Electronic Supplementary Material (ESI) for RSC Advances.

Single-Molecule Magnet Behavior in a Mononuclear Dysprosium(III) Complex with 1-methylimidazole

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Table S1. Selected bond lengths [Å] and angles [deg] for compound **1**.

Dy(1)-O(2)^1	2.346(4)	N(1)^1-Dy(1)-N(1)	141.7(2)
Dy(1)-O(2)	2.346(4)	O(1)-Dy(1)-N(1)^1	74.51(14)
Dy(1)-O(3)^1	2.347(3)	O(1)^1-Dy(1)-N(1)^1	75.96(14)
Dy(1)-O(3)	2.347(3)	O(1)^1-Dy(1)-N(1)	74.51(14)
Dy(1)-O(1)	2.358(4)	O(1)-Dy(1)-N(1)	75.96(14)
Dy(1)-O(1)^1	2.358(4)	O(1)^1-Dy(1)-O(1)	78.12(18)
Dy(1)-N(1)^1	2.467(4)	O(2)^1-Dy(1)-N(1)	110.32(15)
Dy(1)-N(1)	2.467(4)	O(2)-Dy(1)-N(1)	82.12(15)
O(2)^1-Dy(1)-N(1)^1	82.12(15)	O(3)^1-Dy(1)-N(1)	73.57(13)
O(2)^1-Dy(1)-O(1)^1	71.17(14)	O(3)^1-Dy(1)-O(1)^1	120.30(13)
O(2)-Dy(1)-O(1)^1	145.06(15)	O(3)^1-Dy(1)-O(1)	137.37(14)
O(2)-Dy(1)-O(1)	71.17(14)	O(3)-Dy(1)-O(1)	120.30(13)
O(2)^1-Dy(1)-O(1)	145.06(15)	O(3)-Dy(1)-O(1)^1	137.37(14)
O(2)-Dy(1)-O(2)^1	142.7(2)	O(3)-Dy(1)-O(3)^1	74.00(17)
O(2)^1-Dy(1)-O(3)	75.70(15)	C(9)-N(1)-C(10)	104.5(5)
O(2)^1-Dy(1)-O(3)^1	74.69(15)	C(9)-N(1)-Dy(1)	129.0(4)
O(2)-Dy(1)-O(3)	74.68(15)	C(10)-N(1)-Dy(1)	125.9(4)
O(2)-Dy(1)-O(3)^1	75.70(15)	C(2)-O(1)-Dy(1)	134.4(4)
O(3)-Dy(1)-N(1)	143.80(14)	C(4)-O(2)-Dy(1)	134.0(4)
O(3)-Dy(1)-N(1)^1	73.57(13)	C(7)-O(3)-Dy(1)	133.4(3)
O(3)^1-Dy(1)-N(1)^1	143.80(14)		

Table S2. Selected bond lengths [Å] and angles [deg] for compound **2**.

Tb(1)-O(3)[1]	2.354(3)	O(3)-Tb(1)-O(3)[1]	73.49(16)
Tb(1)-O(3)	2.354(3)	O(3)-Tb(1)-O(1)	74.98(15)
Tb(1)-O(1)[1]	2.356(4)	O(3)[1]-Tb(1)-O(1)	75.67(15)
Tb(1)-O(1)	2.346(4)	O(3)-Tb(1)-O(1)[1]	75.67(15)
Tb(1)-O(2)	2.374(3)	O(3)[1]-Tb(1)-O(1)[1]	74.98(15)
Tb(1)-O(2)[1]	2.374(3)	O(1)-Tb(1)-O(1)[1]	143.1(2)
Tb(1)-N(1)[1]	2.481(4)	O(3)-Tb(1)-O(2)[1]	137.39(13)
Tb(1)-N(1)	2.481(4)	O(3)[1]-Tb(1)-O(2)[1]	120.50(13)
O(1)-Tb(1)-O(2)[1]	144.84(14)	O(3)-Tb(1)-N(1)[1]	74.01(13)
O(1)[1]-Tb(1)-O(2)[1]	70.92(13)	O(3)[1]-Tb(1)-N(1)[1]	143.75(14)
O(3)-Tb(1)-O(2)	120.50(13)	O(1)-Tb(1)-N(1)[1]	110.58(15)
O(3)[1]-Tb(1)-O(2)	137.39(13)	O(1)[1]-Tb(1)-N(1)[1]	81.83(15)
O(1)-Tb(1)-O(2)	70.92(13)	O(2)[1]-Tb(1)-N(1)[1]	75.73(14)
O(1)[1]-Tb(1)-O(2)	144.84(14)	O(2)-Tb(1)-N(1)[1]	74.48(14)
O(2)[1]-Tb(1)-O(2)	78.22(16)	N(1)-Tb(1)-N(1)[1]	141.3(2)
O(3)-Tb(1)-N(1)	143.75(14)	C(9)-N(1)-Tb(1)	128.4(3)
O(3)[1]-Tb(1)-N(1)	74.01(13)	C(11)-N(1)-Tb(1)	126.5(4)
O(1)-Tb(1)-N(1)	81.83(15)	C(2)-O(1)-Tb(1)	134.7(4)
O(1)[1]-Tb(1)-N(1)	110.58(15)	C(4)-O(2)-Tb(1)	134.3(4)
O(2)[1]-Tb(1)-N(1)	74.47(14)	C(7)-O(3)-Tb(1)	134.0(3)
O(2)-Tb(1)-N(1)	75.73(14)		

Table S3. Selected bond lengths [Å] and angles [deg] for compound **3**.

Ho(1)-O(2)[1]	2.332(4)	O(2)[1]-Ho(1)-O(2)	142.3(2)
Ho(1)-O(2)	2.332(4)	O(2)[1]-Ho(1)-O(3)	74.49(15)
Ho(1)-O(3)[1]	2.333(3)	O(2)-Ho(1)-O(3)	75.67(15)
Ho(1)-O(3)	2.333(3)	O(2)[1]-Ho(1)-O(3)[1]	75.67(15)
Ho(1)-O(1)	2.347(4)	O(2)-Ho(1)-O(3)[1]	74.49(15)
Ho(1)-O(1)[1]	2.347(4)	O(3)-Ho(1)-O(3)[1]	74.26(16)
Ho(1)-N(1)[1]	2.458(5)	O(2)[1]-Ho(1)-O(1)[1]	71.54(14)
Ho(1)-N(1)	2.458(5)	O(2)-Ho(1)-O(1)[1]	144.99(14)
O(3)-Ho(1)-O(1)[1]	120.08(13)	O(2)[1]-Ho(1)-N(1)[1]	110.58(15)
O(3)[1]-Ho(1)-O(1)[1]	137.66(13)	O(2)-Ho(1)-N(1)[1]	82.08(15)
O(2)[1]-Ho(1)-O(1)	144.99(14)	O(3)-Ho(1)-N(1)[1]	73.67(13)
O(2)-Ho(1)-O(1)	71.54(14)	O(3)[1]-Ho(1)-N(1)[1]	143.98(14)
O(3)-Ho(1)-O(1)	137.66(13)	O(1)[1]-Ho(1)-N(1)[1]	74.23(14)
O(3)[1]-Ho(1)-O(1)	120.08(13)	O(1)-Ho(1)-N(1)[1]	75.93(14)
O(1)[1]-Ho(1)-O(1)	77.86(18)	N(1)-Ho(1)-N(1)[1]	141.4(2)
O(2)[1]-Ho(1)-N(1)	82.08(15)	C(9)-N(1)-Ho(1)	128.4(4)
O(2)-Ho(1)-N(1)	110.58(15)	C(10)-N(1)-Ho(1)	126.3(4)
O(3)-Ho(1)-N(1)	143.98(14)	C(2)-O(1)-Ho(1)	134.5(4)
O(3)[1]-Ho(1)-N(1)	73.67(13)	C(4)-O(2)-Ho(1)	134.2(5)
O(1)[1]-Ho(1)-N(1)	75.93(14)	C(7)-O(3)-Ho(1)	133.7(3)
O(1)-Ho(1)-N(1)	74.23(14)		

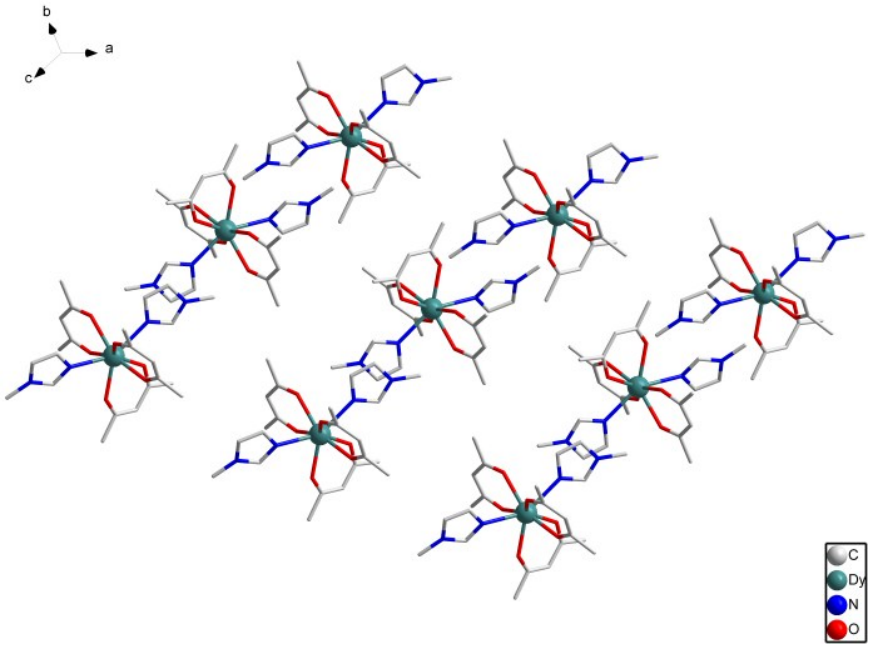

Fig. S1. Packing diagram of complex **1.** The hydrogen atoms and fluorine atoms are omitted for clarity.

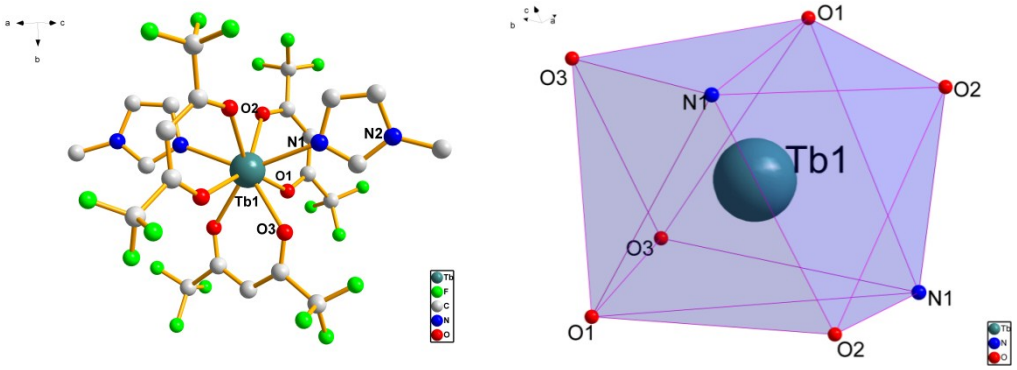

Fig. S2. Perspective view of complex [Tb(hfac)$_3$·(1-MeIm)$_2$] (H atoms were all omitted for clarity, left) and the coordination polyhedron of the Tb^{III} ions (right).

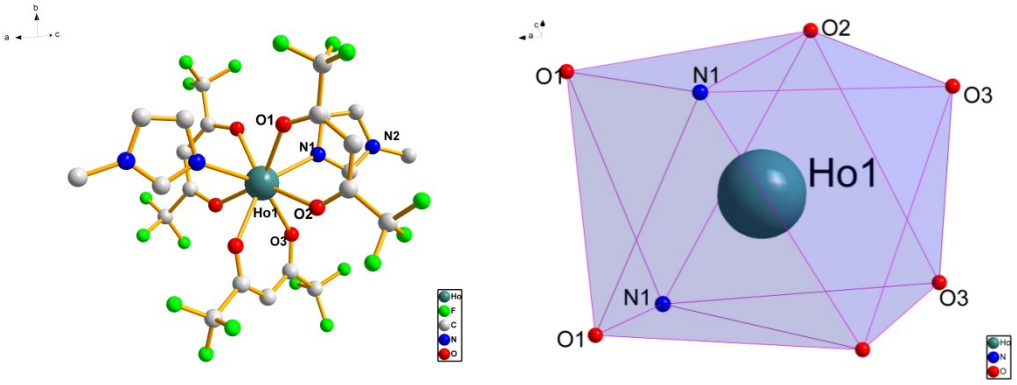

Fig. S3. Perspective view of complex [Ho(hfac)$_3$·(1-MeIm)$_2$] (H atoms were all omitted for clarity, left) and the coordination polyhedron of the Ho^{III} ions (right).

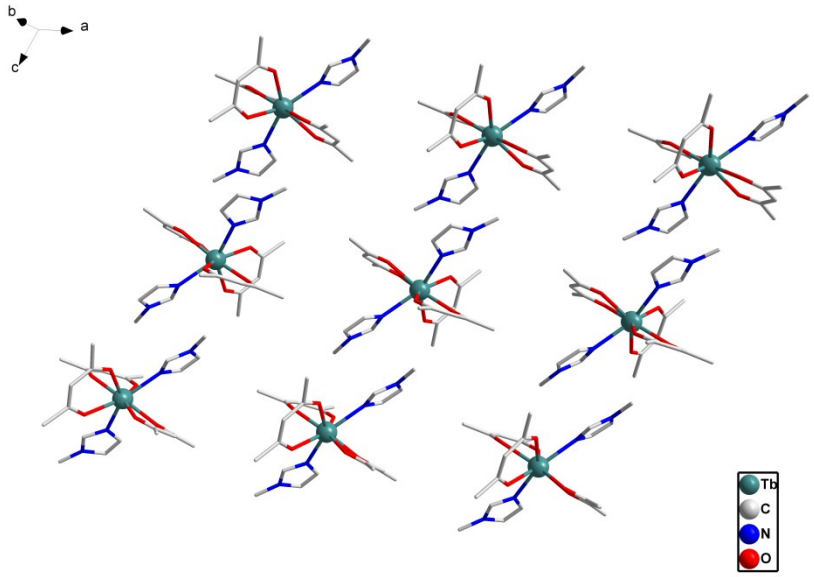

Fig. S4 Packing diagram of complex **2.** The hydrogen atoms and fluorine atoms are omitted for clarity.

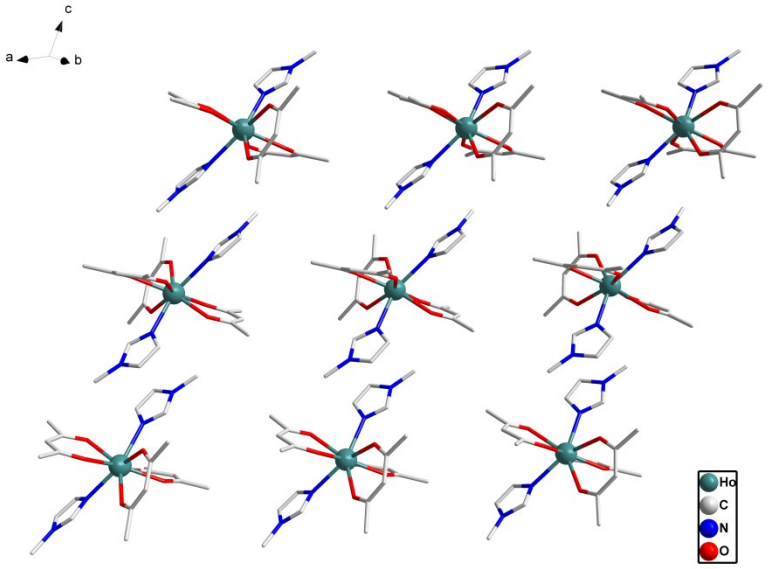

Fig.S5. Packing diagram of complex **3.** The hydrogen atoms and fluorine atoms are omitted for clarity.

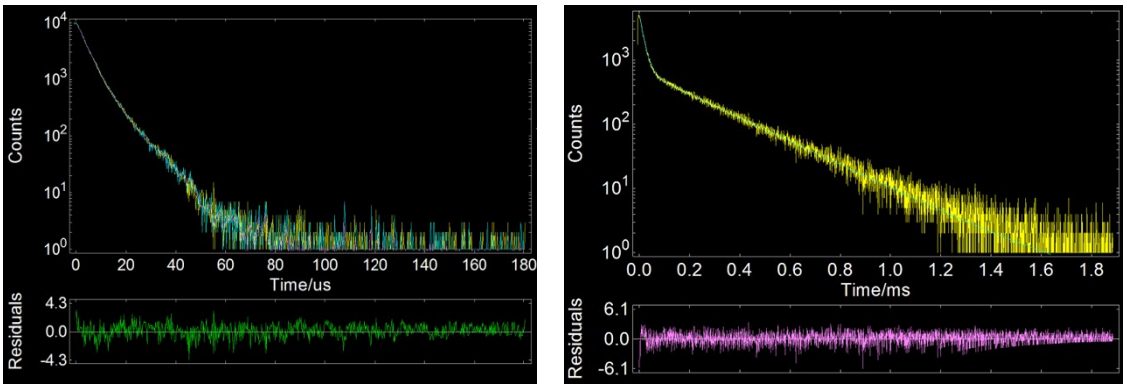

Fig. S6. Lifetime curve of compound Dy **1** (left) and Tb **2** (right).

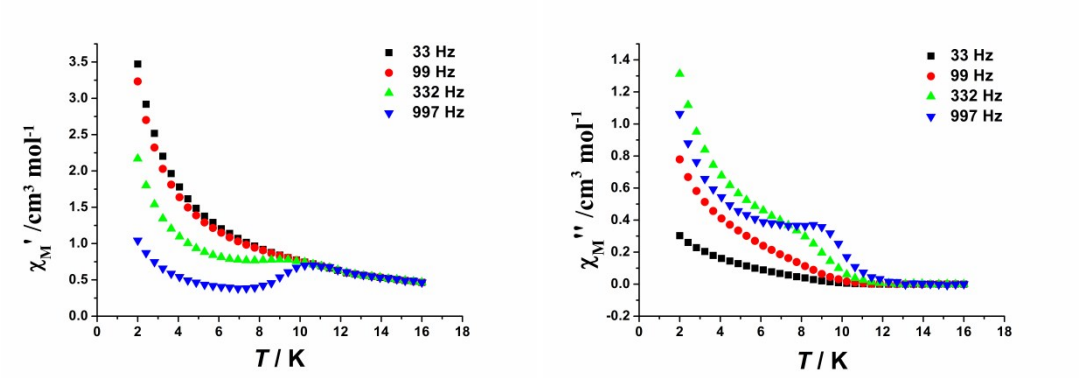

Fig. S7. In-phase and out-of-phase dynamic magnetic susceptibility of **1.**

Table S4 Fitting parameters by Dybye model from 2.0 K to 10.0 K of **1**.

T/K	χ_s/cm^{3}mol^{-1}	χ_t/cm^{3}mol^{-1}	α1
2.0	0.30	3.49	0.1317
3.0	0.24	2.39	0.1190
3.5	0.25	2.04	0.0872
5.0	0.19	1.45	0.0761
6.5	0.17	1.13	0.0464
8.0	0.13	0.92	0.0349
9.0	0.10	0.84	0.0245
9.5	0.08	0.77	0.0210
10	0.03	0.75	0.0180

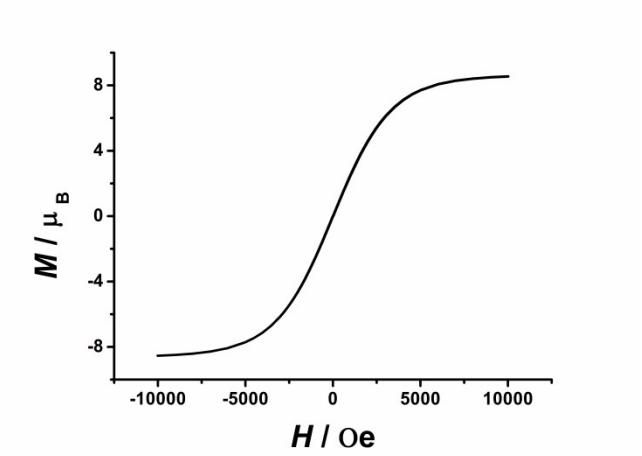

Fig. S8. Field dependence of the magnetization at 2 K showing the absence of hysteresis effect for **1**.

The magnetic data of **2** and **3** can be analyzed by the following approximate treatment of Eqs (2)-(4).

$$\chi_{\mathrm{Tb}} = \frac{2Ng^2\beta^2}{kT}\left[\frac{36\exp\left(\frac{-36\Delta}{kT}\right)+25\exp\left(\frac{-25\Delta}{kT}\right)+16\exp\left(\frac{-16\Delta}{kT}\right)+9\exp\left(\frac{-9\Delta}{kT}\right)+4\exp\left(\frac{-4\Delta}{kT}\right)+\exp\left(\frac{-\Delta}{kT}\right)}{2\exp\left(\frac{-36\Delta}{kT}\right)+2\exp\left(\frac{-25\Delta}{kT}\right)+2\exp\left(\frac{-16\Delta}{kT}\right)+2\exp\left(\frac{-9\Delta}{kT}\right)+2\exp\left(\frac{-4\Delta}{kT}\right)+2\exp\left(\frac{-\Delta}{kT}\right)+1}\right] \quad (2)$$

$$\chi_{\mathrm{Ho}} = \frac{2Ng^2\beta^2}{kT}\left[\frac{64\exp\left(\frac{-64\Delta}{kT}\right)+49\exp\left(\frac{-49\Delta}{kT}\right)+36\exp\left(\frac{-36\Delta}{kT}\right)+25\exp\left(\frac{-25\Delta}{kT}\right)+16\exp\left(\frac{-16\Delta}{kT}\right)+9\exp\left(\frac{-9\Delta}{kT}\right)+4\exp\left(\frac{-4\Delta}{kT}\right)+\exp\left(\frac{-\Delta}{kT}\right)}{2\exp\left(\frac{-64\Delta}{kT}\right)+2\exp\left(\frac{-49\Delta}{kT}\right)+2\exp\left(\frac{-36\Delta}{kT}\right)+2\exp\left(\frac{-25\Delta}{kT}\right)+2\exp\left(\frac{-16\Delta}{kT}\right)+2\exp\left(\frac{-9\Delta}{kT}\right)+2\exp\left(\frac{-4\Delta}{kT}\right)+2\exp\left(\frac{-\Delta}{kT}\right)+1}\right] \quad (3)$$

$$\chi_{\mathrm{M}} = \frac{\chi(\mathrm{Tb\ or\ Ho})}{1-\left(2zJ'/Ng^2\beta^2\right)\chi(\mathrm{Tb\ or\ Ho})} \quad (4)$$

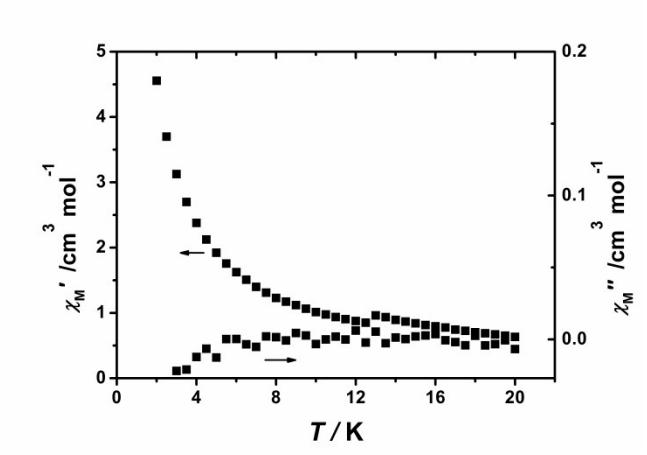

Fig. S9. In-phase and out-of-phase dynamic magnetic susceptibility of **2** under zero-dc field**.**

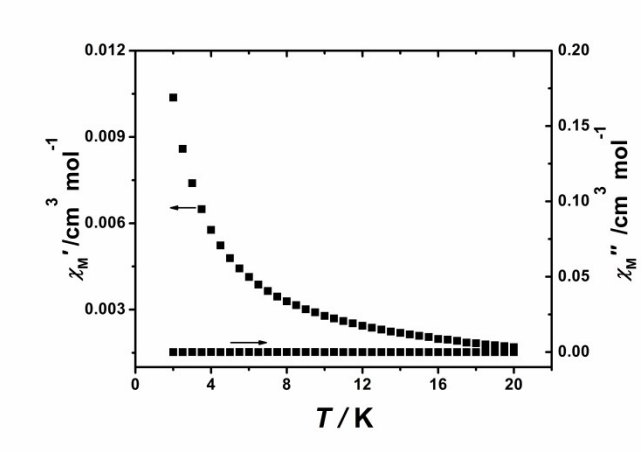

Fig. S10. In-phase and out-of-phase dynamic magnetic susceptibility of **3** under zero-dc field**.**