

## Terbium single-molecule magnets embedded in an inorganic coordination framework showing self-thermometry using luminescence

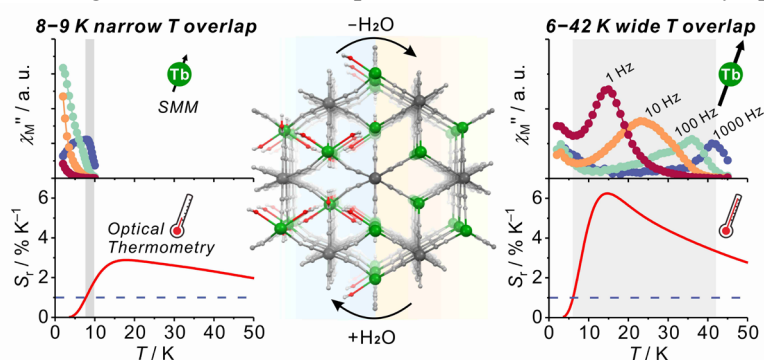
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Research on combining magnetic and optical properties within a single-phase material unveils novel cross-effects, facilitating the development of advanced magneto-optical functional devices. Lanthanide(III) complexes are such materials, which can accommodate both luminescent functionalities and single-molecule magnet (SMM) property, promising for high-density information storage devices with optical features.

In this work, we constructed a three-dimensional cyanido-bridged coordination framework,  $[\text{Tb}^{\text{III}}(\text{H}_2\text{O})_2][\text{Co}^{\text{III}}(\text{CN})_6] \cdot 2.7\text{H}_2\text{O}$  (**1**), and its thermally desolvated phase,  $\text{Tb}^{\text{III}}[\text{Co}^{\text{III}}(\text{CN})_6]$  (**2**), and investigated the conjunction of Tb(III)-centered SMM and luminescent functional properties in them. Upon topotactic transformation between two phases, the terbium complexes underwent a geometry change between an 8-coordinated square antiprism (in **1**) and a 6-coordinated trigonal prism (in **2**), which led to switching of both SMM and luminescent properties. Tb(III) in **1** revealed a moderate magnetic anisotropy with SMM character detectable up to 8.5 K. Upon dehydration, a much larger magnetic anisotropy energy barrier of  $594(18) \text{ cm}^{-1}$  was detectable up to 42 K. Characteristic luminescence observed from Tb(III) exhibited a hue switching of in the emission color. Additionally, their emissions as a function of temperature made both **1** and **2** luminescent ratiometric thermometers, working in the cryogenic temperature regime as low as ca. 6 K, showcasing SMMs with self-temperature monitorable features by optical means.



1) Y. Xin, et al., *J. Am. Chem. Soc.* **2019**, *141*, 18211. 2) J. Wang, et al., *J. Am. Chem. Soc.* **2020**, *142*, 3970. 3) J. Wang, et al., *Angew. Chem., Int. Ed.* **2023**, *62*, e202306372.