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Table S-1. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{Ir}_2(\text{CO})_2(\mu\text{-C}_2\text{Ph}_2)(\eta^5\text{-C}_9\text{H}_7)_2$, **2a**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Ir(1)	2555(1)	822(1)	1435(1)	24(1)
O(1)	679(5)	1907(7)	650(4)	58(2)
C(1)	1397(6)	1539(8)	973(4)	33(2)
Ir(2)	3469(1)	3052(1)	1599(1)	25(1)
O(2)	5157(5)	1914(5)	2541(4)	45(2)
C(2)	4508(6)	2340(7)	2168(4)	29(1)
C(11)	3197(6)	-509(7)	656(4)	35(2)
C(12)	4025(6)	-103(7)	1120(4)	35(2)
C(13)	3846(6)	-507(7)	1793(4)	32(2)
C(14)	2908(6)	-1261(7)	1752(4)	30(2)
C(15)	2383(7)	-1949(7)	2241(4)	36(2)
C(16)	1484(7)	-2606(8)	2035(5)	46(2)
C(17)	1083(6)	-2593(8)	1334(5)	39(2)
C(18)	1571(7)	-1934(8)	850(5)	38(2)
C(19)	2490(6)	-1248(8)	1041(4)	34(2)
C(21)	2522(7)	4158(8)	804(4)	40(2)
C(22)	3010(9)	4995(8)	1296(5)	47(2)
C(23)	4135(7)	4851(7)	1271(4)	36(2)
C(24)	4331(7)	4026(7)	713(4)	32(2)
C(25)	5293(7)	3647(8)	452(5)	43(2)
C(26)	5229(10)	2839(10)	-100(6)	62(3)
C(27)	4256(10)	2414(10)	-378(5)	59(3)
C(28)	3319(8)	2743(9)	-136(4)	45(2)
C(29)	3336(7)	3601(7)	420(4)	33(2)
C(30)	2517(6)	2761(7)	2408(3)	28(2)
C(31)	2383(5)	3720(6)	2939(3)	23(1)
C(32)	3093(6)	4673(7)	3079(4)	32(2)
C(33)	2903(7)	5610(8)	3552(4)	38(2)
C(34)	1968(7)	5592(8)	3896(4)	40(2)
C(35)	1277(7)	4643(8)	3775(4)	38(2)
C(36)	1453(6)	3727(8)	3301(4)	32(2)
C(40)	2145(5)	1608(7)	2348(3)	26(1)
C(41)	1636(6)	857(7)	2859(4)	28(2)
C(42)	2163(7)	650(7)	3503(4)	33(2)
C(43)	1719(7)	-115(8)	3981(4)	37(2)
C(44)	772(7)	-691(8)	3838(5)	39(2)
C(45)	239(6)	-516(8)	3197(5)	39(2)
C(46)	667(6)	225(7)	2706(4)	33(2)

	x	y	z	U(eq)
H(11)	3115(6)	-330(7)	178(4)	42
H(12)	4615(6)	371(7)	999(4)	42
H(13)	4271(6)	-314(7)	2201(4)	38
H(15)	2647(7)	-1959(7)	2710(4)	44
H(16)	1129(7)	-3071(8)	2363(5)	55
H(17)	464(6)	-3052(8)	1200(5)	47
H(18)	1292(7)	-1938(8)	385(5)	46
H(21)	1787(7)	3993(8)	739(4)	48
H(22)	2660(9)	5545(8)	1586(5)	57
H(23)	4658(7)	5236(7)	1572(4)	43
H(25)	5954(7)	3936(8)	649(5)	51
H(26)	5857(10)	2572(10)	-293(6)	74
H(27)	4246(10)	1861(10)	-759(5)	71
H(28)	2673(8)	2410(9)	-332(4)	54
H(32)	3726(6)	4694(7)	2848(4)	38
H(33)	3404(7)	6256(8)	3641(4)	46
H(34)	1822(7)	6236(8)	4209(4)	48
H(35)	660(7)	4608(8)	4022(4)	45
H(36)	942(6)	3090(8)	3215(4)	39
H(42)	2827(7)	1033(7)	3615(4)	40
H(43)	2084(7)	-240(8)	4418(4)	44
H(44)	480(7)	-1206(8)	4172(5)	47
H(45)	-425(6)	-906(8)	3095(5)	47
H(46)	311(6)	309(7)	2263(4)	40

Table S-2. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 2a.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ir(1)	25(1)	25(1)	22(1)	-2(1)	1(1)	4(1)
O(1)	45(4)	59(5)	66(5)	-1(3)	-18(3)	15(3)
C(1)	28(4)	41(4)	29(4)	-13(3)	-1(3)	7(3)
Ir(2)	29(1)	23(1)	22(1)	1(1)	5(1)	4(1)
O(2)	37(3)	36(3)	59(4)	3(3)	-14(3)	-1(2)
C(2)	33(4)	25(4)	29(3)	1(3)	4(3)	-5(3)
C(11)	39(4)	32(4)	36(4)	-7(3)	11(3)	7(3)
C(12)	32(4)	26(4)	49(5)	-4(3)	9(3)	-5(3)
C(13)	28(4)	25(4)	41(4)	-1(3)	-5(3)	7(3)
C(14)	30(4)	23(4)	39(4)	-4(3)	3(3)	9(3)
C(15)	48(5)	27(4)	34(4)	-1(3)	6(3)	14(3)
C(16)	51(5)	28(4)	59(6)	-1(4)	16(4)	0(4)
C(17)	33(4)	28(4)	57(5)	-3(4)	2(4)	-4(3)
C(18)	35(4)	38(5)	42(5)	-18(3)	2(3)	-1(3)
C(19)	32(4)	29(4)	40(4)	-9(3)	1(3)	7(3)
C(21)	37(4)	51(5)	32(4)	19(4)	3(3)	15(4)
C(22)	75(7)	29(4)	40(5)	12(3)	17(5)	15(4)
C(23)	55(5)	24(4)	28(4)	3(3)	3(3)	-10(3)
C(24)	43(4)	23(3)	31(4)	4(3)	5(3)	1(3)
C(25)	42(4)	32(4)	56(5)	18(4)	15(4)	2(4)
C(26)	75(8)	46(6)	71(7)	15(5)	47(6)	32(5)
C(27)	98(9)	46(6)	37(5)	-3(4)	29(5)	14(6)
C(28)	69(6)	38(5)	26(4)	7(3)	-13(4)	-6(4)
C(29)	47(4)	25(4)	27(3)	3(3)	4(3)	6(3)
C(30)	32(4)	32(4)	19(3)	-6(3)	5(3)	4(3)
C(31)	27(3)	25(3)	16(3)	-4(2)	2(2)	5(3)
C(32)	38(4)	26(4)	33(4)	-2(3)	5(3)	-1(3)
C(33)	51(5)	31(4)	32(4)	-8(3)	-9(4)	7(4)
C(34)	53(5)	35(4)	30(4)	-10(3)	-1(4)	6(4)
C(35)	42(4)	48(5)	24(3)	-8(3)	9(3)	7(4)
C(36)	33(4)	40(5)	25(3)	2(3)	5(3)	5(3)
C(40)	22(3)	36(4)	20(3)	-6(3)	4(2)	2(3)
C(41)	25(3)	25(3)	36(4)	0(3)	9(3)	1(3)
C(42)	40(4)	28(4)	32(4)	-3(3)	3(3)	-7(3)
C(43)	42(4)	41(5)	29(4)	5(3)	2(3)	-5(4)
C(44)	47(5)	29(4)	41(5)	-1(3)	5(4)	-4(3)
C(45)	28(4)	40(5)	50(5)	1(4)	4(3)	-12(3)
C(46)	30(4)	33(4)	34(4)	-4(3)	-1(3)	-5(3)

Table S-3. Bond lengths [Å] and angles [°] for 2a.

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Ir(1)-C(1)	1.840(7)	Ir(1)-C(40)	2.069(7)
Ir(1)-C(12)	2.241(8)	Ir(1)-C(13)	2.250(7)
Ir(1)-C(11)	2.279(7)	Ir(1)-C(19)	2.355(8)
Ir(1)-C(14)	2.359(7)	Ir(1)-Ir(2)	2.6750(4)
O(1)-C(1)	1.141(9)	Ir(2)-C(2)	1.830(8)
Ir(2)-C(30)	2.078(7)	Ir(2)-C(23)	2.225(7)
Ir(2)-C(21)	2.237(8)	Ir(2)-C(22)	2.239(8)
Ir(2)-C(24)	2.356(8)	Ir(2)-C(29)	2.368(7)
O(2)-C(2)	1.154(9)	C(11)-C(12)	1.406(12)
C(11)-C(19)	1.448(12)	C(12)-C(13)	1.416(11)
C(13)-C(14)	1.440(11)	C(14)-C(15)	1.413(11)
C(14)-C(19)	1.447(11)	C(15)-C(16)	1.378(12)
C(16)-C(17)	1.424(13)	C(17)-C(18)	1.363(12)
C(18)-C(19)	1.409(11)	C(21)-C(22)	1.425(14)
C(21)-C(29)	1.449(11)	C(22)-C(23)	1.442(14)
C(23)-C(24)	1.438(11)	C(24)-C(25)	1.418(12)
C(24)-C(29)	1.426(11)	C(25)-C(26)	1.38(2)
C(26)-C(27)	1.39(2)	C(27)-C(28)	1.36(2)
C(28)-C(29)	1.422(12)	C(30)-C(40)	1.330(10)
C(30)-C(31)	1.479(9)	C(31)-C(32)	1.380(10)
C(31)-C(36)	1.419(10)	C(32)-C(33)	1.398(10)
C(33)-C(34)	1.405(13)	C(34)-C(35)	1.356(13)
C(35)-C(36)	1.381(11)	C(40)-C(41)	1.468(10)
C(41)-C(42)	1.398(11)	C(41)-C(46)	1.420(10)
C(42)-C(43)	1.393(11)	C(43)-C(44)	1.365(12)
C(44)-C(45)	1.390(12)	C(45)-C(46)	1.387(12)
C(1)-Ir(1)-C(40)	90.5(3)	C(1)-Ir(1)-C(12)	134.9(3)
C(40)-Ir(1)-C(12)	133.1(3)	C(1)-Ir(1)-C(13)	163.5(3)
C(40)-Ir(1)-C(13)	102.5(3)	C(12)-Ir(1)-C(13)	36.8(3)
C(1)-Ir(1)-C(11)	104.4(3)	C(40)-Ir(1)-C(11)	162.3(3)
C(12)-Ir(1)-C(11)	36.2(3)	C(13)-Ir(1)-C(11)	61.3(3)
C(1)-Ir(1)-C(19)	103.2(3)	C(40)-Ir(1)-C(19)	131.4(3)
C(12)-Ir(1)-C(19)	60.1(3)	C(13)-Ir(1)-C(19)	60.5(3)
C(11)-Ir(1)-C(19)	36.4(3)	C(1)-Ir(1)-C(14)	131.1(3)
C(40)-Ir(1)-C(14)	102.6(3)	C(12)-Ir(1)-C(14)	60.2(3)
C(13)-Ir(1)-C(14)	36.3(3)	C(11)-Ir(1)-C(14)	60.4(3)
C(19)-Ir(1)-C(14)	35.8(3)	C(1)-Ir(1)-Ir(2)	90.5(3)
C(40)-Ir(1)-Ir(2)	70.4(2)	C(12)-Ir(1)-Ir(2)	93.9(2)
C(13)-Ir(1)-Ir(2)	103.4(2)	C(11)-Ir(1)-Ir(2)	118.0(2)
C(19)-Ir(1)-Ir(2)	153.1(2)	C(14)-Ir(1)-Ir(2)	138.4(2)
O(1)-C(1)-Ir(1)	174.6(7)	C(2)-Ir(2)-C(30)	85.0(3)
C(2)-Ir(2)-C(23)	105.4(3)	C(30)-Ir(2)-C(23)	127.1(3)
C(2)-Ir(2)-C(21)	166.4(3)	C(30)-Ir(2)-C(21)	107.0(3)
C(23)-Ir(2)-C(21)	62.2(3)	C(2)-Ir(2)-C(22)	135.6(4)
C(30)-Ir(2)-C(22)	100.7(3)	C(23)-Ir(2)-C(22)	37.7(4)
C(21)-Ir(2)-C(22)	37.1(4)	C(2)-Ir(2)-C(24)	106.1(3)
C(30)-Ir(2)-C(24)	161.6(3)	C(23)-Ir(2)-C(24)	36.5(3)
C(21)-Ir(2)-C(24)	60.7(3)	C(22)-Ir(2)-C(24)	61.1(3)
C(2)-Ir(2)-C(29)	133.7(3)	C(30)-Ir(2)-C(29)	140.2(3)
C(23)-Ir(2)-C(29)	60.4(3)	C(21)-Ir(2)-C(29)	36.5(3)
C(22)-Ir(2)-C(29)	60.7(3)	C(24)-Ir(2)-C(29)	35.1(3)
C(2)-Ir(2)-Ir(1)	89.2(2)	C(30)-Ir(2)-Ir(1)	71.6(2)
C(23)-Ir(2)-Ir(1)	156.4(2)	C(21)-Ir(2)-Ir(1)	100.7(3)
C(22)-Ir(2)-Ir(1)	134.7(3)	C(24)-Ir(2)-Ir(1)	122.1(2)

C(29)-Ir(2)-Ir(1)	96.1(2)	O(2)-C(2)-Ir(2)	178.1(7)
C(12)-C(11)-C(19)	107.6(7)	C(12)-C(11)-Ir(1)	70.4(4)
C(19)-C(11)-Ir(1)	74.7(4)	C(11)-C(12)-C(13)	109.7(7)
C(11)-C(12)-Ir(1)	73.3(5)	C(13)-C(12)-Ir(1)	71.9(4)
C(12)-C(13)-C(14)	107.9(7)	C(12)-C(13)-Ir(1)	71.3(4)
C(14)-C(13)-Ir(1)	76.0(4)	C(15)-C(14)-C(13)	133.4(8)
C(15)-C(14)-C(19)	119.5(7)	C(13)-C(14)-C(19)	107.1(7)
C(15)-C(14)-Ir(1)	125.7(5)	C(13)-C(14)-Ir(1)	67.7(4)
C(19)-C(14)-Ir(1)	72.0(4)	C(16)-C(15)-C(14)	119.6(8)
C(15)-C(16)-C(17)	120.5(8)	C(18)-C(17)-C(16)	121.3(8)
C(17)-C(18)-C(19)	120.0(8)	C(18)-C(19)-C(14)	119.2(8)
C(18)-C(19)-C(11)	133.2(8)	C(14)-C(19)-C(11)	107.6(7)
C(18)-C(19)-Ir(1)	126.2(6)	C(14)-C(19)-Ir(1)	72.3(4)
C(11)-C(19)-Ir(1)	68.9(4)	C(22)-C(21)-C(29)	108.5(8)
C(22)-C(21)-Ir(2)	71.5(5)	C(29)-C(21)-Ir(2)	76.7(4)
C(21)-C(22)-C(23)	107.1(8)	C(21)-C(22)-Ir(2)	71.4(5)
C(23)-C(22)-Ir(2)	70.6(5)	C(24)-C(23)-C(22)	108.5(7)
C(24)-C(23)-Ir(2)	76.7(4)	C(22)-C(23)-Ir(2)	71.7(5)
C(25)-C(24)-C(29)	121.8(7)	C(25)-C(24)-C(23)	130.4(8)
C(29)-C(24)-C(23)	107.8(7)	C(25)-C(24)-Ir(2)	126.3(5)
C(29)-C(24)-Ir(2)	72.9(4)	C(23)-C(24)-Ir(2)	66.8(4)
C(26)-C(25)-C(24)	117.1(9)	C(25)-C(26)-C(27)	120.8(9)
C(28)-C(27)-C(26)	123.8(9)	C(27)-C(28)-C(29)	117.9(9)
C(28)-C(29)-C(24)	118.6(8)	C(28)-C(29)-C(21)	133.6(9)
C(24)-C(29)-C(21)	107.7(7)	C(28)-C(29)-Ir(2)	125.0(5)
C(24)-C(29)-Ir(2)	72.0(4)	C(21)-C(29)-Ir(2)	66.8(4)
C(40)-C(30)-C(31)	130.9(6)	C(40)-C(30)-Ir(2)	107.2(5)
C(31)-C(30)-Ir(2)	121.8(5)	C(32)-C(31)-C(36)	117.0(6)
C(32)-C(31)-C(30)	123.4(6)	C(36)-C(31)-C(30)	119.5(7)
C(31)-C(32)-C(33)	121.6(7)	C(32)-C(33)-C(34)	119.7(8)
C(35)-C(34)-C(33)	119.2(7)	C(34)-C(35)-C(36)	121.3(8)
C(35)-C(36)-C(31)	121.1(8)	C(30)-C(40)-C(41)	128.6(6)
C(30)-C(40)-Ir(1)	110.3(5)	C(41)-C(40)-Ir(1)	120.6(5)
C(42)-C(41)-C(46)	117.8(7)	C(42)-C(41)-C(40)	119.4(7)
C(46)-C(41)-C(40)	122.6(7)	C(43)-C(42)-C(41)	120.2(8)
C(44)-C(43)-C(42)	121.7(8)	C(43)-C(44)-C(45)	119.3(8)
C(46)-C(45)-C(44)	120.5(7)	C(45)-C(46)-C(41)	120.5(8)

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Table S-4. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{Ir}(\eta^4\text{-HC}_4\text{Tol}_4\text{Ph})(\eta^5\text{-C}_9\text{H}_7)$, **3b**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Ir (1)	3261 (1)	909 (1)	1011 (1)	24 (1)
C (1)	3654 (7)	-48 (3)	732 (2)	40 (2)
C (2)	4821 (7)	380 (3)	688 (2)	43 (2)
C (3)	5390 (7)	504 (3)	1030 (2)	40 (2)
C (4)	4690 (6)	88 (3)	1282 (2)	37 (1)
C (5)	4885 (8)	-34 (3)	1654 (2)	47 (2)
C (6)	4053 (8)	-492 (3)	1823 (2)	50 (2)
C (7)	2996 (9)	-829 (3)	1638 (2)	52 (2)
C (8)	2744 (8)	-715 (3)	1285 (2)	43 (2)
C (9)	3592 (7)	-253 (3)	1096 (2)	32 (1)
C (10)	1197 (6)	1178 (3)	822 (2)	26 (1)
C (11)	197 (6)	667 (3)	690 (2)	27 (1)
C (12)	-497 (7)	802 (3)	370 (2)	35 (1)
C (13)	-1425 (7)	352 (3)	225 (2)	41 (2)
C (14)	-1674 (6)	-255 (3)	384 (2)	34 (1)
C (15)	-2661 (8)	-762 (4)	221 (2)	52 (2)
C (16)	-972 (7)	-400 (3)	699 (2)	46 (2)
C (17)	-44 (7)	51 (3)	847 (2)	41 (2)
C (20)	1363 (6)	1330 (3)	1199 (2)	25 (1)
C (21)	442 (6)	1052 (3)	1487 (2)	29 (1)
C (22)	891 (6)	615 (3)	1749 (2)	34 (1)
C (23)	-11 (7)	397 (4)	2015 (2)	44 (2)
C (24)	-1388 (7)	631 (4)	2024 (2)	46 (2)
C (25)	-2342 (8)	391 (5)	2323 (2)	78 (3)
C (26)	-1817 (7)	1048 (4)	1755 (2)	51 (2)
C (27)	-934 (6)	1251 (3)	1484 (2)	40 (2)
C (30)	2529 (5)	1741 (3)	1304 (1)	23 (1)
C (31)	2717 (5)	1927 (3)	1691 (1)	25 (1)
C (32)	3808 (6)	1707 (3)	1902 (2)	32 (1)
C (33)	3939 (6)	1931 (3)	2252 (2)	39 (2)
C (34)	3017 (6)	2370 (3)	2406 (2)	37 (2)
C (35)	3144 (8)	2632 (5)	2786 (2)	60 (2)
C (36)	1933 (6)	2588 (3)	2194 (2)	36 (1)
C (37)	1783 (5)	2371 (3)	1843 (2)	30 (1)
C (40)	3430 (5)	1980 (3)	1010 (1)	21 (1)
C (41)	4786 (6)	2321 (3)	1109 (2)	27 (1)
C (42)	6005 (6)	2170 (3)	927 (2)	31 (1)
C (43)	7193 (7)	2546 (3)	989 (2)	37 (2)
C (44)	7202 (6)	3080 (3)	1224 (2)	37 (2)
C (45)	8496 (7)	3499 (4)	1285 (2)	57 (2)
C (46)	5976 (7)	3241 (3)	1398 (2)	37 (1)
C (47)	4784 (6)	2870 (3)	1339 (2)	29 (1)
C (51)	2809 (6)	2374 (3)	701 (2)	28 (1)
C (52)	3340 (7)	2297 (4)	354 (2)	43 (2)
C (53)	2811 (8)	2685 (4)	73 (2)	50 (2)
C (54)	1758 (7)	3141 (4)	136 (2)	51 (2)
C (55)	1237 (8)	3213 (3)	473 (2)	47 (2)
C (56)	1768 (6)	2833 (3)	753 (2)	35 (1)

	x	y	z	U(eq)
H(1)	3025 (7)	-174 (3)	549 (2)	47
H(2)	5157 (7)	551 (3)	467 (2)	51
H(3)	6110 (7)	811 (3)	1084 (2)	48
H(5)	5581 (8)	198 (3)	1784 (2)	56
H(6)	4193 (8)	-584 (3)	2071 (2)	60
H(7)	2444 (9)	-1146 (3)	1763 (2)	62
H(8)	2012 (8)	-941 (3)	1166 (2)	51
H(10)	1203 (6)	1591 (3)	670 (2)	32
H(12)	-328 (7)	1214 (3)	249 (2)	42
H(13)	-1899 (7)	465 (3)	10 (2)	49
H(15A)	-2701 (8)	-1163 (4)	373 (2)	78
H(15B)	-2336 (8)	-888 (4)	-19 (2)	78
H(15C)	-3581 (8)	-563 (4)	202 (2)	78
H(16)	-1129 (7)	-818 (3)	815 (2)	56
H(17)	434 (7)	-66 (3)	1061 (2)	49
H(22)	1819 (6)	463 (3)	1749 (2)	41
H(23)	299 (7)	89 (4)	2192 (2)	53
H(25A)	-1829 (8)	98 (5)	2487 (2)	116
H(25B)	-3114 (8)	141 (5)	2219 (2)	116
H(25C)	-2696 (8)	779 (5)	2456 (2)	116
H(26)	-2744 (7)	1201 (4)	1753 (2)	62
H(27)	-1267 (6)	1528 (3)	1296 (2)	48
H(32)	4466 (6)	1404 (3)	1805 (2)	38
H(33)	4693 (6)	1774 (3)	2392 (2)	47
H(35A)	2376 (8)	2937 (5)	2837 (2)	89
H(35B)	4017 (8)	2875 (5)	2812 (2)	89
H(35C)	3122 (8)	2255 (5)	2954 (2)	89
H(36)	1279 (6)	2893 (3)	2291 (2)	43
H(37)	1028 (5)	2529 (3)	1705 (2)	36
H(42)	6025 (6)	1809 (3)	761 (2)	37
H(43)	8018 (7)	2430 (3)	867 (2)	45
H(45A)	8301 (7)	3853 (4)	1460 (2)	85
H(45B)	8782 (7)	3703 (4)	1057 (2)	85
H(45C)	9236 (7)	3211 (4)	1375 (2)	85
H(46)	5953 (7)	3610 (3)	1559 (2)	45
H(47)	3956 (6)	2994 (3)	1458 (2)	35
H(52)	4055 (7)	1982 (4)	309 (2)	51
H(53)	3175 (8)	2636 (4)	-162 (2)	60
H(54)	1401 (7)	3402 (4)	-56 (2)	61
H(55)	512 (8)	3523 (3)	516 (2)	56
H(56)	1403 (6)	2892 (3)	987 (2)	41

Table S-5. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 3b.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(h a^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ir(1)	27(1)	21(1)	24(1)	0(1)	-1(1)	-1(1)
C(1)	58(4)	25(3)	35(4)	-1(3)	-3(3)	2(3)
C(2)	49(4)	33(3)	46(4)	7(3)	13(3)	14(3)
C(3)	37(3)	33(3)	50(4)	2(3)	2(3)	6(3)
C(4)	36(3)	22(3)	51(4)	-1(3)	-6(3)	9(3)
C(5)	66(5)	32(3)	42(4)	-5(3)	-24(3)	17(3)
C(6)	82(6)	33(4)	34(4)	0(3)	1(4)	8(4)
C(7)	67(5)	24(3)	65(6)	10(3)	13(4)	5(3)
C(8)	62(4)	21(3)	46(4)	0(3)	-6(3)	1(3)
C(9)	45(4)	17(3)	35(3)	-4(2)	-1(3)	1(2)
C(10)	23(3)	25(3)	31(3)	8(2)	-4(2)	-2(2)
C(11)	29(3)	26(3)	27(3)	3(2)	-2(2)	-1(2)
C(12)	45(4)	27(3)	32(3)	4(2)	-7(3)	-5(3)
C(13)	44(4)	48(4)	31(3)	2(3)	-16(3)	-11(3)
C(14)	34(3)	32(3)	36(4)	-5(3)	1(2)	-10(2)
C(15)	52(4)	46(4)	57(5)	-7(3)	-13(4)	-20(3)
C(16)	59(4)	39(4)	41(4)	5(3)	-9(3)	-22(3)
C(17)	50(4)	39(4)	32(4)	12(3)	-12(3)	-6(3)
C(20)	23(3)	30(3)	22(3)	2(2)	-4(2)	2(2)
C(21)	23(3)	41(3)	24(3)	3(2)	0(2)	-12(2)
C(22)	31(3)	38(3)	34(3)	8(3)	-7(2)	-8(3)
C(23)	47(4)	62(4)	25(3)	8(3)	-5(3)	-20(3)
C(24)	37(3)	76(5)	26(4)	6(3)	1(3)	-24(4)
C(25)	48(5)	147(9)	38(4)	22(5)	-3(4)	-43(5)
C(26)	30(4)	76(6)	48(5)	7(4)	1(3)	-9(3)
C(27)	27(3)	54(4)	38(4)	12(3)	-6(3)	-5(3)
C(30)	18(2)	22(3)	29(3)	4(2)	1(2)	5(2)
C(31)	24(3)	25(3)	25(3)	0(2)	1(2)	-4(2)
C(32)	30(3)	30(3)	36(4)	-1(2)	-3(3)	-1(2)
C(33)	37(3)	52(4)	28(3)	2(3)	-11(3)	2(3)
C(34)	40(3)	44(4)	27(3)	-2(3)	-5(2)	-4(3)
C(35)	65(5)	81(6)	33(4)	-15(4)	-3(3)	3(4)
C(36)	41(3)	40(4)	25(3)	-5(3)	4(2)	3(3)
C(37)	26(3)	27(3)	38(3)	-2(2)	2(2)	-1(2)
C(40)	21(3)	18(3)	24(3)	-2(2)	-2(2)	-3(2)
C(41)	30(3)	22(3)	29(3)	3(2)	0(2)	-5(2)
C(42)	32(3)	29(3)	33(3)	2(2)	0(2)	4(2)
C(43)	28(3)	40(4)	44(4)	16(3)	1(3)	1(3)
C(44)	30(3)	44(4)	36(4)	13(3)	-3(3)	-9(3)
C(45)	42(4)	62(5)	67(6)	13(4)	-14(4)	-24(4)
C(46)	45(4)	33(3)	34(4)	-5(3)	-5(3)	-11(3)
C(47)	33(3)	22(3)	33(3)	1(2)	-2(2)	-1(2)
C(51)	29(3)	25(3)	29(3)	4(2)	-1(2)	-7(2)
C(52)	49(4)	44(4)	35(4)	0(3)	5(3)	-5(3)
C(53)	66(5)	55(5)	30(4)	12(3)	-7(3)	-19(4)
C(54)	61(5)	46(4)	46(5)	22(3)	-24(3)	-17(3)
C(55)	50(4)	32(3)	58(5)	7(3)	-16(4)	3(3)
C(56)	45(4)	30(3)	28(3)	4(3)	-4(2)	3(3)

Table S-6. Bond lengths [Å] and angles [°] for 3b.

Ir(1)-C(30)	2.109(5)	Ir(1)-C(40)	2.140(6)
Ir(1)-C(20)	2.143(5)	Ir(1)-C(10)	2.189(5)
Ir(1)-C(2)	2.202(6)	Ir(1)-C(1)	2.204(6)
Ir(1)-C(3)	2.219(6)	Ir(1)-C(9)	2.358(6)
Ir(1)-C(4)	2.371(6)	C(1)-C(9)	1.417(9)
C(1)-C(2)	1.427(9)	C(2)-C(3)	1.412(9)
C(3)-C(4)	1.423(9)	C(4)-C(5)	1.421(9)
C(4)-C(9)	1.441(9)	C(5)-C(6)	1.372(10)
C(6)-C(7)	1.408(11)	C(7)-C(8)	1.356(11)
C(8)-C(9)	1.422(9)	C(10)-C(20)	1.445(8)
C(10)-C(11)	1.489(8)	C(11)-C(17)	1.381(8)
C(11)-C(12)	1.397(8)	C(12)-C(13)	1.380(8)
C(13)-C(14)	1.369(9)	C(14)-C(16)	1.387(9)
C(14)-C(15)	1.519(8)	C(16)-C(17)	1.387(9)
C(20)-C(30)	1.449(7)	C(20)-C(21)	1.501(8)
C(21)-C(22)	1.380(8)	C(21)-C(27)	1.393(8)
C(22)-C(23)	1.391(8)	C(23)-C(24)	1.416(10)
C(24)-C(26)	1.366(11)	C(24)-C(25)	1.527(9)
C(26)-C(27)	1.384(9)	C(30)-C(40)	1.483(7)
C(30)-C(31)	1.498(7)	C(31)-C(37)	1.389(8)
C(31)-C(32)	1.389(8)	C(32)-C(33)	1.386(8)
C(33)-C(34)	1.376(9)	C(34)-C(36)	1.386(8)
C(34)-C(35)	1.514(10)	C(36)-C(37)	1.383(9)
C(40)-C(51)	1.518(7)	C(40)-C(41)	1.526(7)
C(41)-C(47)	1.390(8)	C(41)-C(42)	1.396(8)
C(42)-C(43)	1.394(9)	C(43)-C(44)	1.378(10)
C(44)-C(46)	1.391(9)	C(44)-C(45)	1.524(9)
C(46)-C(47)	1.389(8)	C(51)-C(56)	1.376(8)
C(51)-C(52)	1.400(9)	C(52)-C(53)	1.397(10)
C(53)-C(54)	1.387(11)	C(54)-C(55)	1.360(11)
C(55)-C(56)	1.389(9)		
C(30)-Ir(1)-C(40)	40.8(2)	C(30)-Ir(1)-C(20)	39.9(2)
C(40)-Ir(1)-C(20)	71.1(2)	C(30)-Ir(1)-C(10)	70.5(2)
C(40)-Ir(1)-C(10)	80.0(2)	C(20)-Ir(1)-C(10)	39.0(2)
C(30)-Ir(1)-C(2)	153.0(2)	C(40)-Ir(1)-C(2)	115.1(2)
C(20)-Ir(1)-C(2)	163.3(2)	C(10)-Ir(1)-C(2)	124.8(2)
C(30)-Ir(1)-C(1)	169.2(2)	C(40)-Ir(1)-C(1)	148.1(2)
C(20)-Ir(1)-C(1)	129.9(2)	C(10)-Ir(1)-C(1)	102.6(2)
C(2)-Ir(1)-C(1)	37.8(2)	C(30)-Ir(1)-C(3)	125.6(2)
C(40)-Ir(1)-C(3)	106.9(2)	C(20)-Ir(1)-C(3)	158.7(2)
C(10)-Ir(1)-C(3)	162.1(2)	C(2)-Ir(1)-C(3)	37.3(2)
C(1)-Ir(1)-C(3)	62.6(3)	C(30)-Ir(1)-C(9)	138.3(2)
C(40)-Ir(1)-C(9)	165.5(2)	C(20)-Ir(1)-C(9)	117.2(2)
C(10)-Ir(1)-C(9)	114.0(2)	C(2)-Ir(1)-C(9)	60.7(2)
C(1)-Ir(1)-C(9)	36.0(2)	C(3)-Ir(1)-C(9)	60.8(2)
C(30)-Ir(1)-C(4)	121.2(2)	C(40)-Ir(1)-C(4)	130.1(2)
C(20)-Ir(1)-C(4)	129.3(2)	C(10)-Ir(1)-C(4)	147.2(2)
C(2)-Ir(1)-C(4)	60.0(2)	C(1)-Ir(1)-C(4)	60.2(2)
C(3)-Ir(1)-C(4)	35.9(2)	C(9)-Ir(1)-C(4)	35.5(2)
C(9)-C(1)-C(2)	108.4(6)	C(9)-C(1)-Ir(1)	78.0(3)
C(2)-C(1)-Ir(1)	71.1(3)	C(3)-C(2)-C(1)	108.1(6)
C(3)-C(2)-Ir(1)	72.0(4)	C(1)-C(2)-Ir(1)	71.2(4)
C(2)-C(3)-C(4)	107.8(6)	C(2)-C(3)-Ir(1)	70.7(4)
C(4)-C(3)-Ir(1)	77.9(4)	C(5)-C(4)-C(3)	132.7(6)

C(5)-C(4)-C(9)	119.1(6)	C(3)-C(4)-C(9)	108.1(6)
C(5)-C(4)-Ir(1)	127.7(4)	C(3)-C(4)-Ir(1)	66.2(3)
C(9)-C(4)-Ir(1)	71.8(3)	C(6)-C(5)-C(4)	118.9(6)
C(5)-C(6)-C(7)	121.4(7)	C(8)-C(7)-C(6)	121.8(7)
C(7)-C(8)-C(9)	119.0(7)	C(1)-C(9)-C(8)	133.3(6)
C(1)-C(9)-C(4)	107.0(6)	C(8)-C(9)-C(4)	119.7(6)
C(1)-C(9)-Ir(1)	66.0(3)	C(8)-C(9)-Ir(1)	128.6(5)
C(4)-C(9)-Ir(1)	72.8(3)	C(20)-C(10)-C(11)	122.5(5)
C(20)-C(10)-Ir(1)	68.8(3)	C(11)-C(10)-Ir(1)	122.4(4)
C(17)-C(11)-C(12)	116.8(5)	C(17)-C(11)-C(10)	125.2(5)
C(12)-C(11)-C(10)	117.8(5)	C(13)-C(12)-C(11)	121.6(6)
C(14)-C(13)-C(12)	121.4(6)	C(13)-C(14)-C(16)	117.6(6)
C(13)-C(14)-C(15)	121.7(6)	C(16)-C(14)-C(15)	120.7(6)
C(14)-C(16)-C(17)	121.4(6)	C(11)-C(17)-C(16)	121.1(6)
C(10)-C(20)-C(30)	117.9(5)	C(10)-C(20)-C(21)	123.3(5)
C(30)-C(20)-C(21)	118.7(5)	C(10)-C(20)-Ir(1)	72.2(3)
C(30)-C(20)-Ir(1)	68.8(3)	C(21)-C(20)-Ir(1)	127.0(4)
C(22)-C(21)-C(27)	119.1(5)	C(22)-C(21)-C(20)	123.4(5)
C(27)-C(21)-C(20)	117.5(5)	C(21)-C(22)-C(23)	120.2(6)
C(22)-C(23)-C(24)	120.5(6)	C(26)-C(24)-C(23)	118.1(6)
C(26)-C(24)-C(25)	122.8(7)	C(23)-C(24)-C(25)	119.1(7)
C(24)-C(26)-C(27)	121.5(7)	C(26)-C(27)-C(21)	120.4(6)
C(20)-C(30)-C(40)	116.2(5)	C(20)-C(30)-C(31)	119.6(5)
C(40)-C(30)-C(31)	124.1(4)	C(20)-C(30)-Ir(1)	71.3(3)
C(40)-C(30)-Ir(1)	70.7(3)	C(31)-C(30)-Ir(1)	130.7(4)
C(37)-C(31)-C(32)	117.8(5)	C(37)-C(31)-C(30)	118.1(5)
C(32)-C(31)-C(30)	124.0(5)	C(33)-C(32)-C(31)	120.2(6)
C(34)-C(33)-C(32)	122.4(6)	C(33)-C(34)-C(36)	117.2(6)
C(33)-C(34)-C(35)	123.7(6)	C(36)-C(34)-C(35)	119.1(6)
C(37)-C(36)-C(34)	121.3(6)	C(36)-C(37)-C(31)	121.1(5)
C(30)-C(40)-C(51)	119.6(4)	C(30)-C(40)-C(41)	118.2(4)
C(51)-C(40)-C(41)	107.2(4)	C(30)-C(40)-Ir(1)	68.5(3)
C(51)-C(40)-Ir(1)	119.1(4)	C(41)-C(40)-Ir(1)	120.6(4)
C(47)-C(41)-C(42)	118.0(5)	C(47)-C(41)-C(40)	119.9(5)
C(42)-C(41)-C(40)	121.2(5)	C(43)-C(42)-C(41)	120.3(6)
C(44)-C(43)-C(42)	121.7(6)	C(43)-C(44)-C(46)	117.9(6)
C(43)-C(44)-C(45)	121.4(6)	C(46)-C(44)-C(45)	120.7(6)
C(47)-C(46)-C(44)	121.1(6)	C(46)-C(47)-C(41)	121.0(6)
C(56)-C(51)-C(52)	118.3(6)	C(56)-C(51)-C(40)	121.8(5)
C(52)-C(51)-C(40)	119.8(5)	C(53)-C(52)-C(51)	119.6(7)
C(54)-C(53)-C(52)	120.5(7)	C(55)-C(54)-C(53)	119.9(6)
C(54)-C(55)-C(56)	119.9(7)	C(51)-C(56)-C(55)	121.8(6)

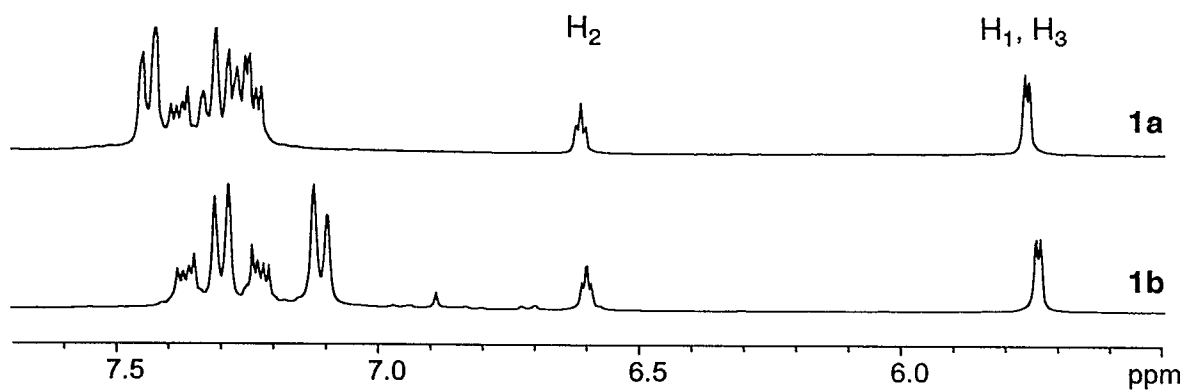
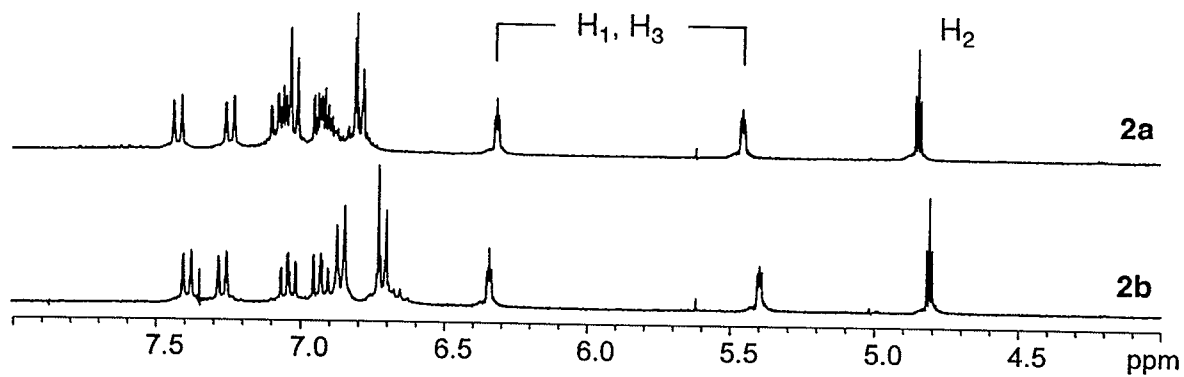
Figure 1.**Figure 2.**

Figure 3.

