

Structure and magnetism of a tetrahedral uranium(III) β -diketiminato complex

Supporting Information -

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Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x

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1. NMR spectra

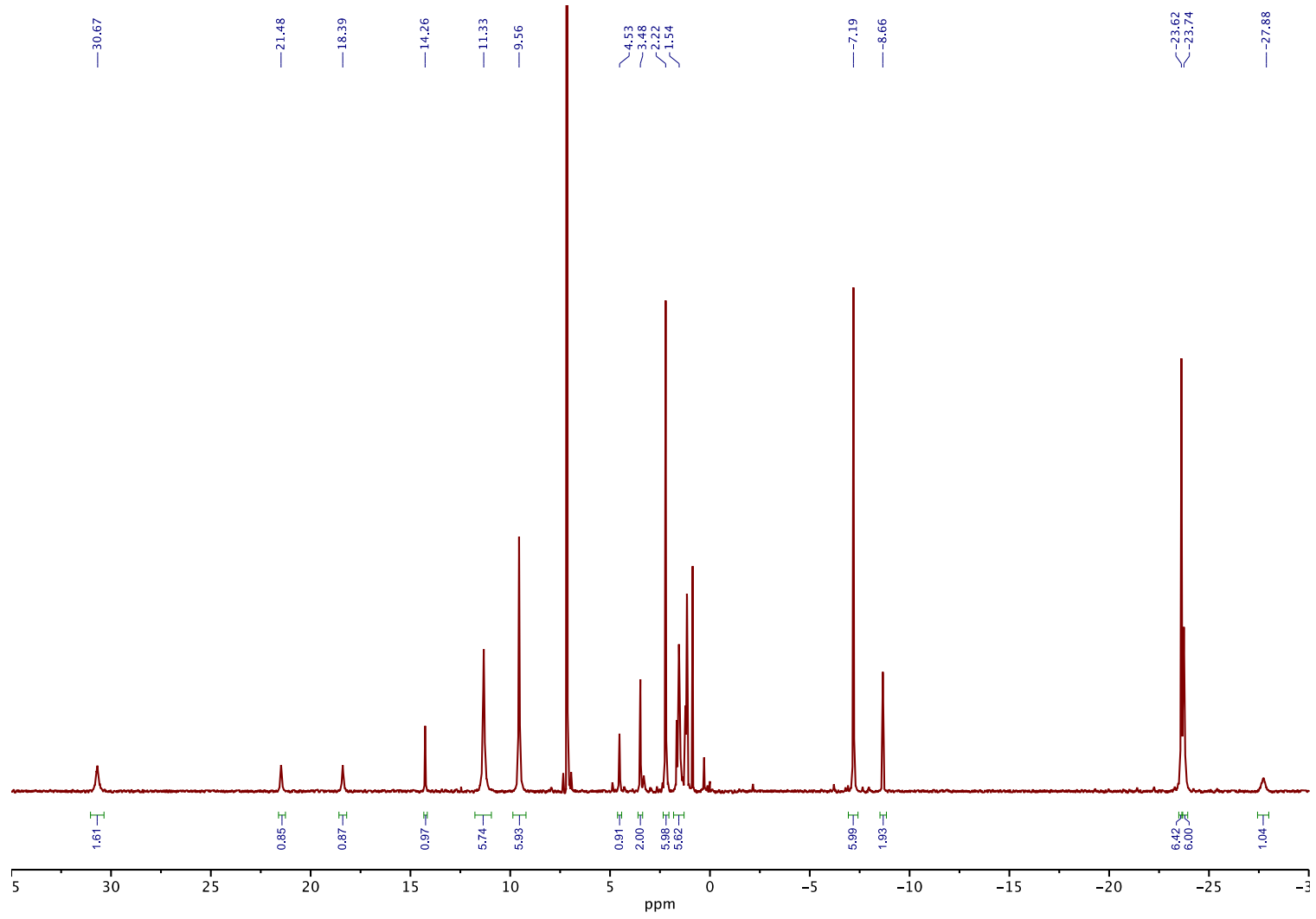
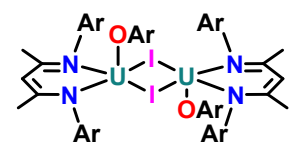


Figure S1: ¹H NMR spectrum of complex 2 in C₆D₆

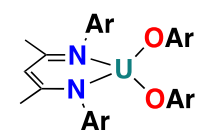
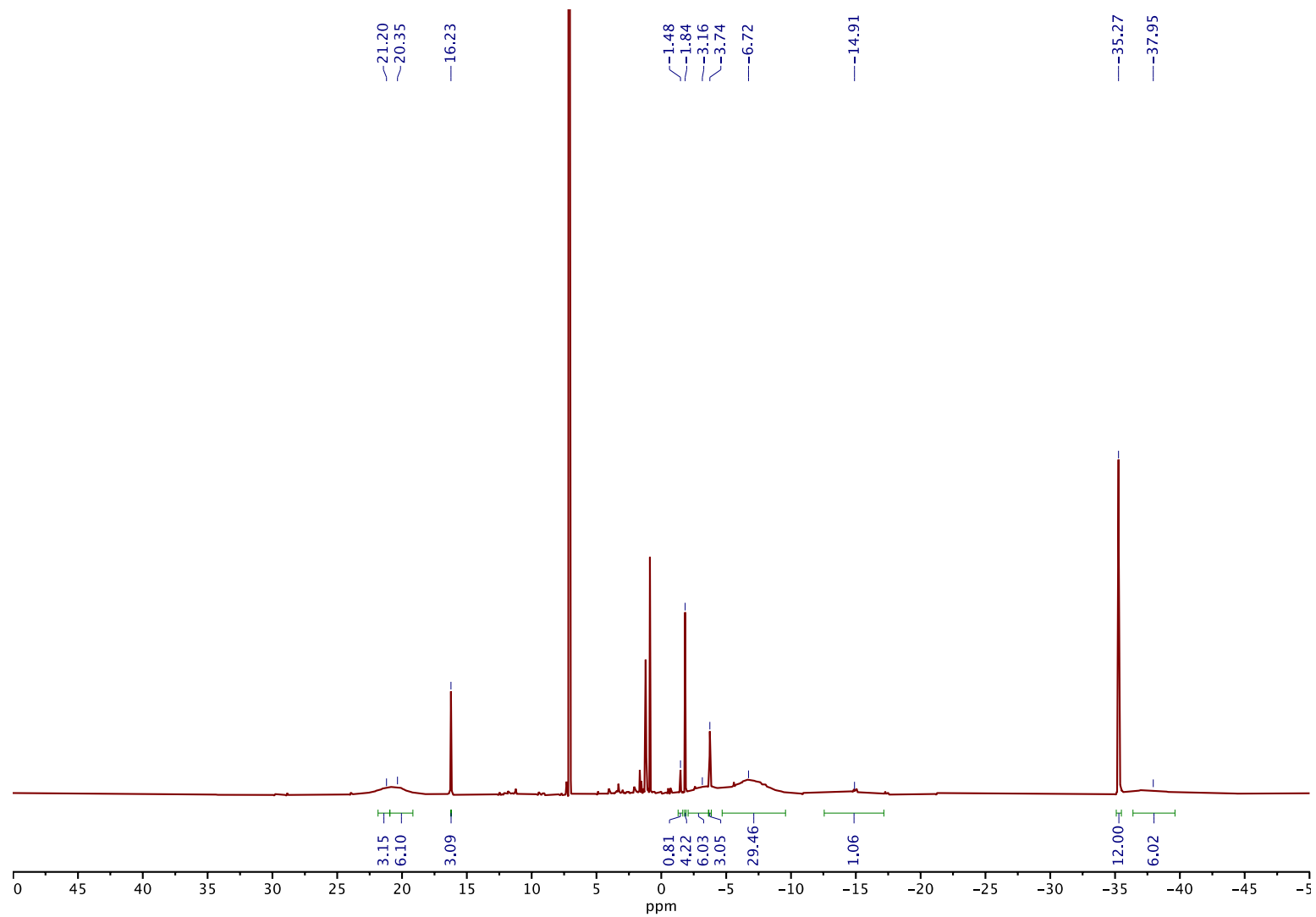


Figure S2: ^1H NMR spectrum of complex **3** in C_6D_6

2. Crystallographic details

Table S1: Crystallographic data for complexes **2** and **3**

	2	3
Chemical formula	C ₈₅ H ₁₂₃ N ₄ O ₂ U ₂ I ₂	C ₅₃ H ₇₅ N ₂ O ₂ U ₁
M_r	1962.736	1010.18
Crystal system	Triclinic	Monoclinic
Space group	P-1	P2 ₁ /c
a (Å)	12.2023(3)	20.5520(7)
b (Å)	16.5876(6)	11.9252(4)
c (Å)	22.5734(8)	21.1347(7)
α (°)	75.346(1)	90
β (°)	80.632(1)	112.708(2)
γ (°)	69.918(1)	90
V (Å ³)	4137.1(2)	4778.3(3)
Z	2	4
Density (g·cm ⁻³)	1.576	1.404
F(000)	1934	2060
λ (Å)	0.71073	0.71073
μ (mm ⁻¹)	4.702	3.437
Crystal size (mm)	0.12x0.03x0.02	0.23x0.08x0.07
Meas. Refl.	11678	87639
Indep. Refl.	15102	8786
Obsvd. [$I > 2\sigma(I)$]	11678	6896
R_{int}	0.0653	0.0616
R_1 [$I > 2\sigma(I)$]	0.0577	0.0298
$wR_2(F^2)$ (all data)	0.1411	0.0687
Goof	1.018	1.036
$\Delta\rho_{max}$ (e·Å ⁻³)	6.415	2.548
$\Delta\rho_{min}$ (e·Å ⁻³)	-0.974	-1.061
CCDC	1991563	1991562

Table S2: Selected bond lengths and angles

	2	3
U1 – I1	3.267(1)	-
U1 – I1A	3.227(1)	-
U1A – I1	3.232(1)	-
U1A – I1A	3.285(1)	-
U1 – U1A	5.087(1)	-
U1 – N1	2.380(8)	2.386(3)
U1 – N2	2.450(7)	2.400(3)
U1 – O1	2.133(6)	2.181(2)
U1 – O2	-	2.162(2)
C4 – C1	1.510(13)	1.517(5)
C1 – C2	1.401(13)	1.355(6)
C2 – C3	1.449(13)	1.426(5)
C3 – C5	1.473(12)	1.497(5)
C1 – N1	1.328(12)	1.346(5)
C3 – N2	1.289(11)	1.332(5)
U1 – O1 – C30	175.2(6)	152.8(2)
U1 – O2 – C4212	-	168.2(2)
N1 – U1 – N2	72.5(2)	77.4(1)
τ_5/τ_4'	0.43/-	-/0.85

3. SQUID magnetometry

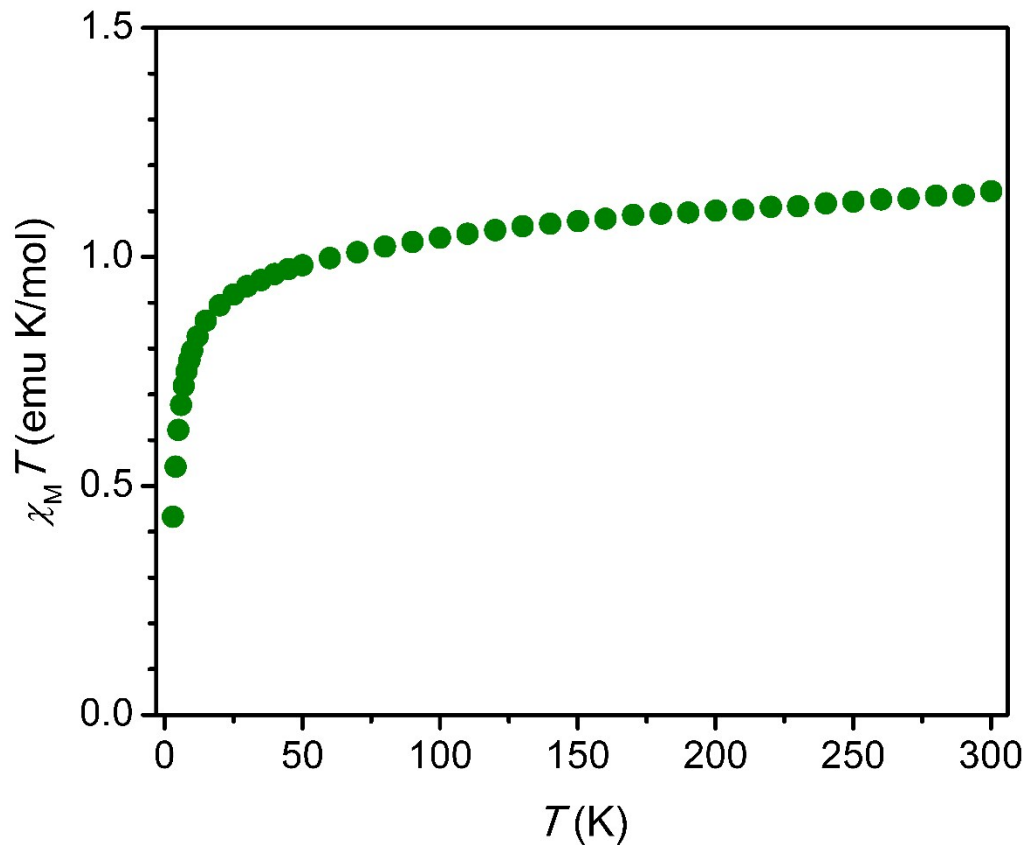


Figure S3: Dc magnetic susceptibility measurements of **3** using a 2-field correction from data collected at 5 kOe and 40 kOe.

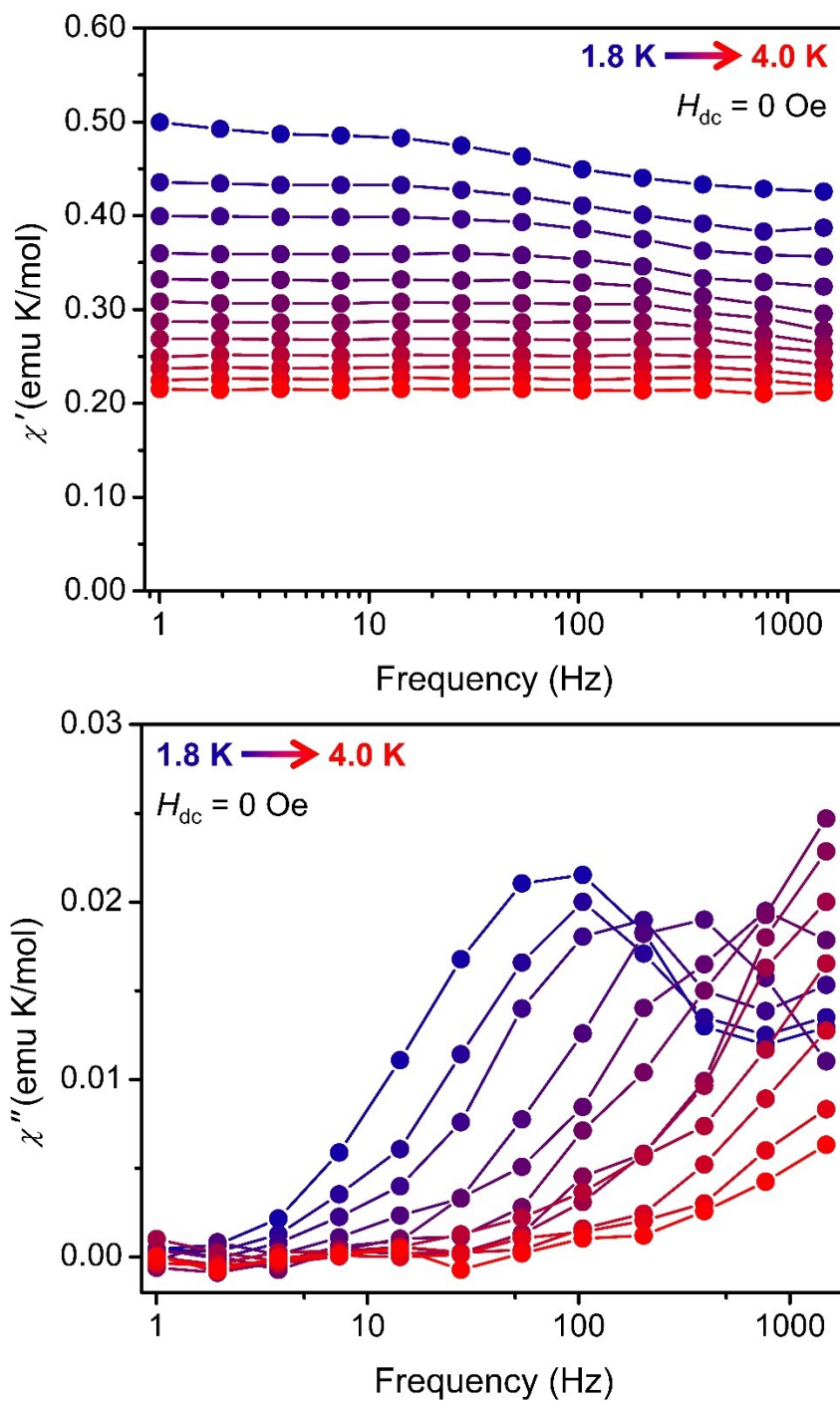


Figure S4: In-phase (χ'_M , top) and out-of-phase (χ''_M , bottom) components of the ac magnetic susceptibility for **3** under zero applied dc field at frequencies ranging from 1–1500 Hz and temperatures from 1.8–4 K (0.2 K steps). The colored lines are guides for the eye.

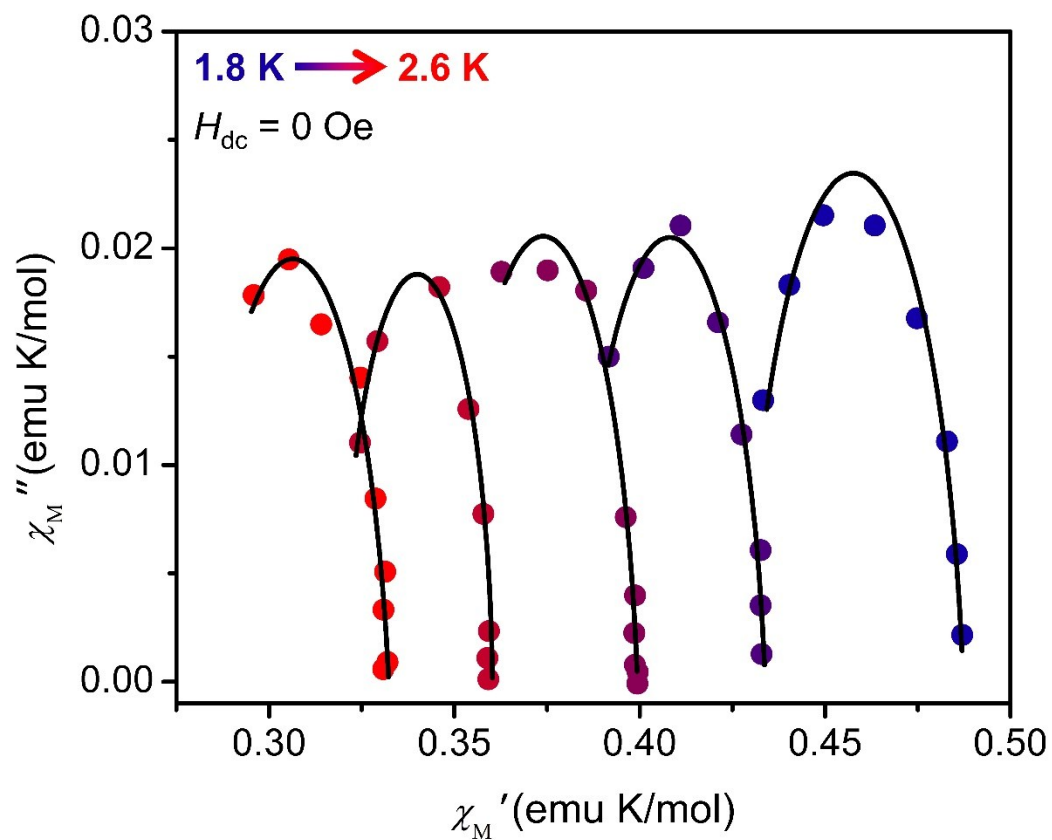


Figure S5: Cole-Cole plots for **3** from 1.8–2.6 K (0.2 K steps) under zero applied dc field. The black lines represent fits to the data using a generalized Debye model, which were used to extract the value of the magnetic relaxation time, τ , at each temperature.

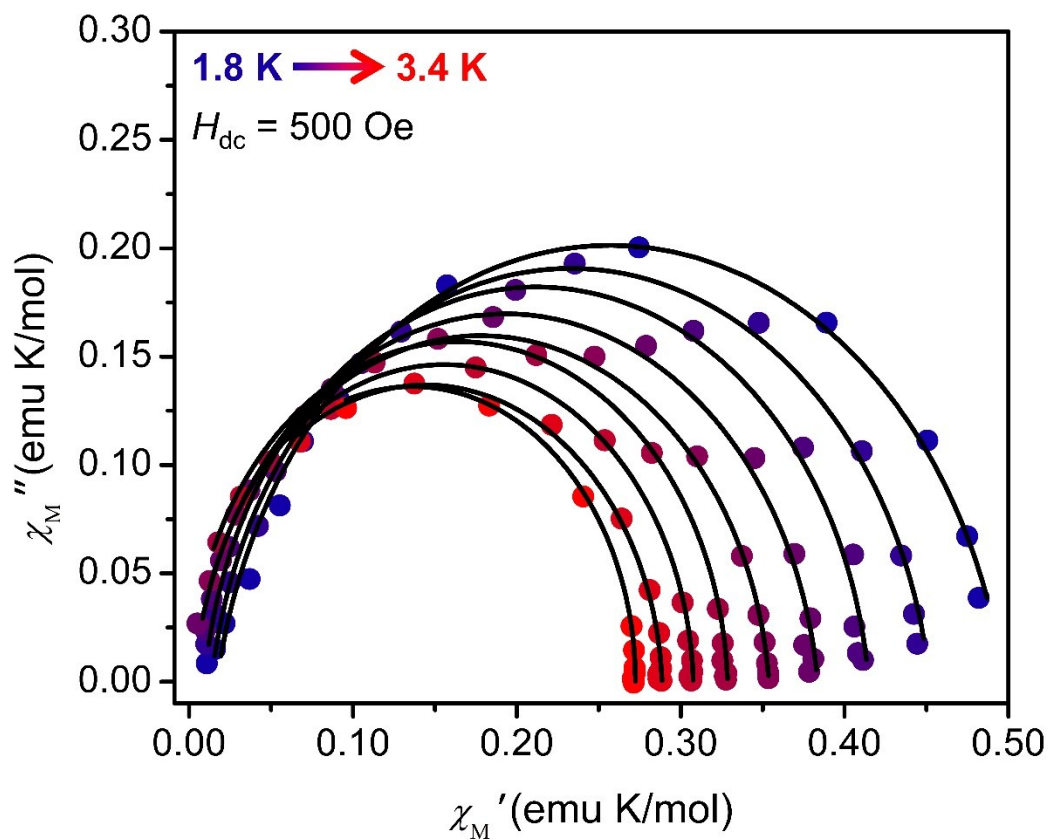


Figure S6: Cole-Cole plots for **3** from 1.8–3.4 K (0.2 K steps) under an applied dc field of 500 Oe. The black lines represent fits to the data using a generalized Debye model, which were used to extract the value of the magnetic relaxation time, τ , at each temperature.

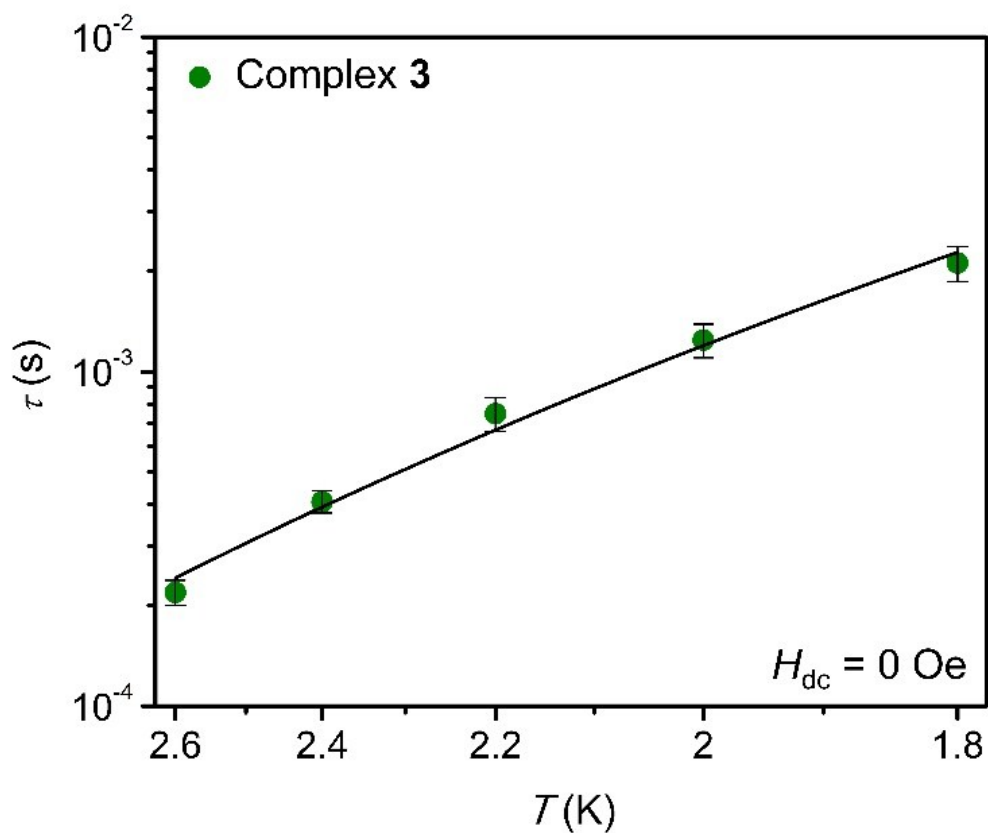


Figure S7: Plot of magnetic relaxation time (log scale) versus temperature (inverse scale) for **3** for data collected under zero applied dc field. The black line represents a fit to the data using the equation $\tau^{-1} = CT^n$, where C and n are free variables that describe Raman relaxation. Values of $C = 12(3) \text{ s}^{-1} \text{ K}^{-n}$ and $n = 6.1(2)$ were extracted from this fit.