Electronic Supplementary Information

Co-crystallized fullerene and mixed (phthalocyaninato)(porphyrinato) dysprosium double-decker SMM

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Caption of Content

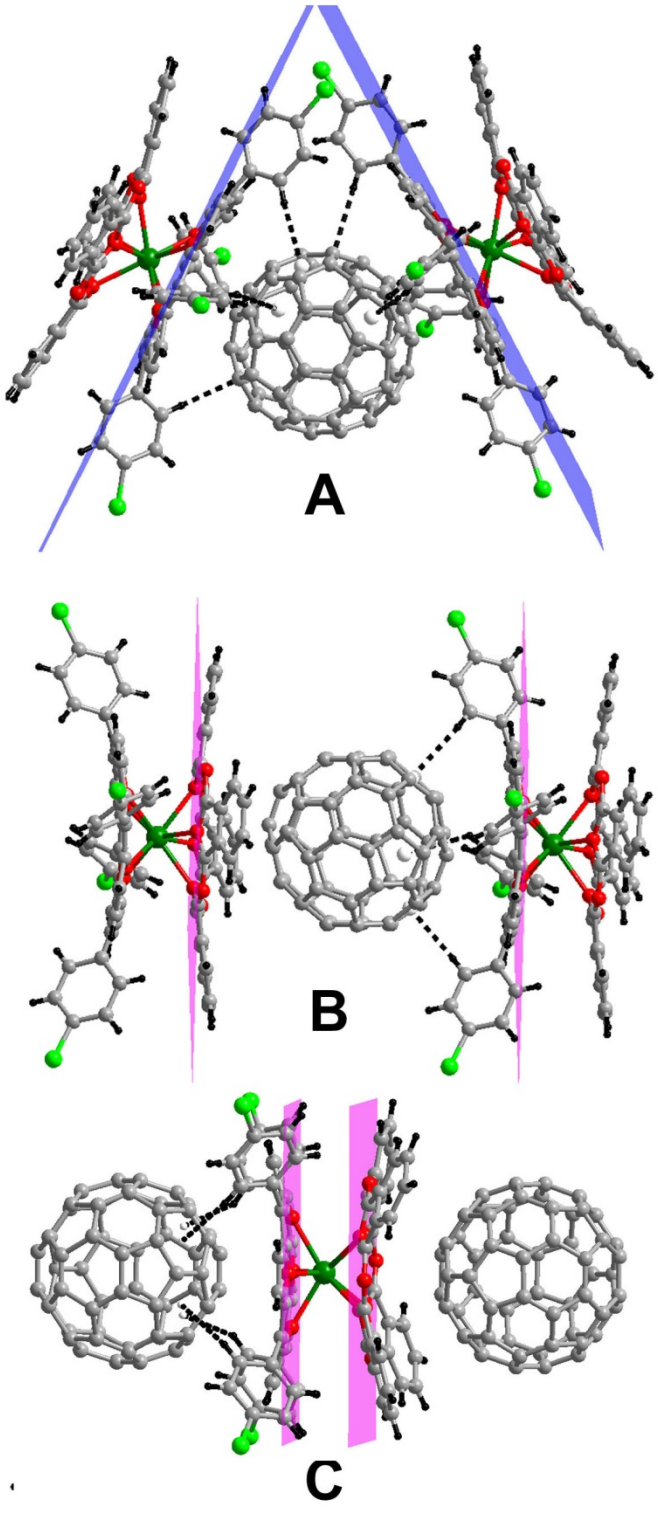


Figure S1. Molecular structures of **2-4** with the detailed C-H…π interaction. Selected hydrogen atoms and all solvent molecules are omitted for clarity.

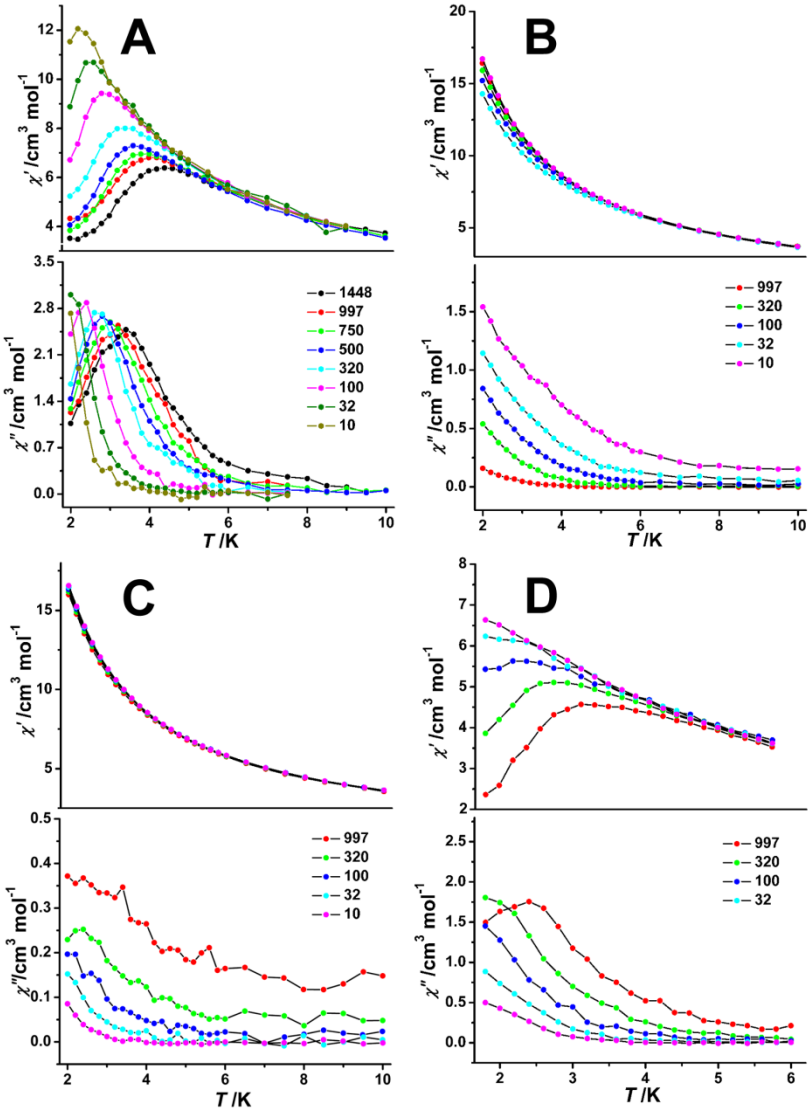


Figure S2. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibility of **1** (A), **2** (B), **3** (C), and **4** (D) at the frequency from 10 to 997 Hz under zero dc field.

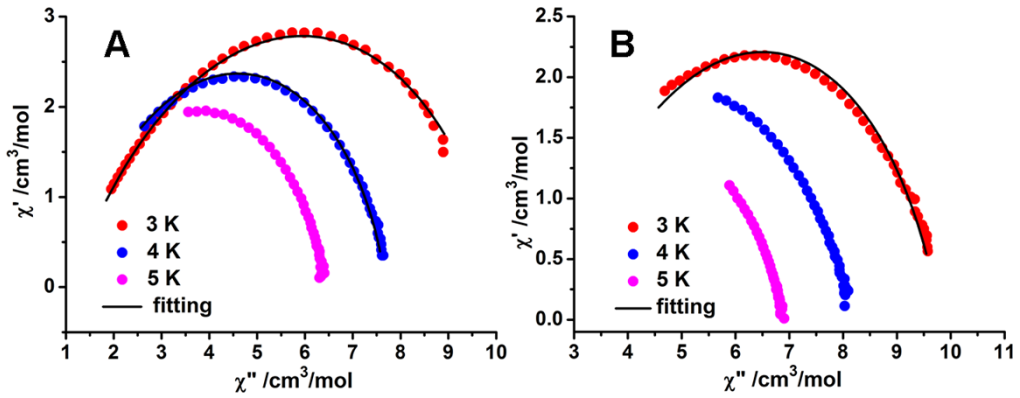


Figure S3. Cole-Cole diagrams of **1** (A) and **4** (B) using the ac susceptibility data at 3.0, 4.0, and 5.0 K under zero applied dc field.

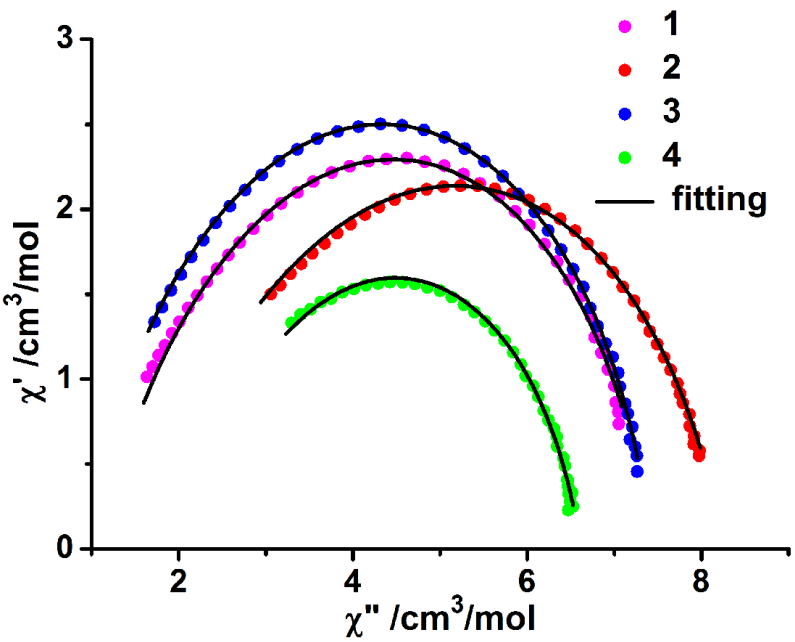


Figure S4. Cole-Cole diagrams of **1**-**4** using the ac susceptibility data at 5.0 K under 2000 Oe applied dc field.

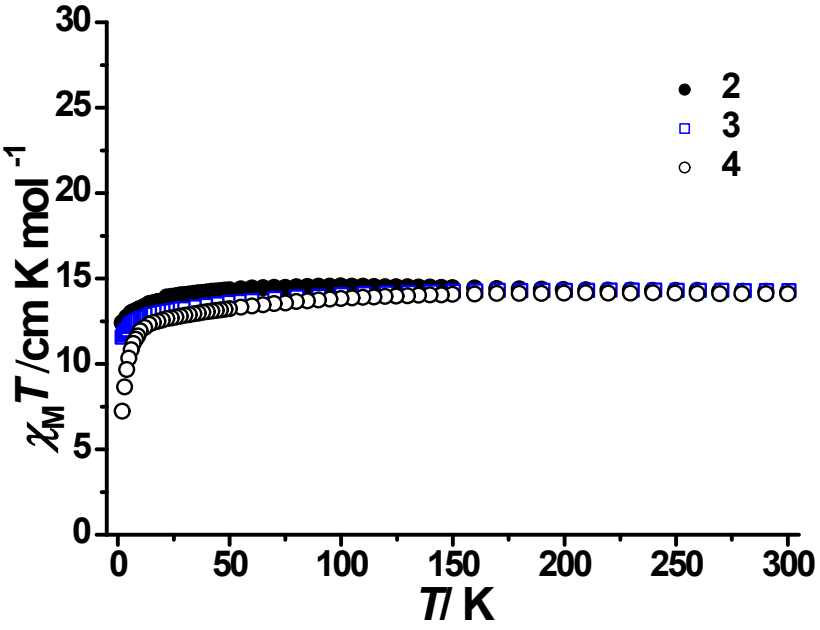


Figure S5. Temperature dependence of $\chi_M T$ curves for **2**-**4**.

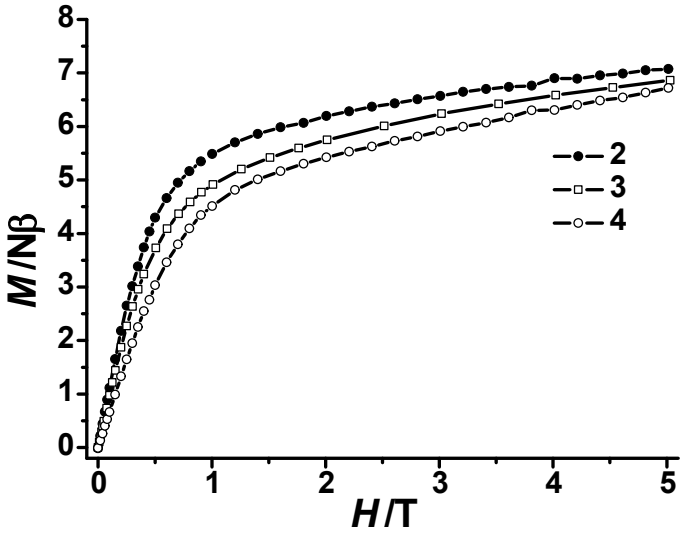


Figure S6. The *M vs. H* curves for **2**-**4** at 2.0 K.

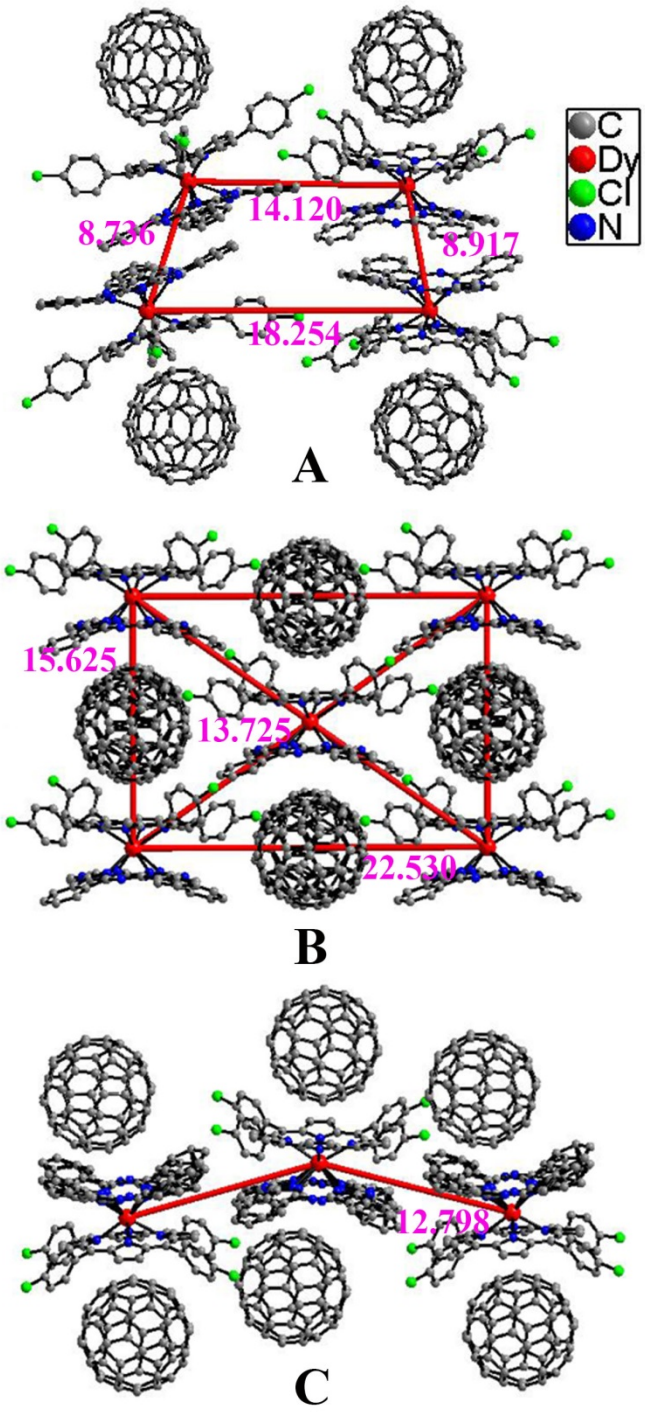
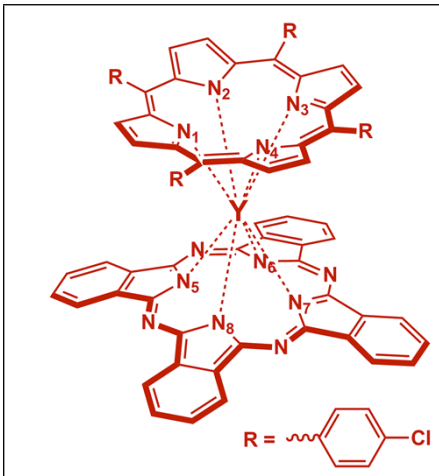


Figure S7. Packing diagrams of **2-4** (A-C) with all hydrogen atoms and all solvent molecules omitted for clarity.



1’		4’	
Y-N_1	0.292	Y-N_1	0.240
Y-N_2	0.287	Y-N_2	0.234
Y-N_3	0.292	Y-N_3	0.240
Y-N_4	0.287	Y-N_4	0.234
Y-Por	1.158	Y-Por	0.948
Y-N_5	0.265	Y-N_5	0.227
Y-N_6	0.265	Y-N_6	0.229
Y-N_7	0.265	Y-N_7	0.226
Y-N_8	0.265	Y-N_8	0.227
Y-Pc	1.060	Y-Pc	0.910
Total	2.218	Total	1.858

Figure S8. Mayer bond order of **1’** and **4’**.

Table S1. Crystal data and structure refinement of complexes **2-4.**

complex	**2**	**3**	**4**
Formula	$C_{217}H_{87}Cl_{23}Dy_2N_{24}O$	$C_{136}H_{40}Cl_4DyN_{12}$	$C_{220}H_{40}Cl_8DyN_{14}$
F.W.	4186.59	2146.10	3324.8
system	monoclinic	monoclinic	orthorhombic
space group	$P2_1/c$	$C2/c$	$Pnma$
a	16.6402(3)	22.5698(4)	24.7203(2)
b	27.6773(7)	15.6246(2)	19.3998(2)
c	39.7657(6)	24.1908(4)	28.3596(3)
α	90	90	90
β	90.466(2)	96.681(2)	90
γ	90	90	90
Z	4	4	4
volume	18313.7(6)	8472.8(2)	13600.4(2)
D_{cald} / g cm^{-3}	1.518	1.682	1.624
F000	8344	4296	6640
R_{int} $I>2\theta$	0.0977	0.0524	0.0936
R_{w2} $I>2\theta$	0.2745	0.1268	0.2108
R_{int} all	0.1192	0.0558	0.0960
R_{w2} all	0.2955	0.1312	0.2117
S	1.061	1.041	1.175