

Ligand-to-ligand charge transfer in heteroleptic Ir-complexes: Comprehensive investigations of its fast dynamics and mechanism

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Figures

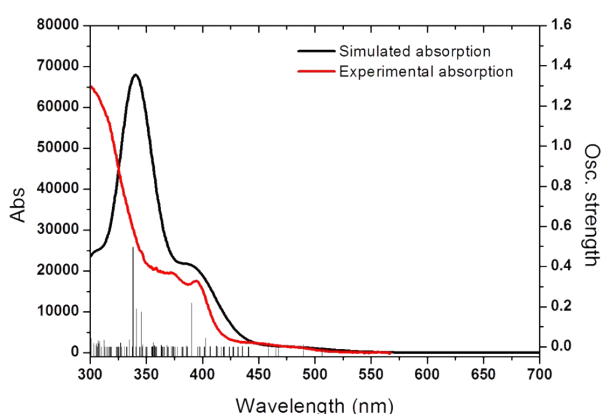


Fig. S1 Simulated absorption spectrum of complex **1** using a TD-DFT with full width at half-maximum of 3000 cm⁻¹ (black) and experimental absorption spectrum. The vertical bars correspond to the individual excited states.

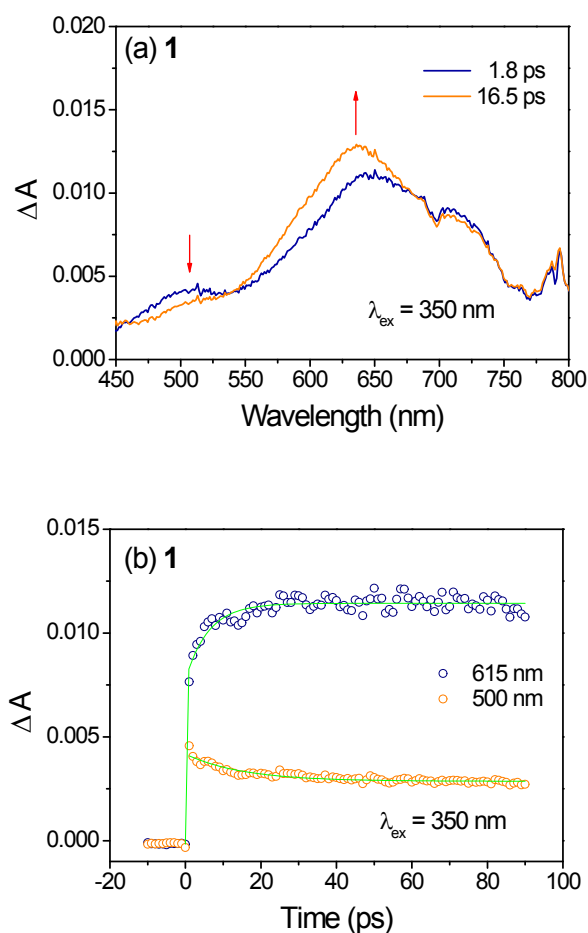


Fig. S2. (a) TA spectra of complex **1** in CH₂Cl₂ measured after selected time delays. All transient spectra were corrected for the chirp. Figure (b) is the temporal profiles monitored at different wavelengths. The excitation wavelengths were 350 nm.

Tables

Table S1 Calculated energy levels of 50-transitions for complex 1

No.	Wavelength (nm)	Oscillation Strength	Symmetry	Major Contributions
1	506.24	0.0	Triplet-A	HOMO→LUMO (54%), HOMO→L+1 (20%)
2	489.51	0.0105	Singlet-A	HOMO→LUMO (79%), HOMO→L+1 (18%)
3	489.43	0.0	Triplet-A	H-6→L+2 (12%), H-5→LUMO (27%), H-5→L+1 (14%), HOMO→LUMO (13%)
4	467.64	0.0	Triplet-A	H-1→LUMO (62%), H-1→L+1 (17%)
5	465.38	0.0	Triplet-A	H-6→LUMO (41%), H-6→L+1 (31%)
6	458.56	0.0115	Singlet-A	H-1→LUMO (75%), H-1→L+1 (16%)
7	441.14	0.0	Triplet-A	H-6→LUMO (10%), HOMO→LUMO (18%), HOMO→L+1 (47%)
8	440.67	0.0	Triplet-A	H-8→LUMO (13%), H-6→L+1 (10%)
9	435.48	0.0013	Singlet-A	HOMO→L+1 (77%), HOMO→LUMO (19%)
10	431.42	0.0	Triplet-A	HOMO→L+3 (35%), HOMO→L+4 (23%)
11	427.49	0.0	Triplet-A	H-3→LUMO (69%), H-3→L+1 (27%)
12	426.99	0.0	Triplet-A	HOMO→L+1 (10%), HOMO→L+2 (53%)
13	424.00	0.0	Singlet-A	H-3→LUMO (72%), H-3→L+1 (26%)
14	423.77	0.0	Triplet-A	H-2→LUMO (11%), H-1→L+3 (18%), H-1→L+4 (20%)
15	419.51	0.0010	Singlet-A	HOMO→L+2 (70%), H-2→LUMO (19%)
16	418.74	0.0003	Singlet-A	H-2→LUMO (55%), HOMO→L+2 (22%)
17	418.62	0.0	Triplet-A	H-2→LUMO (35%), H-2→L+1 (10%), H-1→LUMO (14%)
18	416.58	0.0	Triplet-A	H-9→LUMO (40%), H-9→L+1 (34%)
19	413.42	0.0	Triplet-A	H-6→L+2 (29%), H-5→LUMO (15%), HOMO→L+2 (23%)
20	412.39	0.0035	Singlet-A	H-1→L+1 (71%), H-1→LUMO (14%)
21	412.30	0.0	Triplet-A	H-1→LUMO (11%), H-1→L+1 (55%)
22	406.78	0.0010	Singlet-A	H-5→LUMO (65%), H-5→L+1 (13%), H-4→LUMO (15%)
23	402.54	0.0440	Singlet-A	H-5→LUMO (14%), H-4→LUMO (64%)
24	401.61	0.0	Triplet-A	H-4→LUMO (52%), H-4→L+1 (11%)
25	397.76	0.0	Triplet-A	H-1→L+2 (69%)
26	397.01	0.0027	Singlet-A	H-1→L+2 (87%)
27	395.56	0.0	Triplet-A	H-8→LUMO (11%), H-6→LUMO (13%), H-6→L+1 (14%), H-5→LUMO (10%)
28	390.10	0.2187	Singlet-A	H-6→LUMO (72%)
29	386.40	0.0	Triplet-A	H-2→LUMO (12%), H-2→L+1 (69%)
30	385.26	0.0055	Singlet-A	H-2→L+1 (79%), H-2→LUMO (12%)
31	382.61	0.0	Triplet-A	H-5→L+1 (13%), H-5→L+2 (43%), H-4→L+2 (12%)
32	382.09	0.0	Triplet-A	H-7→LUMO (17%), H-3→L+2 (59%)
33	381.34	0.0	Triplet-A	H-8→LUMO (13%), H-6→L+1 (12%), H-5→L+1 (16%), H-5→L+2 (25%)
34	377.46	0.0	Triplet-A	H-3→LUMO (28%), H-3→L+1 (70%)
35	377.38	0.0	Singlet-A	H-3→LUMO (26%), H-3→L+1 (70%)
36	375.44	0.0001	Singlet-A	H-3→L+2 (53%), H-7→LUMO (27%), H-7→L+1 (11%)
37	374.06	0.0	Triplet-A	H-4→L+1 (31%), H-2→L+2 (35%)
38	373.56	0.0018	Singlet-A	H-5→L+1 (49%), H-4→L+1 (30%), H-5→LUMO (15%)
39	373.36	0.0009	Singlet-A	H-4→L+1 (26%), H-6→L+1 (22%), H-5→L+1 (13%), H-5→L+2 (16%)
40	372.06	0.0019	Singlet-A	H-2→L+2 (46%), H-5→L+1 (16%)
41	369.29	0.0	Triplet-A	H-4→L+1 (26%), H-2→L+2 (52%)
42	369.03	0.0	Triplet-A	H-7→LUMO (51%), H-7→L+1 (19%), H-3→L+2 (22%)
43	368.13	0.0077	Singlet-A	H-2→L+2 (43%), H-8→LUMO (10%), H-4→L+1 (16%)
44	365.70	0.0	Triplet-A	H-2→L+3 (13%), H-1→L+3 (21%), H-1→L+4 (13%)
45	364.32	0.0003	Singlet-A	H-7→LUMO (42%), H-7→L+1 (14%), H-3→L+2 (39%)
46	363.67	0.0	Triplet-A	H-8→L+2 (10%), H-5→L+7 (15%)
47	363.29	0.0095	Singlet-A	H-8→LUMO (47%), H-6→L+1 (35%)
48	359.03	0.0	Triplet-A	H-10→LUMO (15%), H-8→L+1 (13%), H-4→L+2 (26%)
49	358.82	0.0	Triplet-A	H-7→L+2 (13%), H-3→L+7 (64%)
50	357.90	0.0	Triplet-A	H-8→L+1 (14%), HOMO→L+3 (10%)

^a Footnote text.