Electronic supplementary information (ESI)

From mononuclear to two-dimensional Cobalt(II) complexes based on mixed benzimidazole-carboxylate bridges: syntheses, structures, and magnetic properties

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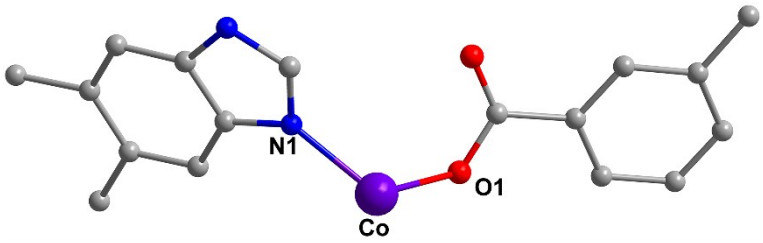

Figure S1. The asymmetric unit of **1**. Hydrogen atoms were omitted for clarity.

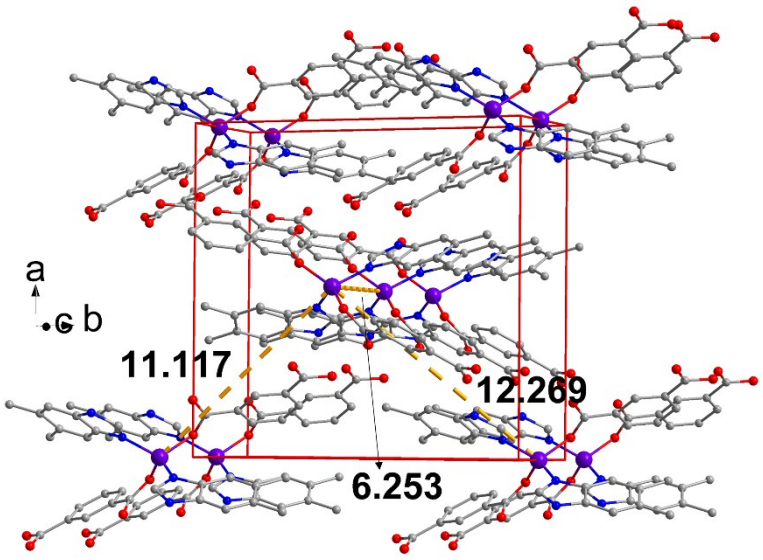

Figure S2. The packing structure of **1**.

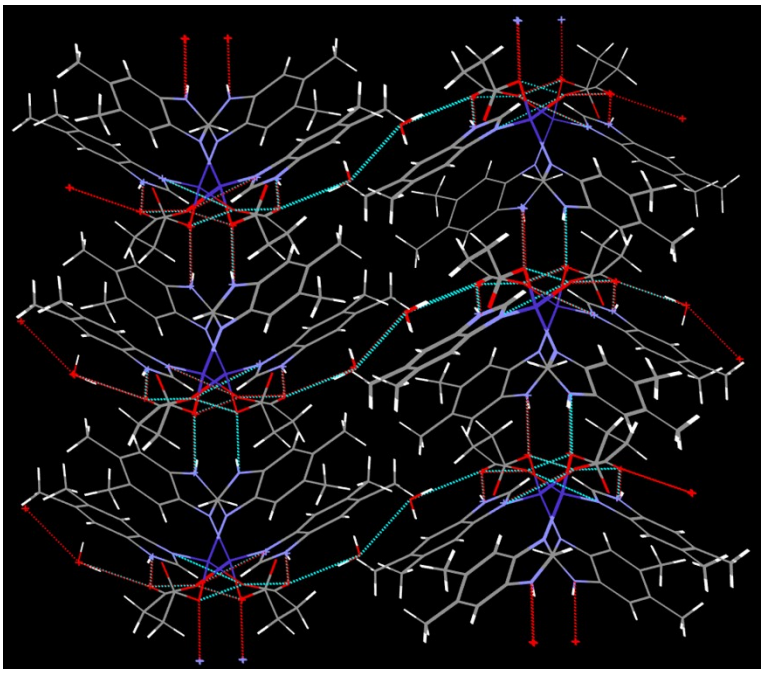

Figure S3. The packing structure of **2**.

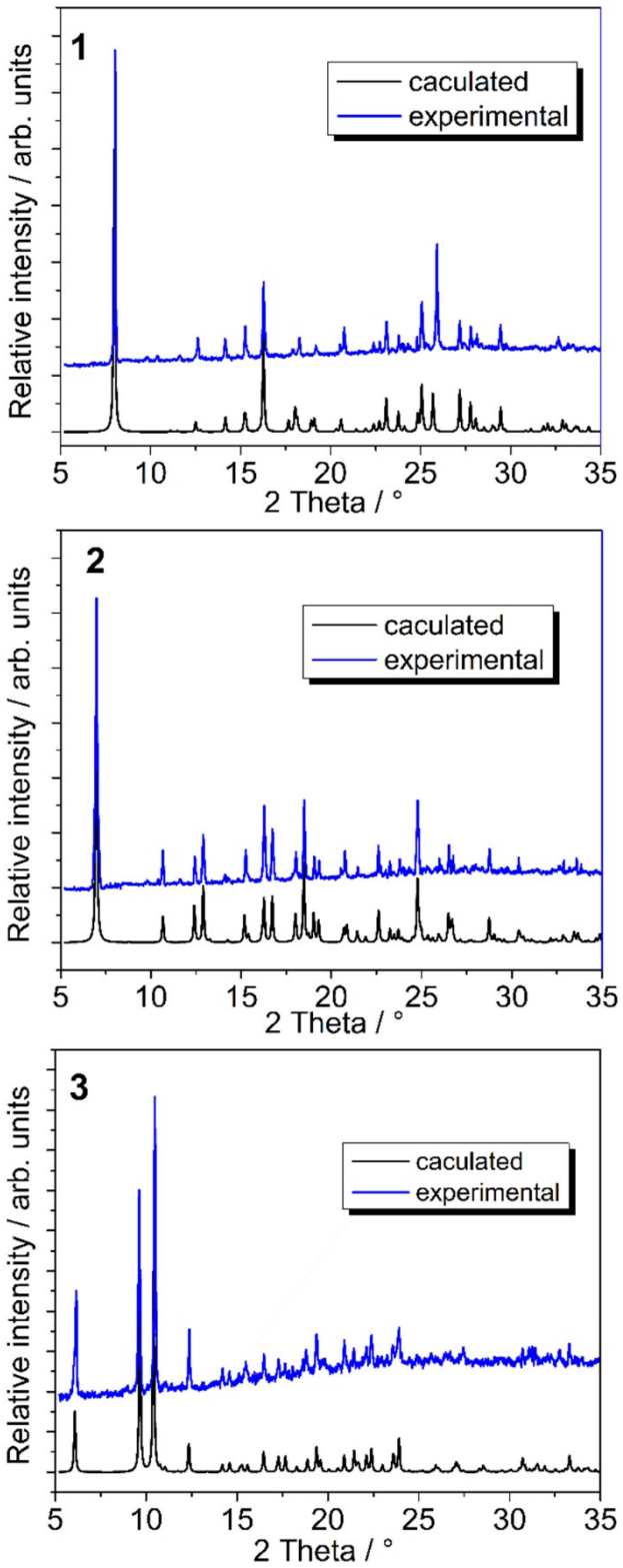

Figure S4. PXRD patterns of **1-3**.

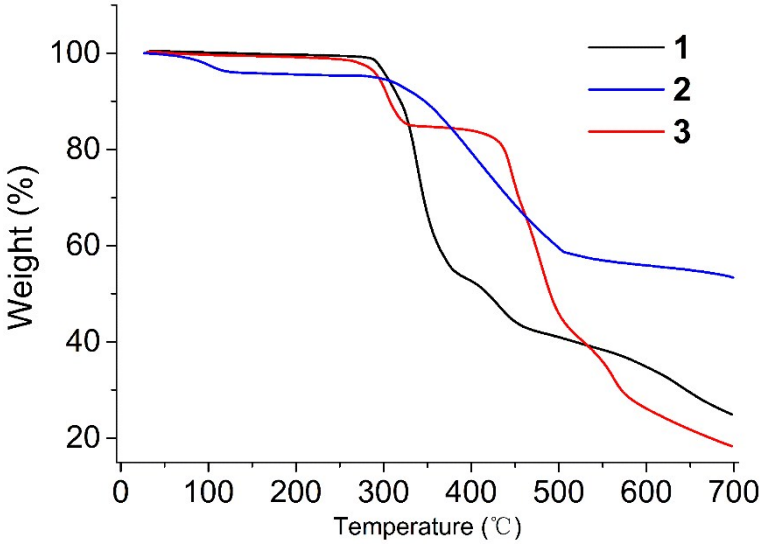

Figure S5. TGA curves of **1-3**.

Table S1. Selected bond lengths (Å) and, angles [°], and structural parameters for **1-3**.

1			
Co(1)-O(1)	1.951(2)	O(1)#1-Co(1)-O(1)	99.20(13)
Co(1)-O(1)#1	1.951(2)	O(1)#1-Co(1)-N(1)	106.99(10)
Co(1)-N(1)	2.011(2)	O(1)-Co(1)-N(1)	121.78(10)
Co(1)-N(1)#1	2.011(2)	O(1)#1-Co(1)-N(1)#1	121.78(10)
Co-X_{aver} (X = N, O)	1.981	O(1)-Co(1)-N(1)#1	106.99(10)
CShM□	1.275	N(1)-Co(1)-N(1)#1	101.64(14)
		C(10)-O(1)-Co(1)	120.22(18)
Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,z □ continuous shape measures calculated by SHAPE 2.0.			

2			
Co(1)-O(1)	1.963(2)	O(1)-Co(1)-O(3)#1	99.73(11)
Co(1)-N(1)	2.005(3)	O(1)-Co(1)-N(2)	119.06(11)
Co(1)-N(2)	2.003(3)	O(3)#1-Co(1)-N(2)	111.74(11)
Co(1)-O(3)#1	1.980(2)	O(1)-Co(1)-N(1)	116.93(11)
Co-X_{aver} (X = N, O)	1.987	O(3)#1-Co(1)-N(1)	94.63(11)
CShM	1.008	N(2)-Co(1)-N(1)	111.04(12)
		C(1)-O(1)-Co(1)	124.8(2)
Symmetry transformations used to generate equivalent atoms: #1 x-1/2,-y+3/2,z-1/2			

3			
Co(1)-O(1)	1.9593(15)	O(1)-Co(1)-O(6)#1	110.89(7)
Co(1)-O(6)#1	1.9866(15)	O(1)-Co(1)-N(1)	109.69(7)
Co(1)-N(1)	2.0083(18)	O(6)#1-Co(1)-N(1)	94.02(7)
Co(1)-O(2)	2.0101(13)	O(1)-Co(1)-O(2)	112.21(6)
Co-X_{aver} (X = N, O)	1.991	O(6)#1-Co(1)-O(2)	96.55(6)

CShM□		N(1)-Co(1)-O(2)	129.31(7)
Co(2)-O(5)#2	2.0391(14)	O(5)#2-Co(2)-O(5)	180.0
Co(2)-O(5)	2.0391(14)	O(5)#2-Co(2)O(4)#3	84.78(6)
Co(2)-O(4)#3	2.0667(14)	O(5)-Co(2)-O(4)#3	95.22(6)
Co(2)-O(4)#4	2.0667(14)	O(5)#2-Co(2)-O(4)#4	95.22(6)
Co(2)-O(2)#4	2.1983(14)	O(5)-Co(2)-O(4)#4	84.78(6)
Co(2)-O(2)#3	2.1983(14)	O(4)#3-Co(2)-O(4)#4	180.00(11)
Co-O_{aver}	2.101	O(5)#2-Co(2)-O(2)#4	90.15(6)
CShM		O(5)-Co(2)-O(2)#4	89.85(6)
		O(4)#3-Co(2)-O(2)#4	88.26(6)
		O(4)#4-Co(2)-O(2)#4	91.74(6)
		O(5)#2-Co(2)-O(2)#3	89.85(6)
		O(5)-Co(2)-O(2)#3	90.15(6)
		O(4)#3-Co(2)-O(2)#3	91.74(6)
		O(4)#4-Co(2)-O(2)#3	88.26(6)
Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z+1/2; #2 -x,-y,-z; #3 x,-y+1/2,z-1/2; #4 -x,y-1/2,-z+1/2			

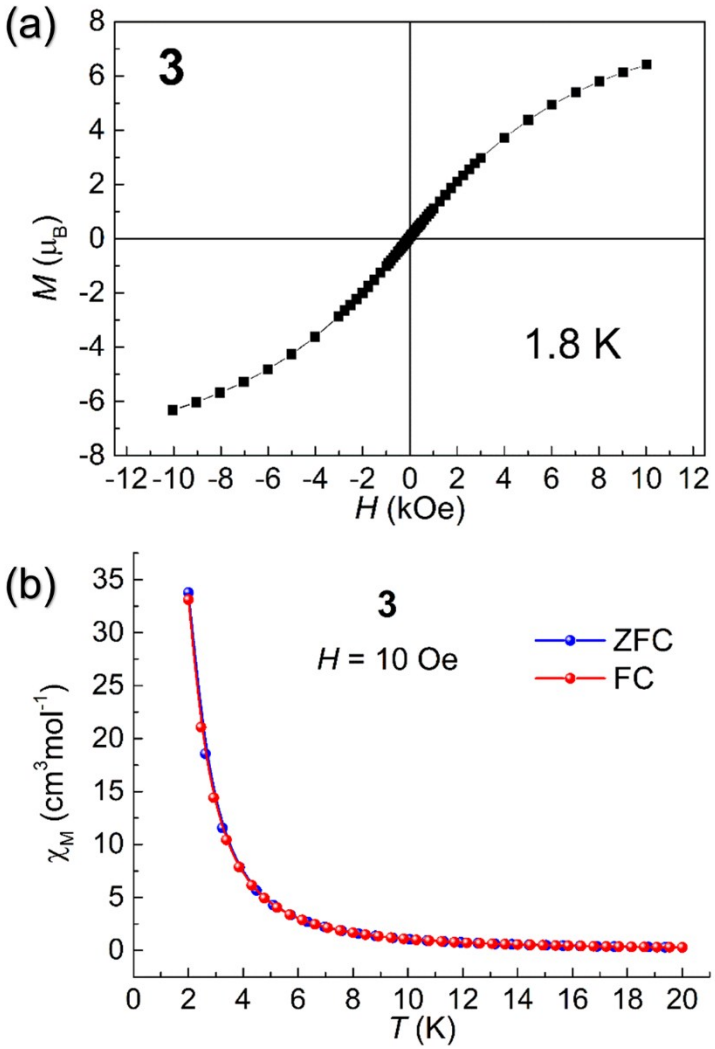

Figure S6 (a) Magnetization curve at 1.8 K for **3**. (b) The field-cooled (FC) and zero-field-cooled (ZFC) magnetizations curves for **3**.

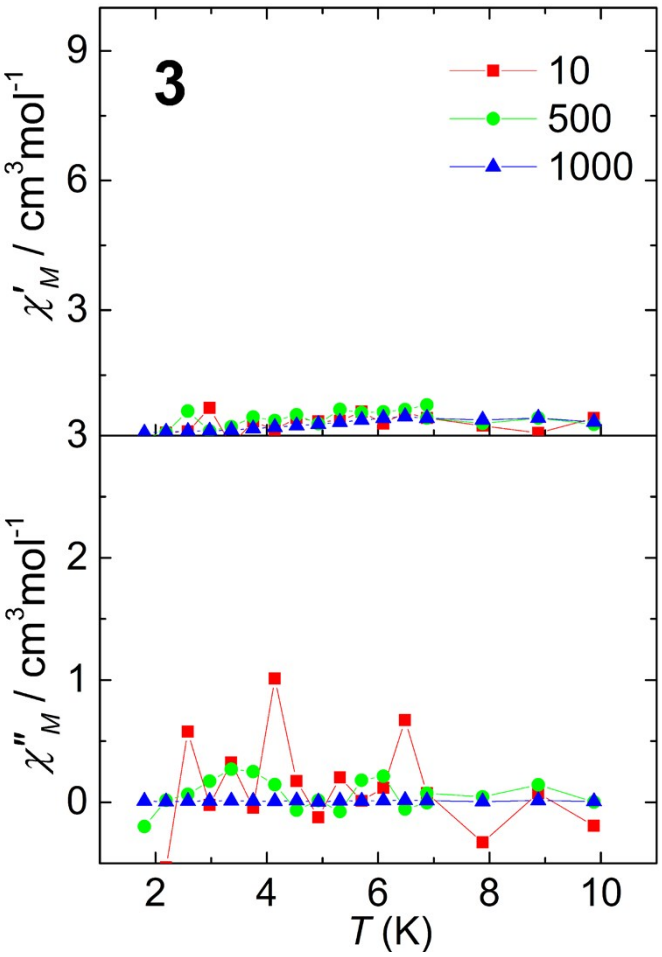

Figure S7. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibilities measured under zero dc field for **3**.

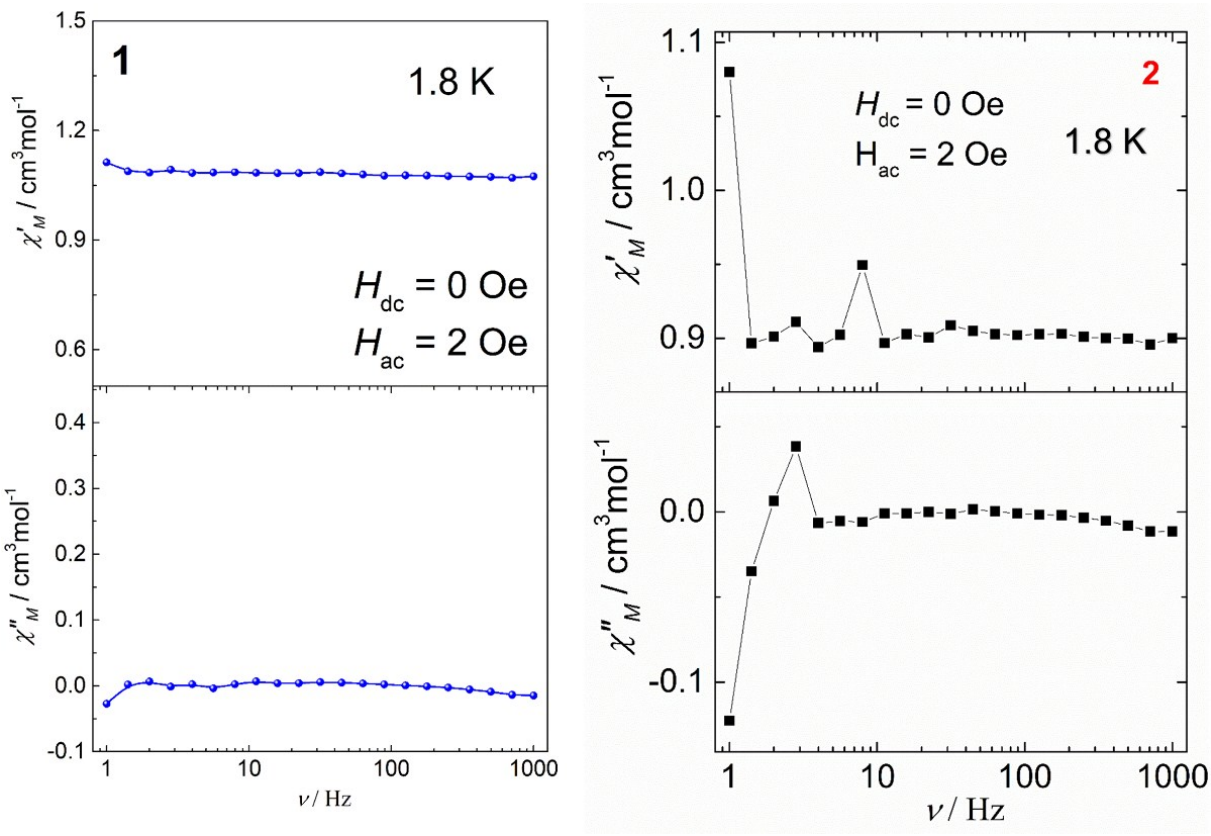

Figure S8. Frequency dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibilities measured under zero dc field at 1.8 K for **1** and **2**.

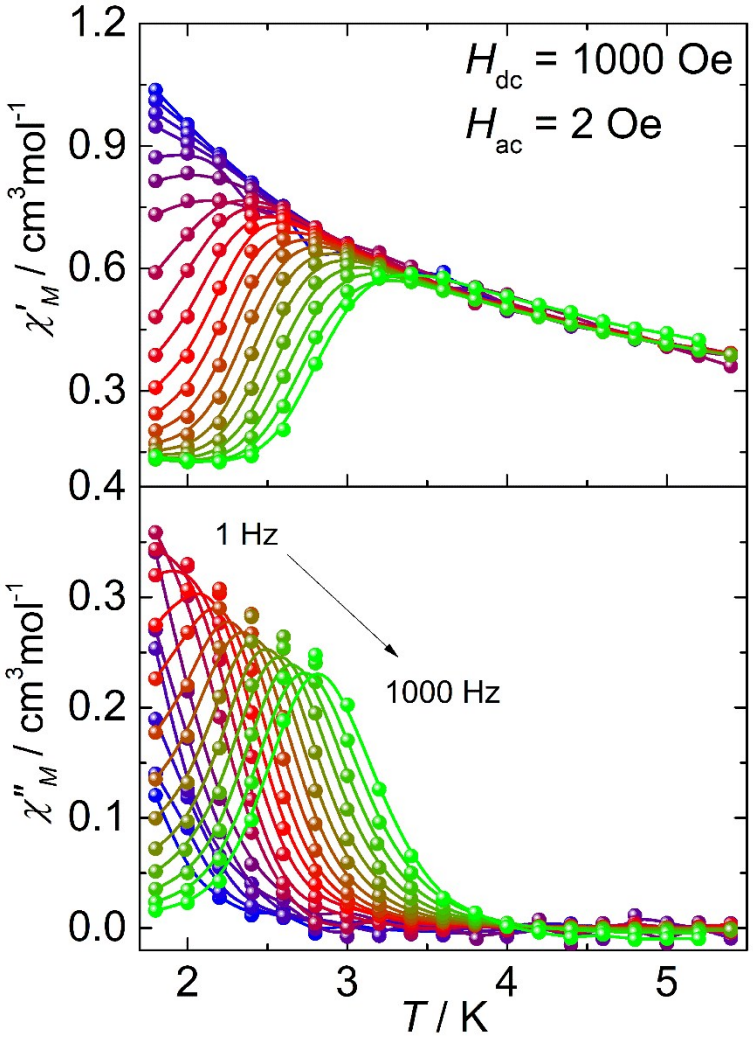

Figure S9. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibilities for **1** under a 1000 Oe dc field.

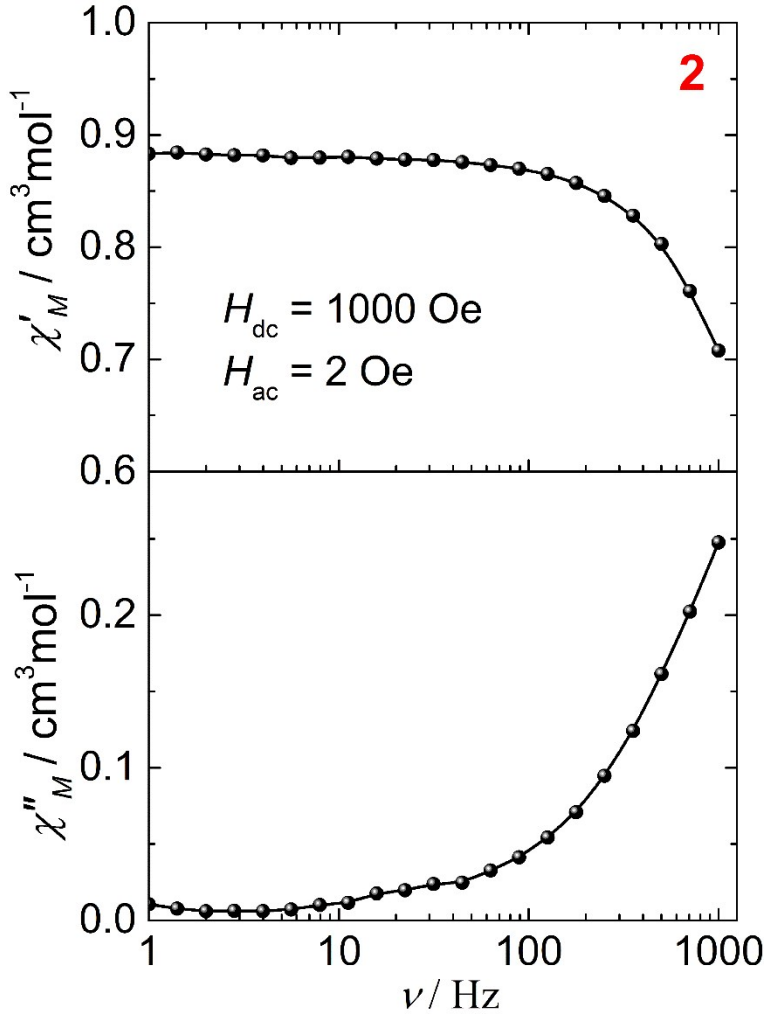

Figure S10. Frequency dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibilities measured under a 1000 Oe dc field at 1.8 K for **2**.

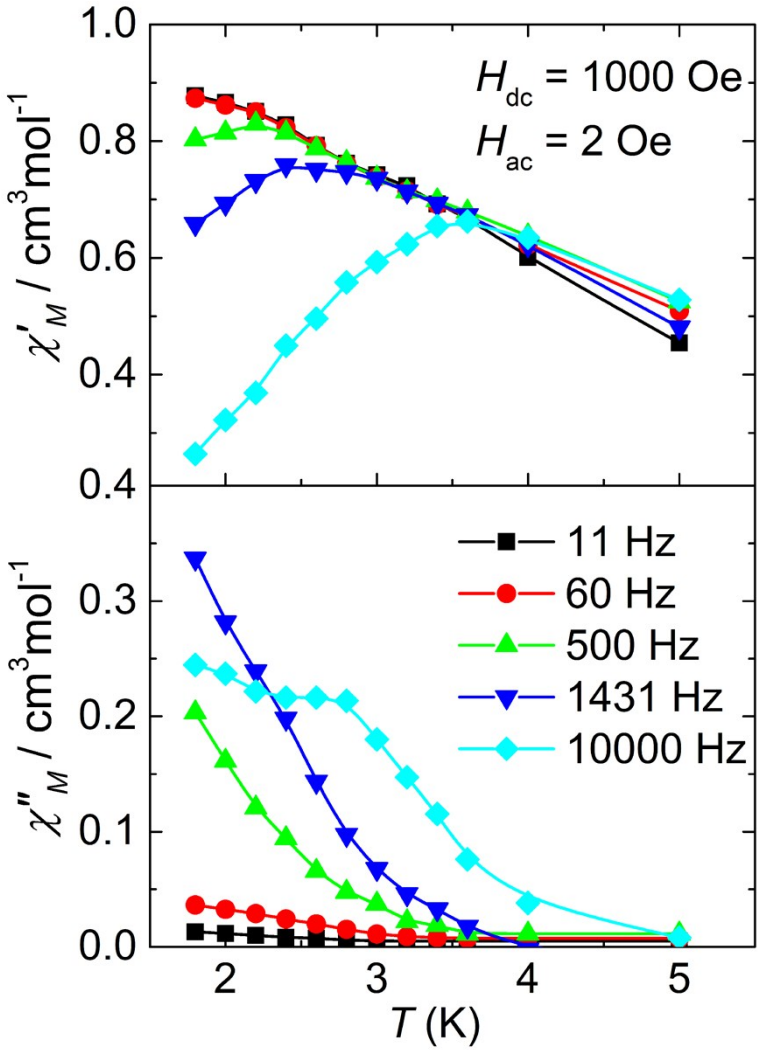

Figure S11. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibilities for **2** under a 1000 Oe dc field.

Table S2. Relaxation fitting parameters at 1.8 K under different dc fields from the least-square fitting of the Cole-Cole plots of **1** according to the generalized Debye model.

H / Oe	χ_S / $cm^3mol^{-1}K$	χ_T / $cm^3mol^{-1}K$	τ / s	α
100	0.99712	1.09803	0.00769	0.2168
200	0.74952	1.09397	0.00859	0.12802
400	0.37771	1.08569	0.01036	0.15719
600	0.22675	1.09895	0.01192	0.14894
800	0.13861	1.08817	0.01329	0.17876
1000	0.13049	1.0462	0.0136	0.10567
1200	0.09234	1.02236	0.01323	0.18174
1400	0.08768	1.04978	0.01263	0.14699
1600	0.07131	0.98656	0.01188	0.13994
1800	0.06351	0.95474	0.01088	0.13945

Table S3. Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **1** according to the generalized Debye model.

T / K	χ_S / $cm^3mol^{-1}K$	χ_T / $cm^3mol^{-1}K$	τ / s	α
1.8	0.06112	0.79145	0.00132	0.1737
1.9	0.05171	0.75523	0.00117	0.17563
2	0.05218	0.71687	0.00102	0.16234
2.2	0.05	0.66094	8.19952E-4	0.15492
2.4	0.06	0.60896	6.63738E-4	0.13177
2.6	0.06	0.5755	5.49856E-4	0.11211
2.8	0.07311	0.53884	4.56748E-4	0.07268
3.0	0.09066	0.50411	3.8486E-4	0.02963
3.2	0.11002	0.48229	3.30516E-4	0.006
3.4	0.14065	0.45959	2.83575E-4	0.00269

Table S4. Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **2** according to the generalized Debye model.

T / K	χ_S / $cm^3mol^{-1}K$	χ_T / $cm^3mol^{-1}K$	τ / s	α
1.8	0.16461	0.89471	6E-5	0.1312
2.0	0.22008	0.88548	6E-5	0.15359
2.2	0.45995	0.99321	5E-5	0.1003
2.4	0.35065	0.83106	4E-5	0.05832
2.6	0.4001	0.80252	3E-5	0.00932
2.8	0.45046	0.76975	2E-5	0.0051

Table S5. Fitting results to the temperature dependence of the magnetic relaxation time by Direct and Raman mechanism, respectively.

Compound	Direct	Raman
1	$A = 1935$	$C = 2.9$; $n = 9$
2	$A = 55036$	$C = 0.02$; $n = 2.2$