

Supporting Information

Synthesis and Structures of Homo- and Heterobimetallic Rhodium(I) and/or Iridium(I) Complexes of Binucleating *Bis(1-pyrazolyl)methane Ligands*

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Part I. Experimental Data – ^1H and ^{13}C NMR data not included in the main document

Dirhodium(I) Dicyclooctadiene Complex with $p\text{-C}_6\text{H}_4[\text{CH}(\text{pz})_2]_2$ Ligand (L_p , **1a**), $[\text{Rh}_2(\text{COD})_2(\text{L}_p)][\text{BAr}^{\text{F}}_4]_2$ (**2**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2 , 298 K): δ 162.11 (q, $^1J(\text{B-C}) = 49.7$ Hz, 8C, quat C *ipso* to B of BAr^{F}_4), 144.39 (s, C3 of Pz), 138.09 (s, C_a), 135.16 (br s, 20C, *ortho*-CH of BAr^{F}_4 and C5 of Pz), 129.22 (q, $^2J(\text{F-C}) = 30.9$ Hz, 16C, C *ipso* to CF_3 of BAr^{F}_4), 127.46 (s, C_b), 124.96 (q, $^1J(\text{F-C}) = 272.7$ Hz, 16C, CF_3 of BAr^{F}_4), 117.87 (br s, 8C, *para*-CH of BAr^{F}_4), 109.41 (s, C4 of Pz), 84.41 (d, $^2J(\text{Rh-C}) = 12.3$ Hz, CH of COD), 75.61 (s, $\text{CH}(\text{Pz})_2$), 30.45 (s, CH_2 of COD), 30.15 (s, CH_2 of COD) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -63.19 ppm.

Iridium(I) Dicyclooctadiene Complex with $p\text{-C}_6\text{H}_4[\text{CH}(\text{pz})_2]_2$ Ligand (L_p , **1a**), $[\text{Ir}_2(\text{COD})_2(\text{L}_p)][\text{BAr}^{\text{F}}_4]_2$ (**3**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2 , 298 K): δ 162.12 (q, $^1J(\text{B-C}) = 49.9$ Hz, 8C, quat C *ipso* to B of BAr^{F}_4), 144.50, 144.43 (2s, C3 of Pz), 137.68 (s, C_a), 135.60, 135.53 (C5 of pz), 135.15 (br s, 16C, *ortho*-CH of BAr^{F}_4), 129.16 (q, $^2J(\text{F-C}) = 31.8$ Hz, 16C, C *ipso* to CF_3 of BAr^{F}_4), 126.66 (s, C_b), 124.94 (q, $^1J(\text{F-C}) = 272.0$ Hz, 16C, CF_3 of BAr^{F}_4), 117.93 (br s, 8C, *para*-CH of BAr^{F}_4), 109.87, 109.81 (2s, C4 of Pz), 76.72 (s, $\text{CH}(\text{Pz})_2$), 70.11, 68.85 (2s, CH of COD), 31.21 (s, CH_2 of COD), 30.80 (s, CH_2 of COD) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -63.19 ppm.

Dirhodium(I) Dicyclooctadiene Complex with $m\text{-C}_6\text{H}_4[\text{CH}(\text{pz})_2]_2$ Ligand (L_m , **1b**), $[\text{Rh}_2(\text{COD})_2(\text{L}_m)][\text{BAr}^{\text{F}}_4]_2$ (**4**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2 , 298 K): δ 162.09 (q, $^1J(\text{B-C}) = 50.4$ Hz, 8C, quat C *ipso* to B of BAr^{F}_4), 144.38 (s, C3 of Pz), 137.34 (s, C_a and c), 135.15 (br s, 16C, *ortho*-CH of BAr^{F}_4), 134.93 (s, C5 of Pz), 131.76 (s, C_e), 129.20 (q, $^2J(\text{F-C}) = 31.7$ Hz, 16C, C *ipso* to CF_3 of BAr^{F}_4), 128.61 (s, C_d and f), 124.94 (q, $^1J(\text{F-C}) = 272.8$ Hz, 16C, CF_3 of BAr^{F}_4), 122.84 (s, C_b), 117.85 (br s, 8C, *para*-CH of BAr^{F}_4), 109.40 (s, C4 of Pz), 84.37 (apparent t, $^2J(\text{Rh-C}) = 14.4$ Hz), CH of COD), 75.57 (s, $\text{CH}(\text{Pz})_2$), 30.43 (s, CH_2 of COD), 30.11 (s, CH_2 of COD) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -63.17 ppm.

Iridium(I) Dicyclooctadiene Complex with $m\text{-C}_6\text{H}_4[\text{CH}(\text{pz})_2]_2$ Ligand (L_m , **1b**), $[\text{Ir}_2(\text{COD})_2(\text{L}_m)][\text{BAr}^{\text{F}}_4]_2$ (**5**).

^1H NMR (600 MHz, CD_2Cl_2 , 298 K): δ 7.99 (d, $^3J(\text{H}_5\text{-H}_4) = 2.5$ Hz, 4H, H5), 7.76 (d, $^3J(\text{H}_4\text{-H}_3/5) = 2.3$ Hz, 4H, H3), 7.72 (s, 16H, *ortho*-CH of BAr^{F}_4), 7.69 (t, $^3J(\text{H}_e\text{-H}_d \text{ and } \text{f}) = 8.0$ Hz, 1H, H_e), 7.56 (s, 8H, *para*-CH of BAr^{F}_4), 7.42 (s, 2H, $\text{CH}(\text{Pz})_2$), 6.81 (d, $^3J(\text{H}_d \text{ and } \text{f-H}_e) = 7.4$

Hz, 2H, H_{d and f}), 6.66 (t, $^3J(\text{H4-H3/H5}) = 2.5$ Hz, 4H, H4), 5.34 (s, 1H, H_b), 4.14 (m, 4H, CH of COD), 3.43 (m, 4H, CH of COD), 2.34 (m, 4H, CH₂ of COD), 1.72 (m, 4H, CH₂ of COD), 1.65 (m, 4H, CH₂ of COD), 1.45 (m, 4H, CH₂ of COD) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD₂Cl₂, 298 K): δ 162.09 (q, $^1J(\text{B-C}) = 49.9$ Hz, 8C, quat C *ipso* to B of BAr^F₄), 144.57 (s, C3 of Pz), 136.81 (s, C_{a and c}), 135.27 (s, C5 of Pz), 135.15 (br s, 16C, *ortho*-CH of BAr^F₄), 131.59 (s, C_e), 129.20 (q, $^2J(\text{F-C}) = 31.7$ Hz, 16C, C *ipso* to CF₃ of BAr^F₄), 127.92 (s, C_{d and f}), 124.93 (q, $^1J(\text{F-C}) = 272.4$ Hz, 16C, CF₃ of BAr^F₄), 121.77 (s, C_b), 117.85 (br s, 8C, *para*-CH of BAr^F₄), 109.90 (s, C4 of Pz), 75.80 (s, CH(Pz)₂), 70.15 (s, CH of COD), 69.20 (s, CH of COD), 31.20 (s, CH₂ of COD), 30.62 (s, CH₂ of COD) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD₂Cl₂, 298 K): δ -63.21 ppm.

Dirhodium(I) Dicyclooctadiene Complex with 1,8-C₆H₄[CH(pz)₂]₂ Ligand (L_{Ant}, **1c**), [Rh₂(COD)₂(L_{Ant})] [BAr^F₄]₂ (**6**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD₂Cl₂, 258 K): δ 161.60 (q, $^1J(\text{B-C}) = 50.0$ Hz, 8C, quat C *ipso* to B of BAr^F₄), 143.23 (s, C3b of Pz), 142.89 (s, C3a of Pz), 135.51 (s, C7), 135.31 (s, C5b of Pz), 135.05 (s, C5), 134.57 (br s, 16C, *ortho*-CH of BAr^F₄), 134.05 (s, quat. C of anthracene), 133.52 (s, C4), 132.61 (br s, C5a of Pz and C10), 132.12 (s, quat. C of anthracene), 132.05 (s, quat. C of anthracene), 131.12 (s, C2), 128.55 (q, $^2J(\text{F-C}) = 31.1$ Hz, 16C, C *ipso* to CF₃ of BAr^F₄), 128.13 (s, quat. C of anthracene), 127.26 (s, quat. C of anthracene), 126.00 (s, C3/6), 125.05 (s, C3/6), 124.35 (q, $^1J(\text{F-C}) = 272.9$ Hz, 16C, CF₃ of BAr^F₄), 122.03 (s, quat. C of anthracene), 118.11 (s, C9), 117.41 (br s, 8C, *para*-CH of BAr^F₄), 108.70 (s, C4a of Pz), 108.14 (s, C4b of Pz), 87.43 (s, CH of COD(b)), 85.09 (s, CH of COD(b)), 83.60 (s, CH of COD(a)), 82.95 (s, CH of COD(a)), 79.24 (s, CH(Pz)₂ at C8), 75.60 (s, CH(Pz)₂ at C1), 30.51 (s, CH₂ of COD(b)), 30.44 (s, CH₂ of COD(b)), 29.63 (s, CH₂ of COD(a)), 29.51 (s, CH₂ of COD(a)) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD₂Cl₂, 298 K): δ -60.16 ppm.

Iridium(I) Dicyclooctadiene Complex with 1,8-C₆H₄[CH(pz)₂]₂ Ligand (L_{Ant}, **1c**), [Ir₂(COD)₂(L_{Ant})] [BAr^F₄]₂ (**7**).

^1H NMR (600 MHz, CD₂Cl₂, 273 K): δ 8.92 (s, 1H, H10), 8.40 (d, $^3J(\text{H5-H6}) = 8.5$ Hz, 1H, H5), 8.38 (d, $^3J(\text{H4-H3}) = 8.5$ Hz, 1H, H4), 8.04 (d, $^3J(\text{H7-H6}) = 6.5$ Hz, 1H, H7), 7.89 (d, $^3J(\text{H3b-H4b}) = 2.0$ Hz, 2H, H3b of Pz), 7.80 (s, 1H, CH(Pz)₂ at C8), 7.73 (br s, 16H, *ortho*-CH of BAr^F₄), 7.66 (m, 1H, H6), 7.61 (m, 1H, H3), 7.54 (s, 8H, *para*-CH of BAr^F₄), 7.48 (s, 1H, CH(Pz)₂ at C1), 7.45 (d, $^3J(\text{H3a-H4a}) = 2.0$ Hz, 2H, H3a of Pz), 7.37 (d, $^3J(\text{H5a-H4a}) = 2.5$ Hz, 2H, H5a of Pz), 7.22 (s, 1H, H9), 7.09 (d, $^3J(\text{H5b-H4b}) = 2.7$ Hz, 2H, H5b of Pz), 6.47 (t, $^3J(\text{H4a-H3a and H5a}) = 2.6$ Hz, 2H, H4a), 6.43 (br s, 1H, H2), 6.40 (t, $^3J(\text{H4b-H3b and H5b}) = 2.5$ Hz, 2H, H4b), 4.45 (m, 2H, CH of COD(b)), 4.23 (m, 2H, CH of COD(b)), 3.91 (m, 2H, CH of COD(a)), 3.14 (m, 2H, CH of COD(a)), 2.50 (m, 2H, CH₂ of COD(b)), 2.40 (m, 2H, CH₂ of COD(b)), 2.21 (m, 2H, CH₂ of COD(a)), 2.00 (m, 4H, CH₂ of COD(b)),

1.56 (m, 2H, CH₂ of COD(a)), 1.34 (m, 2H, CH₂ of COD(a)), 1.21 (m, 2H, CH₂ of COD(a)) ppm. ¹³C{¹H} NMR (150.9 MHz, CD₂Cl₂, 273 K): δ 161.71 (q, ¹J(B-C) = 49.7 Hz, 8C, quat C *ipso* to B of BAr^F₄), 143.88 (s, C3b of Pz), 142.93 (s, C3a of Pz), 136.00 (s, C5b of Pz), 135.82 (s, C7), 135.47 (s, C5), 135.25 (s, quat. C of anthracene), 134.70 (br s, 16C, *ortho*-CH of BAr^F₄), 134.17 (s, quat. C of anthracene), 133.41 (s, C4), 133.07 (br s, C5a of Pz and C10), 132.30 (s, quat. C of anthracene), 132.11 (s, quat. C of anthracene), 130.74 (s, C2), 128.69 (q, ²J(F-C) = 31.7 Hz, 16C, C *ipso* to CF₃ of BAr^F₄), 127.95 (s, quat. C of anthracene), 126.05 (s, C6), 125.12 (s, C3), 124.47 (q, ¹J(F-C) = 272.7 Hz, 16C, CF₃ of BAr^F₄), 121.44 (s, quat. C of anthracene), 117.65 (s, C9), 117.51 (br s, 8C, *para*-CH of BAr^F₄), 109.36 (s, C4a of Pz), 108.89 (s, C4b of Pz), 79.13 (s, CH(Pz)₂ at C8), 75.94 (s, CH(Pz)₂ at C1), 73.37 (s, CH of COD(b)), 70.00 (s, CH of COD(b)), 69.65 (s, CH of COD(a)), 68.10 (s, CH of COD(a)), 31.15 (s, CH₂ of COD(b)), 30.59 (s, CH₂ of COD(b)), 30.40 (s, CH₂ of COD(a)), 30.31 (s, CH₂ of COD(a)) ppm.

Dirhodium(I) Tetracarbonyl Complex with *p*-C₆H₄[CH(pz)₂]₂ Ligand (L_p, **1a**), [Rh₂(CO)₄(L_p)] [BAr^F₄]₂ (**8**).

¹³C{¹H} NMR (150.9 MHz, CD₂Cl₂, 298 K): δ 181.56 (d, ¹J(Rh-CO) = 69.9 Hz, CO), 162.07 (q, ¹J(B-C) = 49.3 Hz, 8C, quat C *ipso* to B of BAr^F₄), 148.55 (s, C3 of Pz), 136.76 (s, C_a), 136.21 (s, C5 of Pz), 135.12 (br s, 16C, *ortho*-CH of BAr^F₄), 129.23 (qq, ²J(F-C) = 31.2 Hz, 16C, C *ipso* to CF₃ of BAr^F₄), 127.16 (s, C_b), 124.91 (q, ¹J(F-C) = 272.8 Hz, 16C, CF₃ of BAr^F₄), 117.90 (br s, 8C, *para*-CH of BAr^F₄), 110.12 (s, C4 of Pz), 75.59 (s, CH(Pz)₂) ppm. ¹⁹F{¹H} NMR (282.4 MHz, CD₂Cl₂, 298 K): δ -63.16 ppm. IR (KBr disc) ν_{CO} = 2113, 2061 (s) cm⁻¹.

Iridium(I) Tetracarbonyl Complex with *p*-C₆H₄[CH(pz)₂]₂ Ligand (L_p, **1a**), [Ir₂(CO)₄(L_p)] [BAr^F₄]₂ (**9**).

¹H NMR (600 MHz, CD₂Cl₂, 298 K): δ 8.17 (d, ³J(H5-H4) = 2.8 Hz, 4H, H5), 8.06 (d, ³J(H5-H4) = 2.4 Hz, 4H, H3), 7.70 (m, 18H, *ortho*-CH of BAr^F₄ and CH(Pz)₂), 7.53 (m, 8H, *para*-CH of BAr^F₄), 6.76 (t, ³J(H4-H3/5) = 2.6 Hz, 4H, H4), 6.46 (s, 4H, H_b) ppm. ¹³C{¹H} NMR (150.9 MHz, CD₂Cl₂, 298 K): δ 168.95 (s, CO), 162.07 (q, ¹J(B-C) = 49.8 Hz, 8C, quat C *ipso* to B of BAr^F₄), 149.66, 149.46, 149.41, 149.20 (4s, C3 of Pz), 136.93 (s, C_a), 136.74, 136.65, 136.55, 136.46 (4s, C5 of Pz), 135.13 (br s, 16C, *ortho*-CH of BAr^F₄), 129.17 (qq, ²J(F-C) = 31.6 Hz, ³J(B-C) = 2.9 Hz, 16C, C *ipso* to CF₃ of BAr^F₄), 126.96 (s, C_b), 124.91 (q, ¹J(F-C) = 272.8 Hz, 16C, CF₃ of BAr^F₄), 117.85 (br s, 8C, *para*-CH of BAr^F₄), 110.70, 110.63 (2s, C4 of Pz), 75.87, 75.82 (2s, CH(Pz)₂) ppm. ¹⁹F{¹H} NMR (282.4 MHz, CD₂Cl₂, 298 K): δ -63.15 ppm. IR (KBr disc) ν_{CO} = 2104, 2047 (s) cm⁻¹.

Dirhodium(I) Tetracarbonyl Complex with *m*-C₆H₄[CH(pz)₂]₂ Ligand (L_m, **1a**), [Rh₂(CO)₄(L_m)] [BAr^F₄]₂ (**10**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2 , 298 K): δ 181.58 (d, $^1J(\text{Rh-CO}) = 69.8$ Hz, CO), 162.11 (q, $^1J(\text{B-C}) = 49.7$ Hz, 8C, quat C *ipso* to B of BAr^{F_4}), 148.71 (s, C3 of Pz), 136.06 (s, C5 of Pz), 135.48 (s, C_a and c), 135.19 (br s, 16C, *ortho*-CH of BAr^{F_4}), 132.38 (s, C_e), 129.23 (q, $^2J(\text{F-C}) = 31.2$ Hz, 16C, C *ipso* to CF_3 of BAr^{F_4}), 128.81 (s, C_d and f), 124.97 (q, $^1J(\text{F-C}) = 272.8$ Hz, 16C, CF_3 of BAr^{F_4}), 121.49 (s, C_b), 117.90 (br s, 8C, *para*-CH of BAr^{F_4}), 110.17 (s, C4 of Pz), 75.54 (s, $\text{CH}(\text{Pz})_2$) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -63.17 ppm. IR (KBr disc) $\nu_{\text{CO}} = 2115, 2055$ (s) cm^{-1} .

Diiridium(I) Tetracarbonyl Complex with *m*- $\text{C}_6\text{H}_4[\text{CH}(\text{pz})_2]_2$ Ligand (L_m , **1a**), $[\text{Ir}_2(\text{CO})_4(\text{L}_m)][\text{BAr}^{\text{F}_4}]_2$ (**11**).

^1H NMR (600 MHz, CD_2Cl_2 , 298 K): δ 8.11 (m, 8H, H5 and H3), 7.73 (s, 16H, *ortho*-CH of BAr^{F_4}), 7.68 (s, 2H, $\text{CH}(\text{Pz})_2$), 7.57 (m, 9H, *para*-CH of BAr^{F_4} and H_e), 6.81 (t, $^3J(\text{H4-H3/5}) = 2.6$ Hz, 4H, H4), 6.74 (br s, 2H, H_d and f), 5.57 (s, 1H, H_b) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2 , 298 K): δ 169.00 (s, CO), 162.07 (q, $^1J(\text{B-C}) = 50.0$ Hz, 8C, quat C *ipso* to B of BAr^{F_4}), 149.62 (s, C3 of Pz), 136.50 (s, C5 of Pz), 135.13 (br s, 17C, *ortho*-CH of BAr^{F_4} and C_a and c), 132.50 (s, C_e), 129.16 (q, $^2J(\text{F-C}) = 31.4$ Hz, 16C, C *ipso* to CF_3 of BAr^{F_4}), 127.62 (s, C_d and f), 124.91 (q, $^1J(\text{F-C}) = 272.7$ Hz, 16C, CF_3 of BAr^{F_4}), 118.43 (s, C_b), 117.86 (br s, 8C, *para*-CH of BAr^{F_4}), 110.75 (s, C4 of Pz), 75.80 (s, $\text{CH}(\text{Pz})_2$) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -63.16 ppm. IR (KBr disc) $\nu_{\text{CO}} = 2101, 2037$ (s) cm^{-1} .

Dirhodium(I) Tetracarbonyl Complex with 1,8- $\text{C}_6\text{H}_4[\text{CH}(\text{pz})_2]_2$ Ligand (L_{Ant} , **1c**), $[\text{Rh}_2(\text{CO})_4(\text{L}_{\text{Ant}})][\text{BAr}^{\text{F}_4}]_2$ (**12**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2 , 258 K): δ 181.25 (d, $^1J(\text{Rh-CO}) = 70.4$ Hz, CO), 161.62 (q, $^1J(\text{B-C}) = 49.4$ Hz, 8C, quat C *ipso* to B of BAr^{F_4}), 148.87, 148.69, 148.13, 147.09 (4s, C3a and C3b of Pz), 136.60 (s, C5a/b of Pz), 137.31 (s, C7), 135.90 (s, C5), 135.17 (s, quat. C of anthracene), 134.64 (br s, 17C, *ortho*-CH of BAr^{F_4} and quat. C of anthracene), 134.04 (s, C4), 133.78 (s, C5a and C5b of Pz), 133.17 (s, C10), 132.19 (s, quat. C of anthracene), 130.33 (s, C2), 128.61 (q, $^2J(\text{F-C}) = 31.1$ Hz, 16C, C *ipso* to CF_3 of BAr^{F_4}), 128.28 (s, quat. C of anthracene), 128.02 (s, quat. C of anthracene), 126.20 (s, C6), 125.03 (s, C3), 124.41 (q, $^1J(\text{F-C}) = 272.7$ Hz, 16C, CF_3 of BAr^{F_4}), 120.23 (s, quat. C of anthracene), 117.47 (br s, 8C, *para*-CH of BAr^{F_4}), 116.91 (s, C9), 109.41, 109.28, 108.98 (m, C4a and C4b of Pz), 108.14 (s, C4b of Pz), 79.44 (s, $\text{CH}(\text{Pz})_2$ at C8), 75.21 (s, $\text{CH}(\text{Pz})_2$ at C1) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -63.17 ppm. IR (KBr disc) $\nu_{\text{CO}} = 2112, 2057$ (s) cm^{-1} .

Diiridium(I) Tetracarbonyl Complex with 1,8- $\text{C}_6\text{H}_4[\text{CH}(\text{pz})_2]_2$ Ligand (L_{Ant} , **1c**), $[\text{Ir}_2(\text{CO})_4(\text{L}_{\text{Ant}})][\text{BAr}^{\text{F}_4}]_2$ (**13**).

^1H NMR (600 MHz, CD_2Cl_2 , 243 K): δ 8.82 (s, 1H, H10), 8.68 (s, 1H, H9), 8.55 (s, 2H, $\text{CH}(\text{Pz})_2$), 8.46 (d, $^3J(\text{H}_{4,5}-\text{H}_{3,6}) = 8.6$ Hz, 2H, H4,5), 8.12 (d, $^3J(\text{H}_{2,7}-\text{H}_{3,6}) = 6.8$ Hz, 2H, H2,7), 8.09 (d, 4H, $^3J(\text{H}_{3'}-\text{H}_{4'}) = 1.90$ Hz, H3'), 7.90 (m, 2H, H3,6), 7.70 (s, 16H, *ortho*-CH of BAr^{F_4}), 7.68 (d, $^3J(\text{H}_{5'}-\text{H}_{4'}) = 2.76$ Hz, 4H, H5'), 7.49 (s, 8H, *para*-CH of BAr^{F_4}), 6.49 (t, $^3J(\text{H}_{4'}-\text{H}_{5'}$ and H3') = 2.43 Hz, 4H, H4'). $^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2 , 243 K): δ 169.58 (s, CO), 161.43 (q, $^1J(\text{B}-\text{C}) = 49.8$ Hz, 8C, quat C *ipso* to B of BAr^{F_4}), 148.83 (s, C3' of Pz), 135.11 (s, C4,5), 134.91 (s, C5' of pz), 134.35 (br s, 16C, *ortho*-CH of BAr^{F_4}), 133.86 (C12,13), 133.25 (C2,7), 132.01 (C10), 128.30 (q, $^2J(\text{F}-\text{C}) = 31.50$ Hz, 16C, C *ipso* to CF_3 of BAr^{F_4}), 125.02 (C3,6), 127.92 (C11,14), 124.12 (q, $^1J(\text{F}-\text{C}) = 272.3$ Hz, 16C, CF_3 of BAr^{F_4}), 119.91 (C1,8), 117.25 (br s, 8C, *para*-CH of BAr^{F_4}), 112.82 (C9), 109.14 (s, C4' of Pz), 71.50 (s, $\text{CH}(\text{Pz})_2$) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -63.21 ppm. IR (KBr disc) $\nu_{\text{CO}} = 2101, 2041$ (s) cm^{-1} .

Rhodium(I) Cyclooctadiene Complex, $[\text{Rh}(\text{COD})(\text{L}_m)]\text{BAr}^{\text{F}_4}$ (**14**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, d_8 -THF, 298 K): δ 162.23 (q, $^1J(\text{B}-\text{C}) = 49.4$ Hz, 4C, quat C *ipso* to B of BAr^{F_4}), 143.80 (s, C3 of Pz), 140.54 (s, C3' of Pz), 140.09 (s, C_c), 137.29 (s, C_a), 135.83 (s, C5 of Pz), 135.00 (br s, 8C, *ortho*-CH of BAr^{F_4}), 130.22 (s, C5' of Pz), 129.84-129.00 (m, 10C, C_e and C_d and C *ipso* to CF_3 of BAr^{F_4}), 126.34 (s, C_f), 124.92 (q, $^1J(\text{F}-\text{C}) = 271.4$ Hz, 8C, CF_3 of BAr^{F_4}), 124.51 (s, C_b), 117.60 (br s, 4C, *para*-CH of BAr^{F_4}), 108.07 (s, C4 of Pz), 106.58 (s, C4' of Pz), 84.61 (br s, CH of COD), 82.61 (br s, CH of COD), 76.90 (s, $\text{CH}(\text{Pz})_2$ at C_c), 75.63 (s, $\text{CH}(\text{Pz})_2$ at C_a), 30.25 (s, CH_2 of COD), 29.91 (s, CH_2 of COD) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -62.10 ppm.

Iridium(I) Cyclooctadiene Complex, $[\text{Ir}(\text{COD})(\text{L}_m)]\text{BAr}^{\text{F}_4}$ (**15**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2 , 298 K): δ 162.08 (q, $^1J(\text{B}-\text{C}) = 50.0$ Hz, 4C, quat C *ipso* to B of BAr^{F_4}), 143.79 (s, C3 of Pz), 141.20 (s, C3' of Pz), 140.09 (s, C_c), 139.43 (s, C_a), 135.26 (s, C5 of Pz), 135.13 (br s, 8C, *ortho*-CH of BAr^{F_4}), 130.19 (s, C5' of pz), 130.07 (s, C_e), 129.72 (s, C_d), 129.18 (qq, $^2J(\text{F}-\text{C}) = 31.9$ Hz, $^3J(\text{B}-\text{C}) = 2.8$ Hz, 8C, C *ipso* to CF_3 of BAr^{F_4}), 125.95 (s, C_f), 124.93 (q, $^1J(\text{F}-\text{C}) = 271.5$ Hz, 8C, CF_3 of BAr^{F_4}), 123.79 (s, C_b), 117.83 (br s, 4C, *para*-CH of BAr^{F_4}), 109.21 (s, C4 of Pz), 107.31 (s, C4' of Pz), 77.09 (s, $\text{CH}(\text{Pz})_2$ at C_c), 76.42 (s, $\text{CH}(\text{Pz})_2$ at C_a), 70.63 (s, CH of COD), 68.10 (s, CH of COD), 30.85 (s, CH_2 of COD), 30.81 (s, CH_2 of COD) ppm. $^{19}\text{F}\{^1\text{H}\}$ NMR (282.4 MHz, CD_2Cl_2 , 298 K): δ -63.24 ppm.

Rhodium(I) Dicarboxyl Complex, $[\text{Rh}(\text{CO})_2(\text{L}_m)]\text{BAr}^{\text{F}_4}$ (**16**).

$^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, d_8 -THF, 298 K): δ 183.16 (d, $^1J(\text{Rh}-\text{CO}) = 70.0$ Hz, CO), 162.82 (q, $^1J(\text{B}-\text{C}) = 49.7$ Hz, 4C, quat C *ipso* to B of BAr^{F_4}), 148.76 (s, C3 of Pz), 141.14 (s, C3' of Pz), 140.62 (s, C_c), 137.37 (s, C5 of Pz), 136.27 (s, C_a), 135.60 (br s, 8C, *ortho*-CH of BAr^{F_4}),

130.81 (s, C5' of pz), 130.62-129.62 (m, 10C, C_e and C_d and C *ipso* to CF₃ of BAr^F₄), 126.60 (s, C_f), 125.52 (q, ¹J(F-C) = 271.6 Hz, 8C, CF₃ of BAr^F₄), 124.90 (s, C_b), 118.19 (br s, 4C, *para*-CH of BAr^F₄), 109.41 (s, C4 of Pz), 107.11 (s, C4' of Pz), 77.31 (s, CH(Pz)₂ at C_c), 76.22 (s, CH(Pz)₂ at C_a) ppm. ¹⁹F{¹H} NMR (282.4 MHz, CD₂Cl₂, 298 K): δ -63.13 ppm. IR (KBr disc) ν_{CO} = 2107, 2049 (s) cm⁻¹.

Iridium(I) Dicarbonyl Complex, [Ir(CO)₂(L_m)]BAr^F₄ (**17**).

¹³C{¹H} NMR (150.9 MHz, CD₂Cl₂, 298 K): δ 169.38 (s, CO), 162.12 (q, ¹J(B-C) = 49.4 Hz, 4C, quat C *ipso* to B of BAr^F₄), 148.92 (s, C3 of Pz), 141.41 (s, C3' of Pz), 139.68 (s, C_c), 136.33 (s, C5 of Pz), 135.69 (s, C_a), 135.18 (br s, 8C, *ortho*-CH of BAr^F₄), 130.80 (br s, C_d and C_e), 130.41 (s, C5' of Pz), 129.26 (q, ²J(F-C) = 32.5 Hz, 8C, C *ipso* to CF₃ of BAr^F₄), 126.36 (s, C_f), 124.96 (q, ¹J(F-C) = 271.5 Hz, 8C, CF₃ of BAr^F₄), 124.07 (s, C_b), 117.87 (br s, 4C, *para*-CH of BAr^F₄), 110.14 (s, C4 of Pz), 107.40 (s, C4' of Pz), 76.89 (s, CH(Pz)₂ at C_c), 76.66 (s, CH(Pz)₂ at C_a) ppm. ¹⁹F{¹H} NMR (282.4 MHz, CD₂Cl₂, 298 K): δ -63.28 ppm. IR (KBr disc) ν_{CO} = 2095, 2033 (s) cm⁻¹.

Rhodium-Iridium Dicyclooctadiene Complex, [Rh(COD)Ir(COD)(L_m)] [BAr^F₄]₂ (**18**).

A CH₂Cl₂ solution of [Rh(COD)₂]BAr^F₄ (0.0578 g, 0.0489 mmol) was added dropwise to a CH₂Cl₂ solution of complex **15** (0.0763 g, 0.0499 mmol). The reaction mixture was stirred for 0.5 h at RT. *n*-Pentane was added slowly to afford a yellow solid which was collected by filtration and washed with *n*-pentane (3 x 5 mL). The crude product was recrystallized from CH₂Cl₂/*n*-pentane to form a mixture of products **18**, **4** and **5** as a yellow solid. Yield: 0.117 g (0.0449 mmol), 92 %. ESI-MS (CH₂Cl₂), *m/z* (%): 1655.0 ([M - BAr^F₄]⁺ of 3.4, 33), 1745.0 ([M - BAr^F₄]⁺ of 3.20, 36), 1833.1 ([M - BAr^F₄]⁺ of 3.5, 26). ¹H NMR (600 MHz, CD₂Cl₂, 298 K): δ 8.00 (m, 4H, H5), 7.92 (m, 4H, H5'), 7.86 (t, ³J(H_e-H_d and _f) = 8.03 Hz, 1H, H_e of [Rh₂]), 7.78 (t, ³J(H_e-H_d and _f) = 8.03 Hz, 1H, H_e of [RhIr]), 7.77 (m, 4H, H3), 7.72 (m, 17H, *ortho*-CH of BAr^F₄, H_e of [Ir₂]), 7.55 (m, 12H, *para*-CH of BAr^F₄ and H3'), 7.47, 7.41 (2s, 2H, CH of [RhIr]), 7.46 (s, 2H, CH of [Ir₂]), 7.42 (s, 2H, CH of [Rh₂]), 6.96 (d, ³J(H_d and _f-H_e) = 7.63 Hz, 2H, H_d and _f of [Rh₂]), 6.91, 6.87 (2d, ³J(H_d and _f-H_e) = 7.39 Hz, 2H, H_d and _f of [RhIr]), 6.82 (d, ³J(H_d and _f-H_e) = 6.87 Hz, 2H, H_d and _f of [Ir₂]), 6.67 (t, ³J(H4-H3/H5) = 2.45 Hz, 4H, H4), 6.57 (t, ³J(H4-H3/H5) = 2.34 Hz, 4H, H4'), 5.46 (s, 1H, H_b of [Rh₂]), 5.40 (s, 1H, H_b of [RhIr]), 5.35 (br s, 1H, H_b of [Ir₂]), 4.35 (m, 4H, CH of [Rh]COD), 4.15 (m, 4H, CH of [Ir]COD), 3.70 (m, 4H, CH of [Rh]COD), 3.44 (m, 4H, CH of [Ir]COD), 2.54 (m, 4H, CH₂ of [Rh]COD), 2.35 (m, 4H, CH₂ of [Ir]COD), 1.91 (m, 4H, CH₂ of [Rh]COD), 1.79 (m, 4H, CH₂ of [Rh]COD), 1.73 (m, 4H, CH₂ of [Ir]COD), 1.66 (m, 4H, CH₂ of [Rh]COD), 1.60 (m, 4H, CH₂ of [Ir]COD), 1.47 (m, 4H, CH₂ of [Ir]COD) ppm.

Part II. Crystal Structure of 1,8-C₁₄H₈[CH(pz)₂]₂ (**L_{Ant}**, **1c**)

The molecular structure of [1,8-*bis*(*bis*(1-pyrazolyl)methyl)anthracene], **L_{Ant}** (**1c**) was determined using single crystal X-ray diffraction. Crystals of **L_{Ant}** (**1c**) suitable for X-ray diffraction were obtained by slow evaporation of a mixture of dichloromethane and toluene solution. The ORTEP diagram of **1c** together with the atom numbering scheme is shown in Figure 1.

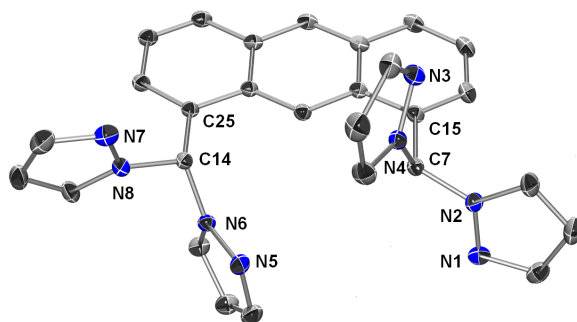


Figure 1: ORTEP depiction of 1,8-C₁₄H₈[CH(pz)₂]₂ (**1c**) with 50% probability ellipsoids for the non-hydrogen atoms.

Part III. Crystallographic Data

Crystallographic data for the solid state structures of ligand 1,8-C₁₄H₈[CH(pz)₂]₂, (**1c**), and complexes [Ir₂(COD)₂(L_m)] [BAr^F₄]₂ (**5**), [Rh₂(CO)₄(L_m)] [BAr^F₄]₂ (**10**), [Ir₂(CO)₄(L_m)] [BAr^F₄]₂ (**11**), [Rh₂(COD)₂(L_p)] [BAr^F₄]₂ (**2**), [Ir₂(COD)₂(L_p)] [BAr^F₄]₂ (**3**), [Ir₂(CO)₄(L_p)] [BAr^F₄]₂ (**9**), [Rh₂(COD)₂(L_{Ant})] [BAr^F₄]₂ (**6**) and [Ir(COD)(L_m)]BAr^F₄ (**5**) are presented in Tables 1-7 as shown below.

Table 1: Crystallographic data for the solid state structure of 1,8-C₁₄H₈[CH(pz)₂]₂ (**1c**).

CCDC-798119

	Anthracene-dibpm (1c)
Empirical formula	C ₂₈ H ₂₂ N ₈
<i>M</i> (g mol ⁻¹)	470.54
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	10.0732(3)
<i>b</i> (Å)	23.3283(5)
<i>c</i> (Å)	10.6167(3)
<i>β</i> (°)	112.066(1)
<i>V</i> (Å ³)	2312.08(11)
<i>D_c</i> (g.cm ⁻³)	1.352
<i>Z</i>	4
<i>T</i> (K)	90(2)
<i>λ</i> Mo-K _α (Å)	0.71073
<i>μ</i> Mo-K _α (mm ⁻¹)	0.085
Crystal size (mm)	0.55 x 0.45 x 0.10
<i>T</i> (Gaussian) _{min,max}	0.9245, 0.9915
2 <i>θ</i> _{max} (°)	32.00
<i>hkl</i> range	-15 ≤ <i>h</i> ≤ 15, -34 ≤ <i>k</i> ≤ 34, -15 ≤ <i>l</i> ≤ 14
<i>N</i>	31238
<i>N</i> _{ind}	8008 (<i>R</i> _{merge} 0.0281)
<i>N</i> _{obs} (<i>I</i> > 2σ(<i>I</i>))	5913
GoF(all data)	1.096
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.0459, 0.1203
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0701, 0.1297

Table 2: Crystallographic data for the solid state structure of $[\text{Ir}_2(\text{COD})_2(\text{L}_m)][\text{BAr}^{\text{F}}_4]_2 \cdot 2\text{CH}_2\text{Cl}_2$ (**5**).

CCDC-798127

	$[\text{Ir}_2(\text{COD})_2(\text{L}_m)][\text{BAr}^{\text{F}}_4]_2 \cdot 2\text{CH}_2\text{Cl}_2$ (5) $\cdot 2\text{CH}_2\text{Cl}_2$
Empirical formula	$\text{C}_{101}\text{H}_{68}\text{B}_2\text{Cl}_2\text{F}_{48}\text{Ir}_2\text{N}_8$
M (g mol^{-1})	2782.55
Crystal system	triclinic
Space group	$P-1$
a (Å)	12.5673(1)
b (Å)	17.6438(2)
c (Å)	24.3971(2)
α (°)	86.700(1)
β (°)	89.240(1)
γ (°)	77.418(1)
V (Å ³)	5271.02(9)
D_c (g.cm^{-3})	1.753
Z	2
T (K)	200(2)
λ Mo- K_α (Å)	0.71073
μ Mo- K_α (mm^{-1})	2.709
Crystal size (mm)	0.55 x 0.23 x 0.05
T (Gaussian) _{min,max}	0.846, 0.980
$2\theta_{\text{max}}$ (°)	27.50
hkl range	$-16 \leq h \leq 15, -22 \leq k \leq 22, -31 \leq l \leq 31$
N	116633
N_{ind}	24176 ($R_{\text{merge}} 0.0694$)
$N_{\text{obs}}(I > 2\sigma(I))$	19570
GoF(all data)	1.053
$R_1, wR_2 [I > 2\sigma(I)]$	0.0389, 0.1019
R_1, wR_2 (all data)	0.0529, 0.1085

Table 3: Crystallographic data for the solid state structures of $[\text{Rh}_2(\text{CO})_4(\text{L}_m)]_2[\text{BAr}^{\text{F}}_4]_2$ (**10**) CCDC-798124.

	$[\text{Rh}_2(\text{CO})_2(\text{L}_m)]_2[\text{BAr}^{\text{F}}_4]_2 \cdot 0.125 \text{ CH}_2\text{Cl}_2$ (10) $\cdot 0.125 \text{ CH}_2\text{Cl}_2$
Empirical formula	$\text{C}_{88.125}\text{H}_{42.25}\text{B}_2\text{Cl}_{0.25}\text{F}_{48}\text{N}_8\text{O}_4\text{Rh}_2$
M (g mol ⁻¹)	2425.35
Crystal system	monoclinic
Space group	$P2_1$
a (Å)	16.1319(3)
b (Å)	19.1238(4)
c (Å)	31.7567(6)
β (°)	103.648(1)
V (Å ³)	9520.4(3)
D_c (g.cm ⁻³)	1.692
Z	4
T (K)	150(2)
λ Mo-K α (Å)	0.71073
μ Mo-K α (mm ⁻¹)	0.503
Crystal size (mm)	0.45 x 0.35 x 0.20
T (Gaussian) _{min,max}	0.8476, 0.9062
$2\theta_{\text{max}}$ (°)	26.00
hkl range	$-19 \leq 19, -22 \leq 23, -39 \leq 39$
N	85461
N_{ind}	33929 (R_{merge} 0.0284)
$N_{\text{obs}}(I > 2\sigma(I))$	28061
GoF(all data)	1.045
$R_1, wR_2 [I > 2\sigma(I)]$	0.0450, 0.1069
R_1, wR_2 (all data)	0.0613, 0.1141

Table 4: Crystallographic data for the solid state structures of $[\text{Rh}_2(\text{COD})_2(\text{L}_p)][\text{BAr}^{\text{F}}_4]_2$ (**2**) and $[\text{Ir}_2(\text{COD})_2(\text{L}_p)][\text{BAr}^{\text{F}}_4]_2$ (**3**). (CCDC-798123 and -798122, respectively)

	$[\text{Rh}_2(\text{COD})_2(\text{L}_p)][\text{BAr}^{\text{F}}_4]_2$ $\cdot 0.3 \text{ CH}_2\text{Cl}_2$ (2) · 0.3 CH₂Cl₂	$[\text{Ir}_2(\text{COD})_2(\text{L}_p)][\text{BAr}^{\text{F}}_4]_2$ $\cdot 0.2 \text{ CH}_2\text{Cl}_2$ (3) · 0.2 CH₂Cl₂
Empirical formula	$\text{C}_{100.3}\text{H}_{66.6}\text{B}_2\text{Cl}_{0.6}\text{F}_{48}\text{N}_8\text{Rh}_2$	$\text{C}_{100.2}\text{H}_{66.4}\text{B}_2\text{Cl}_{0.4}\text{F}_{48}\text{Ir}_2\text{N}_8$
M (g mol ⁻¹)	2544.53	2714.65
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$
a (Å)	13.1485(3)	13.1567(3)
b (Å)	26.1740(5)	26.1697(5)
c (Å)	15.2911(3)	15.2518(3)
β (°)	103.588(1)	103.404(1)
V (Å ³)	5115.12(19)	5108.25(18)
D_c (g.cm ⁻³)	1.652	1.765
Z	2	2
T (K)	150(2)	150(2)
λ Mo-K α (Å)	0.71073	0.71073
μ Mo-K α (mm ⁻¹)	0.478	2.753
Crystal size (mm)	0.50 x 0.30 x 0.20	0.58 x 0.40 x 0.24
T (Gaussian) _{min,max}	0.9105, 0.8658	0.5151, 0.3710
$2\theta_{\text{max}}$ (°)	30.00	32.00
hkl range	$-18 \leq 15, -36 \leq 30, -19 \leq 21$	$-19 \leq 19, -23 \leq 39, -19 \leq 22$
N	54454	61231
N_{ind}	14416 (R_{merge} 0.0204)	17747 (R_{merge} 0.0298)
$N_{\text{obs}}(I > 2\sigma(I))$	11927	14160
GoF(all data)	1.061	1.027
$R_1, wR_2 [I > 2\sigma(I)]$	0.0390, 0.0983	0.0329, 0.0716
R_1, wR_2 (all data)	0.0521, 0.1034	0.0505, 0.0757

Table 5: Crystallographic data for the solid state structure of $[\text{Ir}_2(\text{CO})_4(\text{L}_p)][\text{BAr}^{\text{F}}_4]_2$ (**9**).

CCDC-798121

	$[\text{Ir}_2(\text{CO})_2(\text{L}_p)][\text{BAr}^{\text{F}}_4]_2 \cdot 3\text{THF}$ (9) · 3THF
Empirical formula	$\text{C}_{112}\text{H}_{90}\text{B}_2\text{F}_{48}\text{Ir}_2\text{N}_8\text{O}_{10}$
M (g mol^{-1})	3025.98
Crystal system	triclinic
Space group	$P-1$
a (Å)	12.6310(3)
b (Å)	13.8922(3)
c (Å)	18.4681(4)
α (°)	95.388(1)
β (°)	100.973(1)
γ (°)	108.210(1)
V (Å ³)	2980.90(12)
D_c (g.cm^{-3})	1.686
Z	1
T (K)	150(2)
λ Mo-K α (Å)	0.71073
μ Mo-K α (mm^{-1})	2.365
Crystal size (mm)	0.60 x 0.38 x 0.35
T (Gaussian) _{min,max}	0.4374, 0.3346
$2\theta_{\text{max}}$ (°)	28.00
hkl range	$-16 \leq 16, -18 \leq 18, -24 \leq 24$
N	48457
N_{ind}	14341 (R_{merge} 0.0239)
$N_{\text{obs}}(I > 2\sigma(I))$	11743
GoF(all data)	1.058
R_1, wR_2 [$I > 2\sigma(I)$]	0.0327, 0.0797
R_1, wR_2 (all data)	0.0485, 0.0859

Table 6: Crystallographic data for the solid state structure of $[\text{Rh}_2(\text{COD})_2(\text{L}_{\text{Ant}})][\text{BAR}^{\text{F}}_4]_2$ (**6**).

CCDC-798126

	$[\text{Rh}_2(\text{COD})_2(\text{L}_{\text{Ant}})][\text{BAR}^{\text{F}}_4]_2 \cdot 2.5 \text{ CH}_2\text{Cl}_2$ (6) $\cdot 2.5 \text{ CH}_2\text{Cl}_2$
Empirical formula	$\text{C}_{221}\text{H}_{150}\text{B}_4\text{Cl}_{10}\text{F}_{96}\text{N}_{16}\text{Rh}_4$
M (g mol^{-1})	5662.95
Crystal system	monoclinic
Space group	Cc
a (Å)	38.2718(4)
b (Å)	14.0298(1)
c (Å)	25.8175(3)
β (°)	121.802(2)
V (Å ³)	11781.5(3)
D_c (g cm^{-3})	1.596
Z	2
T (K)	200(2)
λ Mo- K_α (Å)	0.71073
μ Mo- K_α (mm^{-1})	0.520
Crystal size (mm)	0.44 x 0.31 x 0.23
T (Gaussian) _{min,max}	0.920, 0.865
$2\theta_{\text{max}}$ (°)	27.49
hkl range	$-49 \leq 49, -18 \leq 18, -32 \leq 33$
N	126307
N_{ind}	26439 (R_{merge} 0.0359)
$N_{\text{obs}}(I > 2\sigma(I))$	24447
GoF(all data)	1.046
$R_1, wR_2 [I > 2\sigma(I)]$	0.0414, 0.1077
R_1, wR_2 (all data)	0.0466, 0.1113

Table 7: Crystallographic data for the solid state structure of $[\text{Ir}(\text{COD})(\text{L}_m)]\text{BAr}^{\text{F}}_4$ (**15**).

CCDC-798125

	$[\text{Ir}(\text{COD})(\text{L}_m)]\text{BAr}^{\text{F}}_4$ (15)
Empirical formula	$\text{C}_{60}\text{H}_{42}\text{BF}_{24}\text{IrN}_8$
M (g mol^{-1})	1534.03
Crystal system	monoclinic
Space group	$P2_1/c$
a (Å)	13.2724(4)
b (Å)	25.0291(7)
c (Å)	19.2865(5)
β ($^\circ$)	108.476(1)
V (Å ³)	6076.7(3)
D_c (g.cm^{-3})	1.677
Z	4
T (K)	150(2)
λ Mo- K_α (Å)	0.71073
μ Mo- K_α (mm^{-1})	2.318
Crystal size (mm)	0.40 x 0.30 x 0.13
T (Gaussian) _{min,max}	0.7375, 0.5494
θ_{max} ($^\circ$)	27.00
hkl range	$-16 \leq h \leq 11, -30 \leq k \leq 30, -24 \leq l \leq 24$
N	53760
N_{ind}	12893 (R_{merge} 0.0314)
$N_{\text{obs}}(I > 2\sigma(I))$	10498
GoF(all data)	1.107
R_1, wR_2 [$I > 2\sigma(I)$]	0.0477, 0.1228
R_1, wR_2 (all data)	0.0646, 0.1281

Table 8: Crystallographic data for the solid state structure of $[\text{Ir}(\text{COD})(\text{L}_{\text{Ant}})]\text{BAr}^{\text{F}}_4$ (**22**).

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	$[\text{Ir}(\text{COD})(\text{L}_{\text{Ant}})]\text{BAr}^{\text{F}}_4$ (22)
Empirical formula	$\text{C}_{68}\text{H}_{46}\text{BF}_{24}\text{IrN}_8$
M (g mol^{-1})	1634.14
Crystal system	triclinic
Space group	$P-1$
a (Å)	14.0601(4)
b (Å)	14.2130(4)
c (Å)	17.9485(5)
α (°)	79.627(2)
β (°)	73.886(1)
γ (°)	70.046(1)
V (Å ³)	3224.48(16)
D_c (g cm^{-3})	1.683
Z	2
T (K)	150(2)
λ Mo-K α (Å)	0.71073
μ Mo-K α (mm^{-1})	2.190
Crystal size (mm)	0.55 x 0.40 x 0.28
T (Gaussian) _{min,max}	0.5444, 0.4435
θ_{max} (°)	32.00
hkl range	$-18 \leq 20, -21 \leq 20, -26 \leq 26$
N	75016
N_{ind}	22118 (R_{merge} 0.0283)
$N_{\text{obs}}(I > 2\sigma(I))$	18745
GoF(all data)	1.091
R_1, wR_2 [$I > 2\sigma(I)$]	0.0288, 0.0630
R_1, wR_2 (all data)	0.0433, 0.0666