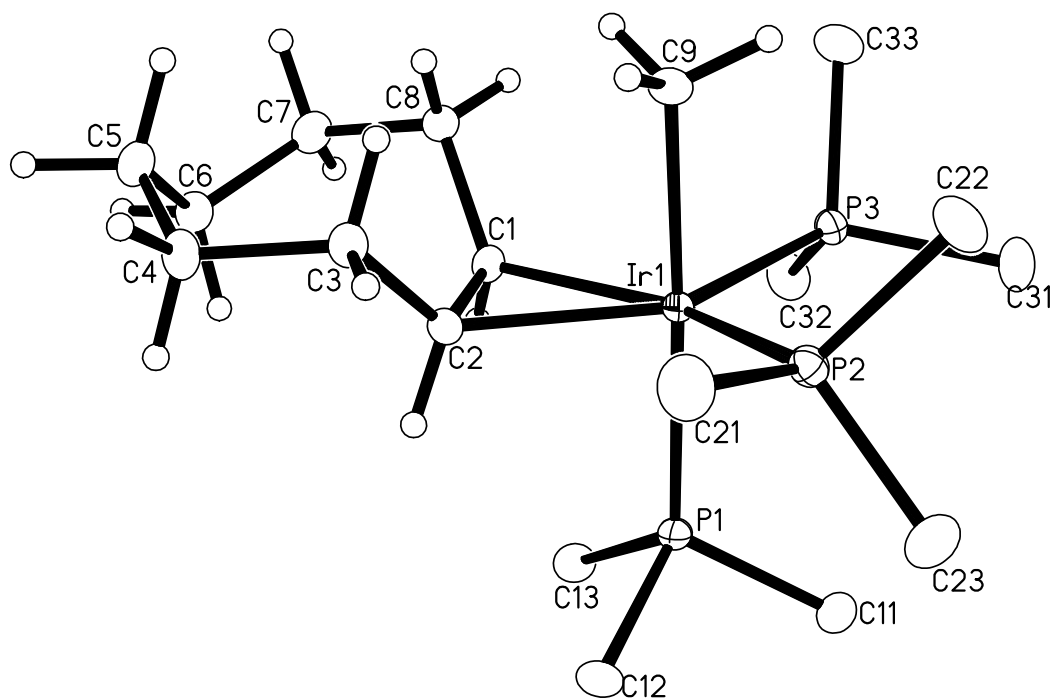


Table 1. Crystal data and structure refinement for jb16907 (compound *fac*-5-acetone).

Identification code	j16907/lt	
Empirical formula	C ₂₀ H ₄₉ Cl Ir O P ₃ Si	
Formula weight	654.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 9.3183(7) Å	α = 90°.
	b = 18.2326(15) Å	β = 104.074(4)°.
	c = 17.2933(15) Å	γ = 90°.
Volume	2849.9(4) Å ³	
Z	4	
Density (calculated)	1.525 Mg/m ³	
Absorption coefficient	4.998 mm ⁻¹	
F(000)	1320	
Crystal size	0.34 x 0.21 x 0.19 mm ³	
Theta range for data collection	3.02 to 36.32°.	
Index ranges	-15 ≤ h ≤ 10, -30 ≤ k ≤ 29, -26 ≤ l ≤ 28	
Reflections collected	115902	
Independent reflections	13806 [R(int) = 0.052]	
Completeness to theta = 36.32°	99.9 %	
Absorption correction	Numerical	
Max. and min. transmission	0.4479 and 0.3488	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	13806 / 0 / 263	
Goodness-of-fit on F ²	1.038	
Final R indices [I > 2σ(I)]	R1 = 0.0256, wR2 = 0.0505	
R indices (all data)	R1 = 0.0387, wR2 = 0.0534	
Largest diff. peak and hole	1.137 and -1.344 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb16907. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ir(1)	2281(1)	8688(1)	1540(1)	12(1)
Cl(1)	-354(1)	7184(1)	1931(1)	33(1)
P(1)	1269(1)	9023(1)	2578(1)	16(1)
P(2)	3957(1)	9663(1)	1575(1)	15(1)
P(3)	4079(1)	7862(1)	2208(1)	18(1)
Si(1)	516(1)	7764(1)	1057(1)	18(1)
C(1)	2464(2)	8732(1)	-1709(1)	20(1)
C(2)	2868(2)	8453(1)	-970(1)	17(1)
C(3)	2225(2)	8718(1)	-315(1)	14(1)
C(4)	2726(2)	8452(1)	431(1)	14(1)
C(5)	4015(2)	7852(1)	-809(1)	25(1)
C(6)	1038(2)	9292(1)	-542(1)	19(1)
C(7)	1096(2)	6934(1)	558(1)	30(1)
C(8)	-1258(2)	8053(1)	351(1)	27(1)
C(11)	1589(2)	8497(1)	3499(1)	26(1)
C(12)	-746(2)	9069(1)	2312(1)	26(1)
C(13)	1649(2)	9947(1)	2982(1)	29(1)
C(21)	4983(2)	10093(1)	2504(1)	27(1)
C(22)	3191(2)	10471(1)	1020(1)	25(1)
C(23)	5478(2)	9458(1)	1115(1)	25(1)
C(31)	5539(2)	8206(1)	3028(1)	27(1)
C(32)	5203(2)	7405(1)	1620(1)	30(1)
C(33)	3502(2)	7068(1)	2702(1)	29(1)
O(1)	1201(2)	10447(1)	5803(1)	59(1)
C(1S)	1903(3)	9928(1)	5663(1)	34(1)
C(2S)	1539(3)	9171(2)	5851(2)	49(1)
C(3S)	3159(3)	10018(2)	5274(2)	45(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for jb16907.

Ir(1)-C(4)	2.1033(17)
Ir(1)-P(1)	2.3046(5)
Ir(1)-P(3)	2.3383(5)
Ir(1)-P(2)	2.3573(5)
Ir(1)-Si(1)	2.3609(5)
Ir(1)-H(1)	1.60(2)
Cl(1)-Si(1)	2.1582(7)
P(1)-C(11)	1.820(2)
P(1)-C(12)	1.8225(19)
P(1)-C(13)	1.825(2)
P(2)-C(22)	1.8083(19)
P(2)-C(23)	1.8247(19)
P(2)-C(21)	1.834(2)
P(3)-C(31)	1.822(2)
P(3)-C(33)	1.827(2)
P(3)-C(32)	1.829(2)
Si(1)-C(8)	1.877(2)
Si(1)-C(7)	1.885(2)
C(1)-C(2)	1.342(3)
C(1)-H(1A)	0.9500
C(1)-H(1B)	0.9500
C(2)-C(3)	1.485(2)
C(2)-C(5)	1.509(3)
C(3)-C(4)	1.349(3)
C(3)-C(6)	1.504(2)
C(4)-H(4)	0.9500
C(5)-H(6A)	0.9800
C(5)-H(6B)	0.9800
C(5)-H(6C)	0.9800
C(6)-H(5A)	0.9800
C(6)-H(5B)	0.9800
C(6)-H(5C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800

C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
O(1)-C(1S)	1.207(3)
C(1S)-C(2S)	1.478(4)
C(1S)-C(3S)	1.494(3)
C(2S)-H(2S1)	0.9800
C(2S)-H(2S2)	0.9800

C(2S)-H(2S3)	0.9800
C(3S)-H(3S1)	0.9800
C(3S)-H(3S2)	0.9800
C(3S)-H(3S3)	0.9800
C(4)-Ir(1)-P(1)	166.83(5)
C(4)-Ir(1)-P(3)	92.44(5)
P(1)-Ir(1)-P(3)	99.517(18)
C(4)-Ir(1)-P(2)	84.33(5)
P(1)-Ir(1)-P(2)	100.056(17)
P(3)-Ir(1)-P(2)	94.735(18)
C(4)-Ir(1)-Si(1)	78.85(5)
P(1)-Ir(1)-Si(1)	94.728(18)
P(3)-Ir(1)-Si(1)	93.939(19)
P(2)-Ir(1)-Si(1)	161.362(18)
C(4)-Ir(1)-H(1)	86.0(8)
P(1)-Ir(1)-H(1)	81.9(8)
P(3)-Ir(1)-H(1)	177.8(8)
P(2)-Ir(1)-H(1)	86.6(8)
Si(1)-Ir(1)-H(1)	84.3(8)
C(11)-P(1)-C(12)	100.68(10)
C(11)-P(1)-C(13)	100.14(10)
C(12)-P(1)-C(13)	98.38(10)
C(11)-P(1)-Ir(1)	122.08(7)
C(12)-P(1)-Ir(1)	114.05(7)
C(13)-P(1)-Ir(1)	117.65(7)
C(22)-P(2)-C(23)	100.58(10)
C(22)-P(2)-C(21)	99.85(10)
C(23)-P(2)-C(21)	100.08(10)
C(22)-P(2)-Ir(1)	115.29(7)
C(23)-P(2)-Ir(1)	114.49(7)
C(21)-P(2)-Ir(1)	123.08(7)
C(31)-P(3)-C(33)	99.06(10)
C(31)-P(3)-C(32)	99.74(10)
C(33)-P(3)-C(32)	99.96(10)
C(31)-P(3)-Ir(1)	118.21(7)

C(33)-P(3)-Ir(1)	119.00(7)
C(32)-P(3)-Ir(1)	117.18(7)
C(8)-Si(1)-C(7)	103.47(10)
C(8)-Si(1)-Cl(1)	99.92(7)
C(7)-Si(1)-Cl(1)	97.26(7)
C(8)-Si(1)-Ir(1)	117.20(7)
C(7)-Si(1)-Ir(1)	118.81(7)
Cl(1)-Si(1)-Ir(1)	116.75(3)
C(2)-C(1)-H(1A)	120.0
C(2)-C(1)-H(1B)	120.0
H(1A)-C(1)-H(1B)	120.0
C(1)-C(2)-C(3)	122.15(17)
C(1)-C(2)-C(5)	118.19(16)
C(3)-C(2)-C(5)	119.66(17)
C(4)-C(3)-C(2)	120.10(16)
C(4)-C(3)-C(6)	124.19(16)
C(2)-C(3)-C(6)	115.70(16)
C(3)-C(4)-Ir(1)	134.29(13)
C(3)-C(4)-H(4)	112.9
Ir(1)-C(4)-H(4)	112.9
C(2)-C(5)-H(6A)	109.5
C(2)-C(5)-H(6B)	109.5
H(6A)-C(5)-H(6B)	109.5
C(2)-C(5)-H(6C)	109.5
H(6A)-C(5)-H(6C)	109.5
H(6B)-C(5)-H(6C)	109.5
C(3)-C(6)-H(5A)	109.5
C(3)-C(6)-H(5B)	109.5
H(5A)-C(6)-H(5B)	109.5
C(3)-C(6)-H(5C)	109.5
H(5A)-C(6)-H(5C)	109.5
H(5B)-C(6)-H(5C)	109.5
Si(1)-C(7)-H(7A)	109.5
Si(1)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
Si(1)-C(7)-H(7C)	109.5

H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
Si(1)-C(8)-H(8A)	109.5
Si(1)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
Si(1)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
P(1)-C(11)-H(11A)	109.5
P(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
P(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
P(1)-C(12)-H(12A)	109.5
P(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
P(1)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
P(1)-C(13)-H(13A)	109.5
P(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
P(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
P(2)-C(21)-H(21A)	109.5
P(2)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
P(2)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
P(2)-C(22)-H(22A)	109.5
P(2)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
P(2)-C(22)-H(22C)	109.5

H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
P(2)-C(23)-H(23A)	109.5
P(2)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
P(2)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
P(3)-C(31)-H(31A)	109.5
P(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
P(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
P(3)-C(32)-H(32A)	109.5
P(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
P(3)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
P(3)-C(33)-H(33A)	109.5
P(3)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
P(3)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
O(1)-C(1S)-C(2S)	121.6(2)
O(1)-C(1S)-C(3S)	121.8(2)
C(2S)-C(1S)-C(3S)	116.6(2)
C(1S)-C(2S)-H(2S1)	109.5
C(1S)-C(2S)-H(2S2)	109.5
H(2S1)-C(2S)-H(2S2)	109.5
C(1S)-C(2S)-H(2S3)	109.5
H(2S1)-C(2S)-H(2S3)	109.5
H(2S2)-C(2S)-H(2S3)	109.5
C(1S)-C(3S)-H(3S1)	109.5

C(1S)-C(3S)-H(3S2)	109.5
H(3S1)-C(3S)-H(3S2)	109.5
C(1S)-C(3S)-H(3S3)	109.5
H(3S1)-C(3S)-H(3S3)	109.5
H(3S2)-C(3S)-H(3S3)	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb16907. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ir(1)	10(1)	11(1)	14(1)	1(1)	3(1)	1(1)
Cl(1)	34(1)	33(1)	34(1)	5(1)	11(1)	-10(1)
P(1)	16(1)	18(1)	16(1)	1(1)	6(1)	0(1)
P(2)	12(1)	14(1)	18(1)	0(1)	3(1)	-1(1)
P(3)	16(1)	16(1)	21(1)	3(1)	1(1)	4(1)
Si(1)	16(1)	15(1)	22(1)	1(1)	3(1)	-3(1)
C(1)	20(1)	23(1)	19(1)	-5(1)	8(1)	-5(1)
C(2)	13(1)	17(1)	21(1)	-5(1)	6(1)	-4(1)
C(3)	12(1)	14(1)	18(1)	-2(1)	5(1)	0(1)
C(4)	13(1)	12(1)	19(1)	-1(1)	5(1)	0(1)
C(5)	24(1)	28(1)	25(1)	-6(1)	9(1)	8(1)
C(6)	18(1)	21(1)	16(1)	2(1)	4(1)	5(1)
C(7)	34(1)	20(1)	35(1)	-5(1)	8(1)	-6(1)
C(8)	20(1)	29(1)	28(1)	4(1)	-2(1)	-8(1)
C(11)	25(1)	35(1)	19(1)	6(1)	7(1)	1(1)
C(12)	19(1)	34(1)	27(1)	2(1)	9(1)	3(1)
C(13)	36(1)	24(1)	33(1)	-6(1)	19(1)	-3(1)
C(21)	28(1)	29(1)	23(1)	-3(1)	5(1)	-12(1)
C(22)	20(1)	18(1)	35(1)	7(1)	4(1)	-2(1)
C(23)	16(1)	26(1)	35(1)	-3(1)	10(1)	-5(1)
C(31)	23(1)	26(1)	27(1)	4(1)	-4(1)	4(1)
C(32)	26(1)	30(1)	34(1)	6(1)	8(1)	16(1)
C(33)	31(1)	19(1)	34(1)	12(1)	2(1)	4(1)
O(1)	77(2)	47(1)	57(1)	-4(1)	25(1)	20(1)
C(1S)	42(1)	36(1)	26(1)	1(1)	10(1)	3(1)
C(2S)	54(2)	42(2)	54(2)	15(1)	20(1)	3(1)
C(3S)	51(2)	54(2)	33(1)	-4(1)	16(1)	-12(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for jb16907.

	x	y	z	U(eq)
H(1A)	1744	9111	-1827	24
H(1B)	2897	8550	-2114	24
H(4)	3440	8074	461	17
H(6A)	4310	7735	-1302	38
H(6B)	3598	7414	-619	38
H(6C)	4882	8016	-403	38
H(5A)	643	9408	-80	28
H(5B)	239	9107	-977	28
H(5C)	1458	9737	-719	28
H(7A)	269	6588	418	44
H(7B)	1938	6697	922	44
H(7C)	1383	7087	73	44
H(8A)	-1050	8235	-144	40
H(8B)	-1720	8444	596	40
H(8C)	-1930	7633	232	40
H(11A)	1032	8716	3854	39
H(11B)	2647	8501	3761	39
H(11C)	1260	7990	3378	39
H(12A)	-1154	8579	2169	39
H(12B)	-1075	9401	1857	39
H(12C)	-1092	9254	2767	39
H(13A)	1435	10303	2545	44
H(13B)	2693	9984	3267	44
H(13C)	1024	10049	3351	44
H(21A)	5898	10309	2423	40
H(21B)	5226	9721	2926	40
H(21C)	4374	10477	2660	40
H(22A)	3984	10826	1025	37
H(22B)	2451	10692	1266	37
H(22C)	2722	10334	469	37

H(23A)	5078	9294	565	37
H(23B)	6097	9070	1417	37
H(23C)	6076	9901	1115	37
H(31A)	5097	8441	3424	41
H(31B)	6139	8564	2824	41
H(31C)	6167	7797	3277	41
H(32A)	5728	7774	1381	45
H(32B)	4561	7115	1196	45
H(32C)	5921	7081	1966	45
H(33A)	4361	6755	2918	43
H(33B)	2758	6789	2317	43
H(33C)	3078	7235	3138	43
H(2S1)	874	9182	6211	73
H(2S2)	2450	8910	6108	73
H(2S3)	1051	8916	5357	73
H(3S1)	3327	10541	5200	68
H(3S2)	2919	9772	4755	68
H(3S3)	4055	9800	5613	68
H(1)	1030(20)	9231(12)	1057(13)	28(6)

Table 6. Torsion angles [°] for jb16907.

C(4)-Ir(1)-P(1)-C(11)	139.3(2)
P(3)-Ir(1)-P(1)-C(11)	-15.60(9)
P(2)-Ir(1)-P(1)-C(11)	-112.19(9)
Si(1)-Ir(1)-P(1)-C(11)	79.20(9)
C(4)-Ir(1)-P(1)-C(12)	18.0(2)
P(3)-Ir(1)-P(1)-C(12)	-136.88(8)
P(2)-Ir(1)-P(1)-C(12)	126.53(8)
Si(1)-Ir(1)-P(1)-C(12)	-42.08(8)
C(4)-Ir(1)-P(1)-C(13)	-96.4(2)
P(3)-Ir(1)-P(1)-C(13)	108.66(9)
P(2)-Ir(1)-P(1)-C(13)	12.07(9)
Si(1)-Ir(1)-P(1)-C(13)	-156.53(9)
C(4)-Ir(1)-P(2)-C(22)	81.37(9)
P(1)-Ir(1)-P(2)-C(22)	-86.09(8)
P(3)-Ir(1)-P(2)-C(22)	173.36(8)
Si(1)-Ir(1)-P(2)-C(22)	55.89(10)
C(4)-Ir(1)-P(2)-C(23)	-34.63(9)
P(1)-Ir(1)-P(2)-C(23)	157.91(8)
P(3)-Ir(1)-P(2)-C(23)	57.36(8)
Si(1)-Ir(1)-P(2)-C(23)	-60.11(10)
C(4)-Ir(1)-P(2)-C(21)	-156.38(10)
P(1)-Ir(1)-P(2)-C(21)	36.16(9)
P(3)-Ir(1)-P(2)-C(21)	-64.40(9)
Si(1)-Ir(1)-P(2)-C(21)	178.13(9)
C(4)-Ir(1)-P(3)-C(31)	123.39(10)
P(1)-Ir(1)-P(3)-C(31)	-62.16(8)
P(2)-Ir(1)-P(3)-C(31)	38.88(8)
Si(1)-Ir(1)-P(3)-C(31)	-157.63(8)
C(4)-Ir(1)-P(3)-C(33)	-116.50(10)
P(1)-Ir(1)-P(3)-C(33)	57.95(9)
P(2)-Ir(1)-P(3)-C(33)	158.99(9)
Si(1)-Ir(1)-P(3)-C(33)	-37.52(9)
C(4)-Ir(1)-P(3)-C(32)	3.96(10)
P(1)-Ir(1)-P(3)-C(32)	178.41(9)

P(2)-Ir(1)-P(3)-C(32)	-80.55(9)
Si(1)-Ir(1)-P(3)-C(32)	82.94(9)
C(4)-Ir(1)-Si(1)-C(8)	-82.78(9)
P(1)-Ir(1)-Si(1)-C(8)	85.61(8)
P(3)-Ir(1)-Si(1)-C(8)	-174.49(8)
P(2)-Ir(1)-Si(1)-C(8)	-56.90(10)
C(4)-Ir(1)-Si(1)-C(7)	42.79(10)
P(1)-Ir(1)-Si(1)-C(7)	-148.83(9)
P(3)-Ir(1)-Si(1)-C(7)	-48.93(9)
P(2)-Ir(1)-Si(1)-C(7)	68.66(10)
C(4)-Ir(1)-Si(1)-Cl(1)	158.81(6)
P(1)-Ir(1)-Si(1)-Cl(1)	-32.81(3)
P(3)-Ir(1)-Si(1)-Cl(1)	67.10(3)
P(2)-Ir(1)-Si(1)-Cl(1)	-175.32(4)
C(1)-C(2)-C(3)-C(4)	-176.10(17)
C(5)-C(2)-C(3)-C(4)	3.9(3)
C(1)-C(2)-C(3)-C(6)	2.9(2)
C(5)-C(2)-C(3)-C(6)	-177.15(16)
C(2)-C(3)-C(4)-Ir(1)	175.77(13)
C(6)-C(3)-C(4)-Ir(1)	-3.1(3)
P(1)-Ir(1)-C(4)-C(3)	28.6(4)
P(3)-Ir(1)-C(4)-C(3)	-176.16(17)
P(2)-Ir(1)-C(4)-C(3)	-81.64(17)
Si(1)-Ir(1)-C(4)-C(3)	90.30(18)

Projection view of the molecule with 50% thermal ellipsoids (acetone solvate not shown):

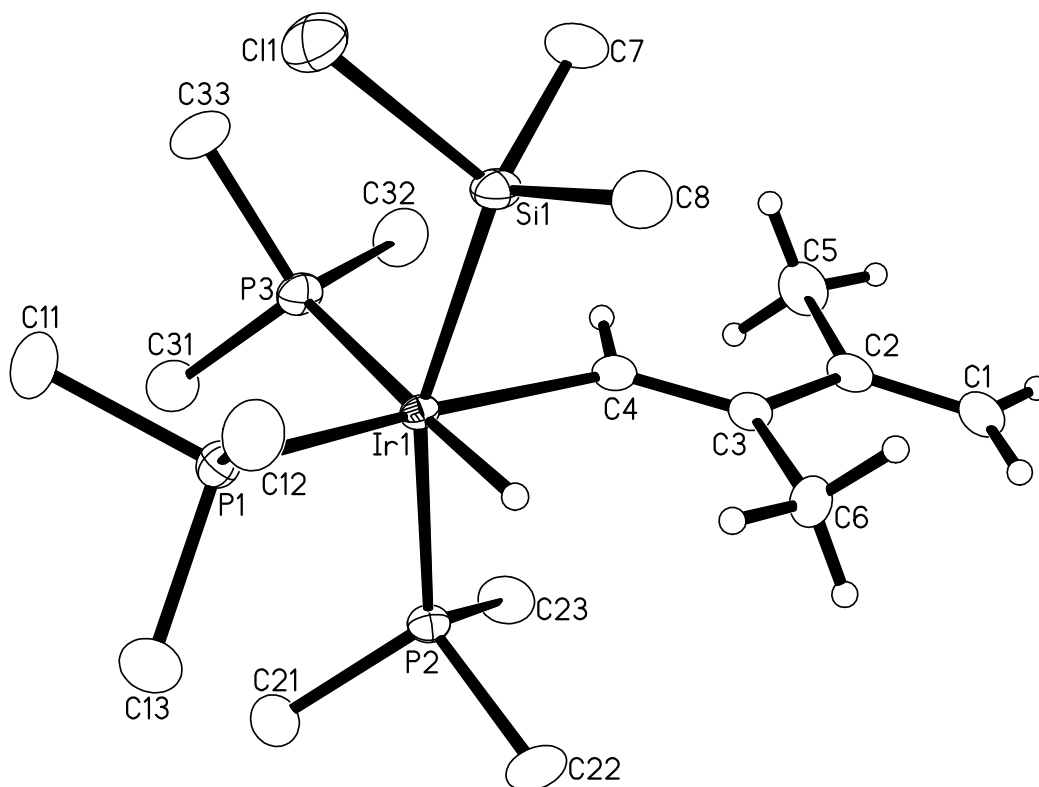


Table 1. Crystal data and structure refinement for jb13907 (compound *fac-6*).

Identification code	b13907/lt	
Empirical formula	C ₁₇ H ₄₃ Cl Ir P ₃ Si	
Formula weight	596.16	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁	
Unit cell dimensions	a = 9.3062(6) Å	α = 90°.
	b = 10.7212(7) Å	β = 94.122(3)°.
	c = 12.1508(7) Å	γ = 90°.
Volume	1209.19(13) Å ³	
Z	2	
Density (calculated)	1.637 Mg/m ³	
Absorption coefficient	5.878 mm ⁻¹	
F(000)	596	
Crystal size	0.18 x 0.15 x 0.14 mm ³	
Theta range for data collection	2.86 to 35.86°.	
Index ranges	-15 ≤ h ≤ 14, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19	
Reflections collected	67549	
Independent reflections	11139 [R(int) = 0.05]	
Completeness to theta = 35.86°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4933 and 0.4176	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11139 / 19 / 233	
Goodness-of-fit on F ²	1.034	
Final R indices [I > 2σ(I)]	R1 = 0.0261, wR2 = 0.0446	
R indices (all data)	R1 = 0.0317, wR2 = 0.0460	
Absolute structure parameter	0.073(6)	
Largest diff. peak and hole	0.996 and -1.017 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb13907. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ir(1)	2023(1)	5(1)	2478(1)	12(1)
P(1)	2165(2)	2215(1)	2371(1)	20(1)
P(2)	-407(1)	-124(2)	2768(1)	17(1)
P(3)	3007(1)	-5(2)	4302(1)	16(1)
Si(1)	2318(2)	-2184(1)	2337(1)	19(1)
C(1)	4065(2)	-6(7)	1774(2)	22(1)
C(3)	2522(3)	57(10)	51(2)	42(1)
C(4)	1425(2)	-13(7)	766(2)	21(1)
C(6)	2263(3)	-46(11)	-1153(2)	52(1)
C(11)	3904(6)	2908(6)	2744(5)	36(1)
C(12)	1739(8)	2927(5)	1037(5)	35(1)
C(21)	-1560(5)	1194(5)	2387(4)	38(1)
C(22)	-977(3)	-447(3)	4134(2)	33(1)
C(23)	-1413(4)	-1332(4)	1976(3)	34(1)
C(31)	2598(6)	1260(6)	5226(4)	28(1)
C(32)	2681(7)	-1301(5)	5245(4)	27(1)
C(33)	4969(2)	28(8)	4449(2)	24(1)
C(41)	1806(8)	-3004(5)	993(4)	32(1)
C(42)	4158(6)	-2870(6)	2738(5)	32(1)
Cl(1)	1061(5)	-3301(3)	3431(3)	33(1)
C(13)	1327(19)	3423(12)	3166(14)	33(1)
C(2)	3953(12)	-320(12)	573(7)	27(2)
C(5)	5254(16)	273(14)	-17(11)	38(3)
Cl(1')	937(7)	3172(5)	3310(6)	46(1)
C(43)	1100(20)	-3295(13)	3268(15)	46(1)
C(2')	4022(11)	217(11)	614(7)	22(2)
C(5')	5192(16)	-296(12)	-22(11)	31(3)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for jb13907.

Ir(1)-C(4)	2.1150(19)
Ir(1)-C(1)	2.140(2)
Ir(1)-P(2)	2.3176(6)
Ir(1)-P(3)	2.3361(5)
Ir(1)-Si(1)	2.3698(16)
Ir(1)-P(1)	2.3776(15)
P(1)-C(11)	1.809(6)
P(1)-C(12)	1.809(6)
P(1)-C(13)	1.825(13)
P(1)-Cl(1')	1.962(6)
P(2)-C(22)	1.813(3)
P(2)-C(21)	1.814(5)
P(2)-C(23)	1.831(4)
P(3)-C(31)	1.818(6)
P(3)-C(33)	1.823(2)
P(3)-C(32)	1.839(5)
Si(1)-C(41)	1.886(5)
Si(1)-C(42)	1.895(5)
Si(1)-C(43)	2.041(11)
Si(1)-Cl(1)	2.189(3)
C(1)-C(2')	1.427(10)
C(1)-C(2)	1.493(9)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(3)-C(4)	1.389(3)
C(3)-C(6)	1.470(3)
C(3)-C(2)	1.489(12)
C(3)-C(2')	1.519(10)
C(4)-H(4A)	0.9500
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800

C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(2)-C(5)	1.584(15)
C(2)-H(2A)	1.0000
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800

C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(2')-C(5')	1.485(16)
C(2')-H(2'A)	1.0000
C(5')-H(5'A)	0.9800
C(5')-H(5'B)	0.9800
C(5')-H(5'C)	0.9800
C(4)-Ir(1)-C(1)	77.59(8)
C(4)-Ir(1)-P(2)	87.59(6)
C(1)-Ir(1)-P(2)	164.75(8)
C(4)-Ir(1)-P(3)	172.18(6)
C(1)-Ir(1)-P(3)	94.63(6)
P(2)-Ir(1)-P(3)	100.136(19)
C(4)-Ir(1)-Si(1)	86.8(2)
C(1)-Ir(1)-Si(1)	81.67(19)
P(2)-Ir(1)-Si(1)	94.10(6)
P(3)-Ir(1)-Si(1)	91.41(6)
C(4)-Ir(1)-P(1)	88.1(2)
C(1)-Ir(1)-P(1)	85.92(19)
P(2)-Ir(1)-P(1)	97.24(6)
P(3)-Ir(1)-P(1)	92.13(6)
Si(1)-Ir(1)-P(1)	167.33(3)
C(11)-P(1)-C(12)	100.7(3)
C(11)-P(1)-C(13)	89.1(6)
C(12)-P(1)-C(13)	95.8(6)
C(11)-P(1)-Cl(1')	100.8(3)
C(12)-P(1)-Cl(1')	101.6(3)
C(13)-P(1)-Cl(1')	14.4(4)
C(11)-P(1)-Ir(1)	116.6(2)
C(12)-P(1)-Ir(1)	117.4(2)
C(13)-P(1)-Ir(1)	130.6(4)
Cl(1')-P(1)-Ir(1)	116.91(19)
C(22)-P(2)-C(21)	100.16(18)
C(22)-P(2)-C(23)	100.00(18)

C(21)-P(2)-C(23)	98.43(16)
C(22)-P(2)-Ir(1)	120.21(10)
C(21)-P(2)-Ir(1)	118.74(16)
C(23)-P(2)-Ir(1)	115.47(14)
C(31)-P(3)-C(33)	100.2(3)
C(31)-P(3)-C(32)	97.33(11)
C(33)-P(3)-C(32)	99.3(3)
C(31)-P(3)-Ir(1)	119.8(2)
C(33)-P(3)-Ir(1)	114.49(7)
C(32)-P(3)-Ir(1)	121.6(2)
C(41)-Si(1)-C(42)	102.0(3)
C(41)-Si(1)-C(43)	95.2(6)
C(42)-Si(1)-C(43)	99.1(6)
C(41)-Si(1)-Cl(1)	99.1(2)
C(42)-Si(1)-Cl(1)	98.3(2)
C(43)-Si(1)-Cl(1)	3.8(6)
C(41)-Si(1)-Ir(1)	120.1(2)
C(42)-Si(1)-Ir(1)	118.2(2)
C(43)-Si(1)-Ir(1)	117.8(4)
Cl(1)-Si(1)-Ir(1)	115.34(12)
C(2')-C(1)-C(2)	22.8(3)
C(2')-C(1)-Ir(1)	115.6(4)
C(2)-C(1)-Ir(1)	113.0(4)
C(2')-C(1)-H(1A)	87.4
C(2)-C(1)-H(1A)	109.0
Ir(1)-C(1)-H(1A)	109.0
C(2')-C(1)-H(1B)	124.6
C(2)-C(1)-H(1B)	109.0
Ir(1)-C(1)-H(1B)	109.0
H(1A)-C(1)-H(1B)	107.8
C(4)-C(3)-C(6)	122.9(3)
C(4)-C(3)-C(2)	113.2(4)
C(6)-C(3)-C(2)	118.8(5)
C(4)-C(3)-C(2')	114.7(4)
C(6)-C(3)-C(2')	122.4(4)
C(2)-C(3)-C(2')	22.2(3)

C(3)-C(4)-Ir(1)	117.46(17)
C(3)-C(4)-H(4A)	121.3
Ir(1)-C(4)-H(4A)	121.3
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
P(1)-C(11)-H(11A)	109.5
P(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
P(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
P(1)-C(12)-H(12A)	109.5
P(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
P(1)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
P(2)-C(21)-H(21A)	109.5
P(2)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
P(2)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
P(2)-C(22)-H(22A)	109.5
P(2)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
P(2)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
P(2)-C(23)-H(23A)	109.5
P(2)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5

P(2)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
P(3)-C(31)-H(31A)	109.5
P(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
P(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
P(3)-C(32)-H(32A)	109.5
P(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
P(3)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
P(3)-C(33)-H(33A)	109.5
P(3)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
P(3)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
Si(1)-C(41)-H(41A)	109.5
Si(1)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
Si(1)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
Si(1)-C(42)-H(42A)	109.5
Si(1)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
Si(1)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
P(1)-C(13)-H(13A)	109.5
P(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5

P(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(3)-C(2)-C(1)	110.6(7)
C(3)-C(2)-C(5)	112.8(10)
C(1)-C(2)-C(5)	110.5(9)
C(3)-C(2)-H(2A)	107.6
C(1)-C(2)-H(2A)	107.6
C(5)-C(2)-H(2A)	107.6
C(2)-C(5)-H(5A)	109.5
C(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(2)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
Si(1)-C(43)-H(43A)	109.5
Si(1)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
Si(1)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(1)-C(2')-C(5')	118.8(10)
C(1)-C(2')-C(3)	112.6(7)
C(5')-C(2')-C(3)	114.1(8)
C(1)-C(2')-H(2'A)	102.8
C(5')-C(2')-H(2'A)	102.8
C(3)-C(2')-H(2'A)	102.8
C(2')-C(5')-H(5'A)	109.5
C(2')-C(5')-H(5'B)	109.5
H(5'A)-C(5')-H(5'B)	109.5
C(2')-C(5')-H(5'C)	109.5
H(5'A)-C(5')-H(5'C)	109.5
H(5'B)-C(5')-H(5'C)	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb13907. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ir(1)	11(1)	13(1)	10(1)	0(1)	1(1)	0(1)
P(1)	26(1)	15(1)	18(1)	0(1)	-4(1)	-2(1)
P(2)	12(1)	24(1)	15(1)	-1(1)	0(1)	0(1)
P(3)	13(1)	22(1)	12(1)	1(1)	0(1)	1(1)
Si(1)	22(1)	15(1)	21(1)	-1(1)	0(1)	3(1)
C(1)	25(1)	23(1)	19(1)	4(3)	7(1)	1(3)
C(3)	24(1)	88(3)	15(1)	-15(3)	1(1)	-1(4)
C(4)	27(1)	23(1)	15(1)	1(3)	4(1)	-2(3)
C(6)	35(2)	108(3)	14(1)	-4(4)	3(1)	-11(5)
C(11)	37(3)	28(3)	40(3)	4(2)	-8(2)	-12(2)
C(12)	48(4)	21(3)	36(3)	10(2)	-8(3)	-9(3)
C(21)	22(2)	40(2)	52(2)	9(2)	-6(2)	7(2)
C(22)	17(1)	63(3)	19(1)	1(1)	6(1)	-2(1)
C(23)	16(2)	46(2)	38(2)	-16(2)	-3(1)	-9(2)
C(31)	25(3)	39(3)	20(2)	-8(2)	-3(2)	3(2)
C(32)	33(3)	34(3)	15(2)	9(2)	0(2)	0(2)
C(33)	14(1)	40(2)	20(1)	0(3)	-2(1)	-2(3)
C(41)	46(4)	22(3)	27(2)	-10(2)	-7(2)	8(2)
C(42)	26(2)	29(3)	40(2)	-7(2)	-9(2)	17(2)
Cl(1)	45(1)	16(1)	39(1)	11(1)	11(1)	-9(1)
C(13)	45(1)	16(1)	39(1)	11(1)	11(1)	-9(1)
C(2)	34(5)	36(5)	13(3)	-15(4)	14(3)	-14(4)
C(5)	26(6)	68(9)	22(5)	4(7)	21(4)	-13(7)
Cl(1')	47(3)	23(2)	71(3)	-15(2)	12(2)	2(2)
C(43)	47(3)	23(2)	71(3)	-15(2)	12(2)	2(2)
C(2')	15(4)	28(6)	23(4)	-19(4)	-8(3)	1(4)
C(5')	26(6)	45(7)	23(6)	4(6)	1(4)	-9(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for jb13907.

	x	y	z	U(eq)
H(1A)	4516	826	1877	26
H(1B)	4702	-621	2173	26
H(4A)	443	-66	496	26
H(6A)	1228	20	-1356	78
H(6B)	2618	-853	-1398	78
H(6C)	2771	628	-1508	78
H(11A)	3834	3817	2672	54
H(11B)	4611	2592	2253	54
H(11C)	4209	2691	3509	54
H(12A)	1833	3835	1103	53
H(12B)	748	2715	775	53
H(12C)	2405	2617	511	53
H(21A)	-2550	1006	2558	57
H(21B)	-1535	1356	1594	57
H(21C)	-1217	1933	2802	57
H(22A)	-2032	-466	4109	49
H(22B)	-614	206	4645	49
H(22C)	-593	-1257	4388	49
H(23A)	-2424	-1313	2152	50
H(23B)	-1000	-2152	2166	50
H(23C)	-1354	-1179	1185	50
H(31A)	3091	1114	5955	43
H(31B)	1556	1297	5293	43
H(31C)	2927	2051	4928	43
H(32A)	3181	-1135	5968	41
H(32B)	3045	-2078	4945	41
H(32C)	1645	-1379	5325	41
H(33A)	5295	20	5234	37
H(33B)	5317	786	4106	37
H(33C)	5351	-706	4087	37

H(41A)	1996	-3899	1078	48
H(41B)	2376	-2667	415	48
H(41C)	779	-2873	789	48
H(42A)	4124	-3777	2638	48
H(42B)	4433	-2676	3513	48
H(42C)	4867	-2513	2270	48
H(13A)	1629	4246	2918	49
H(13B)	1626	3321	3951	49
H(13C)	276	3353	3057	49
H(2A)	4029	-1247	507	32
H(5A)	6166	-6	355	57
H(5B)	5195	1185	18	57
H(5C)	5204	7	-791	57
H(43A)	1319	-4173	3128	69
H(43B)	76	-3138	3070	69
H(43C)	1319	-3108	4051	69
H(2'A)	4180	1138	571	27
H(5'A)	6124	-149	385	47
H(5'B)	5177	118	-742	47
H(5'C)	5047	-1194	-129	47

Table 6. Torsion angles [$^{\circ}$] for jb13907.

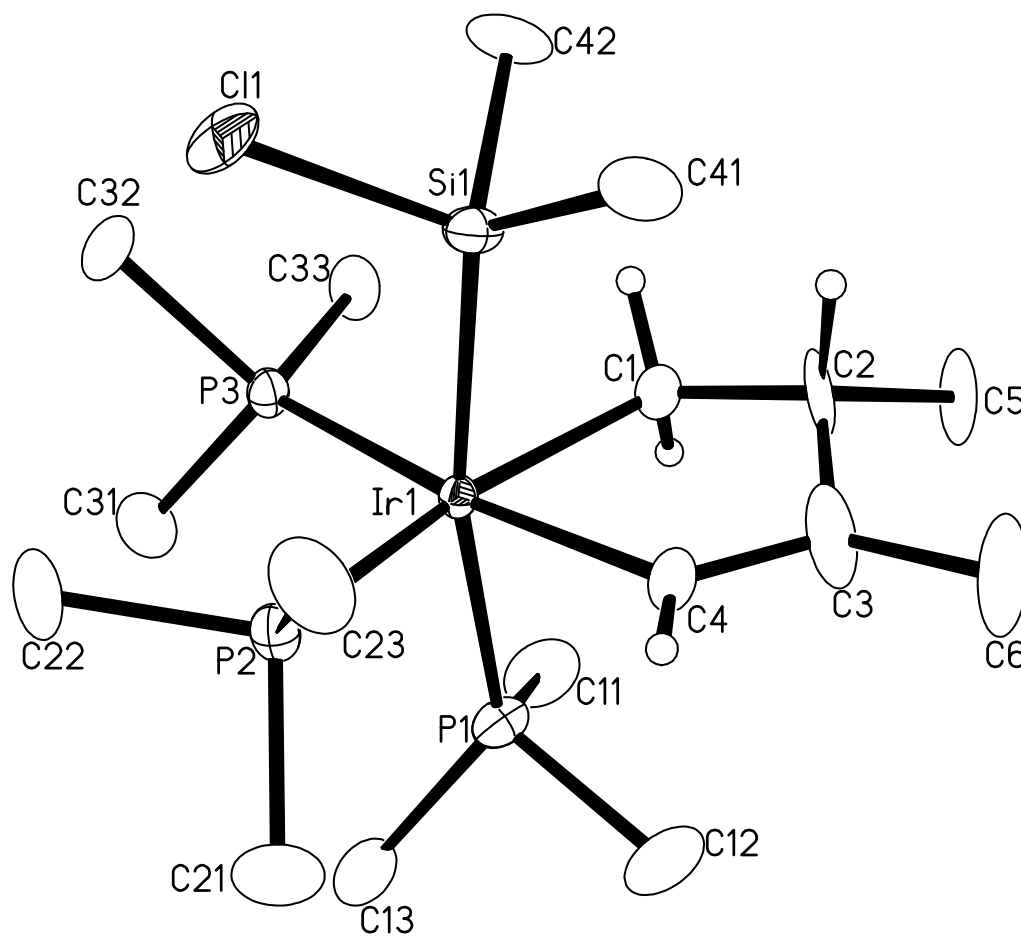
C(4)-Ir(1)-P(1)-C(11)	-119.0(2)
C(1)-Ir(1)-P(1)-C(11)	-41.3(2)
P(2)-Ir(1)-P(1)-C(11)	153.7(2)
P(3)-Ir(1)-P(1)-C(11)	53.2(2)
Si(1)-Ir(1)-P(1)-C(11)	-52.9(3)
C(4)-Ir(1)-P(1)-C(12)	0.6(3)
C(1)-Ir(1)-P(1)-C(12)	78.3(3)
P(2)-Ir(1)-P(1)-C(12)	-86.7(3)
P(3)-Ir(1)-P(1)-C(12)	172.8(3)
Si(1)-Ir(1)-P(1)-C(12)	66.7(3)
C(4)-Ir(1)-P(1)-C(13)	127.0(8)
C(1)-Ir(1)-P(1)-C(13)	-155.3(8)
P(2)-Ir(1)-P(1)-C(13)	39.7(8)
P(3)-Ir(1)-P(1)-C(13)	-60.8(8)
Si(1)-Ir(1)-P(1)-C(13)	-166.9(8)
C(4)-Ir(1)-P(1)-Cl(1')	121.7(3)
C(1)-Ir(1)-P(1)-Cl(1')	-160.6(3)
P(2)-Ir(1)-P(1)-Cl(1')	34.4(3)
P(3)-Ir(1)-P(1)-Cl(1')	-66.1(3)
Si(1)-Ir(1)-P(1)-Cl(1')	-172.2(3)
C(4)-Ir(1)-P(2)-C(22)	168.8(3)
C(1)-Ir(1)-P(2)-C(22)	155.4(7)
P(3)-Ir(1)-P(2)-C(22)	-9.93(17)
Si(1)-Ir(1)-P(2)-C(22)	82.24(16)
P(1)-Ir(1)-P(2)-C(22)	-103.40(16)
C(4)-Ir(1)-P(2)-C(21)	-67.7(3)
C(1)-Ir(1)-P(2)-C(21)	-81.1(8)
P(3)-Ir(1)-P(2)-C(21)	113.57(18)
Si(1)-Ir(1)-P(2)-C(21)	-154.26(18)
P(1)-Ir(1)-P(2)-C(21)	20.09(18)
C(4)-Ir(1)-P(2)-C(23)	48.9(3)
C(1)-Ir(1)-P(2)-C(23)	35.4(8)
P(3)-Ir(1)-P(2)-C(23)	-129.91(19)
Si(1)-Ir(1)-P(2)-C(23)	-37.74(19)

P(1)-Ir(1)-P(2)-C(23)	136.61(19)
C(4)-Ir(1)-P(3)-C(31)	126.0(17)
C(1)-Ir(1)-P(3)-C(31)	120.7(3)
P(2)-Ir(1)-P(3)-C(31)	-63.1(2)
Si(1)-Ir(1)-P(3)-C(31)	-157.5(2)
P(1)-Ir(1)-P(3)-C(31)	34.7(2)
C(4)-Ir(1)-P(3)-C(33)	6.9(17)
C(1)-Ir(1)-P(3)-C(33)	1.7(4)
P(2)-Ir(1)-P(3)-C(33)	177.8(3)
Si(1)-Ir(1)-P(3)-C(33)	83.4(3)
P(1)-Ir(1)-P(3)-C(33)	-84.4(3)
C(4)-Ir(1)-P(3)-C(32)	-112.4(17)
C(1)-Ir(1)-P(3)-C(32)	-117.6(3)
P(2)-Ir(1)-P(3)-C(32)	58.6(2)
Si(1)-Ir(1)-P(3)-C(32)	-35.9(2)
P(1)-Ir(1)-P(3)-C(32)	156.3(2)
C(4)-Ir(1)-Si(1)-C(41)	-5.4(3)
C(1)-Ir(1)-Si(1)-C(41)	-83.3(3)
P(2)-Ir(1)-Si(1)-C(41)	81.9(3)
P(3)-Ir(1)-Si(1)-C(41)	-177.8(3)
P(1)-Ir(1)-Si(1)-C(41)	-71.6(3)
C(4)-Ir(1)-Si(1)-C(42)	120.4(2)
C(1)-Ir(1)-Si(1)-C(42)	42.5(2)
P(2)-Ir(1)-Si(1)-C(42)	-152.3(2)
P(3)-Ir(1)-Si(1)-C(42)	-52.0(2)
P(1)-Ir(1)-Si(1)-C(42)	54.2(3)
C(4)-Ir(1)-Si(1)-C(43)	-120.5(7)
C(1)-Ir(1)-Si(1)-C(43)	161.6(7)
P(2)-Ir(1)-Si(1)-C(43)	-33.2(7)
P(3)-Ir(1)-Si(1)-C(43)	67.1(7)
P(1)-Ir(1)-Si(1)-C(43)	173.3(7)
C(4)-Ir(1)-Si(1)-Cl(1)	-123.80(17)
C(1)-Ir(1)-Si(1)-Cl(1)	158.29(17)
P(2)-Ir(1)-Si(1)-Cl(1)	-36.45(16)
P(3)-Ir(1)-Si(1)-Cl(1)	63.81(16)
P(1)-Ir(1)-Si(1)-Cl(1)	169.98(17)

C(4)-Ir(1)-C(1)-C(2')	11.3(7)
P(2)-Ir(1)-C(1)-C(2')	25.0(13)
P(3)-Ir(1)-C(1)-C(2')	-169.5(7)
Si(1)-Ir(1)-C(1)-C(2')	99.8(7)
P(1)-Ir(1)-C(1)-C(2')	-77.6(7)
C(4)-Ir(1)-C(1)-C(2)	-13.6(7)
P(2)-Ir(1)-C(1)-C(2)	0.1(12)
P(3)-Ir(1)-C(1)-C(2)	165.7(7)
Si(1)-Ir(1)-C(1)-C(2)	74.9(7)
P(1)-Ir(1)-C(1)-C(2)	-102.5(7)
C(6)-C(3)-C(4)-Ir(1)	175.0(8)
C(2)-C(3)-C(4)-Ir(1)	20.7(12)
C(2')-C(3)-C(4)-Ir(1)	-3.6(12)
C(1)-Ir(1)-C(4)-C(3)	-3.9(7)
P(2)-Ir(1)-C(4)-C(3)	179.7(7)
P(3)-Ir(1)-C(4)-C(3)	-9(2)
Si(1)-Ir(1)-C(4)-C(3)	-86.1(7)
P(1)-Ir(1)-C(4)-C(3)	82.3(7)
C(4)-C(3)-C(2)-C(1)	-31.3(13)
C(6)-C(3)-C(2)-C(1)	173.2(8)
C(2')-C(3)-C(2)-C(1)	67.4(16)
C(4)-C(3)-C(2)-C(5)	-155.7(10)
C(6)-C(3)-C(2)-C(5)	48.9(14)
C(2')-C(3)-C(2)-C(5)	-56.9(17)
C(2')-C(1)-C(2)-C(3)	-73.7(19)
Ir(1)-C(1)-C(2)-C(3)	27.9(11)
C(2')-C(1)-C(2)-C(5)	51.9(19)
Ir(1)-C(1)-C(2)-C(5)	153.5(9)
C(2)-C(1)-C(2')-C(5')	-64.8(19)
Ir(1)-C(1)-C(2')-C(5')	-153.5(9)
C(2)-C(1)-C(2')-C(3)	73(2)
Ir(1)-C(1)-C(2')-C(3)	-16.2(12)
C(4)-C(3)-C(2')-C(1)	12.9(14)
C(6)-C(3)-C(2')-C(1)	-165.7(8)
C(2)-C(3)-C(2')-C(1)	-78.4(18)
C(4)-C(3)-C(2')-C(5')	152.3(10)

C(6)-C(3)-C(2)-C(5')	-26.3(16)
C(2)-C(3)-C(2')-C(5')	61.0(16)

Projection view of the molecule with 50% thermal ellipsoids (disorder not shown):



Projection view of the molecule with 50% thermal ellipsoids:

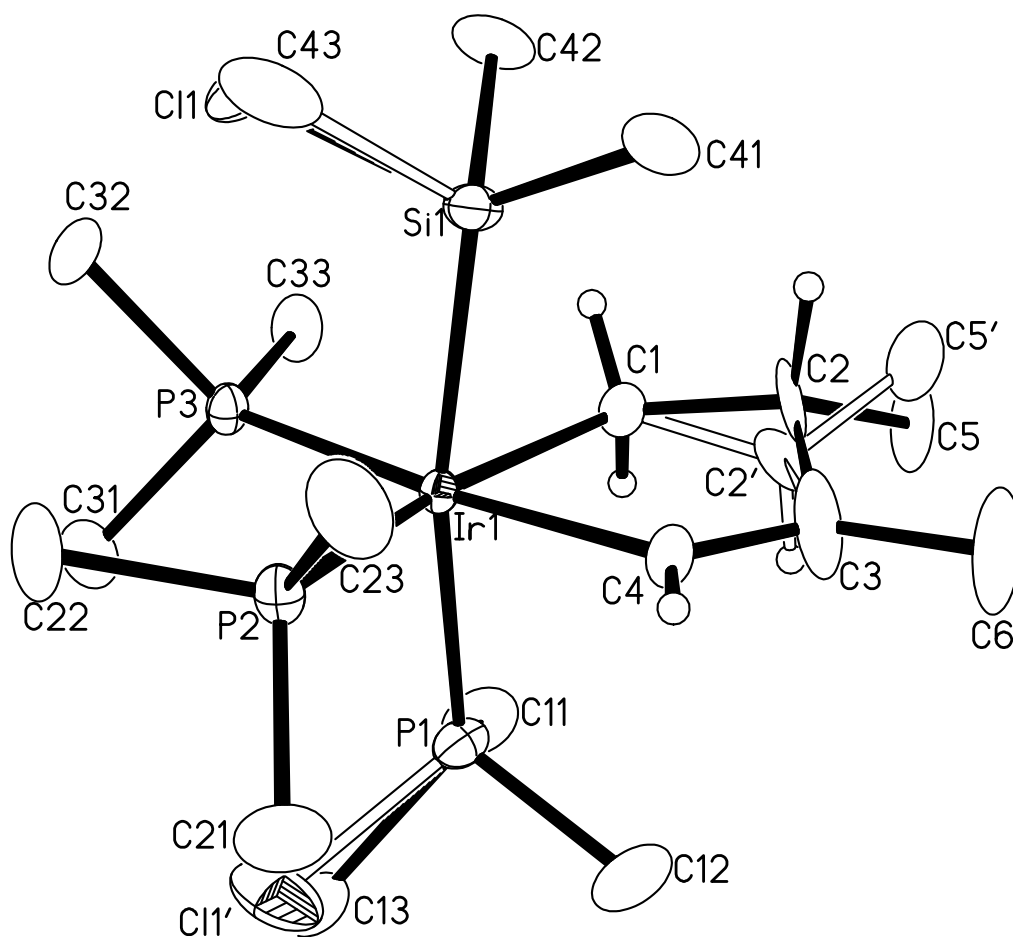


Table 1. Crystal data and structure refinement for jb16707 (compound *fac*-7E).

Identification code	j16707/lt	
Empirical formula	C ₁₈ H ₄₆ Ir P ₃ Si	
Formula weight	575.75	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 15.8275(8) Å	α = 90°.
	b = 17.7785(10) Å	β = 90°.
	c = 17.9098(9) Å	γ = 90°.
Volume	5039.6(5) Å ³	
Z	8	
Density (calculated)	1.518 Mg/m ³	
Absorption coefficient	5.536 mm ⁻¹	
F(000)	2320	
Crystal size	0.18 x 0.14 x 0.14 mm ³	
Theta range for data collection	3.04 to 32.71°.	
Index ranges	-23 ≤ h ≤ 23, -26 ≤ k ≤ 26, -27 ≤ l ≤ 27	
Reflections collected	244958	
Independent reflections	9255 [R(int) = 0.082]	
Completeness to theta = 32.71°	99.7 %	
Absorption correction	Numerical	
Max. and min. transmission	0.6655 and 0.5287	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9255 / 0 / 226	
Goodness-of-fit on F ²	1.030	
Final R indices [I > 2σ(I)]	R1 = 0.0224, wR2 = 0.0390	
R indices (all data)	R1 = 0.0378, wR2 = 0.0419	
Largest diff. peak and hole	0.645 and -0.680 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb16707. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ir(1)	4185(1)	2191(1)	3369(1)	11(1)
P(1)	4244(1)	2332(1)	4645(1)	14(1)
P(2)	3845(1)	3450(1)	3147(1)	15(1)
P(3)	5622(1)	2269(1)	3118(1)	18(1)
Si(1)	3966(1)	853(1)	3511(1)	13(1)
C(1)	1233(1)	186(1)	5245(1)	26(1)
C(2)	2066(1)	181(1)	5124(1)	20(1)
C(3)	2457(1)	572(1)	4480(1)	17(1)
C(4)	3288(1)	525(1)	4330(1)	16(1)
C(5)	2629(2)	-255(1)	5647(1)	30(1)
C(6)	1874(1)	1028(1)	3994(1)	23(1)
C(7)	3435(1)	366(1)	2689(1)	21(1)
C(8)	4882(1)	177(1)	3674(1)	22(1)
C(9)	4049(1)	1963(1)	2185(1)	19(1)
C(11)	4866(1)	1649(1)	5175(1)	21(1)
C(12)	3246(1)	2307(1)	5149(1)	20(1)
C(13)	4676(1)	3198(1)	5046(1)	19(1)
C(21)	2956(1)	3786(1)	3695(1)	21(1)
C(22)	4599(2)	4216(1)	3296(1)	24(1)
C(23)	3481(2)	3702(1)	2216(1)	23(1)
C(31)	6327(2)	2766(2)	3759(1)	34(1)
C(32)	5908(2)	2740(1)	2245(1)	30(1)
C(33)	6236(2)	1413(1)	2994(1)	33(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for jb16707.

Ir(1)-C(9)	2.1688(19)
Ir(1)-P(1)	2.3014(5)
Ir(1)-P(3)	2.3229(5)
Ir(1)-P(2)	2.3372(6)
Ir(1)-Si(1)	2.4166(6)
Ir(1)-H(1)	1.55(3)
P(1)-C(12)	1.820(2)
P(1)-C(11)	1.828(2)
P(1)-C(13)	1.830(2)
P(2)-C(21)	1.817(2)
P(2)-C(23)	1.819(2)
P(2)-C(22)	1.830(2)
P(3)-C(33)	1.819(2)
P(3)-C(31)	1.828(2)
P(3)-C(32)	1.830(2)
Si(1)-C(7)	1.903(2)
Si(1)-C(8)	1.905(2)
Si(1)-C(4)	1.909(2)
C(1)-C(2)	1.336(3)
C(1)-H(1A)	0.9500
C(1)-H(1B)	0.9500
C(2)-C(3)	1.482(3)
C(2)-C(5)	1.507(3)
C(3)-C(4)	1.346(3)
C(3)-C(6)	1.505(3)
C(4)-H(4)	0.9500
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800

C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(9)-Ir(1)-P(1)	174.40(6)

C(9)-Ir(1)-P(3)	85.36(6)
P(1)-Ir(1)-P(3)	98.351(19)
C(9)-Ir(1)-P(2)	89.40(6)
P(1)-Ir(1)-P(2)	94.224(18)
P(3)-Ir(1)-P(2)	97.75(2)
C(9)-Ir(1)-Si(1)	84.56(6)
P(1)-Ir(1)-Si(1)	90.511(18)
P(3)-Ir(1)-Si(1)	102.693(19)
P(2)-Ir(1)-Si(1)	158.107(19)
C(9)-Ir(1)-H(1)	89.6(9)
P(1)-Ir(1)-H(1)	86.5(9)
P(3)-Ir(1)-H(1)	174.4(9)
P(2)-Ir(1)-H(1)	84.6(9)
Si(1)-Ir(1)-H(1)	74.3(9)
C(12)-P(1)-C(11)	101.11(10)
C(12)-P(1)-C(13)	98.60(9)
C(11)-P(1)-C(13)	98.85(10)
C(12)-P(1)-Ir(1)	117.06(7)
C(11)-P(1)-Ir(1)	117.73(7)
C(13)-P(1)-Ir(1)	119.78(7)
C(21)-P(2)-C(23)	99.77(10)
C(21)-P(2)-C(22)	100.45(10)
C(23)-P(2)-C(22)	99.08(10)
C(21)-P(2)-Ir(1)	113.63(7)
C(23)-P(2)-Ir(1)	117.67(7)
C(22)-P(2)-Ir(1)	122.52(8)
C(33)-P(3)-C(31)	98.92(12)
C(33)-P(3)-C(32)	98.39(11)
C(31)-P(3)-C(32)	99.53(11)
C(33)-P(3)-Ir(1)	119.75(8)
C(31)-P(3)-Ir(1)	120.33(8)
C(32)-P(3)-Ir(1)	115.75(8)
C(7)-Si(1)-C(8)	99.62(10)
C(7)-Si(1)-C(4)	101.94(9)
C(8)-Si(1)-C(4)	96.70(9)
C(7)-Si(1)-Ir(1)	115.46(7)

C(8)-Si(1)-Ir(1)	121.89(7)
C(4)-Si(1)-Ir(1)	117.52(6)
C(2)-C(1)-H(1A)	120.0
C(2)-C(1)-H(1B)	120.0
H(1A)-C(1)-H(1B)	120.0
C(1)-C(2)-C(3)	122.3(2)
C(1)-C(2)-C(5)	119.1(2)
C(3)-C(2)-C(5)	118.57(18)
C(4)-C(3)-C(2)	122.23(19)
C(4)-C(3)-C(6)	121.21(18)
C(2)-C(3)-C(6)	116.56(18)
C(3)-C(4)-Si(1)	133.11(16)
C(3)-C(4)-H(4)	113.4
Si(1)-C(4)-H(4)	113.4
C(2)-C(5)-H(5A)	109.5
C(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(2)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
Si(1)-C(7)-H(7A)	109.5
Si(1)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
Si(1)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
Si(1)-C(8)-H(8A)	109.5
Si(1)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
Si(1)-C(8)-H(8C)	109.5

H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
Ir(1)-C(9)-H(9A)	109.5
Ir(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
Ir(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
P(1)-C(11)-H(11A)	109.5
P(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
P(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
P(1)-C(12)-H(12A)	109.5
P(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
P(1)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
P(1)-C(13)-H(13A)	109.5
P(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
P(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
P(2)-C(21)-H(21A)	109.5
P(2)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
P(2)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
P(2)-C(22)-H(22A)	109.5
P(2)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
P(2)-C(22)-H(22C)	109.5

H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
P(2)-C(23)-H(23A)	109.5
P(2)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
P(2)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
P(3)-C(31)-H(31A)	109.5
P(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
P(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
P(3)-C(32)-H(32A)	109.5
P(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
P(3)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
P(3)-C(33)-H(33A)	109.5
P(3)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
P(3)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb16707. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ir(1)	11(1)	12(1)	8(1)	1(1)	0(1)	0(1)
P(1)	16(1)	15(1)	9(1)	-1(1)	0(1)	-2(1)
P(2)	18(1)	13(1)	14(1)	1(1)	-4(1)	0(1)
P(3)	14(1)	25(1)	15(1)	4(1)	2(1)	0(1)
Si(1)	14(1)	13(1)	13(1)	0(1)	0(1)	2(1)
C(1)	27(1)	21(1)	29(1)	-1(1)	10(1)	-2(1)
C(2)	25(1)	16(1)	18(1)	-3(1)	6(1)	-2(1)
C(3)	21(1)	12(1)	17(1)	-2(1)	0(1)	-2(1)
C(4)	20(1)	12(1)	14(1)	-1(1)	-2(1)	-1(1)
C(5)	29(1)	38(1)	21(1)	10(1)	1(1)	-2(1)
C(6)	19(1)	24(1)	27(1)	3(1)	0(1)	-2(1)
C(7)	26(1)	19(1)	19(1)	-2(1)	-2(1)	-1(1)
C(8)	25(1)	19(1)	22(1)	1(1)	2(1)	5(1)
C(9)	28(1)	19(1)	11(1)	1(1)	-1(1)	-1(1)
C(11)	27(1)	24(1)	13(1)	2(1)	-7(1)	1(1)
C(12)	22(1)	21(1)	16(1)	-3(1)	5(1)	-2(1)
C(13)	25(1)	19(1)	14(1)	-2(1)	-3(1)	-6(1)
C(21)	21(1)	18(1)	24(1)	-3(1)	-3(1)	3(1)
C(22)	28(1)	18(1)	25(1)	2(1)	-3(1)	-5(1)
C(23)	32(1)	20(1)	19(1)	2(1)	-8(1)	2(1)
C(31)	17(1)	58(2)	28(1)	0(1)	2(1)	-10(1)
C(32)	26(1)	41(2)	24(1)	11(1)	8(1)	-2(1)
C(33)	20(1)	40(2)	39(1)	7(1)	12(1)	10(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for jb16707.

	x	y	z	U(eq)
H(1A)	869	447	4911	31
H(1B)	1005	-71	5663	31
H(4)	3602	277	4710	19
H(5A)	3057	82	5857	44
H(5B)	2908	-662	5371	44
H(5C)	2288	-469	6051	44
H(6A)	1595	1414	4297	34
H(6B)	1447	697	3772	34
H(6C)	2201	1270	3596	34
H(7A)	3798	405	2247	32
H(7B)	2891	607	2587	32
H(7C)	3344	-166	2810	32
H(8A)	4660	-330	3764	33
H(8B)	5208	342	4108	33
H(8C)	5247	170	3232	33
H(9A)	4427	1551	2043	29
H(9B)	4196	2415	1900	29
H(9C)	3463	1821	2078	29
H(11A)	5443	1633	4977	32
H(11B)	4607	1151	5130	32
H(11C)	4881	1798	5702	32
H(12A)	2985	1811	5089	29
H(12B)	2867	2694	4950	29
H(12C)	3349	2402	5681	29
H(13A)	4664	3164	5592	29
H(13B)	4334	3627	4883	29
H(13C)	5260	3265	4877	29
H(21A)	3112	3793	4225	31
H(21B)	2472	3450	3622	31
H(21C)	2805	4295	3535	31

H(22A)	4327	4698	3182	36
H(22B)	5089	4145	2969	36
H(22C)	4784	4215	3819	36
H(23A)	3045	3346	2056	35
H(23B)	3957	3684	1867	35
H(23C)	3245	4211	2225	35
H(31A)	6301	2529	4253	51
H(31B)	6150	3293	3799	51
H(31C)	6907	2742	3570	51
H(32A)	6524	2764	2202	45
H(32B)	5675	3251	2243	45
H(32C)	5676	2457	1822	45
H(33A)	6813	1544	2844	50
H(33B)	5975	1102	2605	50
H(33C)	6250	1132	3464	50
H(1)	3216(17)	2087(14)	3469(13)	38(8)

Table 6. Torsion angles [°] for jb16707.

C(9)-Ir(1)-P(1)-C(12)	-48.3(6)
P(3)-Ir(1)-P(1)-C(12)	-179.62(8)
P(2)-Ir(1)-P(1)-C(12)	81.89(8)
Si(1)-Ir(1)-P(1)-C(12)	-76.72(8)
C(9)-Ir(1)-P(1)-C(11)	72.5(6)
P(3)-Ir(1)-P(1)-C(11)	-58.76(8)
P(2)-Ir(1)-P(1)-C(11)	-157.25(8)
Si(1)-Ir(1)-P(1)-C(11)	44.14(8)
C(9)-Ir(1)-P(1)-C(13)	-167.4(6)
P(3)-Ir(1)-P(1)-C(13)	61.30(8)
P(2)-Ir(1)-P(1)-C(13)	-37.18(8)
Si(1)-Ir(1)-P(1)-C(13)	164.21(8)
C(9)-Ir(1)-P(2)-C(21)	124.40(9)
P(1)-Ir(1)-P(2)-C(21)	-51.32(8)
P(3)-Ir(1)-P(2)-C(21)	-150.36(8)
Si(1)-Ir(1)-P(2)-C(21)	50.67(9)
C(9)-Ir(1)-P(2)-C(23)	8.39(11)
P(1)-Ir(1)-P(2)-C(23)	-167.33(9)
P(3)-Ir(1)-P(2)-C(23)	93.63(9)
Si(1)-Ir(1)-P(2)-C(23)	-65.34(10)
C(9)-Ir(1)-P(2)-C(22)	-114.68(10)
P(1)-Ir(1)-P(2)-C(22)	69.59(9)
P(3)-Ir(1)-P(2)-C(22)	-29.44(9)
Si(1)-Ir(1)-P(2)-C(22)	171.58(9)
C(9)-Ir(1)-P(3)-C(33)	-77.81(11)
P(1)-Ir(1)-P(3)-C(33)	97.97(10)
P(2)-Ir(1)-P(3)-C(33)	-166.57(10)
Si(1)-Ir(1)-P(3)-C(33)	5.55(10)
C(9)-Ir(1)-P(3)-C(31)	159.40(12)
P(1)-Ir(1)-P(3)-C(31)	-24.81(10)
P(2)-Ir(1)-P(3)-C(31)	70.64(10)
Si(1)-Ir(1)-P(3)-C(31)	-117.24(10)
C(9)-Ir(1)-P(3)-C(32)	39.72(11)
P(1)-Ir(1)-P(3)-C(32)	-144.50(9)

P(2)-Ir(1)-P(3)-C(32)	-49.04(10)
Si(1)-Ir(1)-P(3)-C(32)	123.08(9)
C(9)-Ir(1)-Si(1)-C(7)	-20.21(10)
P(1)-Ir(1)-Si(1)-C(7)	157.12(8)
P(3)-Ir(1)-Si(1)-C(7)	-104.20(8)
P(2)-Ir(1)-Si(1)-C(7)	54.43(9)
C(9)-Ir(1)-Si(1)-C(8)	100.74(10)
P(1)-Ir(1)-Si(1)-C(8)	-81.94(8)
P(3)-Ir(1)-Si(1)-C(8)	16.74(8)
P(2)-Ir(1)-Si(1)-C(8)	175.37(8)
C(9)-Ir(1)-Si(1)-C(4)	-140.63(9)
P(1)-Ir(1)-Si(1)-C(4)	36.69(7)
P(3)-Ir(1)-Si(1)-C(4)	135.37(7)
P(2)-Ir(1)-Si(1)-C(4)	-66.00(9)
C(1)-C(2)-C(3)-C(4)	-175.4(2)
C(5)-C(2)-C(3)-C(4)	2.8(3)
C(1)-C(2)-C(3)-C(6)	4.4(3)
C(5)-C(2)-C(3)-C(6)	-177.35(19)
C(2)-C(3)-C(4)-Si(1)	172.03(15)
C(6)-C(3)-C(4)-Si(1)	-7.8(3)
C(7)-Si(1)-C(4)-C(3)	-56.8(2)
C(8)-Si(1)-C(4)-C(3)	-158.2(2)
Ir(1)-Si(1)-C(4)-C(3)	70.5(2)

Projection view of the molecule with 50% ellipsoids:

