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Supplementary Information

Bright and stable light-emitting electrochemical cells based on an intramolecularly π-stacked, 2-naphthyl-substituted iridium complex

Gabriel E. Schneider,[a] Antonio Pertegás,[b] Edwin C. Constable,[a] Catherine E. Housecroft,*[a] Nik Hostettler,[a] Collin D. Morris,[a] Jennifer A. Zampese,[a] Henk J. Bolink,*[b] José M. Junquera-Hernández,[b] Enrique Ortí[b] and Michele Sessolo[b]

[a] *Department of Chemistry, University of Basel, Spitalstrasse 51, CH–4056 Basel, Switzerland. E-mail: catherine.housecroft@unibas.ch*

[b] *Instituto de Ciencia Molecular, Universidad de Valencia, ES–46980 Paterna (Valencia), Spain. E-mail:henk.bolink@uv.es*

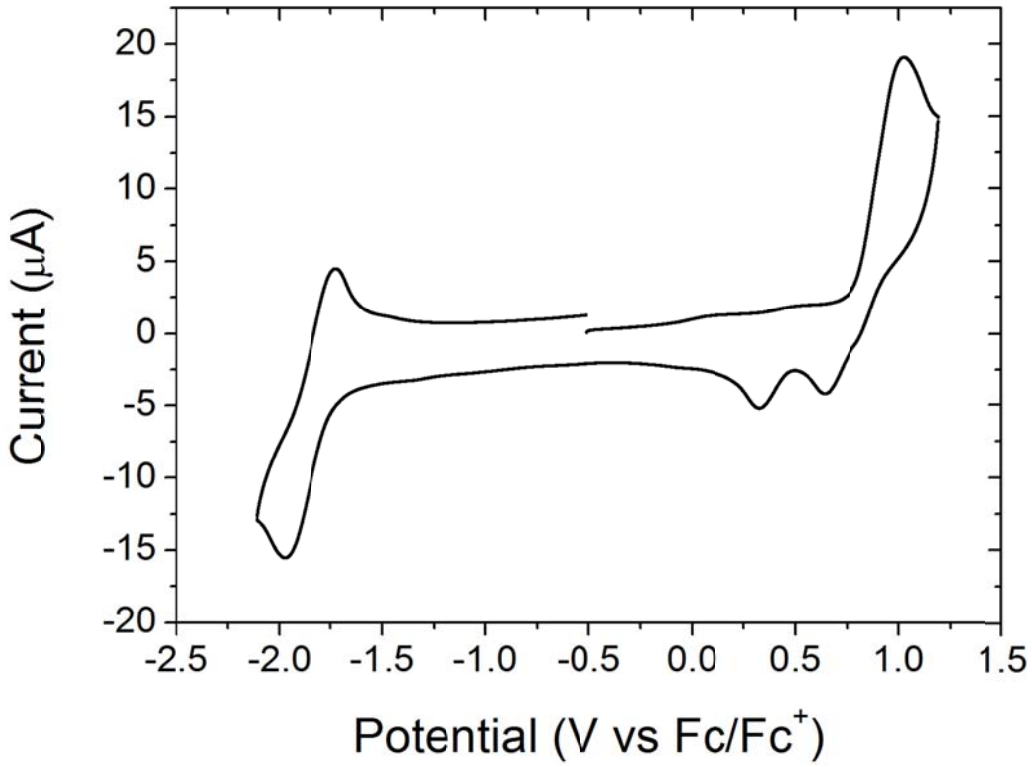

Fig. S1. Cyclic voltammogram of $[Ir(ppy)_2(Naphbpy)][PF_6]$ measured in CH_2Cl_2 solution (with respect to Fc/Fc^+) showing the quasi-reversible oxidation and reduction, as well as the unidentified process at +0.33V. Scan-rate = 0.1 V s^{-1}.

Table S1. Selected bond distances (in Å) and angles (in deg.) calculated for the $[Ir(ppy)_2(Naphbpy)]^+$ complex in the singlet ground state (S_0) and in the lowest-energy triplet states T_1 and T_2. X-ray values are included for comparison.

	Exp.[b]	S_0[c]	T_1[d]	T_2[d]
Ir(1)–N(1)[a]	2.150(5)	2.208	2.226	2.209
Ir(1)–N(2)	2.215(5)	2.356	2.249	2.346
Ir(1)−N(3)	2.064(5)	2.093	2.089	2.097
Ir(1)−N(4)	2.037(5)	2.077	2.073	2.077
Ir(1)−C(21)	2.007(6)	2.013	2.017	2.015
Ir(1)−C(32)	2.019(6)	2.028	1.980	2.026
N(1)−Ir(1)−N(2)	75.60(18)	73.9	74.6	74.1
C(21)−Ir(1)−N(3)	79.9(2)	80.1	80.0	80.1
C(32)−Ir(1)−N(4)	80.4(2)	80.0	81.0	80.1
N(1)−C(5)−C(6)−N(2)	14.4(7)	17.5	11.0	20.4
C(21)−C(26)−C(27)−N(3)	2.7(9)	1.5	–0.1	1.3
C(32)−C(37)−C(38)−N(4)	1.0(8)	–0.8	0.4	0.5
N(2)−C(10)−C(11)−C(20)	61.1(8)	57.5	64.2	45.9

[a] Atom numbering from Figure 1. [b] X-ray values. [c] DFT optimized structure. [d] TD-DFT optimized structure. All calculations performed at the B3LYP/(6-31G**+LANL2DZ) level in the presence of the solvent (CH_2Cl_2).

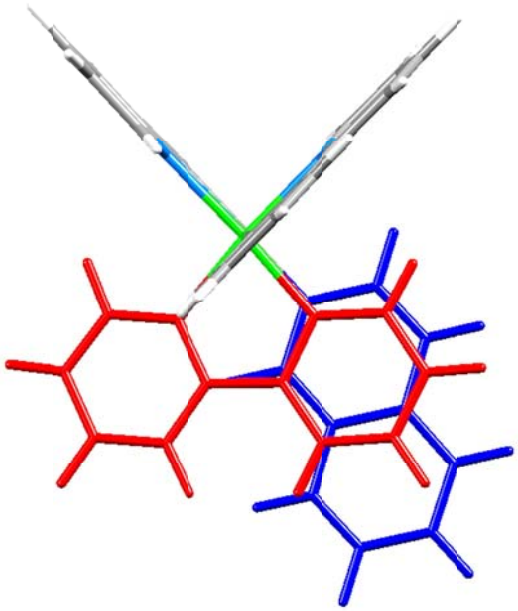

Fig. S2. B3LYP/(6-31G**+LANL2DZ)-optimized structure of the transition state connecting conformers 1 and 2 of the $[Ir(ppy)_2(Naphbpy)]^+$ complex. The transition state presents only one imaginary frequency and the associated vibrational normal mode describes a movement leading to conformers 1 and 2.

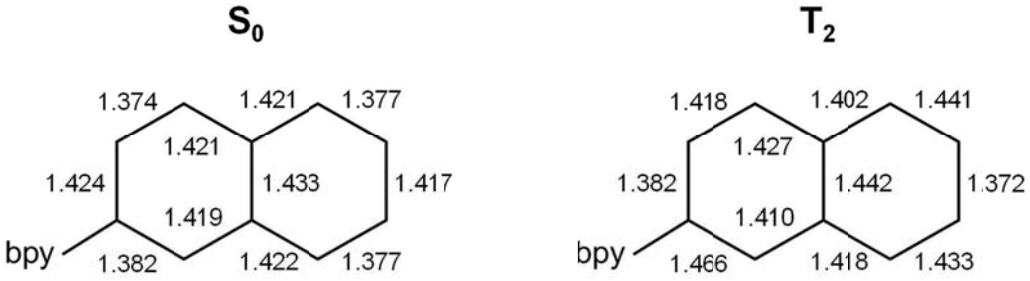

Fig. S3. B3LYP/(6-31G**+LANL2DZ)-optimized bond lengths (in Å) calculated for the pendant naphthyl group of the $[Ir(ppy)_2(Naphbpy)]^+$ complex in the singlet ground state (S_0, DFT optimization) and in the ^{3}LC T_2 triplet state (TD-DFT optimization).