

Supplementary Information

Polyfunctional Yb(III) tropolonate complexes: Slow magnetic relaxation and luminescence

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Table S1. Crystal data and structure refinement for **2**.

Identification code	2
Empirical formula	$C_{46}H_{34}N_2O_{6.50}Yb$
Formula weight	891.81
Temperature, K	296
Wavelength, Å	1.5419
Crystal system	monoclinic
Space group	<i>C2/c</i>
a, Å	22.3808(10)
b, Å	13.42945(62)
c, Å	26.6711(12)
β , °	112.9485(24)
Volume, Å ³	7381.88(61)
Z	8
R _{exp}	5.53
R _{wp}	8.18
R _p	6.23
GOF	1.48
R-Bragg	2.70

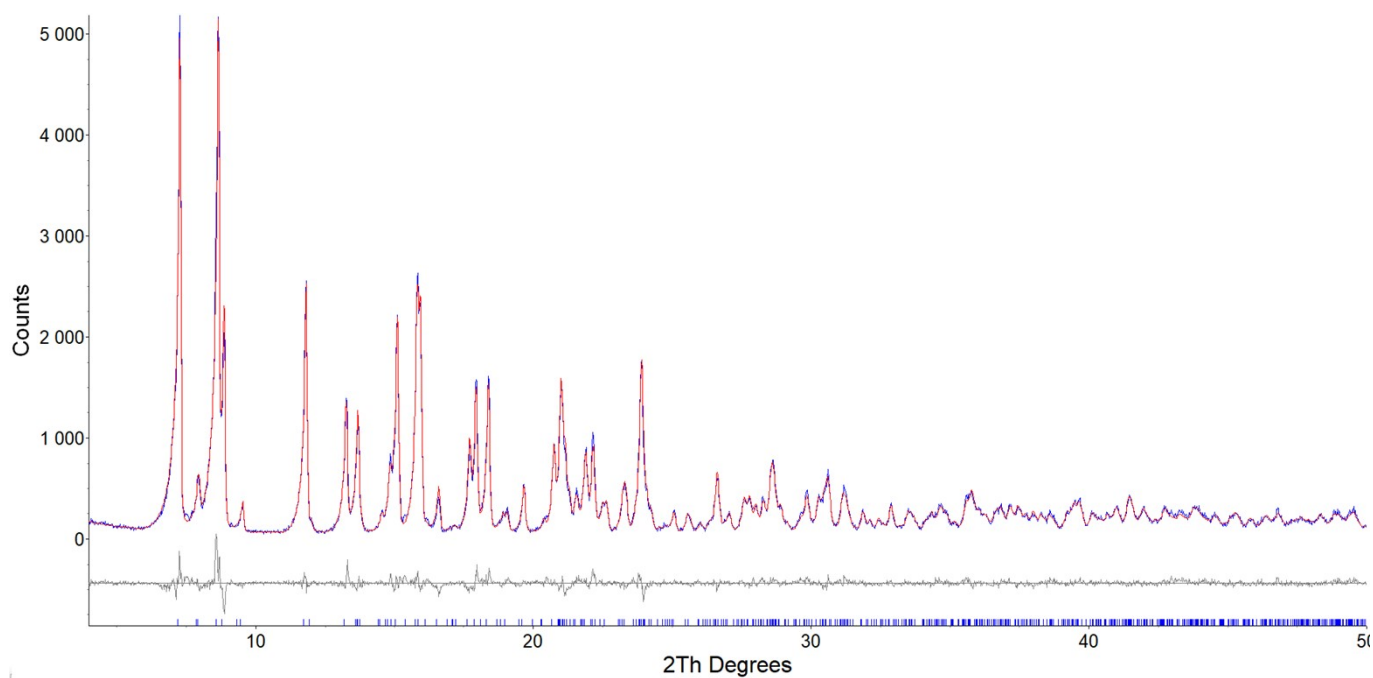


Fig. S1. Rietveld refinement profiles for **2**, for room temperature X-ray data. The calculated (for $[\text{YT}_3(\text{Bath})]\cdot 0.5\text{EtOH}$) and experimental (for **2**) profiles are shown with the red and blue line, respectively. The bottom trace shows the difference curve. The vertical bars indicate the calculated positions of the Bragg peaks.

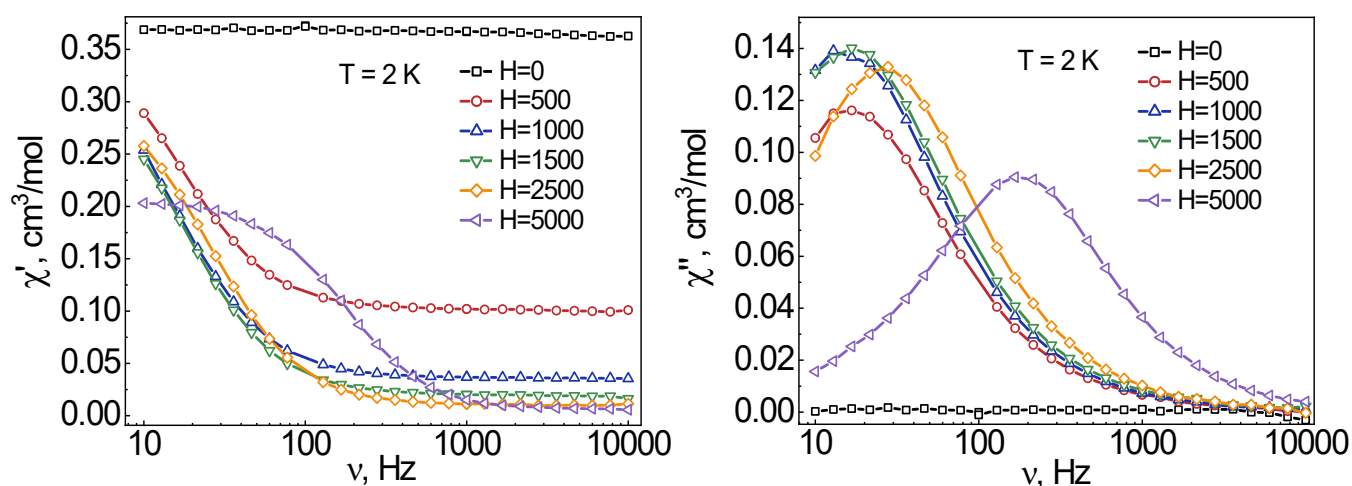
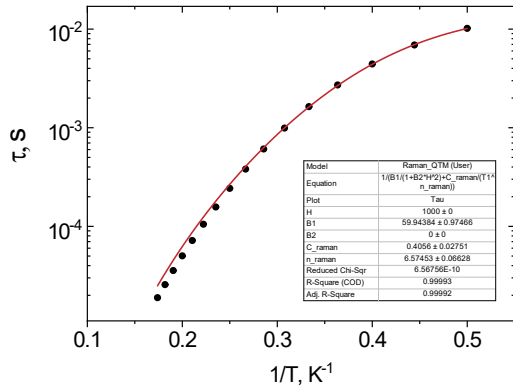


Fig. S2. Frequency dependencies of the real χ' (left) and imaginary χ'' (right) parts of the ac-magnetic susceptibility for complex **2** in dc-magnetic fields up to 5000 Oe at 2 K.

Table S2. Fitting of the τ vs. T dependences for **2**.

Dependence of the relaxation time τ on the reciprocal temperature for complex 2 ($H = 1.0$ kOe, $T = 2.00$ - 5.75 K).	Fit function, temperature range, and the best-fit parameters with uncertainties.																																																
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Raman+ QTM

$$\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}} + B$$

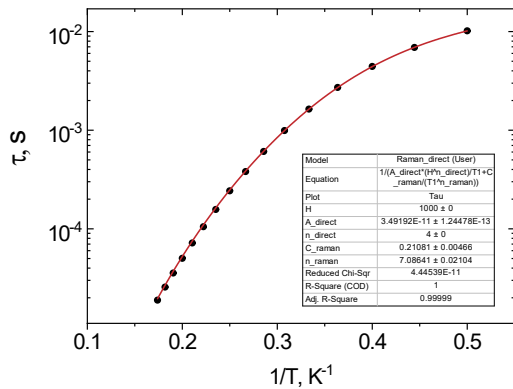
$$C_{\text{Raman}} = 0.41 \pm 0.03 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}$$

$$n_{\text{Raman}} = 6.57 \pm 0.07$$

$$B = 59.9 \pm 1.0 \text{ s}^{-1}$$

$$R^2 = 0.99993$$

Unsatisfactory fit



Raman+Direct

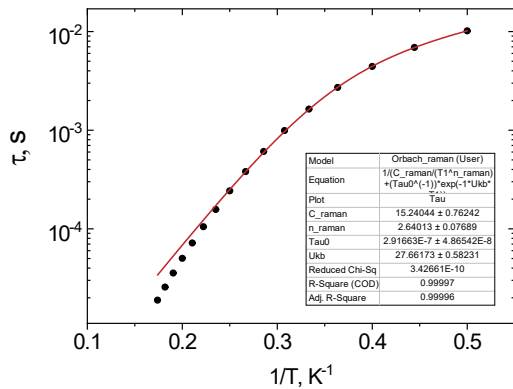
$$\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}} + A_{\text{direct}} T H^4$$

$$C_{\text{Raman}} = 0.211 \pm 0.005 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}$$

$$n_{\text{Raman}} = 7.09 \pm 0.02$$

$$A_{\text{direct}} = 3.49 \cdot 10^{-11} \pm 0.01 \cdot 10^{-11} \text{ K}^{-1} \text{Oe}^{-4} \text{ s}^{-1}$$

$$R^2 = 1$$



Orbach+Raman

$$\tau^{-1} = \tau_0^{-1} \cdot \exp(-\Delta E/kT) + C_{\text{Raman}} T^{n_{\text{Raman}}}$$

$$\Delta E/k = 27.7 \pm 0.6 \text{ K}$$

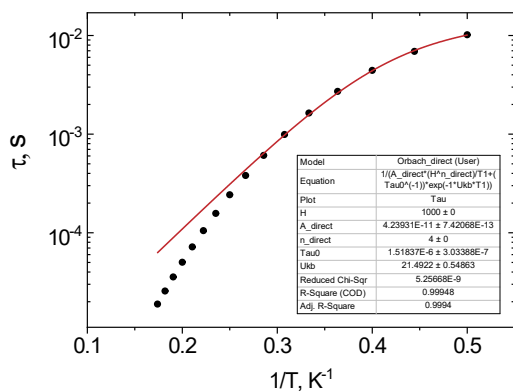
$$\tau_0 = 2.9 \cdot 10^{-7} \pm 0.5 \cdot 10^{-7} \text{ s}$$

$$C_{\text{Raman}} = 15.2 \pm 0.8 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}$$

$$n_{\text{Raman}} = 2.64 \pm 0.08$$

$$R^2 = 0.99997$$

Unsatisfactory fit



Orbach+Direct

$$\tau^{-1} = \tau_0^{-1} \cdot \exp(-\Delta E/kT) + A_{\text{direct}} T H^4$$

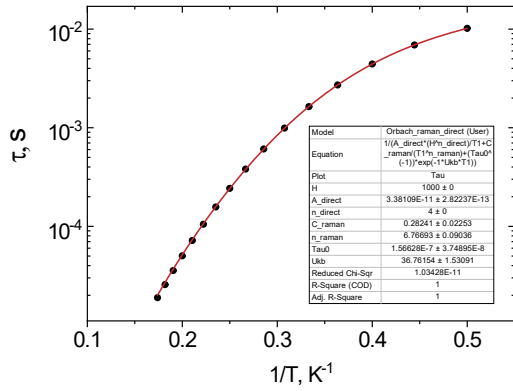
$$\Delta E/k = 21.5 \pm 0.5 \text{ K}$$

$$\tau_0 = 1.5 \cdot 10^{-6} \pm 0.3 \cdot 10^{-6} \text{ s}$$

$$A_{\text{direct}} = 4.24 \cdot 10^{-11} \pm 0.07 \cdot 10^{-11} \text{ K}^{-1} \text{Oe}^{-4} \text{ s}^{-1}$$

$$R^2 = 0.99948$$

Unsatisfactory fit



Orbach+Raman+Direct

$$\tau^{-1} = \tau_0^{-1} \cdot \exp(-\Delta E/kT) + C_{\text{Raman}} T^{n_{\text{Raman}}} + A_{\text{direct}} T H^4$$

$$\Delta E/k = 37 \pm 2 \text{ K}$$

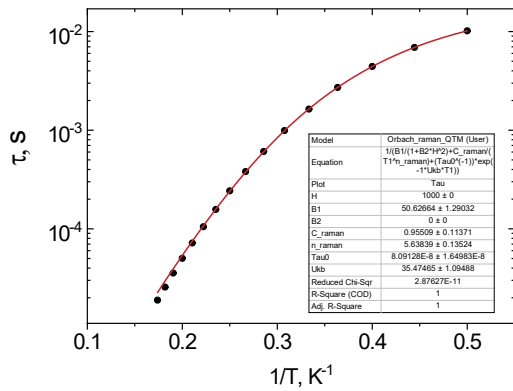
$$\tau_0 = 1.6 \cdot 10^{-7} \pm 0.4 \cdot 10^{-7} \text{ s}$$

$$C_{\text{Raman}} = 0.28 \pm 0.02 \text{ s}^{-1} \text{ K}^{-n_{\text{Raman}}}$$

$$n_{\text{Raman}} = 6.77 \pm 0.09$$

$$A_{\text{direct}} = 3.38 \cdot 10^{-11} \pm 0.03 \cdot 10^{-11} \text{ K}^{-1} \text{ Oe}^{-4} \text{ s}^{-1}$$

$$R^2 = 1$$



Orbach+Raman+QTM

$$\tau^{-1} = \tau_0^{-1} \cdot \exp(-\Delta E/kT) + C_{\text{Raman}} T^{n_{\text{Raman}}} + B$$

$$\Delta E/k = 35 \pm 1 \text{ K}$$

$$\tau_0 = 8 \cdot 10^{-8} \pm 2 \cdot 10^{-8} \text{ s}$$

$$C_{\text{Raman}} = 0.96 \pm 0.11 \text{ s}^{-1} \text{ K}^{-n_{\text{Raman}}}$$

$$n_{\text{Raman}} = 5.6 \pm 0.1$$

$$B = 51 \pm 1 \text{ s}^{-1}$$

$$R^2 = 1$$