

Table S1- Molecular orbital composition of Eu(TTA)₃(phen-X) complexes

Orbital	Eu_TTA	Eu_phen	Eu_phen_methyl	Eu_phen_methoxy	Eu_phen_chloro
H-14	π (TTA)	π (TTA)	π (TTA)	π (phen + TTA)	π (TTA)
H-13	π (TTA)	π (phen)	π (phen)	π (TTA)	π (phen)
H-12	π (TTA)	π (TTA)	π (TTA)	π (phen + TTA)	π (TTA + phen)
H-11	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA + phen)
H-10	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H-9	π (TTA)	π (TTA + phen)	π (TTA)	π (TTA)	π (TTA + phen)
H-8	π (TTA)	π (TTA + phen)	π (TTA + phen)	π (TTA)	π (TTA)
H-7	π (TTA)	π (TTA + phen)	π (TTA)	π (TTA)	π (TTA)
H-6	π (TTA)	π (TTA)	π (TTA + phen)	π (TTA)	π (TTA)
H-5	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H-4	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H-3	π (TTA)	π (TTA)	π (TTA + phen)	π (phen + TTA)	π (TTA)
H-2	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H-1	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
L	π^* (TTA)	π^* (phen)	π^* (TTA)	π^* (TTA)	π^* (phen)
L+1	π^* (TTA)	π^* (TTA)	π^* (phen + TTA)	π^* (TTA)	π^* (phen)
L+2	π^* (TTA)	π^* (phen)	π^* (TTA + phen)	π^* (TTA)	π^* (TTA)
L+3	π^* (TTA)	π^* (TTA)	π^* (TTA)	π^* (phen + TTA)	π^* (TTA)
L+4	π^* (TTA)	π^* (TTA)	π^* (TTA + phen)	π^* (phen + TTA)	π^* (TTA)

Table S1- Molecular orbital composition of Eu(TTA)₃(phen-X) complexes (cont.)

Orbital	Eu_phen_Br	Eu_phen_carboxylate	Eu_phen_phenyl	Eu_phen_1_butin_3_yn	Eu_phen_1_buten_3_yn
H-14	π (TTA)	π (phen + TTA)	π (phen)	π (phen)	π (TTA)
H-13	π (phen)	π (phen)	π (TTA)	π (TTA)	π (TTA + phen)
H-12	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H-11	π (TTA + phen)	π (TTA)	π (TTA)	π (phen)	π (phen + TTA)
H-10	π (TTA)	π (TTA)	π (phen)	π (TTA)	π (TTA)
H-9	π (TTA + phen)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H-8	π (TTA)	π (TTA + phen)	π (TTA)	π (TTA)	π (TTA)
H-7	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H-6	π (TTA)	π (TTA + phen)	π (TTA)	π (TTA)	π (TTA)
H-5	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA)
H-4	π (TTA)	π (TTA)	π (TTA)	π (phen)	π (phen)
H-3	π (TTA)	π (TTA + phen)	π (phen + TTA)	π (phen + TTA)	π (TTA)
H-2	π (TTA)	π (TTA)	π (TTA)	π (TTA + phen)	π (TTA + phen)
H-1	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA + phen)
H	π (TTA)	π (TTA)	π (TTA)	π (TTA)	π (TTA + phen)
L	π^* (phen)	π^* (phen)	π^* (phen)	π^* (phen)	π^* (phen)
L+1	π^* (phen)	π^* (phen)	π^* (TTA)	π^* (phen)	π^* (phen)
L+2	π^* (TTA)	π^* (TTA)	π^* (phen)	π^* (TTA)	π^* (TTA)
L+3	π^* (TTA)	π^* (TTA)	π^* (TTA)	π^* (TTA)	π^* (TTA)
L+4	π^* (TTA)	π^* (TTA)	π^* (TTA)	π^* (TTA)	π^* (TTA)

Table S2- Calculated TD-B3LYP transitions for Eu(TTA)₃(phen-X) complexes

Complexes	transition	$\lambda(\text{nm})^{[a]}$	$f^{[b]}$	composition ^[c]	$CI^{[d]}$
Eu_TTA	S0 → S1	379	0.0058	H → L	0.69578
				H-2 → L+2	0.33363
	S0 → S12	323	0.5975	H → L+2	0.31489
				H-1 → L+2	0.25342
	S0 → T1	524	0.00 ^[e]	H-1 → L+1	0.53595
				H → L+1	0.42899
			H-1 → L+2	0.20884	
Eu_phen	S0 → S1	382	0.0123	H → L	0.67790
				H-1 → L	0.14497
	S0 → S18	320	0.5496	H-2 → L+1	0.32702
				H → L+4	0.26422
				H-2 → L+3	0.25025
	S0 → T1	530	0.00 ^[e]	H → L+1	0.49846
			H-2 → L+4	0.37783	
			H-1 → L+1	0.29100	
Eu_phen_methyl	S0 → S1	374	0.0077	H → L	0.65926
				H-2 → L	0.33533
	S0 → S18	321	0.5252	H-2 → L+3	0.26704
				H → L+4	0.21496
	S0 → T1	531	0.00 ^[e]	H → L	0.46609
				H-2 → L+4	0.30559
			H-1 → L	0.27636	
Eu_phen_methoxy	S0 → S1	374	0.0069	H → L	0.66817
				H-2 → L+1	0.12924
	S0 → S16	323	0.2402	H-2 → L	0.25316
				H-2 → L+2	0.22140
				H-1 → L+1	0.20528
	S0 → T1	531	0.00 ^[e]	H → L	0.46892
			H-2 → L+1	0.33851	
			H-1 → L	0.31465	
Eu_phen_chloro	S0 → S1	412	0.0116	H → L	0.67750
				H-1 → L	0.15608
	S0 → S21	321	0.4720	H-2 → L+2	0.32554
				H → L+4	0.26320
				H-1 → L+3	0.24504
	S0 → T1	530	0.00 ^[e]	H → L+2	0.47737
			H-2 → L+4	0.33689	
			H-1 → L+2	0.30048	

Table S2- Calculated TD-B3LYP transitions for Eu(TTA)₃(phen-X) complexes (cont.)

Complexes	transition	$\lambda(\text{nm})^{[a]}$	$f^{[b]}$	composition ^[c]	$CI^{[d]}$
Eu_phen_bromo	S0 → S1	407	0.0109	H → L	0.68213
				H-1 → L	0.12295
	S0 → S21	321	0.3578	H-5 → L	0.32171
				H-2 → L+2	0.27670
				H → L+4	0.2284
	S0 → T1	530	0.00 ^[e]	H → L+2	0.48675
				H-2 → L+4	0.33861
				H-1 → L+2	0.28702
Eu_phen_carboxylate	S0 → S1	453	0.0061	H → L	0.67484
				H → L+1	0.15096
				H-1 → L	0.12676
	S0 → S33	320	0.5216	H-2 → L+2	0.31392
				H → L+4	0.26184
				H-1 → L+3	0.23571
	S0 → T1	530	0.00 ^[e]	H → L+2	0.49859
				H-2 → L+4	0.35640
H-1 → L+2				0.28743	
Eu_phen_phenyl	S0 → S1	382	0.0176	H → L	0.67985
				H-1 → L	0.13215
	S0 → S19	321	0.4121	H-2 → L+1	0.31647
				H → L+4	0.24910
				H-1 → L+3	0.22549
	S0 → T1	531	0.00 ^[e]	H → L+1	0.48629
				H-2 → L+4	0.36470
				H-1 → L+1	0.29782
Eu_phen_1_butin_3_yn	S0 → S1	414	0.0280	H → L	0.68365
				H → L+1	0.10745
	S0 → S19	338	0.2955	H-4 → L+1	0.35793
				H-1 → L+4	0.29064
				H-3 → L+2	0.23544
	S0 → T1	548	0.00 ^[e]	H-4 → L	0.40728
				H-3 → L+1	0.43422
				H-2 → L+1	0.28278
Eu_phen_1_buten_3_yn	S0 → S1	410	0.0573	H → L	0.66995
				H-2 → L	0.12431
	S0 → S19	345	0.4677	H-4 → L+1	0.42584
				H-4 → L	0.24693

			H-2 → L+4	0.14242
			H → L+1	0.41743
S0 → T1	589	0.00 ^[e]	H-1 → L+1	0.27622
			H-2 → L+1	0.23887

[a] Only the selected low-lying excited states are presented;

[b] Oscillator strength;

[c] Only the three primary transitions are reported; H stands for HOMO and L stands for LUMO

[d] The CI coefficients are in absolute values.

[e] No spin-orbital coupling effect was considered, thus the f values are zero