

Figure S1. PXRD patterns for complex 1.

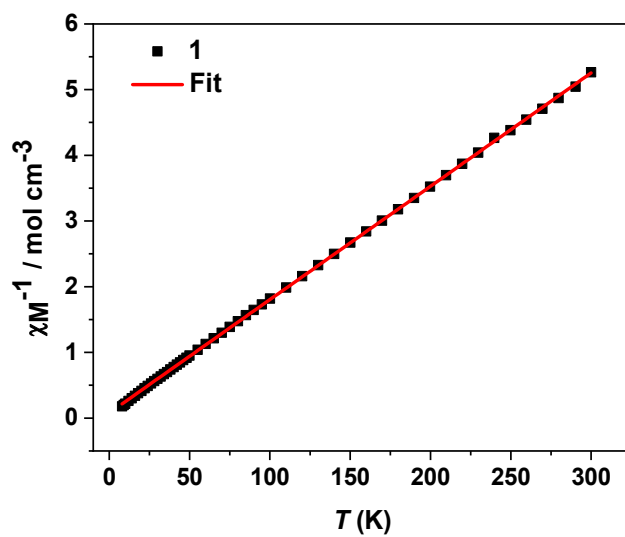
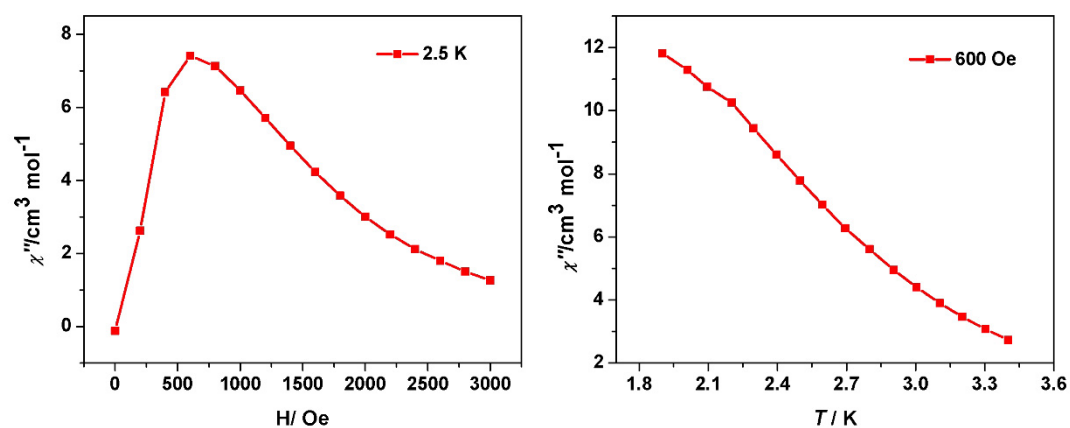
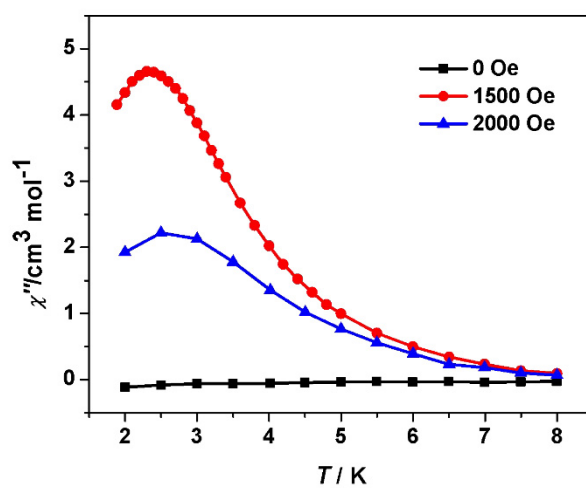


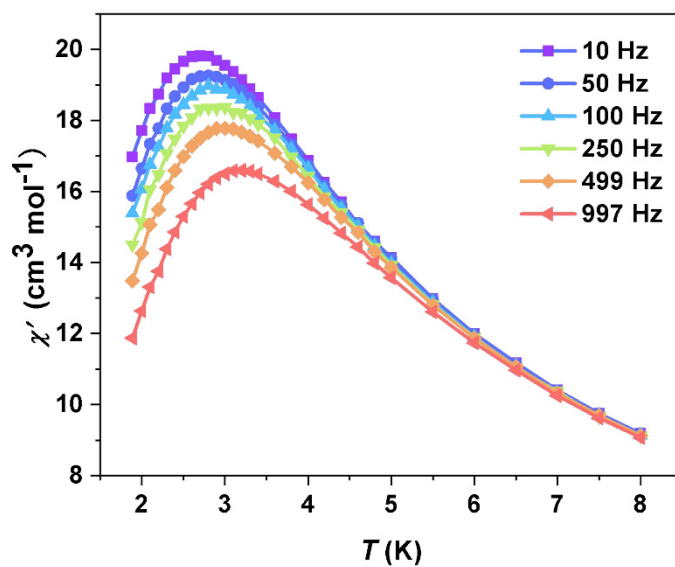
Figure S2. Plot of the  $1/\chi_M$  versus  $T$  for 1. The red solid line represents the linear fit of the data.



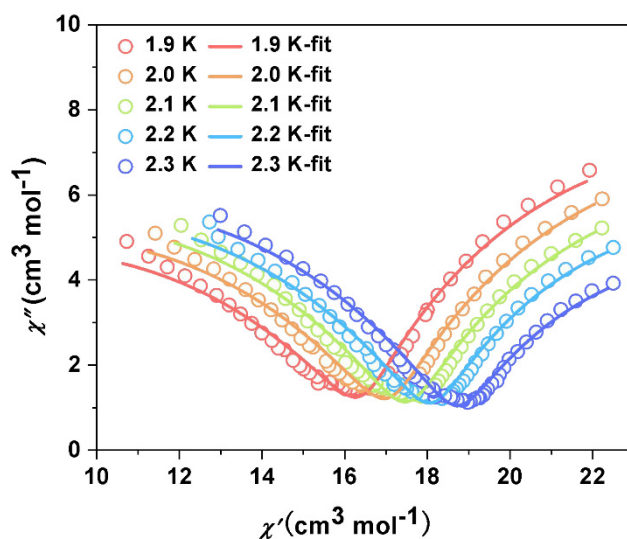
**Figure S3.** (left) Plot of  $\chi''$  versus  $H$  for complex **1** at 997 Hz and (right) plot of  $\chi''$  versus  $T$  for complex **1** at 997 Hz under 600 Oe *dc* field.



**Figure S4.** Plots of  $\chi''$  versus  $T$  for complex **1** at 997 Hz under 0, 1500 and 2000 Oe *dc* field, respectively.



**Figure S5.** Plots of temperature dependent  $\chi'$  ac susceptibility for complex **1** ( $H_{dc} = 1500$  Oe).



**Figure S6.** Cole-Cole curves at 1.9–2.3 K ( $H_{dc} = 1500$  Oe,  $H_{ac} = 2.5$  Oe).

**Table S1.** The coordination geometry of Dyl in **1a** calculated by *SHAPE* software.

Lable	Symmetry	Shape	Calculated results
OP-8	D <sub>8h</sub>	Octagon	31.098
HPY-8	C <sub>7v</sub>	Heptagonal pyramid	22.153
HBPY-8	D <sub>6h</sub>	Hexagonal bipyramid	12.876
CU-8	O <sub>h</sub>	Cube	6.408
SAPR-8	D <sub>4d</sub>	Square antiprism	<b>1.674</b>
TDD-8	D <sub>2d</sub>	Triangular dodecahedron	<b>1.615</b>
JGBF-8	D <sub>2d</sub>	Johnson gyrobifastigium J26	14.411

JETBPY-8	D <sub>3h</sub>	Johnson elongated triangular bipyramid J14	26.247
JBTPR-8	C <sub>2v</sub>	Biaugmented trigonal prism J50	3.706
BTPR-8	C <sub>2v</sub>	Biaugmented trigonal prism	2.903
JSD-8	D <sub>2d</sub>	Snub diphonoid J84	4.986
TT-8	T <sub>d</sub>	Triakis tetrahedron	7.251
ETBPY-8	D <sub>3h</sub>	Elongated trigonal bipyramid	24.020

**Table S2.** Cole-Cole curve fitting parameters for complex **1**.

<b>T</b>	<b><math>\tau_1</math></b>	<b><math>\alpha_1</math></b>	<b><math>\tau_2</math></b>	<b><math>\alpha_2</math></b>	<b><math>\chi_1</math></b>	<b><math>\chi_0</math></b>	<b><math>\chi_2</math></b>
<b>1.9</b>	0.311	0.163	5.457E-5	0.348	18.30	0.0419	34.84
<b>2.0</b>	0.366	0.197	5.271E-5	0.328	18.50	0.0462	35.63
<b>2.1</b>	0.397	0.223	4.970E-5	0.304	17.43	0.0787	34.94
<b>2.2</b>	0.356	0.214	4.919E-5	0.309	15.09	0.126	33.15
<b>2.3</b>	0.395	0.251	4.687E-5	0.299	5.68	0.00909	31.96