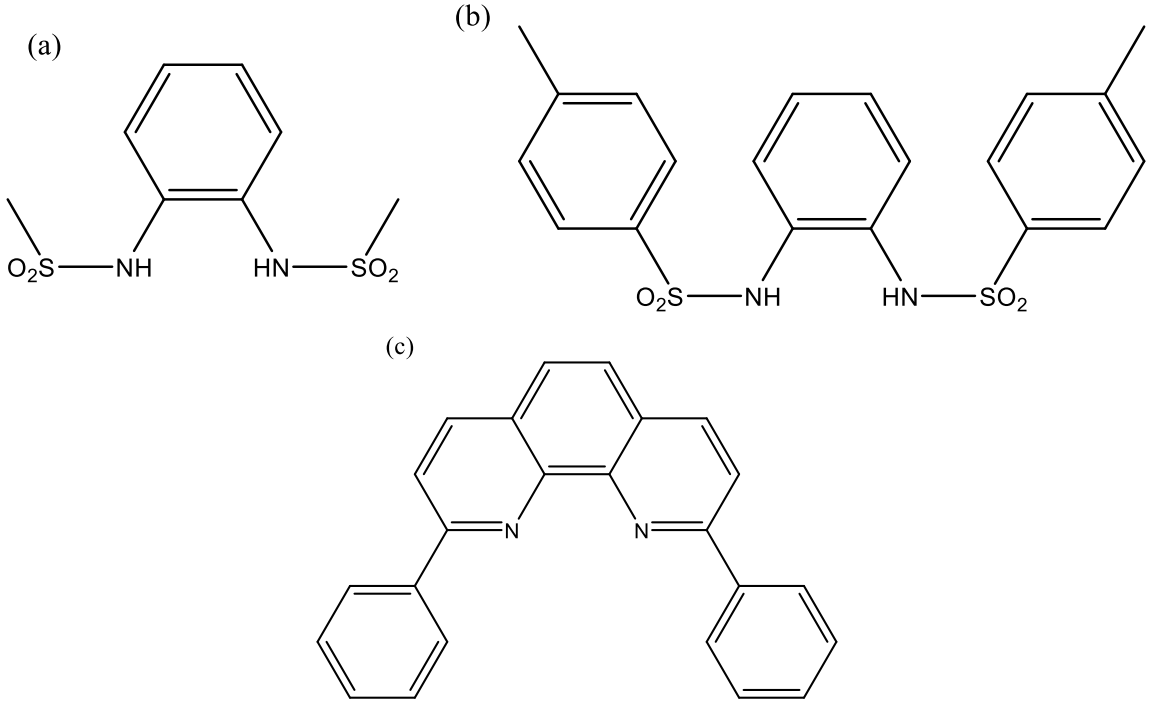
Supporting Information

Phonon-Induced Relaxation Mechanisms are Changed by a Chelating Effect in a Co^{II} Single-Ion Magnet

Yu-Siang, Lou,[a] Bo-Ruei Lin,[a] Chen-Ming Wu,[a] Su-Ying Chien [b] and En-Che Yang*[a]

a Y.-S. Lou, B.-R. Lin, C.-M. Wu and Prof. E.-C. Yang
Department of Chemistry
Fu-Jen Catholic University
Address 1: Hsinchuang, New Taipei City, 24205, Taiwan, Republic of China
E-mail: 071549@mail.fju.edu.tw
b Dr. S.-Y. Chien
Instrumentation Centre t
College of Science, National Taiwan University
Taipei, 10672, Taiwan, Republic of China.



Scheme 1S. Ligands used in the literature. (a) used in ref 13 (b) used in ref 14 (c) used in ref 15. Combining (b) and (c) are the ligands used in current work compound **1**.

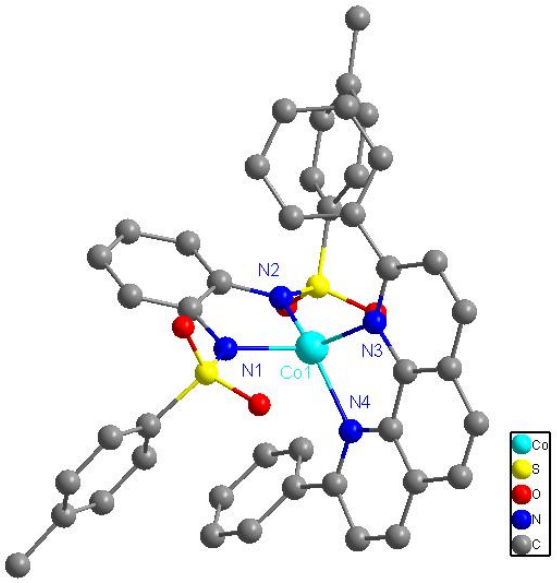
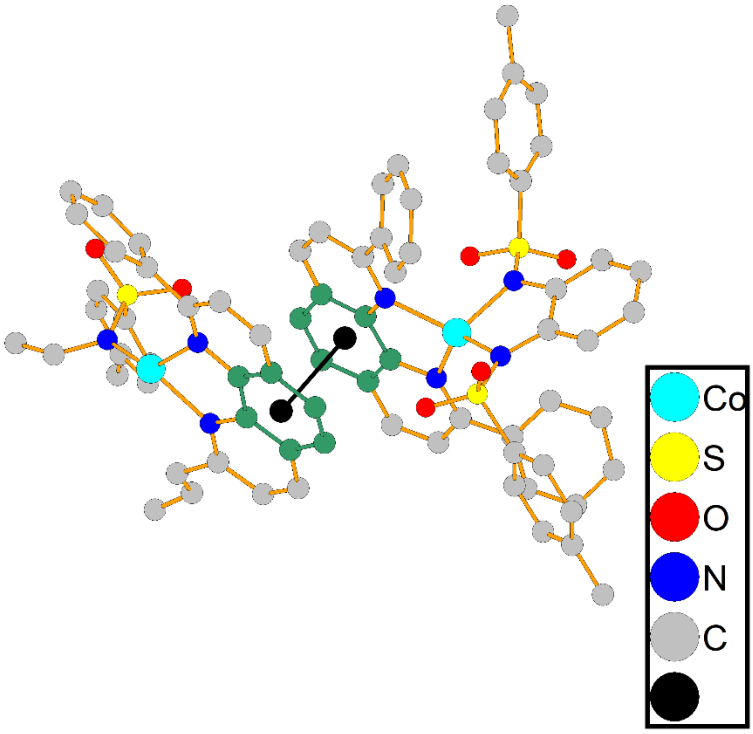


Figure 1S the structures of compounds (**1**)

(*a*)



(*b*)

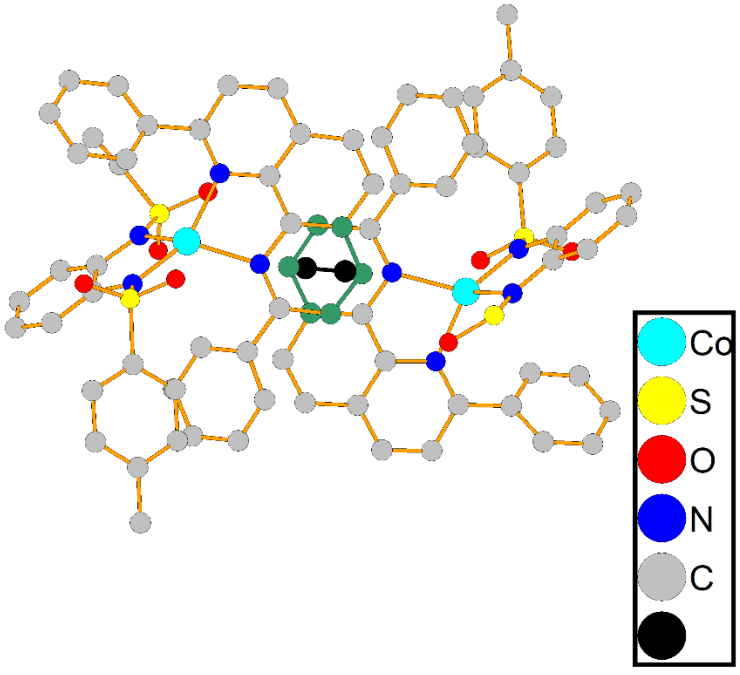


Figure 2S. Different π-π stacking ways are found in the lattice of compound **1**.

Table 1S. Crystal data and structure refinement for Compound **1**.

Identification code	ic20765	
Empirical formula	C45 H39 Co N4 O6 S2	
Formula weight	854.85	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 19.5098(16) Å	α= 90°.
	b = 31.080(3) Å	β= 104.583(3)°.
	c = 14.1457(12) Å	γ = 90°.
Volume	8301.1(12) $Å^3$	
Z	8	
Density (calculated)	1.368 Mg/m^3	
Absorption coefficient	0.568 mm^{-1}	
F(000)	3552	
Crystal size	0.212 x 0.041 x 0.025 mm^3	
Theta range for data collection	1.982 to 25.185°.	
Index ranges	-23<=h<=23, -37<=k<=37, -13<=l<=16	
Reflections collected	65123	
Independent reflections	14807 [R(int) = 0.0941]	
Completeness to theta = 25.185°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8129 and 0.6534	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14807 / 10 / 1036	
Goodness-of-fit on F^2	1.355	
Final R indices [I>2sigma(I)]	R1 = 0.0859, wR2 = 0.2097	
R indices (all data)	R1 = 0.1092, wR2 = 0.2214	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.113 and -1.266 $e.Å^{-3}$	

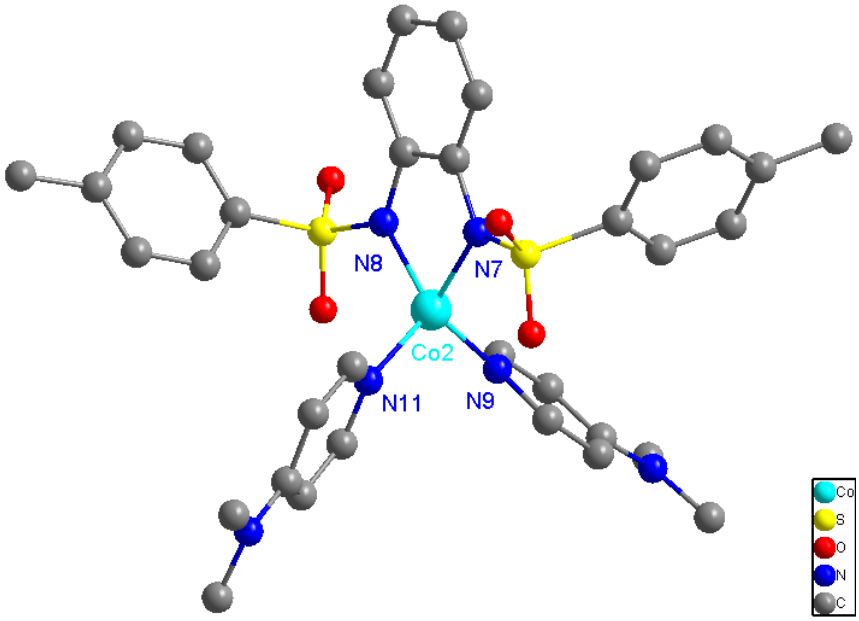


Figure 3S the structures of compounds (**2**)

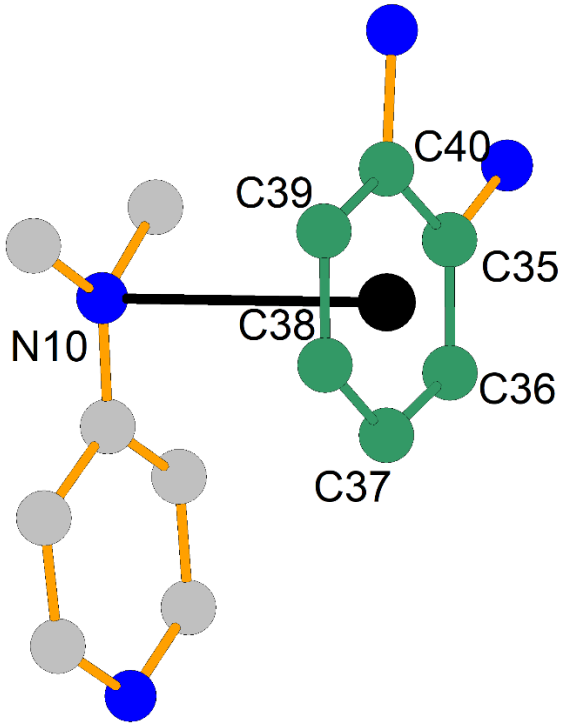


Figure 4S The short contact in compounds (**2**). The nearby aromatic rings are parallel, but no π-π interactions can be seen.

Table 2S. Crystal data and experimental details for Compound **2**.

Empirical formula	C36.50 H44 Cl Co N6 O4.50 S2	
Formula weight	797.27	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 18.7232(14) Å	α= 90°.
	b = 12.8260(9) Å	β= 95.582(7)°.
	c = 32.042(3) Å	γ = 90°.
Volume	7658.3(10) $Å^3$	
Z	8	
F(000)	3336	
Density (calculated)	1.383 Mg/m^3	
Wavelength	0.71073 Å	
Cell parameters reflections used	5594	
Theta range for Cell parameters	3.9800 to 27.1300°.	
Absorption coefficient	0.675 mm^{-1}	
Temperature	100(2) K	
Crystal size	0.15 x 0.10 x 0.10 mm^3	
Data collection		
Diffractometer	Xcalibur, Atlas, Gemini	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.92784	
No. of measured reflections	38187	
No. of independent reflections	17538 [R(int) = 0.0815]	
No. of observed [I>2_igma(I)]	8547	
Completeness to theta = 25.242°	99.8 %	
Theta range for data collection	3.115 to 27.500°.	
Refinement		
Final R indices [I>2sigma(I)]	R1 = 0.0888, wR2 = 0.1993	
R indices (all data)	R1 = 0.1906, wR2 = 0.2873	
Goodness-of-fit on F^2	1.066	
No. of reflections	17538	
No. of parameters	893	
No. of restraints	12	
Largest diff. peak and hole	1.488 and -1.257 e.$Å^{-3}$	

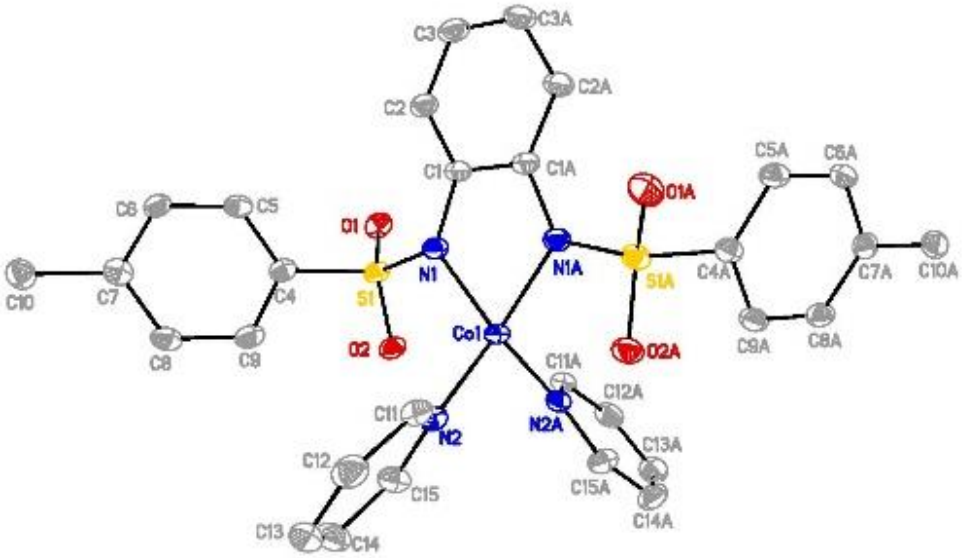


Figure 5S the structures of compounds (**3**)

Table 3S. Crystal data and experimental details for Compound **3**.

Empirical formula	C30 H28 Co N4 O4 S2	
Formula weight	631.61	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 16.6621(18) Å	α= 90°.
	b = 11.5428(12) Å	β= 99.816(10)°.
	c = 14.7676(15) Å	γ = 90°.
Volume	2798.6(5) $Å^3$	
Z	4	
F(000)	1308	
Density (calculated)	1.499 Mg/m^3	
Wavelength	0.71073 Å	
Cell parameters reflections used	3764	
Theta range for Cell parameters	4.1590 to 29.9200°.	
Absorption coefficient	0.807 mm^{-1}	
Temperature	100(2) K	
Crystal size	0.25 x 0.20 x 0.10 mm^3	
	Data collection	
Diffractometer	Xcalibur, Atlas, Gemini	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.92056	
No. of measured reflections	7300	
No. of independent reflections	3215 [R(int) = 0.0359]	
No. of observed [I>2_igma(I)]	2841	
Completeness to theta = 25.242°	99.8 %	
Theta range for data collection	3.363 to 27.496°.	
	Refinement	
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.1108	
R indices (all data)	R1 = 0.0473, wR2 = 0.1179	
Goodness-of-fit on F^2	1.016	
No. of reflections	3215	
No. of parameters	186	
No. of restraints	0	
Largest diff. peak and hole	0.555 and -0.505 e.$Å^{-3}$	

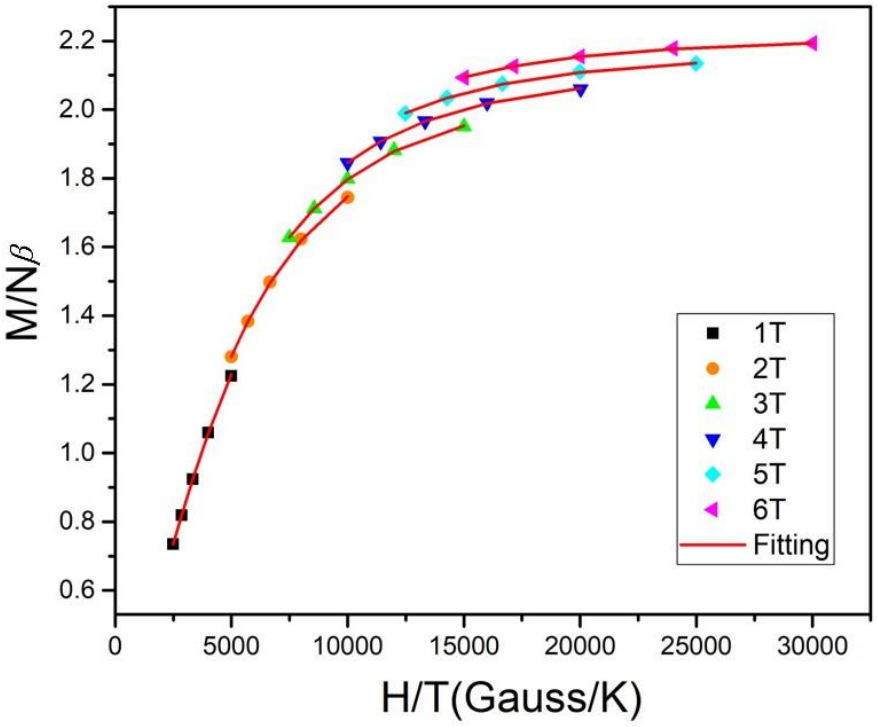


Figure 6S the result of reduced magnetization of compound (**2**)

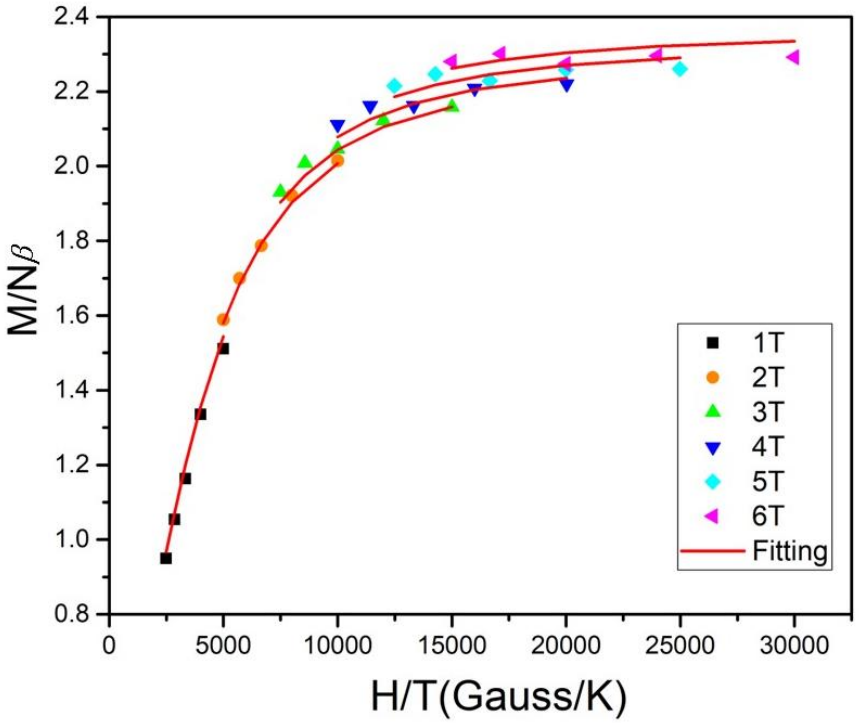


Figure 7S. the result of reduced magnetization of compound (**3**)

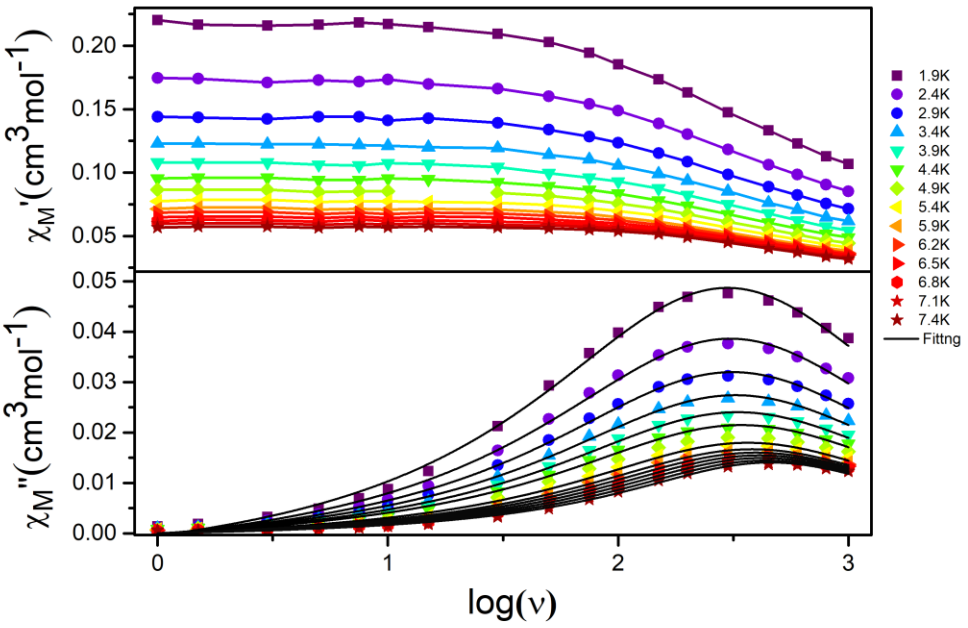


Figure 8S. Frequency dependence of the in-phase (top) and out-of-phase signals (bottom) of compound (**1**) under ***zero*** dc field.

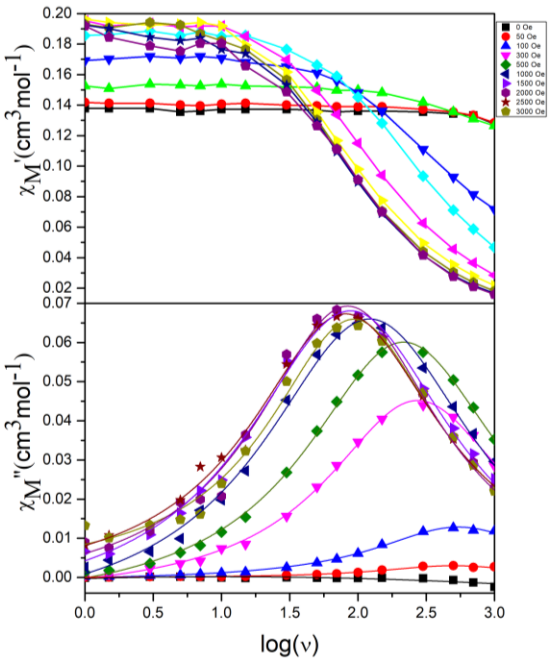


Figure 9S. Field dependence of the in-phase and the out-of-phase signals of compound (**2**) under 0-3000 G dc field at 2.8 K.

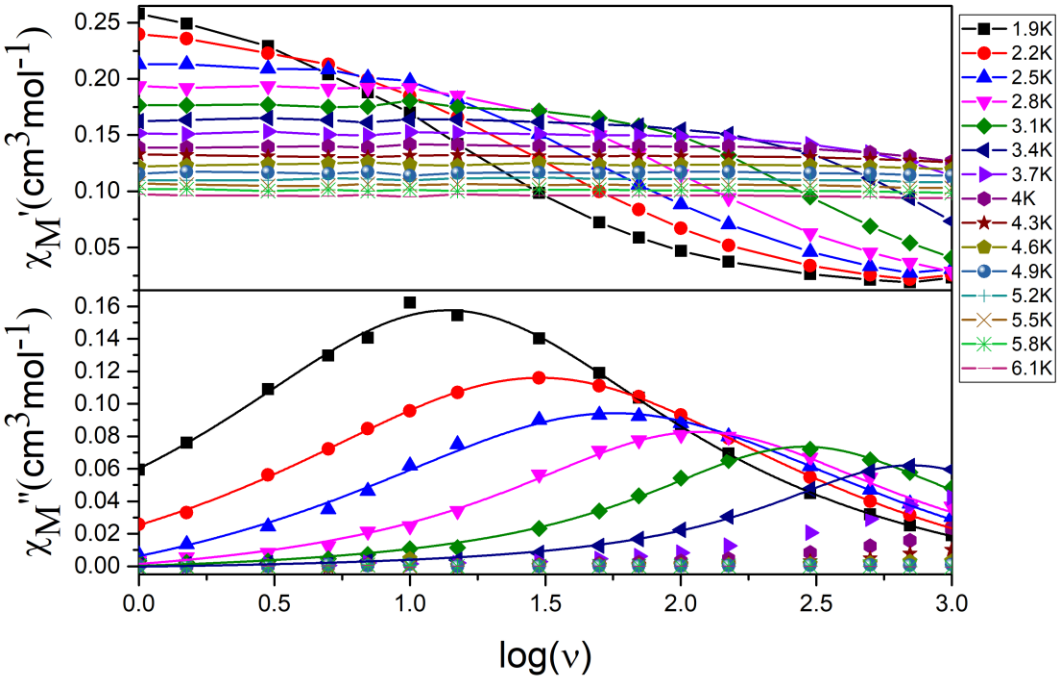


Figure 10S. Frequency dependence of the in-phase and out-of-phase signals of compound (**2**) under 1000 G dc field.

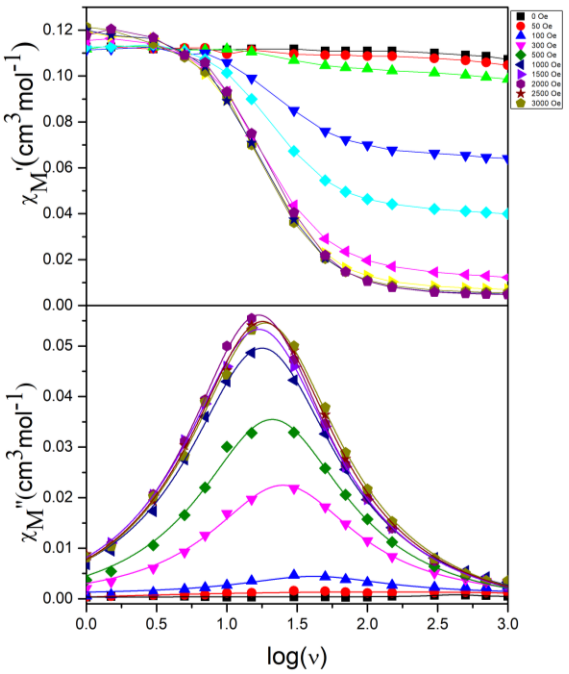


Figure 11S. Field dependence of the in-phase and the out-of-phase signals of compound (**3**) under 0-3000 G dc field at 4.0 K

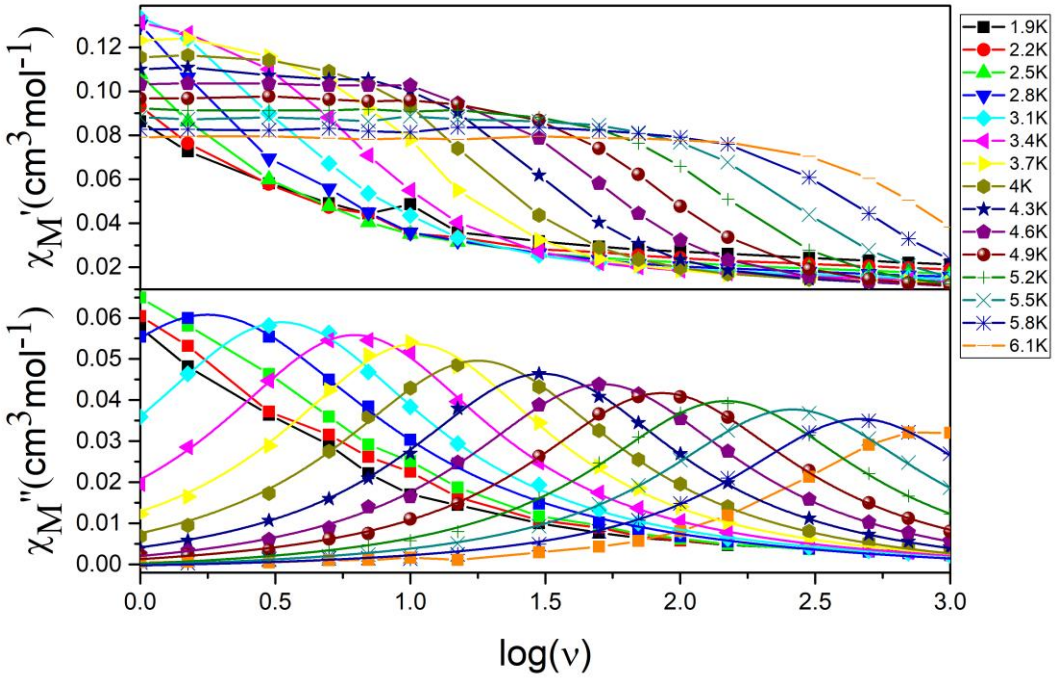


Figure 12S. Frequency dependence of the in-phase and out-of-phase signals of compound (**3**) under 1000 G dc field.

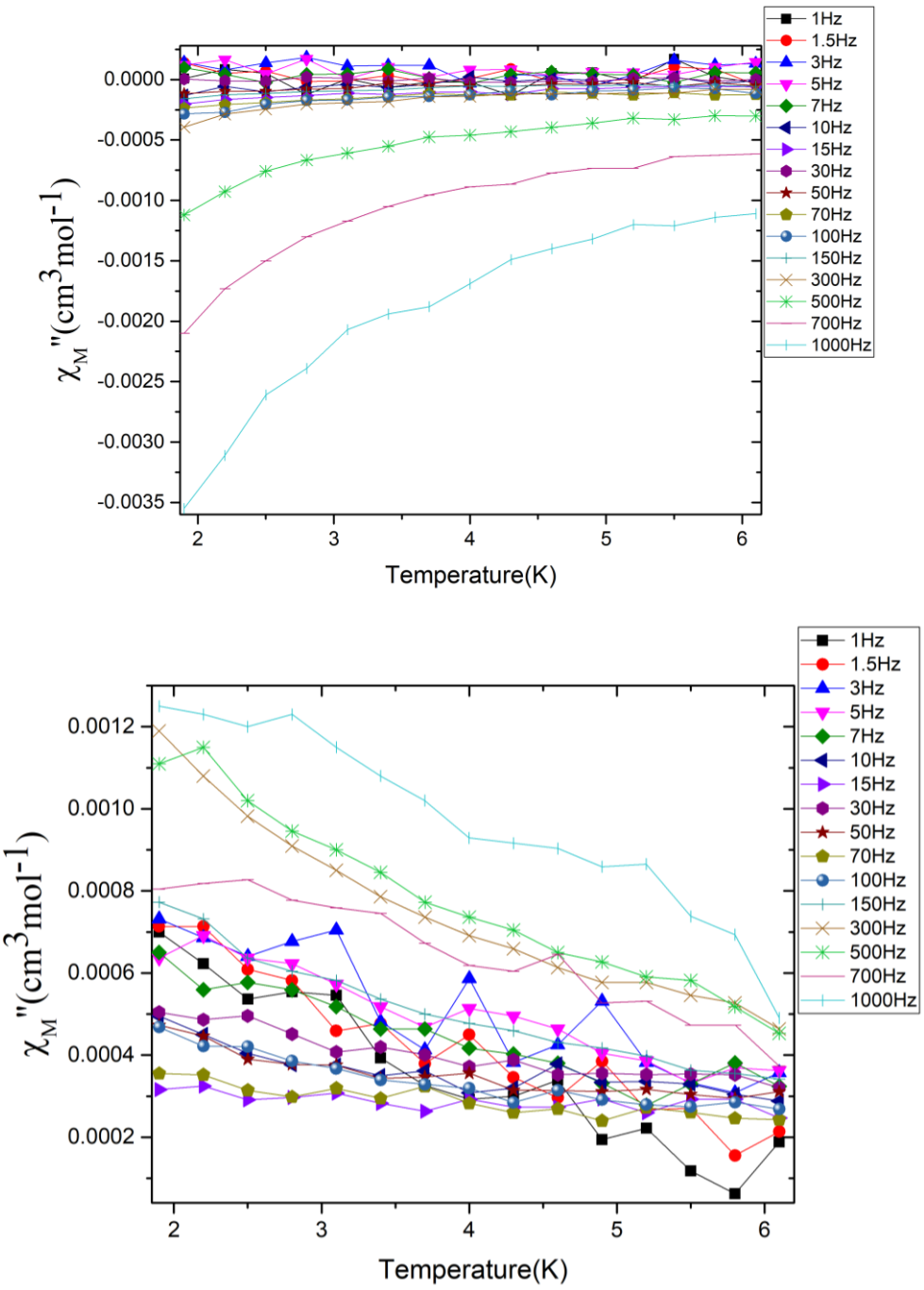


Figure 13S. Temperature dependence of the out-of-phase signals of compound (**2**) and (**3**) under 0 G dc field