Slow magnetic relaxation of a mononuclear dysprosium complex derived from 4,4,4-trifluoro-1-(2-naphthyl)-1,3-butanedione and 1,10-phenanthroline

Shan-Shan Liu,*[a] Qi-Ming Guo[a], Bin Liu,[a] Teng-Hui Jin[a], Zi-Hao Zhang[a], Shijing Lin[a] and Yin-Shan Meng*[b]

[a]Beijing Key Laboratory of Fuels Cleaning and Advanced Catalytic Emission Reduction Technology, College of New Materials and Chemical Engineering, Beijing Institute of Petrochemical Technology, Beijing 102617, P. R. China. E-mail: liushanshan2015@bipt.edu.cn

[b]State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian, 116024, P. R. China. E-mail: mengys@dlut.edu.cn

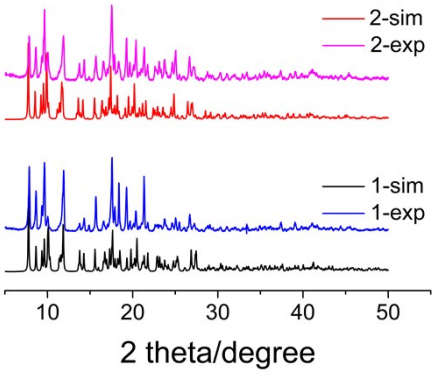


Fig S1 Powder X-ray diffraction data of complexes **1** and **2**

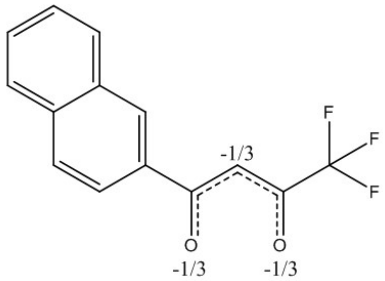


Fig S2 The charge definition of the tfnb$^-$ ligand

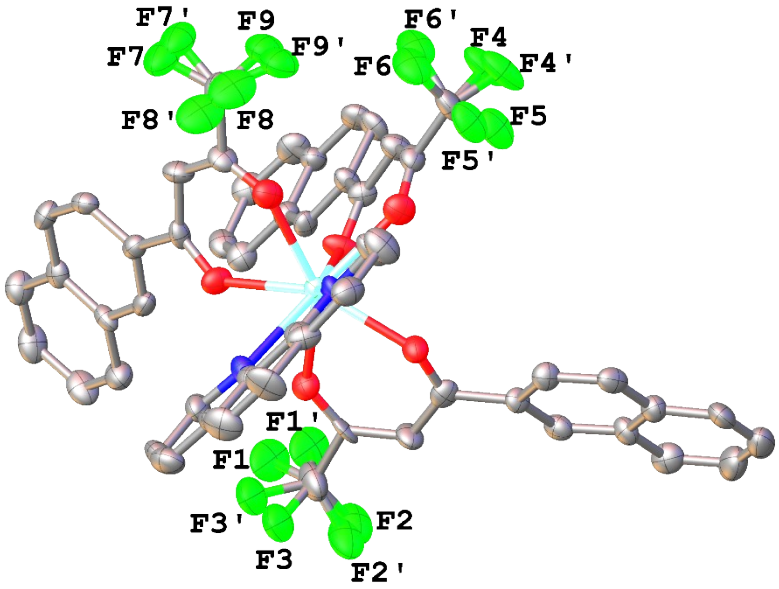
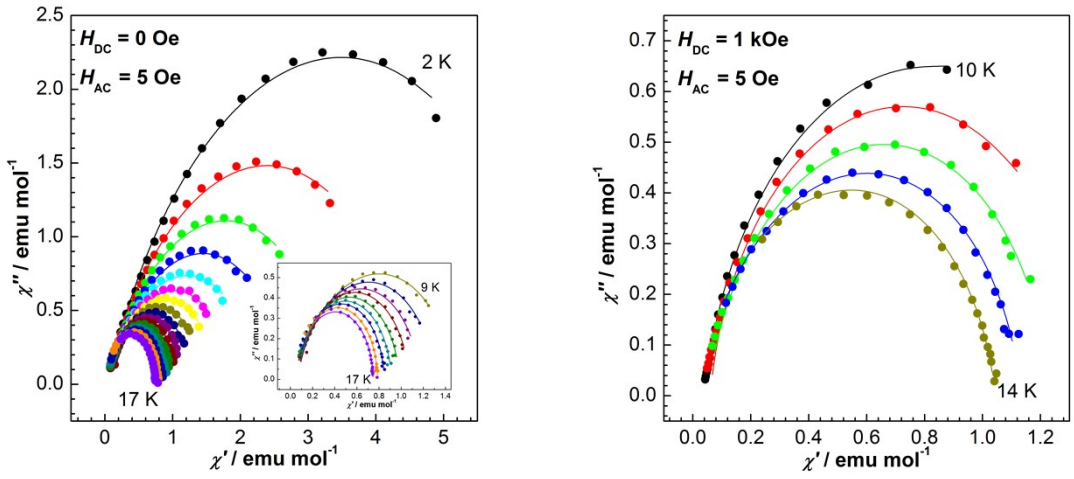


Fig. S3 Molecular structure of complex **2**. Colour code: Tb, turquoise; O, red; N, blue; C, gray; F, green. Hydrogen atoms are omitted for clarity.



(a) (b)

Fig S4. Cole-Cole Plots of complex **1** under zero dc field (a) and under a 1 kOe dc field (b). The inset in (a) shows a zoom-in view on the high temperature curves for clarity. The lines represent the best fits using the generalised Debye model.

Table S1 Extracted parameters from the Cole-Cole plots with the generalized Debye functions for **1** in the absence of a dc field

T (K)	χ_s (cm^{3}mol^{-1})	χ_T (cm^{3}mol^{-1})	α	τ (s)
2	0.03897	6.48500	0.23086	7.2E-4
3	0.00581	4.45679	0.24987	7.1E-4
4	0.01918	3.30879	0.24282	6.4E-4
5	0.01994	2.68108	0.24980	6.2E-4
6	0.00638	2.24754	0.25814	5.9E-4
7	0.02713	1.89137	0.23660	5.3E-4
8	0.04552	1.66509	0.21551	5E-4
9	0.03771	1.47648	0.20339	4.3E-4
10	0.03162	1.31094	0.18158	3.5E-4
11	0.06509	1.16939	0.13397	2.8E-4
12	0.06457	1.07366	0.10275	2.2E-4
13	0.07000	0.98423	0.07568	1.7E-4
14	0.07000	0.91321	0.05491	1.2E-4
15	0.07000	0.84756	0.02634	8E-5
16	0.06966	0.78774	0.00858	5E-5
17	0.07000	0.74707	0.00832	3E-5

Table S2 Extracted parameters from the Cole-Cole plots with the generalized Debye functions for **1** under a 1 kOe dc field

T (K)	χ_s (cm^{3}mol^{-1})	χ_T (cm^{3}mol^{-1})	α	τ (s)
10	0.04055	1.55019	0.09236	0.00144
11	0.05976	1.36827	0.08326	6.7E-4
12	0.05176	1.23378	0.10771	2.9E-4
13	0.01839	1.13381	0.14820	1.1E-4
14	0.00074	1.04422	0.15553	4E-5

The input file of complex **1** for the electrostatic calculations using MAGELLAN software:

```
! sites 1 1
Dy      10.651926     2.867948    17.671808    +3
F       10.202108    -1.306017    15.072404    0
F       11.798855    -1.883849    16.350281    0
F        9.858216    -2.721326    16.622862    0
F       11.716538     7.641297    17.464474    0
F       11.479810     8.012039    15.366355    0
F        9.765742     7.632139    16.588988    0
F        7.885324     5.682586    20.680423    0
F        8.385511     7.078144    19.154291    0
F        6.387426     6.293532    19.300243    0
O       10.657533     0.674353    16.841790    -1/3
O        9.831538     1.475290    19.346166    -1/3
O       11.119210     5.093162    17.215082    -1/3
O       11.254982     3.039219    15.443195    -1/3
O        9.100844     4.192780    18.884893    -1/3
O        8.647309     2.850987    16.532835    -1/3
N       13.089348     2.110518    17.631796    0
N       12.095036     3.684611    19.618746    0
C       10.483411    -1.591911    16.310724    0
C       10.191124    -0.417556    17.258504    0
C        9.521111    -0.682400    18.436579    -1/3
H        9.177276    -1.534371    18.580485    0
C        9.342725     0.308775    19.430736    0
C        8.536662    -0.005233    20.645868    0
C        8.767880     0.749936    21.827808    0
H        9.417382     1.416415    21.831445    0
C        8.040823     0.500905    22.956777    0
H        8.206612     0.998165    23.725186    0
C        7.037582    -0.504068    22.978602    0
C        6.303823    -0.825915    24.148493    0
H        6.481423    -0.376704    24.943728    0
```

C	5.331724	-1.799433	24.115756	0
H	4.856907	-2.004343	24.889166	0
C	5.046392	-2.490415	22.917675	0
H	4.375202	-3.134567	22.902216	0
C	5.750087	-2.218879	21.782794	0
H	5.560880	-2.684375	21.001655	0
C	6.772297	-1.229472	21.782794	0
C	7.550661	-0.964449	20.631545	0
H	7.393225	-1.447045	19.851315	0
C	11.035250	7.274982	16.385746	0
C	11.125387	5.757584	16.142948	0
C	11.134239	5.304270	14.842791	-1/3
H	11.115288	5.919032	14.145085	0
C	11.172587	3.912457	14.547477	0
C	11.083776	3.432801	13.131604	0
C	11.135940	4.312202	12.015138	0
H	11.258189	5.224449	12.149041	0
C	11.005909	3.818760	10.745672	0
H	11.053314	4.402089	10.023414	0
C	10.800238	2.439487	10.511285	0
C	10.629468	1.907183	9.203399	0
H	10.676773	2.471377	8.466136	0
C	10.399594	0.576606	9.025164	0
H	10.303461	0.240331	8.163774	0
C	10.304963	-0.300797	10.127081	0
H	10.118273	-1.201143	9.989313	0
C	10.486443	0.173529	11.396774	0
H	10.447253	-0.412591	12.117214	0
C	10.734497	1.555852	11.623659	0
C	10.898340	2.084020	12.924952	0
H	10.880374	1.509634	13.656304	0
C	7.677966	5.981685	19.399591	0
C	8.110981	4.838714	18.464542	0
C	7.393456	4.687313	17.285558	-1/3
H	6.703038	5.280802	17.093683	0
C	7.687262	3.649055	16.369378	0
C	6.847419	3.444216	15.151064	0
C	5.617470	4.131993	14.936228	0
H	5.297617	4.721701	15.579599	0
C	4.905915	3.927780	13.785661	0
H	4.098144	4.373379	13.665398	0
C	5.372265	3.052729	12.771952	0
C	4.690274	2.880569	11.538406	0
H	3.886991	3.324926	11.389726	0

C	5.203012	2.068191	10.565619	0
H	4.753096	1.979657	9.755153	0
C	6.406250	1.361755	10.776818	0
H	6.743491	0.807097	10.109803	0
C	7.075194	1.493316	11.961486	0
H	7.859734	1.013527	12.099026	0
C	6.591132	2.350726	12.984742	0
C	7.301080	2.564476	14.189416	0
H	8.092646	2.100273	14.336050	0
C	13.583666	1.363500	16.649461	0
H	13.028925	1.144763	15.936523	0
C	14.903885	0.889172	16.639230	0
H	15.208130	0.360022	15.936523	0
C	15.734473	1.210969	17.664760	0
H	16.610325	0.897144	17.673399	0
C	15.262988	2.022329	18.715980	0
C	13.919492	2.451023	18.657099	0
C	13.397364	3.294236	19.698543	0
C	14.244122	3.700493	20.751353	0
C	15.596751	3.224697	20.791820	0
H	16.145433	3.465723	21.501802	0
C	16.085098	2.433040	19.816987	0
H	16.969773	2.149418	19.858135	0
C	13.719671	4.576225	21.716184	0
H	14.246908	4.859021	22.429349	0
C	12.429546	5.009976	21.598422	0
H	12.077693	5.617626	22.208829	0
C	11.643853	4.523032	20.539473	0
H	10.759901	4.804175	20.483320	0