

The role of the excited state dynamic of the antenna ligand in the Lanthanide sensitization mechanism

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Supplementary material

Table 1: Excited states (singlets and triplets) calculated for Cp^{2Ph-} antenna ligand obtained at NEVPT2 level of theory considering an active space of ten electrons in ten π -type orbitals.

State	E(cm ⁻¹)
S ₁	28206.8
S ₁	29253.8
S ₁	30124.0
T ₁	24317.1
T ₂	28245.4
T ₃	30927.8

Table 2: SO-NEVPT2 energies for the low-lying (7F_J) and first excited 5D_4 multiplets derived from the $4f^8$ configuration of the Tb(III). All the energies are given in cm^{-1} .

State	(Cp 2Ph) $_3$ Tb	(Cp 2Ph)TbCl $_2$ (THF) $_3$
7F_6	0.00	0.00
	10.79	3.25
	13.12	36.41
	49.06	40.15
	57.14	91.25
	128.36	103.66
	154.26	130.31
	296.82	199.77
	326.16	279.24
	643.82	296.65
	645.96	343.48
	1358.32	868.55
	1358.82	881.46
7F_5	1964.37	1915.77
	2003.35	1936.36
	2004.53	1983.63
	2083.24	2028.73
	2111.18	2136.22
	2154.50	2145.04
	2289.49	2187.89
	2324.55	2204.03
	2358.41	2276.43
	2725.26	2347.06
	2733.38	2381.13
7F_4	3336.19	3247.60
	3352.37	3257.43
	3409.89	3278.59
	3445.91	3296.65
	3447.11	3341.04
	3462.65	3434.31
	3671.36	3477.98
	3683.90	3518.00
	3809.71	3619.04

Table 3: Continue ...

State	$(\text{Cp}^{2Ph})_3\text{Tb}$	$(\text{Cp}^{2Ph})\text{TbCl}_2(\text{THF})_3$
7F_3	4284.76	4188.73
	4378.64	4196.02
	4392.56	4201.81
	4397.42	4255.91
	4398.25	4295.81
	4415.18	4339.66
	4874.13	4355.89
7F_2	4959.68	4745.49
	4960.59	4858.01
	4961.96	4880.56
	5162.26	4901.53
	5192.77	4995.54
7F_1	5575.64	5172.33
	5576.55	5217.83
	5942.08	5411.42
7F_0	5950.88	5468.30
5D_4	22306.68	21737.6
	22331.53	21862.8
	22331.62	21887.50
	22399.67	21925.7
	22400.43	21945.9
	22490.71	21965.3
	22508.78	21972.2
	22629.79	22006.2
	22626.46	21989.0