Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

3d-4f metallacrown complexes with new sandwich core: synthesis, structures and single molecule magnet behavior

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1: Crystal Data and Structure.

Table S1. Crystal data and structure refinement for **1**-**2**

complex	**1**	**2**
Chemical formula	$C_{33}H_{120}Cl_3Cu_8ErN_{16}O_{43}$	$C_{33}H_{120}Cl_3Cu_8N_{16}O_{43}Yb$
CCDC number	2009454	2009455
M, g mol $^{-1}$	2211.37	2217.15
Crystal system	monoclinic	monoclinic
a /Å	11.3758(8)	11.3776(3)
b/Å	20.6667(11)	20.6630(6)
c/Å	18.5033(10)	18.5000(5)
2Unit cell volume/Å^3	4330.8(4)	4328.1(2)
Temperature/K	132(4)	130(11)
Space group	*P*2(1)	*P*2(1)
Z	2	2
Rint	0.0564	0.0686
R1 a (I > 2σ(I))	0.1126	0.1161
wR2 b (all data)	0.3464	0.3049

Table S2. Selected bond lengths (Å) and angles (deg) for complex **1**.

Er1-O1	2.30(2)	O1-Er1-O3	68.9(7)
Er1-O3	2.342(18)	O1-Er1-O5	107.5(7)
Er1-O5	2.36(2)	O1-Er1-O7	68.6(7)
Er1-O7	2.283(17)	O1-Er1-O9	87.0(7)
Er1-O9	2.315(19)	O1-Er1-O11	82.5(7)
Er1-O11	2.308(19)	O1-Er1-O13	140.8(7)
Er1-O13	2.316(18)	O1-Er1-O15	146.9(7)
Er1-O15	2.312(19)	O3-Er1-O5	69.4(6)
Cu1-O2	1.910(19)	O3-Er1-O7	106.4(6)
Cu1-N3	1.96(2)	O3-Er1-O9	82.4(6)
Cu1-N4	2.01(2)	O1-Cu1-O2	82.1(8)
Cu2-O3	1.895(19)	O1-Cu1-O3	63.1(7)
Cu2-O4	1.982(19)	O1-Cu1-N3	89.5(9)
Cu2-N5	1.96(2)	O1-Cu1-N4	171.8(9)
Cu2-N6	2.01(2)	O2-Cu1-O3	144.7(7)
Cu3-O5	1.871(18)	O2-Cu1-N3	170.7(9)
Cu3-O6	1.98(2)	O2-Cu1-N4	94.7(9)
Cu3-N7	1.92(2)	O3-Cu1-N3	26.5(8)
Cu3-N8	2.04(2)	O3-Cu1-N4	120.6(8)

Table S3. Selected bond lengths (Å) and angles (deg) for complex **2**.

Yb1-O1	2.310(16)	O1-Yb1-O3	69.7(5)
Yb1-O3	2.328(14)	O1-Yb1-O5	108.2(5)
Yb1-O7	2.293(13)	O1-Yb1-O7	70.1(5)
Yb1-O9	2.313(13)	O1-Yb1-O9	85.0(5)

Yb1-O11	2.256(15)	O1-Yb1-O11	81.5(5)
Yb1-O13	2.315(14)	O1-Yb1-O13	141.9(5)
Yb1-O15	2.319(14)	O1-Yb1-O15	146.3(5)
Cu1-O2	1.932(16)	O3-Yb1-O5	69.7(5)
Cu1-N3	1.927(18)	O3-Yb1-O7	107.3(5)
Cu1-N4	1.99(2)	O3-Yb1-O9	81.5(5)
Cu4-N1	1.932(17)	O3-Yb1-O11	140.8(5)
Cu4-N2	1.981(19)	O3-Yb1-O13	146.1(5)
Cu5-O9	1.895(15)	O1-Cu1-O2	81.1(7)
Cu5-O10	1.955(14)	O1-Cu1-O3	64.3(6)
Cu5-N11	1.955(15)	O1-Cu1-N3	90.7(7)
Cu5-N12	1.97(2)	O1-Cu1-N4	172.4(8)
Cu6-O11	1.921(15)	O2-Cu1-O3	144.9(5)
Cu6-N13	1.914(17)	O2-Cu1-N3	170.9(7)
O13-Yb1-O15	69.4(5)	O2-Cu1-N4	95.3(8)

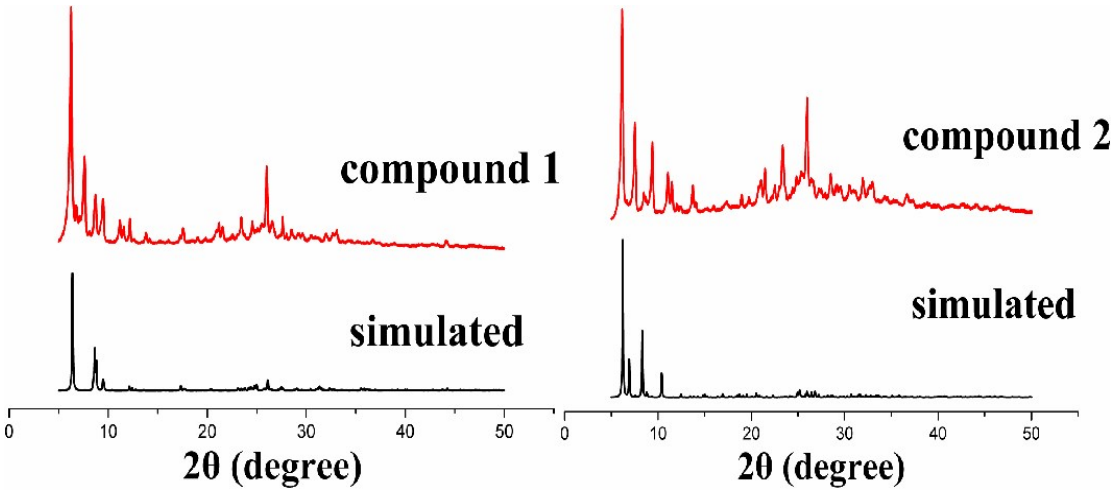

Figure S1. Powder XRD comparison for complexes **1**-**2** against that calculated from crystal data

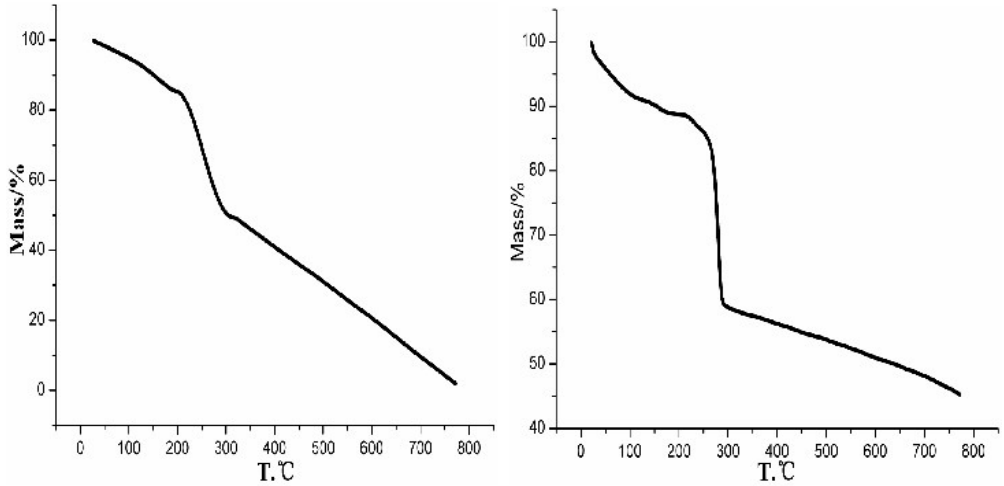

Figure S2. Thermogravimetric analysis of complexes **1**-**2** (from Left to right)

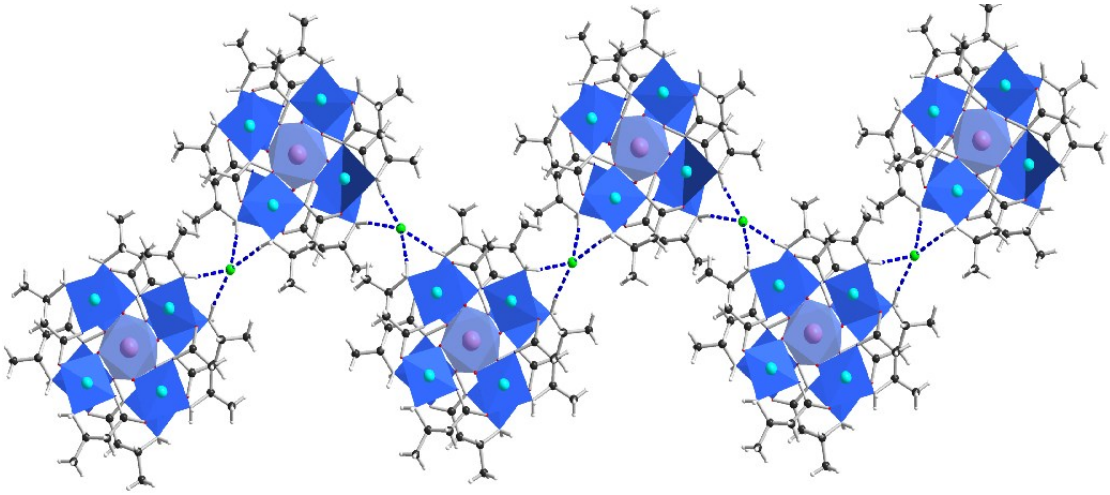

Figure. S3. The 1D chain established by cross-coordinated MC units for **1**.

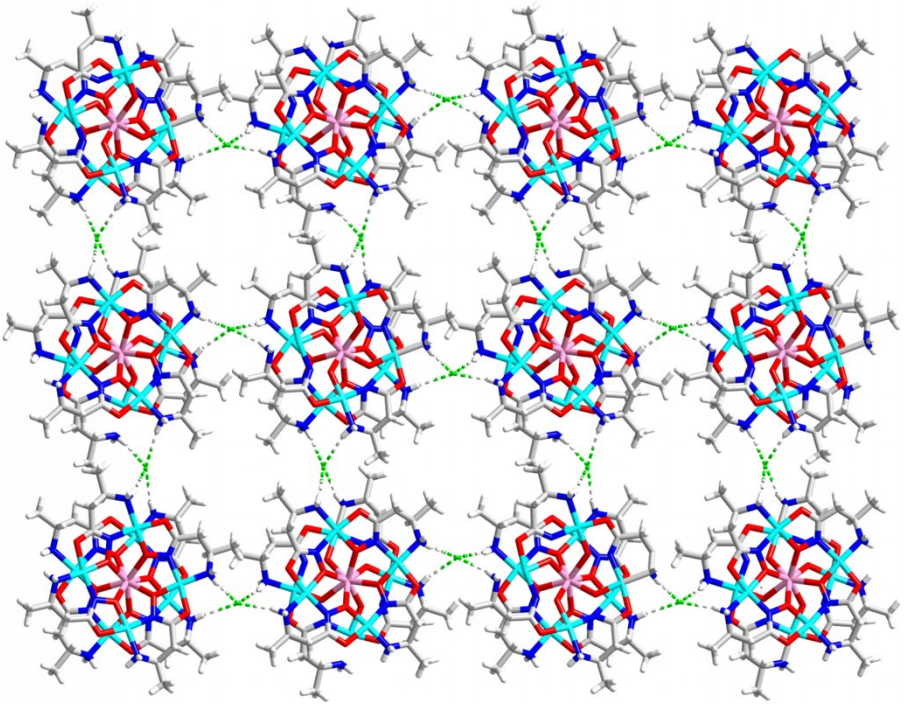

Figure. S4. The 2D network established by cross-coordinated MC units for **1**.

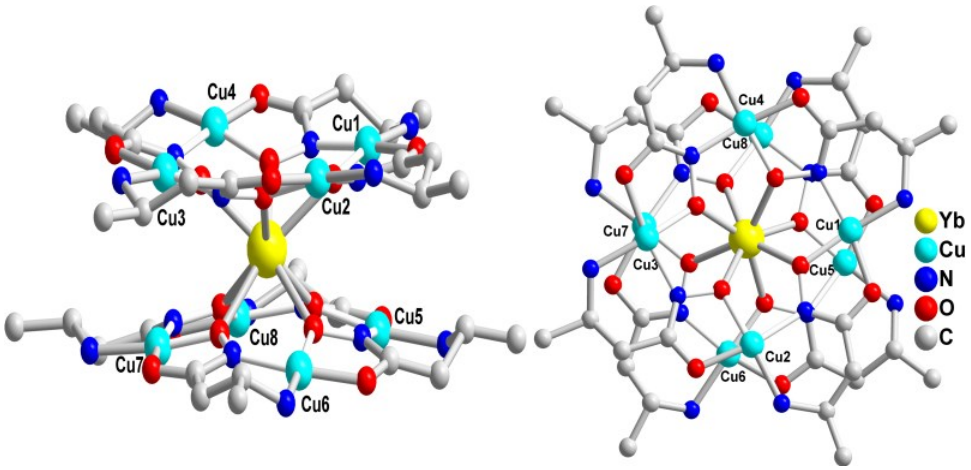

Figure. S5. The structure of complex **2** with hydrogen atoms omitted for clarity

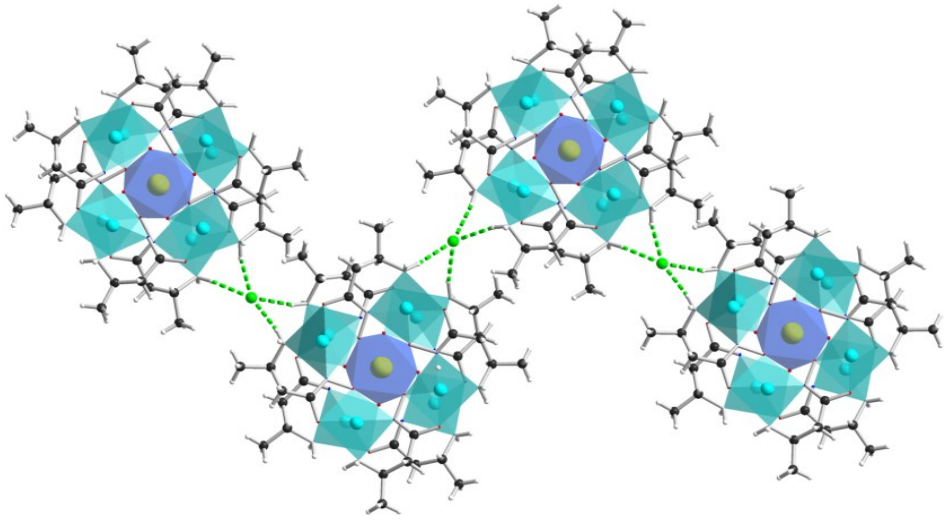

Figure. S6. The 1D network established by cross-coordinated MC units for **2** with extra hydrogen atoms omitted for clarity

2: Magnetic Measurements.

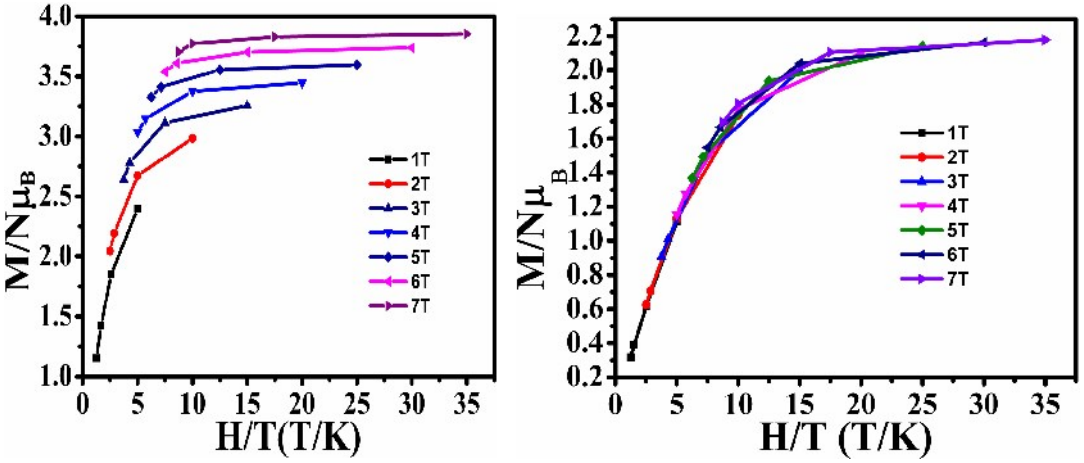

Figure. S7. The plots of reduced magnetization M/Nμ_B vs H/T at the indicated applied fields for

complexes **1**-**2** (from Left to right)

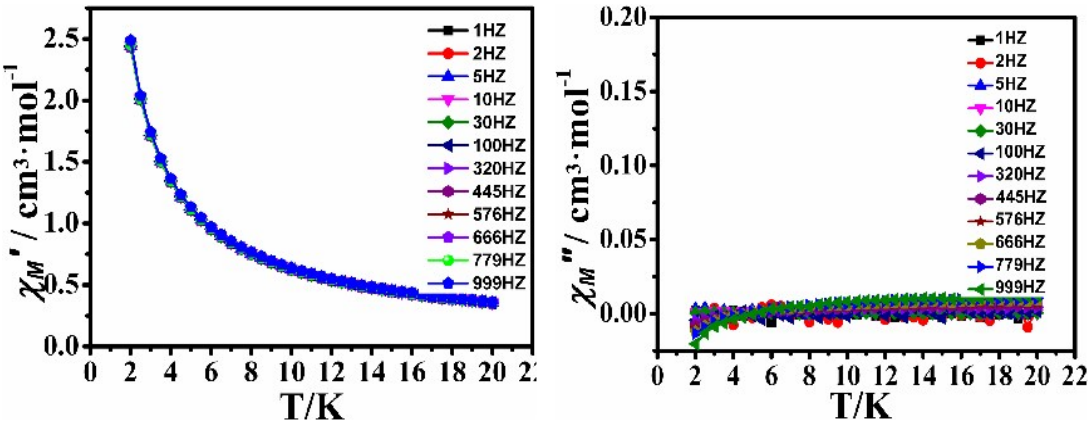

Figure. S8. Temperature-dependent ac susceptibilities under an applied dc field of 0 Oe for complex **1**

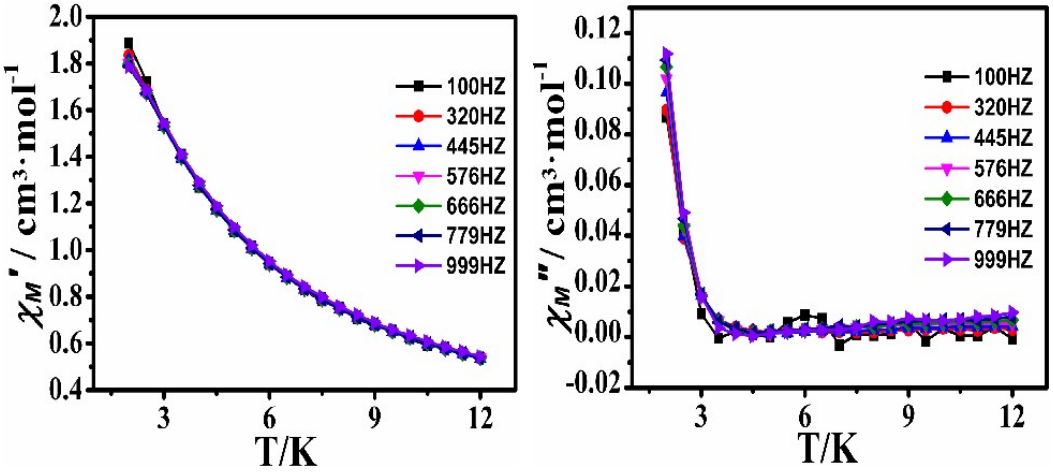

Figure. S9. Temperature-dependent ac susceptibilities under an applied dc field of 1000 Oe for complex

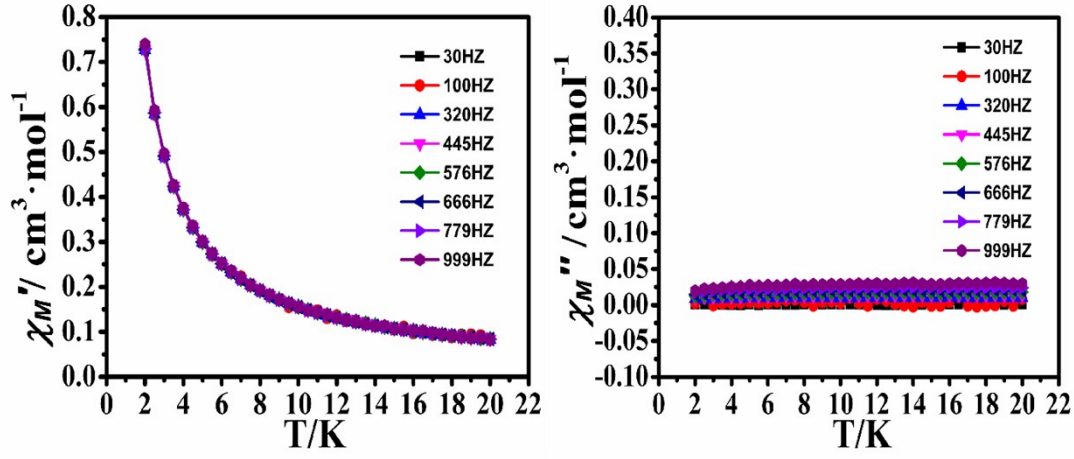

Figure. S10. Temperature-dependent ac susceptibilities under an applied dc field of 0 Oe for

complex **2**

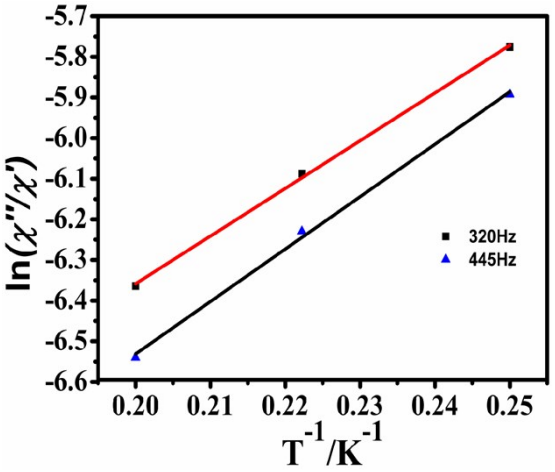

Figure. S11. Plots of ln(χ''/χ') vs. 1/T for complex **1**

Table S4. The energy barrier (ΔE_{eff}) and relaxation time (τ_0) calculated through Debye equation: $\ln(\chi''/\chi') = \ln(\omega\tau_0) + \Delta E_{eff} / k_B T$.

	ΔE_{eff}	τ_0
320Hz	**8.16 K**	**8.21×10^{-8} s**
445 Hz	**8.97 K**	**3.97×10^{-8} s**

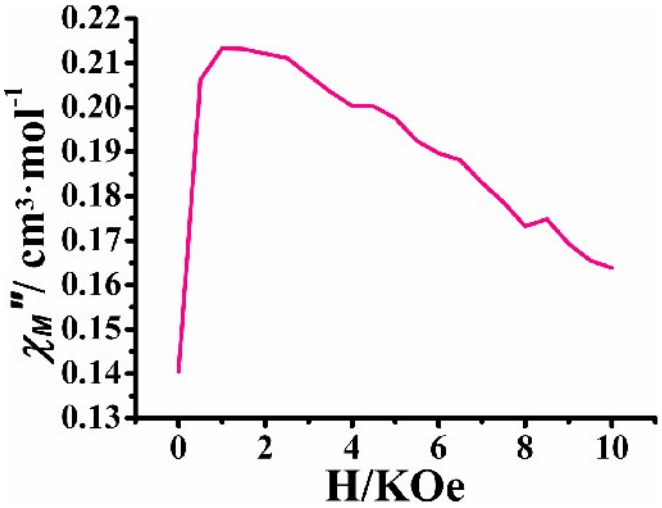

Figure S12. Ac-scan field data of (**2**) at 999 Hz and 2.0 K

Table S5. Relaxation distribution and times fitted from Cole-Cole data for **2**.

T(K)	α	τ (s)
2.0	**0.1795**	**0.706580E-03**
2.5	**0.0978**	**0.421521E-03**

3.0	**0.0977**	**0.262797E-03**
3.5	**0.0404**	**0.178541E-03**
4.0	**0.0033**	**0.128895E-03**
4.5	**0.0011**	**0.946765E-04**
5	**0.555328E-16**	**0.692182E-04**

Table S6. List of AC magnetic susceptibility measurement parameters of the reported discrete dinuclear Cu(II)–Ln(III) complexes

Complex[a]	Energy barrier	τ_0 (s)	Ref	Entry
$[CuL^{A}Dy(NO_3)_3]$	53K	$6(5)\times10^{-9}$	54	1
$[Cu_4Dy_2(OH)_2(NO_3)_8\{(py)_2CO_2\}_2(MeCN)_4]$	20.1(2) K	$8.3(1)\times10^{-9}$	55	2
$[Dy_3Cu_2\text{-}(L^{B})_4(MeOH)]ClO_4$	7.7K	2.6×10^{-5}	56	3
$[Dy_2Cu_4(L^{B})_4](ClO_4)_2$	10.65K	2.5×10^{-7}	56	4
$[CuL^{C}Dy(NO_3)_3]$	15.72K	1.70×10^{-7}	57	5
$[CuL^{D}\ Dy(H_2O)(NO_3)_3]$	122(1)K	$9.9(1)\times10^{-7}$	58	6
$[Na_2Yb\{Cu_4(butyrat)_4\}_2]$	6.84K	1.04×10^{-5}	This work	8

H_2L^{A} : (H2L = N-α-methylsalicylidene-N′-3-methoxysalicylidene-1,3-propanediamine).

H_4L^{B} : 2,2′-{2-hydroxy-3-[(2-hydroxyphenylimino)methyl]-5-methylbenzylazanediyl}diethanol.

H_2L^{C} : (R,R)-N,N′-bis(3-methoxysalicylidene)cyclohexane-1,2-diamine

H_2L^{D}: 1,3-bis(3-ethoxysalicylideneamino)-2-hydroxypropane