

Supporting Information

Slow Magnetic Relaxation in Neutral 0D and 1D Assemblies of a Mn(III) Schiff Base Complex and Heptacyanorhenate(IV)

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Table S1. SCXRD Experimental details

	1	2
Chemical formula	C ₃₁ H ₃₄ MnN ₁₁ O ₂ Re·7H ₂ O	C ₃₁ H ₃₄ MnN ₁₁ O ₂ Re·3H ₂ O
<i>M_w</i>	959.93	887.88
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	150	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.5292 (11) 17.9419 (14) 19.0885 (17)	12.3733(6) 22.9922 (11) 12.7619 (6)
<i>α</i> , <i>β</i> , <i>γ</i> (°)	90 95.031 (3) 90	90 93.070 (2) 90
<i>V</i> (Å ³)	3933.4 (6)	3625.4 (3)
<i>Z</i>	4	4
Radiation type	Mo <i>Kα</i> , λ = 0.71073	Mo <i>Kα</i> , λ = 0.71073
μ (mm ⁻¹)	3.46	3.74
Crystal size (mm)	0.18 × 0.13 × 0.1	0.28 × 0.15 × 0.11
Diffractometer	Bruker Apex DUO	
<i>T_{min}</i> , <i>T_{max}</i>	0.607, 0.745	0.596, 0.745
N ^o of measured, independent observed [<i>I</i> > 2σ(<i>I</i>)] reflections	43075, 7545, 5967	53843, 6903, 6392
<i>R_{int}</i>	0.028	0.019
q values (°)	θ _{max} = 25.8, θ _{min} = 1.6	θ _{max} = 25.7, θ _{min} = 2.4
Range of <i>h</i> , <i>k</i> , <i>l</i>	-14 ≤ <i>h</i> ≤ 14 -21 ≤ <i>k</i> ≤ 21 -23 ≤ <i>l</i> ≤ 23	-15 ≤ <i>h</i> ≤ 15 -28 ≤ <i>k</i> ≤ 28 -15 ≤ <i>l</i> ≤ 15
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.040, 0.111, 1.07	0.040, 0.111, 1.07
No. of reflections, parameters, restraints	7545, 484, 0	6903, 455, 1
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
Weighting scheme	w=1/[σ ² (<i>F_o</i> ²)+(0.049 <i>P</i>) ² +19.910 <i>P</i>] where <i>P</i> = (<i>F_o</i> ² + 2 <i>F_c</i> ²)/3	w=1/[σ ² (<i>F_o</i> ²)+(0.015 <i>P</i>) ² +5.297 <i>P</i>] where <i>P</i> =(<i>F_o</i> ² +2 <i>F_c</i> ²)/3
Δρ _{max} , Δρ _{min} (e Å ⁻³)	3.88, -0.71	0.86, -0.53

Absorption corrections were applied with the use of the SADABS program [APEX2 (Version 2.0), SAINT (Version 8.18c), and SADABS (Version 2.11), Bruker Advanced X-ray Solutions, Bruker AXS Inc., Madison, Wisconsin, USA, 2000–2012.]. The crystal structure was solved by direct methods and refined by full-matrix least squares techniques with the use of the SHELXTL package [Sheldrick, G.M. (2015). *Acta Cryst.* C71, 3–8]. Computer programs: *APEX3* (Bruker-AXS, 2016), *SAINT* (Bruker-AXS, 2016), *SHELXT* 2014/5 (Sheldrick, 2014), *SHELXL* 2017/1 (Sheldrick, 2017). Atomic thermal displacement parameters for non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated corresponding to their geometrical conditions and refined using the riding model.

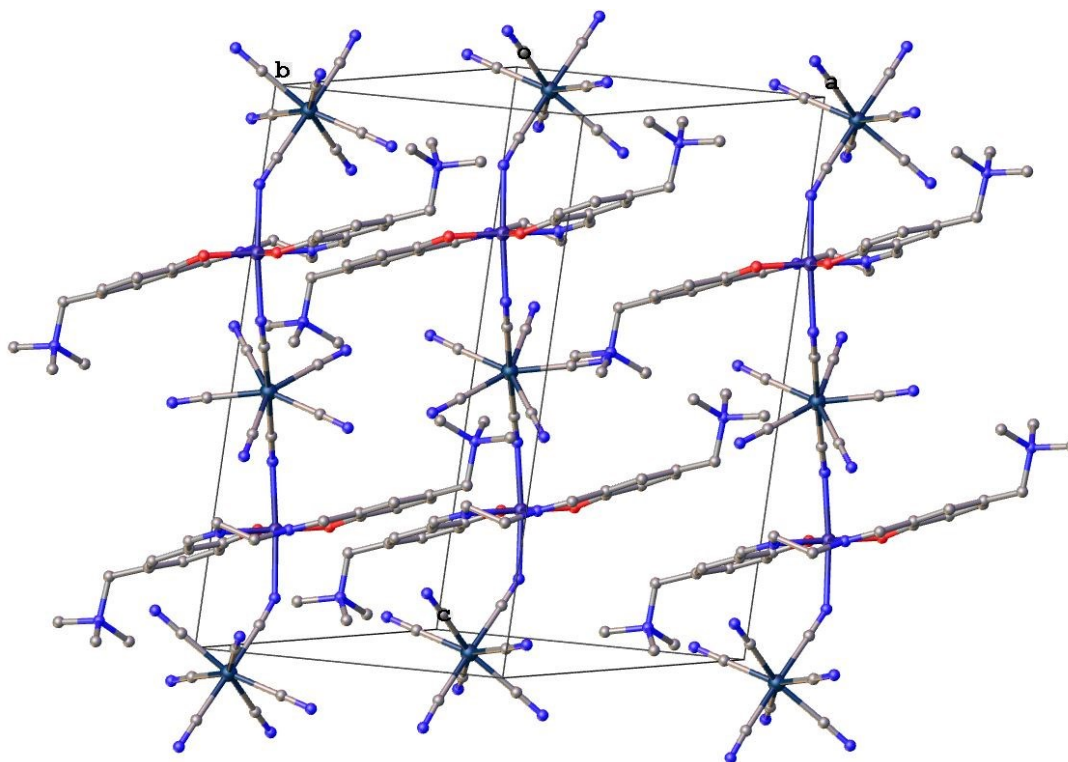


Figure S1. A view of chains packing in a crystal of **1** demonstrating a trans-location of the $[\text{Me}_3\text{N}^+\text{CH}_2]$ substituents relative to a SB^{2+} plane. Hydrogen atoms are omitted for clarity.

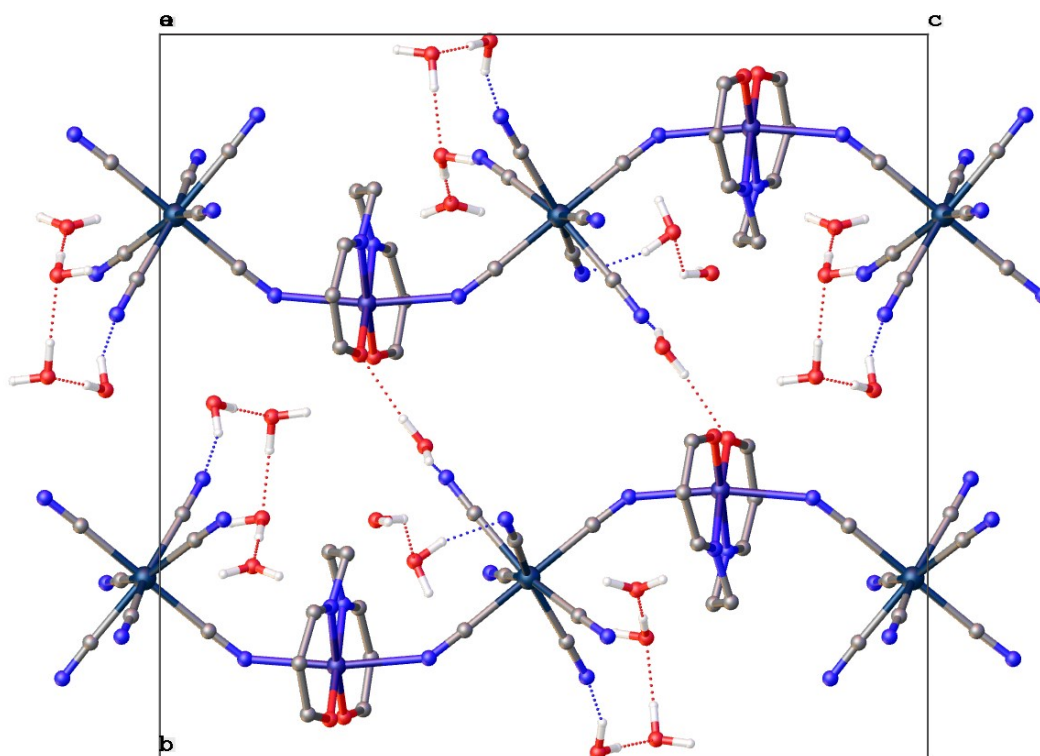


Figure S2. A layer formation in a crystal of **1**: H_2O molecules bind the fragments $[\text{Mn}^{\text{III}}(\text{SB}^{2+})]^{3+}$ and $[\text{Re}(\text{CN})_7]^{3-}$ belonging to the different chains. The layers are interconnecting by means of interstitial water molecules. The SB^{2+} -ligands are reduced for clarity.

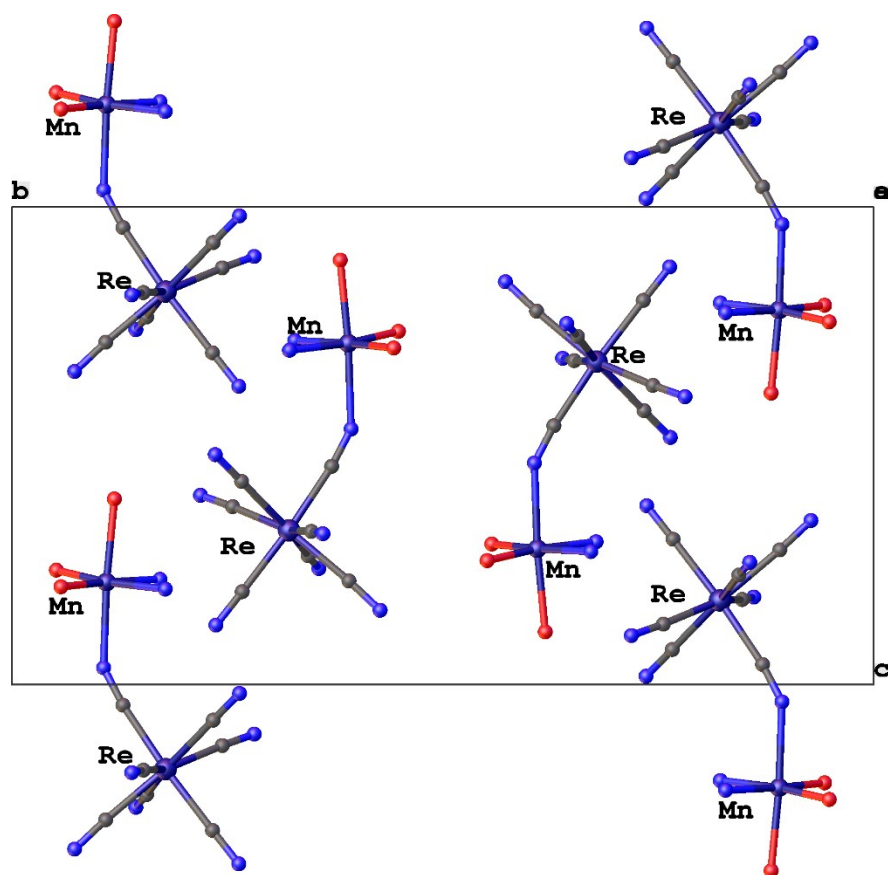


Figure S3. A view of dimers packing in a crystal of **2**. The SB^{2+} -ligands are reduced, and hydrogen atoms are omitted for clarity.

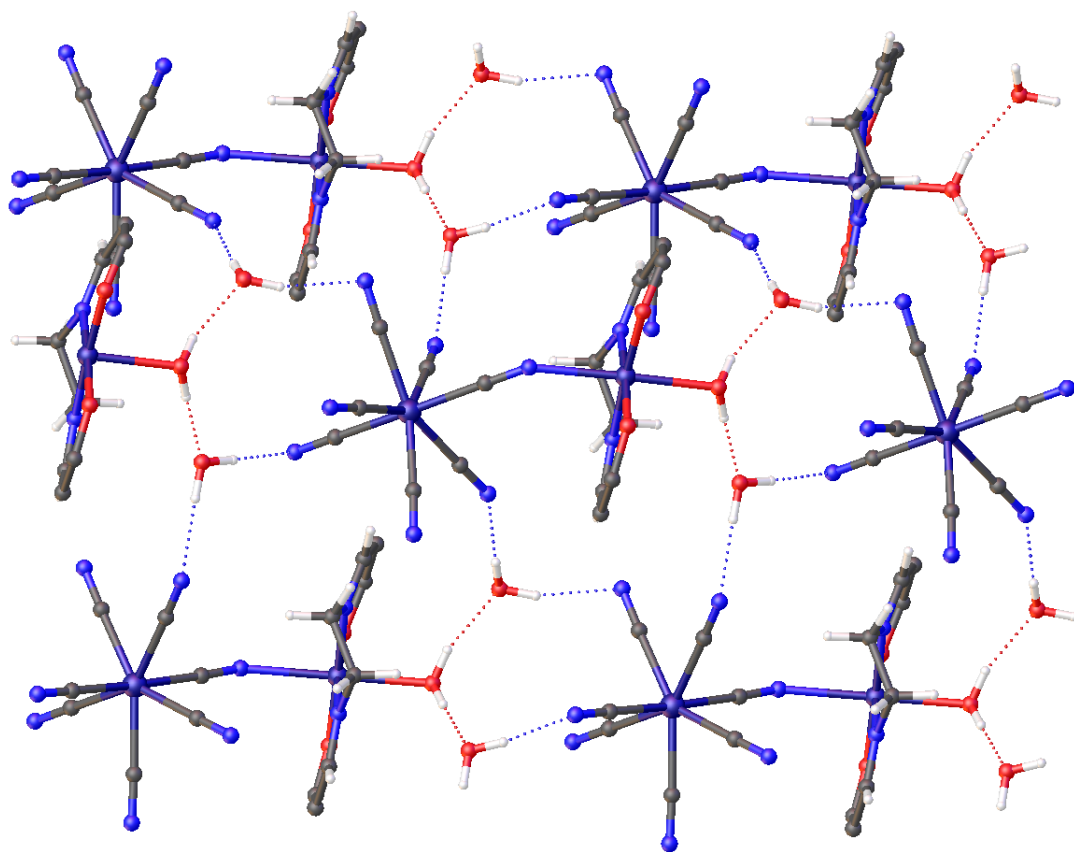
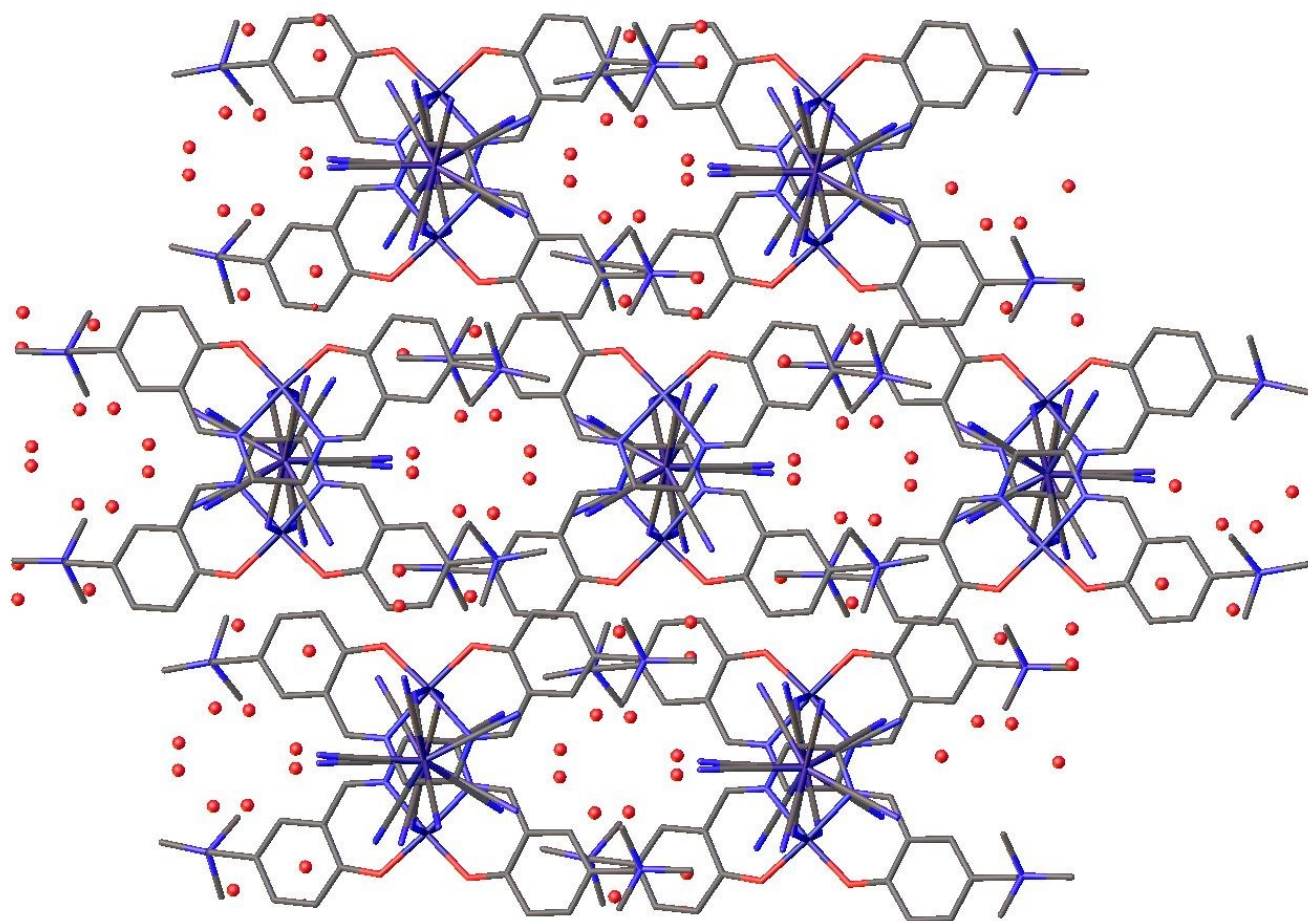
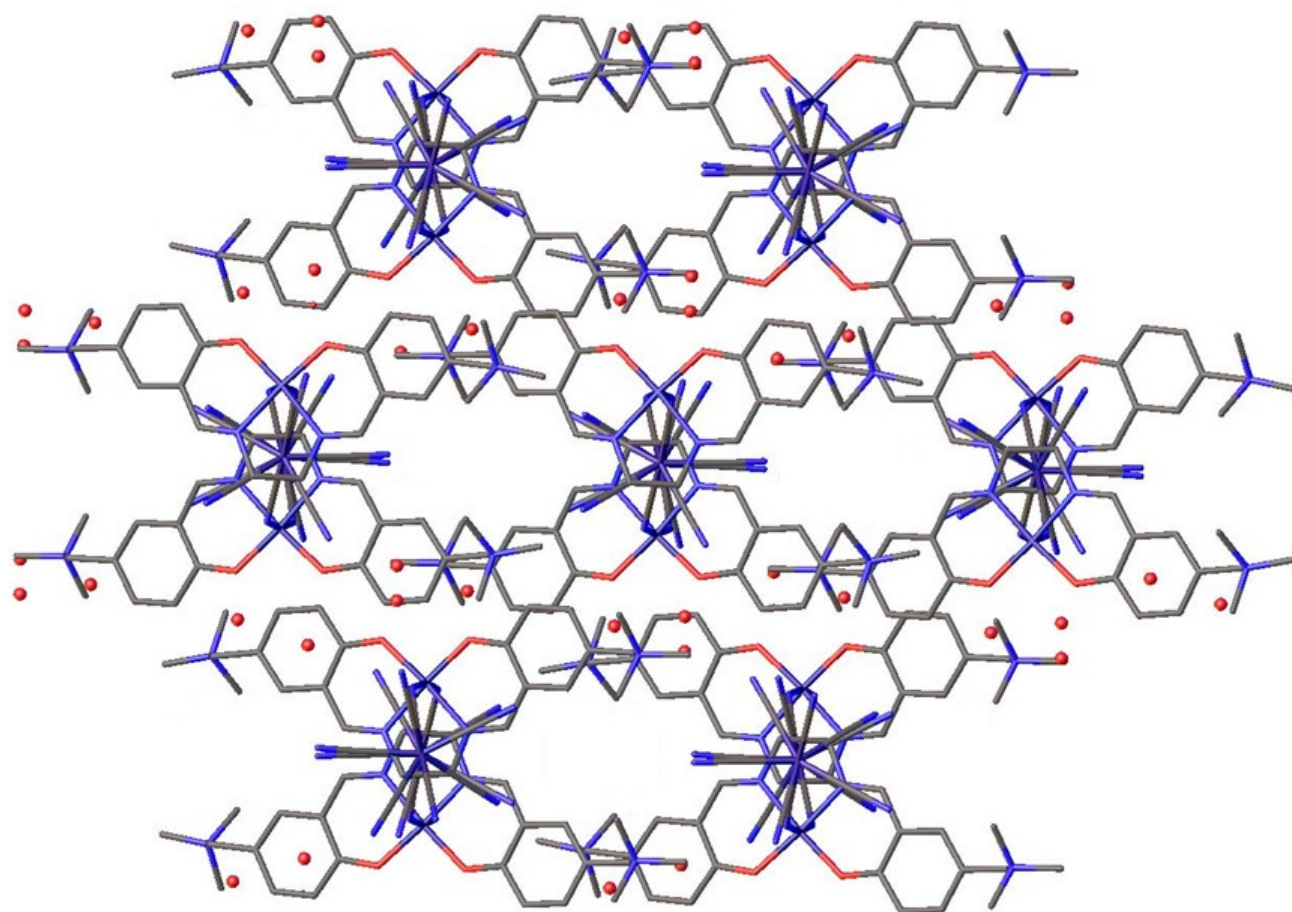


Figure S4. A layer formation in a crystal of **2**: H_2O molecules bind the fragments $[\text{Mn}^{\text{III}}(\text{SB}^{2+})]^{3+}$ and $[\text{Re}(\text{CN})_7]^{3-}$ belonging to the different chains. The layers are interconnecting by means of interstitial water molecules. The hydrogen atoms are partially omitted for clarity.



(a)



(b)

Figure S5. A view (in c-axis direction) of channels in a crystal of **1**: (a) filled by water molecules, (b) empty.

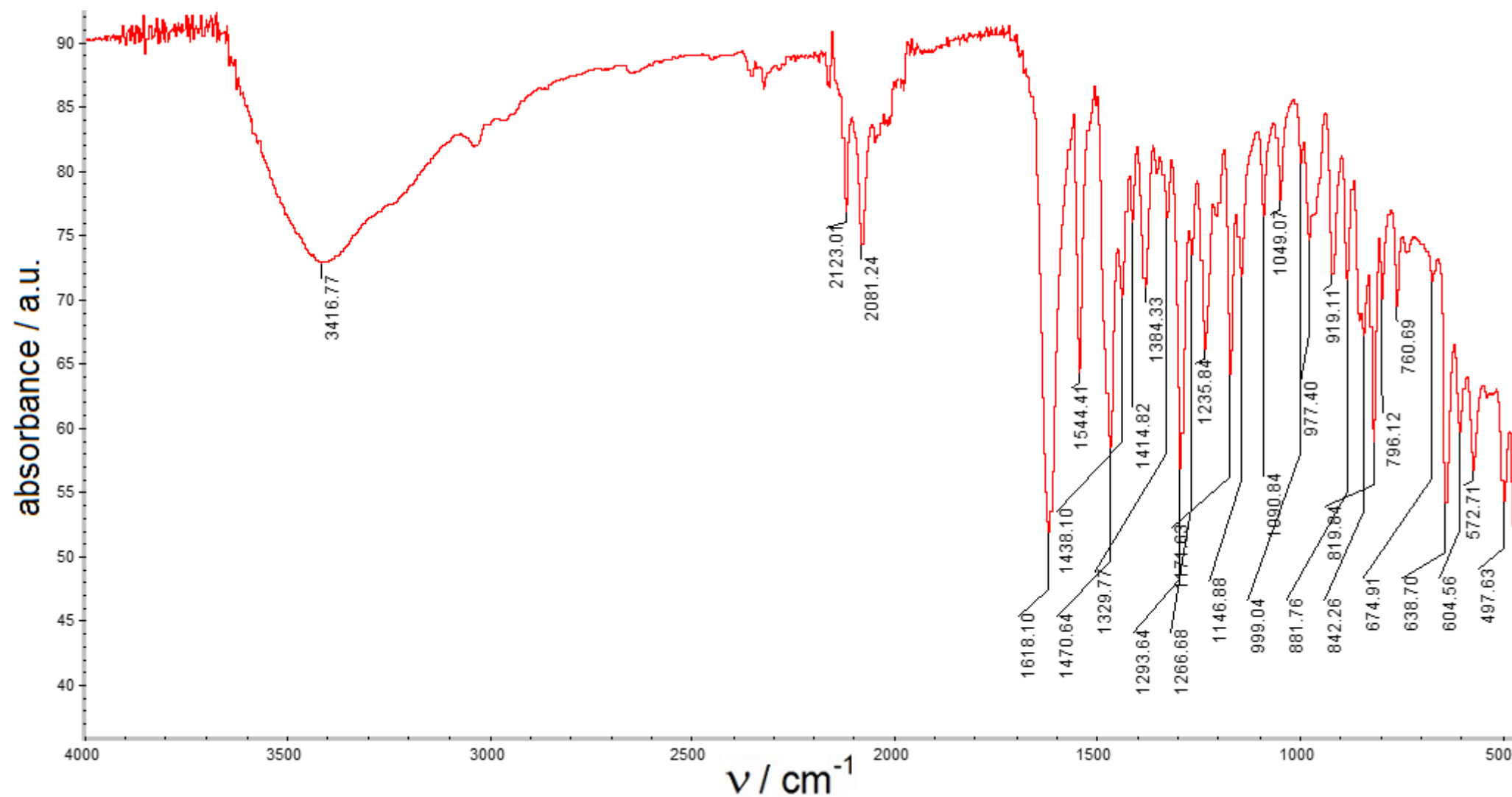


Figure S6. ATR-IR spectrum for {[Mn(SB²⁺)Re(CN)₇](H₂O)₇]_n **1**.

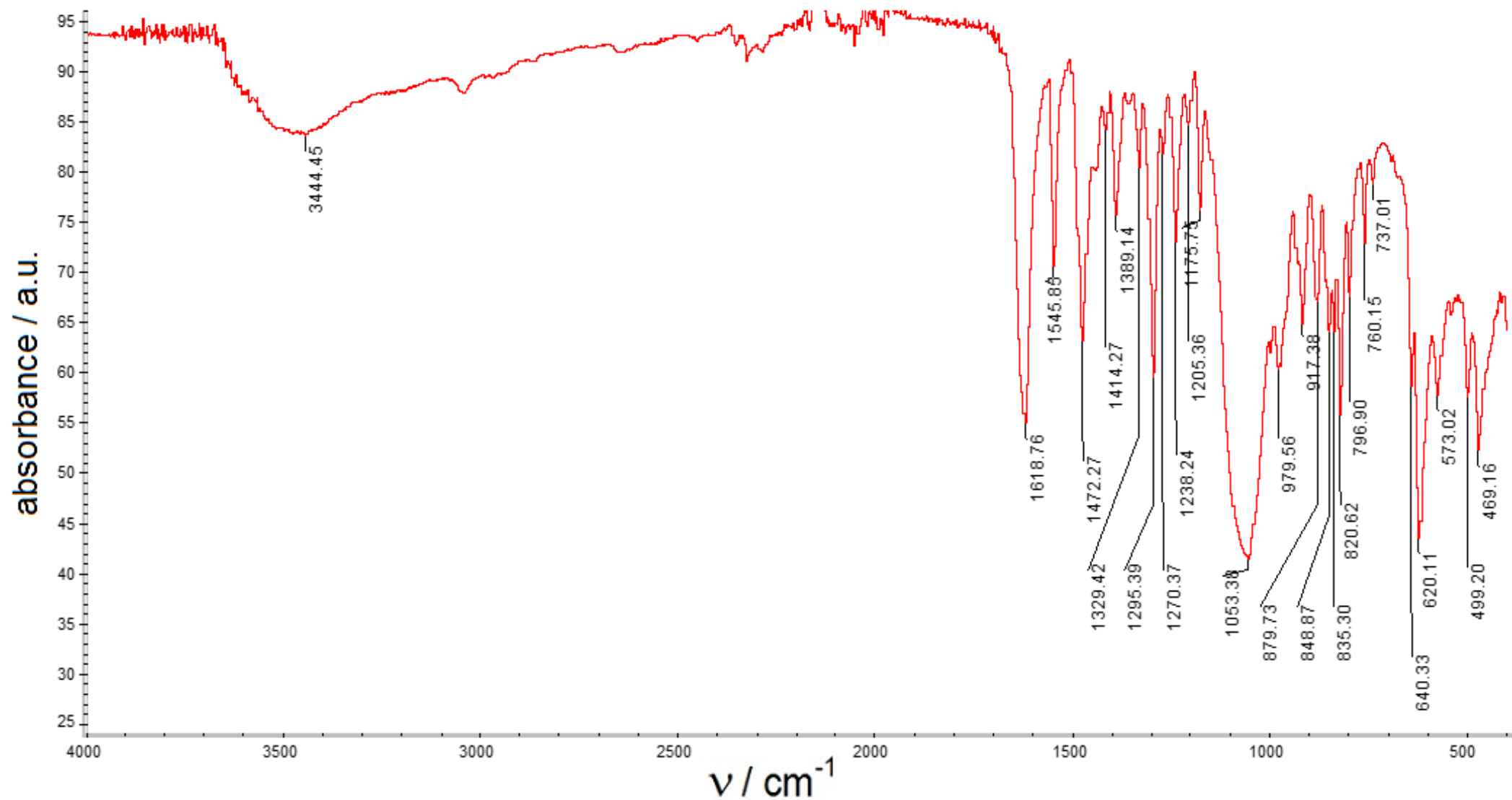


Figure S7. ATR-IR spectrum for the precursor, $[\text{Mn}(\text{SB}^{2+})(\text{H}_2\text{O})_2](\text{ClO}_4)_3 \cdot \text{H}_2\text{O}$.

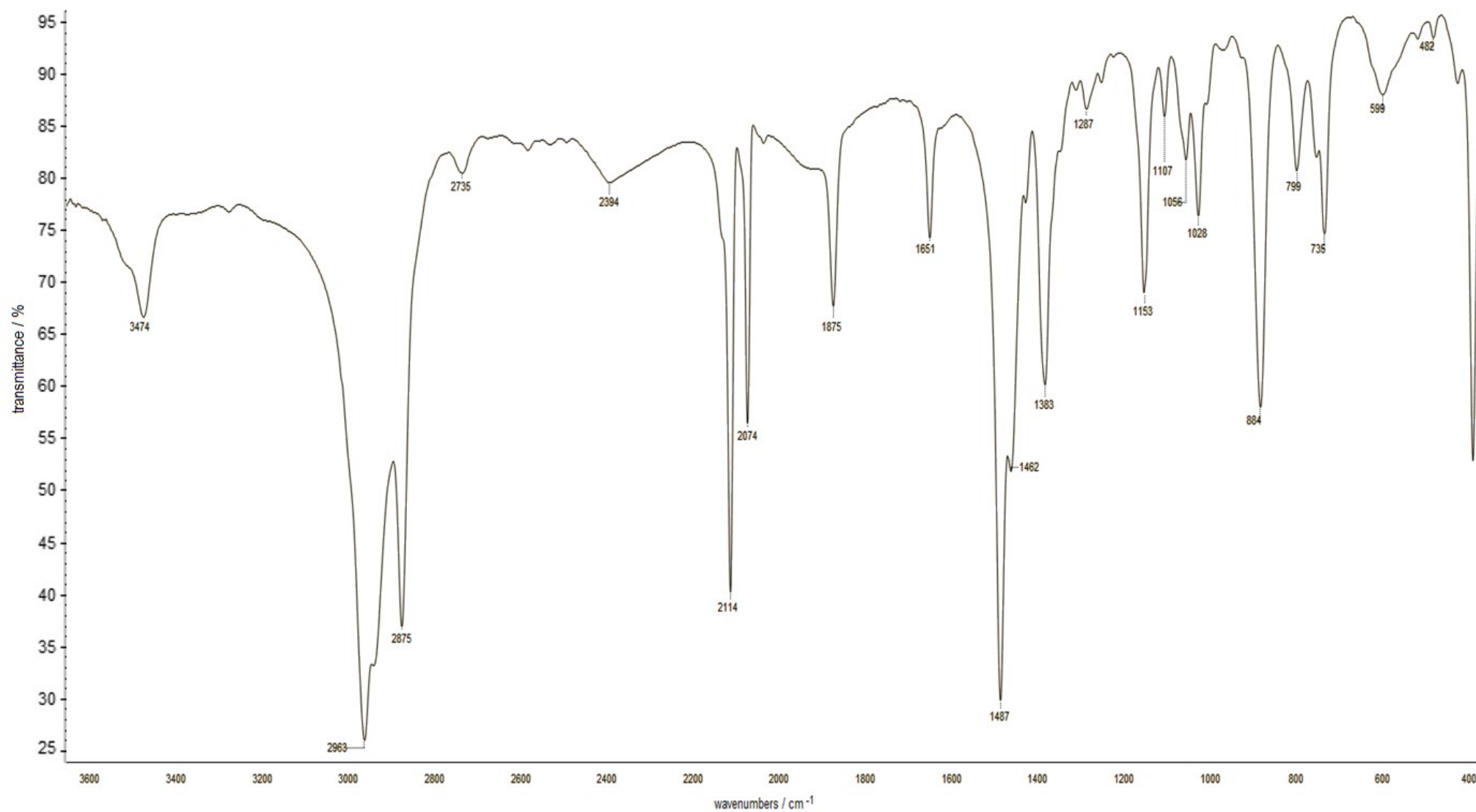


Figure S8. IR spectrum for the precursor, $(\text{Bu}_4\text{N})_3[\text{Re}(\text{CN})_7] \cdot \text{H}_2\text{O}$ (KBr).

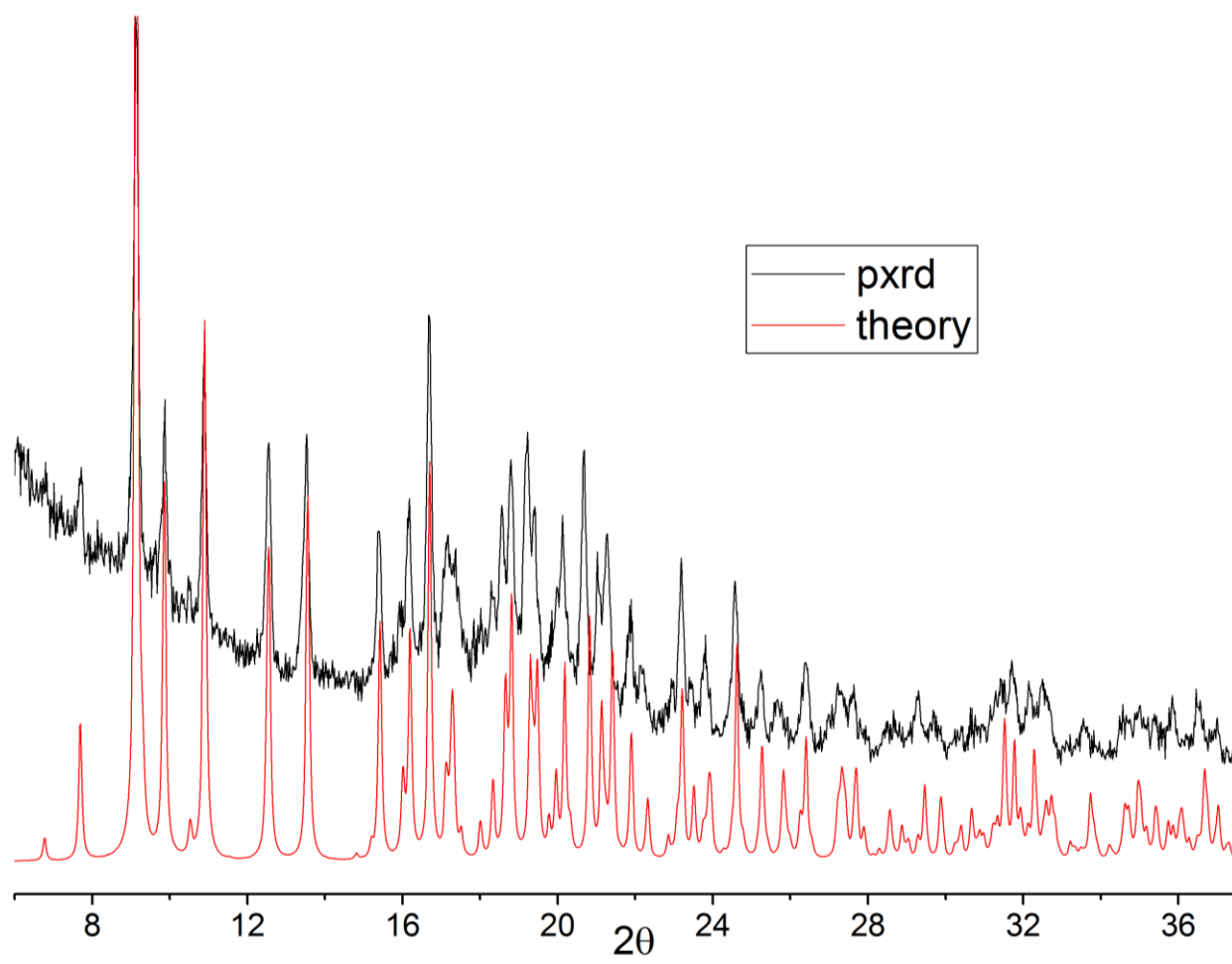


Figure S9. PXRD patterns for the chain compound **1**: polycrystalline sample (black), theoretically calculated (red).

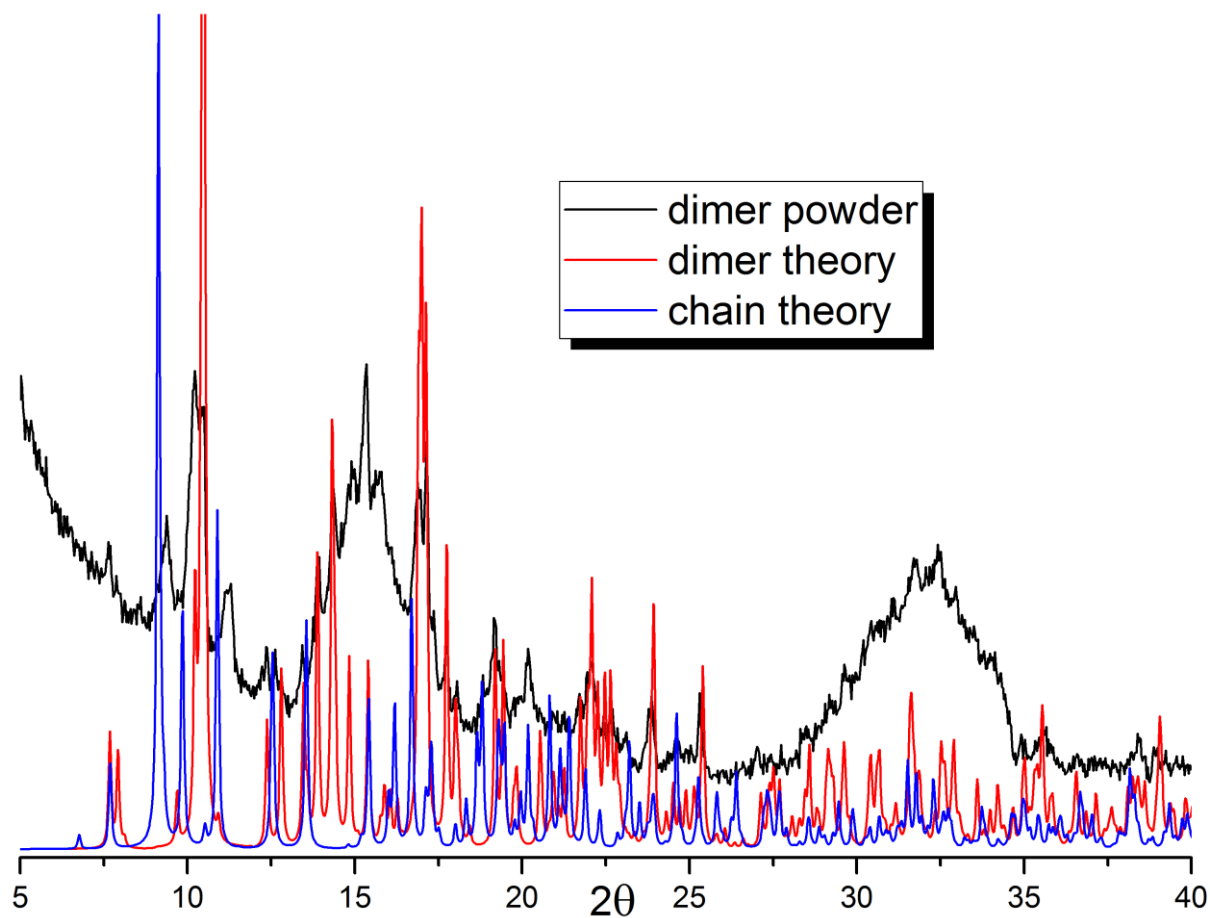


Figure S10. PXRD patterns for the dimer compound **2** (room T) and theoretically calculated (150 K) for **1** and **2**.

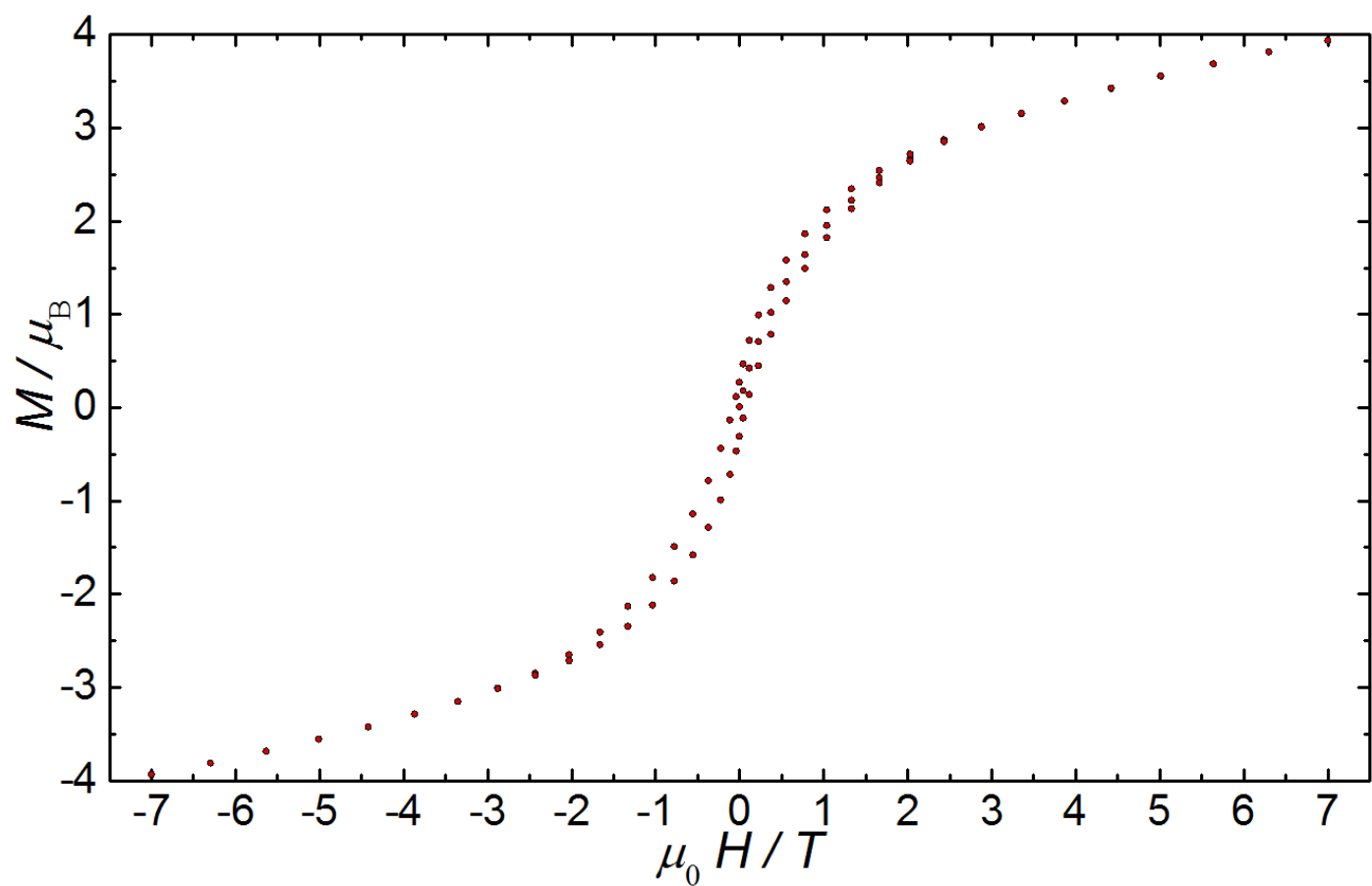


Figure S11. Magnetic hysteresis loop of **2** measured at 1.8 K on a polycrystalline sample (sw. rate – 0.07 T·s⁻¹).

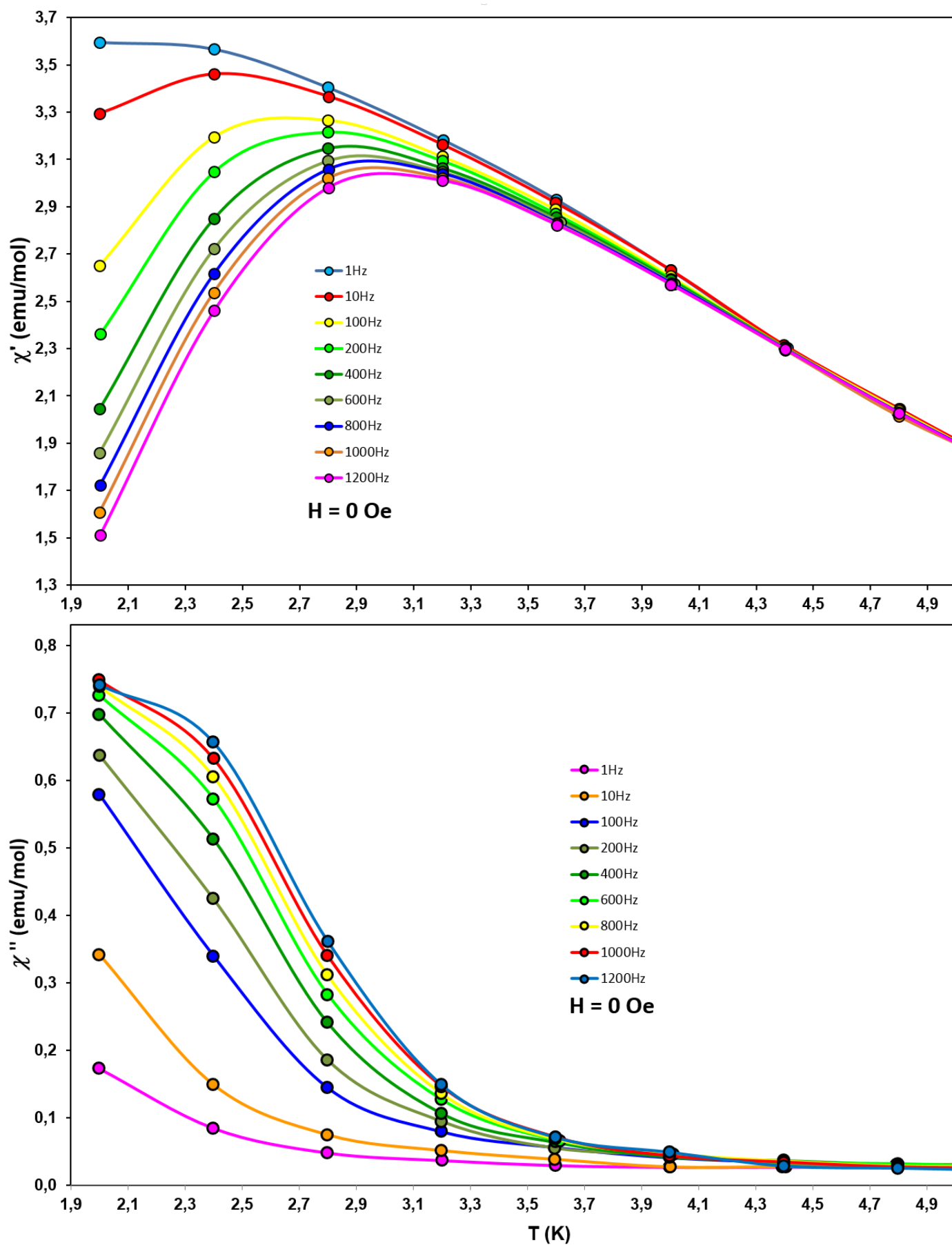


Figure S12. 8. Variable-temperature of the real, χ' (top), and imaginary, χ'' (bottom), parts *ac* molar susceptibility data for **1** under $H_{dc} = 0 \text{ Oe}$, $H_{ac} = 2.7 \text{ Oe}$. Solid lines are guides.

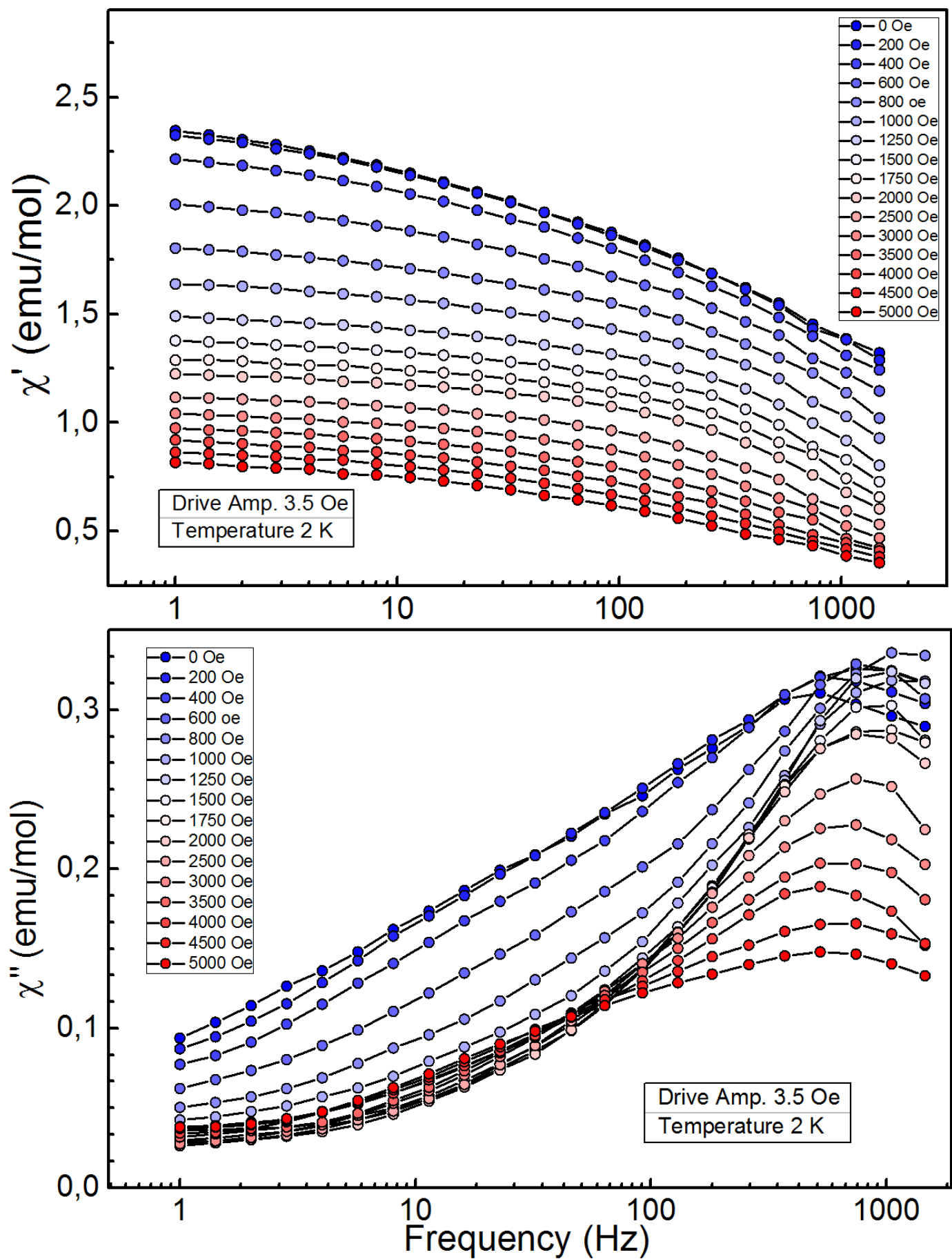


Figure S13. Frequency dependence of the real (χ') (top) and imaginary (χ'') (bottom) parts of the ac susceptibility for a polycrystalline sample of **2** in different dc -fields y and with applied a 3 Oe ac field. Solid lines are guides.

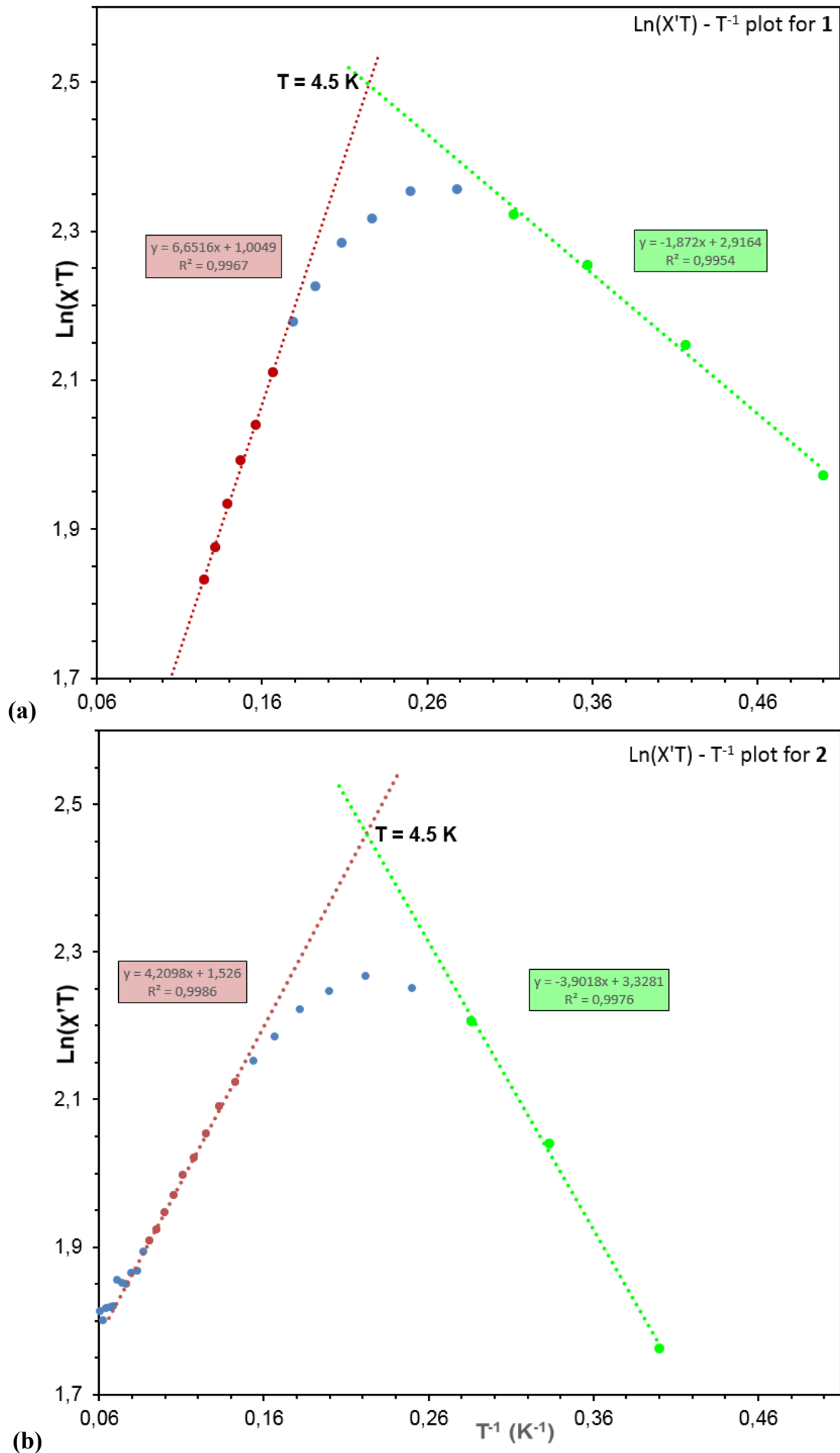


Figure S14. Plots of $\ln(X'T)$ vs $1/T$ (where X' is the molar component of the ac susceptibility) for **1** (top) and **2** (bottom) collected in zero applied dc field and frequency of 1 Hz. The dashed red lines correspond to a linear fit for high temperature region, giving $\Delta\xi/k_B = 6.66$ ($C_{eff}=1.005$ emu·K/mol) and 4.21 K ($C_{eff}=1.526$ emu·K/mol) for **1** and **2** respectively. The dashed green lines corresponds to a linear fit for low temperature region. An intersection of the two linear regions corresponds to the crossover temperature $T^*\approx 4.5$ K equal for both.

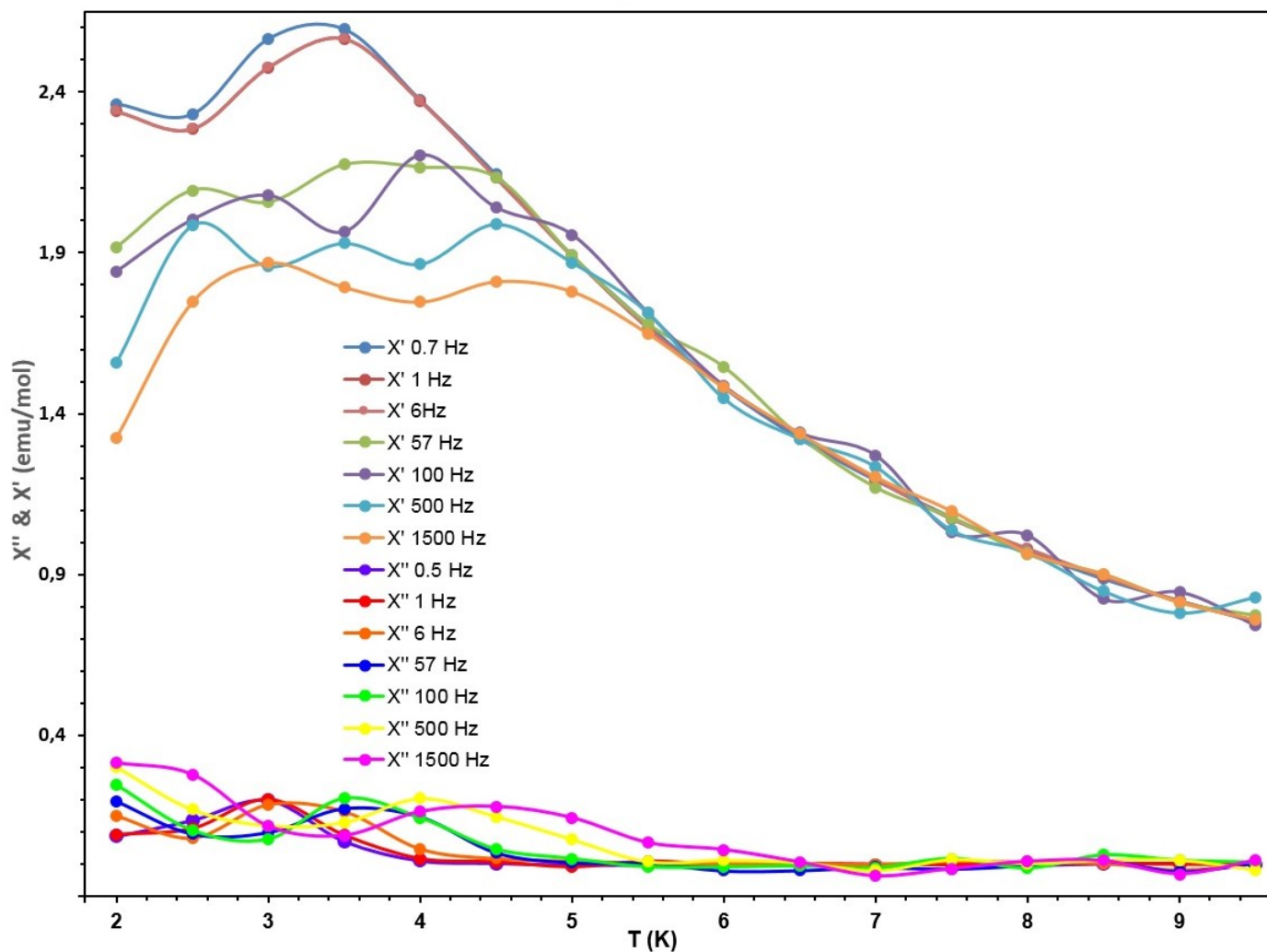


Figure S15. Variable-temperature real, χ' (top) and imaginary, χ'' (bottom) *ac* molar susceptibility data for **2** under $H_{dc}=100$ Oe, $H_{ac}=3.5$ Oe. Solid lines are guides.

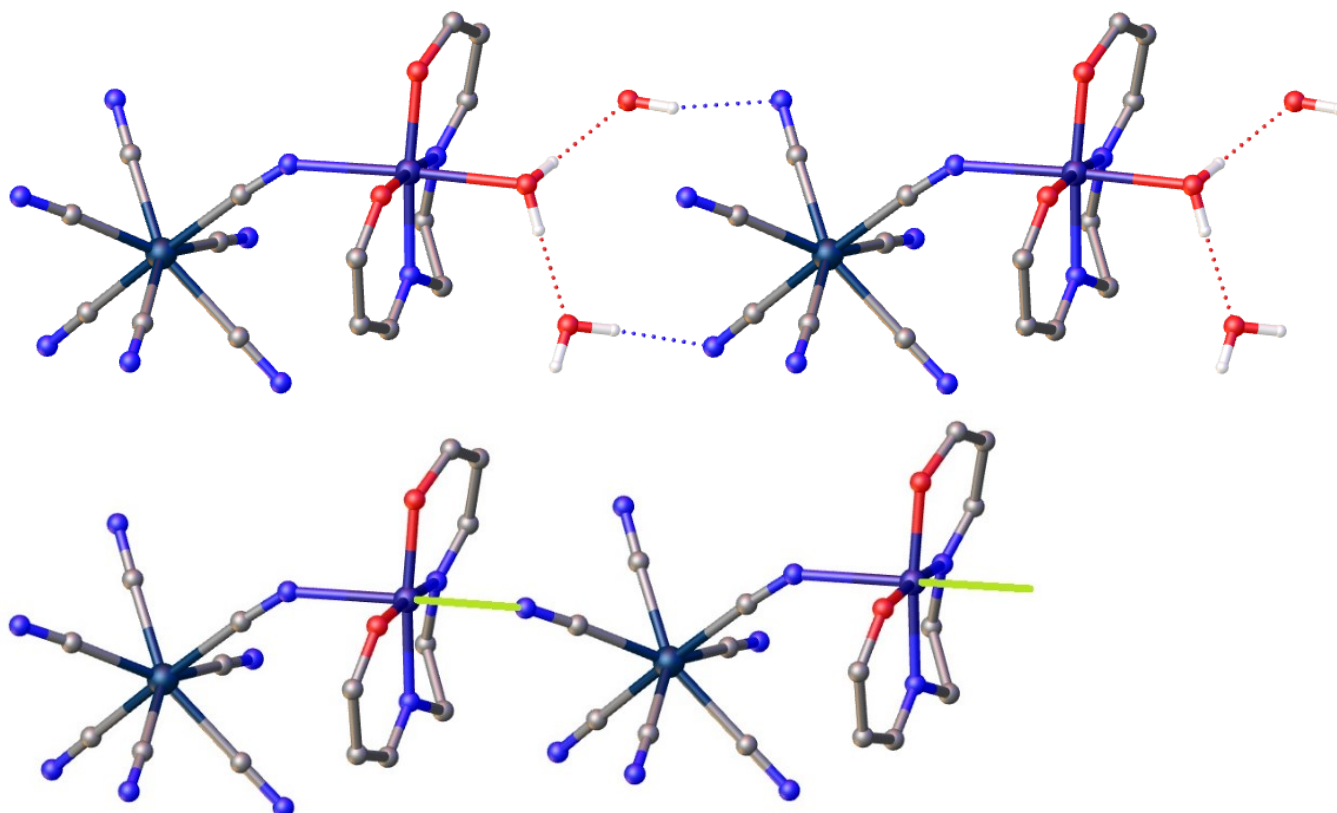


Figure S16. Possible formation of a 1D polymer from **2** by a desolvation. The $[\text{Mn}(\text{SB}^{2+})]^{3+}$ complexes are connected to the Re^{IV} ions by an equatorial and an apical cyanide bridges.

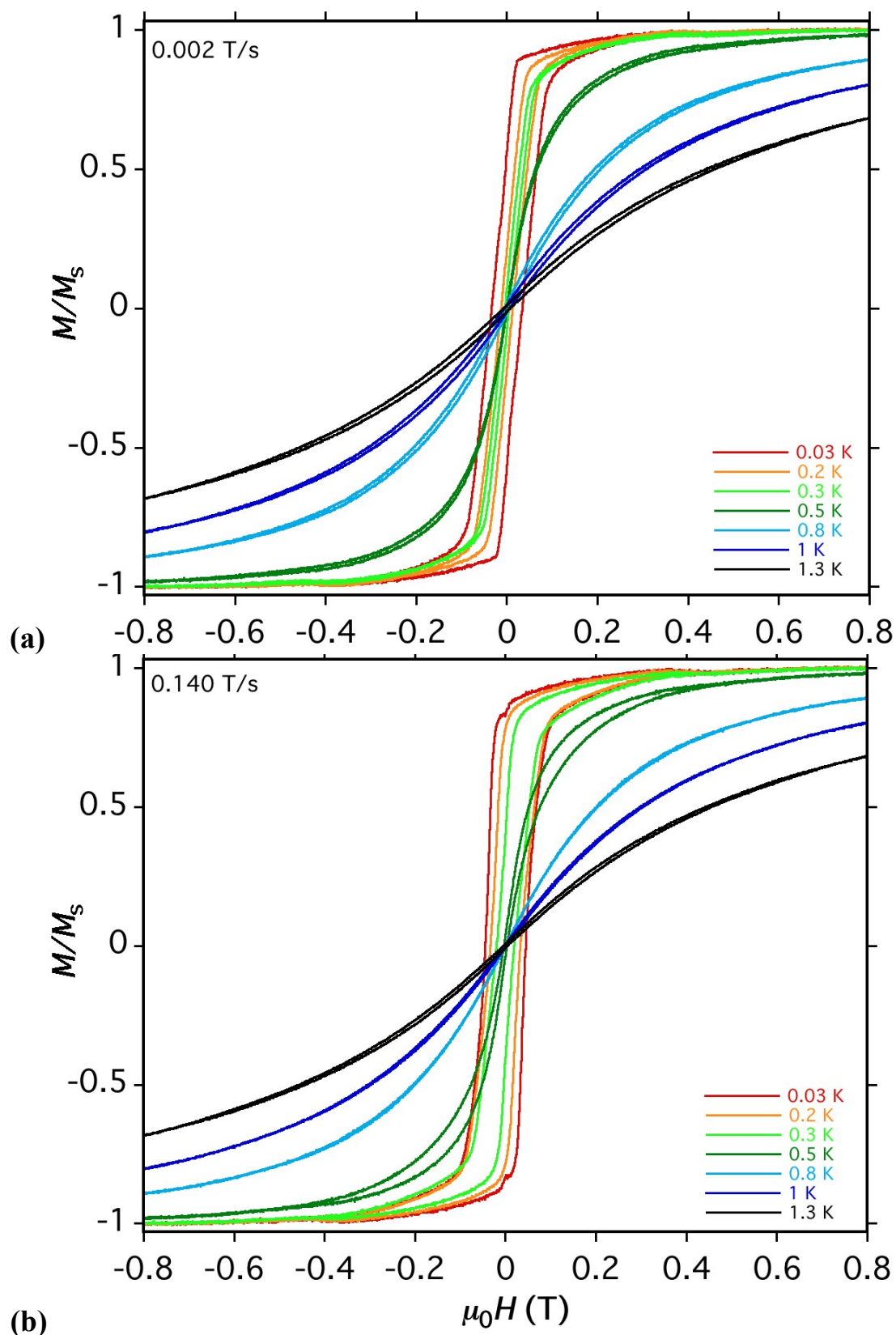


Figure S17. Field dependences of the normalized magnetization at the field sweeping rate of 0.002 T·s⁻¹ (a), and 0.140 T·s⁻¹ (b), measured at different temperatures on an oriented single crystal of **2** with the magnetic field applied along the easy magnetic axis.

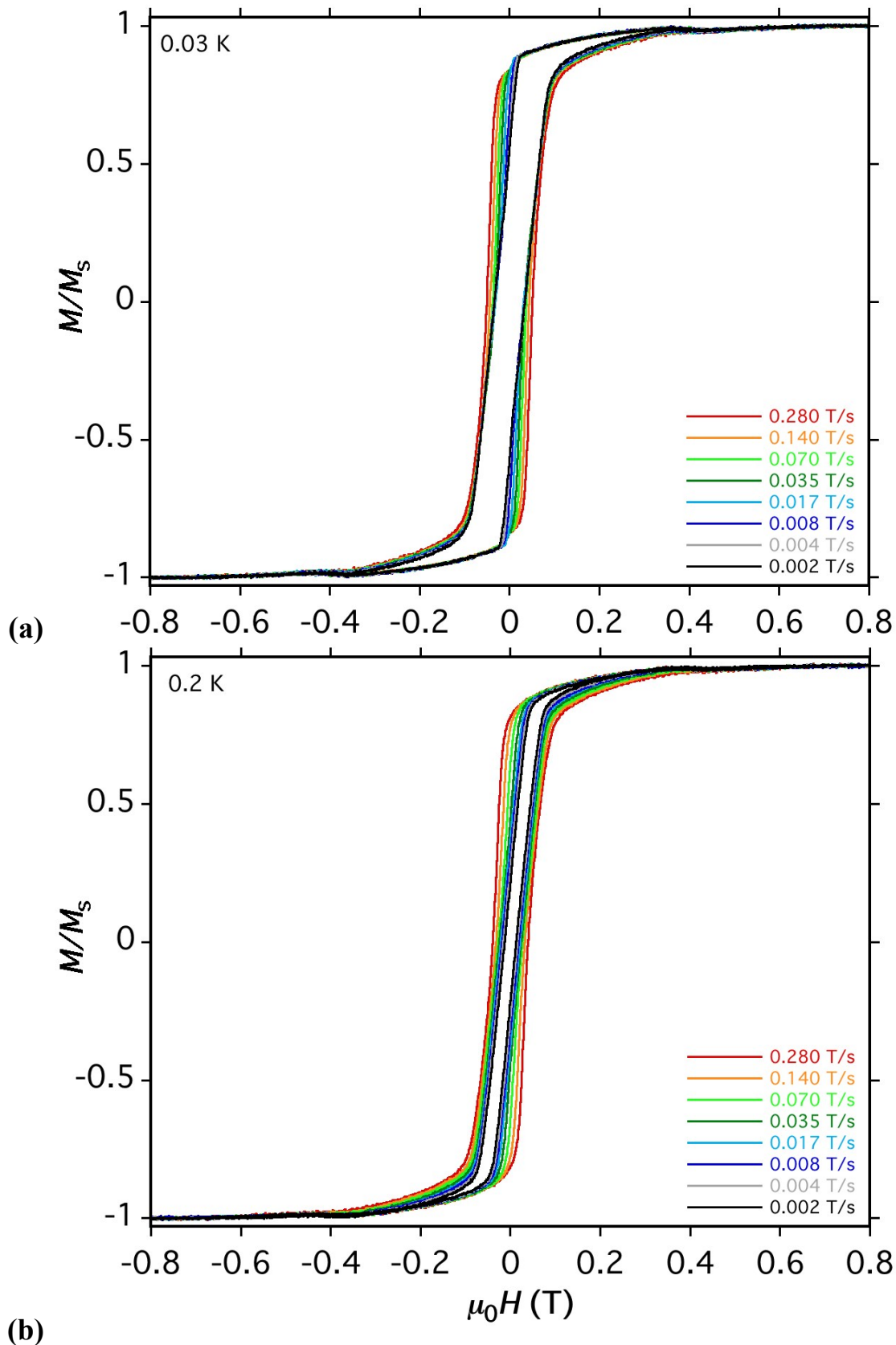


Figure S18. Field dependences of the normalized magnetization at 0.03 K (a), and 0.2 K (b) measured at different field sweeping rates on an oriented single crystal of **2** with the magnetic field applied along the easy magnetic axis. The maximum coercivity reaches 1043.5 Oe at 30 mK and SwRate of 0.280 T·s⁻¹.