

Supporting Information for
Structural phase transformation of quantum spin liquid
herbertsmithite via pressure induced enhancement of cooperative
Jahn-Teller effect and antisite disorder

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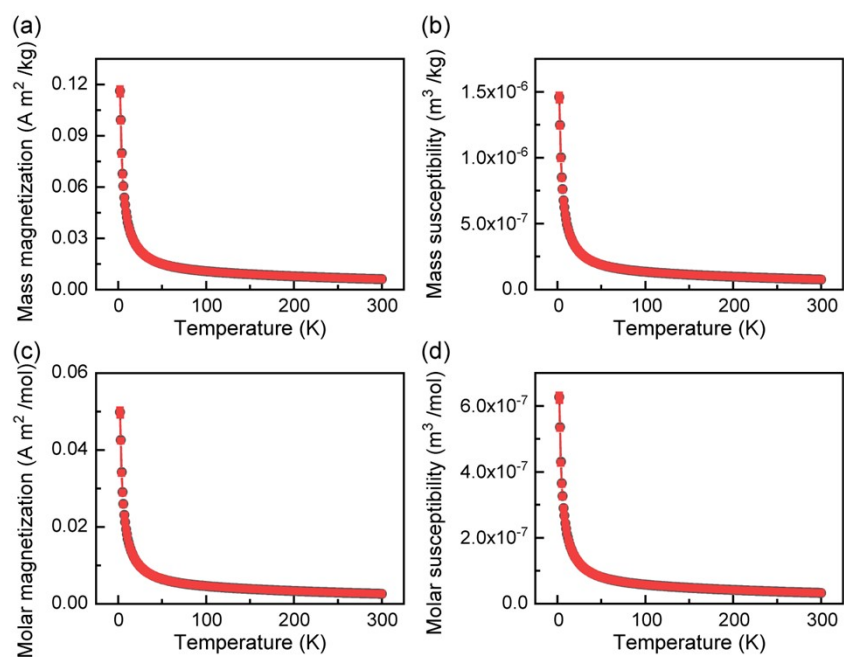


Figure S1 Temperature dependence of (a) mass magnetization, (b) mass susceptibility, (c) molar magnetization, and (d) molar susceptibility measured at 1000 Oe under ZFC-FC conditions.

Note: The cgs units are used in most of the primary literature on magnetism. For example, a series of literature about the magnetic studies on herbertsmithite and its related compounds are still written using cgs units.¹⁻⁵ The data presented in SI units are shown in the Figure S1-S2.

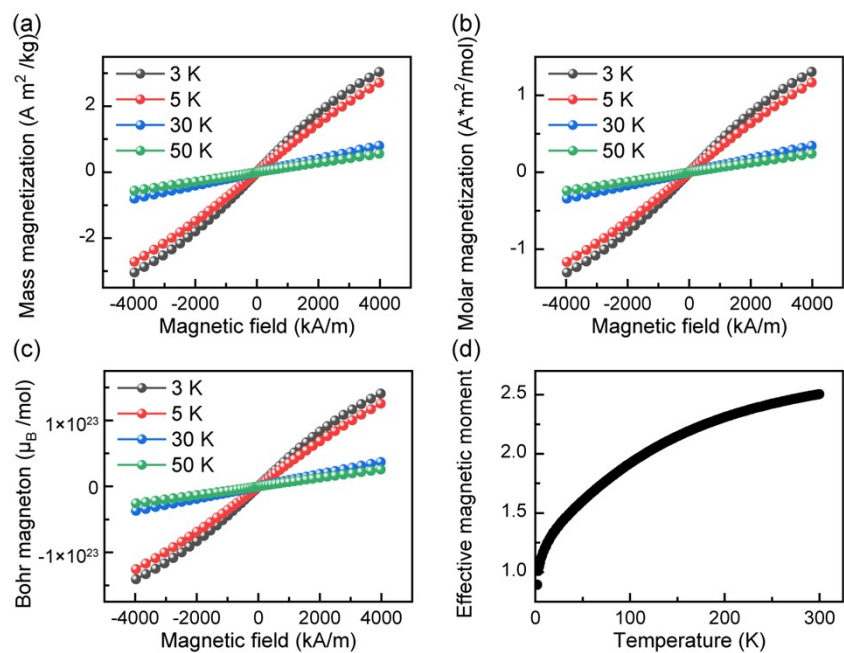


Figure S2 (a-c) Magnetization against applied external field of duplicate sample for several temperatures. (d) The value of effective magnetic moment as a function of temperature.

Note: As shown in Figure S2 a-c, the M-H data were presented in mass magnetization, molar magnetization, and Bohr magneton/mol, respectively. The effective magnetic moment (μ_{eff}) is generally expressed in terms of the Bohr magneton. In fact, the values of μ_{eff} depend on the definitions and the system of units. It is calculated from the molar susceptibility. The dimensionless nature of μ_{eff} in the SI approach is demonstrated below using the equation⁶

$$\chi_M = \frac{N_A \mu_0 \mu_B^2 \mu_{\text{eff}}^2}{3k_B T}$$

where χ_M is the molar susceptibility ($\text{m}^3 \text{mol}^{-1}$), N_A is the Avogadro constant ($N_A = 6.023 \times 10^{23}/\text{mol}$), μ_0 is the permeability of a vacuum ($\mu_0 = 4\pi \times 10^{-7} \text{ kg m s}^{-2} \text{ A}^{-2}$), μ_B the Bohr magneton ($\mu_B = 9.274 \times 10^{-24} \text{ A m}^2$), k_B is the Boltzmann constant ($k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$) and T is the thermodynamic temperature (K), respectively. The SI units of the physical quantities are given in parentheses.

References

- 1 M. M. R. Bhuiyan, X. G. Zheng, M. Hagihala, S. Torii, T. Kamiyama and T. Kawae, *Phys. Rev. B*, 2020, **101**, 134424.
- 2 R. W. Smaha, W. He, J. M. Jiang, J. J. Wen, Y. F. Jiang, J. P. Sheckelton, C. J. Titus, S. G. Wang, Y. S. Chen, S. J. Teat, A. A. Aczel, Y. Zhao, G. Y. Xu, J. W. Lynn, H. C. Jiang and Y. S. Lee, *Npj Quantum Mater*, 2020, **5**, 23.
- 3 P. Malavi, S. Pal, D. V. S. Muthu, S. Sahoo, S. Karmakar and A. K. Sood, *Phys. Rev. B*, 2020, **101**, 214402.
- 4 K. Gupta, A. Dadwal, P. Ninawe, P. A. Joy and N. Ballav, *J Phys Chem C*, 2020, **124**, 19753-19759.
- 5 K. Tustain, E. E. McCabe, A. M. Arevalo-Lopez, A. S. Gibbs, S. P. Thompson, C. A. Murray, C. Ritter and L. Clark, *Chem. Mater.*, 2021, **33**, 9638-9651.
- 6 J. I. Hoppeé, *J. Chem. Educ.*, 1972, **49**, 505.