Supporting Information for

Unsymmetrically Bridging Aryls of Iridium

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Table 1A. Crystal data and structure refinement for (cod)IrBr(μ-2,4,6-$Me_3C_6H_2$)Ir(cod) (**2**).

Empirical formula	$C_{25}H_{35}BrIr_2$
Formula weight	799.84
Temperature	293(2) K
Crystal system	Monoclinc
Space group	$P2_1/c$
Unit cell dimensions	a = 15.383(2) Å α = 90 deg. b = 21.473(2) Å β = 102.942(8) deg. c = 14.5907(10) Å γ = 90 deg.
Volume	4697.1(9) $Å^3$
Z	8
Density (calculated)	2.262 g/cm^3
Absorption coefficient	13.031 mm^{-1}
Absorption correction	Psi-scan
Transmission	0.242 to 0.770
F(000)	2992
Diffractometer	Enraf-Nonius CAD4
Radiation	graphite-monochromated MoKα (0.71073 Å)
Scan type	ω-2θ
Decay	8%, based on 3 standards measured every 7200 s exposure (220 reflections)
Crystal size	0.42 x 0.18 x 0.08 mm
Crystal habit	obelisk
Crystal color	yellow
Theta range for data collection	2.33 to 25.01 deg.
Limiting indices	0<=h<=18, 0<=k<=25, -17<=l<=16
Reflections collected	8482
Independent reflections	8171 [R(int) = 0.0481]
Structure solution method	Patterson
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	8170 / 0 / 505
Goodness-of-fit on F^2	1.039
Final R indices [$I>2\sigma(I)$]	R1 = 0.0516, wR2 = 0.1187
R indices (all data)	R1 = 0.1117, wR2 = 0.1442
Largest diff. peak and hole	1.681 and -1.256 e/Å^3

Table 1B. Atomic coordinates and equivalent isotropic displacement parameters for (cod)IrBr(μ-2,4,6-$Me_3C_6H_2$)Ir(cod) (**2**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ir1	0.98154(4)	0.88360(3)	0.20200(4)	0.0479(2)
Ir2	0.81972(4)	0.77035(3)	-0.00134(4)	0.0427(2)
Ir01	1.39144(4)	0.64852(3)	0.57192(4)	0.0450(2)
Ir02	1.33765(4)	0.83915(3)	0.62106(4)	0.0411(2)
Br1	1.0158(2)	0.77270(9)	0.24513(14)	0.0761(6)
Br01	1.49953(13)	0.71063(10)	0.50680(14)	0.0687(5)
C1	0.8886(10)	0.8608(7)	0.0794(10)	0.046(4)
C2	0.9184(10)	0.8515(7)	-0.0056(10)	0.042(4)
C3	0.8546(11)	0.8461(7)	-0.0914(10)	0.044(4)
C4	0.7633(10)	0.8512(8)	-0.1007(11)	0.053(4)
C5	0.7339(10)	0.8564(7)	-0.0170(11)	0.048(4)
C6	0.7951(10)	0.8579(7)	0.0731(10)	0.045(4)
C7	1.0161(9)	0.8487(9)	-0.0059(12)	0.059(5)
C8	0.6968(13)	0.8506(10)	-0.1952(12)	0.079(6)
C9	0.7555(12)	0.8622(8)	0.1575(11)	0.058(5)
C01	1.3385(9)	0.7254(6)	0.6221(9)	0.034(3)
C02	1.3745(11)	0.7501(7)	0.7092(9)	0.047(4)
C03	1.3293(12)	0.7967(8)	0.7539(11)	0.057(5)
C04	1.2387(12)	0.8108(8)	0.7135(11)	0.052(4)
C05	1.2059(12)	0.7936(9)	0.6233(12)	0.059(5)
C06	1.2556(10)	0.7546(7)	0.5751(10)	0.043(4)
C07	1.4690(12)	0.7293(9)	0.7629(10)	0.063(5)
C08	1.1889(14)	0.8541(10)	0.7683(13)	0.078(6)
C09	1.2152(10)	0.7381(9)	0.4721(10)	0.057(5)
C11	0.7293(12)	0.7127(9)	0.0482(12)	0.059(5)
C12	0.813(2)	0.7034(9)	0.1080(13)	0.075(6)
C13	0.874(2)	0.6526(9)	0.114(2)	0.082(6)
C14	0.937(2)	0.6577(10)	0.050(2)	0.093(7)
C15	0.901(2)	0.6968(8)	-0.0361(14)	0.070(6)
C16	0.8149(14)	0.6955(10)	-0.0957(14)	0.076(7)
C17	0.751(2)	0.6446(11)	-0.090(2)	0.102(8)
C18	0.6922(14)	0.6623(10)	-0.021(2)	0.094(7)
C011	1.4550(12)	0.8923(8)	0.6731(12)	0.059(5)
C012	1.3790(13)	0.9289(9)	0.6732(14)	0.071(5)
C013	1.349(2)	0.9832(10)	0.606(2)	0.098(7)
C014	1.289(2)	0.9610(10)	0.518(2)	0.101(8)
C015	1.2925(12)	0.8930(8)	0.4949(11)	0.057(5)
C016	1.3732(11)	0.8630(7)	0.4926(10)	0.048(4)
C017	1.4626(13)	0.8944(11)	0.5050(13)	0.080(7)
C018	1.5127(13)	0.8971(11)	0.6054(14)	0.082(6)
C21	0.9879(14)	0.9736(9)	0.148(2)	0.078(6)
C22	0.924(2)	0.9693(9)	0.203(2)	0.079(6)
C23	0.942(2)	0.9985(14)	0.303(2)	0.138(12)
C24	1.008(2)	0.9678(13)	0.3752(14)	0.104(8)
C25	1.0486(13)	0.9112(9)	0.3433(11)	0.061(5)
C26	1.1100(13)	0.9132(11)	0.2883(12)	0.069(5)
C27	1.143(2)	0.9693(12)	0.250(2)	0.090(7)
C28	1.077(2)	1.0039(14)	0.178(2)	0.134(12)

C021	1.3425(14)	0.5959(9)	0.670(2)	0.074(6)
C022	1.2791(13)	0.5960(10)	0.5874(14)	0.070(5)
C023	1.259(2)	0.5432(11)	0.519(2)	0.096(7)
C024	1.331(2)	0.5279(10)	0.469(2)	0.093(7)
C025	1.4094(13)	0.5671(7)	0.4901(13)	0.062(5)
C026	1.4743(14)	0.5674(9)	0.570(2)	0.074(6)
C027	1.469(2)	0.5269(13)	0.650(2)	0.135(12)
C028	1.399(2)	0.5398(12)	0.704(2)	0.111(9)

Table 1C. Bond lengths [Å] and angles [deg] for (cod)IrBr(μ-2,4,6-$Me_3C_6H_2$)Ir(cod) (**2**).

Ir1-C22	2.04(2)
Ir1-C1	2.082(15)
Ir1-C21	2.10(2)
Ir1-C25	2.171(15)
Ir1-C26	2.19(2)
Ir1-Br1	2.489(2)
Ir2-C16	2.11(2)
Ir2-C11	2.11(2)
Ir2-C15	2.14(2)
Ir2-C12	2.17(2)
Ir2-C3	2.232(14)
Ir2-C6	2.25(2)
Ir2-C5	2.25(2)
Ir2-C4	2.30(2)
Ir2-C2	2.320(15)
Ir2-C1	2.39(2)
Ir01-C01	2.047(13)
Ir01-C021	2.09(2)
Ir01-C022	2.12(2)
Ir01-C026	2.16(2)
Ir01-C025	2.17(2)
Ir01-Br01	2.481(2)
Ir02-C012	2.12(2)
Ir02-C011	2.13(2)
Ir02-C016	2.129(14)
Ir02-C015	2.153(15)
Ir02-C03	2.17(2)
Ir02-C06	2.227(15)
Ir02-C05	2.26(2)
Ir02-C02	2.304(15)
Ir02-C04	2.33(2)
Ir02-C01	2.443(12)
C1-C6	1.42(2)
C1-C2	1.43(2)
C2-C3	1.41(2)
C2-C7	1.51(2)
C3-C4	1.39(2)
C4-C5	1.40(2)
C4-C8	1.52(2)
C5-C6	1.44(2)
C6-C9	1.49(2)
C01-C02	1.37(2)
C01-C06	1.45(2)
C02-C03	1.45(2)
C02-C07	1.56(2)
C03-C04	1.42(2)
C04-C05	1.35(2)
C04-C08	1.54(2)
C05-C06	1.42(2)
C06-C09	1.53(2)
C11-C12	1.40(3)
C11-C18	1.50(3)

C12-C13	1.43(3)
C13-C14	1.48(3)
C14-C15	1.51(3)
C15-C16	1.41(3)
C16-C17	1.49(3)
C17-C18	1.54(3)
C011-C012	1.41(3)
C011-C018	1.47(2)
C012-C013	1.52(3)
C013-C014	1.49(3)
C014-C015	1.50(3)
C015-C016	1.41(2)
C016-C017	1.51(2)
C017-C018	1.50(2)
C21-C22	1.41(3)
C21-C28	1.49(3)
C22-C23	1.55(3)
C23-C24	1.45(3)
C24-C25	1.49(3)
C25-C26	1.37(2)
C26-C27	1.46(3)
C27-C28	1.49(3)
C021-C022	1.37(3)
C021-C028	1.50(3)
C022-C023	1.50(3)
C023-C024	1.49(3)
C024-C025	1.45(3)
C025-C026	1.36(3)
C026-C027	1.47(3)
C027-C028	1.50(3)

C22-Ir1-C1	90.1(7)
C22-Ir1-C21	39.7(8)
C1-Ir1-C21	88.6(7)
C22-Ir1-C25	82.1(8)
C1-Ir1-C25	165.6(7)
C21-Ir1-C25	93.1(7)
C22-Ir1-C26	94.1(9)
C1-Ir1-C26	157.1(7)
C21-Ir1-C26	80.6(8)
C25-Ir1-C26	36.7(7)
C22-Ir1-Br1	158.0(7)
C1-Ir1-Br1	93.3(4)
C21-Ir1-Br1	162.0(7)
C25-Ir1-Br1	89.5(5)
C26-Ir1-Br1	91.1(6)
C16-Ir2-C11	81.2(7)
C16-Ir2-C15	38.7(7)
C11-Ir2-C15	96.4(7)
C16-Ir2-C12	88.5(9)
C11-Ir2-C12	38.1(7)
C15-Ir2-C12	79.1(7)
C16-Ir2-C3	98.6(7)
C11-Ir2-C3	153.5(7)
C15-Ir2-C3	99.7(6)
C12-Ir2-C3	167.1(7)
C16-Ir2-C6	165.9(8)
C11-Ir2-C6	97.5(6)

C15-Ir2-C6	154.4(7)
C12-Ir2-C6	99.1(7)
C3-Ir2-C6	76.3(5)
C16-Ir2-C5	128.7(8)
C11-Ir2-C5	95.7(6)
C15-Ir2-C5	160.0(6)
C12-Ir2-C5	119.7(7)
C3-Ir2-C5	63.6(6)
C6-Ir2-C5	37.2(5)
C16-Ir2-C4	102.2(8)
C11-Ir2-C4	118.3(6)
C15-Ir2-C4	124.4(7)
C12-Ir2-C4	152.8(7)
C3-Ir2-C4	35.5(6)
C6-Ir2-C4	65.9(6)
C5-Ir2-C4	35.7(6)
C16-Ir2-C2	118.9(6)
C11-Ir2-C2	159.4(6)
C15-Ir2-C2	97.4(7)
C12-Ir2-C2	131.1(7)
C3-Ir2-C2	36.1(5)
C6-Ir2-C2	64.3(5)
C5-Ir2-C2	75.7(5)
C4-Ir2-C2	64.8(5)
C16-Ir2-C1	152.6(6)
C11-Ir2-C1	124.2(6)
C15-Ir2-C1	119.9(7)
C12-Ir2-C1	105.4(7)
C3-Ir2-C1	63.9(5)
C6-Ir2-C1	35.5(5)
C5-Ir2-C1	64.5(5)
C4-Ir2-C1	76.2(5)
C2-Ir2-C1	35.3(5)
C01-Ir01-C021	87.5(6)
C01-Ir01-C022	89.5(7)
C021-Ir01-C022	38.0(7)
C01-Ir01-C026	159.5(7)
C021-Ir01-C026	82.9(7)
C022-Ir01-C026	94.0(8)
C01-Ir01-C025	163.1(7)
C021-Ir01-C025	92.9(8)
C022-Ir01-C025	80.6(8)
C026-Ir01-C025	36.5(7)
C01-Ir01-Br01	93.3(4)
C021-Ir01-Br01	158.0(6)
C022-Ir01-Br01	163.8(6)
C026-Ir01-Br01	88.9(6)
C025-Ir01-Br01	92.5(5)
C012-Ir02-C011	38.8(7)
C012-Ir02-C016	89.0(7)
C011-Ir02-C016	79.6(6)
C012-Ir02-C015	80.3(7)
C011-Ir02-C015	95.9(7)
C016-Ir02-C015	38.3(6)
C012-Ir02-C03	97.7(7)
C011-Ir02-C03	97.0(6)
C016-Ir02-C03	164.8(7)
C015-Ir02-C03	156.4(7)

C012-Ir02-C06	162.7(7)
C011-Ir02-C06	157.4(6)
C016-Ir02-C06	99.8(5)
C015-Ir02-C06	97.3(6)
C03-Ir02-C06	77.5(5)
C012-Ir02-C05	126.0(7)
C011-Ir02-C05	157.0(6)
C016-Ir02-C05	121.7(6)
C015-Ir02-C05	97.3(7)
C03-Ir02-C05	64.7(6)
C06-Ir02-C05	37.0(6)
C012-Ir02-C02	122.6(7)
C011-Ir02-C02	99.4(6)
C016-Ir02-C02	127.7(6)
C015-Ir02-C02	156.2(6)
C03-Ir02-C02	37.8(6)
C06-Ir02-C02	62.8(5)
C05-Ir02-C02	75.0(6)
C012-Ir02-C04	102.3(7)
C011-Ir02-C04	123.1(6)
C016-Ir02-C04	154.5(6)
C015-Ir02-C04	120.5(6)
C03-Ir02-C04	36.5(6)
C06-Ir02-C04	64.0(6)
C05-Ir02-C04	34.2(6)
C02-Ir02-C04	64.6(6)
C012-Ir02-C01	155.2(6)
C011-Ir02-C01	122.1(6)
C016-Ir02-C01	104.1(5)
C015-Ir02-C01	122.8(6)
C03-Ir02-C01	64.9(5)
C06-Ir02-C01	35.7(5)
C05-Ir02-C01	64.5(6)
C02-Ir02-C01	33.5(5)
C04-Ir02-C01	74.8(5)
C6-C1-C2	117.0(13)
C6-C1-Ir1	123.8(11)
C2-C1-Ir1	119.1(11)
C6-C1-Ir2	66.6(9)
C2-C1-Ir2	69.6(8)
Ir1-C1-Ir2	139.2(7)
C3-C2-C1	119.2(13)
C3-C2-C7	119.3(14)
C1-C2-C7	121.5(13)
C3-C2-Ir2	68.5(8)
C1-C2-Ir2	75.1(9)
C7-C2-Ir2	129.0(11)
C4-C3-C2	124.6(14)
C4-C3-Ir2	75.1(9)
C2-C3-Ir2	75.4(8)
C3-C4-C5	116.1(13)
C3-C4-C8	123(2)
C5-C4-C8	121(2)
C3-C4-Ir2	69.4(9)
C5-C4-Ir2	70.2(9)
C8-C4-Ir2	130.2(13)
C4-C5-C6	121.9(14)
C4-C5-Ir2	74.1(10)

C6-C5-Ir2	71.1(9)
C1-C6-C5	120.5(14)
C1-C6-C9	122.5(14)
C5-C6-C9	116.8(14)
C1-C6-Ir2	77.9(10)
C5-C6-Ir2	71.7(9)
C9-C6-Ir2	126.4(11)
C02-C01-C06	113.6(13)
C02-C01-Ir01	122.1(11)
C06-C01-Ir01	123.9(10)
C02-C01-Ir02	67.7(8)
C06-C01-Ir02	64.0(7)
Ir01-C01-Ir02	143.7(6)
C01-C02-C03	123(2)
C01-C02-C07	119.5(14)
C03-C02-C07	117.3(13)
C01-C02-Ir02	78.8(8)
C03-C02-Ir02	66.2(9)
C07-C02-Ir02	127.2(11)
C04-C03-C02	118.9(14)
C04-C03-Ir02	77.8(10)
C02-C03-Ir02	76.1(8)
C05-C04-C03	118(2)
C05-C04-C08	123(2)
C03-C04-C08	118(2)
C05-C04-Ir02	70.0(9)
C03-C04-Ir02	65.7(9)
C08-C04-Ir02	127.5(13)
C04-C05-C06	121(2)
C04-C05-Ir02	75.8(10)
C06-C05-Ir02	70.4(9)
C05-C06-C01	122.3(14)
C05-C06-C09	118.4(14)
C01-C06-C09	119.0(13)
C05-C06-Ir02	72.7(9)
C01-C06-Ir02	80.3(8)
C09-C06-Ir02	124.1(11)
C12-C11-C18	118(2)
C12-C11-Ir2	73.3(10)
C18-C11-Ir2	112.0(13)
C11-C12-C13	130(2)
C11-C12-Ir2	68.6(10)
C13-C12-Ir2	114.0(13)
C12-C13-C14	115(2)
C13-C14-C15	113(2)
C16-C15-C14	128(2)
C16-C15-Ir2	69.3(11)
C14-C15-Ir2	109.8(12)
C15-C16-C17	121(2)
C15-C16-Ir2	72.0(9)
C17-C16-Ir2	116.7(13)
C16-C17-C18	110(2)
C11-C18-C17	115(2)
C012-C011-C018	126(2)
C012-C011-Ir02	70.2(11)
C018-C011-Ir02	112.9(12)
C011-C012-C013	124(2)
C011-C012-Ir02	71.0(11)

C013-C012-Ir02	116.2(13)
C014-C013-C012	111(2)
C013-C014-C015	117(2)
C016-C015-C014	122(2)
C016-C015-Ir02	69.9(8)
C014-C015-Ir02	110.6(13)
C015-C016-C017	125(2)
C015-C016-Ir02	71.7(9)
C017-C016-Ir02	114.2(11)
C018-C017-C016	113(2)
C011-C018-C017	114(2)
C22-C21-C28	125(2)
C22-C21-Ir1	68.0(11)
C28-C21-Ir1	114(2)
C21-C22-C23	120(2)
C21-C22-Ir1	72.3(12)
C23-C22-Ir1	113(2)
C24-C23-C22	117(2)
C23-C24-C25	115(2)
C26-C25-C24	123(2)
C26-C25-Ir1	72.3(10)
C24-C25-Ir1	112.1(13)
C25-C26-C27	126(2)
C25-C26-Ir1	71.1(11)
C27-C26-Ir1	111.5(13)
C26-C27-C28	116(2)
C27-C28-C21	115(2)
C022-C021-C028	122(2)
C022-C021-Ir01	71.9(10)
C028-C021-Ir01	112.8(13)
C021-C022-C023	126(2)
C021-C022-Ir01	70.1(11)
C023-C022-Ir01	112.8(13)
C024-C023-C022	115(2)
C025-C024-C023	117(2)
C026-C025-C024	127(2)
C026-C025-Ir01	71.5(11)
C024-C025-Ir01	112.4(13)
C025-C026-C027	122(2)
C025-C026-Ir01	72.1(10)
C027-C026-Ir01	109.4(14)
C026-C027-C028	118(2)
C027-C028-C021	114(2)

Table 1D. Anisotropic displacement parameters for (cod)IrBr(μ-2,4,6-$Me_3C_6H_2$)Ir(cod) (**2**). 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
Ir1	0.0502(4)	0.0420(4)	0.0450(3)	-0.0015(3)	-0.0029(3)	0.0071(3)
Ir2	0.0421(3)	0.0383(4)	0.0482(3)	0.0012(3)	0.0115(3)	-0.0022(3)
Ir01	0.0462(4)	0.0392(4)	0.0496(4)	0.0004(3)	0.0104(3)	0.0074(3)
Ir02	0.0411(3)	0.0354(4)	0.0418(3)	-0.0001(3)	-0.0014(2)	0.0022(3)
Br1	0.0934(15)	0.0510(12)	0.0696(11)	-0.0010(9)	-0.0124(10)	0.0277(11)
Br01	0.0559(10)	0.0786(14)	0.0748(11)	0.0110(10)	0.0215(9)	-0.0002(10)
C1	0.052(9)	0.033(9)	0.047(9)	0.007(7)	-0.003(7)	0.006(8)
C2	0.042(8)	0.035(9)	0.048(9)	0.006(7)	0.008(7)	0.000(7)
C3	0.068(11)	0.028(8)	0.036(7)	0.003(6)	0.008(7)	-0.009(8)
C4	0.034(8)	0.056(12)	0.058(10)	0.003(8)	-0.011(7)	-0.008(8)
C5	0.036(8)	0.042(10)	0.060(10)	-0.004(8)	-0.001(7)	0.001(7)
C6	0.050(9)	0.034(9)	0.051(9)	0.016(7)	0.008(7)	0.007(7)
C7	0.024(8)	0.066(13)	0.084(12)	0.003(10)	0.006(8)	-0.005(8)
C8	0.083(14)	0.08(2)	0.061(11)	-0.008(10)	-0.010(10)	0.012(12)
C9	0.073(12)	0.047(11)	0.057(10)	0.016(8)	0.022(9)	0.034(9)
C01	0.047(8)	0.011(6)	0.043(7)	0.011(6)	0.007(6)	0.000(6)
C02	0.078(11)	0.028(8)	0.029(7)	0.003(6)	0.003(7)	-0.009(8)
C03	0.075(12)	0.044(10)	0.050(9)	-0.021(8)	0.010(9)	-0.030(10)
C04	0.069(12)	0.037(10)	0.058(10)	-0.002(8)	0.029(9)	0.006(9)
C05	0.052(10)	0.070(13)	0.060(10)	-0.013(9)	0.023(8)	-0.004(10)
C06	0.038(8)	0.034(9)	0.054(9)	0.005(7)	0.006(7)	-0.004(7)
C07	0.076(12)	0.069(13)	0.038(8)	-0.008(8)	-0.001(8)	0.005(11)
C08	0.084(14)	0.080(16)	0.074(12)	-0.005(11)	0.027(11)	0.034(12)
C09	0.039(9)	0.076(14)	0.049(9)	-0.010(9)	-0.005(7)	0.002(9)
C11	0.055(11)	0.049(11)	0.075(11)	-0.007(9)	0.017(9)	0.004(9)
C12	0.106(17)	0.055(13)	0.075(12)	0.040(10)	0.043(12)	0.019(12)
C13	0.099(16)	0.042(12)	0.105(16)	0.012(11)	0.023(13)	0.019(12)
C14	0.108(19)	0.048(13)	0.127(19)	-0.013(13)	0.030(16)	0.011(13)
C15	0.111(17)	0.029(10)	0.090(13)	-0.010(10)	0.065(13)	-0.001(11)
C16	0.084(14)	0.082(15)	0.077(12)	-0.046(11)	0.049(11)	-0.059(12)
C17	0.115(20)	0.068(16)	0.124(19)	-0.020(14)	0.031(16)	-0.036(15)
C18	0.058(13)	0.067(16)	0.152(22)	0.009(15)	0.013(14)	-0.021(12)
C011	0.067(12)	0.044(11)	0.056(10)	0.007(8)	-0.008(9)	-0.002(9)
C012	0.067(13)	0.056(13)	0.084(13)	-0.004(11)	0.005(10)	-0.005(11)
C013	0.094(17)	0.055(14)	0.133(20)	-0.001(14)	0.000(15)	-0.003(13)
C014	0.099(18)	0.055(14)	0.137(20)	0.041(14)	0.002(16)	0.026(13)
C015	0.055(10)	0.043(11)	0.066(11)	0.025(8)	0.000(8)	0.009(9)
C016	0.075(12)	0.012(7)	0.054(9)	0.009(7)	0.010(8)	-0.018(8)
C017	0.071(13)	0.091(17)	0.073(12)	0.021(11)	0.003(10)	-0.043(12)
C018	0.065(13)	0.087(17)	0.091(15)	-0.008(12)	0.013(11)	-0.028(12)
C21	0.084(15)	0.042(12)	0.089(14)	-0.001(10)	-0.022(12)	-0.010(11)
C22	0.085(15)	0.043(12)	0.103(16)	-0.014(11)	0.009(12)	0.008(11)
C23	0.122(22)	0.115(24)	0.160(25)	-0.093(21)	-0.009(20)	0.043(19)
C24	0.130(21)	0.124(23)	0.055(12)	-0.021(14)	0.017(13)	0.013(18)
C25	0.084(13)	0.044(11)	0.046(9)	-0.015(8)	-0.003(9)	0.006(10)
C26	0.074(13)	0.077(15)	0.049(10)	-0.005(10)	-0.001(9)	0.007(12)
C27	0.086(16)	0.106(20)	0.078(14)	-0.027(14)	0.021(12)	-0.021(15)
C28	0.135(24)	0.117(24)	0.128(21)	0.054(19)	-0.018(19)	-0.061(20)

C021	0.099(16)	0.047(12)	0.087(14)	0.030(10)	0.040(13)	0.036(11)
C022	0.070(13)	0.051(12)	0.089(14)	0.008(11)	0.021(11)	-0.014(10)
C023	0.107(18)	0.070(16)	0.120(18)	-0.027(14)	0.047(15)	-0.028(14)
C024	0.107(18)	0.056(14)	0.117(18)	-0.036(13)	0.027(15)	0.005(14)
C025	0.082(14)	0.021(9)	0.085(13)	0.007(9)	0.024(11)	0.013(9)
C026	0.075(14)	0.049(12)	0.096(14)	0.020(11)	0.013(12)	0.036(11)
C027	0.161(28)	0.108(24)	0.125(21)	0.010(18)	0.007(20)	0.091(22)
C028	0.130(22)	0.086(19)	0.133(21)	0.040(16)	0.063(18)	0.029(17)

Table 1E. Hydrogen coordinates and isotropic displacement parameters for (cod)IrBr(μ-2,4,6-$Me_3C_6H_2$)Ir(cod) (**2**).

	x	y	z	U(eq)
H3	0.8754(11)	0.8386(7)	-0.1456(10)	0.044
H5	0.6730(10)	0.8590(7)	-0.0198(11)	0.048
H7A	1.0507(9)	0.8530(9)	0.0573(12)	0.059
H7B	1.0306(9)	0.8819(9)	-0.0440(12)	0.059
H7C	1.0293(9)	0.8094(9)	-0.0312(12)	0.059
H8A	0.6374(13)	0.8547(10)	-0.1854(12)	0.079
H8B	0.7018(13)	0.8121(10)	-0.2269(12)	0.079
H8C	0.7092(13)	0.8847(10)	-0.2329(12)	0.079
H9A	0.6917(12)	0.8593(8)	0.1382(11)	0.058
H9B	0.7716(12)	0.9013(8)	0.1886(11)	0.058
H9C	0.7777(12)	0.8287(8)	0.1999(11)	0.058
H03	1.3593(12)	0.8170(8)	0.8081(11)	0.057
H05	1.1498(12)	0.8075(9)	0.5922(12)	0.059
H07A	1.4846(12)	0.7505(9)	0.8222(10)	0.063
H07B	1.5117(12)	0.7393(9)	0.7262(10)	0.063
H07C	1.4692(12)	0.6851(9)	0.7735(10)	0.063
H08A	1.2242(14)	0.8601(10)	0.8308(13)	0.078
H08B	1.1328(14)	0.8356(10)	0.7714(13)	0.078
H08C	1.1786(14)	0.8936(10)	0.7368(13)	0.078
H09A	1.2556(10)	0.7117(9)	0.4486(10)	0.057
H09B	1.2050(10)	0.7756(9)	0.4354(10)	0.057
H09C	1.1596(10)	0.7167(9)	0.4678(10)	0.057
H11	0.6974(12)	0.7492(9)	0.0510(12)	0.059
H12	0.832(2)	0.7353(9)	0.1510(13)	0.075
H13A	0.841(2)	0.6143(9)	0.100(2)	0.082
H13B	0.909(2)	0.6497(9)	0.178(2)	0.082
H14A	0.949(2)	0.6162(10)	0.030(2)	0.093
H14B	0.992(2)	0.6757(10)	0.084(2)	0.093
H15	0.940(2)	0.7254(8)	-0.0518(14)	0.070
H16	0.7979(14)	0.7270(10)	-0.1397(14)	0.076
H17A	0.784(2)	0.6067(11)	-0.068(2)	0.102
H17B	0.714(2)	0.6367(11)	-0.151(2)	0.102
H18A	0.6345(14)	0.6756(10)	-0.057(2)	0.094
H18B	0.6828(14)	0.6254(10)	0.014(2)	0.094
H31	1.4701(12)	0.8624(8)	0.7201(12)	0.059
H32	1.3452(13)	0.9193(9)	0.7168(14)	0.071
H33A	1.317(2)	1.0133(10)	0.637(2)	0.098
H33B	1.400(2)	1.0036(10)	0.592(2)	0.098
H34A	1.303(2)	0.9846(10)	0.466(2)	0.101
H34B	1.228(2)	0.9710(10)	0.521(2)	0.101
H35	1.2398(12)	0.8701(8)	0.4818(11)	0.057
H36	1.3712(11)	0.8202(7)	0.4826(10)	0.048
H37A	1.4981(13)	0.8721(11)	0.4686(13)	0.080
H37B	1.4538(13)	0.9365(11)	0.4804(13)	0.080
H38A	1.5558(13)	0.8634(11)	0.6169(14)	0.082
H38B	1.5454(13)	0.9360(11)	0.6159(14)	0.082
H21	0.9735(14)	0.9563(9)	0.088(2)	0.078
H22	0.870(2)	0.9487(9)	0.179(2)	0.079
H23A	0.961(2)	1.0413(14)	0.298(2)	0.138

H23B	0.886(2)	0.9995(14)	0.323(2)	0.138
H24A	0.981(2)	0.9563(13)	0.4263(14)	0.104
H24B	1.056(2)	0.9973(13)	0.3998(14)	0.104
H25	1.0314(13)	0.8725(9)	0.3617(11)	0.061
H26	1.1329(13)	0.8754(11)	0.2736(12)	0.069
H27A	1.193(2)	0.9576(12)	0.223(2)	0.090
H27B	1.166(2)	0.9974(12)	0.302(2)	0.090
H28A	1.102(2)	1.0094(14)	0.123(2)	0.134
H28B	1.069(2)	1.0450(14)	0.202(2)	0.134
H41	1.3508(14)	0.6318(9)	0.707(2)	0.074
H42	1.2458(13)	0.6323(10)	0.5724(14)	0.070
H43A	1.246(2)	0.5064(11)	0.552(2)	0.096
H43B	1.205(2)	0.5533(11)	0.472(2)	0.096
H44A	1.350(2)	0.4853(10)	0.484(2)	0.093
H44B	1.306(2)	0.5298(10)	0.402(2)	0.093
H45	1.4161(13)	0.5950(7)	0.4436(13)	0.062
H46	1.5230(14)	0.5938(9)	0.575(2)	0.074
H47A	1.527(2)	0.5286(13)	0.694(2)	0.135
H47B	1.461(2)	0.4845(13)	0.627(2)	0.135
H48A	1.427(2)	0.5457(12)	0.770(2)	0.111
H48B	1.360(2)	0.5037(12)	0.699(2)	0.111

Table 2A. Crystal data and structure refinement for Ir(cod)Br(μ-2,6-$Me_2C_6H_3$)Ir(cod) (**3**).

Empirical formula	$C_{24}H_{33}BrIr_2$
Formula weight	785.81
Temperature	293(2) K
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 7.815(2) Å α = 90 deg. b = 20.328(3) Å β = 105.67(2) deg. c = 14.534(3) Å γ = 90 deg.
Volume	2223.2(7) $Å^3$
Z	4
Density (calculated)	2.348 g/cm^3
Absorption coefficient	13.764 mm^{-1}
Absorption correction	Semi-empirical from psi-scans
Transmission	0.4266 to 0.9678
F(000)	1464
Diffractometer	Enraf-Nonius CAD4
Radiation	graphite-monochromated MoKα (0.71073 Å)
Scan type	ω-2θ scans
Decay	negligible
Crystal size	0.35 x 0.32 x 0.25 mm
Crystal habit	obelisk
Crystal color	yellow
Theta range for data collection	2.00 to 25.00 deg.
Limiting indices	-9<=h<=0, -24<=k<=0, -16<=l<=17
Reflections collected	4199
Independent reflections	3902 [R(int) = 0.0779]
Structure solution method	Patterson
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3902 / 0 / 236

Goodness-of-fit on F^2	1.052
Final R indices [I>2σ(I)]	R1 = 0.0415, wR2 = 0.1076
R indices (all data)	R1 = 0.0582, wR2 = 0.1163
Largest diff. peak and hole	1.236 and -2.659 e/Å^3

Table 2B. Atomic coordinates and equivalent isotropic displacement parameters for Ir(cod)Br(μ-2,6-$Me_2C_6H_3$)Ir(cod) (**3**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ir1	0.62129(5)	0.61615(2)	-0.15406(3)	0.0357(2)
Ir2	0.53900(5)	0.77333(2)	0.01933(3)	0.0335(2)
Br	0.6727(2)	0.72057(6)	-0.23348(9)	0.0597(3)
C1	0.5712(12)	0.6627(5)	-0.0390(7)	0.034(2)
C2	0.7038(12)	0.6786(5)	0.0425(7)	0.034(2)
C3	0.671(2)	0.7016(6)	0.1288(7)	0.044(3)
C4	0.4985(8)	0.7060(3)	0.1372(5)	0.051(3)
C5	0.3605(8)	0.6957(3)	0.0548(5)	0.046(3)
C6	0.3937(8)	0.6797(3)	-0.0338(5)	0.038(2)
C7	0.8981(10)	0.6699(7)	0.0444(6)	0.058(3)
C8	0.2370(10)	0.6737(7)	-0.1208(6)	0.063(3)
C11	0.335(2)	0.8405(7)	-0.0473(10)	0.078(4)
C12	0.441(2)	0.8296(7)	-0.1065(8)	0.069(4)
C13	0.575(3)	0.8804(7)	-0.1231(11)	0.099(7)
C14	0.764(3)	0.8730(9)	-0.0534(13)	0.096(6)
C15	0.755(2)	0.8402(6)	0.0380(10)	0.066(4)
C16	0.644(2)	0.8619(6)	0.0940(8)	0.057(3)
C17	0.525(3)	0.9198(7)	0.0711(11)	0.089(5)
C18	0.337(3)	0.8985(7)	0.0133(12)	0.087(5)
C21	0.666(2)	0.5286(5)	-0.0727(8)	0.049(3)
C22	0.486(2)	0.5335(6)	-0.1226(9)	0.053(3)
C23	0.393(2)	0.4954(7)	-0.2089(12)	0.077(4)
C24	0.493(2)	0.4972(8)	-0.2884(10)	0.084(5)
C25	0.604(2)	0.5588(7)	-0.2832(8)	0.063(4)
C26	0.775(2)	0.5624(7)	-0.2340(8)	0.059(3)
C27	0.883(2)	0.5105(6)	-0.1721(11)	0.068(4)
C28	0.788(2)	0.4813(6)	-0.1018(11)	0.068(4)

Table 2C. Bond lengths [Å] and angles [deg] for Ir(cod)Br(μ-2,6-$Me_2C_6H_3$)Ir(cod) (**3**).

Ir1-C1	2.049(9)
Ir1-C22	2.100(11)
Ir1-C21	2.113(11)
Ir1-C26	2.176(11)
Ir1-C25	2.182(11)
Ir1-Br	2.5000(12)
Ir2-C12	2.117(12)
Ir2-C11	2.122(11)
Ir2-C15	2.125(12)
Ir2-C16	2.148(12)
Ir2-C3	2.200(10)
Ir2-C6	2.244(6)
Ir2-C5	2.256(6)
Ir2-C4	2.280(6)
Ir2-C2	2.290(9)
Ir2-C1	2.441(10)
C1-C2	1.385(14)
C1-C6	1.451(11)
C2-C3	1.425(14)
C2-C7	1.522(12)
C3-C4	1.391(12)
C4-C5	1.39
C5-C6	1.42
C6-C8	1.509(10)
C11-C12	1.36(2)
C11-C18	1.47(2)
C12-C13	1.54(2)
C13-C14	1.55(2)
C14-C15	1.51(2)
C15-C16	1.41(2)
C16-C17	1.48(2)
C17-C18	1.54(2)
C21-C22	1.40(2)
C21-C28	1.49(2)
C22-C23	1.49(2)
C23-C24	1.56(2)
C24-C25	1.51(2)
C25-C26	1.34(2)
C26-C27	1.49(2)
C27-C28	1.54(2)
C1-Ir1-C22	88.5(4)
C1-Ir1-C21	88.4(4)
C22-Ir1-C21	38.9(5)
C1-Ir1-C26	157.2(4)
C22-Ir1-C26	95.6(5)
C21-Ir1-C26	81.0(5)
C1-Ir1-C25	165.2(5)
C22-Ir1-C25	80.9(5)
C21-Ir1-C25	89.6(5)
C26-Ir1-C25	35.7(5)
C1-Ir1-Br	94.3(3)
C22-Ir1-Br	158.9(4)

C21-Ir1-Br	161.9(3)
C26-Ir1-Br	90.0(4)
C25-Ir1-Br	92.1(4)
C12-Ir2-C11	37.5(6)
C12-Ir2-C15	81.6(6)
C11-Ir2-C15	96.8(6)
C12-Ir2-C16	89.1(5)
C11-Ir2-C16	80.2(6)
C15-Ir2-C16	38.4(5)
C12-Ir2-C3	166.6(5)
C11-Ir2-C3	154.8(5)
C15-Ir2-C3	97.5(5)
C16-Ir2-C3	98.6(4)
C12-Ir2-C6	97.5(4)
C11-Ir2-C6	98.1(5)
C15-Ir2-C6	153.7(4)
C16-Ir2-C6	166.9(4)
C3-Ir2-C6	77.4(4)
C12-Ir2-C5	118.3(5)
C11-Ir2-C5	96.9(5)
C15-Ir2-C5	159.4(4)
C16-Ir2-C5	130.3(4)
C3-Ir2-C5	64.5(3)
C6-Ir2-C5	36.76(10)
C12-Ir2-C4	151.9(5)
C11-Ir2-C4	119.3(5)
C15-Ir2-C4	123.7(4)
C16-Ir2-C4	103.6(4)
C3-Ir2-C4	36.1(3)
C6-Ir2-C4	65.8(2)
C5-Ir2-C4	35.77(9)
C12-Ir2-C2	129.7(5)
C11-Ir2-C2	158.5(5)
C15-Ir2-C2	97.1(5)
C16-Ir2-C2	120.4(4)
C3-Ir2-C2	36.9(4)
C6-Ir2-C2	63.2(3)
C5-Ir2-C2	74.7(3)
C4-Ir2-C2	64.6(3)
C12-Ir2-C1	104.2(4)
C11-Ir2-C1	124.7(5)
C15-Ir2-C1	118.8(4)
C16-Ir2-C1	152.4(4)
C3-Ir2-C1	64.4(4)
C6-Ir2-C1	35.8(3)
C5-Ir2-C1	64.1(3)
C4-Ir2-C1	75.9(3)
C2-Ir2-C1	33.9(3)
C2-C1-C6	113.9(8)
C2-C1-Ir1	122.8(7)
C6-C1-Ir1	123.3(6)
C2-C1-Ir2	67.1(6)
C6-C1-Ir2	64.7(4)
Ir1-C1-Ir2	140.3(4)
C1-C2-C3	124.0(9)
C1-C2-C7	120.0(8)
C3-C2-C7	115.9(9)
C1-C2-Ir2	79.0(6)

C3-C2-Ir2	68.1(5)
C7-C2-Ir2	128.3(8)
C4-C3-C2	120.4(9)
C4-C3-Ir2	75.1(5)
C2-C3-Ir2	75.0(6)
C3-C4-C5	117.4(5)
C3-C4-Ir2	68.8(5)
C5-C4-Ir2	71.2(2)
C4-C5-C6	121.7
C4-C5-Ir2	73.1(2)
C6-C5-Ir2	71.2(2)
C5-C6-C1	120.9(4)
C5-C6-C8	118.2(4)
C1-C6-C8	120.6(6)
C5-C6-Ir2	72.1(2)
C1-C6-Ir2	79.5(5)
C8-C6-Ir2	125.3(6)
C12-C11-C18	127(2)
C12-C11-Ir2	71.0(7)
C18-C11-Ir2	111.0(10)
C11-C12-C13	123.1(14)
C11-C12-Ir2	71.5(7)
C13-C12-Ir2	113.4(10)
C12-C13-C14	113.5(11)
C15-C14-C13	110.9(13)
C16-C15-C14	123.7(14)
C16-C15-Ir2	71.7(7)
C14-C15-Ir2	113.3(10)
C15-C16-C17	124.5(13)
C15-C16-Ir2	69.9(7)
C17-C16-Ir2	114.8(10)
C16-C17-C18	110.4(12)
C11-C18-C17	113.9(14)
C22-C21-C28	121.8(11)
C22-C21-Ir1	70.0(6)
C28-C21-Ir1	114.0(9)
C21-C22-C23	126.2(12)
C21-C22-Ir1	71.0(6)
C23-C22-Ir1	113.1(9)
C22-C23-C24	112.8(11)
C25-C24-C23	112.0(11)
C26-C25-C24	123.2(14)
C26-C25-Ir1	71.9(6)
C24-C25-Ir1	112.8(9)
C25-C26-C27	127.4(14)
C25-C26-Ir1	72.4(7)
C27-C26-Ir1	109.8(8)
C26-C27-C28	111.9(11)
C21-C28-C27	113.6(10)

Table 2D. Anisotropic displacement parameters for Ir(cod)Br(μ-2,6-$Me_2C_6H_3$)Ir(cod) (**3**). 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
Ir1	0.0373(2)	0.0405(3)	0.0314(2)	-0.0011(2)	0.0127(2)	-0.0011(2)
Ir2	0.0328(2)	0.0359(2)	0.0305(2)	0.0025(2)	0.0061(2)	0.0045(2)
Br	0.0726(8)	0.0601(8)	0.0546(7)	0.0152(6)	0.0314(6)	-0.0019(6)
C1	0.034(5)	0.035(5)	0.038(5)	0.008(4)	0.020(4)	-0.003(4)
C2	0.031(5)	0.033(5)	0.039(5)	0.004(4)	0.009(4)	0.005(4)
C3	0.053(6)	0.046(6)	0.032(5)	0.011(5)	0.009(5)	0.014(5)
C4	0.073(8)	0.049(7)	0.037(6)	0.006(5)	0.027(6)	0.005(6)
C5	0.037(5)	0.057(7)	0.053(6)	-0.004(6)	0.028(5)	-0.014(5)
C6	0.033(5)	0.039(6)	0.047(6)	0.003(5)	0.018(4)	-0.004(4)
C7	0.029(5)	0.080(9)	0.063(8)	-0.012(7)	0.010(5)	0.009(6)
C8	0.043(7)	0.074(9)	0.067(8)	-0.017(7)	0.006(6)	-0.002(6)
C11	0.082(10)	0.072(10)	0.067(9)	0.015(8)	-0.004(8)	0.046(8)
C12	0.100(11)	0.064(9)	0.034(6)	0.006(6)	0.004(7)	0.016(8)
C13	0.21(2)	0.043(8)	0.059(9)	0.022(7)	0.066(12)	0.020(10)
C14	0.11(2)	0.089(12)	0.093(12)	0.005(10)	0.041(11)	-0.051(11)
C15	0.076(9)	0.034(6)	0.091(10)	-0.012(6)	0.027(8)	-0.025(6)
C16	0.078(9)	0.055(7)	0.033(6)	-0.001(5)	0.007(6)	0.007(7)
C17	0.16(2)	0.043(8)	0.056(8)	-0.003(6)	0.024(10)	0.018(10)
C18	0.116(14)	0.056(9)	0.091(12)	0.000(8)	0.029(11)	0.029(9)
C21	0.062(7)	0.028(6)	0.054(7)	0.003(5)	0.010(6)	-0.008(5)
C22	0.067(8)	0.037(6)	0.061(7)	-0.003(5)	0.029(6)	-0.009(6)
C23	0.057(8)	0.053(8)	0.117(13)	-0.013(8)	0.017(8)	-0.016(7)
C24	0.075(10)	0.106(13)	0.063(9)	-0.037(9)	0.004(7)	-0.016(9)
C25	0.075(9)	0.069(9)	0.042(6)	-0.026(6)	0.009(6)	-0.001(7)
C26	0.071(9)	0.062(8)	0.052(7)	-0.020(6)	0.028(7)	0.004(7)
C27	0.058(8)	0.057(8)	0.090(10)	-0.018(7)	0.021(7)	0.020(7)
C28	0.078(9)	0.037(7)	0.081(9)	-0.003(6)	0.008(8)	0.006(6)

Table 2E. Hydrogen coordinates and isotropic displacement parameters for Ir(cod)Br(μ-2,6-$Me_2C_6H_3$)Ir(cod) (**3**).

	x	y	z	U(eq)
H3	0.766(2)	0.7137(6)	0.1799(7)	0.044
H4	0.4759(8)	0.7155(3)	0.1954(5)	0.051
H5	0.2437(8)	0.6994(3)	0.0580(5)	0.046
H7A	0.9315(13)	0.6246(8)	0.0571(14)	0.058
H7B	0.9709(10)	0.6971(13)	0.0937(12)	0.058
H7C	0.9146(11)	0.6824(6)	-0.0163(9)	0.058
H8A	0.1767(10)	0.6329(6)	-0.1183(9)	0.063
H8B	0.2779(10)	0.6748(7)	-0.1774(6)	0.063
H8C	0.1567(10)	0.7096(7)	-0.1220(7)	0.063
H11	0.253(2)	0.8078(7)	-0.0451(10)	0.078
H12	0.432(2)	0.7895(7)	-0.1383(8)	0.069
H13A	0.531(3)	0.9242(7)	-0.1162(11)	0.099
H13B	0.584(3)	0.8761(7)	-0.1882(11)	0.099
H14A	0.838(3)	0.8470(9)	-0.0835(13)	0.096
H14B	0.818(3)	0.9161(9)	-0.0392(13)	0.096
H15	0.826(2)	0.8035(6)	0.0586(10)	0.066
H16	0.647(2)	0.8383(6)	0.1492(8)	0.057
H17A	0.572(3)	0.9513(7)	0.0344(11)	0.089
H17B	0.518(3)	0.9409(7)	0.1299(11)	0.089
H18A	0.266(3)	0.8891(7)	0.0573(12)	0.087
H18B	0.281(3)	0.9349(7)	-0.0269(12)	0.087
H21	0.711(2)	0.5556(5)	-0.0201(8)	0.049
H22	0.418(2)	0.5635(6)	-0.0995(9)	0.053
H23A	0.275(2)	0.5131(7)	-0.2344(12)	0.077
H23B	0.382(2)	0.4501(7)	-0.1908(12)	0.077
H24A	0.569(2)	0.4589(8)	-0.2820(10)	0.084
H24B	0.407(2)	0.4950(8)	-0.3505(10)	0.084
H25	0.550(2)	0.5961(7)	-0.3159(8)	0.063
H26	0.833(2)	0.6016(7)	-0.2389(8)	0.059
H27A	0.996(2)	0.5293(6)	-0.1364(11)	0.068
H27B	0.908(2)	0.4756(6)	-0.2121(11)	0.068
H28A	0.719(2)	0.4433(6)	-0.1312(11)	0.068
H28B	0.876(2)	0.4664(6)	-0.0451(11)	0.068

Table 3A. Crystal data and structure refinement for $Ir(CO)_2Br(\mu\text{-}2,4,6\text{-}Me_3C_6H_2)Ir(cod)$ (**5**).

Empirical formula	$C_{19}H_{23}BrIr_2O_2$
Formula weight	747.68
Temperature	293(2) K
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 14.1633(11) Å α = 90 deg. b = 14.7640(11) Å β = 90 deg. c = 18.7081(14) Å γ = 90 deg.
Volume	3912.0(5) $Å^3$
Z	8
Density (calculated)	2.539 g/cm^3
Absorption coefficient	15.644 mm^{-1}
Absorption correction	SADABS
Transmission	0.0254 to 0.0656
F(000)	2736
Diffractometer	Bruker SMART APEX
Radiation	graphite-monochromated MoKα (0.71073 Å)
Scan type	ω scans
Decay	negligible
Crystal size	0.5 x 0.5 x 0.3 mm
Crystal habit	irregular
Crystal color	yellow
Theta range for data collection	2.18 to 28.28 deg.
Limiting indices	-18<=h<=18, -19<=k<=19, -23<=l<=23
Reflections collected	32944
Independent reflections	4719 [R(int) = 0.0701]
Structure solution method	Patterson
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	4719 / 0 / 217
Goodness-of-fit on F^2	1.117
Final R indices [$I>2\sigma(I)$]	R1 = 0.0366, wR2 = 0.0886
R indices (all data)	R1 = 0.0421, wR2 = 0.0905
Largest diff. peak and hole	1.264 and -3.433 e/Å^3

Table 3B. Atomic coordinates and equivalent isotropic displacement parameters for $Ir(CO)_2Br(\mu\text{-}2,4,6\text{-}Me_3C_6H_2)Ir(cod)$ (**5**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ir1	0.22583(2)	0.95811(2)	0.068050(13)	0.02117(9)
Ir2	0.45905(2)	0.82686(2)	0.155544(12)	0.01674(8)
Br	0.11922(5)	0.99935(4)	0.16882(4)	0.0312(2)
O1	0.3535(4)	0.8996(4)	-0.0484(3)	0.0434(13)
O2	0.1007(5)	1.0561(4)	-0.0379(4)	0.062(2)
C1	0.3046(4)	0.8900(4)	0.1456(3)	0.0178(12)
C2	0.2987(4)	0.7951(4)	0.1551(3)	0.0176(12)
C3	0.3471(4)	0.7520(4)	0.2132(3)	0.0209(12)
C4	0.3962(5)	0.8006(4)	0.2675(3)	0.0237(13)
C5	0.4039(3)	0.8948(3)	0.2575(2)	0.0231(13)
C6	0.3639(3)	0.9374(3)	0.1962(2)	0.0184(12)
C7	0.2442(5)	0.7371(4)	0.1051(4)	0.029(2)
C8	0.4374(6)	0.7545(5)	0.3314(4)	0.035(2)
C9	0.3807(5)	1.0390(4)	0.1883(4)	0.028(2)
C11	0.5824(5)	0.9089(5)	0.1393(4)	0.0282(14)
C12	0.5313(5)	0.8990(5)	0.0743(4)	0.028(2)
C13	0.5675(6)	0.8425(5)	0.0127(4)	0.031(2)
C14	0.5278(6)	0.7448(5)	0.0157(4)	0.033(2)
C15	0.5034(5)	0.7163(4)	0.0904(3)	0.0238(13)
C16	0.5648(5)	0.7235(5)	0.1498(4)	0.0274(14)
C17	0.6649(5)	0.7569(5)	0.1435(5)	0.039(2)
C18	0.6728(5)	0.8585(6)	0.1571(4)	0.041(2)
C31	0.3068(5)	0.9224(4)	-0.0042(4)	0.0282(14)
C32	0.1468(6)	1.0206(5)	0.0027(4)	0.036(2)

Table 3C. Bond lengths [Å] and angles [deg] for $Ir(CO)_2Br(\mu\text{-}2,4,6\text{-}Me_3C_6H_2)Ir(cod)$ (**5**).

Ir1-C31	1.849(7)
Ir1-C32	1.897(7)
Ir1-C1	2.088(6)
Ir1-Br	2.4909(8)
Ir2-C12	2.119(6)
Ir2-C15	2.132(6)
Ir2-C16	2.141(7)
Ir2-C11	2.147(7)
Ir2-C3	2.213(6)
Ir2-C6	2.248(4)
Ir2-C5	2.292(4)
Ir2-C4	2.309(6)
Ir2-C2	2.319(6)
Ir2-C1	2.385(6)
O1-C31	1.112(8)
O2-C32	1.130(9)
C1-C2	1.414(8)
C1-C6	1.446(7)
C2-C3	1.435(8)
C2-C7	1.484(9)
C3-C4	1.424(9)
C4-C5	1.408(7)
C4-C8	1.495(9)
C5-C6	1.43
C6-C9	1.526(7)
C11-C12	1.421(10)
C11-C18	1.518(11)
C12-C13	1.512(9)
C13-C14	1.550(9)
C14-C15	1.498(9)
C15-C16	1.416(10)
C16-C17	1.505(10)
C17-C18	1.525(11)
C31-Ir1-C32	91.9(3)
C31-Ir1-C1	92.2(3)
C32-Ir1-C1	175.7(3)
C31-Ir1-Br	177.1(2)
C32-Ir1-Br	90.6(2)
C1-Ir1-Br	85.2(2)
C12-Ir2-C15	80.4(3)
C12-Ir2-C16	89.1(3)
C15-Ir2-C16	38.7(3)
C12-Ir2-C11	38.9(3)
C15-Ir2-C11	96.4(3)
C16-Ir2-C11	80.0(3)
C12-Ir2-C3	161.2(3)
C15-Ir2-C3	96.2(2)
C16-Ir2-C3	99.8(2)
C11-Ir2-C3	159.0(3)
C12-Ir2-C6	99.6(2)
C15-Ir2-C6	157.7(2)
C16-Ir2-C6	162.5(2)

C11-Ir2-C6	97.2(2)
C3-Ir2-C6	76.6(2)
C12-Ir2-C5	122.8(2)
C15-Ir2-C5	155.7(2)
C16-Ir2-C5	126.3(2)
C11-Ir2-C5	98.5(2)
C3-Ir2-C5	64.5(2)
C6-Ir2-C5	36.57(7)
C12-Ir2-C4	157.1(3)
C15-Ir2-C4	120.3(2)
C16-Ir2-C4	101.3(2)
C11-Ir2-C4	122.5(2)
C3-Ir2-C4	36.6(2)
C6-Ir2-C4	65.4(2)
C5-Ir2-C4	35.6(2)
C12-Ir2-C2	124.9(3)
C15-Ir2-C2	97.6(2)
C16-Ir2-C2	122.8(2)
C11-Ir2-C2	155.5(2)
C3-Ir2-C2	36.8(2)
C6-Ir2-C2	64.0(2)
C5-Ir2-C2	76.0(2)
C4-Ir2-C2	65.9(2)
C12-Ir2-C1	101.0(2)
C15-Ir2-C1	121.6(2)
C16-Ir2-C1	156.4(2)
C11-Ir2-C1	121.0(2)
C3-Ir2-C1	64.9(2)
C6-Ir2-C1	36.2(2)
C5-Ir2-C1	65.2(2)
C4-Ir2-C1	77.4(2)
C2-Ir2-C1	34.9(2)
C2-C1-C6	115.6(5)
C2-C1-Ir1	122.2(5)
C6-C1-Ir1	122.1(4)
C2-C1-Ir2	70.0(3)
C6-C1-Ir2	66.7(3)
Ir1-C1-Ir2	137.1(3)
C1-C2-C3	120.4(6)
C1-C2-C7	121.5(6)
C3-C2-C7	118.1(5)
C1-C2-Ir2	75.1(4)
C3-C2-Ir2	67.6(3)
C7-C2-Ir2	128.9(5)
C4-C3-C2	123.4(5)
C4-C3-Ir2	75.3(4)
C2-C3-Ir2	75.6(4)
C5-C4-C3	116.1(5)
C5-C4-C8	121.8(6)
C3-C4-C8	122.1(6)
C5-C4-Ir2	71.5(3)
C3-C4-Ir2	68.0(3)
C8-C4-Ir2	130.7(5)
C4-C5-C6	120.8(3)
C4-C5-Ir2	72.9(3)
C6-C5-Ir2	70.04(11)
C5-C6-C1	122.9(3)
C5-C6-C9	116.7(3)

C1-C6-C9	120.2(5)
C5-C6-Ir2	73.38(11)
C1-C6-Ir2	77.1(3)
C9-C6-Ir2	126.0(4)
C12-C11-C18	124.5(6)
C12-C11-Ir2	69.5(4)
C18-C11-Ir2	112.2(5)
C11-C12-C13	122.4(7)
C11-C12-Ir2	71.6(4)
C13-C12-Ir2	115.6(4)
C12-C13-C14	111.3(5)
C15-C14-C13	112.3(6)
C16-C15-C14	124.6(6)
C16-C15-Ir2	71.0(4)
C14-C15-Ir2	112.7(4)
C15-C16-C17	122.8(6)
C15-C16-Ir2	70.3(4)
C17-C16-Ir2	115.4(5)
C16-C17-C18	112.2(6)
C11-C18-C17	112.6(6)
O1-C31-Ir1	178.1(7)
O2-C32-Ir1	177.9(7)

Table 3D. Anisotropic displacement parameters for $Ir(CO)_2Br(\mu\text{-}2,4,6\text{-}Me_3C_6H_2)Ir(cod)$ (**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
Ir1	0.0297(2)	0.01568(13)	0.01809(14)	0.00325(8)	-0.00250(10)	0.00122(9)
Ir2	0.02283(14)	0.01576(13)	0.01162(13)	0.00060(8)	0.00019(9)	-0.00064(8)
Br	0.0338(4)	0.0281(3)	0.0318(4)	0.0075(3)	0.0076(3)	0.0053(3)
O1	0.058(4)	0.044(3)	0.027(3)	-0.001(2)	0.006(3)	0.007(3)
O2	0.075(5)	0.066(4)	0.044(4)	0.018(3)	-0.010(4)	0.034(4)
C1	0.022(3)	0.016(3)	0.015(3)	0.002(2)	0.005(2)	0.002(2)
C2	0.019(3)	0.016(3)	0.017(3)	0.000(2)	0.001(2)	-0.001(2)
C3	0.023(3)	0.019(3)	0.021(3)	0.003(2)	0.000(3)	0.002(2)
C4	0.027(3)	0.030(3)	0.015(3)	0.004(2)	0.010(3)	0.006(3)
C5	0.028(3)	0.027(3)	0.014(3)	-0.006(2)	-0.001(3)	-0.001(3)
C6	0.026(3)	0.014(2)	0.015(3)	-0.003(2)	0.002(2)	0.000(2)
C7	0.036(4)	0.020(3)	0.030(4)	0.006(3)	-0.009(3)	-0.008(3)
C8	0.040(4)	0.044(4)	0.020(3)	0.012(3)	-0.007(3)	0.005(3)
C9	0.042(4)	0.014(3)	0.028(4)	-0.004(2)	-0.004(3)	-0.005(3)
C11	0.031(4)	0.026(3)	0.028(3)	-0.005(3)	0.008(3)	-0.008(3)
C12	0.035(4)	0.024(3)	0.026(4)	0.007(3)	0.007(3)	-0.003(3)
C13	0.039(4)	0.032(3)	0.022(3)	-0.002(3)	0.010(3)	-0.003(3)
C14	0.051(5)	0.028(3)	0.019(3)	-0.003(3)	0.005(3)	0.008(3)
C15	0.033(3)	0.016(3)	0.023(3)	-0.004(2)	0.007(3)	0.001(3)
C16	0.028(3)	0.030(3)	0.024(3)	0.005(3)	0.004(3)	0.007(3)
C17	0.034(4)	0.043(4)	0.039(4)	-0.002(3)	-0.005(4)	0.008(3)
C18	0.024(4)	0.056(5)	0.041(5)	-0.011(4)	0.003(3)	-0.011(4)
C31	0.036(4)	0.024(3)	0.025(3)	0.002(3)	-0.003(3)	0.006(3)
C32	0.049(5)	0.032(3)	0.027(4)	0.005(3)	0.001(4)	0.013(3)

Table 3E. Hydrogen coordinates and isotropic displacement parameters for $Ir(CO)_2Br(\mu\text{-}2,4,6\text{-}Me_3C_6H_2)Ir(cod)$ (**5**).

	x	y	z	U(eq)
H3	0.3465(4)	0.6891(4)	0.2156(3)	0.021
H5	0.4355(3)	0.9297(3)	0.2913(2)	0.023
H7A	0.1790(7)	0.737(2)	0.1191(14)	0.029
H7B	0.269(2)	0.6765(8)	0.107(2)	0.029
H7C	0.250(3)	0.761(2)	0.0575(5)	0.029
H8A	0.457(3)	0.6943(12)	0.3187(7)	0.035
H8B	0.3909(11)	0.752(3)	0.3687(9)	0.035
H8C	0.491(2)	0.788(2)	0.348(2)	0.035
H9A	0.331(2)	1.0715(4)	0.212(2)	0.028
H9B	0.382(3)	1.0546(6)	0.1385(4)	0.028
H9C	0.4400(14)	1.0547(6)	0.210(2)	0.028
H11	0.5588(5)	0.9490(5)	0.1732(4)	0.028
H12	0.4736(5)	0.9284(5)	0.0696(4)	0.028
H13A	0.6359(6)	0.8404(5)	0.0144(4)	0.031
H13B	0.5492(6)	0.8706(5)	-0.0320(4)	0.031
H14A	0.4718(6)	0.7411(5)	-0.0139(4)	0.033
H14B	0.5744(6)	0.7033(5)	-0.0036(4)	0.033
H15	0.4436(5)	0.6922(4)	0.0982(3)	0.024
H16	0.5424(5)	0.7069(5)	0.1946(4)	0.027
H17A	0.6885(5)	0.7435(5)	0.0960(5)	0.039
H17B	0.7042(5)	0.7249(5)	0.1776(5)	0.039
H18A	0.6883(5)	0.8685(6)	0.2069(4)	0.041
H18B	0.7239(5)	0.8828(6)	0.1284(4)	0.041

Table 4A. Crystal data and structure refinement for $Ir(CO)_2(2,6\text{-}Me_2C_6H_3)(\mu\text{-}2,6\text{-}Me_2C_6H_3)Ir(cod)$ (**8**).

Empirical formula	$C_{26}H_{30}Ir_2O_2$
Formula weight	758.90
Temperature	170(2) K
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 14.2533(6) Å α = 90 deg. b = 14.6197(6) Å β = 90 deg. c = 21.3585(8) Å γ = 90 deg.
Volume	4450.7(3) $Å^3$
Z	8
Density (calculated)	2.265 g/cm^3
Absorption coefficient	11.968 mm^{-1}
Absorption correction	SADABS
Transmission	0.7438 to 0.7495
F(000)	2848
Diffractometer	Bruker SMART APEX
Radiation	graphite-monochromated MoKα (0.71073 Å)
Scan type	ω scans
Decay	negligible
Crystal size	0.27 x 0.28 x 0.35 mm
Crystal habit	prism
Crystal color	orange
Theta range for data collection	1.91 to 30.52 deg.
Limiting indices	-20<=h<=20, -20<=k<=20, -30<=l<=29
Reflections collected	54340
Independent reflections	6802 [R(int) = 0.0337]
Structure solution method	Patterson
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	6802 / 0 / 271
Goodness-of-fit on F^2	1.083
Final R indices [$I>2\sigma(I)$]	R1 = 0.0232, wR2 = 0.0617
R indices (all data)	R1 = 0.0260, wR2 = 0.0630
Largest diff. peak and hole	1.818 and -0.659 e/Å^3

Table 4B. Atomic coordinates and equivalent isotropic displacement parameters for $Ir(CO)_2(2,6\text{-}Me_2C_6H_3)(\mu\text{-}2,6\text{-}Me_2C_6H_3)Ir(cod)$ (**8**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ir1	-0.231441(9)	0.812890(9)	0.081531(6)	0.01703(4)
Ir2	0.024354(9)	0.905306(9)	0.155372(6)	0.01613(4)
C1	-0.0939(2)	0.8686(2)	0.0786(2)	0.0162(6)
C2	-0.0773(2)	0.9654(2)	0.0862(2)	0.0190(6)
C3	0.0121(3)	1.0070(3)	0.0751(2)	0.0222(7)
C4	0.0908(3)	0.9525(3)	0.0631(2)	0.0239(7)
C5	0.0791(2)	0.8561(3)	0.0646(2)	0.0225(7)
C6	-0.0116(2)	0.8142(2)	0.0706(2)	0.0188(6)
C7	-0.1575(3)	1.0286(3)	0.1023(2)	0.0230(7)
C8	-0.0142(3)	0.7116(3)	0.0697(2)	0.0251(7)
C11	0.1470(3)	0.8877(3)	0.2111(2)	0.0257(7)
C12	0.0954(3)	0.8049(3)	0.2094(2)	0.0267(8)
C13	0.0355(4)	0.7680(3)	0.2618(2)	0.0373(10)
C14	-0.0313(4)	0.8411(4)	0.2885(2)	0.0376(10)
C15	-0.0582(3)	0.9106(3)	0.2385(2)	0.0265(8)
C16	-0.0092(3)	0.9950(3)	0.2304(2)	0.0261(7)
C17	0.0763(3)	1.0226(3)	0.2682(2)	0.0351(10)
C18	0.1526(3)	0.9491(3)	0.2688(2)	0.0347(9)
C51	-0.2630(2)	0.8734(3)	-0.0073(2)	0.0212(7)
C52	-0.3252(3)	0.9488(3)	-0.0129(2)	0.0239(7)
C53	-0.3467(3)	0.9859(3)	-0.0718(2)	0.0328(9)
C54	-0.3094(3)	0.9493(3)	-0.1259(2)	0.0376(11)
C55	-0.2510(3)	0.8732(4)	-0.1217(2)	0.0347(10)
C56	-0.2274(2)	0.8346(3)	-0.0601(2)	0.0241(7)
C57	-0.3757(3)	0.9885(3)	0.0425(2)	0.0346(9)
C58	-0.1683(3)	0.7511(4)	-0.0620(2)	0.0354(10)
C31	-0.2094(3)	0.7589(3)	0.1600(2)	0.0269(8)
C32	-0.3533(3)	0.7687(3)	0.0770(2)	0.0221(7)
O1	-0.2003(3)	0.7258(3)	0.2076(2)	0.0441(8)
O2	-0.4292(2)	0.7424(2)	0.0737(2)	0.0335(7)

Table 4C. Bond lengths [Å] and angles [deg] for $Ir(CO)_2(2,6\text{-}Me_2C_6H_3)(\mu\text{-}2,6\text{-}Me_2C_6H_3)Ir(cod)$ (**8**).

Ir1-C32	1.856(4)
Ir1-C31	1.878(4)
Ir1-C1	2.124(3)
Ir1-C51	2.142(4)
Ir2-C12	2.123(4)
Ir2-C16	2.126(4)
Ir2-C11	2.131(4)
Ir2-C15	2.132(4)
Ir2-C5	2.210(4)
Ir2-C2	2.247(3)
Ir2-C3	2.276(4)
Ir2-C4	2.292(4)
Ir2-C6	2.306(3)
Ir2-C1	2.411(3)
C1-C6	1.428(5)
C1-C2	1.444(5)
C2-C3	1.432(5)
C2-C7	1.510(5)
C3-C4	1.399(6)
C4-C5	1.419(6)
C5-C6	1.436(5)
C6-C8	1.501(5)
C11-C12	1.417(6)
C11-C18	1.526(6)
C12-C13	1.508(6)
C13-C14	1.541(7)
C14-C15	1.523(6)
C15-C16	1.428(6)
C16-C17	1.516(6)
C17-C18	1.528(6)
C51-C56	1.360(5)
C51-C52	1.420(5)
C52-C53	1.404(6)
C52-C57	1.501(6)
C53-C54	1.380(7)
C54-C55	1.392(8)
C55-C56	1.471(6)
C56-C58	1.483(6)
C31-O1	1.135(5)
C32-O2	1.150(5)
C32-Ir1-C31	93.3(2)
C32-Ir1-C1	174.88(14)
C31-Ir1-C1	91.9(2)
C32-Ir1-C51	84.33(14)
C31-Ir1-C51	177.5(2)
C1-Ir1-C51	90.55(13)
C12-Ir2-C16	97.1(2)
C12-Ir2-C11	38.9(2)
C16-Ir2-C11	80.6(2)
C12-Ir2-C15	80.6(2)
C16-Ir2-C15	39.2(2)
C11-Ir2-C15	89.5(2)

C12-Ir2-C5	94.8(2)
C16-Ir2-C5	160.4(2)
C11-Ir2-C5	99.30(14)
C15-Ir2-C5	159.6(2)
C12-Ir2-C2	159.1(2)
C16-Ir2-C2	96.28(14)
C11-Ir2-C2	160.6(2)
C15-Ir2-C2	100.21(14)
C5-Ir2-C2	77.19(13)
C12-Ir2-C3	153.8(2)
C16-Ir2-C3	98.5(2)
C11-Ir2-C3	124.3(2)
C15-Ir2-C3	124.2(2)
C5-Ir2-C3	65.1(2)
C2-Ir2-C3	36.90(13)
C12-Ir2-C4	118.5(2)
C16-Ir2-C4	123.8(2)
C11-Ir2-C4	100.25(14)
C15-Ir2-C4	158.9(2)
C5-Ir2-C4	36.7(2)
C2-Ir2-C4	65.41(13)
C3-Ir2-C4	35.67(14)
C12-Ir2-C6	97.65(14)
C16-Ir2-C6	153.99(14)
C11-Ir2-C6	123.48(14)
C15-Ir2-C6	123.56(14)
C5-Ir2-C6	37.00(13)
C2-Ir2-C6	64.31(13)
C3-Ir2-C6	76.61(14)
C4-Ir2-C6	65.81(13)
C12-Ir2-C1	123.26(14)
C16-Ir2-C1	119.50(14)
C11-Ir2-C1	157.89(14)
C15-Ir2-C1	100.86(14)
C5-Ir2-C1	65.05(12)
C2-Ir2-C1	35.89(12)
C3-Ir2-C1	65.15(12)
C4-Ir2-C1	76.79(12)
C6-Ir2-C1	35.15(11)
C6-C1-C2	115.1(3)
C6-C1-Ir1	123.3(2)
C2-C1-Ir1	121.6(2)
C6-C1-Ir2	68.4(2)
C2-C1-Ir2	65.8(2)
Ir1-C1-Ir2	135.3(2)
C3-C2-C1	122.9(3)
C3-C2-C7	116.9(3)
C1-C2-C7	120.1(3)
C3-C2-Ir2	72.7(2)
C1-C2-Ir2	78.3(2)
C7-C2-Ir2	125.3(2)
C4-C3-C2	120.1(3)
C4-C3-Ir2	72.8(2)
C2-C3-Ir2	70.4(2)
C3-C4-C5	117.9(3)
C3-C4-Ir2	71.5(2)
C5-C4-Ir2	68.5(2)
C4-C5-C6	122.1(3)

C4-C5-Ir2	74.8(2)
C6-C5-Ir2	75.1(2)
C1-C6-C5	120.8(3)
C1-C6-C8	122.5(3)
C5-C6-C8	116.6(3)
C1-C6-Ir2	76.4(2)
C5-C6-Ir2	67.9(2)
C8-C6-Ir2	126.3(3)
C12-C11-C18	123.4(4)
C12-C11-Ir2	70.3(2)
C18-C11-Ir2	115.0(3)
C11-C12-C13	125.4(4)
C11-C12-Ir2	70.8(2)
C13-C12-Ir2	112.4(3)
C12-C13-C14	112.1(4)
C15-C14-C13	111.1(3)
C16-C15-C14	122.5(4)
C16-C15-Ir2	70.2(2)
C14-C15-Ir2	114.8(3)
C15-C16-C17	124.0(4)
C15-C16-Ir2	70.7(2)
C17-C16-Ir2	112.6(3)
C16-C17-C18	112.9(3)
C11-C18-C17	111.6(3)
C56-C51-C52	119.2(4)
C56-C51-Ir1	118.9(3)
C52-C51-Ir1	121.7(3)
C53-C52-C51	120.7(4)
C53-C52-C57	116.9(4)
C51-C52-C57	122.3(4)
C54-C53-C52	121.1(4)
C53-C54-C55	119.1(4)
C54-C55-C56	120.1(4)
C51-C56-C55	119.7(4)
C51-C56-C58	125.3(4)
C55-C56-C58	115.0(4)
O1-C31-Ir1	176.9(4)
O2-C32-Ir1	179.1(4)

Table 4D. Anisotropic displacement parameters for $Ir(CO)_2(2,6\text{-}Me_2C_6H_3)(\mu\text{-}2,6\text{-}Me_2C_6H_3)Ir(cod)$ (**8**). 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
Ir1	0.01397(6)	0.01850(7)	0.01862(7)	0.00089(4)	-0.00003(4)	-0.00144(4)
Ir2	0.01537(6)	0.01815(7)	0.01487(6)	0.00042(4)	-0.00118(4)	-0.00020(4)
C1	0.0155(14)	0.018(2)	0.0153(14)	-0.0003(11)	-0.0009(11)	-0.0015(11)
C2	0.018(2)	0.020(2)	0.019(2)	0.0031(12)	-0.0036(12)	0.0010(12)
C3	0.026(2)	0.024(2)	0.017(2)	0.0044(13)	-0.0027(13)	-0.0067(14)
C4	0.019(2)	0.034(2)	0.019(2)	0.0022(14)	0.0008(13)	-0.0072(14)
C5	0.016(2)	0.032(2)	0.019(2)	-0.0035(14)	-0.0018(12)	0.0004(13)
C6	0.0137(14)	0.023(2)	0.019(2)	-0.0045(12)	-0.0014(12)	-0.0003(12)
C7	0.023(2)	0.018(2)	0.029(2)	0.0009(14)	-0.0028(14)	0.0016(13)
C8	0.023(2)	0.023(2)	0.029(2)	-0.005(2)	-0.0012(14)	0.0049(14)
C11	0.022(2)	0.034(2)	0.022(2)	0.000(2)	-0.0045(14)	0.005(2)
C12	0.034(2)	0.025(2)	0.021(2)	0.0011(14)	-0.007(2)	0.009(2)
C13	0.052(3)	0.030(2)	0.030(2)	0.011(2)	-0.009(2)	-0.003(2)
C14	0.046(3)	0.048(3)	0.018(2)	0.010(2)	0.002(2)	-0.006(2)
C15	0.025(2)	0.037(2)	0.017(2)	-0.0004(14)	0.0012(14)	0.003(2)
C16	0.033(2)	0.024(2)	0.021(2)	-0.0054(14)	-0.0030(14)	0.006(2)
C17	0.044(2)	0.033(2)	0.028(2)	-0.012(2)	-0.010(2)	0.000(2)
C18	0.037(2)	0.037(2)	0.030(2)	-0.004(2)	-0.014(2)	-0.001(2)
C51	0.016(2)	0.023(2)	0.025(2)	0.0018(14)	-0.0003(13)	-0.0053(13)
C52	0.020(2)	0.022(2)	0.030(2)	0.0023(14)	-0.0043(14)	-0.0030(13)
C53	0.026(2)	0.033(2)	0.039(2)	0.013(2)	-0.010(2)	-0.007(2)
C54	0.036(2)	0.046(3)	0.031(2)	0.015(2)	-0.012(2)	-0.016(2)
C55	0.031(2)	0.052(3)	0.021(2)	0.000(2)	-0.001(2)	-0.018(2)
C56	0.0112(14)	0.024(2)	0.037(2)	-0.004(2)	0.0054(13)	-0.0113(12)
C57	0.027(2)	0.035(2)	0.041(2)	-0.002(2)	-0.004(2)	0.012(2)
C58	0.026(2)	0.046(3)	0.034(2)	-0.013(2)	0.005(2)	0.005(2)
C31	0.020(2)	0.033(2)	0.027(2)	0.004(2)	-0.0026(14)	-0.003(2)
C32	0.023(2)	0.024(2)	0.019(2)	0.0022(13)	-0.0009(13)	-0.0011(13)
O1	0.040(2)	0.054(2)	0.038(2)	0.021(2)	-0.004(2)	-0.003(2)
O2	0.0196(13)	0.044(2)	0.037(2)	0.0039(14)	-0.0020(12)	-0.0074(13)

Table 4E. Hydrogen coordinates and isotropic displacement parameters for $Ir(CO)_2(2,6\text{-}Me_2C_6H_3)(\mu\text{-}2,6\text{-}Me_2C_6H_3)Ir(cod)$ (**8**).

	x	y	z	U(eq)
H3	0.0180(3)	1.0717(3)	0.0758(2)	0.027
H4	0.1501(3)	0.9791(3)	0.0543(2)	0.029
H5	0.1330(2)	0.8181(3)	0.0615(2)	0.027
H7A	-0.2146(3)	0.9926(3)	0.1089(2)	0.034
H7B	-0.1674(3)	1.0718(3)	0.0678(2)	0.034
H7C	-0.1425(3)	1.0625(3)	0.1406(2)	0.034
H8A	0.0494(3)	0.6878(3)	0.0637(2)	0.038
H8B	-0.0545(3)	0.6908(3)	0.0354(2)	0.038
H8C	-0.0393(3)	0.6891(3)	0.1096(2)	0.038
H11	0.1798(3)	0.9060(3)	0.1745(2)	0.031
H12	0.0987(3)	0.7698(3)	0.1720(2)	0.032
H13A	0.0767(4)	0.7452(3)	0.2958(2)	0.045
H13B	-0.0019(4)	0.7157(3)	0.2461(2)	0.045
H14A	-0.0886(4)	0.8112(4)	0.3048(2)	0.045
H14B	-0.0003(4)	0.8730(4)	0.3238(2)	0.045
H15	-0.1096(3)	0.8974(3)	0.2117(2)	0.032
H16	-0.0316(3)	1.0363(3)	0.1995(2)	0.031
H17A	0.0568(3)	1.0355(3)	0.3118(2)	0.042
H17B	0.1026(3)	1.0796(3)	0.2504(2)	0.042
H18A	0.2149(3)	0.9788(3)	0.2703(2)	0.042
H18B	0.1457(3)	0.9112(3)	0.3070(2)	0.042
H53	-0.3876(3)	1.0371(3)	-0.0744(2)	0.039
H54	-0.3234(3)	0.9756(3)	-0.1655(2)	0.045
H55	-0.2262(3)	0.8463(4)	-0.1587(2)	0.042
H57A	-0.3551(3)	0.9574(3)	0.0808(2)	0.052
H57B	-0.4434(3)	0.9801(3)	0.0373(2)	0.052
H57C	-0.3615(3)	1.0539(3)	0.0457(2)	0.052
H58A	-0.1518(3)	0.7372(4)	-0.1055(2)	0.053
H58B	-0.2031(3)	0.6997(4)	-0.0440(2)	0.053
H58C	-0.1109(3)	0.7615(4)	-0.0377(2)	0.053

Table 5A. Crystal data and structure refinement for $Ir(CO)_2BrI_2(\mu\text{-}2,6\text{-}Me_2C_6H_3)Ir(cod)$ (**12**).

Empirical formula	$C_{18}H_{21}BrI_2Ir_2O_2$
Formula weight	987.46
Temperature	170(2) K
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 9.1441(3) Å α = 90 deg. b = 15.8388(6) Å β = 92.5990(10) deg. c = 15.0766(6) Å γ = 90 deg.
Volume	2181.32(14) $Å^3$
Z	4
Density (calculated)	3.007 g/cm^3
Absorption coefficient	16.860 mm^{-1}
Absorption correction	SADABS
Transmission	0.6221 to 1.0000
F(000)	1760
Diffractometer	Bruker SMART APEX
Radiation	graphite-monochromated MoKα (0.71073 Å)
Scan type	ω scans
Decay	negligible
Crystal size	0.02 x 0.08 x 0.15 mm
Crystal habit	needle
Crystal color	orange
Theta range for data collection	1.87 to 28.28 deg.
Limiting indices	-12<=h<=12, -20<=k<=21, -20<=l<=20
Reflections collected	23765
Independent reflections	5409 [R(int) = 0.0626]
Structure solution method	Patterson
Refinement method	Full-matrix least-squares on F^2