Slow magnetic relaxation in mononuclear seven-coordinate cobalt(II) complexes with easy plane anisotropy

Lei Chen,[a] Shu-Yang Chen,[a] Yi-Chen Sun,[b] Yu-Mei Guo,[b] Lu Yu,[c] Xue-Tai Chen,[a] Zhenxing Wang,[b] Z. W. Ouyang,[b] You Song,[a] and Zi-Ling Xue[d]*

[a]State Key Laboratory of Coordination Chemistry, Nanjing National Laboratory of Microstructures, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China. E-mail: xtchen@netra.nju.edu.cn; Fax: +86 25 83314502

[b]Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan 430074, China

[c]High Magnetic Field Laboratory, Hefei Institutes of Physical Science, Chinese Academy of Sciences, Hefei 230031, China

[d]Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37996, USA.

Electronic Supplementary Information

Table S1. Summary of crystal data and refinement for **1** and **2**.

	1	**2**
Molecular formula	$C_{27}H_{39}CoN_5O_6$	$C_{27}H_{21}CoN_5O_6$
CCDC no	1033355	1033356
Formula weight	588.56	570.42
Temperature / K	296	296
Wavelength / Å	0.71073	0.71073
crystal system	Monoclinic	Monoclinic
Space group	C2/c	P2(1)/n
a / Å	21.205(3)	11.8781(10)
b / Å	13.3419(18)	10.8093(9)
c / Å	22.253(3)	20.5482(18)
a / deg	90	90
β / deg	95.851(3)	102.7700(10)
γ / deg	90	90
V / Å^3	6263.0(14)	2573.0(4)
Z	8	4
D_{calc}, g/cm^3	1.248	1.473
μ / mm^{-1}	0.592	0.719
F (000)	2488	1172
Goodness-of-fit on F^2	1.321	1.109
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0774 wR2 =0.2268	R1 = 0.0429 wR2 = 0.1164
R indices (all data)	R1 = 0.1114 wR2 = 0.2492	R1 = 0.0557 wR2 = 0.1245

Table S2. The parameters obtained by fitting Cole-Cole plot under 1.0 KOe for **1**.

T (K)	χ_S	χ_T	τ	α
1.8	0.06935	0.94960	0.00538	0.27340
2.0	0.06784	0.85145	0.00396	0.25889
2.2	0.06816	0.77479	0.00304	0.24060
2.4	0.06929	0.71070	0.00239	0.21861
2.6	0.07147	0.65641	0.00191	0.19338
2.8	0.07284	0.60999	0.00155	0.17000
3.0	0.07181	0.57028	0.00125	0.15226
3.2	0.07202	0.53647	0.00102	0.13131
3.4	0.07075	0.50599	0.00082	0.11190
3.6	0.07250	0.47686	0.00066	0.08460
3.8	0.07202	0.45277	0.00053	0.06706
4.0	0.06969	0.43260	0.00042	0.05855
4.2	0.06820	0.41212	0.00033	0.04570
4.4	0.06563	0.39473	0.00026	0.03959
4.6	0.06190	0.37781	0.00021	0.03349
4.8	0.05504	0.36312	0.00016	0.03514
5.0	0.04416	0.34947	0.00012	0.03977
5.2	0.01754	0.33720	0.00009	0.05415

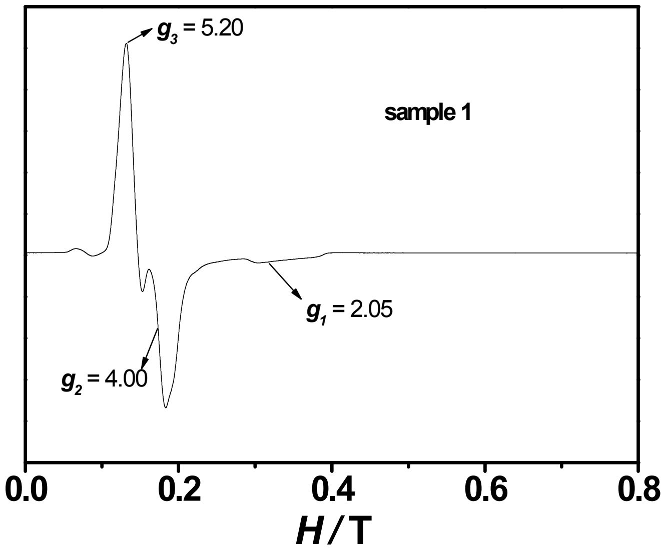

Figure S1. X-band EPR spectrum (υ = 9.4 GHz) of a polycrystalline sample of **1** at 4.2 K.

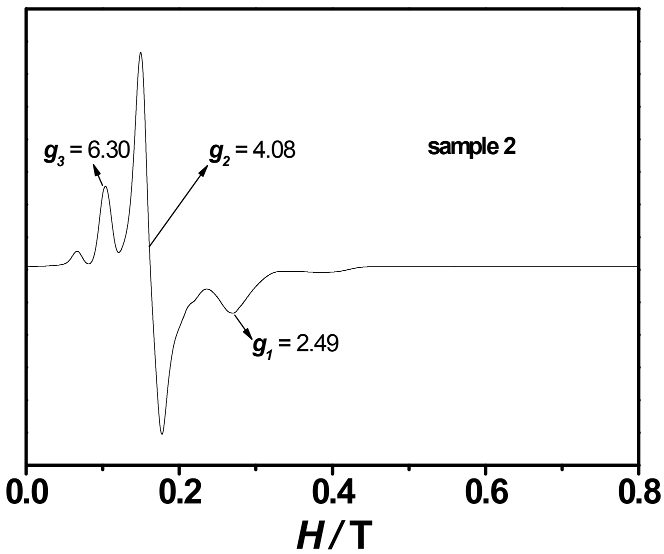

Figure S2. X-band EPR spectrum (υ = 9.4 GHz) of a polycrystalline sample of **2** at 4.2 K.

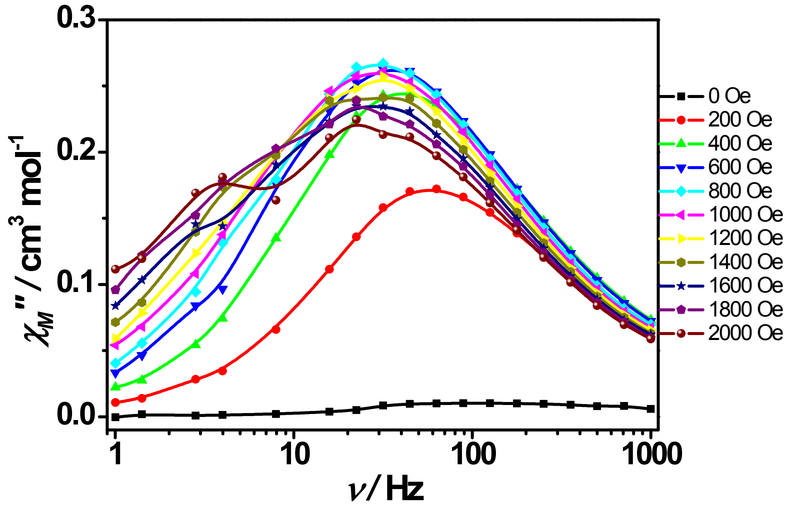

Figure S3. Frequency dependence of the out-of-phase (χ_M'') ac susceptibility at 1.8 K under the applied dc fields from 0 to 2000 Oe for complex **1**. The solid lines are for eye guide.

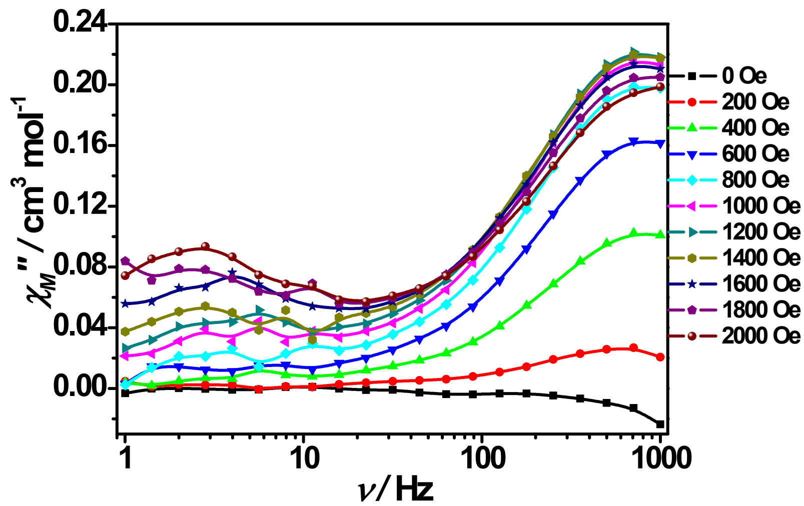

Figure S4. Frequency dependence of the out-of-phase (χ_M'') ac susceptibility at 1.8 K under the applied dc fields from 0 to 2000 Oe for complex **2**. The solid lines are for eye guide.

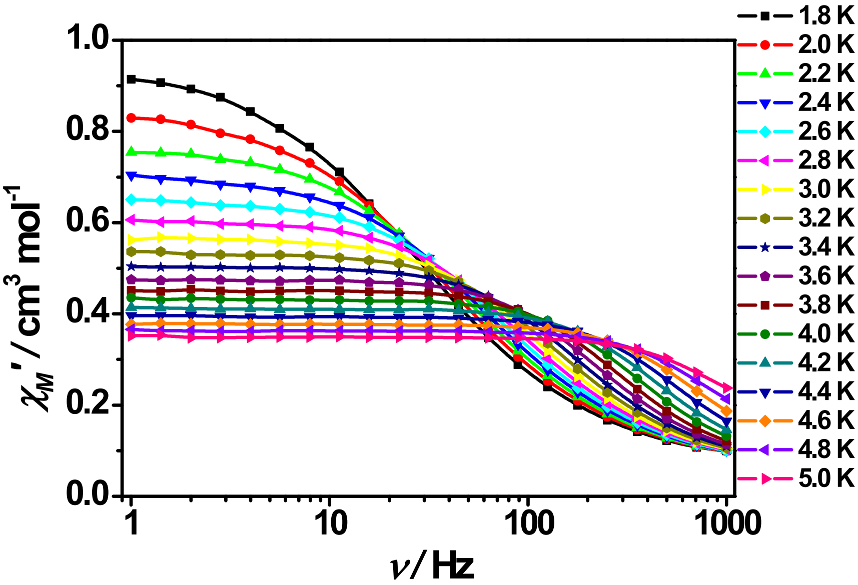

Figure S5. Frequency dependence of in-phase ac susceptibility from 1 to 1000 Hz under 1.0 KOe dc field for complex **1**. The solid lines are for eye guide.

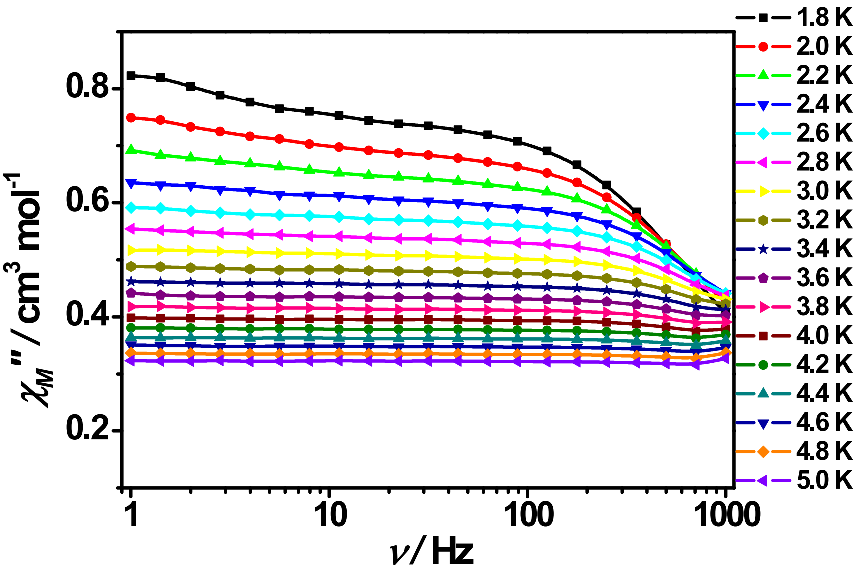

Figure S6. Frequency dependence of in-phase ac susceptibility from 1 to 1000 Hz under 1.2 KOe dc field for complex **2**. The solid lines are for eye guide.

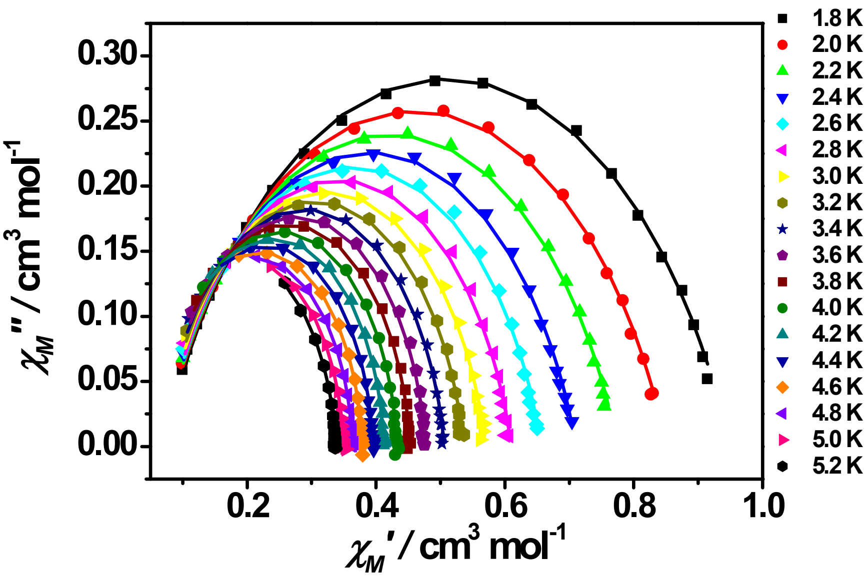

Figure S7. Cole-Cole plots obtained from the ac susceptibility data under 1.0 KOe dc field in the temperature range of 1.8-5.2 K for complex **1**. Solid lines represent best fits to a generalized Debye model.

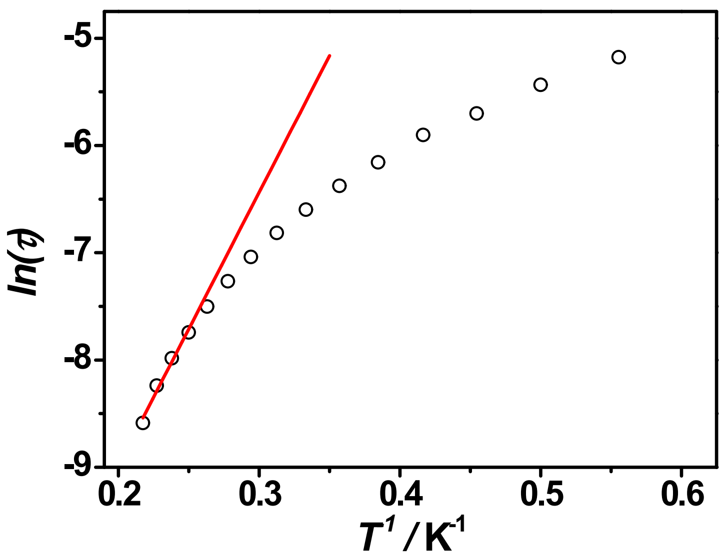

Figure S8. Relaxation time of the magnetization *ln(τ)* vs T^{-1} plot under the 1.0 KOe applied field for **1**.

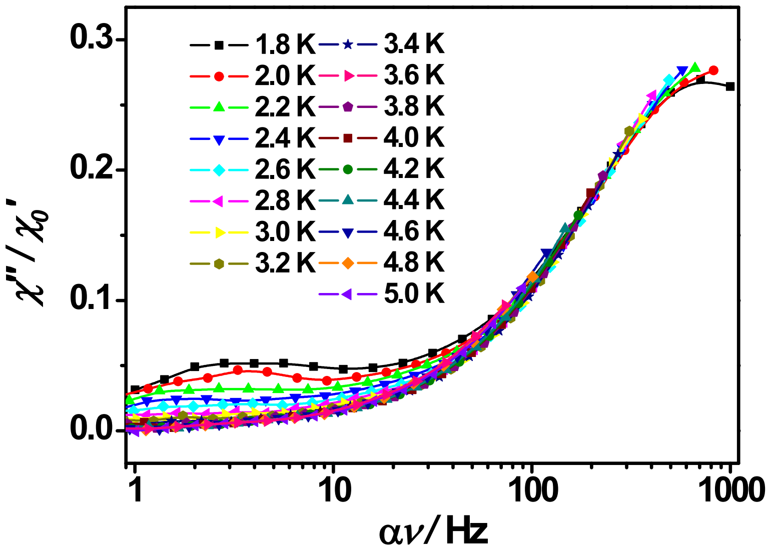

Figure S9. Scaled frequency dependence of χ_M'' normalized by the zero-frequency in-phase susceptibility (take experimentally at 1 Hz) between 1.8 and 5 K (with H = 1.2 KOe) for **2**. α is the scaling parameter equals to 1 for the data at 1.8 K.

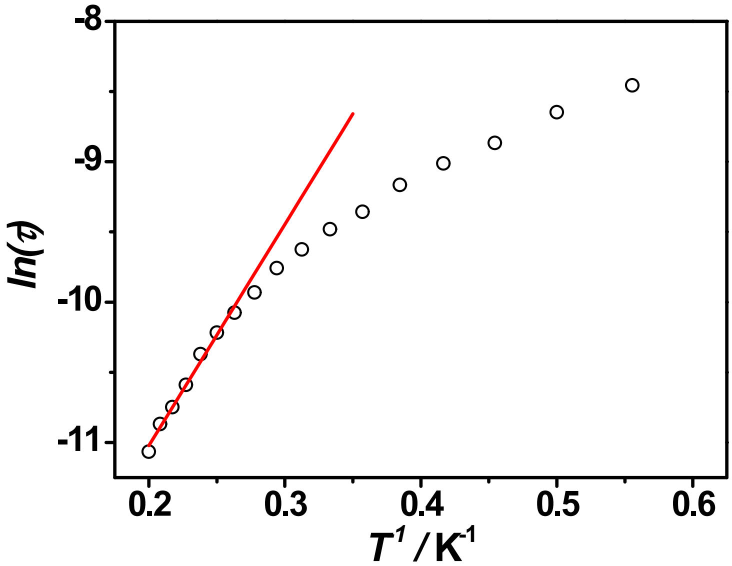

Figure S10. Relaxation time of the magnetization *ln(τ)* vs T^{-1} plot under the 1.2 KOe applied field for **2**.

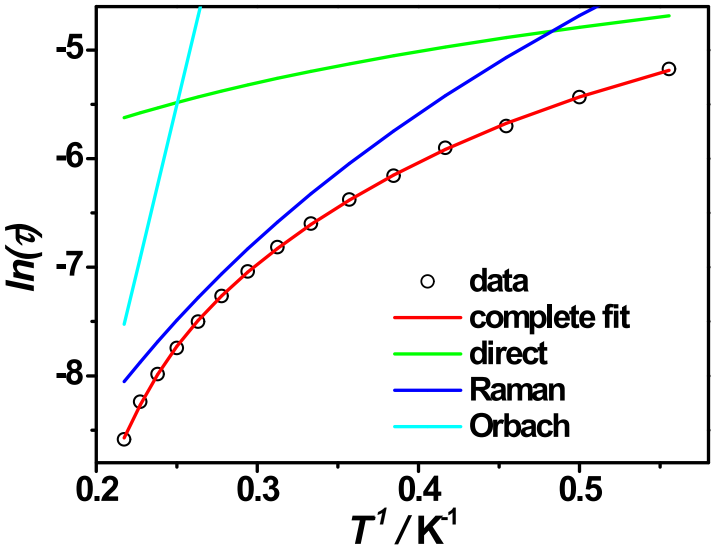

Figure S11. Temperature dependence of the magnetization relaxation rates of **1** under the applied dc field of 1.0 KOe. The solid red lines represent the best fit by using eqn (1). The other solid lines represent data fits using individual direct (cyan), Orbach (pink), and Raman (blue) process, respectively.

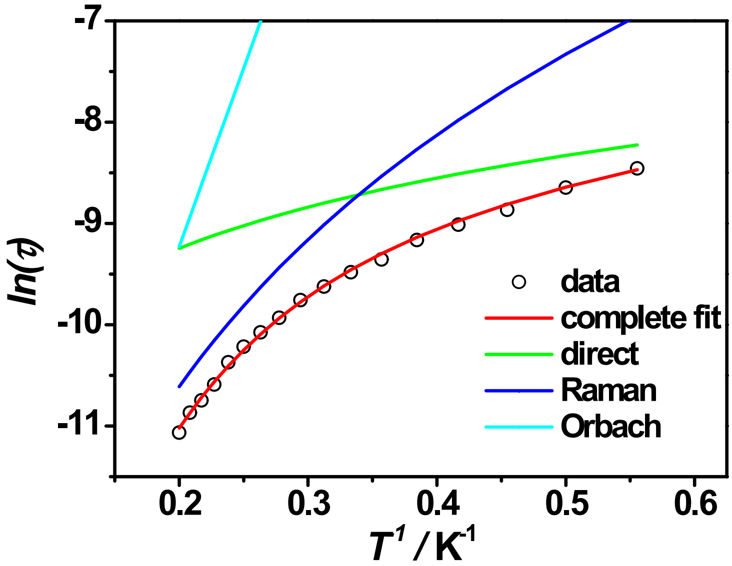

Figure S12. Temperature dependence of the magnetization relaxation rates of **2** under the applied dc field of 1.2 KOe. The solid red lines represent the best fit by using eqn (1). The other solid lines represent data fits using individual direct (cyan), Orbach (pink), and Raman (blue) process, respectively.

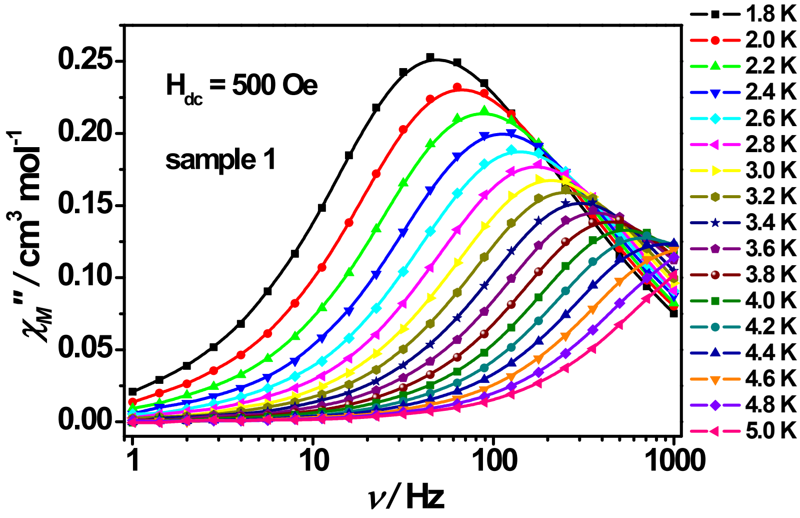

Figure S13. Frequency dependence of the out-of-phase ac magnetic susceptibility from 1 to 1000 Hz under 500 Oe dc field on pure polycrystalline samples of **1**. The solid lines are for eye guide.

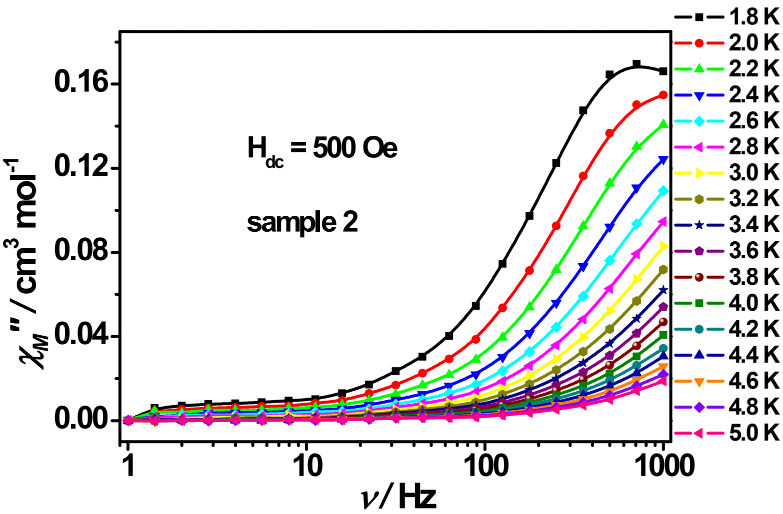

Figure S14. Frequency dependence of the out-of-phase ac magnetic susceptibility from 1 to 1000 Hz under 500 Oe dc field on pure polycrystalline samples of **2** (bottom). The solid lines are for eye guide.

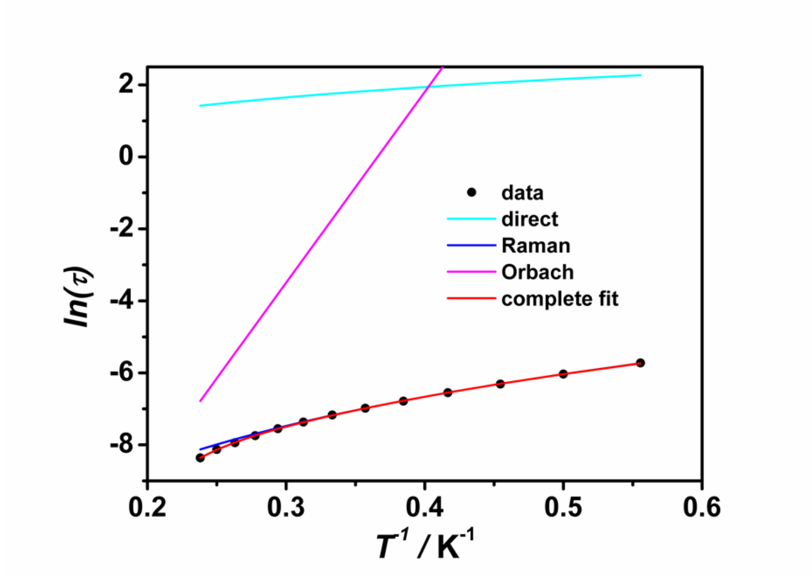

Figure S15. Temperature dependence of the magnetization relaxation rates of **1** under the applied dc field of 0.5 KOe. The solid red lines represent the best fit by using eqn (1). The other solid lines represent data fits using individual direct (cyan), Orbach (pink), and Raman (blue) process, respectively.

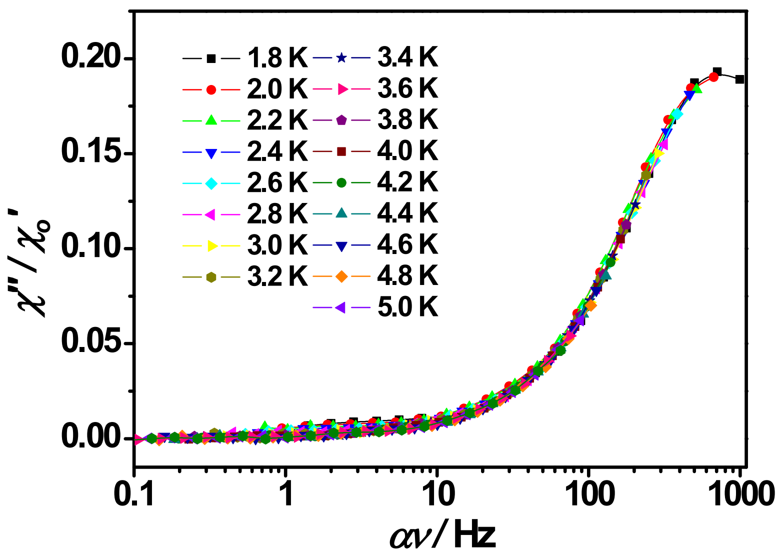

Figure S16. Scaled frequency dependence of χ_M'' normalized by the zero-frequency in-phase susceptibility (take experimentally at 1.41 Hz) between 1.8 and 5 K (with H = 0.5 KOe) for **2**. α is the scaling parameter equals to 1 for the data at 1.8 K.

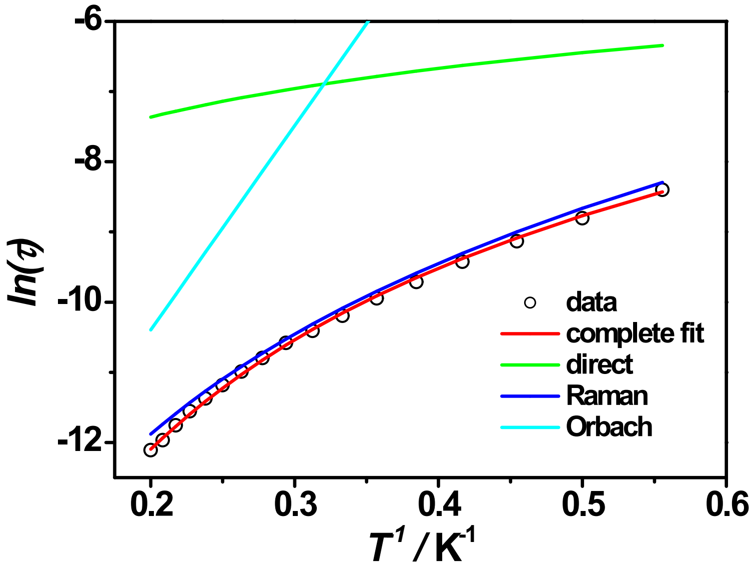

Figure S17. Temperature dependence of the magnetization relaxation rates of **2** under the applied dc field of 0.5 KOe. The solid red lines represent the best fit by using eqn (1). The other solid lines represent data fits using individual direct (cyan), Orbach (pink), and Raman (blue) process, respectively.

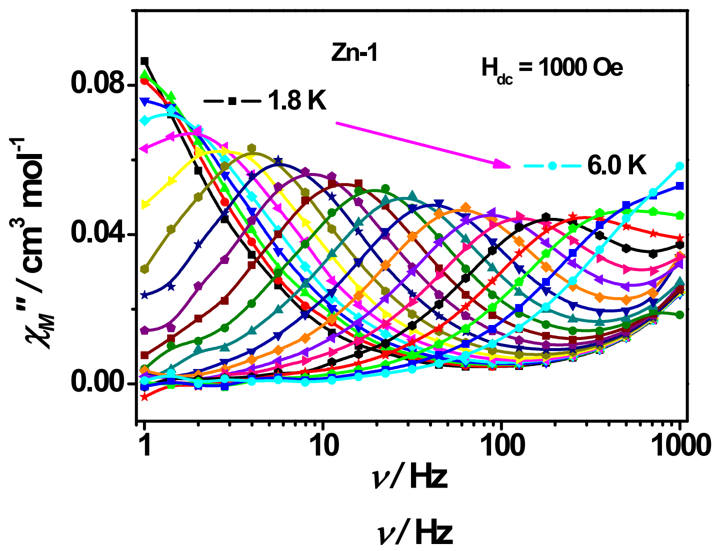

Figure S18. Frequency dependence of the out-of-phase ac magnetic susceptibility from 1 to 1000 Hz under 1.0 KOe dc field on pure polycrystalline samples of **Zn-1**. The solid lines are for eye guide.

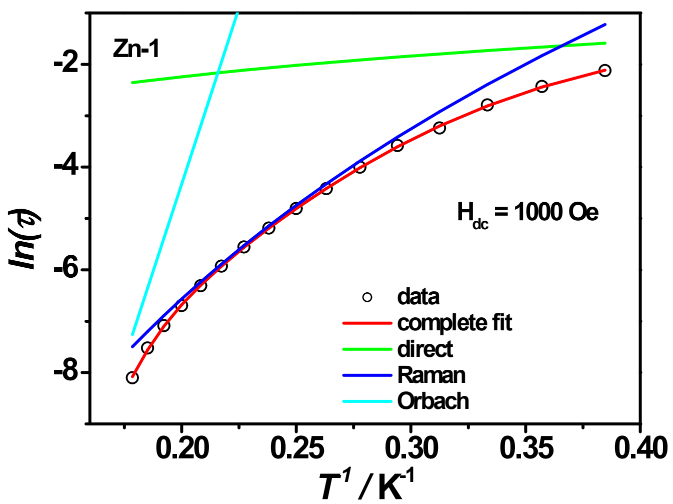

Figure S19. Temperature dependence of the magnetization relaxation rates of **Zn-1** under the applied dc field of 1.0 KOe. The solid red lines represent the best fit by using eqn (1). The other solid lines represent data fits using individual direct (cyan), Orbach (pink), and Raman (blue) process, respectively.