Electronic Supplementary Information for Dalton Transactions

Sandwich-type Mixed (Phthalocyaninato)(porphyrinato) Rare Earth Double-decker Complexes with Decreased Molecular Symmetry of C_s: Single Crystal Structure and Self-assembled Nano-structure

Xingcui Wu, Wei Lv, Quanbo Wang, Hailong Wang, Xiaomei Zhang,* and Jianzhuang Jiang*

Department of Chemistry, University of Science and Technology Beijing, Beijing 100083, P. R. China.

Department of Chemistry, Shandong University, Jinan 250100, P. R. China.

Electronic supplementary information

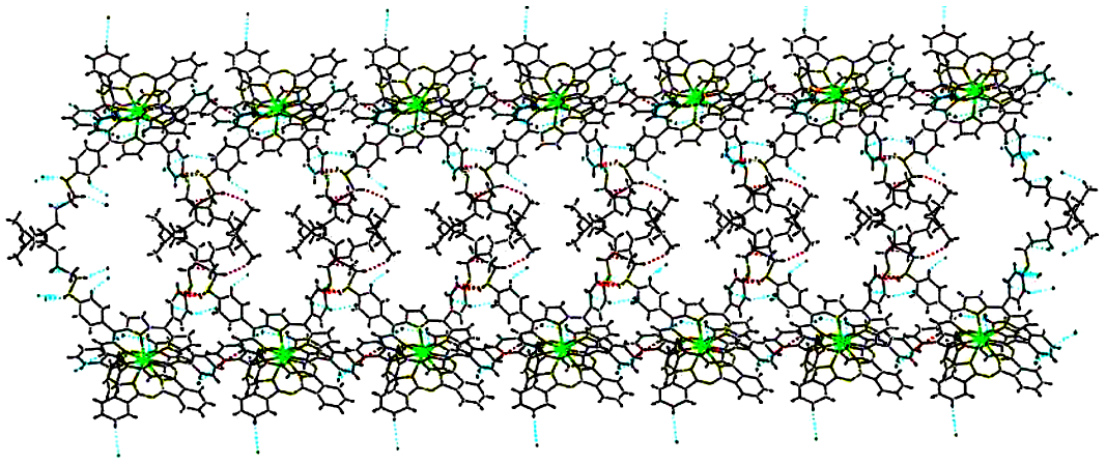

Figure S1. The crystal stacking image for Eu(Pc)[D(NHC8H17)2PP] (1) viewed in b axis. Hydrogen atoms and alkyl atoms are omitted for clarity.

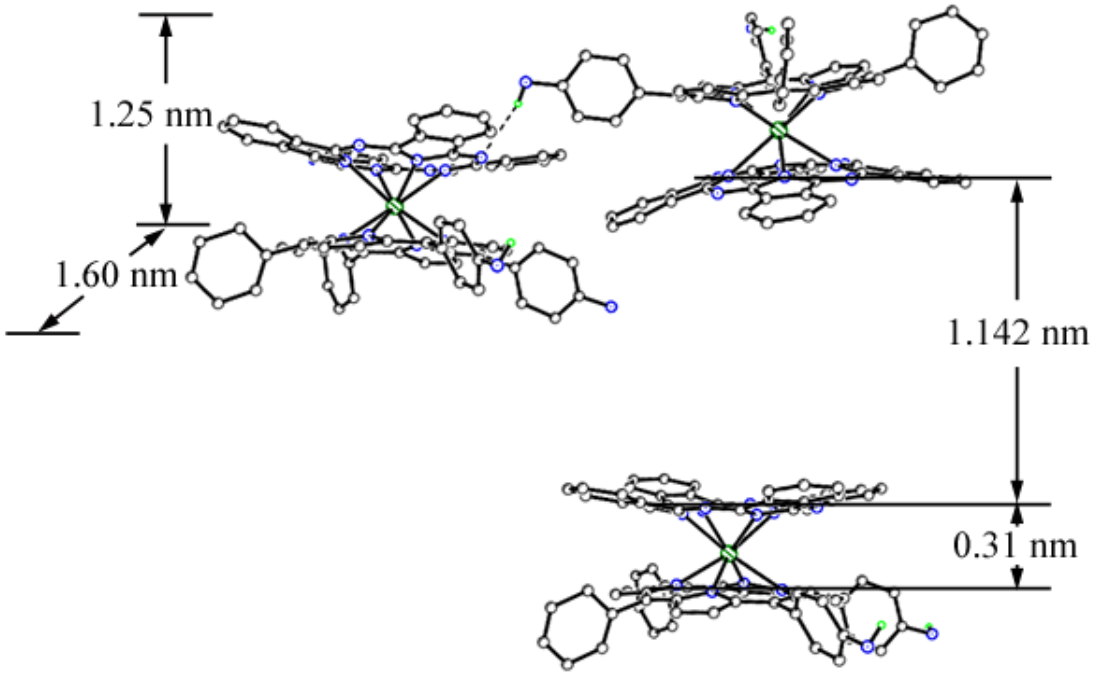

Figure S2. The crystal packing diagrams for Eu(Pc)[D(NHC_8H_{17})$_2$PP] (**1**) in side view. Hydrogen atoms and alkyl atoms are omitted for clarity.

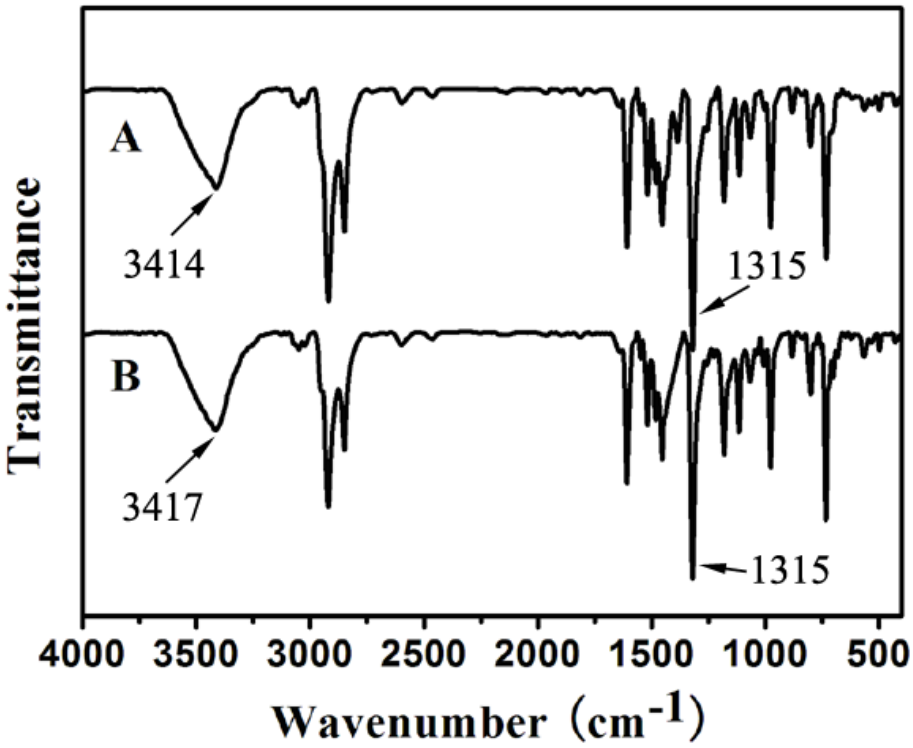

Figure S3. IR spectra of **2** and nano-structures with leaf morphology fabricated from **2** in the region of 400-4000 cm^{-1} with 2 cm^{-1} resolution.

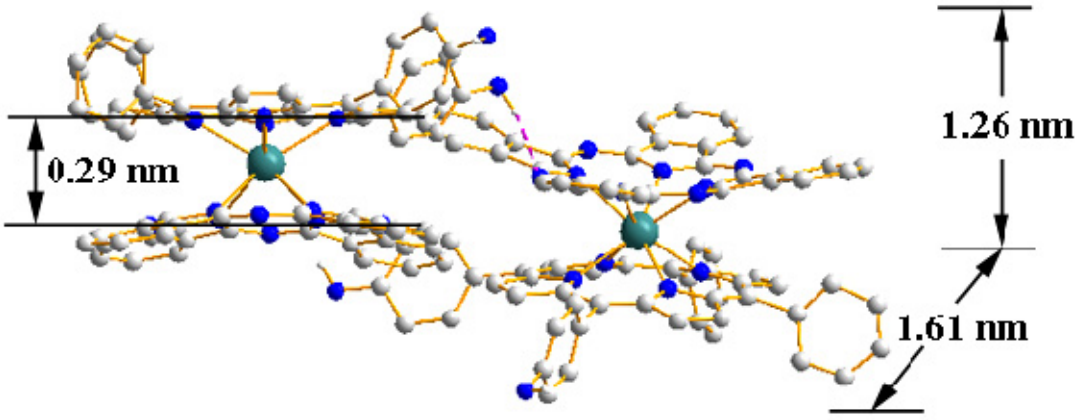

Figure S4. Schematic representation of the unit cell in the aggregate of Lu(Pc)[D(NHC_8H_{17})$_2$PP] (**2**).

Table S1. Analytical and mass spectroscopic data for **1** and **2**. [a]

Compound	Yield (%)	M^+ (*m/z*)[a,b]	Analysis (%)[a]		
			C	H	N
Eu(Pc)[D(NHC_8H_{17})$_2$PP] (**1**)	40	1531.7 (1531.7)	71.37 (71.43)	5.10 (5.29)	12.45 (12.54) [c]
Lu(Pc)[D(NHC_8H_{17})$_2$PP] (**2**)	32	1554.9 (1554.6)	70.13 (69.93)	5.14 (4.98)	12.19 (12.38) [c]

[a] Calculated values given in parentheses.

[b] By MALDI-TOF mass spectrometry. The value corresponds to the most abundant isotopic peak of the molecular ion (M^+).

[c] For **1**·CH_3OH, **2**·1/4 $CHCl_3$.

Table S2. ^{1}H NMR spectroscopic data (δ) for **1** and **2** recorded in $CDCl_3$–DMSO-d_6 (1:1) with the addition of ca. 10% (by volume) hydrazine hydrate. [a]

Compound	Pc-α	Pc-β	Por endo o-Ph	Por endo m-Ph	Por exo o-Ph	Por exo m-Ph	Por p-Ph	Por-β	Por NH	Por alkyl
Eu(Pc)[D(NHC_8H_{17})$_2$PP] (**1**)	10.33 (m, 8H)	8.56 (m, 8H)	10.82 (br, 2H)	8.67 (m, 2H)	7.89 (br, 2H)	6.56 (br, 2H)	5.96 (br, 2H)	7.20 (m, 4H)	5.68 (br, 2H)	3.61 (t, 4H)
			10.58 (br, 2H)	8.54 (m, 2H)	7.30 (m, 2H)	6.10 (d, 2H)		7.05 (m, 4H)		1.03-2.14 (m, 30H)
Lu(Pc)[D(NHC_8H_{17})$_2$PP] (**2**)	9.04 (br, 8H)	8.06 (m, 8H)	8.08 (m, 4H)	7.90 (m, 4H)	7.57 (m, 2H)	7.25 (d, 2H)	6.16 (m, 2H)	7.08 (m, 4H)	5.26 (br, 2H)	3.24 (m, 4H)
					7.45 (t , 2H)	6.78 (br, 2H)		6.36 (m, 4H)		0.93-1.78 (m, 30H)

[a] Multiplicities: d, = doublet, t = triplet, br=broad, m = multiple

Table S3. Electronic absorption data for **1** and **2** in toluene and their nano-aggregates dispersed in methanol.

Compound	λ_{max} / nm (log ε)					
Eu(Pc)[D(NHC_8H_{17})$_2$PP] (**1**)[a]	321 (4.71)	409 (4.81)	480 (4.51)	733 (3.39)	1018 (3.45)	1402 (3.80)
Eu(Pc)[D(NHC_8H_{17})$_2$PP] (**1**)[b]	327	412	484	763	1051	1405
Lu(Pc)[D(NHC_8H_{17})$_2$PP] (**2**)[a]	328 (4.92)	398 (4.96)	473 (4.72)	732 (3.59)	1230 (4.07)	
Lu(Pc)[D(NHC_8H_{17})$_2$PP] (**2**)[b]	333	406	484	746	1205	

[a] The electronic absorption data in toluene. [b] The electronic absorption data in methanol.