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PCCP



Electronic Supplementary Information

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

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Fig. S2. (a) TA spectra of complex 1 in CH_2CI_2 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

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	No.	Wavelength (nm)	Oscillation Strength	Symmetry	Major Contributions
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1	506.24	0.0	Triplet-A	HOMO→LUMO (54%), HOMO→L+1 (20%)
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	2	489.51	0.0105	Singlet-A	HOMO→LUMO (79%), HOMO→L+1 (18%)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	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%)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6	458.56	0.0115	Singlet-A	H-1→LUMO (75%), H-1→L+1 (16%)
8 440.67 0.0 Triplet-A H-3-LUMO (13%), H-5-L+1 (10%) 9 435.48 0.0013 Singlet-A H0MO-L+1 (75%), HOMO-LUMO (19%) 10 431.42 0.0 Triplet-A H-3-LUMO (19%), H-3-L+1 (25%) 11 427.49 0.0 Triplet-A H-3-LUMO (19%), H-3-L+1 (25%) 13 424.00 0.0 Singlet-A H-3-LUMO (17%), H-3-L+1 (25%) 14 423.77 0.0 Triplet-A H-3-LUMO (17%), H-1-L+3 (18%), H-1-L+4 (20%) 15 419.51 0.0010 Singlet-A H-2-LUMO (17%), H-3-L+1 (25%) 16 418.74 0.0003 Singlet-A H-2-LUMO (15%), HOMO-L+2 (25%) 17 418.62 0.0 Triplet-A H-2-LUMO (15%), H-3-L-1 (10%), H-1-L-10 (14%) 19 413.42 0.0 Triplet-A H-2-LUMO (35%), H-3-L-1 (10%), H-1-L-10 (14%) 19 413.42 0.0 Triplet-A H-2-LUMO (35%), H-3-L-1 (10%), H-1-L-10 (14%) 10 413.42 0.0 Triplet-A H-2-LUMO (15%), H-3-L-1 (10%), H-1-L-10 (14%) 12 440.67 8 0.0010 Singlet-A H-1-1-1/17%, H-1-L-10 (14%), H-3-LUMO (15%) 23 402.54 0.0040 Singlet-A H-1-L-11/1%), H-3-LUMO (15%), H-3/L-1 (15%) 24 401.61 0.0 Triplet-A H-3-LUMO (15%), H-3-H-1 (15%), H-3/L-10 (15%) 25 397.76 0.0 Triplet-A H-3-LUMO (15%), H-3-L-1 (15%), H-3/L-10 (15%) 25 397.76 0.0 Triplet-A H-3-LUMO (15%), H-3-L-1 (15%), H-3-LUMO (15%) 25 397.10 0.0227 Singlet-A H-1-1-2 (26%) 26 397.01 0.0227 Singlet-A H-1-1-2 (26%) 27 395.55 0.0 Triplet-A H-3-LUMO (12%), H-3-L-1 (15%), H-3-LUMO (10%) 28 390.10 0.2187 Singlet-A H-3-LUMO (12%), H-3-L-1 (15%), H-3-LUMO (10%) 28 390.10 0.2187 Singlet-A H-3-LUMO (12%), H-3-L-1 (15%), H-3-LUMO (10%) 29 386.40 0.0 Triplet-A H-3-LUMO (12%), H-3-L-1 (16%), H-5-LUMO (10%) 30 385.26 0.0055 Singlet-A H-3-LUMO (12%), H-3-L-1 (16%), H-5-LUMO (10%) 31 382.61 0.0 Triplet-A H-3-LUMO (12%), H-3-L-1 (16%), H-5-LUMO (10%) 34 377.46 0.0 Triplet-A H-3-LUMO (12%), H-3-L-1 (16%), H-5-L+2 (25%) 34 377.46 0.0 Triplet-A H-3-LUMO (12%), H-3-L-1 (16%), H-5-L+2 (25%) 34 377.46 0.0 Triplet-A H-3-LUMO (12%), H-3-L+1 (16%), H-5-L+2 (25%) 34 377.46 0.0 Triplet-A H-3-LUMO (25%), H-3-L+1 (16%), H-5-L+2 (25%) 34 377.46 0.0 Triplet-A H-3-LUMO (25%), H-3-L+1 (16%), H-5-L+2 (25%) 34 377.46 0.0 Triplet-A H-3-LUMO (25%), H-3-L+1 (16%), H-5-L+2 (25%	7	441.14	0.0	Triplet-A	H-6→LUMO (10%), HOMO→LUMO (18%), HOMO→L+1 (47%)
9 435 48 0.0013 Singlet-A HOMO-L+1 (77%), HOMO-LUNO (19%), 10 431 42 0.0 Triplet-A HOMO-L+3 (35%), HOMO-L+4 (23%) 11 427.49 0.0 Triplet-A HOMO-H-1 (27%), HOMO-L+2 (35%) 13 424.00 0.0 Singlet-A H-3-LUNO (09%), H-3-L+1 (27%) 14 423.77 0.0 Triplet-A H-2-LUNO (12%), H-1-L+2 (35%) 15 419.51 0.0010 Singlet-A HOMO-L+2 (77%), H-2-LUNO (19%), H-1-L+4 (20%) 16 418.74 0.0003 Singlet-A H-2-LUNO (15%), H-1-L+1 (25%) 17 418.62 0.0 Triplet-A H-2-LUNO (15%), H-1-L-1 (15%), H-1-L-1 (23%) 18 416.58 0.0 Triplet-A H-2-LUNO (15%), H-1-L-1 (10%), H-1-LUNO (14%) 18 416.58 0.0 Triplet-A H-2-LUNO (15%), H-1-L-1 (10%), H-1-LUNO (14%) 19 413.42 0.0 Triplet-A H-2-LUNO (55%), H-2-L-1 (10%), H-1-LUNO (14%) 21 412.30 0.0 Triplet-A H-2-LUNO (55%), H-2-L-1 (15%), H-2-LUNO (15%) 22 406.78 0.0010 Singlet-A H-1-LUNO (11%), H-1-L-1 (15%) 23 402.54 0.0440 Singlet-A H-3-LUNO (55%), H-3-L-1 (15%) 24 401.61 0.0 Triplet-A H-4-LUNO (15%), H-3-L-1 (15%) 25 397.76 0.0 Triplet-A H-4-LUNO (15%), H-3-L-1 (15%) 25 397.76 0.0 Triplet-A H-4-LUNO (15%), H-3-L-1 (15%) 26 397.01 0.0027 Singlet-A H-3-LUNO (12%), H-3-LUNO (15%), H-5-LUNO (10%) 28 380.10 0.2187 Singlet-A H-3-LUNO (12%), H-3-LUNO (12%), H-5-LUNO (10%) 29 386.40 0.0 Triplet-A H-4-LUNO (12%), H-2-LUNO (12%), H-5-LUNO (10%) 20 385.26 0.0057 Singlet-A H-2-LUNO (12%), H-3-LLUNO (12%), H-5-LLUNO (10%) 21 31 382.61 0.0 Triplet-A H-3-LUNO (12%), H-3-LLUNO (12%), H-5-LLUNO (10%) 31 382.61 0.0 Triplet-A H-3-LUNO (12%), H-3-LLUNO (12%), H-5-LLUNO (10%) 33 381.34 0.0 Triplet-A H-3-LUNO (12%), H-3-LLUNO (12%), H-5-LL1 (15%), H-5-LL2 (25%) 34 377.36 0.0 Singlet-A H-3-LLUNO (12%), H-3-LL1 (15%), H-5-LL2 (25%) 35 377.38 0.0 Singlet-A H-3-LLUNO (12%), H-3-LL1 (15%), H-5-LL2 (25%) 34 377.46 0.0 Triplet-A H-3-LLUNO (12%), H-3-LL1 (10%), H-5-LL2 (25%) 35 377.36 0.00 Singlet-A H-3-LLUNO (12%), H-3-LL1 (15%), H-5-LL2 (25%) 35 377.36 0.00 Singlet-A H-3-LLUNO (15%), H-3-LL1 (15%), H-5-LL2 (25%) 35 377.36 0.00 Singlet-A H-3-LLUNO (15%), H-3-LL1 (15%), H-5-LL2 (25%) 45 364.32 0.0007 Singlet-A H-3	8	440.67	0.0	Triplet-A	H-8→LUMO (13%), H-6→L+1 (10%)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	9	435.48	0.0013	Singlet-A	HOMO→L+1 (77%), HOMO→LUMO (19%)
11 427.49 0.0 Triplet-A HOMO-H-1(10%), HOMO-H-2(13%) 12 424.00 0.0 Singlet-A H-3-ULWO (72%), H-3-L+1 (26%) 13 424.00 0.0 Singlet-A H-3-ULWO (72%), H-3-L+1 (26%) 14 423.77 0.0 Triplet-A H-2-ULWO (15%), H-1-L+2 (25%) 15 419.51 0.0010 Singlet-A H-2-ULWO (55%), H-2-ULWO (19%), H-1-L-ULWO (14%) 17 418.62 0.0 Triplet-A H-2-ULWO (55%), H-2-ULWO (15%), H-1-ULWO (14%) 19 413.42 0.0 Triplet-A H-2-ULWO (15%), H-3-ULWO (15%), H-1-ULWO (14%) 20 412.39 0.003 Singlet-A H-3-ULWO (15%), H-3-ULWO (15%), H-3-ULWO (15%) 21 412.30 0.0 Triplet-A H-3-ULWO (15%), H-3-ULUMO (15%), H-3-ULMO (15%) 22 406.78 0.0010 Singlet-A H-3-ULWO (15%), H-3-UL-1 (10%), H-3-ULMO (15%) 24 40.61 0 Triplet-A H-4-ULWO (15%), H-3-UL-1 (10%), H-3-ULMO (15%), H-3-ULMO (10%) 25 397.76 0.0 Triplet-A H-3-ULWO (15%), H-3-UL-1 (10%), H-3-ULMO (15%), H-3-ULMO (10%) 26 397.01 0.0227	10	431.42	0.0	Triplet-A	HOMO→L+3 (35%), HOMO→L+4 (23%)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	11	427.49	0.0	Triplet-A	H-3→LUMO (69%), H-3→L+1 (27%)
13 424.00 0.0 Singlet-A H3→LUMO (72%), H3→L1 (26%) 14 423.77 0.0 Triplet-A H2→LUMO (11%), H1→L1+3 (18%), H1→L1+4 (20%) 15 419.51 0.0010 Singlet-A HOMO→L+2 (70%), H2→LUMO (19%), H1→L1+4 (20%) 16 418.74 0.0003 Singlet-A H2→LUMO (5%), H2→L1 (10%), H1→L1+4 (10%), H1→L1 17 418.62 0.0 Triplet-A H3→LUMO (40%), H3→L1 (10%), H1→L1+1 (10%), H1→L1+1 (10%), H1→L1+1 (11%) 19 413.42 0.0 Triplet-A H5→LUMO (40%), H3→L1+1 (15%) 20 412.39 0.0035 Singlet-A H1→L1+1 (11%), H1→L1+1 (15%) 21 410.23 0.0010 Singlet-A H5→LUMO (65%), H3→L1+1 (15%) 23 402.54 0.0440 Singlet-A H4→LUMO (52%), H4→L1+1 (15%) 24 401.61 0.0 Triplet-A H4→LUMO (12%), H4→L1+1 (15%) 25 397.76 0.0 Triplet-A H4→LUMO (12%), H4→L1+1 (15%) 26 397.01 0.02187 Singlet-A H5→LUMO (12%), H3→L2+1 (15%) 26 397.01 0.02187 Singlet-A H5→LUMO (12%), H3→L1+1 (15%) <tr< td=""><td>12</td><td>426.99</td><td>0.0</td><td>Triplet-A</td><td>HOMO\rightarrowL+1 (10%), HOMO\rightarrowL+2 (53%)</td></tr<>	12	426.99	0.0	Triplet-A	HOMO \rightarrow L+1 (10%), HOMO \rightarrow L+2 (53%)
14 423.77 0.0 Triplet-A H=2→LUMO (11%), H=1→L+2 (12%), H=1→L+4 (20%) 15 419.51 0.0010 Singlet-A H=2→LUMO (55%), HOMO→L+2 (22%) 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 (13%), H=1→LUMO (14%) 19 413.42 0.0 Triplet-A H=0→LUMO (40%), H=3→LUMO (14%), H=1→LUMO (14%) 20 412.39 0.003 Singlet-A H=1→L+1 (17%), H=1→LUMO (14%), H=4→LUMO (15%) 21 412.39 0.001 Singlet-A H=5→LUMO (14%), H=4→LUMO (14%) 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 (15%), H=4→L+1 (11%) 25 397.76 0.0 Triplet-A H=4→LUMO (12%), H=4→L+1 (11%) 26 397.01 0.0027 Singlet-A H=4→LUMO (12%), H=4→L+1 (11%) 27 395.56 0.0 Triplet-A H=4→LUMO (12%), H=4→L+1 (14%), H=5→LUMO (10%) 28 390.10 0.2187 Singlet-A H=5→LUMO (12%), H=4→L+1 (16%) <	13	424.00	0.0	Singlet-A	H-3→LUMO (72%), H-3→L+1 (26%)
15 419.51 0.0010 Singlet-A HOMO-L-2 (70%), H-2-LUMO (15%), 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 (15%), H-2-L+1 (10%), H-1→LUMO (14%), 18 416.58 0.0 Triplet-A H-2-LUMO (14%), H-1→LUMO (14%), 19 411.342 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 (1%), H-1→LUMO (14%), H-4→LUMO (15%), 21 412.30 0.0 Triplet-A H-5-LUMO (15%), H-5-L+1 (13%), H-4→LUMO (15%) 23 402.54 0.0440 Singlet-A H-5-LUMO (12%), H-4-LUMO (14%), H-4→LUMO (15%) 24 401.61 0.0 Triplet-A H-1-L+2 (6%) 25 397.66 0.0 Triplet-A H-3-LUMO (12%), H-6→LUMO (13%), H-6→L+1 (14%), H-5→LUMO (10%) 27 395.56 0.0 Triplet-A H-2→LUMO (12%), H-2→L+1 (6%) 38 390.10 0.2187 Singlet-A H-2→LUMO (12%), H-2→L+1 (16%), H-5→L+1 (14%), H-5→L+1 (10%), H-5→L+2 (25%) 31 382.61 0.0 Triplet-A	14	423.77	0.0	Triplet-A	H-2 \rightarrow LUMO (11%), H-1 \rightarrow L+3 (18%), H-1 \rightarrow L+4 (20%)
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 (35%), H-9→L+1 (34%) 19 413.42 0.0 Triplet-A H-9→LUMO (15%), H-1→L+1 (35%) 20 412.39 0.003 Singlet-A H-1→L1 (17%), H-1→LUMO (14%) 21 412.30 0.0 Triplet-A H-1→L1 (17%), H-1→L1 (15%), H-4→LUMO (15%) 22 406.78 0.0010 Singlet-A H-5→LUMO (14%), H-4→L1 (11%) 23 402.54 0.0440 Singlet-A H-5→LUMO (14%), H-4→L1 (11%) 24 401.61 0.0 Triplet-A H-4→L2 (69%) 25 397.76 0.0 Triplet-A H-4→L2 (69%) 26 397.01 0.0218 Singlet-A H-2→LUMO (12%), H-4→L+1 (11%) 27 395.56 0.0 Triplet-A H-2→LUMO (12%), H-4→L+1 (69%) 30 385.26 0.0055 Singlet-A H-2→LUMO (12%), H-4→L+1 (69%) 31 382.61 0.0 Triplet-A	15	419.51	0.0010	Singlet-A	HOMO→L+2 (70%), H-2→LUMO (19%)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	16	418.74	0.0003	Singlet-A	H-2 \rightarrow LUMO (55%), HOMO \rightarrow L+2 (22%)
18 416.58 0.0 Triplet-A H→→UUMO (40%), H→→U+I (3%), H→O→L+1 (23%), H→O→L+2 (23%) 19 413.42 0.0 Triplet-A H→=-L+1 (1%), H→=-LUMO (15%), H→O→LMO (15%), HOMO→L+2 (23%) 20 412.39 0.003 Singlet-A H→=-L+1 (1%), H→=-LUMO (14%) 21 412.30 0.0 Triplet-A H→=-LUMO (14%), H→=-L+1 (15%), H→=-LUMO (15%) 23 402.54 0.0440 Singlet-A H→=-L+2 (6%) 24 401.61 0.0 Triplet-A H→=-L+2 (6%) 25 397.76 0.0 Triplet-A H→=-L+2 (6%) 26 397.01 0.0027 Singlet-A H→=-L+2 (8%) 27 395.56 0.0 Triplet-A H=-L+2 (8%) 30 38.26 0.00 Triplet-A H=L+1 (1%), H=L+1 (6%) 30 38.26 0.00 Triplet-A H=L+1 (1%), H=L+1 (6%) 31 382.61 0.0 Triplet-A H=L+1 (1%), H=L+1 (6%) 33 381.34 0.0 Triplet-A H=L+1 (1%), H=L+1 (1%), H=L+1 (1%), H=L+1 (1%), H=L+2 (25%) 34 377.46 0.0 Tripl	17	418.62	0.0	Triplet-A	H-2→LUMO (35%), H-2→L+1 (10%), H-1→LUMO (14%)
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→LUMO (14%), H-1→LUMO (14%) 21 412.30 0.0 Triplet-A H-1→LUMO (14%), H-1→LUMO (15%), H-3→LUMO (15%) 22 406.78 0.0010 Singlet-A H-5→LUMO (5%), H-5→LUMO (64%) 23 402.54 0.0440 Singlet-A H-3→LUMO (5%), H-4→LUMO (64%) 24 401.61 0.0 Triplet-A H-4→LUMO (5%), H-4→LUMO (64%) 24 397.01 0.0027 Singlet-A H-1→L+2 (67%) 26 397.01 0.0027 Singlet-A H-1→L+2 (87%) 27 395.56 0.0 Triplet-A H-2→LUMO (12%), H-2→L+1 (69%) 30 385.26 0.0055 Singlet-A H-2→LUMO (12%), H-2→L+1 (69%) 31 382.61 0.0 Triplet-A H-3→LUMO (12%), H-3→L+2 (59%) 33 381.34 0.0 Triplet-A H-3→LUMO (12%), H-3→L+1 (10%), 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 (10%), H-1→L+1 (11%) 35 377.33	18	416.58	0.0	Triplet-A	H-9 \rightarrow LUMO (40%), H-9 \rightarrow L+1 (34%)
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 (15%), H-4-LUMO (15%), 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 (62%), H-4-L+1 (11%) 25 397.76 0.0 Triplet-A H-1-L+2 (69%) 26 397.01 0.0227 Singlet-A H-3-LUMO (12%), H-4-L+1 (11%), H-5-LUMO (10%) 28 390.10 0.2187 Singlet-A H-3-LUMO (12%), H-6-LUMO (13%), H-6-L+1 (14%), H-5-LUMO (10%) 28 390.10 0.2187 Singlet-A H-3-LUMO (12%), H-2-LUMO (12%) 29 386.40 0.0 Triplet-A H-2-L+1 (79%), H-2-LUMO (12%) 31 382.61 0.0 Triplet-A H-2-L+1 (19%), H-2-LUMO (12%) 33 381.34 0.0 Triplet-A H-3-LUMO (13%), H-6-L+1 (16%), H-5-L+2 (25%) 34 377.46 0.0 Triplet-A H-3-LUMO (28%), H-3-L+2 (59%) 35 377.38 0.0 Singlet-A H-3-LUMO (28%), H-3-L+1 (10%), H-5-L+2 (25%) 36 375.44 0.0001 Singlet-A H-3-LUMO (28%), H-3-L+1 (10%), H-5-L+2 (25%) 37 374.06 0.0 Triplet-A H-3-LUMO (28%), H-3-L+1 (10%), H-5-L+2 (16%) 38 373.56 0.0018 Singlet-A H-3-LUMO (27%), H-7-LUMO (15%), H-5-L+2 (16%) 41 369.29 0.0 Triplet-A H-3-LUMO (26%), H-5-L+1 (10%), H-5-L+2 (16%) 41 369.29 0.0 Triplet-A H-2-L+1 (26%), H-6-L+1 (26%), H-5-L+1 (16%) 41 369.29 0.0 Triplet-A H-2-L+1 (26%), H-6-L+1 (10%), H-5-L+2 (16%) 41 369.29 0.0 Triplet-A H-2-L+1 (26%), H-2-L+2 (25%) 42 369.03 0.0 Triplet-A H-2-L+1 (26%), H-2-L+2 (25%) 44 365.70 0.0 Triplet-A H-2-L+1 (26%), H-2-L+2 (25%) 45 364.32 0.0003 Singlet-A H-2-L+1 (26%), H-2-L+1 (16%), H-3-L+2 (26%) 46 363.67 0.0 Triplet-A H-2-L+2 (13%), H-2-L+1 (16%), H-3-L+2 (26%) 47 363.29 0.005 Singlet-A H-2-L+2 (16%), H-2-L+1 (26%), H-2-L+2 (25%) 48 359.03 0.0 Triplet-A H-2-L+2 (15%), H-2-L+1 (16%), H-3-L+2 (26%) 49 358.82 0.0 Triplet-A H-2-L+2 (13%), H-3-L+1 (16%), H-3-L+2 (26%) 49 358.82 0.0 Triplet-A H-2-L+2 (15%), H-3-L+1 (16%), H-3-L+2 (26%) 49 358.82 0.0 Triplet-A H-2-L+2 (15%), H-3-L+1 (15%) 49 358.82 0.0 Triplet-A H-3-L+1 (14%), H-3-L+2 (26%) 49 358.82 0.0 Triplet-A H-3-L+1 (14%), H-3-L+2 (26%)	19	413.42	0.0	Triplet-A	H-6 \rightarrow L+2 (29%), H-5 \rightarrow LUMO (15%), HOMO \rightarrow L+2 (23%)
21 412.30 0.0 Triplet-A H-1→LUNO (1 ⁵ %), H-1→L+1 (55%) 22 406.78 0.0010 Singlet-A H-5→LUNO (65%), H-3→LUNO (64%), 33 402.54 0.0440 Singlet-A H-5→LUNO (14%), H-3→LUNO (64%) 24 401.61 0.0 Triplet-A H-3→LUNO (12%), H-4→LUNO (64%) 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→LUNO (12%), H-6→LUNO (13%), H-6→L+1 (14%), H-5→LUNO (10%) 28 390.10 0.2187 Singlet-A H-2→LUNO (12%), H-2→L+1 (69%) 30 385.26 0.0055 Singlet-A H-2→LUNO (12%), H-2→LUNO (12%) 31 382.61 0.0 Triplet-A H-2→LUNO (12%), H-3→L+2 (43%), H-4→L+2 (12%) 32 382.09 0.0 Triplet-A H-7→LUNO (13%), H-3→L+2 (59%) 33 381.34 0.0 Triplet-A H-7→LUNO (13%), H-3→L+2 (59%), H-3→L+1 (16%), H-5→L+2 (25%) 34 377.46 0.0 Singlet-A H-3→LUNO (26%), H-3→L+1 (10%), H-5→L+1 (16%), H-5→L+2 (25%) 35 377.38 0.0 Singlet-A H-3→LUNO (26%), H-3→L+1 (70%) 36 375.44 0.001 Singlet-A H-3→LUNO (26%), H-3→L+1 (10%), H-5→LL+2 (16%) 39 373.36 0.0009 Singlet-A H-3→LUNO (26%), H-3→L+1 (13%), H-5→LUNO (15%) 39 373.36 0.0009 Singlet-A H-4→L+1 (26%), H-5→L+1 (13%), H-5→LL+2 (16%) 41 369.29 0.0 Triplet-A H-4→L+1 (26%), H-5→L+1 (13%), H-5→LL+1 (13%), H-5→L+2 (16%) 41 369.29 0.0 Triplet-A H-2→L+2 (25%), H-5→L+1 (13%), H-5→L+2 (25%) 42 369.03 0.0 Triplet-A H-2→L+2 (26%), H-5→L+1 (13%), H-5→L+2 (26%) 43 368.13 0.0077 Singlet-A H-2→L+2 (26%), H-5→L+1 (16%) 44 365.70 0.0 Triplet-A H-2→L+2 (26%), H-5→L+1 (16%) 45 364.32 0.0003 Singlet-A H-2→L+2 (26%), H-5→L+1 (16%) 46 363.67 0.0 Triplet-A H-2→L+2 (10%), H-3→L+2 (22%) 46 363.67 0.0 Triplet-A H-2→L+2 (10%), H-3→L+2 (26%) 47 363.29 0.0095 Singlet-A H-2→L+2 (10%), H-3→L+2 (26%) 48 359.03 0.0 Triplet-A H-3→L+100 (47%), H-3→L+1 (16%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-8→LUNO (47%), H-3→L+1 (16%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-8→LUNO (47%), H-3→L+7 (64%) 50 357.90 0.0 Triplet-A H-8→LUNO (47%), H-3→L+7 (64%) 50 357.90 0.0 Triplet-A H-3→L+1 (14%), HONO→L+3 (10%)	20	412.39	0.0035	Singlet-A	H-1 \rightarrow L+1 (71%), H-1 \rightarrow LUMO (14%)
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 (65%) 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-8→LUMO (11%), H-6→LUMO (13%), H-6→L+1 (14%), H-5→LUMO (10%) 28 390.10 0.2187 Singlet-A H-8→LUMO (12%), H-2→LUMO (12%) H-2→LUMO (12%) 29 386.40 0.0 Triplet-A H-3→LUMO (12%), H-2→LUMO (12%) H-2→LUMO (12%) 30 385.26 0.005 Singlet-A H-5→L+1 (13%), H-5→L+2 (43%), H-4→L+2 (12%) 31 382.61 0.0 Triplet-A H-3→LUMO (12%), H-3→L+2 (2%) 33 381.34 0.0 Triplet-A H-3→LUMO (12%), H-3→L+1 (2%), H-5→L+1 (16%), H-5→L+2 (25%) 34 377.46 0.0 Tiplet-A H-3→LUMO (28%), H-3→L+1 (70%) H-3→L+2 (25%) 35 377.38 0.0 Singlet-A H-3→LUMO (28%), H-3→L+1 (10%), H-5→L+1 (11%) H-3→L+2 (25%) 36	21	412.30	0.0	Triplet-A	$H-1 \rightarrow LUMO(11\%), H-1 \rightarrow L+1(55\%)$
23 402.54 0.040 Singlet-A H-5→LUMO (14%), H-4→LUNO (64%) 24 401.61 0.0 Triplet-A H-1→LUMO (12%), 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-6→LUMO (12%), H-6→L+1 (14%), H-5→LUMO (10%) 28 390.10 0.2187 Singlet-A H-6→LUMO (12%), H-2→LUMO (13%), H-6→L+1 (14%), H-5→LUMO (10%) 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→LUMO (12%), H-2→LUMO (12%) 31 382.61 0.0 Triplet-A H-5→LL/1 (13%), H-5→L+2 (43%), H-4→L+2 (12%) 32 382.09 0.0 Triplet-A H-7→LUMO (12%), H-3→L+2 (59%) 33 381.34 0.0 Triplet-A H-3→LUMO (28%), H-3→L+1 (15%), H-5→L+1 (16%), H-5→L+2 (25%) 44 377.46 0.0 Triplet-A H-3→LUMO (26%), H-3→L+1 (10%), H-5→L+1 (16%), H-5→L+2 (25%) 35 377.38 0.0 Singlet-A H-3→LUMO (26%), H-3→L+1 (10%), H-5→L+1 (11%) 37 374.06 0.0 Triplet-A H-3→LUMO (26%), H-3→L+1 (10%), H-5→L+1 (11%) 38 373.56 0.0018 Singlet-A H-3→LUMO (26%), H-3→L+1 (10%), H-5→L+2 (16%) 40 372.06 0.0019 Singlet-A H-4→L+1 (24%), H-4→L+1 (25%), H-5→L+1 (15%), H-5→L+2 (16%) 41 369.29 0.0 Triplet-A H-4→L+1 (26%), H-3→L+1 (15%), H-5→L+2 (16%) 42 369.03 0.0 Triplet-A H-2→L+2 (44%), H-3→L+1 (25%), H-5→L+1 (15%) 43 368.13 0.0077 Singlet-A H-2→L+2 (45%), H-3→L+1 (16%) 44 365.70 0.0 Triplet-A H-2→L+2 (45%), H-3→L+1 (16%), H-3→L+2 (25%) 43 368.13 0.0077 Singlet-A H-2→L+2 (45%), H-3→L+1 (16%), H-3→L+2 (25%) 44 365.70 0.0 Triplet-A H-2→L+2 (45%), H-3→L+1 (16%) 45 364.32 0.0003 Singlet-A H-2→L+2 (45%), H-3→L+1 (16%) 46 363.67 0.0 Triplet-A H-2→L+2 (16%), H-3→L+2 (25%) 48 359.03 0.0 Triplet-A H-2→L+2 (16%), H-3→L+2 (25%) 48 359.03 0.0 Triplet-A H-2→L+2 (16%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-2→L+2 (16%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→L+2 (10%), H-3→L+7 (15%) 47 363.29 0.005 Singlet-A H-2→L+2 (13%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→L+2 (14%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→L+1 (14%), HOMO→L+3 (10%)	22	406.78	0.0010	Singlet-A	H-5 \rightarrow LUMO (65%), H-5 \rightarrow L+1 (13%), H-4 \rightarrow LUMO (15%)
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 (69%) 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-5→L+1 (13%), H-5→L+2 (43%), H-4→L+2 (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-5→L+1 (13%), H-5→L+2 (43%), H-4→L+2 (12%) 33 381.34 0.0 Triplet-A H-3→LUMO (28%), H-3→L+1 (70%) 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 (28%), H-3→L+1 (70%) 36 375.44 0.0001 Singlet-A H-3→LUMO (28%), H-3→L+1 (70%) 38 373.56 0.0018 Singlet-A H-3→L+2 (53%), H-7→LUMO (15%), H-5→L+1 (11%) 39 373.36 0.0009 Singlet-A H-4→L+1 (31%), H-3→L+2 (35%) 31 368.13 0.0077 Singlet-A H-2→L+2 (46%), H-5→L+1 (12%), H-5→L+2 (16%) 41 369.29 0.0 Triplet-A H-2→L+2 (46%), H-5→L+1 (19%), H-3→L+2 (22%) 43 368.13 0.0077 Singlet-A H-2→L+2 (43%), H-6→L+1 (16%), H-1→L+2 (22%) 44 365.70 0.0 Triplet-A H-2→L+2 (43%), H-2→L+2 (52%) 45 364.32 0.0003 Singlet-A H-2→L+2 (43%), H-3→L+2 (52%) 46 363.67 0.0 Triplet-A H-2→L+2 (13%), H-1→L+3 (19%), H-3→L+2 (22%) 47 363.29 0.0003 Singlet-A H-2→L+2 (10%), H-3→L+2 (22%) 48 359.03 0.0 Triplet-A H-2→L+2 (13%), H-3→L+2 (25%) 48 359.03 0.0 Triplet-A H-2→L+2 (10%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-2→L+2 (10%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→LUMO (15%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→LUMO (15%), H-3→L+1 (13%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→LUMO (15%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→LUMO (15%), H-3→L+1 (13%), H-4→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→LUMO (15%), H-3→L+1 (13%), H-4→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→LUMO (15%), H-3→L+1 (13%), H-4→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→LUMO (15%), H-3→L+1 (14%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→LUMO (15%), H-3→L+1 (14%), H-3→L+2 (26%) 49 358.82 0.0 Trip	23	402.54	0.0440	Singlet-A	H-5→LUMO (14%). H-4→LUMO (64%)
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-8→LUMO (12%), H-2→LUMO (12%) 30 385.26 0.0055 Singlet-A H-2→LUMO (12%), 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-5→L+1 (13%), H-5→L+2 (43%), H-4→L+2 (12%) 33 381.34 0.0 Triplet-A H-3→LUMO (12%), H-3→L+2 (59%) 34 377.46 0.0 Triplet-A H-3→LUMO (12%), H-3→L+1 (10%), H-5→L+1 (16%), H-5→L+2 (25%) 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→LUMO (26%), H-3→L+1 (70%) 38 373.56 0.0018 Singlet-A H-3→LUMO (26%), H-3→L+1 (10%), H-7→L+1 (11%) 39 373.36 0.0009 Singlet-A H-4→L+1 (31%), H-2→L+1 (30%), H-5→L+2 (16%) 40 372.06 0.0019 Singlet-A H-4→L+1 (26%), H-3→L+1 (25%), H-3→L+2 (22%) 42 369.03 0.0 Triplet-A H-4→L+1 (26%), H-3→L+1 (19%), H-3→L+2 (22%) 43 368.13 0.0077 Singlet-A H-2→L+2 (46%), H-3→L+1 (19%), H-3→L+2 (22%) 43 368.13 0.0077 Singlet-A H-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (22%) 45 364.32 0.0003 Singlet-A H-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (22%) 46 365.77 0.0 Triplet-A H-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (22%) 47 368.13 0.0077 Singlet-A H-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (22%) 48 359.03 0.0 Triplet-A H+2→L+1 (14%), H-3→L+2 (22%) 49 358.82 0.00 Triplet-A H-2→L+2 (10%), H-3→L+1 (13%), H-3→L+2 (26%) 48 359.03 0.0 Triplet-A H+2→L+1 (10%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-8→L+1 (10%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H+2→L+1 (14%), H-3→L+2 (26%) 40 Triplet-A H+2→L+1 (14%), H-3→L+2 (26%) 41 359.03 0.0 Triplet-A H+2→L+1 (14%), H-3→L+2 (26%) 42 369.03 0.0 Triplet-A H+2→L+2 (10%), H-3→L+2 (26%) 43 368.13 0.0077 Singlet-A H+2→L+2 (10%), H-3→L+2 (26%) 44 365.70 0.0 Triplet-A H+2→L+1 (14%), H-3→L+2 (26%) 45 364.32 0.0003 Singlet-A H+2→L+1 (14%), H-3→L+2 (26%) 46 363.67 0.0 Triplet-A H+2→L+2 (10%), H-3→L+7 (15%) 47 363.29 0.0005 Singlet-A H+2→L+1 (14%), H-3→L+2 (26%) 48 359.0	24	401.61	0.0	Triplet-A	H-4→LUMO (52%), H-4→L+1 (11%)
26397.010.0027Singlet-AH-1→L+2 (87%)27395.560.0Triplet-AH-8→UUMO (11%), H-6→UUMO (13%), H-6→L+1 (14%), H-5→LUMO (10%)28390.100.2187Singlet-AH-6→UUMO (12%), H-2→UHO (12%)29386.400.0Triplet-AH-2→UUMO (12%), H-2→UUMO (12%)30385.260.0055Singlet-AH-2→UUMO (17%), H-3→UUMO (12%)31382.610.0Triplet-AH-5→L+1 (13%), H-5→L+2 (39%)32382.090.0Triplet-AH-7→UUMO (17%), H-3→L+2 (59%)33381.340.0Triplet-AH-3→UUMO (28%), H-3→L+1 (70%)35377.380.0Singlet-AH-3→LUMO (28%), H-3→L+1 (70%)36375.440.0001Singlet-AH-3→LUMO (26%), H-3→L+1 (70%)37374.060.0Triplet-AH-4→L+1 (31%), H-2→L+2 (35%)38373.560.0018Singlet-AH-3→LUMO (26%), H-3→L+1 (70%)39373.360.0009Singlet-AH-4→L+1 (26%), H-5→L+1 (13%), H-5→L+2 (16%)40372.060.0019Singlet-AH-2→L+2 (45%), H-5→L+1 (15%)41368.130.0077Singlet-AH-2→L+2 (45%), H-3→L+1 (19%), H-3→L+2 (22%)42369.030.0Triplet-AH-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (22%)43368.130.0077Singlet-AH-2→L+2 (43%), H-3→L+1 (16%)44365.700.0Triplet-AH-2→L+2 (19%), H-3→L+2 (29%)45364.320.0003Singlet-AH-3→LUMO (42%), H-3→L+2 (19%) <td>25</td> <td>397.76</td> <td>0.0</td> <td>Triplet-A</td> <td>H-1→L+2 (69%)</td>	25	397.76	0.0	Triplet-A	H-1→L+2 (69%)
27395.560.0Triplet-AH-8→LUMO (11%), H-6→LUMO (13%), H-6→L+1 (14%), H-5→LUMO (10%)28390.100.2187Singlet-AH-6→LUMO (12%), H-2→L+1 (69%)30385.260.0055Singlet-AH-2→LUMO (12%), H-2→LUMO (12%)31382.610.0Triplet-AH-5→L+1 (13%), H-5→L+2 (43%), H-4→L+2 (12%)32382.090.0Triplet-AH-7→LUMO (17%), H-3→L+2 (59%)33381.340.0Triplet-AH-3→LUMO (28%), H-3→L+1 (10%), H-5→L+1 (16%), H-5→L+2 (25%)34377.460.0Triplet-AH-3→LUMO (28%), H-3→L+1 (70%)35377.380.0Singlet-AH-3→LUMO (26%), H-3→L+1 (70%)36375.440.0001Singlet-AH-3→L+2 (53%)39373.560.0018Singlet-AH-5→L+1 (49%), H-4→L+1 (30%), H-5→LUMO (15%)39373.360.0009Singlet-AH-4→L+1 (26%), H-5→L+1 (10%), H-5→L+2 (16%)41369.290.0Triplet-AH-4→L+1 (26%), H-5→L+1 (10%), H-5→L+2 (16%)42369.030.0Triplet-AH-2→L+2 (43%), H-4→L+1 (30%), H-3→L+2 (22%)43368.130.0077Singlet-AH-2→L+2 (43%), H-3→L+1 (10%), H-3→L+2 (22%)44365.700.0Triplet-AH-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (22%)45364.320.0003Singlet-AH-2→L+1 (11%), H-1→L+1 (19%), H-3→L+2 (29%)46363.670.0Triplet-AH-2→L+2 (13%), H-1→L+1 (14%), H-3→L+2 (39%)46363.670.0Triplet-AH-8→L+1 (00%), H-1→L+1 (13	26	397.01	0.0027	Singlet-A	H-1→L+2 (87%)
28390.100.2187Singlet-AH-6→LUMO (72%)H C (2, y)H C (2, y)H C (2, y)H C (2, y)H (2, y)	27	395.56	0.0	Triplet-A	H-8 \rightarrow LUMO (11%), H-6 \rightarrow LUMO (13%), H-6 \rightarrow L+1 (14%), H-5 \rightarrow LUMO (10%)
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-3→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 (26%), H-3→L+1 (70%) 36 375.44 0.0001 Singlet-A H-3→LUMO (26%), H-3→L+1 (70%) 38 373.56 0.0018 Singlet-A H-3→LUMO (26%), H-3→L+1 (70%) 38 373.56 0.0019 Singlet-A H-3→L+1 (31%), H-2→L+2 (35%) 40 372.06 0.0019 Singlet-A H-3→L+1 (26%), H-3→L+1 (10%), H-5→L+2 (16%) 41 369.29 0.0 Triplet-A H-4→L+1 (26%), H-3→L+1 (16%) 41 369.29 0.0 Triplet-A H-4→L+1 (26%), H-3→L+1 (16%) 42 369.03 0.0 Triplet-A H-2→L+2 (43%), H-3→L+1 (16%) 44 365.70 0.0 Triplet-A H-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (22%) 45 364.32 0.0003 Singlet-A H-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (39%) 46 363.67 0.0 Triplet-A H-2→L+2 (10%), H-3→L+2 (39%) 46 363.67 0.0 Triplet-A H-2→L+2 (10%), H-3→L+2 (39%) 47 363.29 0.0003 Singlet-A H-2→L+2 (10%), H-3→L+2 (39%) 48 359.03 0.0 Triplet-A H-2→L+2 (10%), H-3→L+2 (39%) 48 359.03 0.0 Triplet-A H-3→LUMO (15%), H-3→L+2 (39%) 48 359.03 0.0 Triplet-A H-8→L+2 (10%), H-3→L+2 (39%) 48 359.03 0.0 Triplet-A H-8→L+2 (10%), H-3→L+1 (13%), H-4→L+2 (26%) 49 358.82 0.0 Triplet-A H-10→LUMO (15%), H-3→L+1 (13%), H-4→L+2 (26%) 49 358.82 0.0 Triplet-A H-8→L+1 (14%), H-3→L+2 (26%)	28	390.10	0.2187	Singlet-A	H-6→LUMO (72%)
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-3→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 (26%), 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-3→L+2 (53%), H-7→LUMO (27%), H-5→L+1 (11%) 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-5→L+1 (49%), H-4→L+1 (30%), H-5→L+2 (16%) 40 372.06 0.0019 Singlet-A H-2→L+2 (46%), H-6→L+1 (12%), H-5→L+2 (16%) 41 369.29 0.0 Triplet-A H-2→L+2 (46%), H-5→L+1 (16%) 42 369.03 0.0 Triplet-A H-2→L+2 (46%), H-3→L+1 (16%), 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+2 (43%), H-8→LUMO (10%), H-3→L+2 (23%) 45 364.32 0.0003 Singlet-A H-2→L+2 (10%), H-3→L+2 (15%) 46 63.67 0.0 Triplet-A H-2→L+2 (10%), H-3→L+1 (14%), H-3→L+2 (39%) 46 363.67 0.0 Triplet-A H-2→L+2 (10%), H-3→L+1 (14%), H-3→L+2 (39%) 47 363.29 0.0095 Singlet-A H-8→L+2 (10%), H-3→L+1 (13%), H-4→L+2 (26%) 48 359.03 0.0 Triplet-A H-8→L+2 (10%), H-3→L+2 (26%) 49 358.82 0.0 Triplet-A H-3→L+2 (13%), H-3→L+7 (64%) 50 357.90 0.0 Triplet-A H-8→L+1 (14%), HOMO→L+3 (10%)	29	386.40	0.0	Triplet-A	H-2→LUMO (12%), H-2→L+1 (69%)
31382.610.0Triplet-AH-5→L+1 (13%), H-5→L+2 (43%), H-4→L+2 (12%)32382.090.0Triplet-AH-7→LUMO (17%), H-3→L+2 (59%)33381.340.0Triplet-AH-8→LUMO (28%), H-3→L+1 (12%), H-5→L+1 (16%), H-5→L+2 (25%)34377.460.0Triplet-AH-3→LUMO (28%), H-3→L+1 (70%)35377.380.0Singlet-AH-3→LUMO (26%), H-3→L+1 (70%)36375.440.0001Singlet-AH-3→LL4 (53%), H-7→LUMO (27%), H-7→L+1 (11%)37374.060.0Triplet-AH-4→L+1 (30%), H-5→L+1 (13%), H-5→L+2 (16%)38373.560.0018Singlet-AH-5→L+1 (49%), H-4→L+1 (30%), H-5→L+1 (13%), H-5→L+2 (16%)40372.060.0019Singlet-AH-2→L+2 (46%), H-5→L+1 (16%)41369.290.0Triplet-AH-2→L+2 (46%), H-5→L+1 (16%)43368.130.0077Singlet-AH-2→L+2 (42%), H-7→L+1 (19%), H-3→L+2 (22%)43368.130.0077Singlet-AH-2→L+2 (43%), H-8→LUMO (10%), H-4→L+1 (16%)44365.700.0Triplet-AH-2→L+2 (43%), H-8→LUMO (10%), H-3→L+2 (22%)45364.320.0003Singlet-AH-2→L+2 (13%), H-1→L+1 (14%), H-3→L+2 (39%)46363.670.0Triplet-AH-8→LUMO (47%), H-6→L+1 (13%)47363.290.0095Singlet-AH-8→LUMO (47%), H-6→L+1 (13%)48359.030.0Triplet-AH-8→LUMO (15%), H-8→L+7 (15%)49358.820.0Triplet-AH-8→LUMO (15%), H-3→L+7 (64%) <tr< td=""><td>30</td><td>385.26</td><td>0.0055</td><td>Singlet-A</td><td>$H-2\rightarrow L+1$ (79%), $H-2\rightarrow LUMO$ (12%)</td></tr<>	30	385.26	0.0055	Singlet-A	$H-2\rightarrow L+1$ (79%), $H-2\rightarrow LUMO$ (12%)
32382.090.0Triplet-AH-7→LUMO (17%), H-3→L+2 (59%)33381.340.0Triplet-AH-8→LUMO (13%), H-6→L+1 (12%), H-5→L+1 (16%), H-5→L+2 (25%)34377.460.0Triplet-AH-3→LUMO (28%), H-3→L+1 (70%)35377.380.0Singlet-AH-3→LUMO (27%), H-7→LUMO (27%), H-7→L+1 (11%)36375.440.0001Singlet-AH-3→L+2 (53%), H-7→LUMO (27%), H-7→L+1 (11%)37374.060.0Triplet-AH-4→L+1 (31%), H-2→L+2 (35%)38373.560.0018Singlet-AH-5→L+1 (49%), H-4→L+1 (30%), H-5→LUMO (15%)39373.360.0009Singlet-AH-2→L+2 (46%), H-6→L+1 (22%), H-5→L+1 (13%), H-5→L+2 (16%)41369.290.0Triplet-AH-4→L+1 (26%), H-2→L+2 (52%)42369.030.0Triplet-AH-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (22%)43368.130.0077Singlet-AH-2→L+2 (43%), H-8→LUMO (10%), H-4→L+1 (16%)44365.700.0Triplet-AH-2→L+2 (43%), H-3→L+1 (19%), H-3→L+2 (39%)46363.670.0Triplet-AH-7→LUMO (42%), H-5→L+1 (14%), H-3→L+2 (39%)47363.290.0095Singlet-AH-8→L+2 (10%), H-5→L+1 (13%), H-4→L+2 (26%)48359.030.0Triplet-AH-8→L+2 (13%), H-3→L+7 (55%)48359.030.0Triplet-AH-7→L+2 (13%), H-3→L+7 (56%)50357.900.0Triplet-AH-7→L+2 (13%), H-3→L+1 (13%), H-4→L+2 (26%)50357.900.0Triplet-AH-7→L+2 (13%), H-3→	31	382.61	0.0	Triplet-A	H-5 \rightarrow L+1 (13%), H-5 \rightarrow L+2 (43%), H-4 \rightarrow L+2 (12%)
33381.340.0Triplet-AH-8→LUMO (13%), H-6→L+1 (12%), H-5→L+1 (16%), H-5→L+2 (25%)34377.460.0Triplet-AH-3→LUMO (28%), H-3→L+1 (70%)35377.380.0Singlet-AH-3→LUMO (26%), H-3→L+1 (70%)36375.440.0001Singlet-AH-3→LUQ (26%), H-3→L+1 (70%)37374.060.0Triplet-AH-4→L+1 (31%), H-2→L+2 (35%)38373.560.0018Singlet-AH-5→L+1 (49%), H-4→L+1 (30%), H-5→LUMO (15%)39373.360.0009Singlet-AH-4→L+1 (26%), H-6→L+1 (22%), H-5→L+1 (13%), H-5→L+2 (16%)40372.060.0019Singlet-AH-4→L+1 (26%), H-2→L+2 (52%)41369.290.0Triplet-AH-4→L+1 (26%), H-7→L+1 (19%), H-3→L+2 (22%)43368.130.0077Singlet-AH-2→L+2 (43%), H-8→LUMO (10%), H-1→L+4 (13%)44365.700.0Triplet-AH-2→L+2 (43%), H-1→L+1 (14%), H-3→L+2 (39%)46363.670.0Triplet-AH-2→L+2 (10%), H-1→L+1 (14%), H-3→L+2 (39%)47363.290.0095Singlet-AH-8→LUMO (47%), H-6→L+1 (13%), H-1→L+2 (26%)48359.030.0Triplet-AH-8→LUMO (15%), H-3→L+7 (15%)48359.030.0Triplet-AH-8→LUMO (15%), H-3→L+7 (64%)50357.900.0Triplet-AH-7→L+2 (13%), H-3→L+7 (64%)50357.900.0Triplet-AH-7→L+2 (13%), H-3→L+7 (64%)	32	382.09	0.0	Triplet-A	H-7→LUMO (17%), H-3→L+2 (59%)
34377.460.0Triplet-AH-3 \rightarrow LUMO (28%), H-3 \rightarrow L+1 (70%)35377.380.0Singlet-AH-3 \rightarrow LUMO (26%), H-3 \rightarrow L+1 (70%)36375.440.0001Singlet-AH-3 \rightarrow L+2 (53%), H-7 \rightarrow LUMO (27%), H-7 \rightarrow L+1 (11%)37374.060.0Triplet-AH-4 \rightarrow L+1 (31%), H-2 \rightarrow L+2 (35%)38373.560.0018Singlet-AH-5 \rightarrow L+1 (49%), H-4 \rightarrow L+1 (30%), H-5 \rightarrow LUMO (15%)39373.360.0009Singlet-AH-4 \rightarrow L+1 (26%), H-6 \rightarrow L+1 (22%), H-5 \rightarrow L+1 (13%), H-5 \rightarrow L+2 (16%)40372.060.0019Singlet-AH-2 \rightarrow L+2 (46%), H-5 \rightarrow L+1 (16%)41369.290.0Triplet-AH-4 \rightarrow L+1 (26%), H-2 \rightarrow L+2 (52%)42369.030.0Triplet-AH-7 \rightarrow LUMO (51%), H-3 \rightarrow L+2 (22%)43368.130.0077Singlet-AH-2 \rightarrow L+2 (43%), H-3 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)44365.700.0Triplet-AH-2 \rightarrow L+2 (43%), H-3 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)45364.320.0003Singlet-AH-2 \rightarrow L+2 (10%), H-1 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%)46363.670.0Triplet-AH-8 \rightarrow L+2 (10%), H-5 \rightarrow L+7 (15%)47363.290.0095Singlet-AH-8 \rightarrow LUMO (47%), H-6 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)48359.030.0Triplet-AH-8 \rightarrow LUMO (15%), H-3 \rightarrow L+7 (64%)50357.900.0Triplet-AH-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)6" Footnote text	33	381.34	0.0	Triplet-A	H-8 \rightarrow LUMO (13%), H-6 \rightarrow L+1 (12%), H-5 \rightarrow L+1 (16%), H-5 \rightarrow L+2 (25%)
35377.380.0Singlet-AH-3→LUMO (26%), H-3→L+1 (70%)36375.440.0001Singlet-AH-3→L+2 (53%), H-7→LUMO (27%), H-7→L+1 (11%)37374.060.0Triplet-AH-4→L+1 (31%), H-2→L+2 (35%)38373.560.0018Singlet-AH-5→L+1 (49%), H-4→L+1 (20%), H-5→LUMO (15%)39373.360.0009Singlet-AH-4→L+1 (26%), H-6→L+1 (22%), H-5→L+1 (13%), H-5→L+2 (16%)40372.060.0019Singlet-AH-4→L+1 (26%), H-2→L+2 (52%)41369.290.0Triplet-AH-4→L+1 (26%), H-2→L+2 (52%)42369.030.0Triplet-AH-2→L+2 (43%), H-8→LUMO (10%), H-3→L+2 (22%)43368.130.0077Singlet-AH-2→L+3 (13%), H-1→L+3 (21%), H-1→L+4 (13%)44365.700.0Triplet-AH-2→L+2 (10%), H-7→L+1 (14%), H-3→L+2 (39%)46363.670.0Triplet-AH-8→LUMO (42%), H-7→L+1 (14%), H-3→L+2 (39%)47363.290.0095Singlet-AH-8→LUMO (15%), H-8→L+1 (13%)48359.030.0Triplet-AH-8→L10MO (15%), H-8→L+1 (13%), H-4→L+2 (26%)49358.820.0Triplet-AH-7→L2(13%), H-3→L+7 (64%)50357.900.0Triplet-AH-8→L+1 (14%), HOMO→L+3 (10%)	34	377.46	0.0	Triplet-A	H-3→LUMO (28%), H-3→L+1 (70%)
36375.440.0001Singlet-AH-3→L+2 (53%), H-7→LUMO (27%), H-7→L+1 (11%)37374.060.0Triplet-AH-4→L+1 (31%), H-2→L+2 (35%)38373.560.0018Singlet-AH-5→L+1 (49%), H-4→L+1 (30%), H-5→LUMO (15%)39373.360.0009Singlet-AH-4→L+1 (26%), H-6→L+1 (22%), H-5→L+1 (13%), H-5→L+2 (16%)40372.060.0019Singlet-AH-2→L+2 (46%), H-6→L+1 (22%), H-5→L+1 (13%), H-5→L+2 (16%)41369.290.0Triplet-AH-4→L+1 (26%), H-2→L+2 (52%)42369.030.0Triplet-AH-7→LUMO (51%), H-7→L+1 (19%), H-3→L+2 (22%)43368.130.0077Singlet-AH-2→L+2 (43%), H-8→LUMO (10%), H-4→L+1 (16%)44365.700.0Triplet-AH-2→L+3 (13%), H-1→L+3 (21%), H-1→L+4 (13%)45364.320.0003Singlet-AH-7→LUMO (42%), H-7→L+1 (14%), H-3→L+2 (39%)46363.670.0Triplet-AH-8→L+2 (10%), H-5→L+7 (15%)47363.290.0095Singlet-AH-8→LUMO (15%), H-8→L+1 (13%), H-4→L+2 (26%)48359.030.0Triplet-AH-8→L+2 (13%), H-3→L+7 (64%)50357.900.0Triplet-AH-8→L+1 (14%), HOMO→L+3 (10%)650357.900.0Triplet-A650357.900.0Triplet-A650357.900.0Triplet-A650357.900.0Triplet-A650357.900.0Triplet-A750357.90	35	377.38	0.0	Singlet-A	H-3→LUMO (26%), H-3→L+1 (70%)
37374.060.0Triplet-AH-4 \rightarrow L+1 (31%), H-2 \rightarrow L+2 (35%)38373.560.0018Singlet-AH-5 \rightarrow L+1 (49%), H-4 \rightarrow L+1 (30%), H-5 \rightarrow LUMO (15%)39373.360.0009Singlet-AH-4 \rightarrow L+1 (26%), H-6 \rightarrow L+1 (22%), H-5 \rightarrow L+1 (13%), H-5 \rightarrow L+2 (16%)40372.060.0019Singlet-AH-2 \rightarrow L+2 (46%), H-5 \rightarrow L+1 (16%)41369.290.0Triplet-AH-4 \rightarrow L+1 (26%), H-2 \rightarrow L+2 (52%)42369.030.0Triplet-AH-7 \rightarrow LUMO (51%), H-7 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)43368.130.0077Singlet-AH-2 \rightarrow L+2 (43%), H-8 \rightarrow LUMO (10%), H-4 \rightarrow L+1 (16%)44365.700.0Triplet-AH-2 \rightarrow L+3 (13%), H-1 \rightarrow L+3 (21%), H-1 \rightarrow L+4 (13%)45364.320.0003Singlet-AH-7 \rightarrow LUMO (42%), H-7 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%)46363.670.0Triplet-AH-8 \rightarrow L+2 (10%), H-5 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)48359.030.0Triplet-AH-8 \rightarrow LUMO (15%), H-8 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)49358.820.0Triplet-AH-7 \rightarrow L+2 (13%), H-3 \rightarrow L+2 (26%)49358.820.0Triplet-AH-7 \rightarrow L+2 (13%), H-3 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)4° Evotrote text	36	375.44	0.0001	Singlet-A	H-3→L+2 (53%), H-7→LUMO (27%), H-7→L+1 (11%)
38373.560.0018Singlet-AH-5 \rightarrow L+1 (49%), H-4 \rightarrow L+1 (30%), H-5 \rightarrow LUMO (15%)39373.360.0009Singlet-AH-4 \rightarrow L+1 (26%), H-6 \rightarrow L+1 (22%), H-5 \rightarrow L+1 (13%), H-5 \rightarrow L+2 (16%)40372.060.0019Singlet-AH-2 \rightarrow L+2 (46%), H-5 \rightarrow L+1 (16%)41369.290.0Triplet-AH-4 \rightarrow L+1 (26%), H-2 \rightarrow L+2 (52%)42369.030.0Triplet-AH-7 \rightarrow LUMO (51%), H-7 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)43368.130.0077Singlet-AH-2 \rightarrow L+2 (43%), H-8 \rightarrow LUMO (10%), H-4 \rightarrow L+1 (16%)44365.700.0Triplet-AH-2 \rightarrow L+2 (43%), H-1 \rightarrow L+3 (21%), H-1 \rightarrow L+4 (13%)45364.320.0003Singlet-AH-2 \rightarrow L+2 (10%), H-7 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%)46363.670.0Triplet-AH-8 \rightarrow L+2 (10%), H-6 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)48359.030.0Triplet-AH-8 \rightarrow LUMO (15%), H-8 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)49358.820.0Triplet-AH-7 \rightarrow L+2 (13%), H-3 \rightarrow L+7 (64%)50357.900.0Triplet-AH-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)	37	374.06	0.0	Triplet-A	$H-4 \rightarrow L+1 (31\%), H-2 \rightarrow L+2 (35\%)$
39373.360.0009Singlet-AH-4 \rightarrow L+1 (26%), H-6 \rightarrow L+1 (22%), H-5 \rightarrow L+1 (13%), H-5 \rightarrow L+2 (16%)40372.060.0019Singlet-AH-2 \rightarrow L+2 (46%), H-5 \rightarrow L+1 (16%)41369.290.0Triplet-AH-4 \rightarrow L+1 (26%), H-2 \rightarrow L+2 (52%)42369.030.0Triplet-AH-7 \rightarrow LUMO (51%), H-7 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)43368.130.0077Singlet-AH-2 \rightarrow L+2 (43%), H-8 \rightarrow LUMO (10%), H-4 \rightarrow L+1 (16%)44365.700.0Triplet-AH-2 \rightarrow L+3 (13%), H-1 \rightarrow L+3 (21%), H-1 \rightarrow L+4 (13%)45364.320.0003Singlet-AH-7 \rightarrow LUMO (42%), H-7 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%)46363.670.0Triplet-AH-8 \rightarrow LUMO (47%), H-6 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)48359.030.0Triplet-AH-10 \rightarrow LUMO (15%), H-3 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)49358.820.0Triplet-AH-7 \rightarrow LL2 (13%), H-3 \rightarrow L+1 (14%), H-4 \rightarrow L+2 (26%)50357.900.0Triplet-AH-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)	38	373.56	0.0018	Singlet-A	$H-5 \rightarrow L+1$ (49%), $H-4 \rightarrow L+1$ (30%), $H-5 \rightarrow LUMO$ (15%)
40372.060.0019Singlet-AH-2 \rightarrow L+2 (46%), H-5 \rightarrow L+1 (16%)41369.290.0Triplet-AH-4 \rightarrow L+1 (26%), H-2 \rightarrow L+2 (52%)42369.030.0Triplet-AH-7 \rightarrow LUMO (51%), H-7 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)43368.130.0077Singlet-AH-2 \rightarrow L+2 (43%), H-8 \rightarrow LUMO (10%), H-4 \rightarrow L+1 (16%)44365.700.0Triplet-AH-2 \rightarrow L+3 (13%), H-1 \rightarrow L+3 (21%), H-1 \rightarrow L+4 (13%)45364.320.0003Singlet-AH-7 \rightarrow LUMO (42%), H-7 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%)46363.670.0Triplet-AH-8 \rightarrow LUMO (42%), H-7 \rightarrow L+1 (15%)47363.290.0095Singlet-AH-8 \rightarrow LUMO (47%), H-6 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)48359.030.0Triplet-AH-10 \rightarrow LUMO (15%), H-3 \rightarrow L+7 (64%)50357.900.0Triplet-AH-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)	39	373.36	0.0009	Singlet-A	$H-4 \rightarrow L+1$ (26%), $H-6 \rightarrow L+1$ (22%), $H-5 \rightarrow L+1$ (13%), $H-5 \rightarrow L+2$ (16%)
41369.290.0Triplet-AH-4 \rightarrow L+1 (26%), H-2 \rightarrow L+2 (52%)42369.030.0Triplet-AH-7 \rightarrow LUMO (51%), H-7 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)43368.130.0077Singlet-AH-2 \rightarrow L+2 (43%), H-8 \rightarrow LUMO (10%), H-4 \rightarrow L+1 (16%)44365.700.0Triplet-AH-2 \rightarrow L+3 (13%), H-1 \rightarrow L+3 (21%), H-1 \rightarrow L+4 (13%)45364.320.0003Singlet-AH-7 \rightarrow LUMO (42%), H-7 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%)46363.670.0Triplet-AH-8 \rightarrow L+2 (10%), H-5 \rightarrow L+7 (15%)47363.290.0095Singlet-AH-8 \rightarrow LUMO (47%), H-6 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)48359.030.0Triplet-AH-10 \rightarrow LUMO (15%), H-3 \rightarrow L+7 (64%)50357.900.0Triplet-AH-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)	40	372.06	0.0019	Singlet-A	$H-2 \rightarrow L+2$ (46%), $H-5 \rightarrow L+1$ (16%)
42369.030.0Triplet-AH-7 \rightarrow LUMO (51%), H-7 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)43368.130.0077Singlet-AH-2 \rightarrow L+2 (43%), H-8 \rightarrow LUMO (10%), H-4 \rightarrow L+1 (16%)44365.700.0Triplet-AH-2 \rightarrow L+3 (13%), H-1 \rightarrow L+3 (21%), H-1 \rightarrow L+4 (13%)45364.320.0003Singlet-AH-7 \rightarrow LUMO (42%), H-7 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%)46363.670.0Triplet-AH-8 \rightarrow L+2 (10%), H-5 \rightarrow L+7 (15%)47363.290.0095Singlet-AH-8 \rightarrow LUMO (47%), H-6 \rightarrow L+1 (35%)48359.030.0Triplet-AH-10 \rightarrow LUMO (15%), H-8 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)49358.820.0Triplet-AH-7 \rightarrow L+2 (13%), H-3 \rightarrow L+7 (64%)50357.900.0Triplet-AH-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)	41	369.29	0.0	Triplet-A	$H-4 \rightarrow L+1$ (26%), $H-2 \rightarrow L+2$ (52%)
43 368.13 0.0077 Singlet-A $H-2 \rightarrow L+2$ (43%), $H-8 \rightarrow LUMO (10%), H-4 \rightarrow L+1 (16%)$ 44 365.70 0.0 Triplet-A $H-2 \rightarrow L+3 (13\%), H-1 \rightarrow L+3 (21\%), H-1 \rightarrow L+4 (13\%)$ 45 364.32 0.0033 Singlet-A $H-7 \rightarrow LUMO (42\%), H-7 \rightarrow L+1 (14\%), H-3 \rightarrow L+2 (39\%)$ 46 363.67 0.0 Triplet-A $H-8 \rightarrow L+2 (10\%), H-5 \rightarrow L+7 (15\%)$ 47 363.29 0.0095 Singlet-A $H-8 \rightarrow LUMO (47\%), H-6 \rightarrow L+1 (35\%)$ 48 359.03 0.0 Triplet-A $H-10 \rightarrow LUMO (15\%), H-8 \rightarrow L+1 (13\%), H-4 \rightarrow L+2 (26\%)$ 49 358.82 0.0 Triplet-A $H-7 \rightarrow L+2 (13\%), H-3 \rightarrow L+7 (64\%)$ 50 357.90 0.0 Triplet-A $H-8 \rightarrow L+1 (14\%), HOMO \rightarrow L+3 (10\%)$	42	369.03	0.0	Triplet-A	H-7 \rightarrow LUMO (51%), H-7 \rightarrow L+1 (19%), H-3 \rightarrow L+2 (22%)
44 365.70 0.0 Triplet-A H-2 \rightarrow L+3 (13%), H-1 \rightarrow L+3 (21%), H-1 \rightarrow L+4 (13%) 45 364.32 0.0003 Singlet-A H-7 \rightarrow LUMO (42%), H-7 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%) 46 363.67 0.0 Triplet-A H-8 \rightarrow L+2 (10%), H-5 \rightarrow L+7 (15%) 47 363.29 0.0095 Singlet-A H-8 \rightarrow LUMO (47%), H-6 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%) 48 359.03 0.0 Triplet-A H-10 \rightarrow LUMO (15%), H-8 \rightarrow L+7 (64%) 49 358.82 0.0 Triplet-A H-7 \rightarrow L+2 (13%), H-3 \rightarrow L+7 (64%) 50 357.90 0.0 Triplet-A H-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)	43	368.13	0.0077	Singlet-A	$H-2 \rightarrow L+2$ (43%), $H-8 \rightarrow LUMO$ (10%), $H-4 \rightarrow L+1$ (16%)
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+1 (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-8→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%)	44	365.70	0.0	Triplet-A	$H-2 \rightarrow L+3$ (13%), $H-1 \rightarrow L+3$ (21%), $H-1 \rightarrow L+4$ (13%)
46 363.67 0.0 Triplet-A H-8 \rightarrow L+2 (10%), H-5 \rightarrow L+7 (15%) 47 363.29 0.0095 Singlet-A H-8 \rightarrow LUMO (47%), H-6 \rightarrow L+1 (35%) 48 359.03 0.0 Triplet-A H-10 \rightarrow LUMO (15%), H-8 \rightarrow L+7 (64%) 49 358.82 0.0 Triplet-A H-7 \rightarrow L+2 (13%), H-3 \rightarrow L+7 (64%) 50 357.90 0.0 Triplet-A H-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)	45	364.32	0.0003	Singlet-A	H-7 \rightarrow LUMO (42%), H-7 \rightarrow L+1 (14%), H-3 \rightarrow L+2 (39%)
47 363.29 0.0095 Singlet-A $H-8 \rightarrow LUMO(47\%), H-6 \rightarrow L+1(35\%)$ 48 359.03 0.0 Triplet-A $H-10 \rightarrow LUMO(15\%), H-8 \rightarrow L+1(13\%), H-4 \rightarrow L+2(26\%)$ 49 358.82 0.0 Triplet-A $H-7 \rightarrow L+2(13\%), H-3 \rightarrow L+7(64\%)$ 50 357.90 0.0 Triplet-A $H-8 \rightarrow L+1(14\%), HOMO \rightarrow L+3(10\%)$	46	363.67	0.0	Triplet-A	$H-8 \rightarrow L+2$ (10%), $H-5 \rightarrow L+7$ (15%)
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%)	47	363.29	0.0095	Singlet-A	$H-8 \rightarrow LUMO(47\%), H-6 \rightarrow L+1(35\%)$
49 358.82 0.0 Triplet-A H-7 \rightarrow L+2 (13%), H-3 \rightarrow L+7 (64%) 50 357.90 0.0 Triplet-A H-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%) ^a Footnote text 436.82 436.82 436.82	48	359.03	0.0	Triplet-A	H-10 \rightarrow LUMO (15%), H-8 \rightarrow L+1 (13%), H-4 \rightarrow L+2 (26%)
50 357.90 0.0 Triplet-A H-8 \rightarrow L+1 (14%), HOMO \rightarrow L+3 (10%)	49	358.82	0.0	Triplet-A	$H-7 \rightarrow L+2$ (13%), $H-3 \rightarrow L+7$ (64%)
^a Footnote text	50	357.90	0.0	Triplet-A	$H-8 \rightarrow L+1$ (14%), HOMO $\rightarrow L+3$ (10%)
	^a Footno	ote text.		1	