Supporting Information

Low coordinated mononuclear erbium(III) single-molecule magnets with C_{3v} symmetry: a method for altering single-molecule magnet properties by incorporating hard and soft donors

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1.1 Syntheses Details

$Er(dbpc)_3$ (**1**), $Er(btmsm)_3$ (**2**), and their precursor were synthesized according to the literatures[1-5]. All reagents were purchased from Wako Chemicals (Osaka, Japan), Kanto Chemical CO. INC. and used without further purification. All manipulation carried out by using standard Schlenk technique or in N_2 filled glovebox (MBraun UNIlab). The elemental analysis was performed on J−SCIENCE LAB CO., Ltd. JM−11 microanalyzer.

1.1.1 Tris(2,6−Di−*tert*−butyl−*p*−cresolate)erbium, $Er(dbpc)_3$ (1)

Deoxidized tetrahydrofuran (THF) (80 mL) was placed in a 200 mL Schlenk flask containing a magnetic stirring bar. Erbium (III) chloride anhydrous (2.20 g, 8.04 mmol) was added slowly into THF with stirring. Keep this mixture under stirring for 2h at ambient temperature. $[Li(OC_6H_2Me{-}4{-}Bu^t{}_2{-}2,6)(OEt_2)]_2$ (7.37g, 12.3 mmol) was added and the mixture was heated under reflux overnight yielded orchid suspension liquid. After cooling down to room temperature, the solvent was removed by liquid nitrogen cold trap, and genially warmed the viscous oil to get dry solid. The mashed residue was transferred to a sublimation tube. The sublimation at 250 °C (rapid heating−up) under 10^{-4} torr afforded pink crystalline product of (**1**) Yield: 2.84 g (42.8%). Elemental analysis: Calculated (%) for $C_{45}H_{69}O_3Er$: C, 65.49; H, 8.43. found: C, 65.42; H, 8.54.*

1.1.2 Tris(bis(trimethylsilyl)methyl)erbium, $Er(btmsm)_3$ (2) & diluted $Er_{0.05}Y_{0.95}(btmsm)_3$ (2')

$Er(dbpc)_3$ (0.537 g, 0.651 mmol) was dissolved in pentane (20 mL) to yield a clear solution, afterwards [Bis(trimethylsilyl)methyl]lithium (0.321 g, 1.93 mmol) was added with stirring. Maintain the mixture under stirring overnight at ambient temperature. White precipitate was removed by filtration through the diatomite bed. The filtrate was concentrated to half volume and frozen, harvested pink needle−like crystal. Repeat above procedure to yield the second crop. Product was combined and dried under vacuum. Yield: 0.163 g (38.8 %). Elemental analysis: Calculated (%) for $C_{21}H_{57}Si_6Er$: C, 39.08; H, 8.90. found: C, 39.16; H, 8.95. The diluted sample $Er_{0.05}Y_{0.95}(btmsm)_3$ was recrystallized from proportional mixture of $Er(dbpc)_3$ and $Y(dbpc)_3$ in pentane, which was prepared by the same method with $Er(dbpc)_3$. The erbium concentration was confirmed by magnetic susceptibility and single crystal X-ray diffraction data.

1.2 X−ray Crystallography

Single crystal X−ray diffraction data were collected on a Bruker APEX−II diffractometer with an APEX II CCD detector with Mo Kα radiation (λ = 0.71075 Å) at 120 K for (**1**) wrapped in Paratone−N (Hampton Research Corp., Aliso Viejo, CA, USA), at 110 K for (**2**), and at 163K for (**2'**). The structures were solved by Patterson methods. SHELXL−2014/7 was used for structure refinement[6]. Full-matrix least-squares refinements on F^2 based on unique reflections with unweighted and weighted agreement factors of $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ ($I > 2.00\ \sigma(I)$) and $wR = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$ were performed. Due to the existence of highly disordered solvent molecular in (**2**) and (**2'**), the squeeze processes were applied by PLATON[7]. Mercury 3.8 was used for visualization and analysis of the structure[8].

1.3 Magnetic Susceptibility Measurement

Magnetic susceptibility measurements were performed on a Quantum Design SQUID magnetometer MPMS−5L (Quantum Design, San Diego, CA, USA). The polycrystalline samples were sealed in NMR tubes with n−eicosane to avoid flip−flop. The temperature depended magnetic susceptibility data were collected from 280 K to 1.82 K in *H* of 1 kOe for (**1**) and (**2'**), and various strength (100 Oe, 1kOe, 3kOe, 6kOe) for (**2**). *M* vs *H* / *T* measurement were performed from 1.82 K to 5 K with follow direct field sequence: 0 Oe → 50 kOe → −50 kOe → 50 kOe. The background form sample tube was subtracted from data. The diamagnetic components of the sample and n−eicosane were corrected by Pascal's constants. The AC temperature depended susceptibility were collected with an AC field amplitude of 3.6 Oe from 30 K to 2 K, in zero and 1 kOe direct field for (**1**), in zero and 2 kOe direct field for (**2**), in zero and 1 kOe direct field for (**2'**).The AC frequency depended susceptibility were collected with an AC field amplitude of 3 Oe in the range of 0.1 − 1500 Hz, the same extra field was applied for both. The frequency scan data were fitted by the generalized Debye model (Eqn S1, S2)

$$\chi_M{}' = \chi_S + (\chi_T - \chi_S)\frac{(2\pi\tau)^{1-\alpha}\sin(\frac{\pi\alpha}{2})}{1 + 2(2\pi\tau)^{1-\alpha}\sin\left(\frac{\pi\alpha}{2}\right) + (2\pi\tau)^{2-2\alpha}} \quad \text{(Eqn.S1)}$$

$$\chi_M{}'' = (\chi_T - \chi_S)\frac{(2\pi\tau)^{1-\alpha}\cos(\frac{\pi\alpha}{2})}{1 + 2(2\pi\tau)^{1-\alpha}\sin\left(\frac{\pi\alpha}{2}\right) + (2\pi\tau)^{2-2\alpha}} \quad \text{(Eqn.S2)}$$

$$\tau^{-1} = cB^4 + d\frac{1 + eB^2}{1 + fB^2} \quad \text{(Eqn.S3)}$$

where χ_S is the adiabatic susceptibility, χ_T is the isothermal susceptibility, $\omega = 2\pi\upsilon$, (υ is the frequency) is the angular frequency, τ is the magnetization relaxation time, and α is the quantitative parameter for the width of the τ distribution. The field scan data were fitted by above equation (Eqn.S3) whose first term described direct process and the second term for Raman[9].

1.4 Theoretical calculation

The (**1**) and (**2**) model were built from X-ray diffraction determined structures (Table S12). The single point calculations carried out via Gaussian09 program package[10] under B3LYP functional[11] with small core Stuttgart basis set for (Er) including Effective Core Potentials (28 core electrons) and Def2-TZVP for others (H, C, N, O, Si), which were taken from the EMSL Basis Set Exchange Database[12]. Quartet is selected as ground state. Superfine integration grid was applied for numerical integrations and tight convergence condition were used for the SCF procedure. The achieved wavefunction was used for Localized orbital locator (LOL) analysis via Multiwfn v3.4. Visualization of the molecule and orbitals was achieved by GaussView 5.0. From the gross population analysis for erbium centre, 4f orbitals contribute the spin dominantly (Table S13).

Table S1. Selected X-ray crystallography information

	$Er(dbpc)_3$ (1)	**$Er(btmsm)_3$ (2)**	**$Er_{0.05}Y_{0.95}(btmsm)_3$ (2')**
Temperature / K	120(2)	110(2)	163(2)
formula	$C_{45}H_{69}O_3Er$	$C_{21}H_{57}Si_6Er$	$C_{21}H_{57}Si_6Er_{0.05}Y_{0.95}$
crystal system	triclinic	trigonal	trigonal
space group	$P\bar{1}$	$P\,3\,1\,c$	$P\,3\,1\,c$
***a* / Å**	9.6885(3)	16.2788(3)	16.3386(4)
***b* / Å**	14.9921(6)	16.2788(3)	16.3386(4)
***c* / Å**	15.9119(6)	8.5882(2)	8.6228(3)
α / °	70.604(3)	90	90
β / °	84.413(3)	90	90
γ / °	81.472(3)	120	120
***V* / Å³**	2153.07(14)	1970.96(9)	1993.46(12)
Z	2	2	2
***R*1 (*I* > 2σ (*I*))**	0.0573	0.0205	0.0338
***wR*2 (*I* > 2σ(*I*))**	0.1291	0.0444	0.0786
GooF	1.086	1.043	1.054

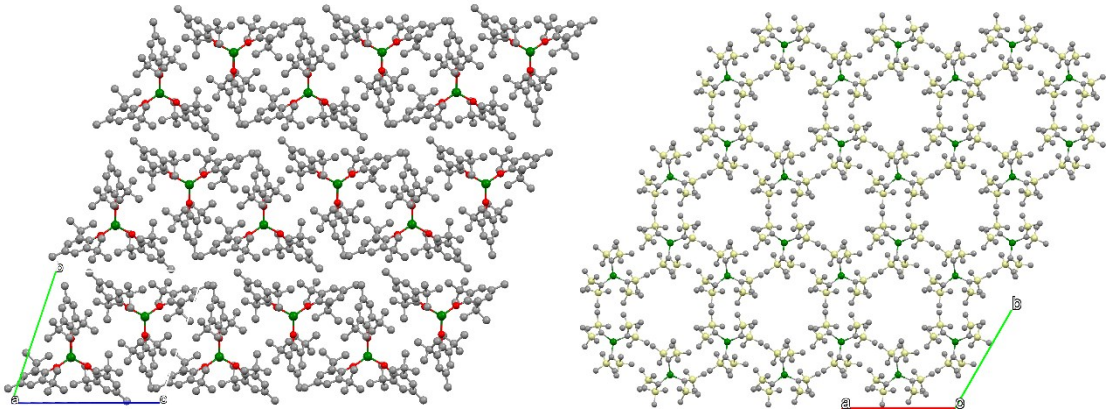

Fig.S1. Packing structure for $Er(dbpc)_3$ (**1**) alone the *a* axis (left), and $Er(btmsm)_3$ (**2**) alone the *c* axis (right). Hydrogen have been omitted for clarity. Color code: green, erbium; red, oxygen; gray, carbon; citrine, silicon.

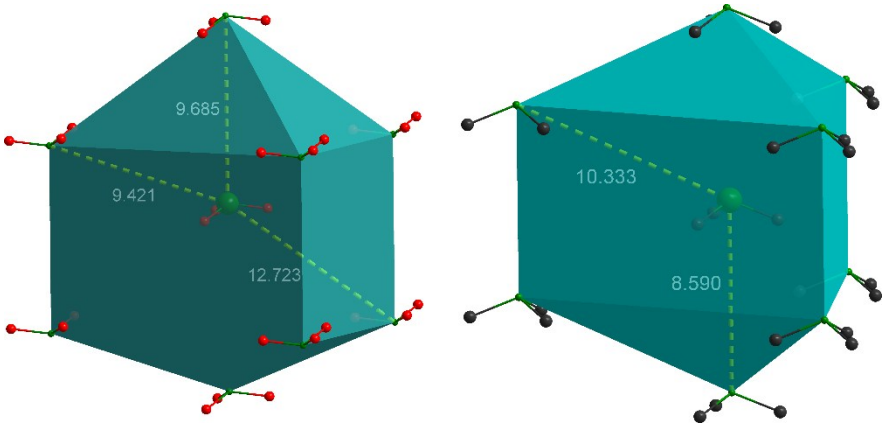

Fig.S2. The adjacent magnetic center environments of $Er(dbpc)_3$ (**1**) with the distance form 9.421 Å to 12.723 Å (left) , and $Er(btmsm)_3$ (**2**) with the distance 8.590 Å or 10.333 Å (right).

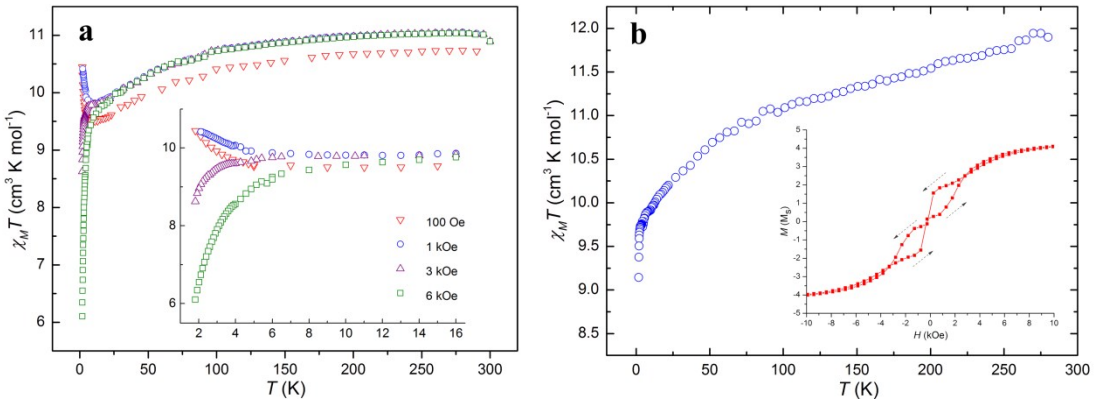

Fig.S3. (a) Temperature dependence of the $\chi_m T$ of Er(btmsm)$_3$ (**2**) in 100 Oe,1 kOe,3 kOe, and 6 kOe applied field respectively. Inset: enlarged view of the low temperature region. (b) The $\chi_m T$ of $Er_{0.05}Y_{0.95}$(btmsm)$_3$ (**2'**) under 1 kOe applied field. Inset: filed dependent magnetization at 1.82 K.

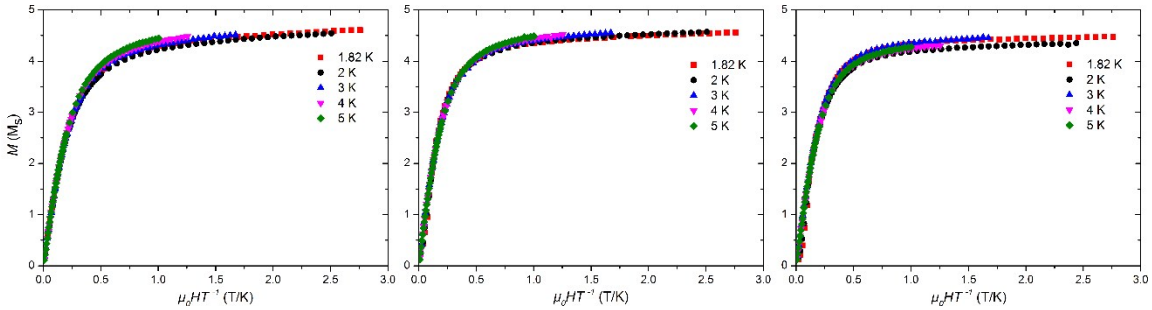

Fig.S4. Temperature reduced filed dependent magnetization for Er(dbpc)$_3$ (**1**) (left), Er(btmsm)$_3$ (**2**) (middle), and $Er_{0.05}Y_{0.95}$(btmsm)$_3$ (**2'**) (right).

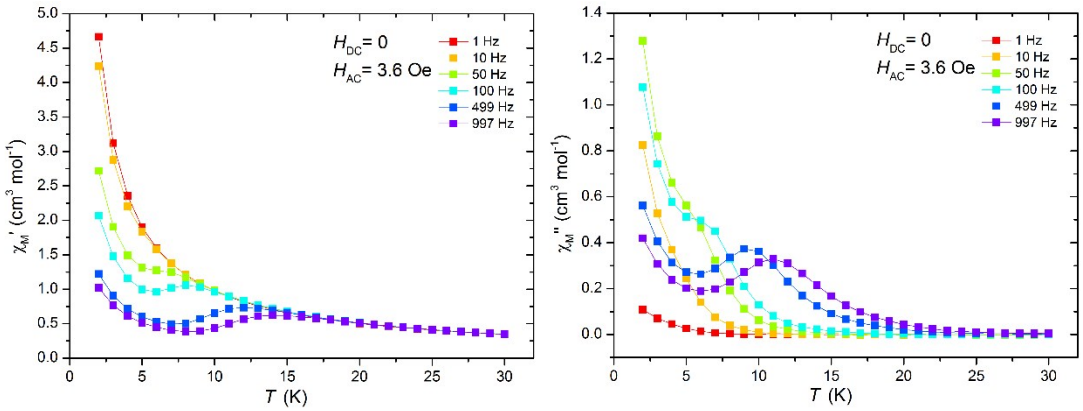

Fig.S5. The temperature dependent in-phase (χ_M') (left) and out-of-phase (χ_M'') (right) molar susceptibility in zero field for Er(dbpc)$_3$ (**1**).

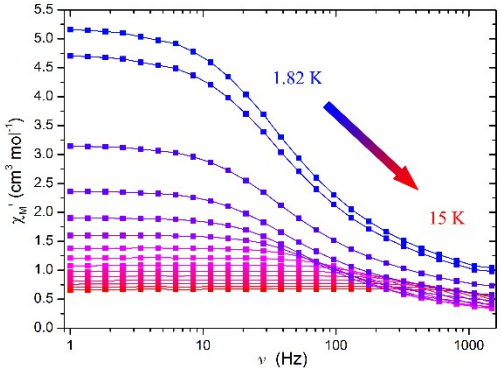

Fig.S6. The frequency dependent in-phase molar susceptibility (χ_M') for Er(dbpc)$_3$ (**1**) in zero field (left).

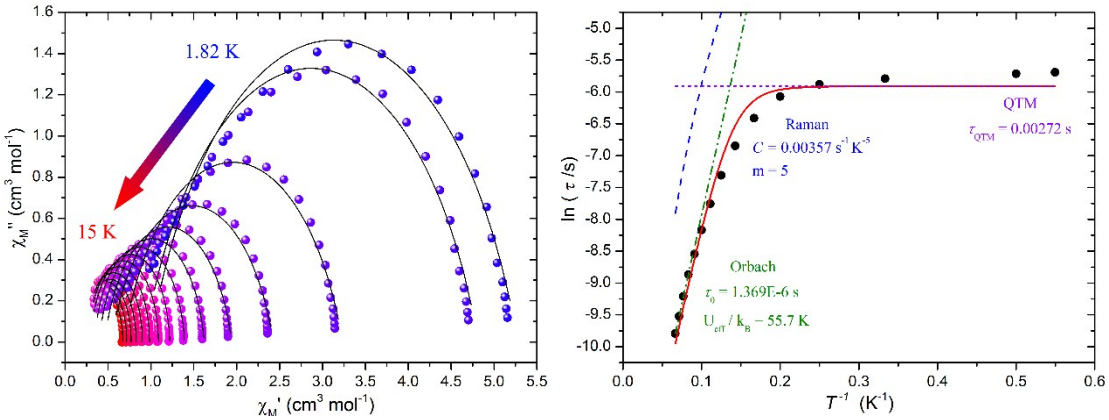

Fig.S7. Cole-Cole plot for Er(dbpc)$_3$ (**1**) in zero field (left). Relaxation times of the magnetization ln(τ) vs T^{-1} in zero field of Er(dbpc)$_3$ (**1**) (black circle). The red curve is the best fitting of Orbach (olive dash dot), Raman (blue dash), and QTM (violet short dash) process components.

Table S2. The fitting parameter from ac susceptibility of $Er(dbpc)_3$ (**1**) in zero field by the Debye model.

Temperature (K)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
1.82	3.36E-03	8.29E-05	0.24	1.12E-02	4.06E-03	0.99859
2	3.30E-03	8.18E-05	0.24	1.12E-02	3.37E-03	0.99859
3	3.05E-03	8.16E-05	0.24	1.21E-02	1.68E-03	0.99846
4	2.79E-03	7.81E-05	0.22	1.29E-02	1.09E-03	0.99829
5	2.30E-03	5.89E-05	0.18	1.27E-02	6.96E-04	0.99841
6	1.64E-03	3.47E-05	0.13	1.13E-02	4.07E-04	0.99879
7	1.06E-03	1.64E-05	0.08	8.78E-03	1.83E-04	0.99933
8	6.68E-04	8.08E-06	0.05	7.18E-03	8.97E-05	0.99961
9	4.28E-04	3.73E-06	0.02	5.22E-03	3.37E-05	0.99983
10	2.84E-04	2.31E-06	0.00	4.69E-03	1.86E-05	0.99989
11	1.94E-04	2.39E-06	0.00	6.22E-03	2.07E-05	0.99986
12	1.41E-04	3.53E-06	0.00	1.06E-02	3.56E-05	0.99974
13	1.00E-04	3.03E-06	0.00	1.01E-02	1.92E-05	0.99984
14	7.33E-05	3.46E-06	0.00	1.22E-02	1.60E-05	0.99986
15	5.57E-05	4.27E-06	0.00	1.57E-02	1.51E-05	0.99985

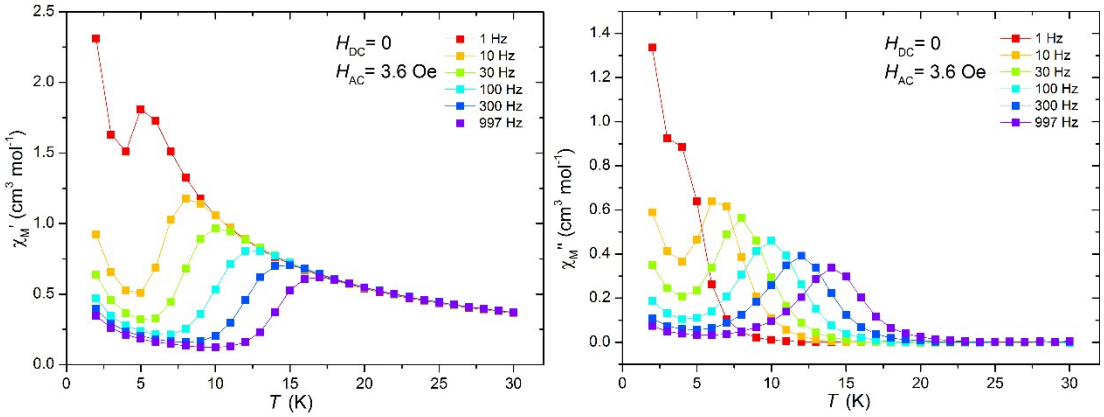

Fig.S8. The temperature dependent in-phase (χ_M') (left) and out-of-phase (χ_M'') (right) molar susceptibility in zero field for Er(btmsm)$_3$ (**2**).

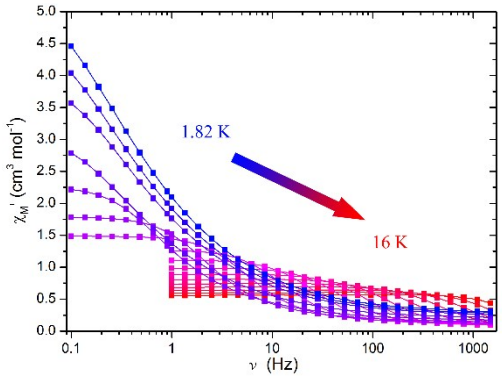

Fig.S9. The frequency dependent in-phase molar susceptibility (χ_M') for Er(btmsm)$_3$ (**2**) in zero field.

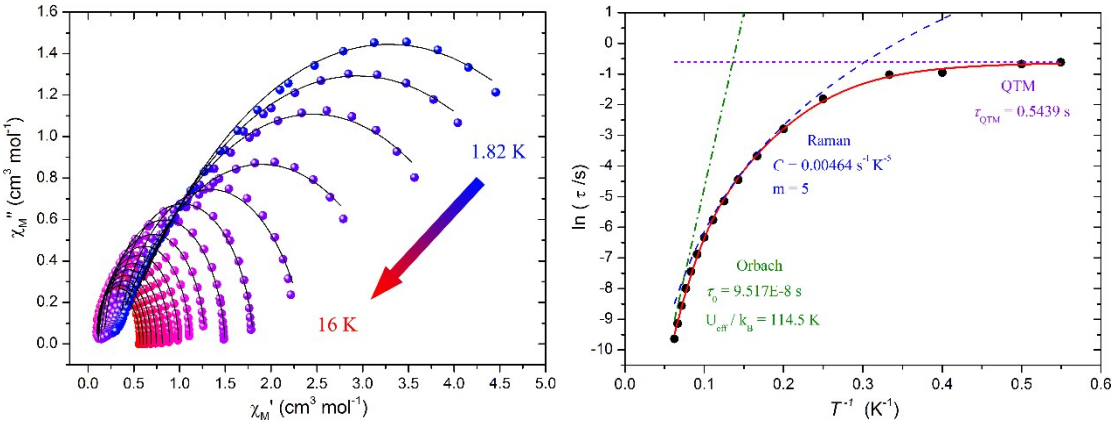

Fig.S10. Cole-Cole plot for (**2**) in zero field (left). Relaxation times of the magnetization ln(τ) vs T^{-1} in zero field of (**2**) (black circle). The red curve is the best fitting of Orbach (olive dash dot), Raman (blue dash), and QTM (violet short dash) process components.

Table S3. The fitting parameter from ac susceptibility of $Er(btmsm)_3$ (**2**) in zero field by the Debye model.

Temperature (K)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
1.82	5.38E-01	1.37E-02	0.44	3.80E-03	4.23E-04	0.99960
2	5.09E-01	1.34E-02	0.43	4.02E-03	3.87E-04	0.99955
2.5	3.85E-01	1.14E-02	0.41	5.28E-03	5.33E-04	0.99924
3	3.69E-01	1.16E-02	0.40	5.94E-03	4.10E-04	0.99904
4	1.64E-01	4.68E-03	0.27	1.02E-02	9.30E-04	0.99720
5	6.13E-02	9.83E-04	0.14	8.10E-03	4.72E-04	0.99842
6	2.53E-02	2.49E-04	0.08	5.42E-03	1.62E-04	0.99937
7	1.16E-02	8.77E-05	0.06	4.47E-03	6.41E-05	0.99956
8	5.82E-03	3.37E-05	0.04	3.53E-03	3.32E-05	0.99975
9	3.15E-03	1.42E-05	0.03	2.81E-03	1.69E-05	0.99986
10	1.79E-03	7.07E-06	0.02	2.51E-03	1.07E-05	0.99990
11	1.03E-03	4.26E-06	0.01	2.67E-03	9.39E-06	0.99990
12	5.87E-04	2.58E-06	0.00	2.82E-03	7.75E-06	0.99991
13	3.37E-04	2.29E-06	0.00	4.09E-03	1.09E-05	0.99987
14	1.92E-04	2.31E-06	0.00	6.05E-03	1.36E-05	0.99982
15	1.07E-04	2.55E-06	0.00	8.35E-03	1.21E-05	0.99983
16	6.52E-05	4.99E-06	0.00	1.80E-02	2.14E-05	0.99970

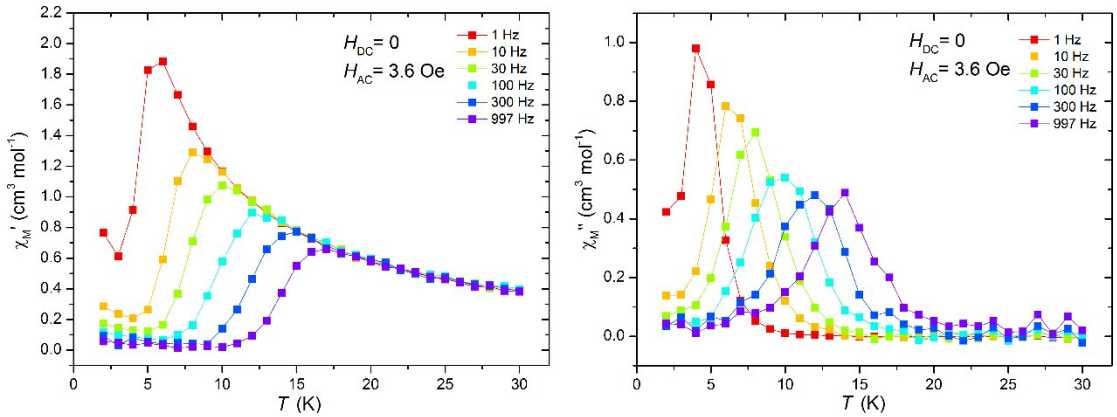

Fig.S11. The temperature dependent in-phase (χM′) (left) and out-of-phase (χM″) (right) molar susceptibility in zero field for $Er_{0.05}Y_{0.95}(btmsm)_3$ (2').

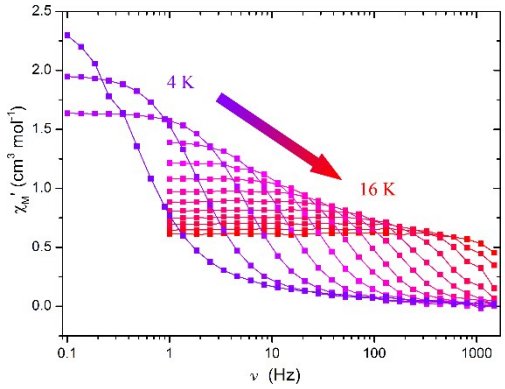

Fig.S12. The frequency dependent in-phase molar susceptibility (χ_M') for $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**) in zero field.

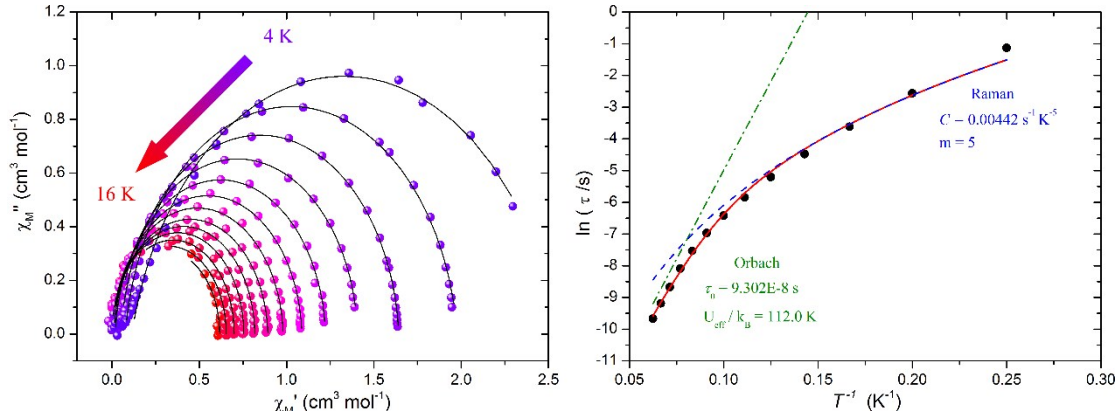

Fig.S13. Cole-Cole plot for (**2'**) in zero field (left). Relaxation times of the magnetization ln(τ) vs T^{-1} in zero field of (**2'**) (black circle). The red curve is the best fitting of Orbach (olive dash dot), and Raman (blue dash) process components.

Table S4. The fitting parameter from ac susceptibility of $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**) in zero field by the Debye model.

Temperature (K)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
4	3.23E-01	6.59E-03	0.18	8.26E-03	7.14E-04	0.99773
5	7.73E-02	8.05E-04	0.09	5.76E-03	3.43E-04	0.99907
6	2.68E-02	2.53E-04	0.06	5.39E-03	2.36E-04	0.99928
7	1.14E-02	9.47E-05	0.04	5.09E-03	1.24E-04	0.99936
8	5.49E-03	5.66E-05	0.03	6.40E-03	1.61E-04	0.99908
9	2.90E-03	3.36E-05	0.03	7.22E-03	1.64E-04	0.99894
10	1.62E-03	1.69E-05	0.03	6.49E-03	1.05E-04	0.99923
11	9.39E-04	1.25E-05	0.03	8.29E-03	1.30E-04	0.99891
12	5.34E-04	6.64E-06	0.01	7.75E-03	8.40E-05	0.99921
13	3.07E-04	4.91E-06	0.00	9.47E-03	8.48E-05	0.99912
14	1.70E-04	5.50E-06	0.00	1.53E-02	1.20E-04	0.99867
15	1.02E-04	5.82E-06	0.00	1.93E-02	9.06E-05	0.99894
16	6.34E-05	6.90E-06	0.00	2.50E-02	6.44E-05	0.99922

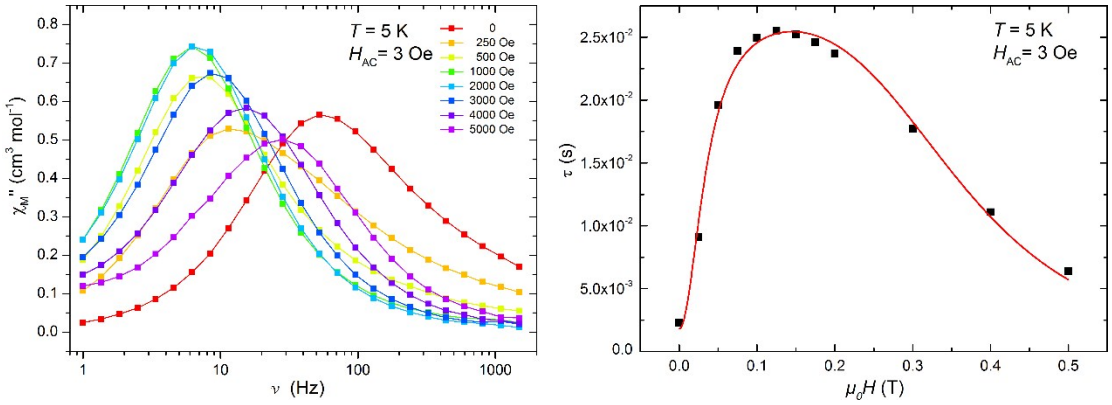

Fig.S14. The frequency dependent out-of-phase molar susceptibility (χM″) at 5 K for Er(dbpc)3 (1) under various applied field (left). Relaxation time of the magnetization τ vs H for (**1**) at 5 K and the fitted by Eqn. S3.(right).

Table S5. The fitting parameter from ac susceptibility of $Er(dbpc)_3$ (**1**) at 5K under various field by the Debye model.

Field (Oe)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
0	2.30E-03	5.89E-05	0.18	1.27E-02	6.96E-04	0.99841
250	9.10E-03	3.39E-04	0.29	1.50E-02	9.13E-04	0.99724
500	1.96E-02	5.19E-04	0.13	1.36E-02	8.69E-04	0.99684
750	2.39E-02	2.76E-04	0.06	6.76E-03	2.41E-04	0.99907
1000	2.50E-02	1.87E-04	0.04	4.51E-03	1.07E-04	0.99956
1250	2.55E-02	1.01E-04	0.03	2.45E-03	3.34E-05	0.99987
1500	2.52E-02	7.01E-05	0.02	1.72E-03	1.64E-05	0.99993
1750	2.46E-02	6.27E-05	0.02	1.57E-03	1.36E-05	0.99994
2000	2.37E-02	4.67E-05	0.03	1.21E-03	7.93E-06	0.99997
3000	1.77E-02	5.67E-05	0.06	1.90E-03	1.75E-05	0.99993
4000	1.11E-02	7.88E-05	0.10	3.98E-03	6.56E-05	0.99971
5000	6.41E-03	8.80E-05	0.13	7.34E-03	1.79E-04	0.99916

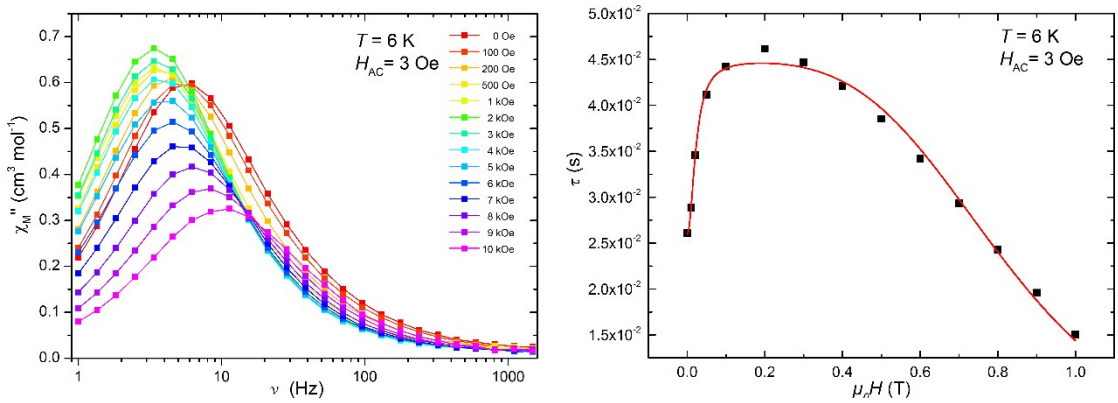

Fig.S15. The frequency dependent out-of-phase molar susceptibility (χ_M'') at 6 K for Er(btmsm)$_3$ (**2**) under various applied field (left). Relaxation time of the magnetization τ vs *H* for (**2**) at 6 K and the fitted by Eqn. S3 (right).

Table S6. The fitting parameter from ac susceptibility of Er(btmsm)$_3$ (**2**) at 6K under various field by the Debye model.

Field (Oe)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
0	2.61E-02	3.06E-04	0.10	6.28E-03	1.39E-04	0.99905
100	2.88E-02	3.21E-04	0.10	5.88E-03	1.18E-04	0.99916
200	3.46E-02	3.54E-04	0.09	5.37E-03	9.40E-05	0.99927
500	4.11E-02	3.99E-04	0.07	5.18E-03	8.52E-05	0.99929
1000	4.42E-02	3.91E-04	0.06	4.75E-03	6.96E-05	0.99939
2000	4.62E-02	1.94E-04	0.04	2.47E-03	1.91E-05	0.99986
3000	4.47E-02	2.71E-04	0.04	3.39E-03	3.69E-05	0.99968
4000	4.21E-02	2.41E-04	0.05	3.23E-03	3.05E-05	0.99972
5000	3.85E-02	2.37E-04	0.05	3.46E-03	3.13E-05	0.99968
6000	3.42E-02	2.17E-04	0.06	3.59E-03	2.95E-05	0.99966
7000	2.93E-02	1.87E-04	0.07	3.61E-03	2.61E-05	0.99967
8000	2.43E-02	1.64E-04	0.07	3.82E-03	2.52E-05	0.99965
9000	1.96E-02	1.31E-04	0.09	3.75E-03	2.06E-05	0.99968
10000	1.51E-02	9.41E-05	0.10	3.44E-03	1.46E-05	0.99974

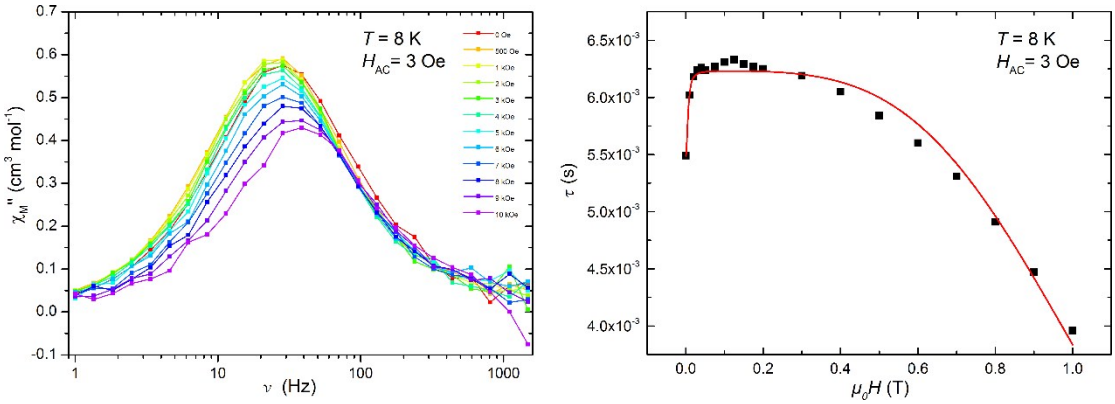

Fig.S16. The frequency dependent out-of-phase molar susceptibility (χ_M'') at 8 K for $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**) under various applied field (left). Relaxation time of the magnetization τ vs *H* for (**2'**) at 8 K and the fitted by Eqn. S3 (right).

Table S7. The fitting parameter from ac susceptibility of $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**) at 8K under various field by the Debye model.

Field (Oe)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
0	5.49E-03	5.66E-05	0.03	6.40E-03	1.61E-04	0.99908
100	6.02E-03	5.82E-05	0.03	6.08E-03	1.28E-04	0.99921
200	6.18E-03	6.70E-05	0.03	6.85E-03	1.66E-04	0.99898
300	6.24E-03	6.25E-05	0.03	6.33E-03	1.40E-04	0.99914
400	6.26E-03	4.89E-05	0.03	4.94E-03	8.66E-05	0.99947
500	6.24E-03	5.83E-05	0.03	5.81E-03	1.40E-04	0.99921
750	6.27E-03	5.35E-05	0.02	5.43E-03	1.05E-04	0.99936
1000	6.31E-03	5.43E-05	0.02	5.39E-03	1.17E-04	0.99932
1250	6.33E-03	5.21E-05	0.03	5.22E-03	9.62E-05	0.99941
1500	6.29E-03	4.97E-05	0.02	5.08E-03	9.09E-05	0.99944
1750	6.27E-03	5.41E-05	0.02	5.50E-03	1.06E-04	0.99934
2000	6.25E-03	4.47E-05	0.02	4.50E-03	8.05E-05	0.99953
3000	6.19E-03	7.81E-05	0.01	8.08E-03	2.51E-04	0.99848
4000	6.05E-03	5.81E-05	0.02	6.03E-03	1.35E-04	0.99916
5000	5.84E-03	7.78E-05	0.03	8.26E-03	2.37E-04	0.99842
6000	5.60E-03	7.67E-05	0.03	8.52E-03	2.34E-04	0.99832
7000	5.31E-03	5.41E-05	0.03	6.37E-03	1.22E-04	0.99909
8000	4.91E-03	8.42E-05	0.04	1.05E-02	2.98E-04	0.99755
9000	4.47E-03	4.38E-05	0.04	6.00E-03	8.76E-05	0.99922
10000	3.96E-03	8.65E-05	0.02	1.36E-02	4.06E-04	0.99606

Table S8. The fitting parameter from filed scan ac susceptibility by Eqn.S3.

Compound	$Er(dbpc)_3$ (1)	$Er(btmsm)_3$ (2)	$Er_{0.05}Y_{0.95}(btmsm)_3$ (2')
c	2.21E+03	4.73E+01	1.00E+02
c (error)	1.97E+02	1.97E+00	4.03E+00
d	5.54E+02	3.85E+01	1.82E+02
d (error)	2.49E+02	1.13E+00	2.90E+00
e	8.09E+02	1.93E+03	2.93E+04
e (error)	1.17E+02	3.86E+02	1.92E+04
f	1.23E+04	3.33E+03	3.33E+04
f (error)	6.53E+03	7.15E+02	2.17E+04
Reduced Chi-Sqr	6.86E-07	7.33E-07	7.53E-09
Adj. R-Square	0.99030	0.99251	0.98364

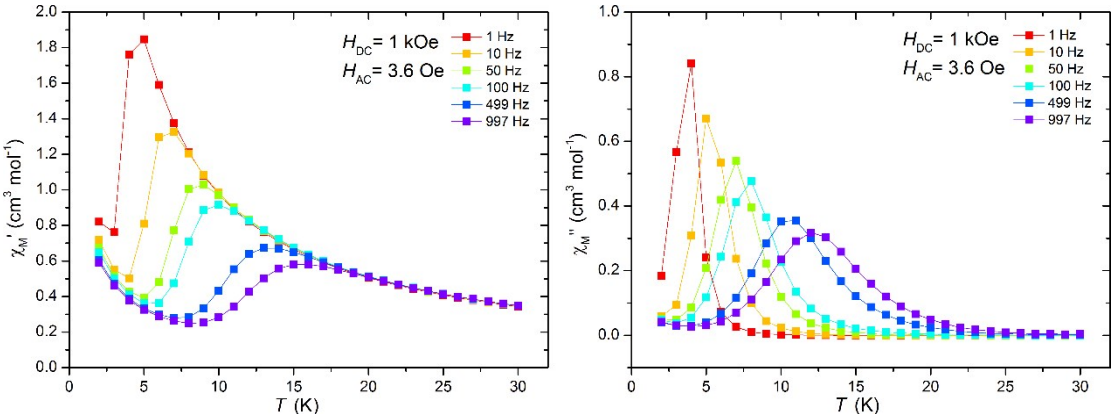

Fig.S17. The temperature dependent in-phase (χ_M') (left) and out-of-phase (χ_M'') (right) molar susceptibility in a 1 kOe applied field for Er(dbpc)$_3$ (**1**).

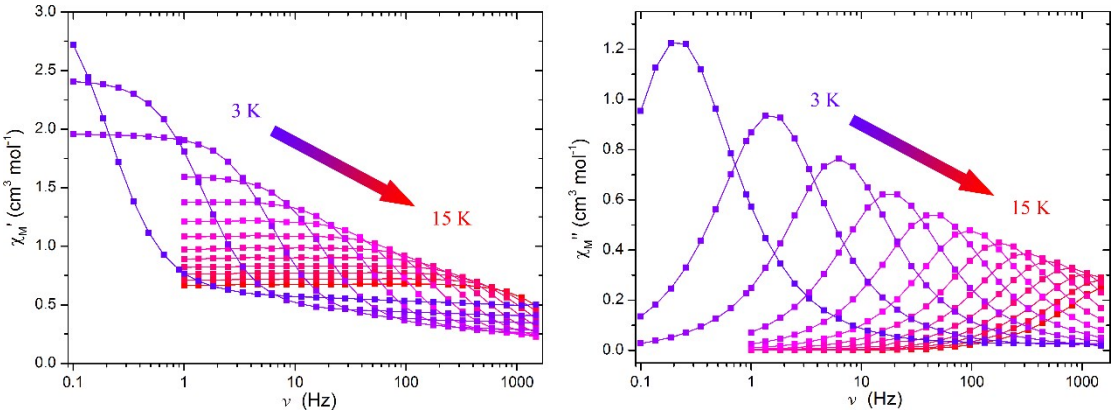

Fig.S18. The frequency dependent in-phase (χ_M') (left) and out-of-phase (χ_M'') (right) molar susceptibility for Er(dbpc)$_3$ (**1**) and in a 1 kOe applied field.

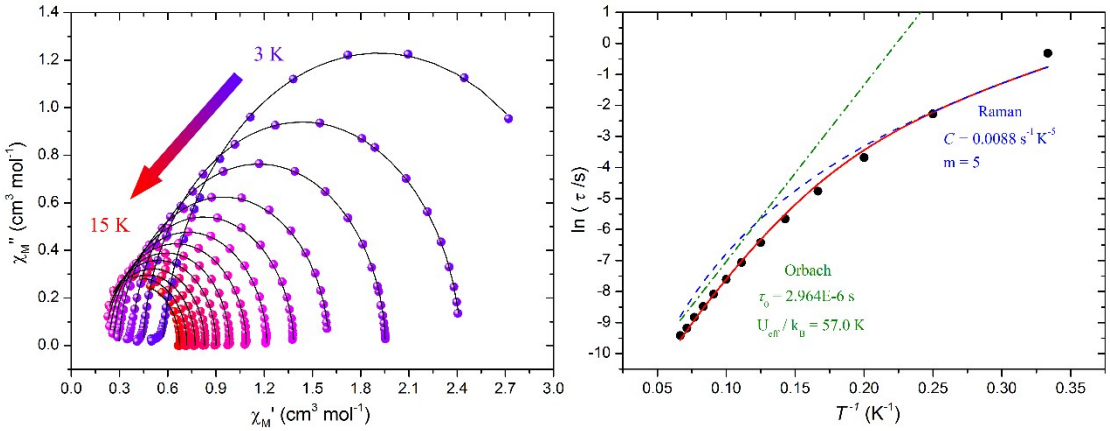

Fig.S19. Cole-Cole plot for Er(dbpc)$_3$ (**1**) in a 1 kOe applied field (left). Relaxation times of the magnetization ln(τ) vs T^{-1} in a 1 kOe applied field of Er(dbpc)$_3$ (**1**) (black circle). The red curve is the best fitting of Orbach (olive dash dot), and Raman (blue dash) process components.

Table S9. The fitting parameter from ac susceptibility of $Er(dbpc)_3$ (**1**) in a 1 kOe applied field by the Debye model.

Temperature (K)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
3	7.29E-01	5.69E-03	0.06	3.82E-03	1.16E-04	0.99970
4	1.03E-01	5.88E-04	0.04	3.41E-03	1.33E-04	0.99972
5	2.52E-02	1.15E-04	0.03	2.72E-03	6.14E-05	0.99986
6	8.51E-03	4.85E-05	0.03	3.53E-03	5.65E-05	0.99977
7	3.47E-03	1.65E-05	0.02	2.98E-03	3.06E-05	0.99987
8	1.63E-03	7.79E-06	0.02	3.01E-03	2.31E-05	0.99989
9	8.57E-04	4.34E-06	0.01	3.21E-03	1.89E-05	0.99989
10	4.96E-04	2.93E-06	0.00	3.72E-03	1.76E-05	0.99989
11	3.08E-04	2.28E-06	0.00	4.37E-03	1.63E-05	0.99988
12	2.07E-04	2.54E-06	0.00	6.38E-03	2.11E-05	0.99983
13	1.46E-04	2.85E-06	0.00	8.47E-03	2.24E-05	0.99981
14	1.03E-04	2.69E-06	0.00	8.88E-03	1.44E-05	0.99987
15	8.11E-05	4.37E-06	0.00	1.52E-02	2.37E-05	0.99976

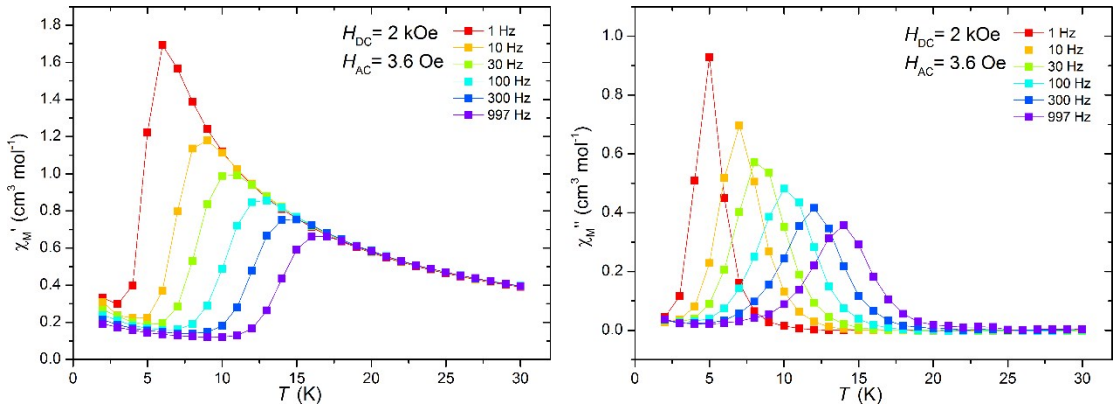

Fig.S20. The temperature dependent in-phase (χ_M') (left) and out-of-phase (χ_M'') (right) molar susceptibility in a 2 kOe applied field for Er(btmsm)$_3$ (**2**).

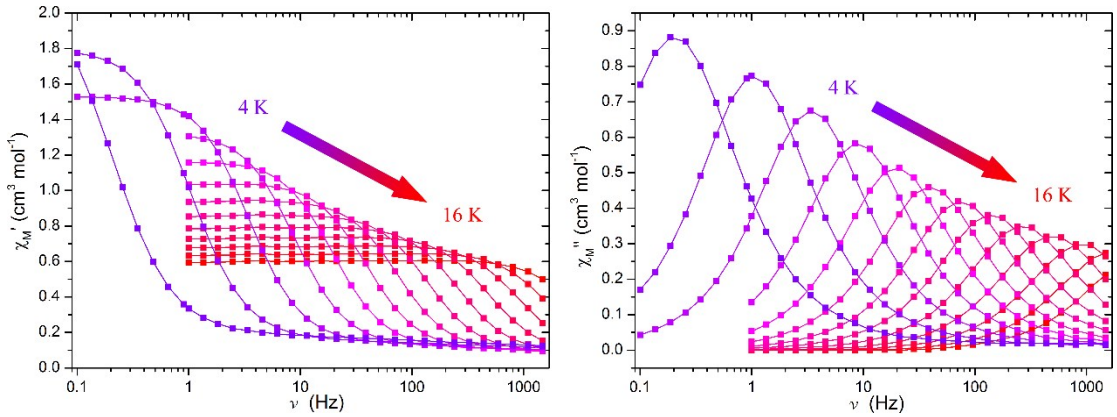

Fig.S21. The frequency dependent in-phase (χ_M') (left) and out-of-phase (χ_M'') (right) for Er(btmsm)$_3$ (**2**) and in a 2 kOe applied field (right).

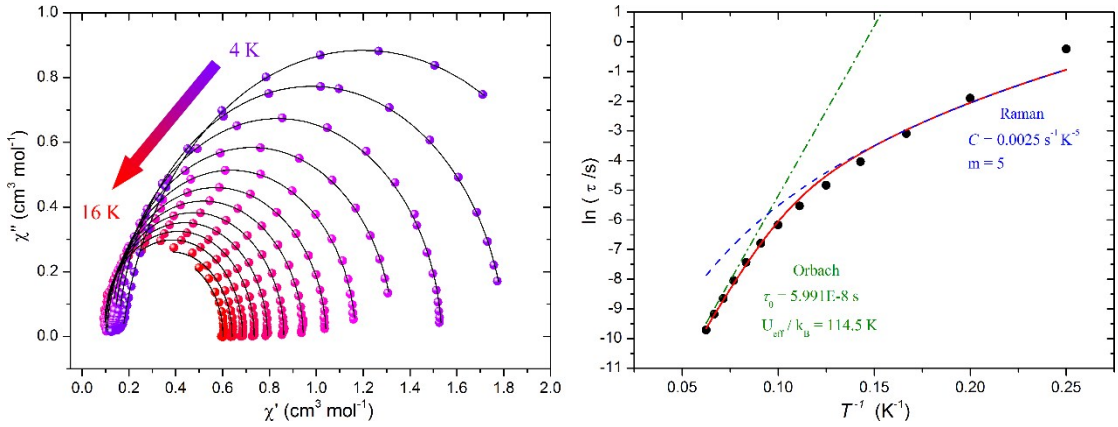

Fig.S22. Cole-Cole plot for Er(btmsm)$_3$ (**2**) in a 2 kOe applied field (left). Relaxation times of the magnetization ln(τ) vs T^{-1} in a 2 kOe applied field of Er(btmsm)$_3$ (**2**) (black circle). The red curve is the best fitting of Orbach (olive dash dot), and Raman (blue dash) process components.

Table S10. The fitting parameter from ac susceptibility of $Er(btmsm)_3$ (**2**) in a 2 kOe applied field by the Debye model.

Temperature (K)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
4	7.87E-01	7.08E-03	0.10	3.57E-03	5.79E-05	0.99962
5	1.50E-01	5.57E-04	0.05	2.23E-03	3.43E-05	0.99987
6	4.54E-02	1.65E-04	0.03	2.22E-03	2.88E-05	0.99989
7	1.76E-02	7.79E-05	0.03	2.75E-03	2.67E-05	0.99981
8	7.94E-03	2.87E-05	0.02	2.27E-03	1.57E-05	0.99989
9	3.97E-03	1.37E-05	0.02	2.19E-03	1.19E-05	0.99991
10	2.09E-03	8.72E-06	0.01	2.66E-03	1.41E-05	0.99988
11	1.12E-03	4.69E-06	0.00	2.70E-03	1.12E-05	0.99990
12	5.92E-04	3.04E-06	0.00	3.28E-03	1.19E-05	0.99988
13	3.19E-04	2.17E-06	0.00	4.05E-03	1.18E-05	0.99987
14	1.74E-04	1.92E-06	0.00	5.28E-03	1.06E-05	0.99988
15	1.03E-04	3.74E-06	0.00	1.24E-02	2.41E-05	0.99972
16	6.06E-05	5.54E-06	0.00	2.02E-02	2.39E-05	0.99971

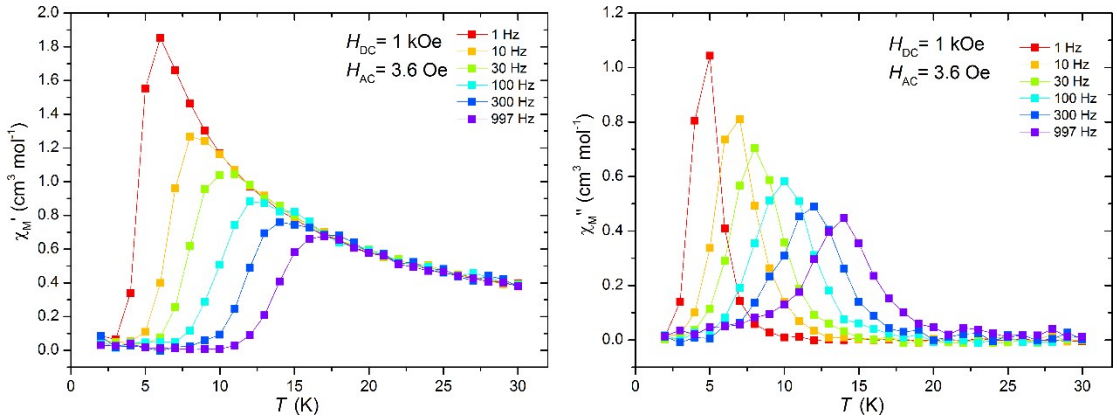

Fig.S23. The temperature dependent in-phase (χ_M') (left) and out-of-phase (χ_M'') (right) molar susceptibility in a 1 kOe applied field for $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**).

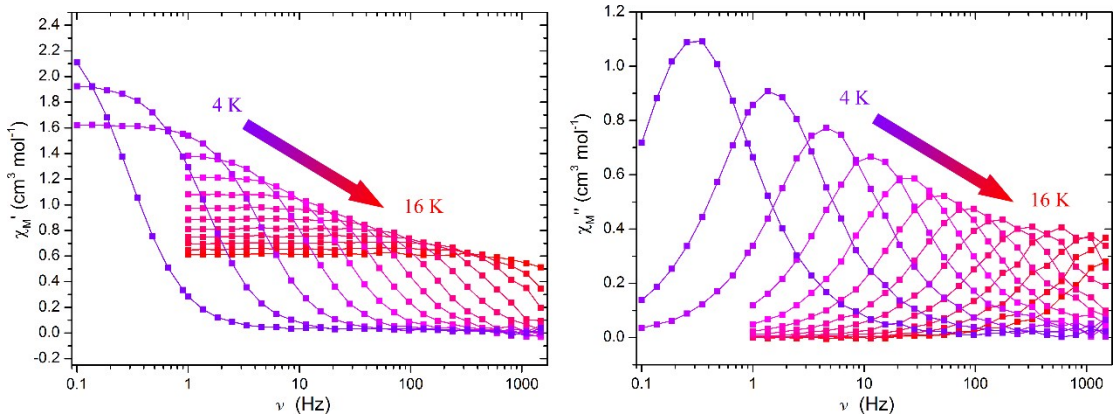

Fig.S24. The frequency dependent in-phase (χ_M') (left) and out-of-phase (χ_M'') (right) for $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**) and in a 1 kOe applied field (right).

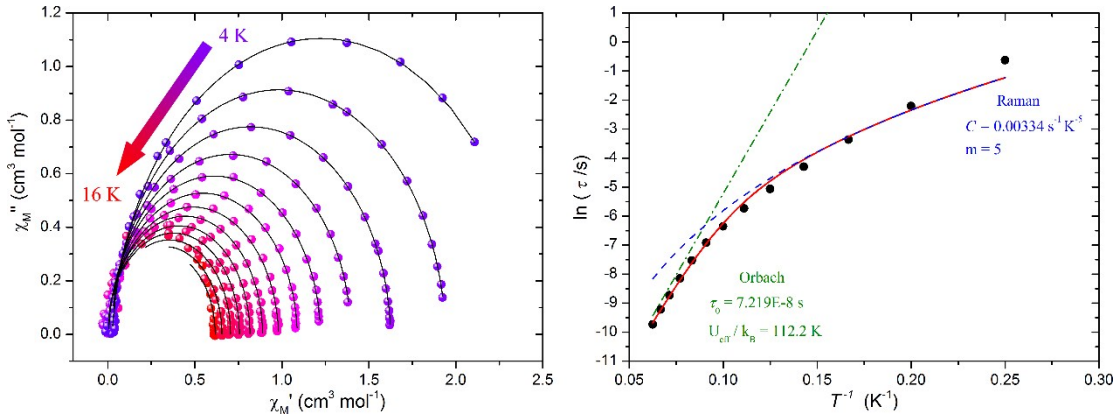

Fig.S25. Cole-Cole plot for $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**) in a 1 kOe applied field (left). Relaxation times of the magnetization ln(τ) vs T^{-1} in a 1 kOe applied field of $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**) (black circle). The red curve is the best fitting of Orbach (olive dash dot), and Raman (blue dash) process components.

Table S11. The fitting parameter from ac susceptibility of $Er_{0.05}Y_{0.95}(btmsm)_3$ (**2'**) in a 1 kOe applied field by the Debye model.

Temperature (K)	τ (s)	τ (error)	α	α (error)	Reduced Chi-Sqr	Adj. R-Square
4	5.35E-01	3.61E-03	0.05	3.34E-03	1.07E-04	0.99957
5	1.10E-01	6.27E-04	0.03	3.45E-03	1.27E-04	0.99963
6	3.45E-02	1.75E-04	0.02	3.04E-03	7.80E-05	0.99976
7	1.36E-02	1.39E-04	0.03	6.38E-03	1.99E-04	0.99894
8	6.30E-03	4.87E-05	0.02	4.87E-03	9.67E-05	0.99945
9	3.24E-03	2.68E-05	0.02	5.21E-03	8.86E-05	0.99943
10	1.74E-03	1.56E-05	0.02	5.65E-03	8.14E-05	0.99940
11	9.87E-04	1.23E-05	0.00	8.03E-03	1.29E-04	0.99892
12	5.38E-04	6.19E-06	0.00	7.28E-03	7.56E-05	0.99929
13	2.89E-04	7.59E-06	0.00	1.53E-02	2.14E-04	0.99780
14	1.62E-04	5.41E-06	0.00	1.54E-02	1.17E-04	0.99872
15	9.92E-05	6.50E-06	0.00	2.17E-02	1.10E-04	0.99872
16	5.92E-05	1.02E-05	0.00	3.73E-02	1.28E-04	0.99844

Table S12. The atom list for calculation of $Er(dbpc)_3$, $Er[N(SiMe_3)_2]_3$, and $Er(btmsm)_3$.

$Er(dbpc)_3$ (1)			
Atom	x (Å)	y (Å)	z (Å)
Er	0.0066	-0.4873	0.0604
O	-0.4271	-0.0180	-1.8304
O	1.9472	0.0984	0.5035
O	-1.2940	0.1593	1.4755
C	-1.8655	-2.9221	4.5779
C	-1.7193	-1.1274	-3.5081
C	-0.9105	-0.0466	-3.0913
C	-0.5886	1.0136	-3.9660
C	0.3348	2.1679	-3.5399
C	-4.2940	1.3242	3.1508
C	3.2732	0.0936	0.7626
C	-0.2160	2.8941	-2.2864
C	5.2389	1.2127	1.5668
C	4.0461	-1.0578	0.4584
C	3.0384	2.5082	1.6618
C	3.4131	-2.3183	-0.1365
C	1.7436	1.6413	-3.2506
C	-1.1234	0.9791	-5.2547
C	3.8713	1.2515	1.3201
C	2.8324	-2.0230	-1.5243
C	6.0046	0.1119	1.2637
C	5.4070	-1.0028	0.7139
C	-1.9185	-0.0539	-5.6654
C	3.9134	3.6489	2.2307

C	1.9928	2.1590	2.7287
C	0.4536	3.2377	-4.6311
C	2.3325	-2.8649	0.8119
C	-2.0679	-2.3247	-2.6092
C	-2.2051	-1.0862	-4.8118
C	-2.8200	-1.8764	-1.3132
C	4.4314	-3.4430	-0.3460
C	2.3724	3.0555	0.3888
C	-0.7161	-3.0217	-2.0751
C	-3.1151	2.3670	1.1666
C	-2.4552	-0.7780	3.3392
C	-2.3265	0.2270	2.3429
C	-3.2383	1.2915	2.2510
C	-3.2944	1.7470	-0.2224
C	-4.4479	0.3580	4.1238
C	-3.5499	-0.6805	4.1996
C	-4.1935	3.4636	1.2859
C	-1.4525	-1.9217	3.4730
C	-1.3698	-2.7379	2.1712
C	-0.0646	-1.3998	3.8353
C	-1.7559	3.0898	1.2573
C	-2.8469	-3.4395	-3.2112
C	-5.6178	0.4437	5.1217
C	7.5204	0.1251	1.5357
C	-2.4943	-0.0555	-7.0938
H	-1.9134	-2.4562	5.4384
H	-1.2036	-3.6418	4.6314
H	-2.7441	-3.3012	4.3640
H	-4.9282	2.0284	3.0947
H	0.4929	3.4379	-1.8861
H	-0.5279	2.2320	-1.6341
H	-0.9637	3.4733	-2.5461
H	5.6567	1.9699	1.9579
H	2.1277	1.2651	-4.0704
H	1.6986	0.9441	-2.5620
H	2.3093	2.3778	-2.9337
H	-0.9307	1.6869	-5.8574
H	3.5581	-1.7753	-2.1363
H	2.1939	-1.2826	-1.4605
H	2.3757	-2.8214	-1.8629
H	5.9455	-1.7563	0.5043
H	3.3463	4.4186	2.4490
H	4.5793	3.9124	1.5617
H	4.3685	3.3372	3.0406
H	1.3581	1.5071	2.3631
H	1.5117	2.9707	2.9918

H	2.4399	1.7757	3.5112
H	0.9456	2.8717	-5.3950
H	0.9336	4.0142	-4.2760
H	-0.4425	3.5104	-4.9197
H	1.8645	-3.6105	0.3796
H	1.6912	-2.1536	1.0207
H	2.7524	-3.1800	1.6396
H	-2.7527	-1.7993	-5.1208
H	-3.6384	-1.3963	-1.5607
H	-2.2420	-1.2891	-0.7870
H	-3.0542	-2.6675	-0.7824
H	4.8234	-3.6928	0.5182
H	5.1398	-3.1358	-0.9494
H	3.9835	-4.2195	-0.7370
H	2.0022	2.3124	-0.1305
H	3.0397	3.5280	-0.1504
H	1.6534	3.6719	0.6358
H	-0.9462	-3.7572	-1.4672
H	-0.1732	-2.3611	-1.5971
H	-0.2080	-3.3764	-2.8345
H	-2.5823	1.0944	-0.3823
H	-3.2519	2.4500	-0.9027
H	-4.1664	1.2994	-0.2697
H	-3.6778	-1.3524	4.8563
H	-5.0788	3.0667	1.1496
H	-4.0366	4.1543	0.6072
H	-4.1519	3.8674	2.1783
H	-2.2526	-3.1047	1.9584
H	-0.7292	-3.4709	2.2869
H	-1.0722	-2.1578	1.4403
H	0.2408	-0.7774	3.1438
H	0.5603	-2.1517	3.8987
H	-0.1043	-0.9352	4.6979
H	-1.7606	3.7005	2.0255
H	-1.6031	3.6013	0.4357
H	-1.0413	2.4278	1.3689
H	-2.8756	-4.1940	-2.5854
H	-2.4186	-3.7237	-4.0464
H	-3.7595	-3.1372	-3.3983
H	-5.9558	-0.5430	5.3605
H	-5.2899	0.9342	6.0144
H	-6.4203	0.9994	4.6836
H	7.8884	1.1266	1.4556
H	7.7092	-0.2466	2.5211
H	8.0167	-0.4956	0.8192
H	-2.7367	0.9461	-7.3817

H	-1.7683	-0.4553	-7.7705
H	-3.3778	-0.6583	-7.1215
$Er[N(SiMe_3)_2]_3$			
Atom	x (Å)	y (Å)	z (Å)
Er	0.0000	0.0000	-0.4606
N	0.0000	-2.1338	0.1175
N	1.8479	1.0669	0.1175
N	-1.8479	1.0669	0.1175
Si	-2.0629	2.3069	1.2755
Si	-3.0299	0.6328	-1.0405
Si	-0.9664	-2.9400	1.2755
Si	0.9669	-2.9404	-1.0405
Si	3.0293	0.6331	1.2755
Si	2.0630	2.3075	-1.0405
C	-2.0061	4.0319	0.5415
C	-0.6939	2.2170	2.5034
C	-3.6099	2.1878	2.2235
C	-4.4938	-0.2793	-0.3075
C	-2.2668	-0.5071	-2.2685
C	-3.7000	2.0318	-1.9885
C	-2.4887	-3.7533	0.5415
C	-1.5730	-1.7094	2.5034
C	-0.0897	-4.2202	2.2235
C	2.4888	-3.7521	-0.3075
C	1.5726	-1.7096	-2.2685
C	0.0904	-4.2202	-1.9885
C	4.4948	-0.2786	0.5415
C	2.2669	-0.5075	2.5034
C	3.6996	2.0324	2.2235
C	2.0050	4.0314	-0.3075
C	0.6942	2.2167	-2.2685
C	3.6096	2.1884	-1.9885
H	-2.1451	4.6979	1.2295
H	-2.7101	4.1168	-0.1205
H	-1.1541	4.1730	0.1255
H	-0.7920	2.8970	3.1654
H	0.1471	2.3301	2.0534
H	-0.7108	1.3520	2.9364
H	-3.6760	2.9258	2.8515
H	-4.3549	2.2307	1.6205
H	-3.6268	1.3658	2.6985
H	-5.1408	-0.4923	-0.9955
H	-4.9198	0.2877	0.3545
H	-4.1907	-1.0873	0.1085
H	-2.9048	-0.7622	-2.9315

H	-1.9437	-1.2931	-1.8185
H	-1.5259	-0.0611	-2.7015
H	-4.3720	1.7197	-2.6165
H	-4.1100	2.6557	-1.3855
H	-2.9960	2.4578	-2.4645
H	-2.9959	-4.2067	1.2295
H	-2.2102	-4.4054	-0.1205
H	-3.0368	-3.0860	0.1255
H	-2.1129	-2.1343	3.1654
H	-2.0914	-1.0377	2.0534
H	-0.8154	-1.2916	2.9364
H	-0.6958	-4.6464	2.8515
H	0.2456	-4.8868	1.6205
H	0.6306	-3.8238	2.6985
H	2.9968	-4.2059	-0.9955
H	2.2108	-4.4045	0.3545
H	3.0370	-3.0856	0.1085
H	2.1125	-2.1345	-2.9315
H	2.0917	-1.0368	-1.8185
H	0.8158	-1.2909	-2.7015
H	0.6967	-4.6461	-2.6165
H	-0.2449	-4.8873	-1.3855
H	-0.6305	-3.8236	-2.4645
H	5.1410	-0.4912	1.2295
H	4.9203	0.2886	-0.1205
H	4.1909	-1.0870	0.1255
H	2.9048	-0.7626	3.1654
H	1.9444	-1.2924	2.0534
H	1.5263	-0.0604	2.9364
H	4.3718	1.7206	2.8515
H	4.1093	2.6561	1.6205
H	2.9962	2.4581	2.6985
H	2.1440	4.6982	-0.9955
H	2.7090	4.1168	0.3545
H	1.1538	4.1729	0.1085
H	0.7923	2.8967	-2.9315
H	-0.1480	2.3299	-1.8185
H	0.7100	1.3520	-2.7015
H	3.6753	2.9264	-2.6165
H	4.3550	2.2315	-1.3855
H	3.6266	1.3657	-2.4645
$Er(btmsm)_3$ (2)			
Atom	x (Å)	y (Å)	z (Å)
Er	0.0000	0.0000	0.4916
Si	-1.0568	-3.0670	-1.4505

Si	-2.6137	-1.9574	1.1216
Si	3.1845	0.6183	-1.4505
Si	3.0020	-1.2848	1.1216
Si	-2.1277	2.4487	-1.4505
Si	-0.3883	3.2422	1.1216
C	-1.5193	-1.6034	-0.2584
C	0.2537	-4.1939	-0.7246
C	-0.3292	-2.3156	-3.0965
C	-2.5147	-4.1562	-1.8615
C	-4.4296	-1.8431	0.7936
C	-2.2735	-3.5720	2.0035
C	-2.3048	-0.5197	2.3977
C	2.1482	-0.5140	-0.2584
C	-0.6290	2.1174	-0.2584
C	3.5052	2.3167	-0.7246
C	2.1699	0.8727	-3.0965
C	4.8567	-0.0997	-1.8615
C	3.8110	-2.9146	0.7936
C	4.2302	-0.1829	2.0035
C	1.6025	-1.7362	2.3977
C	-3.7589	1.8772	-0.7246
C	-1.8408	1.4429	-3.0965
C	-2.3420	4.2559	-1.8615
C	0.6186	4.7577	0.7936
C	-1.9567	3.7549	2.0035
C	0.7023	2.2558	2.3977
H	0.5344	-3.8368	0.2442
H	-0.1367	-5.1865	-0.6394
H	1.1115	-4.2018	-1.3641
H	-0.3237	-1.2477	-3.0291
H	0.6707	-2.6691	-3.2385
H	-0.9353	-2.6176	-3.9249
H	-3.3867	-3.7883	-1.3622
H	-2.3146	-5.1566	-1.5392
H	-2.6790	-4.1482	-2.9188
H	-4.9689	-2.0750	1.6882
H	-4.6732	-0.8503	0.4776
H	-4.6977	-2.5378	0.0253
H	-2.9715	-3.6945	2.8052
H	-1.2781	-3.5613	2.3958
H	-2.3764	-4.3837	1.3139
H	-2.1398	-0.9350	3.3699
H	-3.1598	0.1230	2.4248
H	3.0555	2.3812	0.2442
H	4.5600	2.4748	-0.6394
H	3.0831	3.0635	-1.3641

H	1.2424	0.3435	-3.0291
H	1.9762	1.9154	-3.2385
H	2.7346	0.4988	-3.9249
H	4.9741	-1.0388	-1.3622
H	5.6231	0.5738	-1.5392
H	4.9319	-0.2460	-2.9188
H	4.2815	-3.2657	1.6882
H	3.0730	-3.6220	0.4776
H	4.5467	-2.7994	0.0253
H	4.6853	-0.7261	2.8052
H	3.7232	0.6738	2.3958
H	4.9845	0.1338	1.3139
H	1.8797	-1.3856	3.3699
H	1.4734	-2.7980	2.4248
H	-3.5900	1.4555	0.2442
H	-4.4233	2.7117	-0.6394
H	-4.1946	1.1383	-1.3641
H	-0.9187	0.9042	-3.0291
H	-2.6469	0.7537	-3.2385
H	-1.7992	2.1188	-3.9249
H	-1.5874	4.8271	-1.3622
H	-3.3085	4.5828	-1.5392
H	-2.2529	4.3942	-2.9188
H	0.6874	5.3407	1.6882
H	1.6002	4.4722	0.4776
H	0.1510	5.3373	0.0253
H	-1.7138	4.4207	2.8052
H	-2.4451	2.8875	2.3958
H	-2.6082	4.2498	1.3139
H	0.2601	2.3206	3.3699
H	1.6864	2.6750	2.4248
H	0.6860	-1.2734	2.0995
H	0.7598	1.2308	2.0995
H	-1.4458	0.0426	2.0995
H	1.9564	-1.3489	-0.8983
H	0.1899	2.3687	-0.8983
H	-2.1463	-1.0199	-0.8983

Table S13. The gross population analysis of Er in $Er(dbpc)_3$, $Er[N(SiMe_3)_2]_3$, and $Er(btmsm)_3$.

$Er(dbpc)_3$ (1)				
Basis function	Total	Alpha	Beta	Spin
4S	2.0009	1.0005	1.0004	0.0001
5S	2.0852	1.0457	1.0395	0.0062
6S	0.1544	0.0780	0.0764	0.0017
7S	-0.0105	-0.0048	-0.0056	0.0008

8S	-0.1086	-0.0583	-0.0503	-0.0080
4PX	1.0885	0.5431	0.5454	-0.0024
4PY	1.0932	0.5455	0.5478	-0.0023
4PZ	1.0877	0.5427	0.5450	-0.0024
5PX	0.8670	0.4360	0.4309	0.0051
5PY	0.8591	0.4321	0.4270	0.0051
5PZ	0.8683	0.4367	0.4316	0.0051
6PX	0.3479	0.1682	0.1797	-0.0115
6PY	0.3827	0.1862	0.1966	-0.0104
6PZ	0.3335	0.1609	0.1727	-0.0118
7PX	1.1269	0.5614	0.5655	-0.0042
7PY	1.1314	0.5636	0.5678	-0.0042
7PZ	1.1251	0.5605	0.5646	-0.0041
8PX	0.5789	0.2959	0.2830	0.0130
8PY	0.5573	0.2849	0.2724	0.0124
8PZ	0.5827	0.2979	0.2848	0.0131
4D 0	0.6309	0.3167	0.3142	0.0025
4D+1	0.6311	0.3167	0.3144	0.0023
4D-1	0.6293	0.3159	0.3135	0.0024
4D+2	0.6295	0.3160	0.3135	0.0026
4D-2	0.6291	0.3157	0.3133	0.0024
5D 0	0.0968	0.0484	0.0484	0.0000
5D+1	0.0974	0.0487	0.0487	0.0000
5D-1	0.0739	0.0367	0.0372	-0.0005
5D+2	0.0798	0.0396	0.0401	-0.0005
5D-2	0.0708	0.0351	0.0357	-0.0007
6D 0	0.4693	0.2331	0.2362	-0.0031
6D+1	0.4691	0.2331	0.2360	-0.0029
6D-1	0.4711	0.2340	0.2371	-0.0031
6D+2	0.4706	0.2337	0.2369	-0.0032
6D-2	0.4714	0.2341	0.2373	-0.0031
7D 0	0.8507	0.4264	0.4244	0.0020
7D+1	0.8505	0.4263	0.4243	0.0020
7D-1	0.8498	0.4260	0.4238	0.0021
7D+2	0.8503	0.4262	0.4241	0.0021
7D-2	0.8497	0.4259	0.4238	0.0021
4F 0	1.2323	0.8754	0.3569	0.5186
4F+1	1.3525	0.8752	0.4773	0.3979
4F-1	1.5762	0.8725	0.7038	0.1687
4F+2	1.1326	0.8754	0.2572	0.6182
4F-2	1.6207	0.8723	0.7484	0.1239
4F+3	1.1178	0.8749	0.2429	0.6319
4F-3	1.6344	0.8718	0.7626	0.1092
5F 0	0.0463	0.0252	0.0212	0.0040
5F+1	0.0475	0.0244	0.0231	0.0013
5F-1	0.0465	0.0229	0.0236	-0.0006

5F+2	0.0421	0.0245	0.0175	0.0070
5F-2	0.0439	0.0212	0.0227	-0.0016
5F+3	0.0377	0.0232	0.0145	0.0087
5F-3	0.0487	0.0237	0.0250	-0.0013
6F 0	0.1552	0.1053	0.0499	0.0554
6F+1	0.1706	0.1055	0.0650	0.0405
6F-1	0.2009	0.1071	0.0938	0.0132
6F+2	0.1423	0.1053	0.0370	0.0684
6F-2	0.2071	0.1072	0.1000	0.0072
6F+3	0.1402	0.1057	0.0345	0.0712
6F-3	0.2086	0.1074	0.1012	0.0062
f electron number				11.2043
Spin (f excluded)		0.0071	**Spin (f)**	2.8481
$Er[N(SiMe_3)_2]_3$				
Basis function	Total	Alpha	Beta	Spin
4S	2.0009	1.0005	1.0004	0.0001
5S	2.0868	1.0465	1.0403	0.0062
6S	0.2256	0.1160	0.1097	0.0063
7S	0.0159	0.0085	0.0073	0.0012
8S	-0.1985	-0.1085	-0.0901	-0.0184
4PX	1.0880	0.5428	0.5452	-0.0024
4PY	1.0880	0.5428	0.5452	-0.0024
4PZ	1.0927	0.5452	0.5475	-0.0023
5PX	0.8678	0.4365	0.4313	0.0052
5PY	0.8678	0.4365	0.4313	0.0052
5PZ	0.8601	0.4326	0.4274	0.0052
6PX	0.3303	0.1597	0.1707	-0.0110
6PY	0.3303	0.1597	0.1707	-0.0110
6PZ	0.3725	0.1812	0.1914	-0.0102
7PX	1.1291	0.5619	0.5672	-0.0053
7PY	1.1291	0.5619	0.5672	-0.0053
7PZ	1.1313	0.5634	0.5679	-0.0045
8PX	0.5815	0.2975	0.2840	0.0135
8PY	0.5815	0.2975	0.2840	0.0135
8PZ	0.5608	0.2867	0.2740	0.0127
4D 0	0.6292	0.3158	0.3134	0.0024
4D+1	0.6296	0.3161	0.3134	0.0027
4D-1	0.6296	0.3161	0.3134	0.0027
4D+2	0.6315	0.3170	0.3145	0.0025
4D-2	0.6315	0.3170	0.3145	0.0025
5D 0	0.0678	0.0338	0.0340	-0.0002
5D+1	0.0745	0.0371	0.0374	-0.0003
5D-1	0.0745	0.0371	0.0374	-0.0003
5D+2	0.0986	0.0500	0.0486	0.0014
5D-2	0.0986	0.0500	0.0486	0.0014

6D 0	0.4713	0.2341	0.2372	-0.0031
6D+1	0.4707	0.2337	0.2370	-0.0034
6D-1	0.4707	0.2337	0.2370	-0.0034
6D+2	0.4687	0.2328	0.2359	-0.0031
6D-2	0.4687	0.2328	0.2359	-0.0031
7D 0	0.8501	0.4261	0.4240	0.0021
7D+1	0.8503	0.4262	0.4240	0.0022
7D-1	0.8503	0.4262	0.4240	0.0022
7D+2	0.8509	0.4265	0.4244	0.0021
7D-2	0.8509	0.4265	0.4244	0.0021
4F 0	1.6545	0.8732	0.7813	0.0920
4F+1	1.1846	0.8761	0.3085	0.5676
4F-1	1.1815	0.8761	0.3053	0.5708
4F+2	1.4444	0.8754	0.5690	0.3064
4F-2	1.4467	0.8754	0.5714	0.3040
4F+3	1.4561	0.8766	0.5795	0.2972
4F-3	1.2785	0.8765	0.4019	0.4746
5F 0	0.0477	0.0232	0.0245	-0.0013
5F+1	0.0333	0.0214	0.0118	0.0096
5F-1	0.0332	0.0214	0.0118	0.0097
5F+2	0.0421	0.0228	0.0193	0.0035
5F-2	0.0422	0.0228	0.0194	0.0035
5F+3	0.0542	0.0275	0.0267	0.0009
5F-3	0.0381	0.0216	0.0165	0.0051
6F 0	0.2095	0.1067	0.1029	0.0038
6F+1	0.1466	0.1049	0.0417	0.0632
6F-1	0.1462	0.1049	0.0413	0.0636
6F+2	0.1799	0.1052	0.0747	0.0305
6F-2	0.1802	0.1052	0.0750	0.0302
6F+3	0.1806	0.1046	0.0759	0.0287
6F-3	0.1590	0.1041	0.0549	0.0493
f electron number				11.1388
Spin (f excluded)		0.0055	**Spin (f)**	2.9127
$Er(btmsm)_3$ (2)				
Basis function	Total	Alpha	Beta	Spin
4S	2.0009	1.0005	1.0004	0.0001
5S	2.0842	1.0450	1.0392	0.0059
6S	0.3464	0.1797	0.1668	0.0129
7S	-0.0527	-0.0265	-0.0262	-0.0003
8S	0.1518	0.0717	0.0801	-0.0085
4PX	1.0888	0.5432	0.5457	-0.0025
4PY	1.0888	0.5432	0.5457	-0.0025
4PZ	1.0926	0.5451	0.5474	-0.0023
5PX	0.8663	0.4358	0.4305	0.0053
5PY	0.8663	0.4358	0.4305	0.0053

5PZ	0.8602	0.4327	0.4275	0.0052
6PX	0.3263	0.1573	0.1690	-0.0117
6PY	0.3263	0.1573	0.1690	-0.0117
6PZ	0.3679	0.1790	0.1889	-0.0098
7PX	1.1237	0.5593	0.5644	-0.0050
7PY	1.1237	0.5593	0.5644	-0.0050
7PZ	1.1304	0.5629	0.5675	-0.0046
8PX	0.5788	0.2962	0.2826	0.0136
8PY	0.5788	0.2962	0.2826	0.0136
8PZ	0.5604	0.2865	0.2740	0.0125
4D 0	0.6290	0.3157	0.3133	0.0023
4D+1	0.6298	0.3162	0.3135	0.0027
4D-1	0.6298	0.3162	0.3135	0.0027
4D+2	0.6311	0.3168	0.3143	0.0025
4D-2	0.6311	0.3168	0.3143	0.0025
5D 0	0.0649	0.0322	0.0327	-0.0004
5D+1	0.0795	0.0398	0.0397	0.0000
5D-1	0.0795	0.0398	0.0397	0.0000
5D+2	0.0964	0.0492	0.0473	0.0019
5D-2	0.0964	0.0492	0.0473	0.0019
6D 0	0.4715	0.2343	0.2373	-0.0030
6D+1	0.4704	0.2335	0.2369	-0.0034
6D-1	0.4704	0.2335	0.2369	-0.0034
6D+2	0.4691	0.2330	0.2361	-0.0030
6D-2	0.4691	0.2330	0.2361	-0.0030
7D 0	0.8498	0.4259	0.4239	0.0020
7D+1	0.8502	0.4262	0.4240	0.0022
7D-1	0.8502	0.4262	0.4240	0.0022
7D+2	0.8505	0.4263	0.4243	0.0020
7D-2	0.8505	0.4263	0.4243	0.0020
4F 0	1.6366	0.8719	0.7647	0.1072
4F+1	1.2086	0.8747	0.3340	0.5407
4F-1	1.2028	0.8747	0.3281	0.5467
4F+2	1.4317	0.8739	0.5579	0.3160
4F-2	1.4349	0.8739	0.5611	0.3128
4F+3	1.2001	0.8758	0.3244	0.5514
4F-3	1.5419	0.8738	0.6680	0.2058
5F 0	0.0468	0.0226	0.0241	-0.0015
5F+1	0.0343	0.0219	0.0124	0.0095
5F-1	0.0341	0.0219	0.0123	0.0096
5F+2	0.0400	0.0218	0.0182	0.0035
5F-2	0.0401	0.0218	0.0183	0.0035
5F+3	0.0373	0.0222	0.0151	0.0072
5F-3	0.0422	0.0218	0.0204	0.0014
6F 0	0.2086	0.1070	0.1016	0.0055
6F+1	0.1510	0.1055	0.0455	0.0599

6F-1	0.1502	0.1054	0.0448	0.0607
6F+2	0.1801	0.1057	0.0744	0.0313
6F-2	0.1805	0.1057	0.0748	0.0309
6F+3	0.1495	0.1047	0.0449	0.0598
6F-3	0.1937	0.1059	0.0878	0.0181
f electron number				11.1450
Spin (f excluded)		0.0210	**Spin (f)**	2.8798

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