Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Near Infrared-Emitting Tris-Bidentate Os(II) Phosphors: Control of Excited State Characters and Fabrication of OLEDs

Jia-Ling Liao,[a] Yun Chi,[a,*] Chia-Chi Yeh,[b] Hao-Che Kao,[b] Chih-Hao Chang,[b,*] Mark A. Fox,[c] Paul J. Low,[d,*] and Gene-Hsiang Lee[e]

[a] Department of Chemistry and Low Carbon Energy Research Center, National Tsing Hua University, Hsinchu 30013, Taiwan; E-mail: ychi@mx.nthu.edu.tw mailto:ychi@mx.nthu.edu.tw[b] Department of Photonics Engineering, Yuan Ze University, Chungli 32003, Taiwan; E-mail: chc@saturn.yzu.edu.tw

[c] Department of Chemistry, Durham University, South Rd, Durham, DH1 3LE, UK

[d] School of Chemistry and Biochemistry, University of Western Australia, 35 Stirling Highway, Crawley, 6009, Western Australia, Australia; E-mail paul.low@uwa.edu.au

[e] Instrumentation Center, National Taiwan University, Taipei 10617, Taiwan

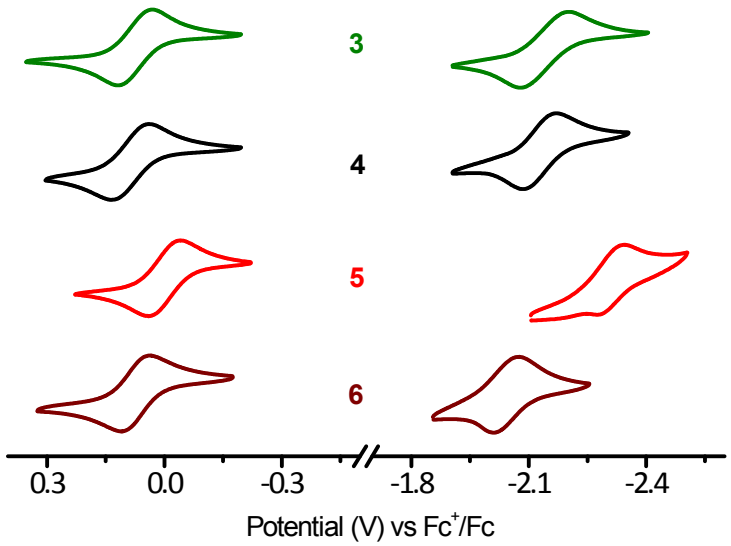

Figure S1. Cyclic voltammograms of Os(II) complexes **3** – **6**.

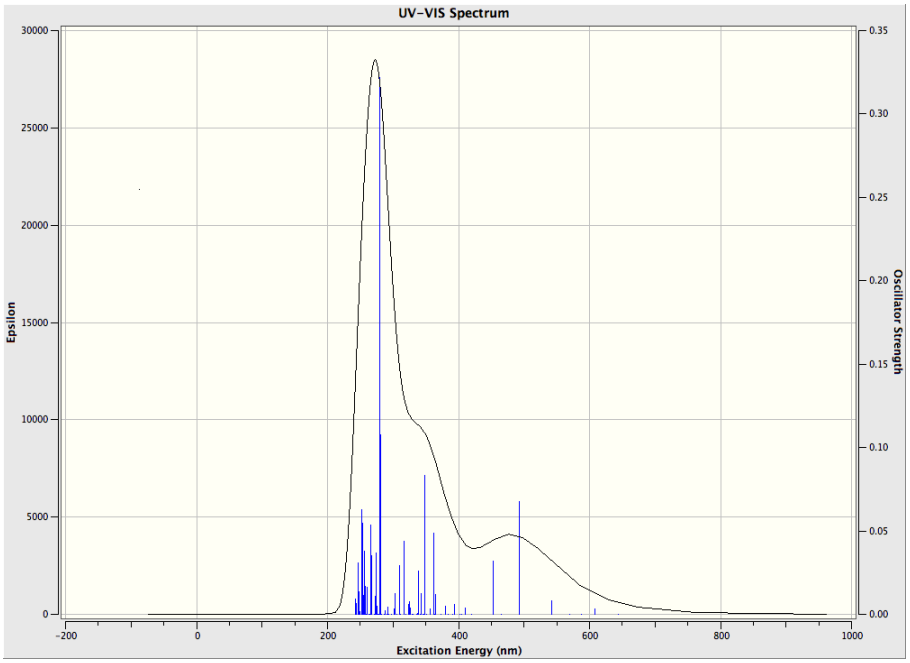

Figure S2. The simulated absorption spectra for Os(II) complex **3'**. In this and all subsequent Figures, the stick graph representation of the TD DFT results from the first 50 (singlet and triplet) excited states. The simulated electronic absorption spectrum overlaid on the stick spectrum was obtained using a 0.333 eV peak half-width at half height

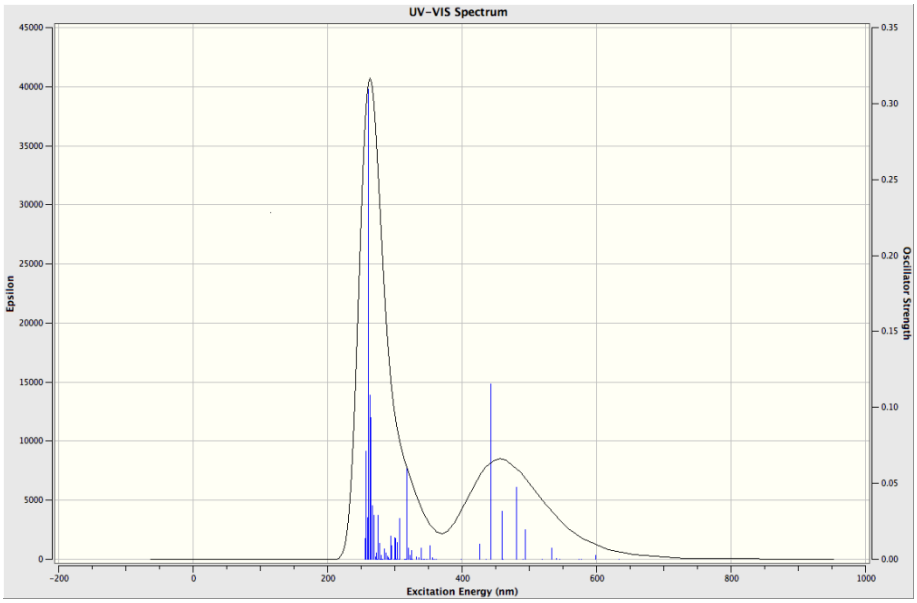

Figure S3. The simulated absorption spectra for Os(II) complex **4'**.

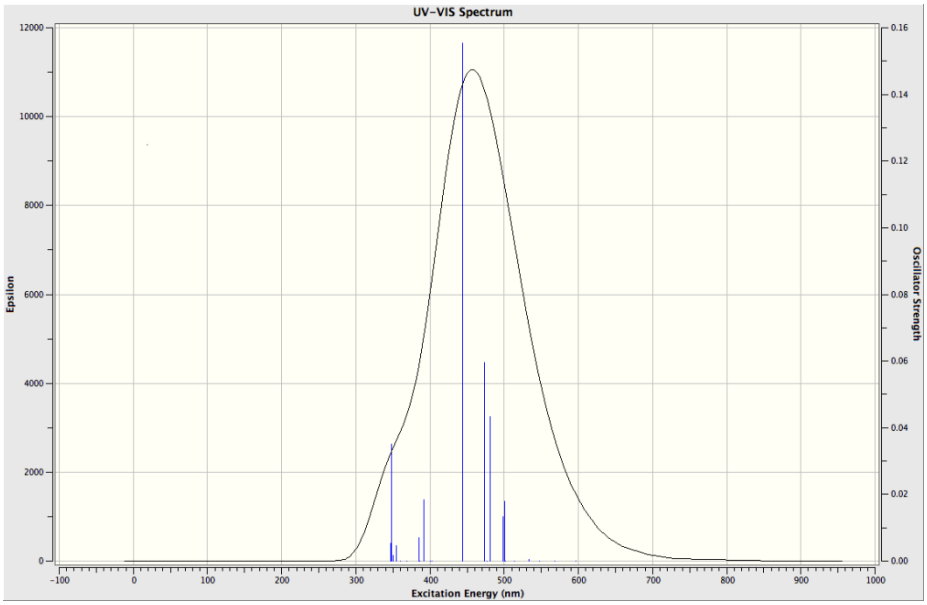

Figure S4. The simulated absorption spectra for Os(II) complex **5'**.

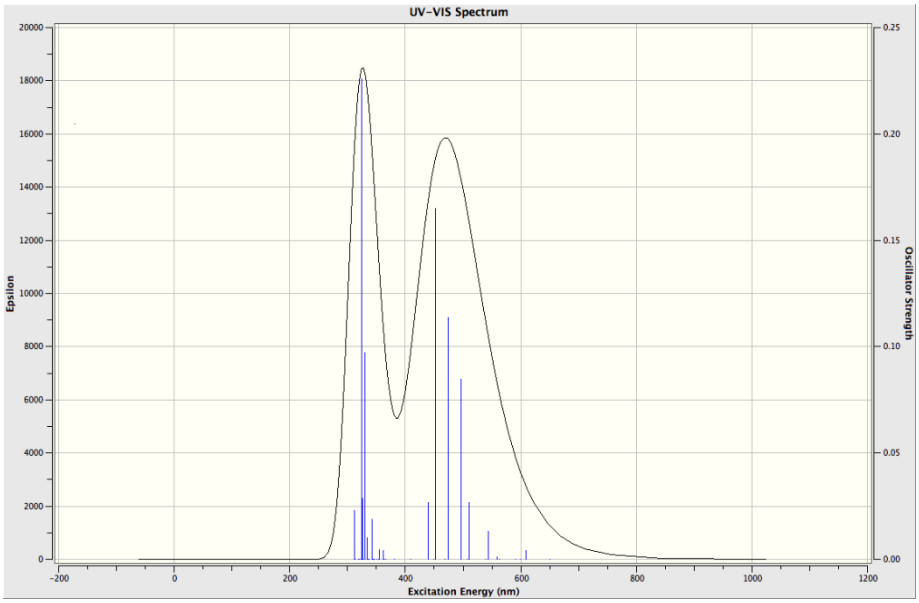

Figure S5. The simulated absorption spectra for Os(II) complex **6'**.

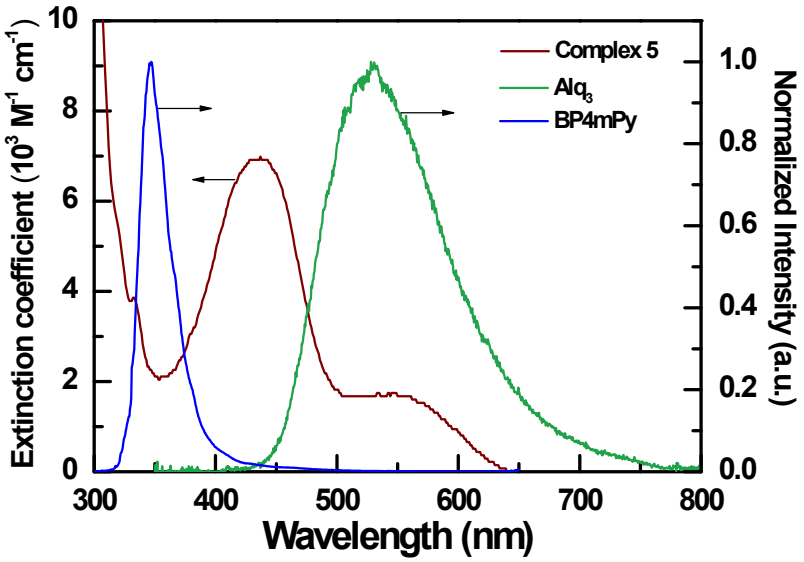

Figure S6. UV-Vis absorption spectrum of Os(II) complex **5** and the PL spectra of Alq_3 and BP4mPy recorded in CH_2Cl_2 solutions.

Table S1. Orbital energies (eV) and composition (%) for Os(II) complex **3**´.

MO		eV	Os	PP	bpy	bipz
188	L+5	0.22	3	4	58	35
187	L+4	-0.76	2	92	5	1
186	L+3	-0.88	1	98	1	0
185	L+2	-1.12	1	3	96	0
184	L+1	-1.27	3	5	92	0
183	LUMO	-2.16	6	1	92	1
182	HOMO	-5.00	49	5	2	44
181	H-1	-5.22	51	7	7	35
180	H-2	-5.37	64	7	8	21
179	H-3	-5.54	37	5	5	52
178	H-4	-6.71	14	8	8	71
177	H-5	-6.88	13	14	4	69

Table S2. Orbital energies (eV) and composition (%) for Os(II) complex **4**´.

MO		eV	Os	PP	phen	bipz
194	L+5	-0.04	1	1	98	0
193	L+4	-0.70	3	51	46	0
192	L+3	-0.84	1	65	33	1
191	L+2	-0.87	1	82	18	0
190	L+1	-2.05	1	1	98	0
189	LUMO	-2.13	6	1	92	1
188	HOMO	-5.00	48	5	2	45
187	H-1	-5.22	51	7	7	35
186	H-2	-5.37	65	7	8	20
185	H-3	-5.53	36	5	6	54
184	H-4	-6.67	9	7	27	57
183	H-5	-6.83	13	11	18	59

Table S3. Orbital energies (eV) and composition (%) for Os(II) complex **5**´.

MO		eV	Os	PP	Me_4phen	bipz
210	L+5	-0.11	6	5	3	85
209	L+4	-0.51	3	13	83	1
208	L+3	-0.75	2	84	12	2
207	L+2	-0.82	0	99	1	0
206	L+1	-1.85	3	1	95	1
205	LUMO	-1.91	3	1	95	1
204	HOMO	-5.03	57	8	3	32
203	H-1	-5.05	52	7	14	26
202	H-2	-5.29	75	8	11	7
201	H-3	-5.64	11	2	3	85
200	H-4	-6.55	2	5	60	33
199	H-5	-6.80	3	2	94	1

Table S4. Orbital energies (eV) and composition (%) for Os(II) complex **6**´.

MO		eV	Os	PP	Ph_2phen	bipz
234	L+5	-0.65	0	1	98	0
233	L+4	-0.75	2	85	12	1
232	L+3	-0.85	1	94	5	0
231	L+2	-0.94	1	14	84	0
230	L+1	-2.13	1	1	98	0
229	LUMO	-2.18	6	1	92	1
228	HOMO	-4.98	49	5	2	44
227	H-1	-5.19	51	7	9	33
226	H-2	-5.33	66	7	10	16
225	H-3	-5.50	32	5	6	58
224	H-4	-6.51	3	4	62	31
223	H-5	-6.77	15	7	22	56