Electronic Supplementary Information for Dalton Transactions

Functionalized phosphorus analogues of the β-diketiminato ligand systems: Bis(*N*-arylphosphinimino)acetonitrile-derived complexes of rhodium and iridium

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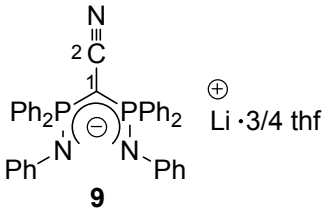
Supporting Informations

General

All reactions were carried out in an inert atmosphere (argon) in Schlenk-type glassware or in a glovebox. Solvents were dried and distilled under argon prior use. Bis(*N*-phenylimino-diphenylphosphoranyl)acetonitrile[1] was prepared using the known procedure. The following instruments were used for the physical characterization of the compounds. NMR: Bruker AC 200 P-FT (^{31}P: 81.0 MHz), Varian Inova 500 (^{1}H: 499.8 MHz, ^{13}C: 125.7 MHz), Unity Plus 600 (^{1}H: 599.9 MHz, ^{13}C: 150.8 MHz). Most NMR assignments were supported by additional 2D experiments. Melting points: DSC 2010 (TA-Instrument). IR: Varian 3100 FT-IR spectrometer.

Lithium[cyano-bis(*N*-phenylimino-diphenylphosphoranyl)methanide] (9)



9

A solution of bis(*N*-phenylimino-diphenylphosphoranyl)acetonitrile (**6**) (568 mg, 960 mmol) and lithiumdiisopropylamide (97 mg, 960 mmol) in tetrahydrofuran (60 ml) was stirred overnight at room temperature. The solvent was removed *in vacuo* and the residue washed with pentane (three times, 30 ml each). The solid light-yellow product was dried *in vacuo* (485 mg, 77%). Mp: 129.5 °C (DSC). Found: C, 74.79; H, 5.65; N, 6.23. Calc. for $C_{38}H_{30}LiN_3P_2 \cdot 3/4$ thf: C, 75.57; H, 5.57; N, 6.45%.

δ_H(499.8 MHz; d_6-DMSO; 298 K) 7.60 (m, 8H, *o*-Ph^P), 7.22 (m, 4H, *p*-Ph^P), 7.09 (m, 8H, *m*-Ph^P), 7.05 (m, 4H, *m*-Ph^N), 6.85 (m, 4H, *o*-Ph^N), 6.53 (m, 2H, *p*-Ph^N), 3.59 (m, 3H, α-THF), 1.75 (m, 3H, β-THF).

[1] L. Braun, G. Kehr, R. Fröhlich, G. Erker, *Inorg. Chim. Acta* **2007**, doi: 10.1016/j.ica.2007.02.028.

δ_C(125.7 MHz; d_6-DMSO; 298 K) 153.6 (s, *i*-Ph^N), 135.3 (pd, $^1J_{PC}$ + $^3J_{PC}$ = 117.9 Hz, *i*-Ph^P), 132.3 (m, *o*-Ph^P), 129.5 (s, *p*-Ph^P), 128.3 (m, C2), 128.1 (s, *m*-Ph^N), 127.0 (m, *m*-Ph^P), 123.6 (m, *o*-Ph^N), 114.4 (s, *p*-Ph^N), 67.0 (s, α-THF), 25.1 (s, β-THF), 18.0 (t, $^1J_{PC}$= 97.8 Hz, C1).

$\delta_{P\{1H\}}$(81.0 MHz; d_6-DMSO; 298 K) 4.8 (s, $\nu_{1/2}$ = 11.9 Hz).

δ_{Hirr} / δ_{Hres} (1D-TOCSY, 499.8 MHz, d_6-DMSO, 298 K) 7.60 / 7.22, 7.09 (*o*-Ph^P / *p*-Ph^P, *m*-Ph^P), 6.53 / 7.05, 6.85 (*p*-Ph^N / *m*-Ph^N, *o*-Ph^N).

δ_H / δ_H (GCOSY, 599.6 MHz / 599.6 MHz, d_6-DMSO, 298 K) 7.60 / 7.09 (*o*-Ph^P / *m*-Ph^P), 7.22 / 7.09 (*p*-Ph^P / *m*-Ph^P), 7.09 / 7.60, 7.22 (*m*-Ph^P / *o*-Ph^P, *p*-Ph^P), 7.05 / 6.85, 6.53 (*m*-Ph^N / *o*-Ph^N, *p*-Ph^N), 6.85 / 7.05 (*o*-Ph^N / *m*-Ph^N), 6.53 / 7.05 (*p*-Ph^N / *m*-Ph^N), 3.59 / 1.67 (α-THF / β-THF).

δ_H / δ_C (^{1}H,^{13}C-GHSQC, 499.8 MHz / 125.7 MHz, d_6-DMSO, 298 K) 7.60 / 132.3 (*o*-Ph^P), 7.22 / 129.5 (*p*-Ph^P), 7.09 / 127.0 (*m*-Ph^P), 7.05 / 128.1 (*m*-Ph^N), 6.85 / 123.6 (*o*-Ph^N), 6.53 / 114.4 (*p*-Ph^N), 3.59 / 67.0 (α-THF), 1.75 / 25.1 (β-THF).

δ_H / δ_C (^{1}H,^{13}C-GHMBC, 599.6 MHz / 150.7 MHz, d_6-DMSO, 298 K) 7.60 / 135.3, 132.3, 129.5, 127.0 (*o*-Ph^P / *i*-Ph^P, *o*-Ph^P, *p*-Ph^P, *m*-Ph^P), 7.22 / 132.3, 127.0 (*p*-Ph^P / *o*-Ph^P, *m*-Ph^P), 7.09 / 135.3, 132.3, 129.5, 127.0 (*p*-Ph^P / *i*-Ph^P, *o*-Ph^P, *p*-Ph^P, *m*-Ph^P), 7.05 / 153.6, 128.1 (*m*-Ph^N / *i*-Ph^N, *m*-Ph^N), 6.85 / 114.4 (*o*-Ph^N / *p*-Ph^N), 6.53 / 123.6, 128.1 (*p*-Ph^N / *o*-Ph^N, *m*-Ph^N)

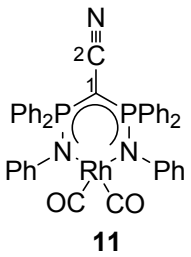
ν_{max}(KBr)/cm^{-1} 3054, 3006, 2972, 2873, 2159, 1590, 1483, 1436, 1288, 1262, 1205, 1179, 1106, 1036, 1012, 746, 717, 693.

General procedure for the synthesis of the complexes 11, 12, and 13

Either $[(CO)_2RhCl]_2$ (**10a**) or [(nbd)]$RhCl_2$ (**10b**) or [(cod)]$IrCl_2$ (**10c**) (93.3 µmol, 0.5 equiv.) was added to a suspension of lithium[cyano-bis(*N*-phenylimino-diphenylphosphoranyl)-methanide] (**9**) (186.6 µmol, 1.0 equiv.) in toluene (15 ml). The reaction mixture was stirred for 12 hours at room temperature. Subsequently the insoluble LiCl was removed by filtration, the solvent removed *in vacuo* and the solid washed with pentane (three times, 6 ml each). The resulting yellow solid was dried *in vacuo*.

Dicarbonyl[cyano-bis(*N*-phenylimino-diphenylphosphoranyl)methanide]rhodium(I) (11)

A mixture of the lithium salt **9** (118 mg, 186.6 µmol, 1.0 equiv.) and *µ*-dichlorotetracarbonyldirhodium (I) (**10a**) (36 mg, 93.3 µmol, 0.5 equiv.) in toluene (15 ml) formed the yellow, air-stable product **11** (90 mg, 64%). Single crystals were obtained from a



11

toluene/pentane mixture at −35 °C. Mp: > 200°C (DSC). Found: C, 63.30; H, 4.03; N, 5.13. Calc. for $C_{40}H_{30}N_3O_2P_2Rh$: C, 64.10; H, 4.03; N, 5.61%.

δ_H(499.8 MHz; CD_2Cl_2; 298 K) 7.71 (m, 8H, *o*-Ph^P), 7.48 (m, 4H, *p*-Ph^P), 7.33 (m, 8H, *m*-Ph^P), 7.12 (m, 4H, *o*-Ph^N), 7.02 (m, 4H, *m*-Ph^N), 6.84 (m, 2H, *p*-Ph^N).

δ_C(125.7 MHz; CD_2Cl_2; 298 K) 185.1 (d, $^1J_{RhC}$ = 69.9 Hz, Rh-CO), 152.0 (s, *i*-Ph^N), 133.2 (m, *o*-Ph^P), 132.3 (s, *p*-Ph^P), 129.2 (pd, $^1J_{PC} + {}^3J_{PC}$ = 95.1 Hz, *i*-Ph^P), 128.8 (m, *m*-Ph^P), 128.8 (s, *m*-Ph^N), 124.4 (m, *o*-Ph^N), 121.5 (s, *p*-Ph^N), 123.1 (t, $^2J_{PC}$ = 9.3 Hz, C2), 21.6 (t, $^1J_{PC}$ = 145.6 Hz, C1).

$\delta_{P\{1H\}}$(81.0 MHz; CD_2Cl_2; 298 K) 29.3 (s, $\nu_{1/2}$ = 2.3 Hz).

δ_{Hirr} / δ_{Hres} (1D-TOCSY, 499.8 MHz, CD_2Cl_2, 298 K) 7.48 / 7.71, 7.33 (*p*-Ph^P / *o*-Ph^P, *m*-Ph^P), 7.02 / 7.12, 6.84 (*m*-Ph^N / *o*-Ph^N, *p*-Ph^N).

δ_H / δ_H (GCOSY, 499.8 MHz / 499.8 MHz, CD_2Cl_2, 298 K) 7.71 / 7.33 (*o*-Ph^P / *m*-Ph^P), 7.48 / 7.33 (*p*-Ph^P / *m*-Ph^P), 7.33 / 7.71, 7.48 (*m*-Ph^P / *o*-Ph^P, *p*-Ph^P), 7.12 / 7.02 (*o*-Ph^N / *m*-Ph^N), 7.02 / 7.12, 6.84 (*m*-Ph^N / *o*-Ph^N, *p*-Ph^N), 6.84 / 7.02 (*p*-Ph^N / *m*-Ph^N).

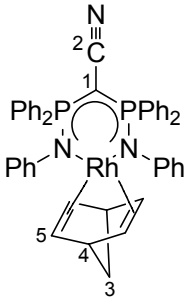
δ_H / δ_C (^{1}H,^{13}C-GHSQC, 499.8 MHz / 125.7 MHz, CD_2Cl_2, 298 K) 7.71 / 133.2 (*o*-Ph^P), 7.48 / 132.3 (*p*-Ph^P), 7.33 / 128.8 (*m*-Ph^P), 7.12 / 124.4 (*o*-Ph^N), 7.02 / 128.8 (*m*-Ph^N), 6.84 / 121.5 (*p*-Ph^N).

δ_H / δ_C (^{1}H,^{13}C-GHMBC, 499.8 MHz / 125.7 MHz, CD_2Cl_2, 298 K) 7.71 / 133.2, 132.3, 129.2, 128.8 (*o*-Ph^P / *o*-Ph^P, *p*-Ph^P, *i*-Ph^P, *m*-Ph^P), 7.48 / 133.2, 128.8 (*p*-Ph^P / *o*-Ph^P, *m*-Ph^P), 7.33 / 133.2, 132.3, 129.2, 128.8 (*m*-Ph^P / *o*-Ph^P, *p*-Ph^P, *i*-Ph^P, *m*-Ph^P), 7.12 / 128.8, 124.4, 121.5 (*o*-Ph^N / *m*-Ph^N, *o*-Ph^N, *p*-Ph^N), 7.02 / 152.0, 128.8 (*m*-Ph^N / *i*-Ph^N, *m*-Ph^N), 6.84 / 128.8, 124.4 (*p*-Ph^N / *m*-Ph^N, *o*-Ph^N).

ν_{max}(KBr)/cm^{-1} 3057, 2165, 2061, 1989, 1589, 1483, 1435, 1259, 1175, 1102, 1009, 989, 803, 721, 690.

Crystal data for $C_{40}H_{30}N_3O_2P_2Rh$, M = 749.52, monoclinic, space group $P2_1/c$ (No. 14), a = 9.8125(2), b = 20.4272(5), c = 17.5318(2) Å, β = 102.278(2)°, V = 3433.73(12) $Å^3$, D_c = 1.450 g cm^{-3}, μ = 0.631 mm^{-1}, Z = 4, λ = 0.71073 Å, T = 198(2) K, 22757 reflections collected (±h, ±k, ±l), [(sinθ)/λ] = 0.66 $Å^{-1}$, 8114 independent (R_{int} = 0.056), and 5740 observed reflections [I ≥ 2σ(I)], 433 refined parameters, R = 0.044, wR^2 = 0.100. CCDC.

Norbornadiene[cyano-bis(*N*-phenylimino-diphenylphosphoranyl)-methanide]-rhodium(I) (12)



12

A mixture of the lithium salt **9** (118 mg, 186.6 µmol, 1.0 equiv.) and μ-dichlorobis(norbornadiene)dirhodium(I) (**10b**) (43 mg, 93.3 µmol, 0.5 Äq.) in toluene (15 ml) formed the yellow, air-stable product **12** (109 mg, 74%). Single crystals of **12** suited for the X-ray crystal structure analysis were obtained from a toluene/pentane mixture at ─35 °C. Mp: > 200°C (DSC). Found: C, 68.11; H, 5.11; N, 5.14. Calc. for $C_{45}H_{38}N_3P_2Rh$: C, 68.79; H, 4.88; N, 5.35%.

δ_H(599.6 MHz; CD_2Cl_2; 298 K) 7.93 (m, 8H, *o*-Ph^P), 7.55 (m, 4H, *p*-Ph^P), 7.47 (m, 8H, *m*-Ph^P), 6.76 (m, 4H, *m*-Ph^N), 6.63 (m, 2H, *p*-Ph^N), 6.16 (m, 4H, *o*-Ph^N), 3.44 (m, 2H, 4-H), 2.78 (m, 4H, 5-H), 0.94 (m, 2H, 3-H).

δ_C(125.7 MHz; CD_2Cl_2; 298 K) 149.3 (s, *i*-Ph^N), 133.8 (m, *o*-Ph^P), 132.9 (pd, $^1J_{PC}$ + $^3J_{PC}$ = 102.4 Hz, *i*-Ph^P), 131.9 (s, *p*-Ph^P), 128.5 (m, *o*-Ph^N), 128.4 (m, *m*-Ph^P), 127.7 (s, *m*-Ph^N), 124.6 (t, $^2J_{PC}$ = 9.4 Hz, C2), 121.5 (s, *p*-Ph^N), 61.3 (d, $^3J_{RhC}$ = 7.0 Hz, C3), 52.5 (d, $^1J_{RhC}$ = 10.6 Hz, C5), 49.0 (d, $^2J_{RhC}$ = 2.8 Hz, C4), 25.3 (t, $^1J_{PC}$ = 136.5 Hz, C1).

$\delta_{P\{1H\}}$(81.0 MHz, CD_2Cl_2, 298 K) 29.4 (s, $\nu_{1/2}$ = 3.9 Hz).

δ_{Hirr} / δ_{Hres} (1D-TOCSY, 599.6 MHz, CD_2Cl_2, 298 K) 7.93 / 7.55, 7.47 (*o*-Ph^P / *p*-Ph^P, *m*-Ph^P), 6.76 / 6.63, 6.16 (*m*-Ph^N / *p*-Ph^N, *o*-Ph^N), 3.44 / 2.78, 0.94 (4-H / 5-H, 3-H).

δ_H / δ_H (GCOSY, 599.6 MHz, CD_2Cl_2, 298 K) 7.93 / 7.47 (*o*-Ph^P / *m*-Ph^P), 7.55 / 7.47 (*p*-Ph^P / *m*-Ph^P), 7.47 / 7.93, 7.55 (*m*-Ph^P / *o*-Ph^P, *p*-Ph^P), 6.76 / 6.63, 6.16 (*m*-Ph^N / *p*-Ph^N, *o*-Ph^N), 6.63 / 6.76 (*p*-Ph^N / *m*-Ph^N), 6.16 / 6.76 (*o*-Ph^N / *m*-Ph^N), 3.44 / 2.78, 0.94 (4-H / 5-H, 3-H), 2.78 / 3.44 (5-H / 4-H), 0.94 / 3.44 (3-H / 4-H).

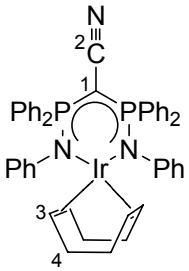
δ_H / δ_C (^{1}H,^{13}C-GHSQC, 599.6 MHz / 150.8 MHz, CD_2Cl_2, 298 K) 7.93 / 133.8 (*o*-Ph^P), 7.55 / 131.9 (*p*-Ph^P), 7.47 / 128.4 (*m*-Ph^P), 6.76 / 127.7 (*m*-Ph^N), 6.63 / 121.5 (*p*-Ph^N), 6.16 / 128.5 (*o*-Ph^N), 3.44 / 49.0 (4-H / C4), 2.78 / 52.5 (5-H / C5), 0.94 / 61.3 (3-H / C3).

δ_H / δ_C (^{1}H,^{13}C-GHMBC, 599.6 MHz / 150.8 MHz, CD_2Cl_2, 298 K) 7.93 / 133.8, 132.9, 131.9, 128.4 (*o*-Ph^P / *o*-Ph^P, *i*-Ph^P, *p*-Ph^P, *m*-Ph^P), 7.55 / 133.8, 132.7, 128.4 (*p*-Ph^P / *o*-Ph^P, *i*-Ph^P, *m*-Ph^P), 7.47 / 133.8, 132.9, 128.4 (*m*-Ph^P / *o*-Ph^P, *i*-Ph^P, *m*-Ph^P), 6.76 / 149.3, 128.5, 127.7, 121.5 (*m*-Ph^N / *i*-Ph^N, *o*-Ph^N, *m*-Ph^N, *p*-Ph^N), 6.63 / 128.5, 127.7 (*p*-Ph^N / *o*-Ph^N, *m*-Ph^N), 6.16 / 149.3, 128.5, 127.7, 121.5 (*m*-Ph^N / *i*-Ph^N, *o*-Ph^N, *m*-Ph^N, *p*-Ph^N), 2.78 / 61.3, 52.5, 49.0 (5-H / C3, C5, C4), 0.94 / 52.5, 49.0 (3-H / C5, C4).

ν_{max}(KBr)/cm^{-1} 3054, 3003, 2953, 2908, 2851, 2148, 1588, 1482, 1435, 1257, 1233, 1196, 1107, 1010, 986, 803, 745, 668.

Crystal data for $C_{45}H_{38}N_3P_2Rh \cdot C_7H_8$, M = 877.77, monoclinic, space group $P2_1/c$ (No. 14), a = 9.9780(1), b = 20.7312(3), c = 41.3429(7) Å, β = 91.050(1)°, V = 8550.6(2) Å^3, D_c = 1.364 g cm^{-3}, μ = 4.237 mm^{-1}, Z = 8, λ = 1.54178 Å, T = 223(2) K, 78803 reflections collected (±h, ±k, ±l), [(sinθ)/λ] = 0.60 Å^{-1}, 15282 independent (R_{int} = 0.128), and 10879 observed reflections [I ≥ 2σ(I)], 1018 refined parameters, R = 0.063, wR^2 = 0.165. CCDC.

Cyclooctadiene[cyano-bis(*N*-phenylimino-diphenylphosphoranyl)methanide]iridium(I) (13)



13

Reaction of the lithium salt **9** (120 mg, 186.6 μmol, 1.0 equiv.) and μ-dichlorobis(1,5-cyclooctadiene)diiridium(I) (**10c**) (63 mg, 93.3 μmol, 0.5 equiv.) in toluene (15 ml) yielded the yellow, air-stable product **13** (110 mg, 66%). Single crystals were obtained from a toluene/pentane mixture at ─35 °C. Mp: > 200°C (DSC). Found: C, 61.42; H, 4.92; N, 4.22. Calc. for $C_{46}H_{42}IrN_3P_2$: C, 62.01; H, 4.75; N, 4.72%.

δ_H(499.8 MHz; CD_2Cl_2; 298 K) 7.84 (m, 8H, *o*-Ph^P), 7.55 (m, 4H, *p*-Ph^P), 7.44 (m, 8H, *m*-Ph^P), 6.75 (m, 4H, *m*-Ph^N), 6.68 (m, 2H, *p*-Ph^N), 6.12 (m, 4H, *o*-Ph^N), 2.95 (m, 4H, 3-H), 2.00 (m, 4H, 4-H), 1.24 (m, 4H, 4'-H).

δ_C(125.7 MHz; CD_2Cl_2; 298 K) 148.4 (s, *i*-Ph^N), 134.2 (m, *o*-Ph^P), 132.9 (pd, $^1J_{PC}$ + $^3J_{PC}$ = 104.8 Hz, *i*-Ph^P), 132.2 (s, *p*-Ph^P), 129.9 (m, *o*-Ph^N), 128.5 (m, *m*-Ph^P), 127.5 (s, *m*-Ph^N), 122.5 (s, *p*-Ph^N), 124.1 (t, $^2J_{PC}$ = 7.9 Hz, C2), 60.4 (s, C3), 31.1 (s, C4), 24.6 (t, $^1J_{PC}$ = 130.7 Hz, C1).

$\delta_{P\{1H\}}$(81.0 MHz; CD_2Cl_2; 298 K) 32.0 (s, $\nu_{1/2}$ = 1.9 Hz).

δ_{Hirr} / δ_{Hres} (1D-TOCSY, 499.8 MHz, CD_2Cl_2, 298 K) 7.55 / 7.84, 7.44 (*p*-Ph^P / *o*-Ph^P, *m*-Ph^P), 6.68 / 6.75, 6.12 (*p*-Ph^N / *m*-Ph^N, *o*-Ph^N), 1.24 / 2.95, 2.00 (4'-H / 3-H, 4-H).

δ_H / δ_H (GCOSY, 499.8 MHz, CD_2Cl_2, 298 K) 7.84 / 7.44 (*o*-Ph^P / *m*-Ph^P), 7.55 / 7.44 (*p*-Ph^P / *m*-Ph^P), 7.44 / 7.84, 7.55 (*m*-Ph^P / *o*-Ph^P, *p*-Ph^P), 6.75 / 6.68, 6.12 (*m*-Ph^N / *p*-Ph^N, *o*-Ph^N), 6.68 / 6.75 (*p*-Ph^N / *m*-Ph^N), 6.12 / 6.75 (*o*-Ph^N / *m*-Ph^N), 2.95 / 2.00, 1.24 (3-H / 4-H, 4'-H), 2.00 / 2.95, 1.24 (4-H / 3-H, 4'-H), 1.24 / 2.95, 1.24 (4'-H / 3-H, 4-H).

δ_H / δ_C (^{1}H,^{13}C-GHSQC, 499.8 MHz / 125.7 MHz, CD_2Cl_2, 298 K) 7.84 / 134.2 (*o*-Ph^P), 7.55 / 132.2 (*p*-Ph^P), 7.44 / 128.5 (*m*-Ph^P), 6.75 / 127.5 (*m*-Ph^N), 6.68 / 122.5 (*p*-Ph^N), 6.12 / 129.9 (*o*-Ph^N), 2.95 / 60.4 (3-H / C3), 2.00 / 31.1 (4-H / C4), 1.24 / 31.1 (4'-H / C4).

δ_H / δ_C (^{1}H,^{13}C-GHMBC, 499.8 MHz / 125.7 MHz, CD_2Cl_2, 298 K) 7.84 / 134.2, 132.9, 132.2 (*o*-Ph^P / *o*-Ph^P, *i*-Ph^P, *p*-Ph^P), 7.55 / 134.2 (*p*-Ph^P / *o*-Ph^P), 7.44 / 134.2, 132.9, 132.2, 128.5 (*m*-Ph^P / *o*-Ph^P, *i*-Ph^P, *p*-Ph^P, *m*-Ph^P), 6.75 / 148.4, 127.5 (*m*-Ph^N / *i*-Ph^N, *m*-Ph^N), 6.68 / 129.9

(*p*-Ph^N / *o*-Ph^N), 6.12 / 148.4, 129.9, 122.5 (*m*-Ph^N / *i*-Ph^N, *o*-Ph^N, *p*-Ph^N), 2.95 / 31.1 (3-H / C4), 2.00 / 60.4, 31.1 (4-H / C3, C4), 1.24 / 60.4, 31.1 (4'-H / C3, C4).

ν_{max}(KBr)/cm^{-1} 3052, 2911, 2878, 2830, 2154, 1588, 1482, 1436, 1231, 1206, 1108, 1012, 982, 808, 748, 693.

Crystal data for $C_{46}H_{42}IrN_3P_2$ * C_7H_8, M = 983.10, monoclinic, space group $P2_1/c$ (No. 14), a = 19.7081(2), b = 11.3012(1), c = 21.4893(2) Å, β = 111.446(1)°, V = 4454.82(7) Å^3, D_c = 1.466 g cm^{-3}, μ = 3.108 mm^{-1}, Z = 4, λ = 0.71073 Å, T = 223(2) K, 41726 reflections collected (±h, ±k, ±l), [(sinθ)/λ] = 0.66 Å^{-1}, 10575 independent (R_{int} = 0.053), and 8671 observed reflections [I ≥ 2σ(I)], 533 refined parameters, R = 0.029, wR^2 = 0.072.