

Supporting Information

Table S1. Amount of reagent used and product formed for reaction scheme 1.

Table S2. Amounts of reagents used and product formed for aerial oxidation, protonation and deprotonation reactions.

Table S3. ESI, hi-resolution MS data and elemental analysis for **4-7**.

Table S4. ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR data for **4-7**.

Table S5. Crystal and refinement data for **4c.Cl**, **4c'**, **5e.Cl**, **5g.Cl**, **6b** and **7e**.

Figure S1. Computationally optimised geometry for intermediates **A-C**, **4** and **4'**.

Table S1

Aminopyridine	Amount (mg)	Alkyne	Product	Yield (mg, (%))
2-NH ₂ -pyridine	10.0	tBuCCH (125 μ l)	C ₂₁ H ₃₁ Cl ₂ IrN ₂ , 4a	45.0 (80)
5-Br-2-NH ₂ -pyridine	17.5	tBuCCH (125 μ l)	C ₂₁ H ₃₀ BrCl ₂ IrN ₂ , 4b	47.1 (76)
6-Br-2-NH ₂ -pyridine	17.5	tBuCCH (125 μ l)	C ₂₁ H ₃₀ BrCl ₂ IrN ₂ , 4c	50.7 (82)
6-CH ₃ -2-NH ₂ -pyridine	11.5	tBuCCH (125 μ l)	C ₂₂ H ₃₃ Cl ₂ IrN ₂ , 4d	34.0 (59)
6-Br-2-NH ₂ -pyridine	17.5	PhCCH (110 μ l)	C ₂₃ H ₂₆ BrCl ₂ IrN ₂ , 4e	50.8 (79)
6-Br-2-NH ₂ -pyridine	17.5	4-BrC ₆ H ₄ CCH (180 mg)	C ₂₃ H ₂₅ Br ₂ Cl ₂ IrN ₂ , 4f	49.6 (69)
6-Br-2-NH ₂ -pyridine	17.5	4-CH ₃ C ₆ H ₄ CCH (125 μ l)	C ₂₄ H ₂₈ BrCl ₂ IrN ₂ , 4g	42.0 (64)

All reactions were carried out with **1** (40 mg, 50 μ mol), aminopyridines (100 μ mol) and alkynes (1 mmol).

Table S2

Compound	Amount (mg, μmol)	Reagent	Amount (μl, μmol)	Product	Yield (mg, (%))
6c	20 (32.5)	$\text{HBF}_4 \cdot \text{OEt}_2$	5 (39)	4c.BF₄	22.0 (96)
4e.Cl	20 (29.7)	-	-	5e.Cl	15.1 (74)
4g.Cl	20 (29.7)	-	-	5g.Cl	16.9 (83)
4a.Cl	20 (34.8)	Triethylamine	6 (41.8)	6a	17.0 (91)
4b.Cl	22.7 (34.8)	Triethylamine	6 (41.8)	6b	19.9 (93)
4c.Cl	22.7 (34.8)	Triethylamine	6 (41.8)	6c	20.0 (94)
5e.Cl	23.9 (34.8)	Triethylamine	6 (41.8)	7e	20.3 (90)
5g.Cl	24.4 (34.8)	Triethylamine	6 (41.8)	7g	21.2 (92)

Table S3

Product	Melting point, °C (dec with melting)	ESI-MS [†]	HRMS (Found (calc))	Elemental analysis Found (calc)
C ₂₁ H ₃₁ Cl ₂ IrN ₂ , 4a.Cl	268-270	539 [M] ⁺	540.1882 (540.1883)	C: 43.79; H: 5.35; N: 4.53 (C: 43.90; H: 5.44; N: 4.88)
C ₂₁ H ₃₀ BrCl ₂ IrN ₂ , 4b.Cl	197-199	617 [M] ⁺	618.0958 (618.0988)	C: 38.32; H: 4.49; N: 4.02 (C: 38.60; H: 4.63; N: 4.29)
C ₂₁ H ₃₀ BrCl ₂ IrN ₂ , 4c.Cl	214-216	617 [M] ⁺	618.0980 (618.0988)	C: 38.41; H: 4.52; N: 4.12 (C: 38.60; H: 4.63; N: 4.29)
C ₂₁ H ₃₀ BrClIrN ₂ BF ₄ , 4c.BF₄	240-242	539 [M] ⁺	618.0972 (618.0988)	-
C ₂₂ H ₃₃ Cl ₂ IrN ₂ , 4d.Cl	195-196	553 [M] ⁺	554.2029 (554.2040)	-
C ₂₃ H ₂₆ BrCl ₂ IrN ₂ , 4e.Cl	238-240	637 [M] ⁺	638.0676 (638.0676)	-
C ₂₃ H ₂₅ Br ₂ Cl ₂ IrN ₂ , 4f.Cl	224-226	717 [M] ⁺	719.9765 (719.9740)	-
C ₂₄ H ₂₈ BrCl ₂ IrN ₂ , 4g.Cl	231-233	651 [M] ⁺	652.0811 (652.0832)	-
C ₂₃ H ₂₄ BrCl ₂ IrN ₂ O, 5e.Cl	248-250	651 [M] ⁺	652.0441 (652.0468)	C: 40.37; H: 3.19; N: 3.77 (C: 40.18; H: 3.52; N: 4.07)
C ₂₄ H ₂₆ BrCl ₂ IrN ₂ O, 5g.Cl	230-232	665 [M] ⁺	666.0662 (666.0625)	C: 41.36; H: 4.01; N: 3.76 (C: 41.09; H: 3.74; N: 3.99)
C ₂₁ H ₃₀ ClIrN ₂ , 6a	191-193	539 [M+H] ⁺	504.2111 (504.2117)	C: 46.72; H: 5.39; N: 5.01 (C: 46.87; H: 5.62; N: 5.21)
C ₂₁ H ₂₉ BrClIrN ₂ , 6b	198-200	617 [M+H] ⁺	582.1206 (582.1222)	C: 40.81; H: 4.56; N: 4.43 (C: 40.88; H: 4.74; N: 4.54)
C ₂₁ H ₂₉ BrClIrN ₂ , 6c	201-203	617 [M+H] ⁺	582.1208 (582.1222)	-
C ₂₃ H ₂₃ BrClIrN ₂ O, 7e	228-230	651 [M+H] ⁺	616.0673 (616.0701)	-
C ₂₄ H ₂₅ BrClIrN ₂ O, 7g	224-226	665 [M+H] ⁺	630.0828 (630.0858)	-

[†] M = Complex cation for ionic products.

Table S4

4a.Cl	1.17 (s, 9H, ^t Bu), 1.70 (s, 15H, Cp*), 3.51 (d, ² J _{HH} = 10.6 Hz, 1H, CH ₂), 3.65 (d, 1H, CH ₂), 7.35 (t, ³ J _{HH} = 6.4 Hz, 1H, aromatic), 7.85 (t, ³ J _{HH} = 7.6 Hz, 1H, aromatic), 8.25 (d, ³ J = 5.5 Hz, 1H, aromatic), 8.55 (d, ³ J _{HH} = 8.2 Hz, 1H, aromatic).	9.47 (CH ₃ , Cp*), 31.08 (CH ₃ , ^t Bu), 37.22 (C, ^t Bu), 58.14 (CH ₂), 95.49 (C, Cp*), 116.52, 123.13, 141.29, 148.99 and 158.72 (C, aromatic), 241.51 (Ir=C).
4b.Cl	1.19 (s, 9H, ^t Bu), 1.73 (s, 15H, Cp*), 3.52 (d, ² J _{HH} = 10.5 Hz, 1H, CH ₂), 3.65 (d, 1H, CH ₂), 7.96 (d, ³ J _{HH} = 7.8 Hz, 1H, aromatic), 8.27 (s, 1H, aromatic), 8.56 (d, ³ J _{HH} = 8.7 Hz, 1H, aromatic).	9.52 (CH ₃ , Cp*), 31.16 (CH ₃ , ^t Bu), 37.53 (C, ^t Bu), 58.49 (CH ₂), 95.82 (C, Cp*), 117.27, 117.51, 143.97, 149.15 and 157.73 (C, aromatic), 242.39 (Ir=C).
4c.Cl	1.17 (s, 9H, ^t Bu), 1.72 (s, 15H, Cp*), 3.57 (d, ² J _{HH} = 10.5 Hz, 1H, CH ₂), 3.79 (d, 1H, CH ₂), 7.68 (m, 2H, aromatic), 8.62 (d, ³ J _{HH} = 5.0 Hz, 1H, aromatic).	10.76 (CH ₃ , Cp*), 31.18 (CH ₃ , ^t Bu), 37.71 (C, ^t Bu), 57.61 (CH ₂), 96.83 (C, Cp*), 114.81, 127.41, 142.24, 144.04 and 159.21 (C, aromatic), 242.31 (Ir=C).
4d.Cl	1.18 (s, 9H, ^t Bu), 1.70 (s, 15H, Cp*), 2.96 (s, 3H, CH ₃), 3.58 (d, ² J _{HH} = 10.5 Hz, 1H, CH ₂), 3.84 (d, 1H, CH ₂), 7.28 (d, ³ J _{HH} = 7.3 Hz, 1H, aromatic), 7.7 (t, ³ J _{HH} = 7.3 Hz, 1H, aromatic), 8.43 (d, ³ J _{HH} = 7.3 Hz, 1H, aromatic).	10.32 (CH ₃ , Cp*), 26.61 (CH ₃), 31.21 (CH ₃ , ^t Bu), 37.46 (C, ^t Bu), 57.66 (CH ₂), 95.65 (C, Cp*), 113.80, 122.23, 141.00, 145.57 and 160.44 (C, aromatic), 239.78 (Ir=C).
4e.Cl	1.74 (s, 15H, Cp*), 4.81 (d, ² J _{HH} = 13.3 Hz, 1H, CH ₂), 5.20 (d, 1H, CH ₂), 7.18 (t, ³ J _{HH} = 7.3 Hz, 1H, aromatic), 7.24-7.28 (m, 2H, aromatic), 7.53 (d, ³ J _{HH} = 7.8 Hz, 2H, aromatic), 7.60-7.64 (m, 2H, aromatic), 8.58 (d, ³ J _{HH} = 7.8 Hz, 1H, aromatic).	10.66 (CH ₃ , Cp*), 51.90 (CH ₂), 96.94 (C, Cp*), 115.18, 127.11, 127.69, 128.69, 130.92, 132.75, 142.04, 144.18 and 159.87 (C, aromatic), 237.91 (Ir=C).
4f.Cl	1.76 (s, 15H, Cp*), 4.77 (d, ² J _{HH} = 12.8 Hz, 1H, CH ₂), 5.16 (d, 1H, CH ₂), 7.38 (d, ³ J _{HH} = 8.2 Hz, 2H, aromatic), 7.47 (d, ³ J _{HH} = 8.2 Hz, 2H, aromatic), 7.62-7.66 (m, 2H, aromatic), 8.53 (d, ³ J _{HH} = 7.4 Hz, 1H, aromatic).	10.73 (CH ₃ , Cp*), 51.11 (CH ₂), 97.06 (C, Cp*), 115.13, 121.97, 127.25, 131.68, 131.77, 132.70, 142.17, 144.28 and 159.81 (C, aromatic), 237.08 (Ir=C).
4g.Cl	1.75 (s, 15H, Cp*), 2.23 (s, 3H, CH ₃), 4.81 (d, ² J _{HH} = 13.3 Hz, 1H, CH ₂), 5.13 (d, 1H, CH ₂), 7.06 (d, ³ J _{HH} = 7.8 Hz, 2H, aromatic), 7.43 (d, ³ J _{HH} = 8.2 Hz, 2H, aromatic), 7.59-7.64 (m, 2H, aromatic), 8.56 (d, ³ J _{HH} = 7.3 Hz, 1H, aromatic).	10.67 (CH ₃ , Cp*), 21.30 (CH ₃), 51.62 (CH ₂), 96.89 (C, Cp*), 115.09, 127.01, 129.37, 129.58, 130.77, 137.23, 142.01, 144.14 and 159.88 (C, aromatic), 238.17 (Ir=C).
4c. BF₄	1.13 (s, 9H, ^t Bu), 1.75 (s, 15H, Cp*), 3.33 (d, ² J _{HH} = 11.5 Hz, 1H, CH ₂), 3.72 (d, 1H, CH ₂), 7.70 (d, ³ J _{HH} = 8.0 Hz, 1H, aromatic), 7.77 (t, ³ J _{HH} = 8.0 Hz, 1H, aromatic), 8.06 (d, ³ J _{HH} = 8.0 Hz, 1H, aromatic).	10.58 (CH ₃ , Cp*), 31.08 (CH ₃ , ^t Bu), 37.79 (C, ^t Bu), 58.96 (CH ₂), 97.54 (C, Cp*), 113.69, 127.68, 142.97, 144.54 and 158.01 (C, aromatic), 244.37 (Ir=C).

Table S4 (continued)

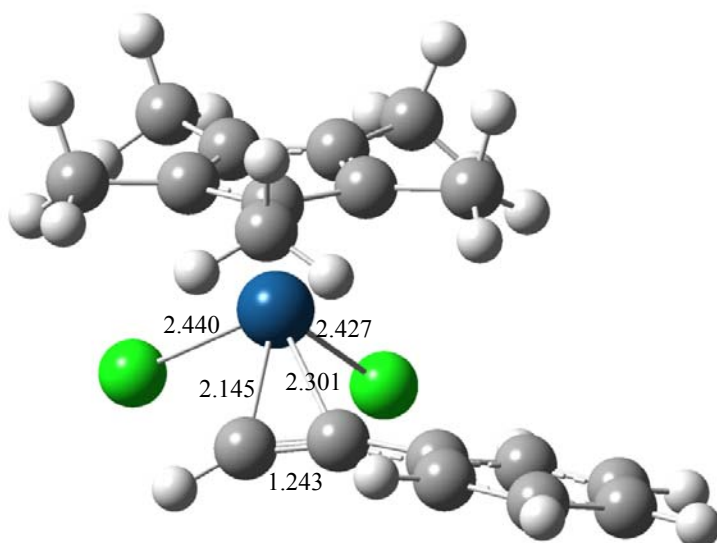
5e.Cl	1.67 (s, 15H, Cp*), 7.48 (t, $^3J_{\text{HH}} = 7.6$ Hz, 2H, aromatic), 7.61 (t, $^3J_{\text{HH}} = 7.3$ Hz, 1H, aromatic), 7.76-7.79 (m, 2H, aromatic), 8.17 (d, $^3J_{\text{HH}} = 7.8$ Hz, 2H, aromatic), 8.77 ((d, $^3J_{\text{HH}} = 6.9$ Hz, 1H, aromatic).	10.16 (CH ₃ , Cp*), 98.00 (C, Cp*), 116.93, 128.46, 129.28, 130.67, 133.57, 135.51, 142.53 and 144.62, 159.66 (C, aromatic), 193.95 (C=O), 231.26 (Ir=C).
5g.Cl	1.66 (s, 15H, Cp*), 2.39 (s, 3H, CH ₃), 7.27 (d, $^3J_{\text{HH}} = 6.4$ Hz, 2H, aromatic), 7.75-7.83 (m, 2H, aromatic), 8.05 (d, $^3J_{\text{HH}} = 7.8$ Hz, 2H, aromatic), 8.76 (d, $^3J_{\text{HH}} = 5.0$ Hz 1H, aromatic).	10.20 (CH ₃ , Cp*), 22.27 (CH ₃), 97.94 (C, Cp*), 116.84, 128.43, 130.01, 130.74, 131.21, 142.49, 144.63 and 146.80, 159.68 (C, aromatic), 193.46 (C=O), 231.54 (Ir=C).
6a	1.17 (s, 9H, ^t Bu), 1.69 (s, 15H, Cp*), 3.16 (d, $^2J_{\text{HH}} = 16.0$ Hz, 1H, CH ₂), 3.32 (d, 1H, CH ₂), 6.91 (t, $^3J_{\text{HH}} = 6.4$ Hz, 1H, aromatic), 7.59 (t, $^3J_{\text{HH}} = 8.0$ Hz, 1H, aromatic), 7.68 (d, $^3J_{\text{HH}} = 7.8$ Hz, 1H, aromatic), 8.29 (d, $^3J_{\text{HH}} = 5.9$ Hz, 1H, aromatic).	9.32 (CH ₃ , Cp*), 30.81 (CH ₃ , ^t Bu), 33.84 (C, ^t Bu), 61.92 (CH ₂), 91.08 (C, Cp*), 118.34, 118.89, 138.98, 148.08 and 173.94 (C, aromatic), 231.16 (Ir=C).
6b	1.16 (s, 9H, ^t Bu), 1.69 (s, 15H, Cp*), 3.14 (d, $^2J_{\text{HH}} = 16.0$ Hz, 1H, CH ₂), 3.29 (d, 1H, CH ₂), 7.55 (d, $^3J_{\text{HH}} = 8.7$ Hz, 1H, aromatic), 7.68 (d, $^3J_{\text{HH}} = 9.2$ Hz, 1H, aromatic), 8.34 (s, 1H, aromatic).	9.31 (CH ₃ , Cp*), 30.77 (CH ₃ , ^t Bu), 33.74 (C, ^t Bu), 62.17 (CH ₂), 91.33 (C, Cp*), 112.24, 119.13, 141.50, 148.31 and 173.26 (C, aromatic), 237.76 (Ir=C).
6c	1.13 (s, 9H, ^t Bu), 1.66 (s, 15H, Cp*), 3.19 (d, $^2J_{\text{HH}} = 16.9$ Hz, 1H, CH ₂), 3.34 (d, 1H, CH ₂), 7.22 (d, $^3J_{\text{HH}} = 7.3$ Hz, 1H, aromatic), 7.37 (t, $^3J_{\text{HH}} = 7.8$ Hz, 1H, aromatic), 7.53 (d, $^3J_{\text{HH}} = 8.2$ Hz, 1H, aromatic).	10.36 (CH ₃ , Cp*), 30.67 (CH ₃ , ^t Bu), 33.54 (C, ^t Bu), 61.97 (CH ₂), 92.03 (C, Cp*), 116.25, 122.14, 139.49, 142.08 and 173.99 (C, aromatic), 233.53 (Ir=C).
7e	1.63 (s, 15H, Cp*), 7.40-7.54 (m, 5H, aromatic), 7.77 (d, $^3J_{\text{HH}} = 7.8$ Hz, 1H, aromatic), 8.24 (d, $^3J_{\text{HH}} = 8.24$ Hz, 2H, aromatic).	10.05 (CH ₃ , Cp*), 93.59 (C, Cp*), 118.38, 124.70, 128.54, 130.80, 133.73, 134.43, 140.58, 142.84, 173.51 (C, aromatic), 198.95 (C=O), 226.19 (Ir=C).
7g	1.63 (s, 15H, Cp*), 2.37 (s, 3H, CH ₃), 7.22 (d, $^3J_{\text{HH}} = 7.8$ Hz, 2H, aromatic), 7.43-7.51 (m, 2H, aromatic), 7.76 (d, $^3J_{\text{HH}} = 7.8$ Hz, 2H, aromatic), 8.12 (d, $^3J_{\text{HH}} = 8.2$ Hz 1H, aromatic).	10.03 (CH ₃ , Cp*), 22.07 (CH ₃), 93.54 (C, Cp*), 118.33, 124.62, 129.29, 130.90, 132.00, 140.54, 142.82, 144.57 and 173.58 (C, aromatic), 198.69 (C=O), 226.53 (Ir=C).

Table S5

Identification code	4c.Cl	4c.BF₄	5e.Cl	5g.Cl	6b	7e
Empirical formula	C ₂₃ H ₃₄ BrCl ₆ Ir N ₂	C ₂₁ H ₂₉ BBrClF ₄ Ir N ₂	C ₂₅ H ₂₇ BrCl ₅ Ir N ₂ O	C ₂₆ H ₃₀ BrCl ₆ Ir N ₂ O	C ₂₁ H ₂₉ BrClIr N ₂	C ₂₃ H ₂₃ BrClIr N ₂ O
Formula weight	823.33	703.83	814.84	850.10	617.02	650.99
Temperature, K	103(2)	296(2)	103(2)	103(2)	296(2)	103(2)
Crystal system	Monoclinic	orthorhombic	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	P2(1)/c	Pbca	P2(1)/c	P2(1)/c	P-1	P2(1)/n
a, Å	17.1605(7)	13.5702(11)	9.6911(4)	9.4513(2)	8.0767(5)	15.1691(7)
b, Å	10.9386(3)	13.1705(10)	22.7375(7)	22.3781(5)	11.9633(9)	9.8575(3)
c, Å	15.6735(6)	27.7649(18)	27.3923(8)	29.0848(6)	12.6252(9)	16.1962(6)
β, deg	96.499(10)	90.0	95.046(10)	92.5970(10)	96.291(4)	117.412(10)
Volume, Å ³	2923.19(18)	4964.0(6)	6012.4(4)	6145.2(2)	1129.83(14)	2149.88(9)
Z	4	8	8	8	2	4
Density(calc) Mg/m ³	1.871	1.884	1.800	1.838	1.814	2.011
Abs coefficient, mm ⁻¹	6.499	7.138	6.235	6.147	7.802	8.210
F(000)	1600	2712	3144	3292	596	1248
Crystal size, mm ³	0.30 x 0.20 x 0.12	0.30 x 0.30 x 0.20	0.40 x 0.14 x 0.02	0.20 x 0.20 x 0.10	0.40 x 0.22 x 0.20	0.12 x 0.08 x 0.06
Reflections collected	35751	47498	91092	64543	22240	31091
Independent reflections	5966 [R(int) = 0.0374]	5072 [R(int) = 0.0624]	12236 [R(int) = 0.0636]	15631 [R(int) = 0.0937]	6855 [R(int) = 0.0565]	4389 [R(int) = 0.0457]
Completeness (to θ, deg)	99.7 % (26.37°)	99.9 % (26.37°)	99.7 % (26.37°)	98.7 % (28.66°)	99.0 % (30.56°)	99.9 % (26.37°)
Max. and min. transmission	0.5093 and 0.2459	0.3294 and 0.2233	0.8854 and 0.1894	0.5785 and 0.3728	0.3044 and 0.1464	0.6386 and 0.4391
Data / restraints / parameters	5966/6/306	5072/316/300	12236/54/662	15631/0/679	6855/669/373	4389/0/268
Goodness-of-fit on F ²	1.191	1.125	1.108	1.019	1.046	1.131
Final R indices [I>2σ(I)]	R1 = 0.0518, wR2 = 0.1252	R1 = 0.0404, wR2 = 0.1067	R1 = 0.0497, wR2 = 0.1081	R1 = 0.0479, wR2 = 0.1019	R1 = 0.0420, wR2 = 0.1003	R1 = 0.0278, wR2 = 0.0769
R indices (all data)	R1 = 0.0600, wR2 = 0.1287	R1 = 0.0711, wR2 = 0.1362	R1 = 0.0790, wR2 = 0.1287	R1 = 0.1105, wR2 = 0.1296	R1 = 0.0820, wR2 = 0.1360	R1 = 0.0387, wR2 = 0.0847
Largest diff. peak and hole, e.Å ⁻³	4.146 and -3.269	1.775 and -1.817	3.294 and -2.815	1.850 and -2.025	1.113 and -1.983	2.485 and -1.568

Figure S1

Intermediate A



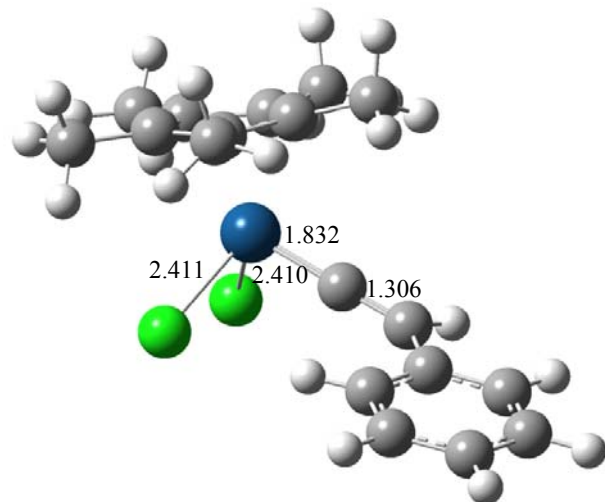
Charge = 0 Multiplicity = 1

C	0.18362	1.12672	1.42909
C	1.33267	0.36041	1.84623
C	1.90833	1.53552	-0.08873
C	0.56657	1.89293	0.25703
C	-0.26274	2.94673	-0.40226
H	-1.32681	2.72765	-0.32455
H	-0.08498	3.91332	0.07984
H	-0.01702	3.04801	-1.45872
C	2.75968	2.13966	-1.1581
H	2.15773	2.66351	-1.8998
H	3.45832	2.86126	-0.72217
H	3.33685	1.3733	-1.67597
C	1.37939	-0.51955	3.05044
H	2.22002	-1.20932	3.01157
H	1.48006	0.09402	3.95185
H	0.47004	-1.11355	3.13766
C	-1.06902	1.29147	2.22897
H	-1.36495	0.35455	2.70004
H	-0.91375	2.03088	3.02206
H	-1.90244	1.63031	1.61593
Cl	-0.05074	-2.44423	0.46553
C	2.37789	0.57768	0.90901
C	3.7593	0.01294	0.96099
H	4.44456	0.74789	1.39621

H	3.80175	-0.89191	1.56489
H	4.11259	-0.24135	-0.03768
C	-0.54564	-0.18557	-2.03413
H	-0.14734	-0.29763	-3.02187
C	-1.4595	-0.18762	-1.19184
Cl	2.16429	-1.371	-1.76494
C	-2.78262	-0.11669	-0.63314
C	-3.24669	-1.04235	0.31179
C	-3.64941	0.89213	-1.08584
C	-4.54762	-0.95467	0.78701
H	-2.57623	-1.82137	0.64932
C	-4.95	0.96791	-0.6057
H	-3.29774	1.60352	-1.82285
C	-5.40289	0.0468	0.334
H	-4.89892	-1.6795	1.51181
H	-5.61093	1.74621	-0.96834
H	-6.41818	0.10621	0.70754
Ir	0.63687	-0.22719	-0.24436

Sum of electronic and zero-point Energies= -1723.639580
Sum of electronic and thermal Energies= -1723.614654
Sum of electronic and thermal Enthalpies= -1723.613710
Sum of electronic and thermal Free Energies= -1723.694810

Intermediate B



Charge = 0 Multiplicity = 1

C	3.13163	0.13204	0.42008
C	2.72693	1.21691	-0.39726
C	1.29805	1.18613	1.5018
C	2.20951	0.04888	1.5774
C	2.39241	-0.89172	2.73544
H	2.60264	-1.9064	2.38143
H	3.23293	-0.57003	3.36781
H	1.49681	-0.93802	3.36327
C	0.34427	1.63624	2.5725
H	-0.01204	0.79628	3.17655
H	0.84621	2.34604	3.24524
H	-0.53246	2.13737	2.15063
C	3.32143	1.66363	-1.70095
H	2.60608	1.50838	-2.51976
H	3.56907	2.73306	-1.66631
H	4.23303	1.11001	-1.94311
C	4.25659	-0.83321	0.18444
H	4.79892	-0.60882	-0.73828
H	4.97099	-0.80332	1.01875
H	3.87159	-1.85825	0.10488
C	1.53549	1.84587	0.21881
C	0.90354	3.11644	-0.27745
H	-0.065	3.29955	0.1991
H	1.55164	3.97939	-0.06474
H	0.73967	3.074	-1.35933
Cl	0.25625	-0.01159	-2.53634
C	-0.96579	-0.54721	0.33949
C	-3.45057	-0.11382	0.33207
C	-4.66245	-0.85013	0.17344
C	-5.86837	-0.14816	-0.07033

C	-4.67026	1.97726	-0.08569
C	-5.87305	1.24911	-0.19297
H	-6.79527	-0.70785	-0.18469
H	-4.66913	3.05824	-0.19504
H	-6.80999	1.76702	-0.38483
Cl	1.22772	-2.64432	-0.49578
C	-3.47506	1.2899	0.17809
H	-2.54499	1.84324	0.28694
C	-2.20939	-0.84462	0.68572
H	-2.31279	-1.73562	1.31646
H	-4.66141	-1.91802	0.24054
Ir	0.96387	-0.21473	-0.19601

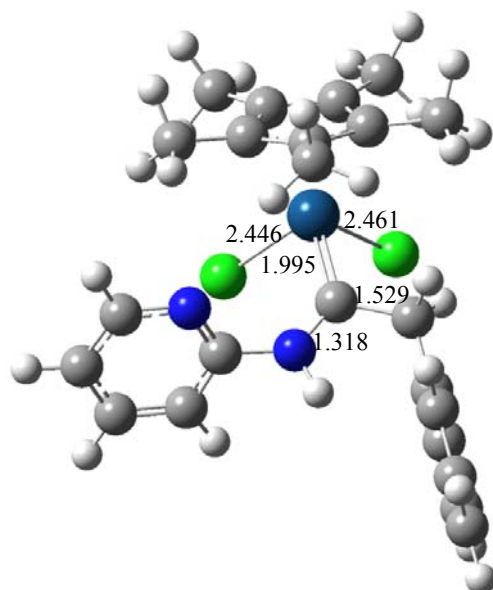
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Sum of electronic and thermal Energies= -1723.626057

Sum of electronic and thermal Enthalpies= -1723.625113

Sum of electronic and thermal Free Energies= -1723.707102

Intermediate C



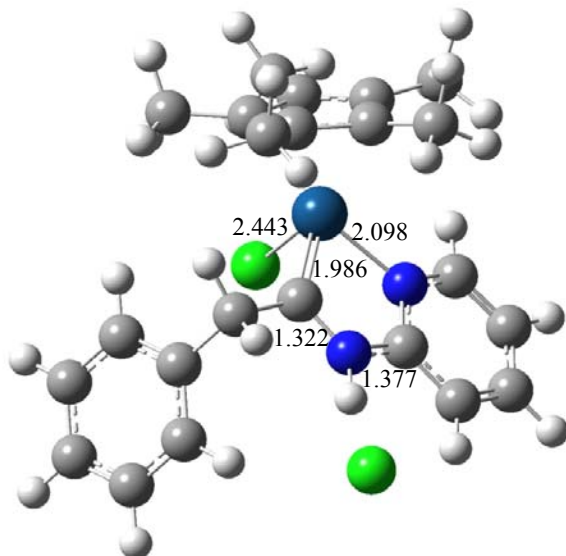
Charge = 0 Multiplicity = 1

C	1.66957	-0.29275	1.83012
C	1.9624	-1.58723	1.26079
C	3.21196	-0.00461	0.09449
C	2.37573	0.69749	1.06655
C	2.48844	2.15685	1.36544
H	1.6744	2.49265	2.00344
H	3.43531	2.36285	1.87721
H	2.46304	2.7472	0.44873
C	4.13896	0.68047	-0.85736
H	3.6153	1.46454	-1.40764
H	4.97173	1.13877	-0.31466
H	4.55227	-0.01491	-1.58625
C	1.58053	-2.92582	1.81066
H	1.39897	-3.64298	1.00939
H	2.37852	-3.32676	2.44559
H	0.67721	-2.87012	2.41859
C	0.85793	-0.02309	3.05849
H	0.14534	-0.82434	3.25588
H	1.51888	0.0465	3.92877
H	0.30546	0.91236	2.9721
Cl	0.44334	-2.02525	-1.95961
C	2.97076	-1.38323	0.22299
C	3.58835	-2.49347	-0.56239
H	4.19276	-3.12441	0.09688
H	2.8181	-3.11339	-1.02417
H	4.23127	-2.11757	-1.35637

C	-0.99814	-0.24375	0.11656
C	-3.26278	-1.51865	0.28709
C	-3.87708	-1.70463	-0.95683
C	-4.07385	-1.30657	1.40561
C	-5.26159	-1.68238	-1.07512
H	-3.25907	-1.87545	-1.8315
C	-5.46151	-1.28379	1.28899
H	-3.61609	-1.16926	2.37992
C	-6.05812	-1.47073	0.04747
H	-5.72046	-1.83534	-2.04481
H	-6.0739	-1.12509	2.16882
H	-7.1375	-1.45701	-0.04543
N	-1.78365	0.81412	0.14242
H	-2.77981	0.62547	0.24454
Ir	0.96425	-0.35775	-0.22658
C	-1.75518	-1.54376	0.39241
H	-1.4557	-1.83952	1.40389
H	-1.33684	-2.29269	-0.28059
Cl	0.78652	1.34232	-1.97692
C	-1.4878	2.21804	0.07276
C	-2.03708	2.95891	-0.96973
C	-1.84983	4.32987	-0.96006
H	-2.55917	2.46032	-1.77485
C	-0.62487	4.06614	1.06965
C	-1.1233	4.90004	0.08046
H	-2.24867	4.94195	-1.75955
H	-0.05772	4.47485	1.89988
H	-0.94707	5.9671	0.12588
N	-0.81382	2.74168	1.08328

Sum of electronic and zero-point Energies= -2027.320656
Sum of electronic and thermal Energies= -2027.290177
Sum of electronic and thermal Enthalpies= -2027.289233
Sum of electronic and thermal Free Energies= -2027.384341

Iridium amino-carbene 4



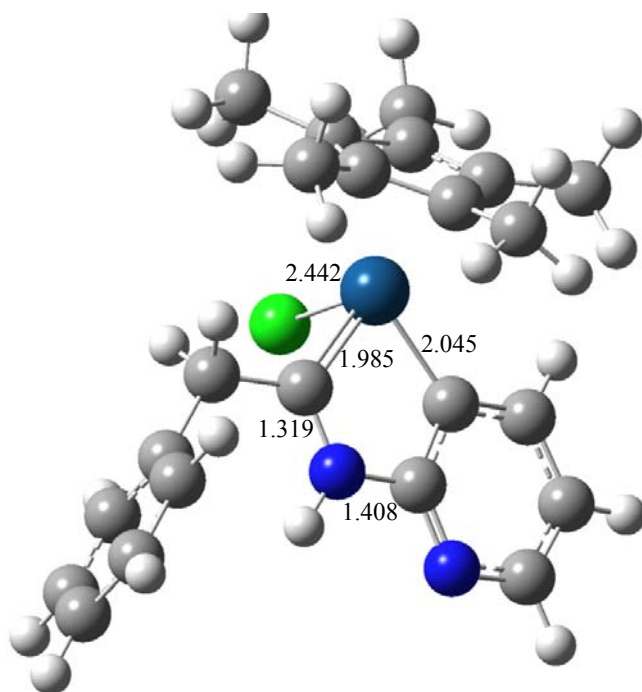
Charge = 0 Multiplicity = 1

C	-1.89189	-2.01294	0.54251
C	-1.71556	-1.19065	1.70189
C	-2.43141	0.04233	1.48172
C	-3.20122	-0.11388	0.25012
C	-2.87235	-1.35073	-0.3204
Cl	-0.09264	-0.83414	-2.22444
C	-3.3845	-1.93302	-1.59692
H	-2.56019	-2.15265	-2.27901
H	-3.91782	-2.86699	-1.39671
H	-4.07163	-1.25736	-2.10442
C	-4.19619	0.88107	-0.26049
H	-4.37192	0.7713	-1.33039
H	-5.15651	0.74448	0.2471
H	-3.87875	1.90701	-0.0704
C	-2.63454	1.13099	2.4907
H	-2.77786	2.10129	2.01423
H	-3.52106	0.92872	3.10144
H	-1.78148	1.21875	3.1628
C	-1.05499	-1.58493	2.98464
H	-0.51425	-0.75935	3.44662
H	-1.82394	-1.91266	3.69187
H	-0.36321	-2.41508	2.8536
C	-1.4164	-3.41831	0.34443
H	-0.55436	-3.64474	0.97121
H	-2.20719	-4.13225	0.59791
H	-1.12702	-3.59	-0.69277
H	2.39307	1.73317	0.91508
C	0.73961	2.26277	-0.2991
C	-1.21081	2.57235	-1.50801

C	1.20573	3.53619	-0.61986
H	-2.13856	2.13968	-1.85272
H	2.17013	3.84633	-0.23564
C	-0.81623	3.84194	-1.87753
H	-1.45486	4.43276	-2.52002
C	0.40601	4.33441	-1.41429
H	0.73381	5.33012	-1.68556
N	1.47264	1.36139	0.43937
C	0.96485	0.15549	0.62766
C	1.89181	-0.80927	1.32499
H	2.40309	-0.27367	2.13145
H	1.32091	-1.62509	1.75796
C	2.93892	-1.38298	0.37322
C	2.67597	-2.5483	-0.34622
C	4.1749	-0.75272	0.22086
C	3.6326	-3.08278	-1.20163
H	1.71441	-3.03771	-0.24818
C	5.13093	-1.28931	-0.63555
H	4.38974	0.15879	0.76963
C	4.8643	-2.45386	-1.34813
H	3.41281	-3.98708	-1.75693
H	6.08818	-0.79263	-0.74156
H	5.61141	-2.86884	-2.01458
Ir	-0.88161	-0.14471	-0.04016
N	-0.4592	1.80053	-0.70392
Cl	3.73828	2.59944	1.79645

Sum of electronic and zero-point Energies= -2027.343840
Sum of electronic and thermal Energies= -2027.313941
Sum of electronic and thermal Enthalpies= -2027.312997
Sum of electronic and thermal Free Energies= -2027.406129

Iridium amino-carbene 4'



Charge = 0 Multiplicity = 1

C	-1.95104	-2.13353	-0.21949
C	-1.36398	-1.97495	1.05401
C	-1.88802	-0.75163	1.64586
C	-2.9298	-0.25872	0.75967
C	-2.924	-1.05793	-0.39943
Cl	-0.43895	0.07116	-2.54277
C	-3.7966	-0.91934	-1.60704
H	-3.19881	-0.90961	-2.52051
H	-4.49778	-1.75788	-1.66896
H	-4.37875	0.00123	-1.58099
C	-3.87977	0.84836	1.09202
H	-4.32063	1.28993	0.19859
H	-4.69905	0.46286	1.70866
H	-3.39219	1.64445	1.65404
C	-1.70073	-0.31895	3.06908
H	-1.82128	0.75942	3.17392
H	-2.43236	-0.80254	3.72664
H	-0.70652	-0.57232	3.43814
C	-0.45122	-2.93526	1.75006
H	0.27131	-2.41995	2.3845
H	-1.03345	-3.5991	2.39808
H	0.09661	-3.56381	1.04793
C	-1.7355	-3.24218	-1.20225
H	-0.86156	-3.84259	-0.94823
H	-2.60084	-3.91324	-1.22872

H	-1.58694	-2.84927	-2.20988
H	2.7253	1.2395	0.23054
C	-0.47856	1.90569	0.02085
C	0.86669	2.25146	0.21481
C	-1.36888	2.97667	-0.07467
H	-2.41672	2.79486	-0.27837
C	-0.9371	4.29621	0.06602
H	-1.65667	5.10418	-0.00782
C	0.40598	4.58978	0.2882
H	0.73376	5.61666	0.39361
N	1.71676	1.12907	0.21054
C	1.15613	-0.05512	0.04917
C	2.07983	-1.2368	-0.13537
H	1.78957	-2.0066	0.58197
H	1.82819	-1.63981	-1.12215
C	3.56617	-0.9725	-0.04212
C	4.28821	-0.56895	-1.16912
C	4.24574	-1.10513	1.17153
C	5.65236	-0.30832	-1.08536
H	3.77537	-0.46318	-2.11902
C	5.60985	-0.84548	1.25861
H	3.70303	-1.42162	2.05615
C	6.31695	-0.4456	0.12925
H	6.19635	-0.00166	-1.9709
H	6.12064	-0.95902	2.20757
H	7.37975	-0.24565	0.19456
Ir	-0.8134	-0.11116	-0.13519
N	1.32978	3.55283	0.35338

Sum of electronic and zero-point Energies= -1566.490741
 Sum of electronic and thermal Energies= -1566.462975
 Sum of electronic and thermal Enthalpies= -1566.462031
 Sum of electronic and thermal Free Energies= -1566.549448