# Supporting information

# Synthesis, Crystal Structure and Study of Magnetocaloric Effect and Single Molecular Magnetic Behaviour in Discrete Lanthanide Complexes

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**Table S1. Selected hydrogen bonding distances (Å) and angles (deg) for the complex 1**

| D-H….A | Symmetry operation | D-H(Å) | A…H(Å) | D….A(Å) | <D-H-A(deg) |
|---|---|---|---|---|---|
| C7-H7….O2 | x,y,z | 0.930 | 2.607 | 3.179 | 120 |
| O1-H1A-...Cl2 | x,y,z | 0.851 | 2.258 | 2.934 | 136 |
| O9-H9A-...Cl2 | x,y,z | 0.850 | 2.154 | 2.845 | 138 |
| O3-H3A-...Cl3 | -x,+y,-z+1/2 +1 | 0.850 | 2.631 | 3.202 | 126 |
| O11-H11A...N3 | -x,-y+1,-z+1 | 0.930 | 2.355 | 2.881 | 120 |

**Table S2. Selected hydrogen bonding distances (Å) and angles (deg) for the complex 2**

| D-H….A | Symmetry operation | D-H(Å) | A…H(Å) | D….A(Å) | <D-H-A(deg) |
|---|---|---|---|---|---|
| O21- H21B…Cl3 | x,y,z | 0.901 | 2.319 | 3.077 | 141 |
| O9 –H9A ...O6 | x,y,z | 0.880 | 2.157 | 2.776 | 129 |
| C18-H18…O10 | x,y,z | 0.930 | 2.576 | 3.158 | 121 |
| O3w-H3wA…Cl2 | x,y,z | 0.850 | 2.517 | 3.057 | 122 |
| O1-H1B…Cl5 | x-1,+y,+z | 0.873 | 2.314 | 3.012 | 137 |
| C30-H30…O10 | -x,-y,-z+1 | 0.930 | 2.649 | 3.261 | 124 |

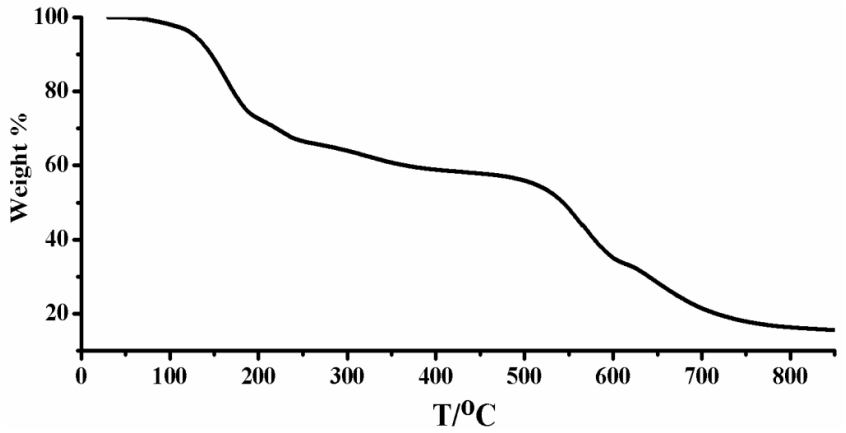


**Fig. S1.** Thermogravimetric analysis plot for complex **1**.

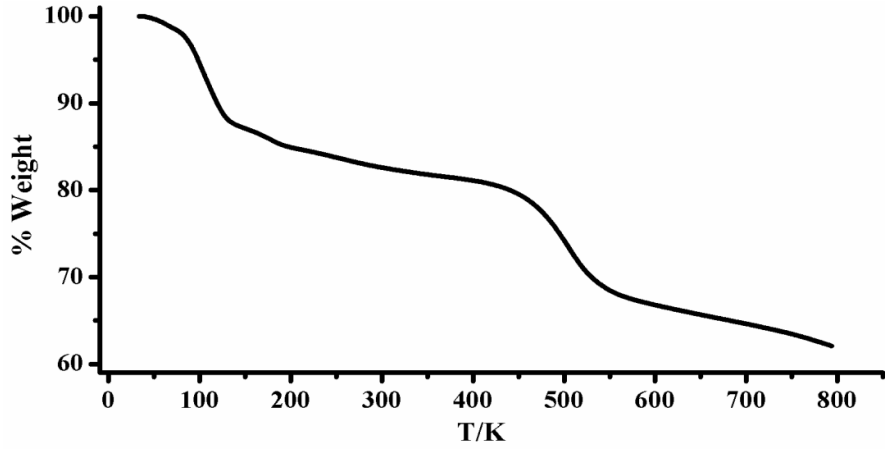


**Fig. S2.** Thermogravimetric analysis plot for complex **2**.

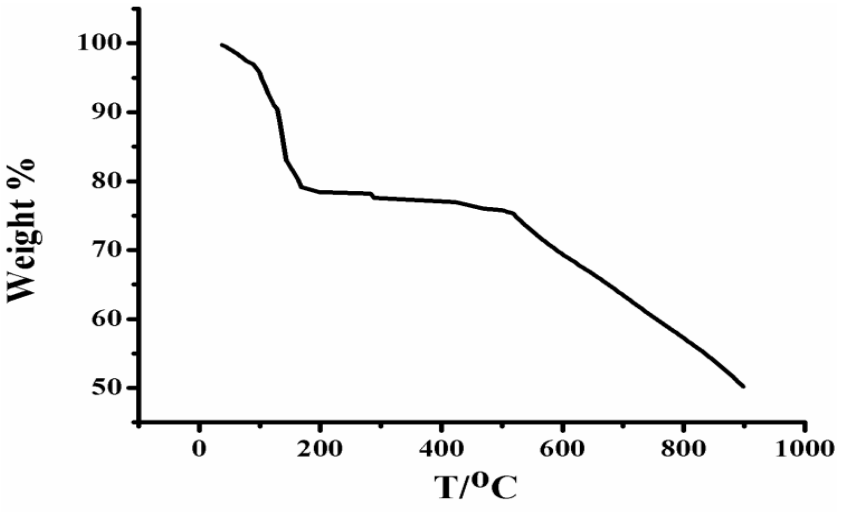


**Fig. S3.** Thermogravimetric analysis plot for complex **3**.

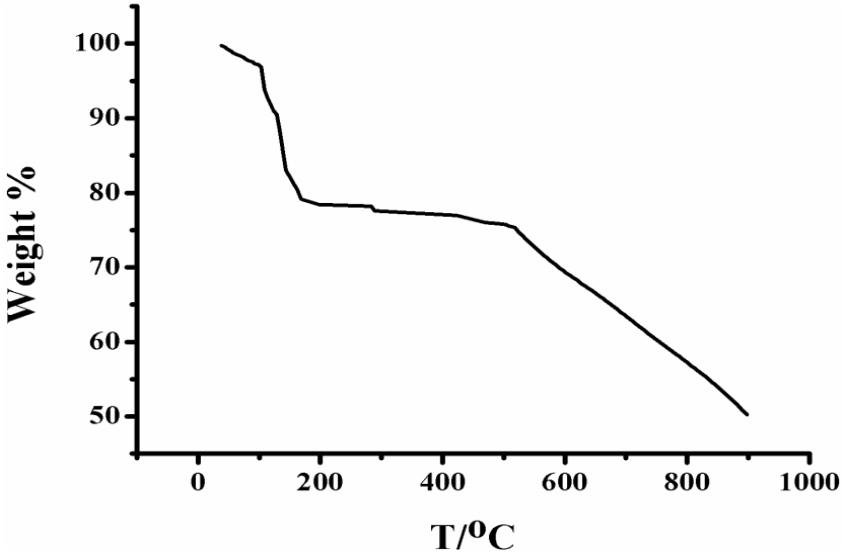


**Fig. S4.** Thermogravimetric analysis plot for complex **4**.

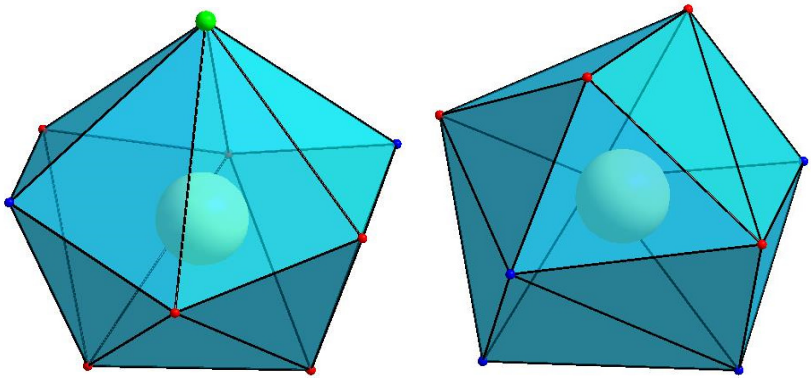

**Fig. S5.** Tri-capped trigonal prismatic geometry around $Gd^{3+}$ with $N_2O_6Cl$ coordination (left) and $N_4O_5$ coordination (right) in complex **1**.

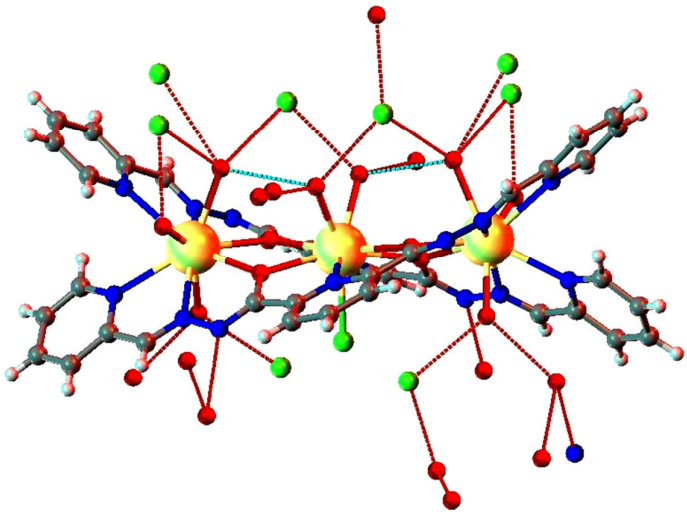

**Fig. S6.** Intra-molecular H-bonding of complex **1**

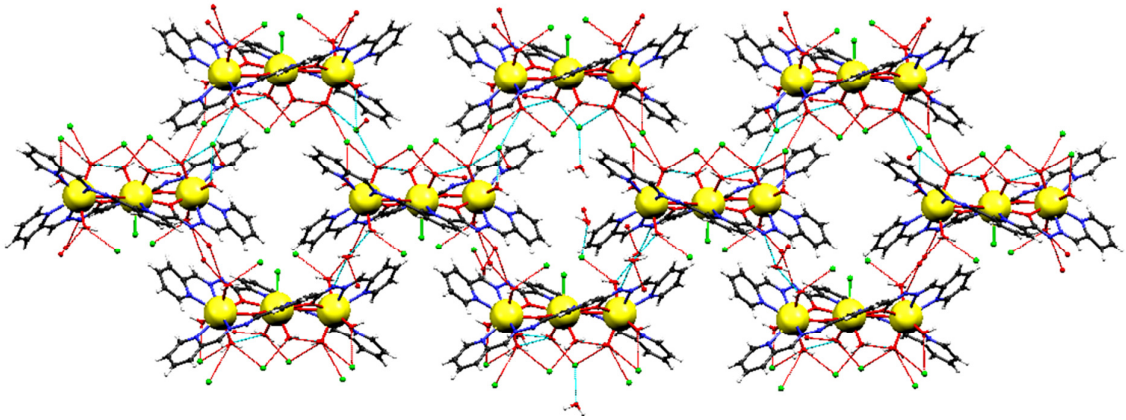

**Fig. S7.** Inter-molecular H-bonding of complex **1** along a-axis

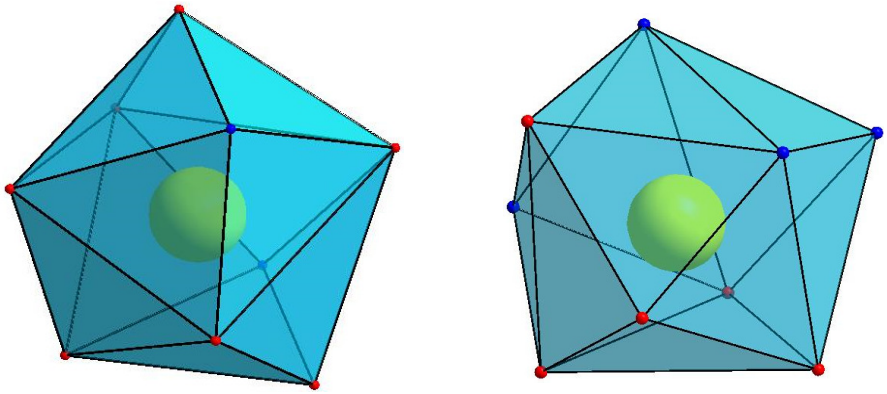

**Fig. S8.** Tri-capped trigonal prismatic geometry around $Dy^{3+}$ with $N_2O_7$ (left) and $N_4O_5$ coordination (right) in complex **2**.

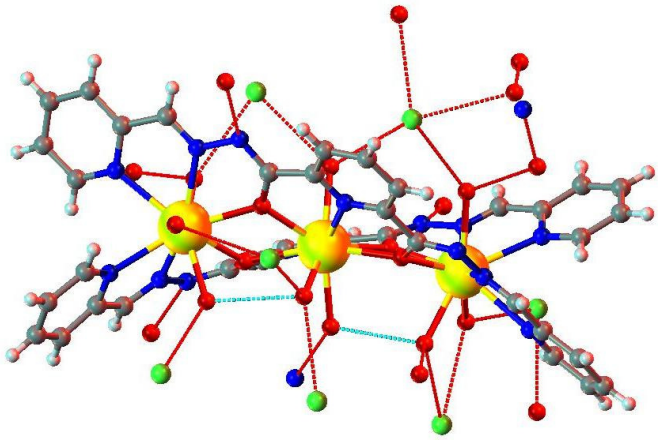

**Fig. S9.** Intra-molecular H-bonding of complex **2**

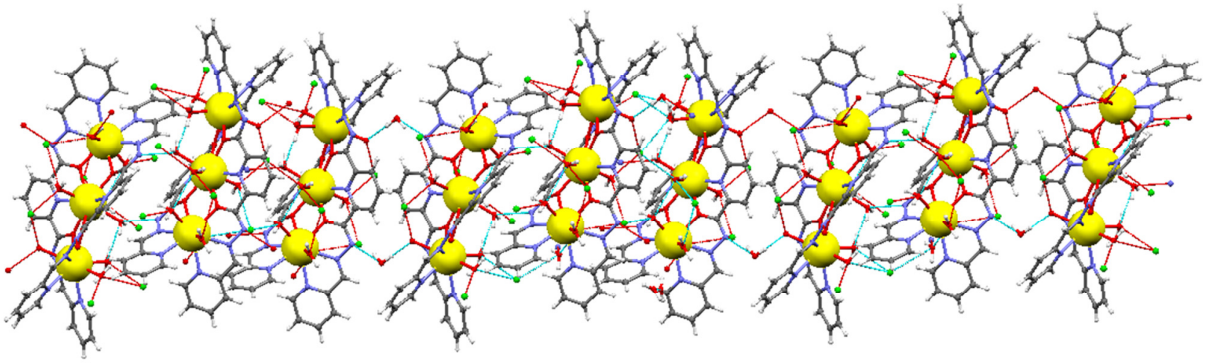

**Fig. S10.** Inter-molecular H-bonding of complex **2** along a-axis.

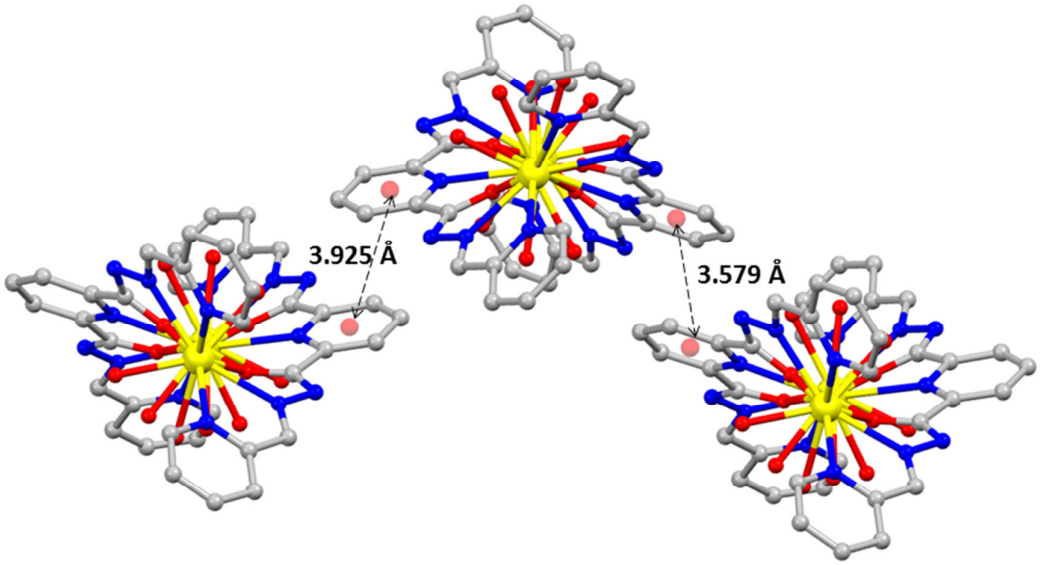


**Fig. S11.** π- π stacking between pyridine ring of complex **2**.

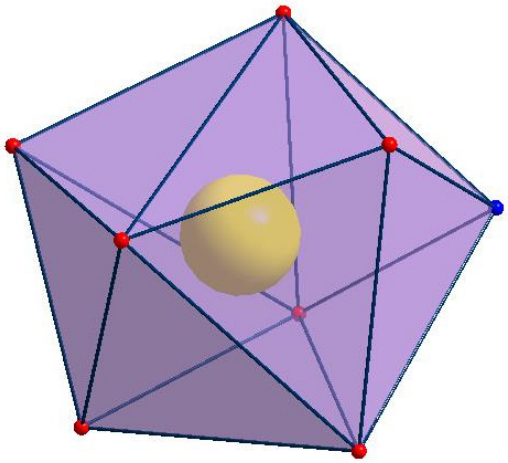

**Fig. S12.** Square antiprismatic geometry around $Ln^{3+}$( $Ln^{3+}$ = $Gd^{3+}$, $Dy^{3+}$) in complexes **3** and **4**.

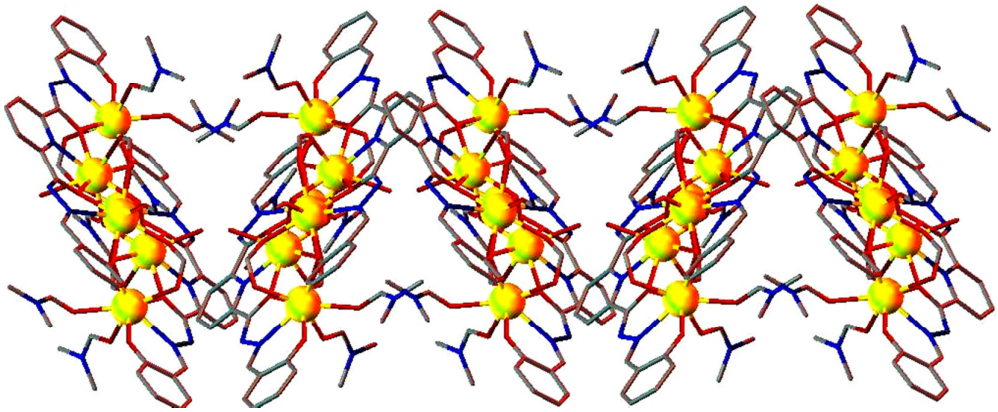

**Fig. S13.** Packing diagram of complex **3** (isostrcural complex **4**) showing zig-zag like arrangement along c-axis.

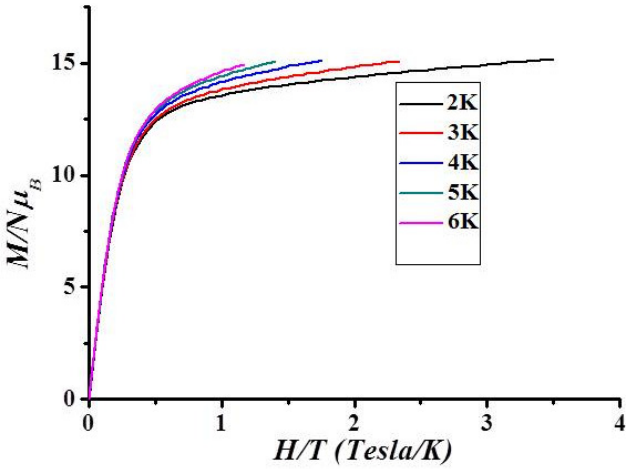


**Fig. S14.** M/NμB *vs* H/T plots for complex **2** at 2-6 K.

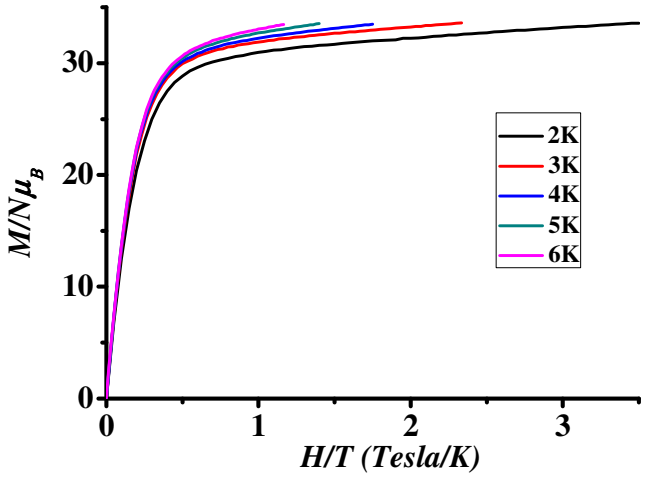


**Fig. S15.** M/NμB *vs* H/T plots for complex **4** from at 2-6 K.

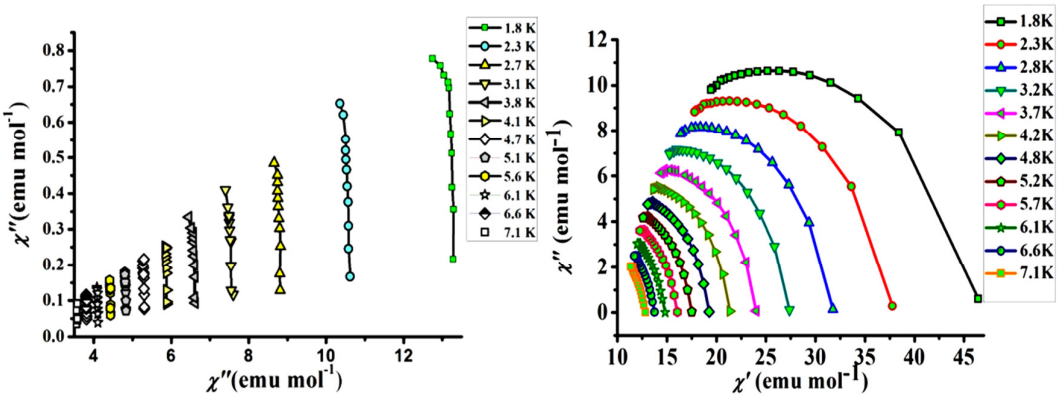


**Fig. S16.** Cole–Cole plots for complex **2** (left) and **4** (right) using the ac susceptibility data at zero field. The solid lines are to guide the eye.

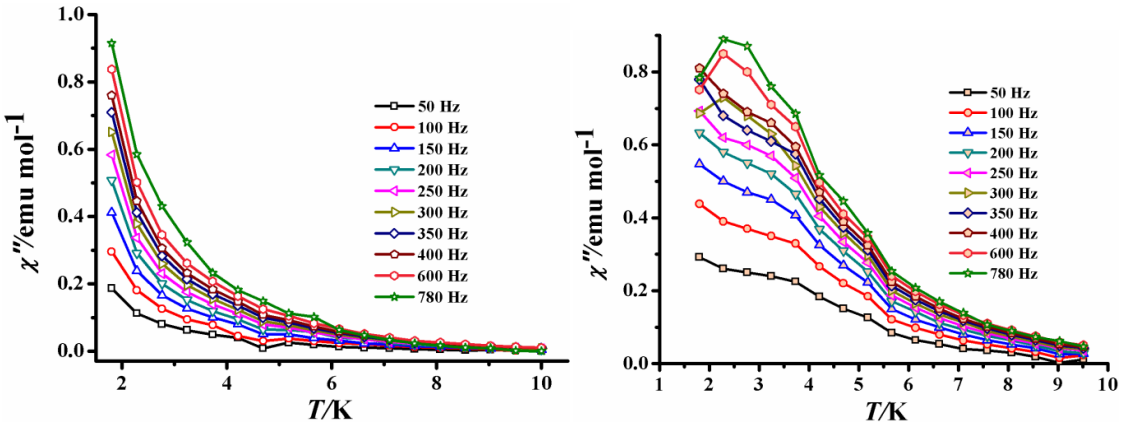


**Fig. S17.** Frequency dependence of the out of phase ($\chi$'') ac susceptibility for complex **2** under a field of 1200 Oe (left) and 1600 Oe (right).

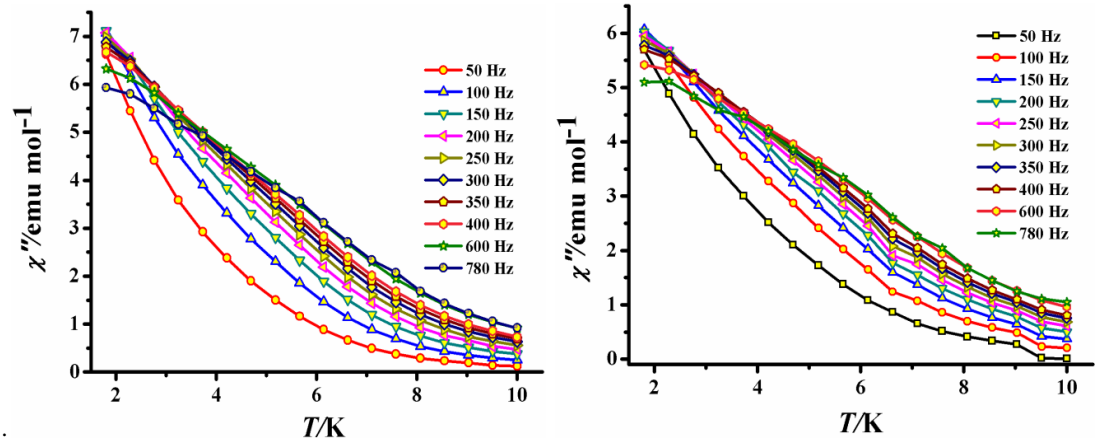


**Fig. S18.** Frequency dependence of the out of phase ($\chi$'') ac susceptibility for complex **4** under a field of 1400 Oe (left) and 1600 Oe (right).

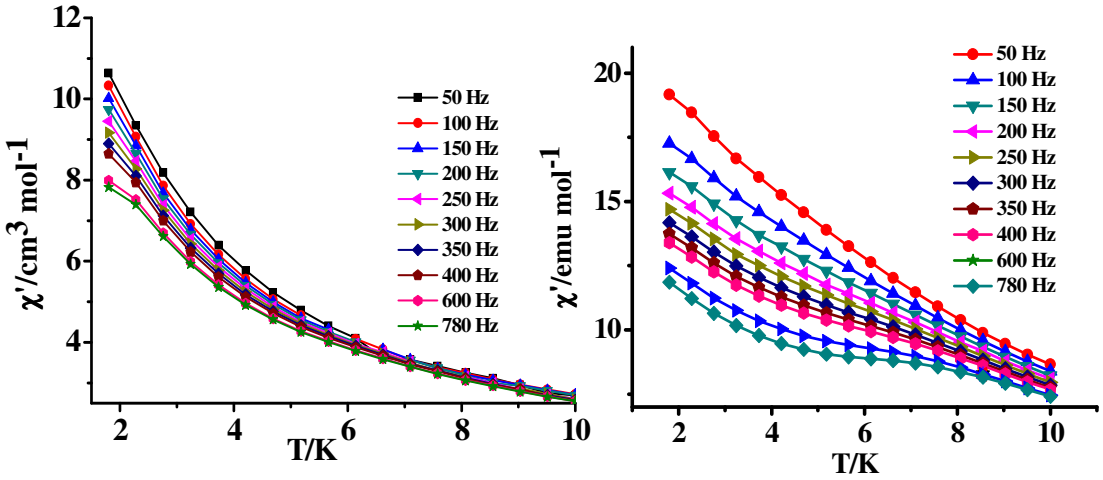


**Fig. S19.** Frequency dependence of the in phase ($\chi$') ac susceptibility for complex **2** (left) and complex **4** (right) under optimized dc fields.