

Supplementary Materials

Slow Magnetic Relaxation in Tetranuclear Co(II) Complexes Derived from Tridentate *NNO*-Schiff Base Ligands with [Co₄O₄] Cubane Metal Core

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Table S1. Crystallographic data and refinement parameters.

	1	2
Moiety formula	C ₅₂ H ₄₄ Cl ₄ Co ₄ N ₈ O ₄ , 4CH ₃ OH, 4H ₂ O, 8[H ₂ O]	C ₆₆ H ₅₄ Co ₄ N ₈ O ₈ , 2Cl, 12[CH ₃ OH]
Empirical formula	C ₅₆ H ₈₄ Cl ₄ Co ₄ N ₈ O ₂₀	C ₇₈ H ₁₀₂ Cl ₂ Co ₄ N ₈ O ₂₀
Formula weight	1566.83	1778.29
Temperature / K	113	113
Crystal system	tetragonal	tetragonal
Space group	<i>I</i> 4 ₁ / <i>a</i>	<i>I</i> 4 ₂ <i>d</i>
<i>a</i> / Å	14.3434(3)	19.329(4)
<i>b</i> / Å	14.3434(3)	19.329(4)
<i>c</i> / Å	33.6052(10)	22.582(5)
α / °	90	90
β / °	90	90
γ / °	90	90
<i>V</i> / Å ³	6913.7(4)	8437(4)
<i>Z</i>	4	4
<i>D</i> _{calc} / g cm ⁻³	1.505	1.400
μ (MoK α) / mm ⁻¹	1.172	0.909
<i>F</i> (0 0 0)	3248.0	3712.0
Crystal dimensions / mm ³	0.2 × 0.2 × 0.2	0.2 × 0.2 × 0.2
Radiation	MoK α (λ = 0.71073)	MoK α (λ = 0.71075)
2 θ range for data collection / °	6.176 to 54.946	6.576 to 54.952
Reflections collected	11649	25877
Independent reflections	2597 [<i>R</i> _{int} = 0.0422]	4399 [<i>R</i> _{int} = 0.0464]
Data/Restraints/Params	2597 / 2 / 195	4399 / 36 / 202
Goodness of fit indicator	1.027	1.034
<i>R</i> indices [<i>I</i> > 2.00 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0489, <i>wR</i> ₂ = 0.1051	<i>R</i> ₁ = 0.0848, <i>wR</i> ₂ = 0.2212
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0754, <i>wR</i> ₂ = 0.1143	<i>R</i> ₁ = 0.0954, <i>wR</i> ₂ = 0.2338
Largest diff. peak, hole / e Å ⁻³	0.43 / -0.30	1.85 / -0.76
Flack parameter	----	0.48(4)
CCDC deposition number	2387207	2387208

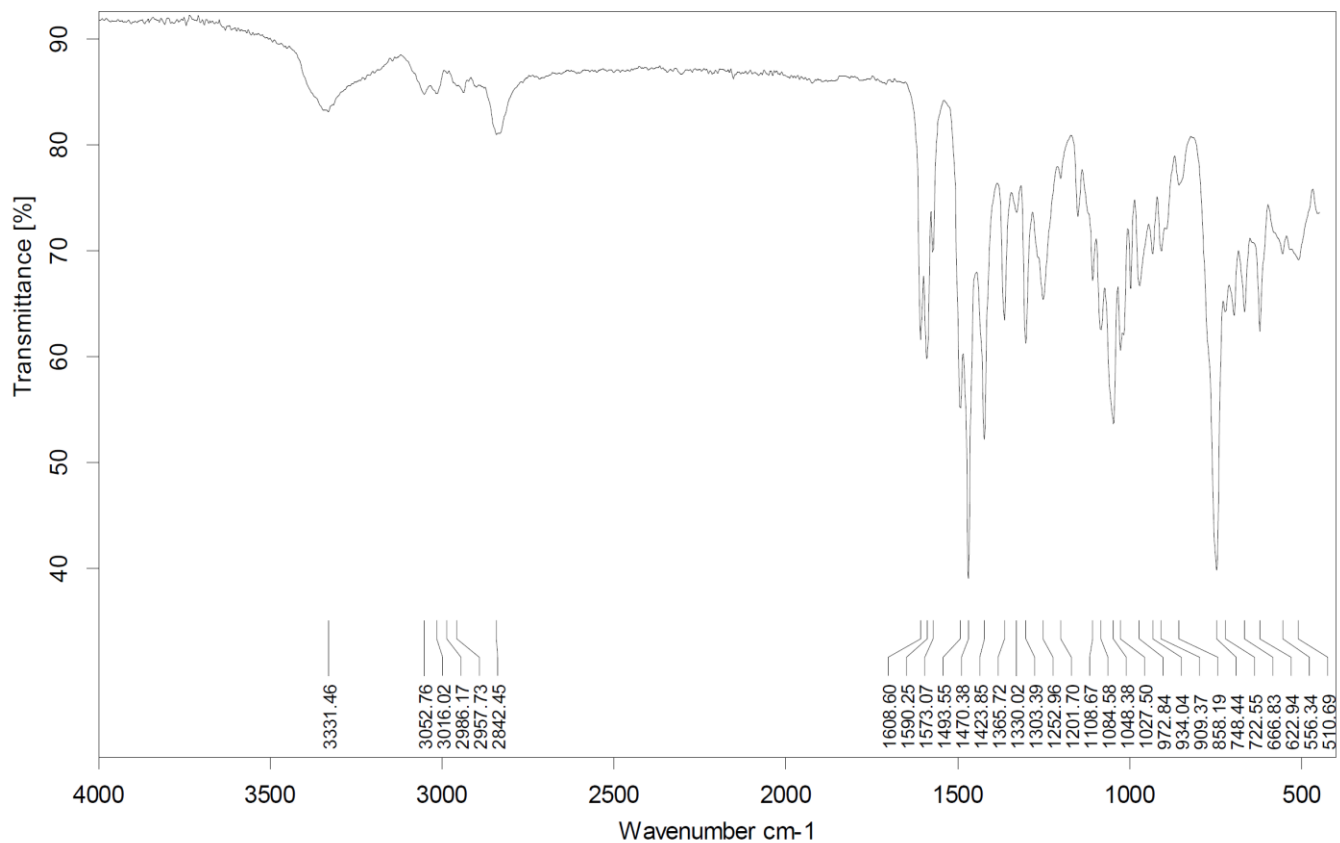


Figure S1. IR spectrum of Hpmab.

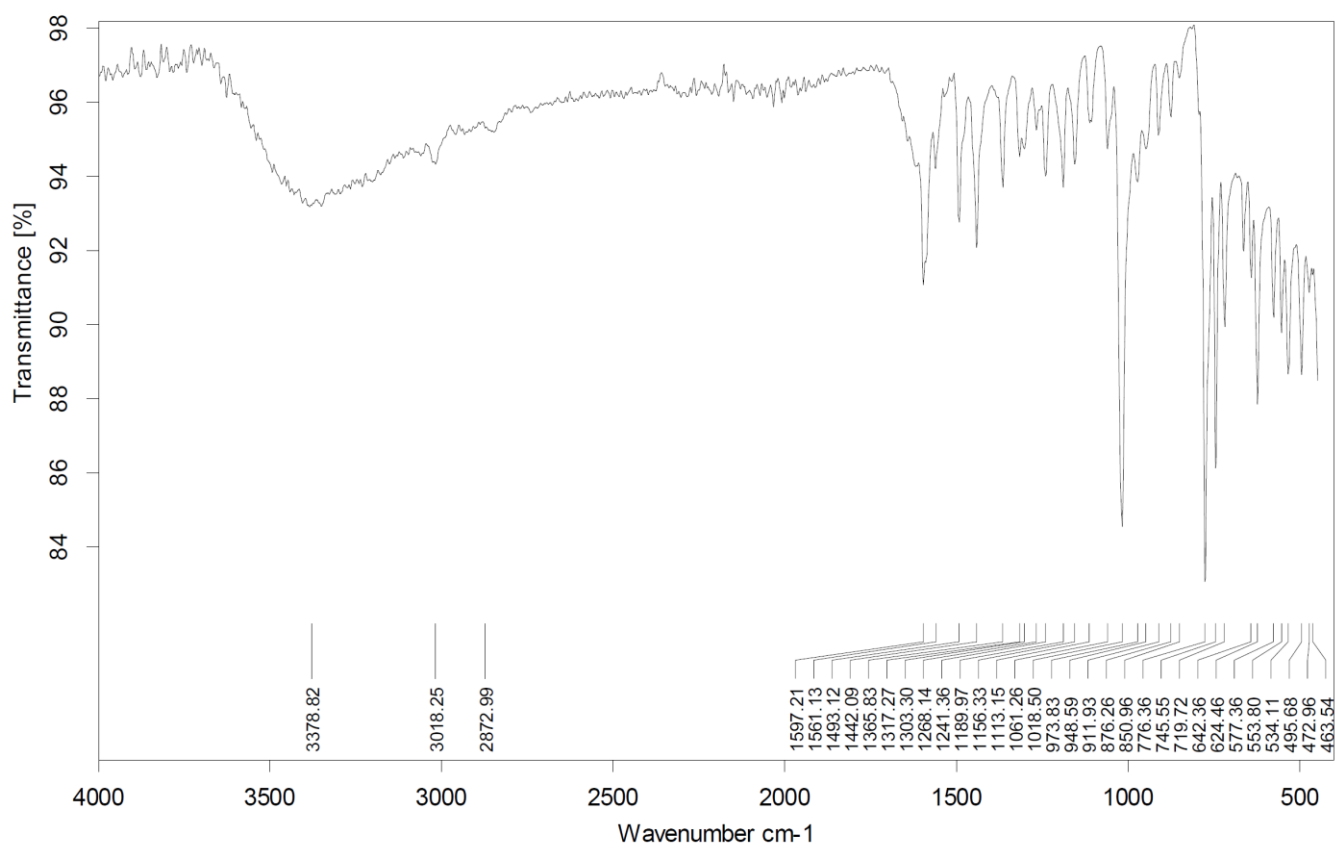


Figure S2. IR spectrum of 1.

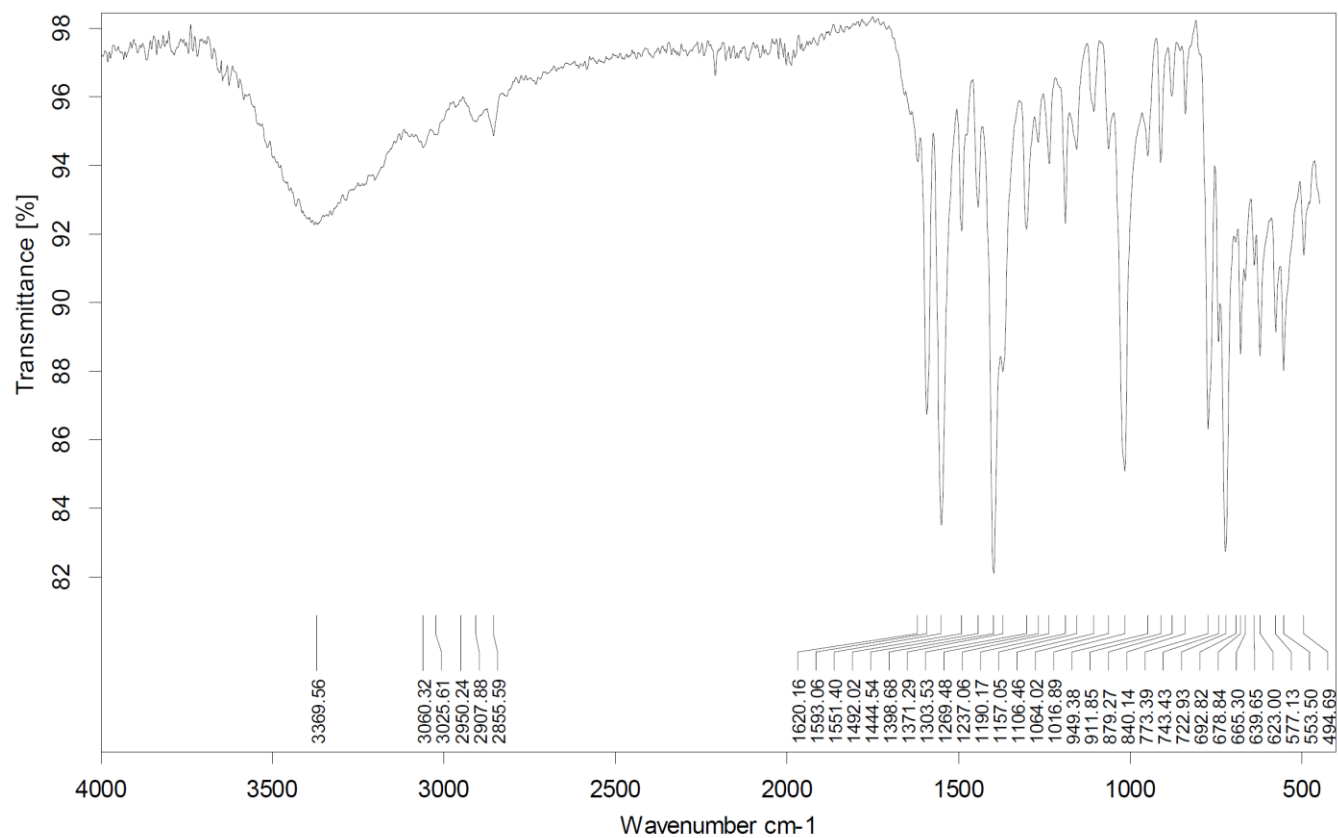


Figure S3. IR spectrum of **2**.

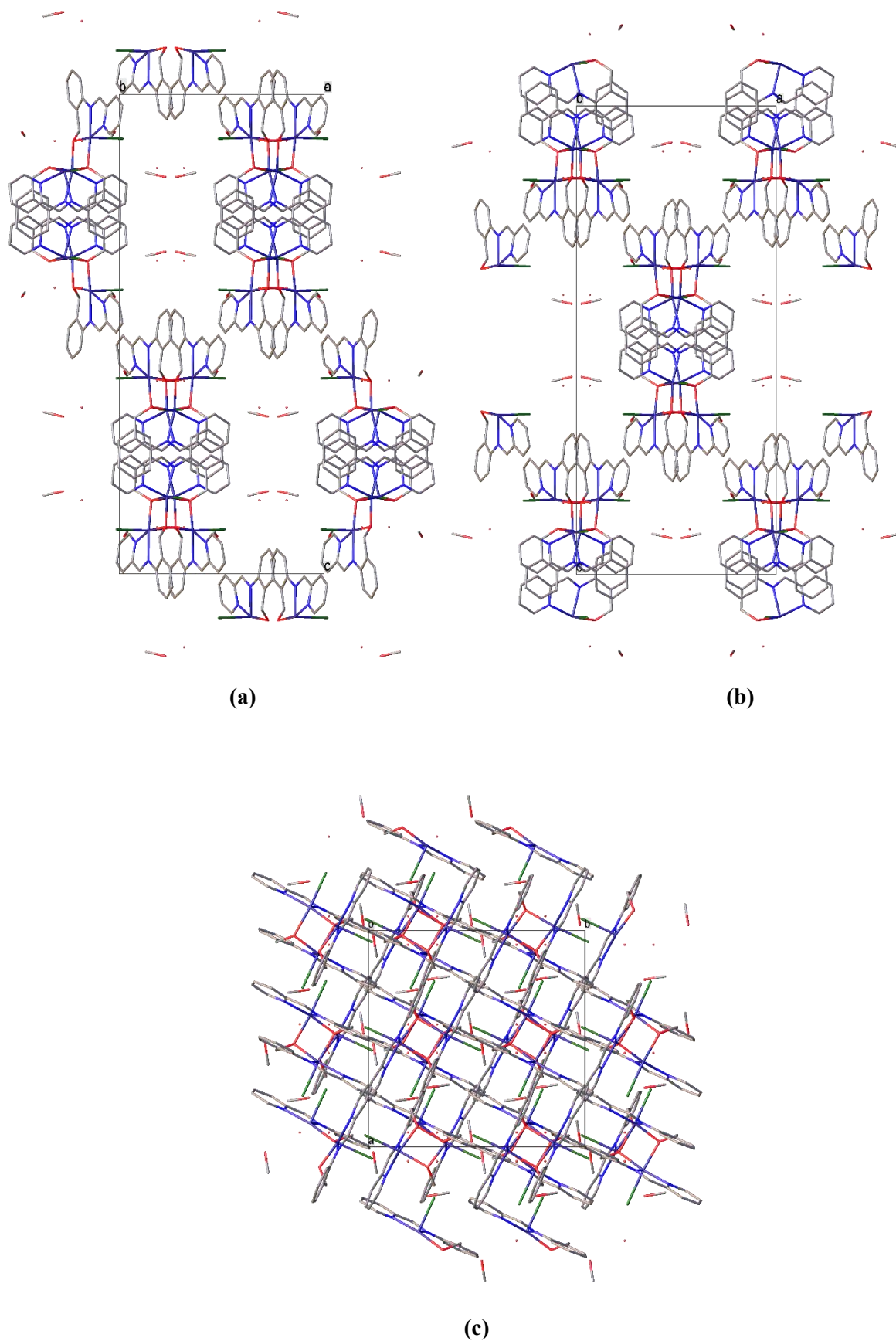


Figure S4. Crystal packing diagram of **1**. Hydrogen atoms are omitted for clarity. (a) view along the a -axis. (b) view along the b -axis. (c) view along the c -axis.

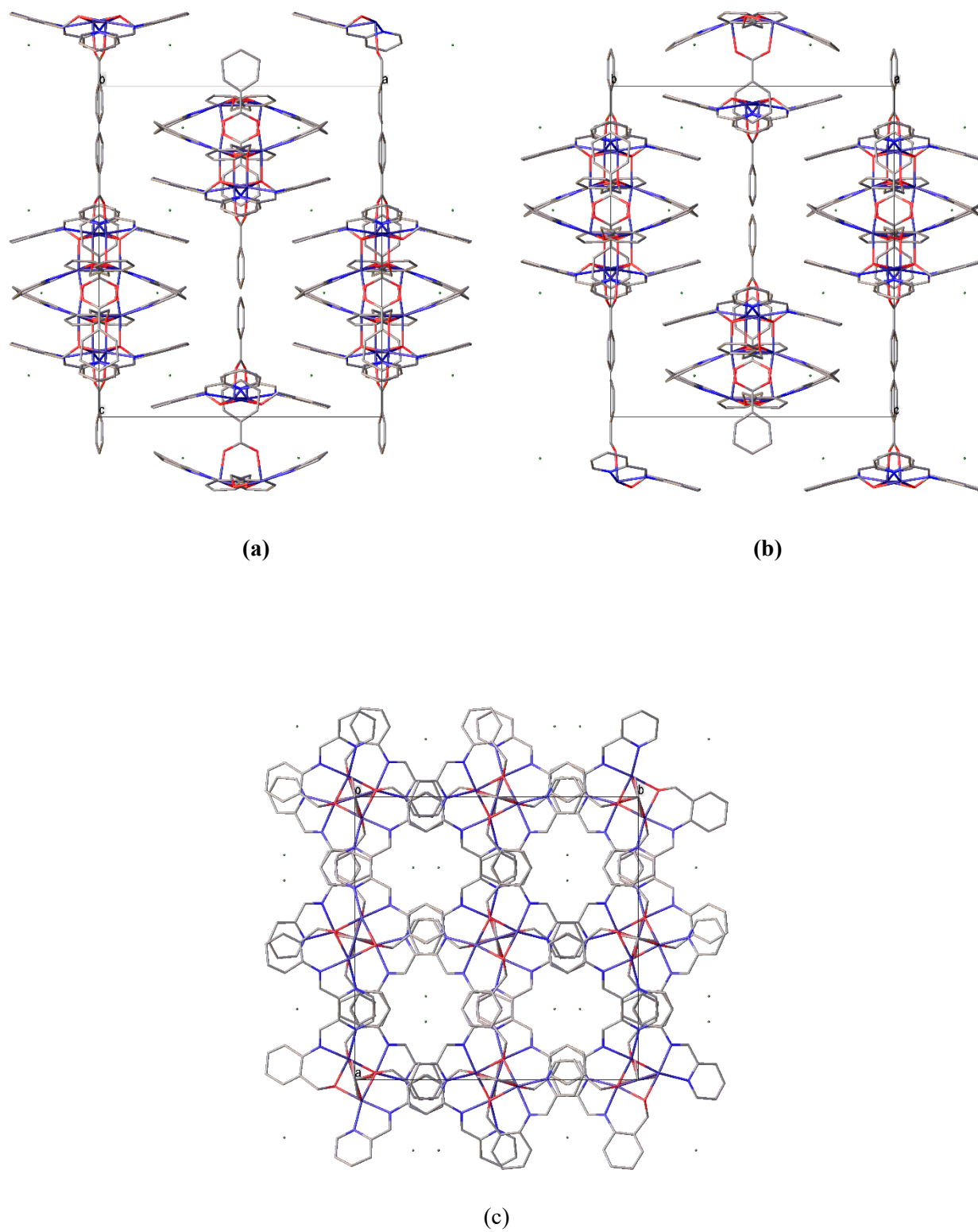


Figure S5. Crystal packing diagram of **2**. Hydrogen atoms are omitted for clarity. (a) view along the *a*-axis. (b) view along the *b*-axis. (c) view along the *c*-axis.

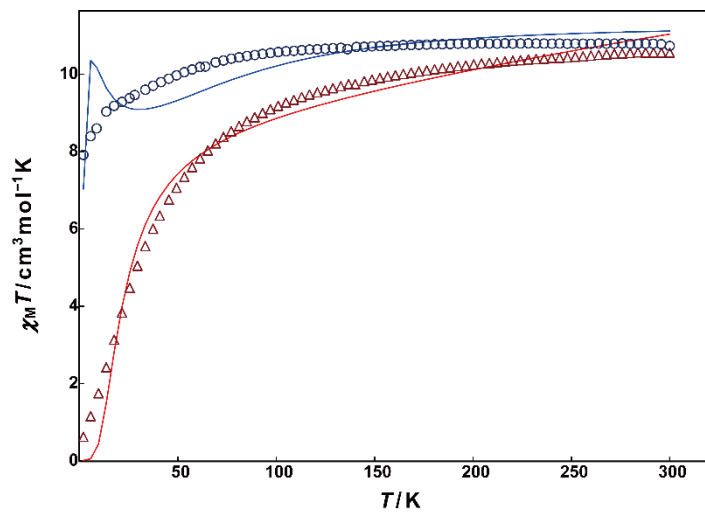
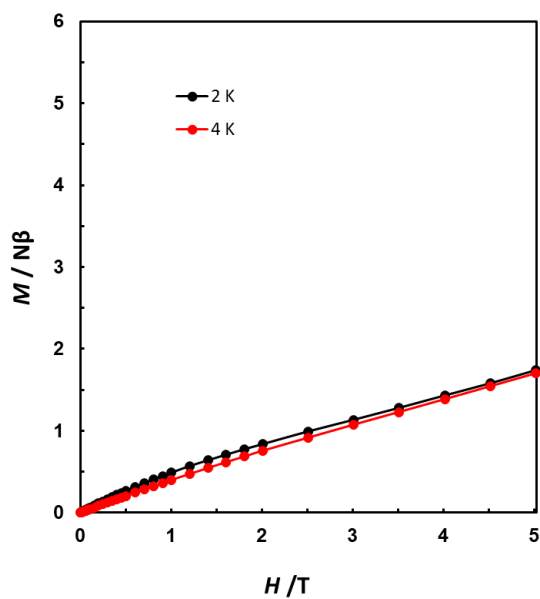
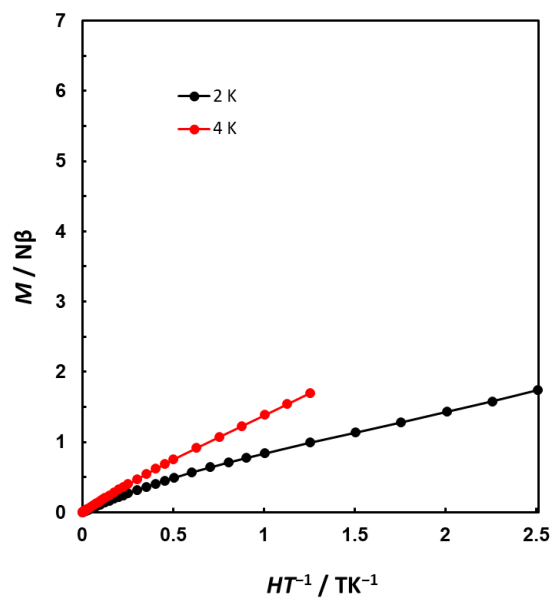


Figure S6. Fitting of the χT curve using an $S = 3/2$ tetranuclear cubane model. For **1**, the parameters are $J = 0.989 \text{ cm}^{-1}$, $J' = -0.041 \text{ cm}^{-1}$, $g = 2.45$, $D = -85 \text{ cm}^{-1}$. For **2**, the parameters are $J = 1.157 \text{ cm}^{-1}$, $J' = -1.186 \text{ cm}^{-1}$, $g = 2.80$, $D = -488 \text{ cm}^{-1}$.

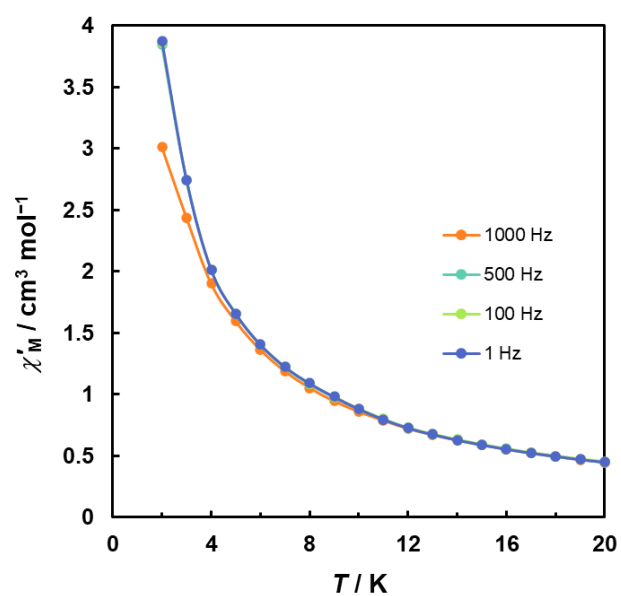


(a)

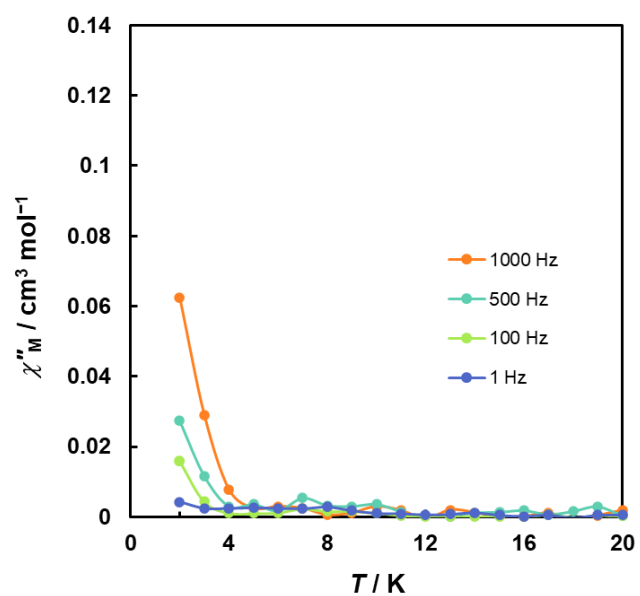


(b)

Figure S7. Magnetization plots of **2**. (a) M vs. H plot at 2 and 4 K; (b) M vs. H/T plot. Solid lines are guides for the eye.



(a)



(b)

Figure S8. Variable temperature AC susceptibility data in a 3 Oe AC field oscillating at 1, 100, 500, and 1000 Hz under zero applied DC field for **1**. **(a)** Plot of in-phase (χ'_M) signal. **(b)** Plot of out-of-phase (χ''_M) signal. Solid lines are guides for the eye.