Electronic Supplementary Information (ESI)

Synthesis, Characterization, Photophysics and Electrochemical Study of Luminescent Iridium(III) Complexes with Isocyanoborate Ligands

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Table S1. Crystal and structure determination data for **1**, **3**, **8** and **12**.

	1	**3**	**8**
Formula	$C_{59}H_{31}BF_{15}IrN_3P$	$C_{48}H_{16}BClF_{19}IrN_4 \cdot 0.5CH_2Cl_2$	$C_{48}H_{31}BClF_4IrN_4 \cdot 1.5C_4H_{10}O$
M_r	1300.85	1290.57	1089.41
T, [K]	173	173 (2)	133
a, [Å]	23.3783 (4)	21.9289 (3)	16.5174 (6)
b, [Å]	10.11539 (14)	13.81974 (14)	17.2287 (4)
c, [Å]	23.8296 (4)	16.7040 (2)	17.8271 (5)
α, [deg]	90.0	90.0	90.0
β, [deg]	99.119 (2)	112.2864 (15)	105.839 (3)
γ, [deg]	90.0	90.0	90.0
V, [Å^3]	5015.22(14)	4684.04 (10)	4880.5 (2)
Crystal color	Yellow	Yellow	Yellowish green
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/c$
Z	4	4	4
F(000)	2552	2492	2180
$D_{c,}$ [gcm^{-3}]	1.723	1.830	1.483
Crystal dimensions [mm]	0.74 × 0.33 × 0.09	0.22 × 0.11 × 0.02	0.79 × 0.21 × 0.02
λ, [Å]	1.54178	1.54178	1.54178
μ / mm^{-1}	6.35	7.64	6.29
Collection range	$3.6 \le \theta \le 71.7°$ (h: –28 to 28; k: –13 to 11; l: –29 to 29)	$3.9 \le \theta \le 71.6°$ (h: –26 to 19; k: –13 to 16; l: –15 to 20)	$3.8 \le \theta \le 71.7°$ (h: –18 to 20; k: –20 to 15; l: –21 to 20)
Completeness to theta	99.9%	99.5%	98.5%
No. of data collected	37126	21237	20142
No. of unique data	9683	8305	9406
No. of data used in refinement, m	9405	7382	8898
No. of parameters refined, p	721	721	626
R^a	0.0317	0.0340	0.0271
wR^a	0.0816	0.0949	0.0729
Goodness-of-fit, S	1.11	1.06	1.05
Maximum shift, $(\Delta/\sigma)_{max}$	0.003	0.001	0.005
Residual extrema in final difference map, eÅ^{-3}	+1.44, –1.92	+1.29, –1.01	+1.71, –1.29

Table S2. Selected bond distances (Å), angles and torsions (°) with estimated standard deviations (e.s.d.s) in parentheses for **1**, **3**, **8** and **12**.

1	Ir(1)–C(1)	2.033 (3)	Ir(1)–C(12)	2.060 (3)
	Ir(1)–C(23)	2.048 (3)	Ir(1)–N(3)	2.087 (2)
	Ir(1)–N(2)	2.059 (2)	N(1)–B(1)	1.559 (4)
	C(1)–N(1)	1.143 (4)		
	C(12)–Ir(1)–N(2)	79.77 (11)	C(23)–Ir(1)–N(3)	79.55 (11)
	C(1)–N(1)–B(1)	165.3 (3)		
3	Ir(1)–C(1)	2.032 (5)	Ir(1)–C(2)	2.001 (4)
	Ir(1)–C(3)	2.047 (4)	Ir(1)–C(14)	2.056 (4)
	Ir(1)–N(3)	2.058 (4)	Ir(1)–N(4)	2.053 (4)
	C(1)–N(1)	1.146 (6)	C(2)–N(2)	1.159 (6)
	N(1)–B(1)	1.550 (6)		
	C(3)–Ir(1)–N(3)	80.06 (18)	C(14)–Ir(1)–N(4)	80.05 (17)
	C(1)–N(1)–B(1)	174.0 (4)	C(2)–N(2)–C(25)	178.1 (5)
8	Ir(1)–C(1)	2.036 (2)	Ir(1)–C(2)	2.011 (2)
	Ir(1)–C(27)	2.051 (2)	Ir(1)–C(38)	2.047 (2)
	Ir(1)–N(3)	2.056 (2)	Ir(1)–N(4)	2.058 (2)
	C(1)–N(1)	1.153 (3)	C(2)–N(2)	1.149 (3)
	N(1)–B(1)	1.580 (3)		
	C(27)–Ir(1)–N(3)	80.30 (9)	C(38)–Ir(1)–N(4)	80.02 (10)
	C(1)–N(1)–B(1)	172.5 (2)	C(2)–N(2)–C(21)	170.8 (3)

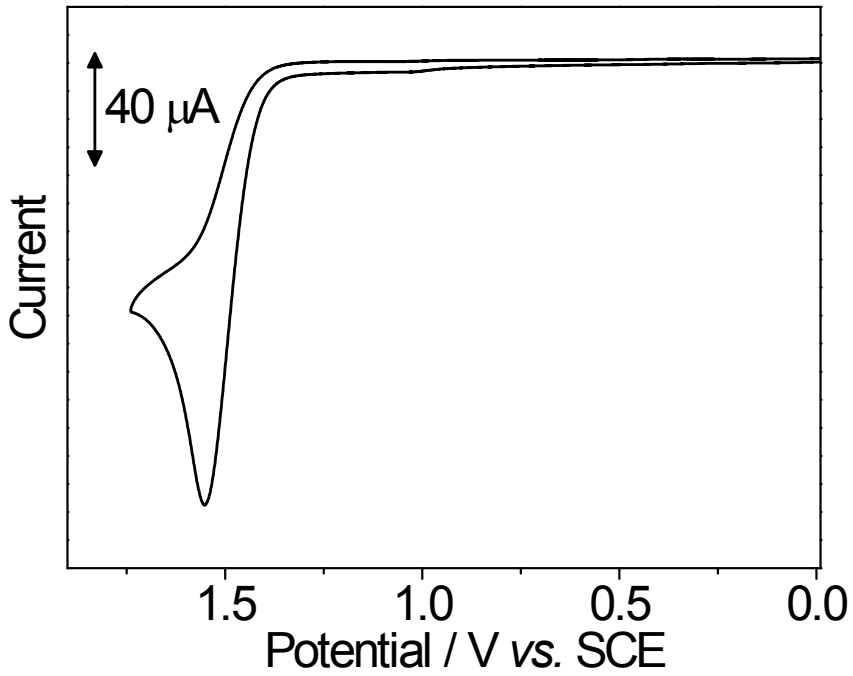

Figure S1. Cyclic voltammogram of oxidative scan of **2** in acetonitrile solution (0.1 M $^{n}Bu_4NPF_6$). Scan rate: 100 mV s^{-1}.

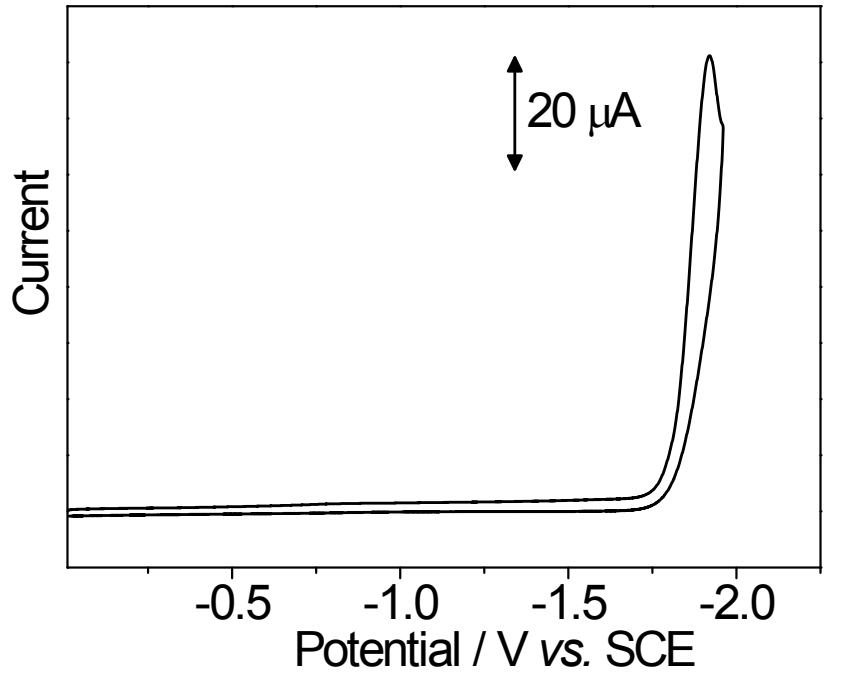

Figure S2. Cyclic voltammogram of reductive scan of **2** in acetonitrile solution (0.1 M $^{n}Bu_4NPF_6$). Scan rate: 100 mV s^{-1}.