Supporting Information

Mixed (Phthalocyaninato)(Porphyrinato) Rare Earth Double-Decker Complexes with C_4-chirality: Synthesis, Resolution, and Absolute Configuration Assignment

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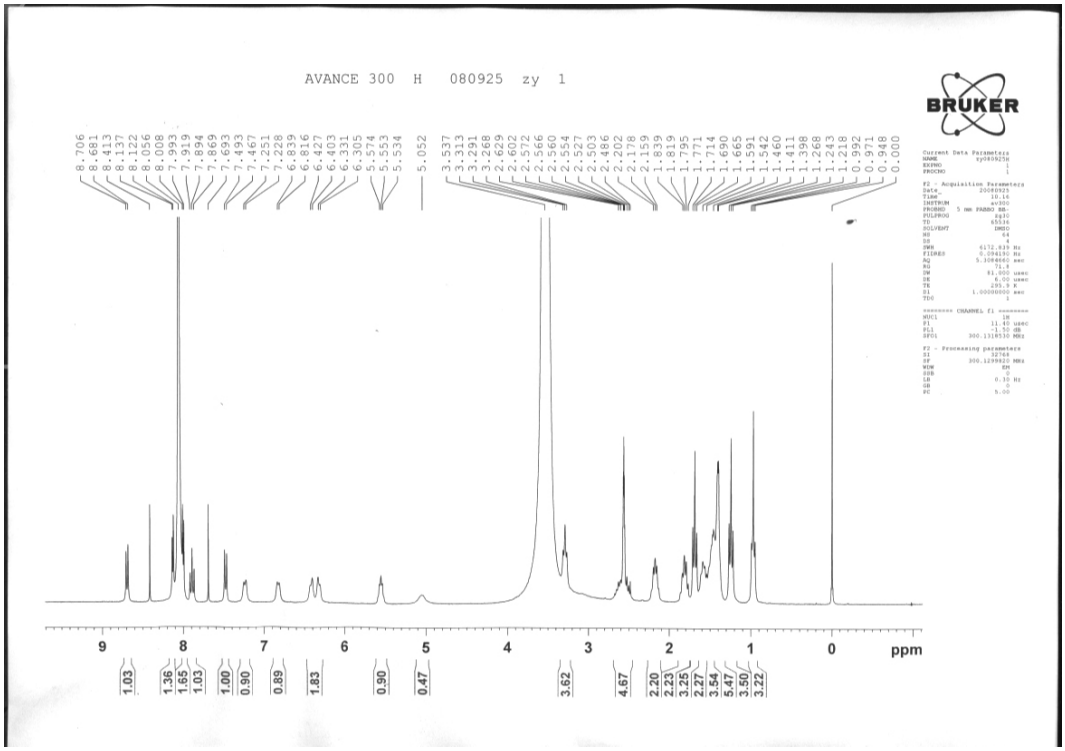


Figure S1. ^{1}H NMR spectrum of [Y^{III}{Pc(α-OC_5H_{11})$_4$}{TOAPP}] (**1**).

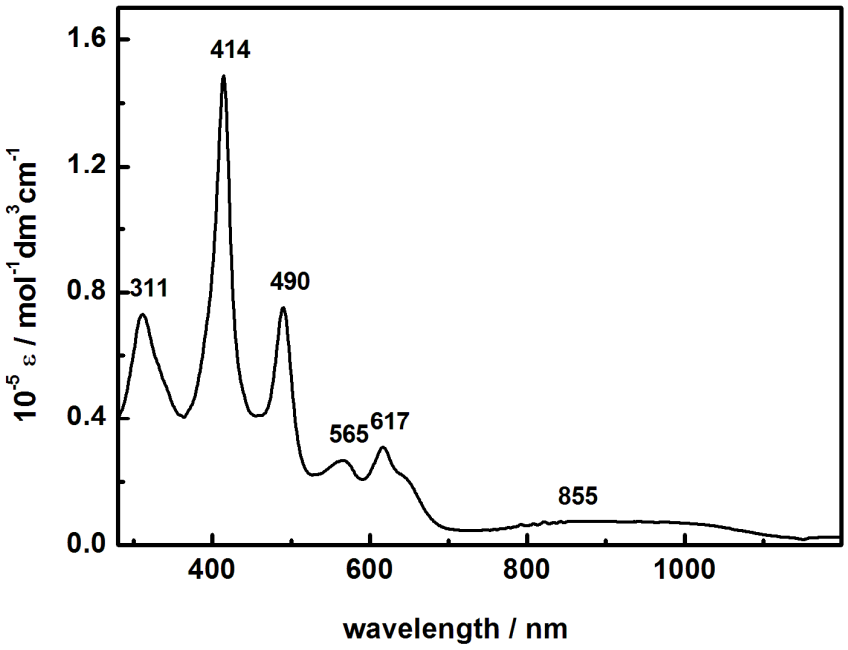


Figure S2. Electronic absorption spectrum of [$Ho^{III}H\{Pc(\alpha\text{-}OC_5H_{11})_4\}\{TOAPP\}$] (**2**) in $CHCl_3$.

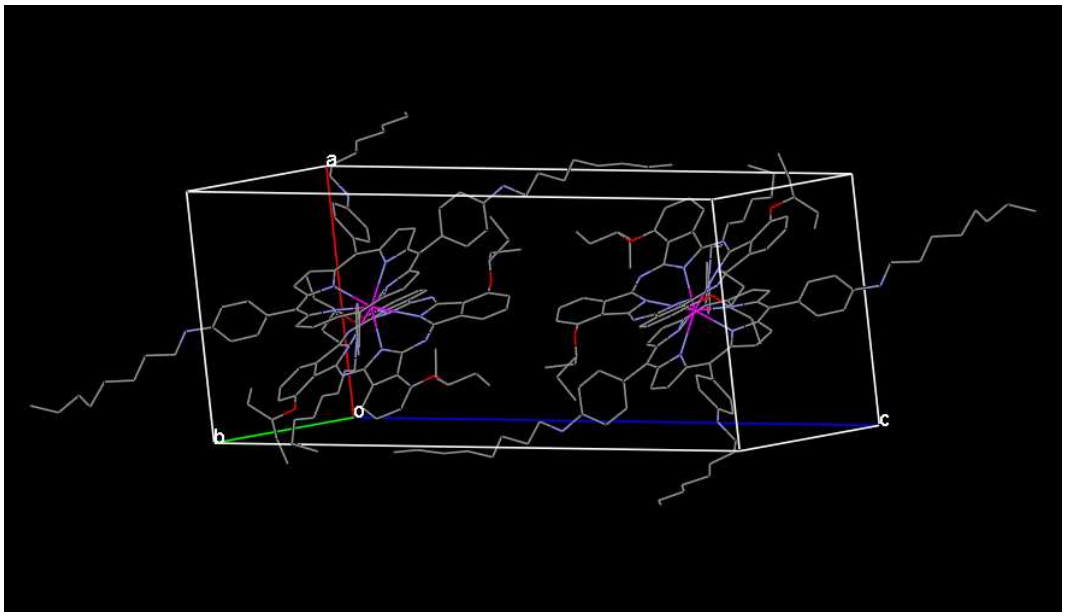
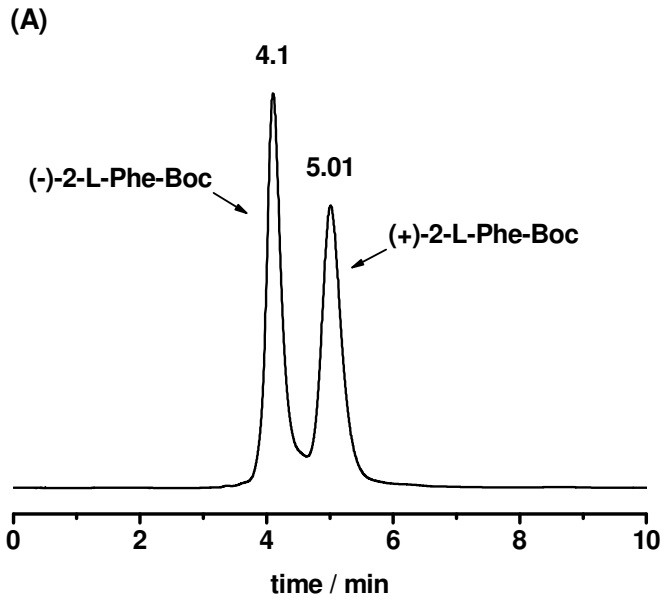


Figure S3. Unit cell of $[Y^{III}H\{Pc(\alpha\text{-}OC_5H_{11})_4\}\{TOAPP\}]$ (**1**) shows one pair of enantiomers.



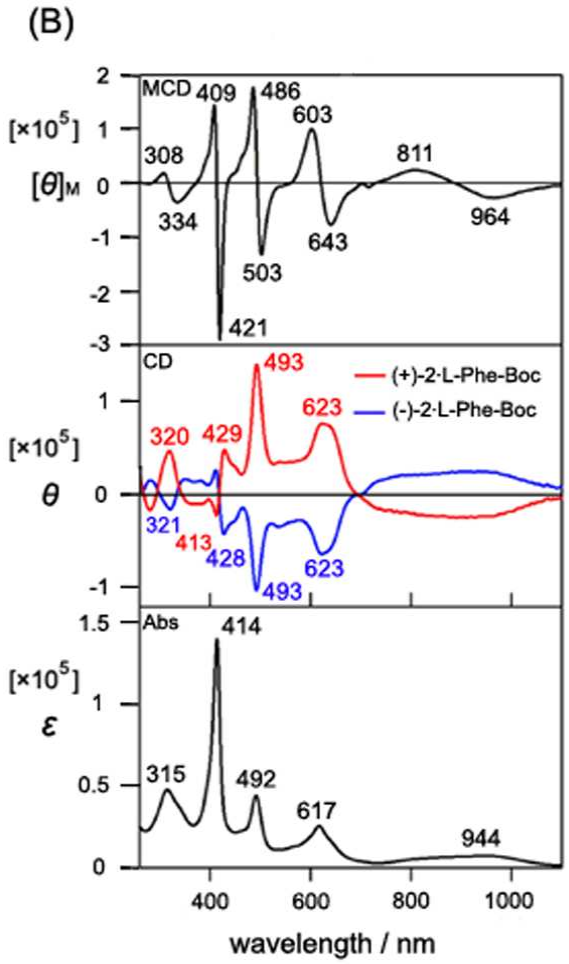


Figure S4. (A) Chromatogram of **2**·L-Phe-Boc monitored at 400 nm; (B) Electronic absorption, CD, and MCD spectra of (-)-**2**·L-Phe-Boc and (+)-**2**·L-Phe-Boc measured in $CHCl_3$.

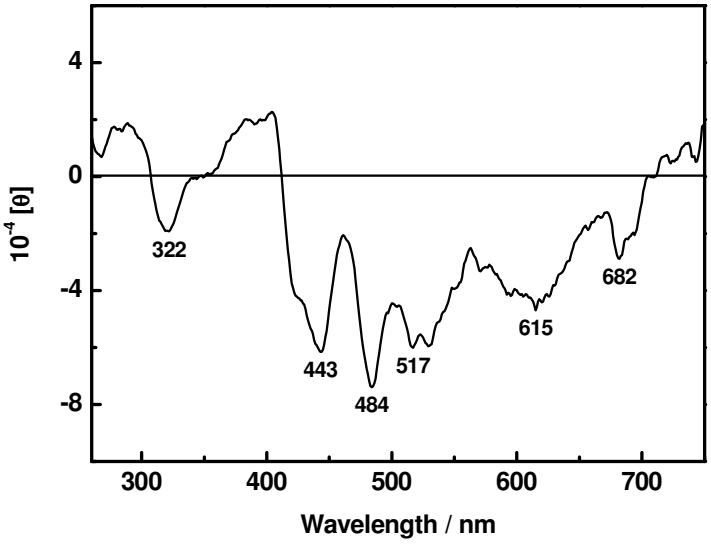


Figure S5. CD spectra of a precipitate, in which (-)-**2**·L-Phe-Boc was enriched by reprecipitation of **2**·L-Phe-Boc five times, with a mixed solvent of $CHCl_3$ and CH_3OH (1:9, v/v), measured in $CHCl_3$.

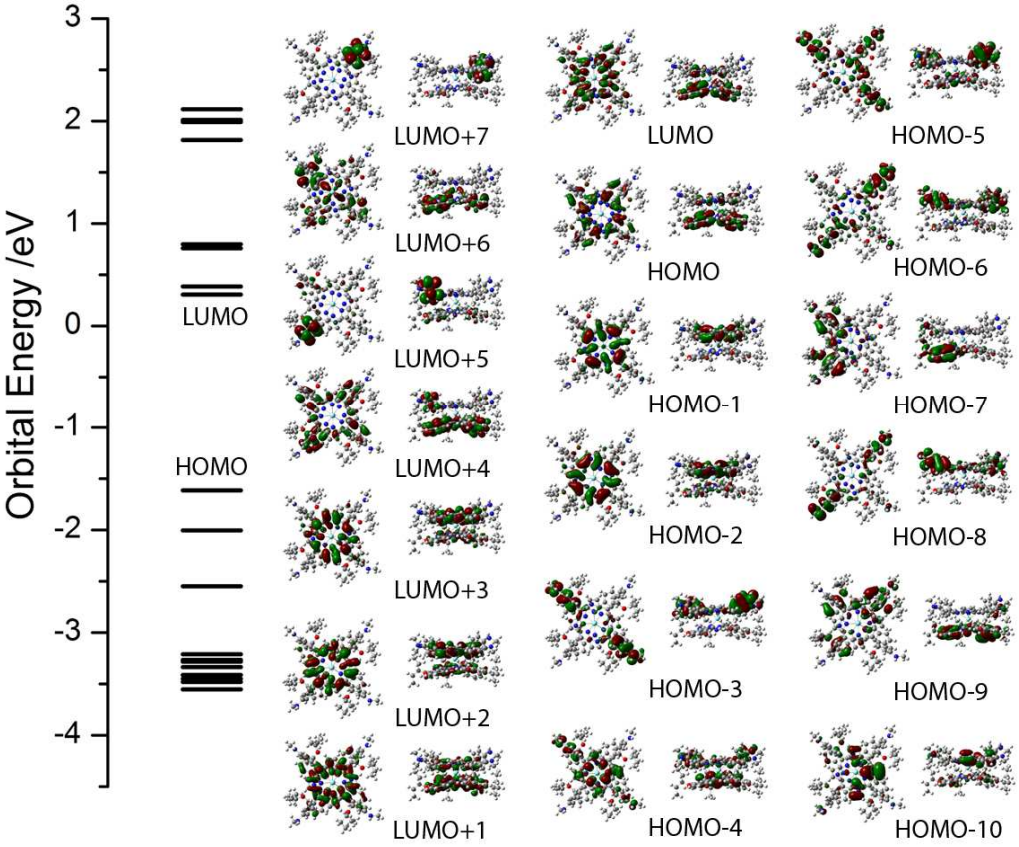


Figure S6. Energy level scheme (left) and maps (right) of the molecular orbitals for *(R)*-[Y^{III}{Pc(α-3-OC_5H_{11})$_4$}{TMAPP}]$^-$.

Table S1. Major contributions (in %) from occupied-unoccupied orbital pairs to the transition dipole moments of some excitations of (*R*)-[Y^{III}{Pc(α-3-OC_5H_{11})$_4$}{TMAPP}]$^-$ (B3LYP functional, LANL2DZ/6-31G(d) basis set).

no.	λ / nm	*f*	*R* /10^{-40} cgs (velocity)	major contribution to transition dipole moment
1	786.8	0.0544	158.4652	H-0->L+0(+64%) H-0->L+1(+13%)
2	763.4	0.0519	62.2968	H-0->L+1(+63%) H-0->L+0(11%)
3	684.9	0.0019	-5.5167	H-1->L+0(+81%) H-0->L+2(+7%)
4	661	0.0011	14.5146	H-1->L+1(+71%) H-0->L+3(+20%)
5	631.1	0.0825	-18.3397	H-0->L+2(+70%) H-1->L+3(+8%)
6	614	0.0807	-141.4767	H-0->L+3(+58%) H-1->L+1(13%)
7	542	0.0016	18.6379	H-2->L+0(+45%) H-1->L+3(+24%)
8	535.2	0.0141	35.2023	H-2->L+1(+42%) H-1->L+2(26%)
9	494.1	0.2692	-155.121	H-2->L+0(+36%) H-2->L+2(+13%)
10	479.2	0.251	-149.745	H-2->L+1(+38%) H-2->L+2(+15%)
11	408.3	0.0027	0.5219	H-0->L+4(+90%)
12	406.7	0.0775	-243.6538	H-2->L+2(+25%) H-4->L+0(+22%)
13	400.1	0.1196	47.4538	H-4->L+1(+21%) H-2->L+3(+19%)
14	398.5	0.0199	-28.2058	H-0->L+6(+32%) H-7->L+0(20%)
15	396.6	0.0014	-5.2954	H-3->L+0(+72%) H-0->L+6(14%)
16	396.4	0.0143	-3.4633	H-0->L+6(+44%) H-7->L+0(+12%)
17	390.1	0.007	12.2167	H-3->L+1(+27%) H-7->L+1(22%)
18	388.4	0.0275	27.5351	H-3->L+1(+54%) H-5->L+0(+9%)
19	387.4	0.0027	12.7048	H-0->L+5(+86%)
20	386.5	0.0255	9.2618	H-5->L+0(+32%) H-6->L+0(14%)
21	383.7	0.0215	-20.6124	H-6->L+0(+33%) H-5->L+0(+18%)
22	382.3	0.4405	192.5627	H-4->L+1(+19%) H-2->L+3(13%)
23	380.4	0.3025	164.7169	H-5->L+1(+9%) H-7->L+1(+8%)
24	377.4	0.0078	-4.3034	H-9->L+0(+24%) H-7->L+0(21%)
25	376.8	0.0895	86.4132	H-5->L+1(+45%) H-6->L+1(14%)
26	374.6	0.0037	-12.6255	H-6->L+1(+38%) H-10->L+0(25%)
27	373.8	0.0359	44.7782	H-0->L+7(+65%) H-9->L+0(+8%)
28	372.9	0.013	26.7495	H-0->L+7(27%) H-9->L+0(+20%)
29	371.5	0.0005	4.8447	H-1->L+4(+61%) H-9->L+1(7%)
30	369.3	0.0239	12.0922	H-10->L+1(+24%) H-7->L+1(12%)

Complete ref. 37:

[37] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Jr. Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M. Gill,; P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision B.05; Gaussian, Inc.: Pittsburgh, PA, 2004.