# 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 | C2/c |
| 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 |
| Rexp | 5.53 |
| Rwp | 8.18 |
| Rp | 6.23 |
| GOF | 1.48 |
| R-Bragg | 2.70 |

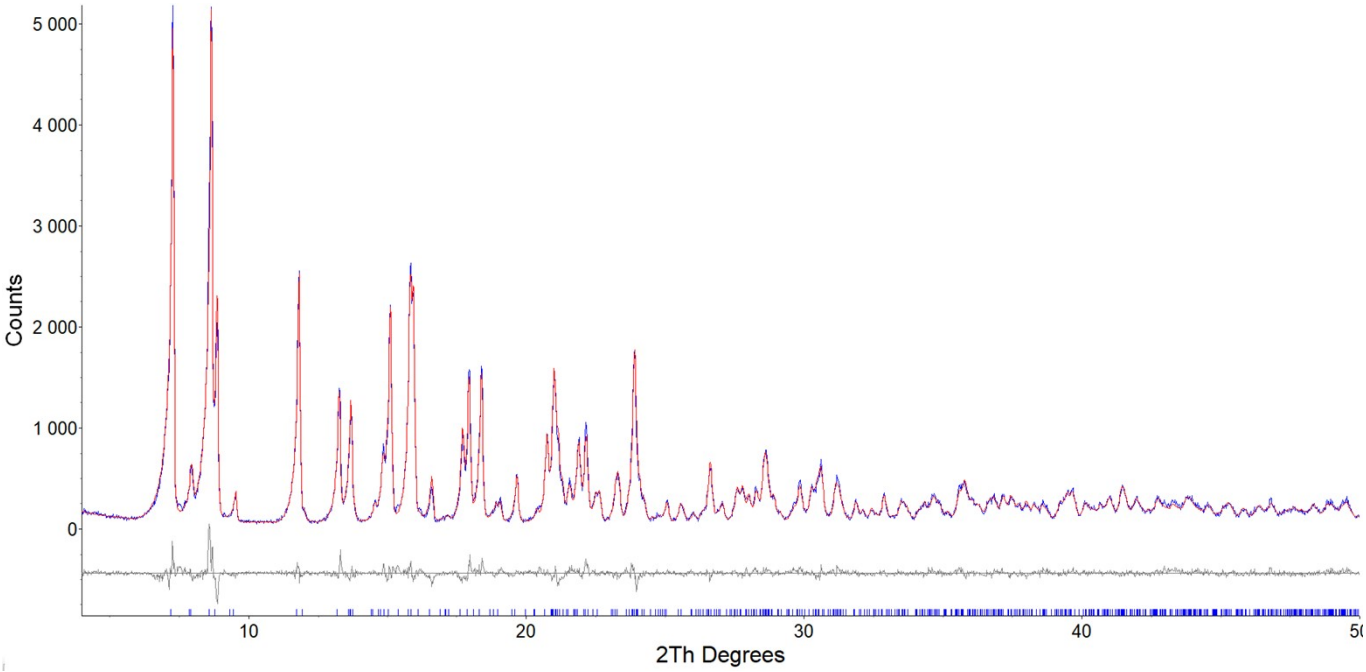



**Fig. S1**. Rietveld refinement profiles for **2**, for room temperature X-ray data. The calculated (for $[YT_3(Bath)]\cdot 0.5EtOH$) and experimental (for **2**) profiles are shown with the red and blue line, respectively. The bottom trace shows the difference curve. The vertical bars indicate the calculated positions of the Bragg peaks.

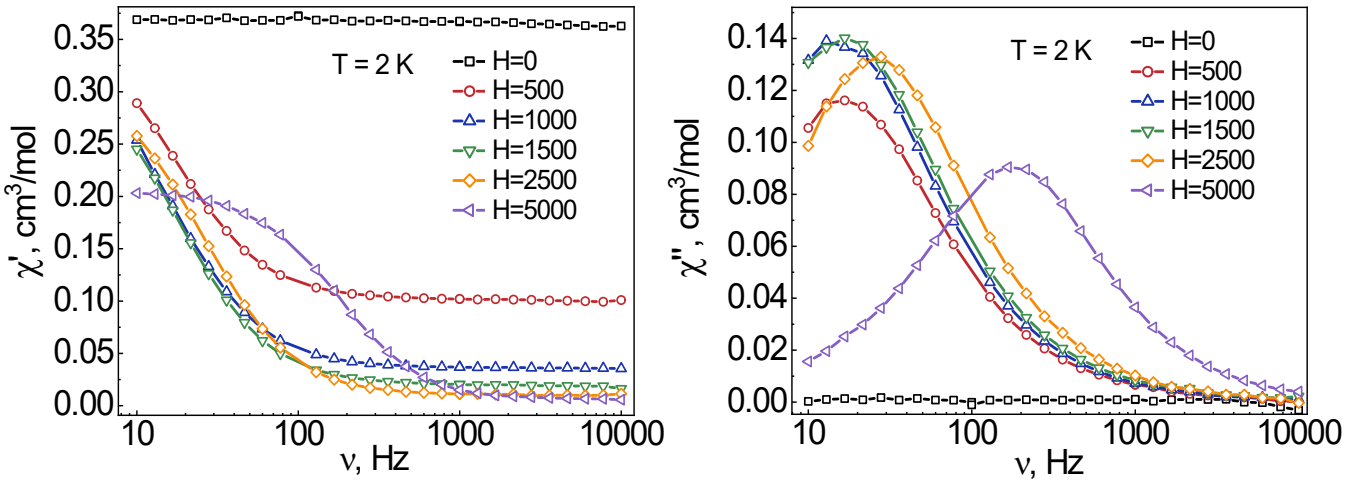
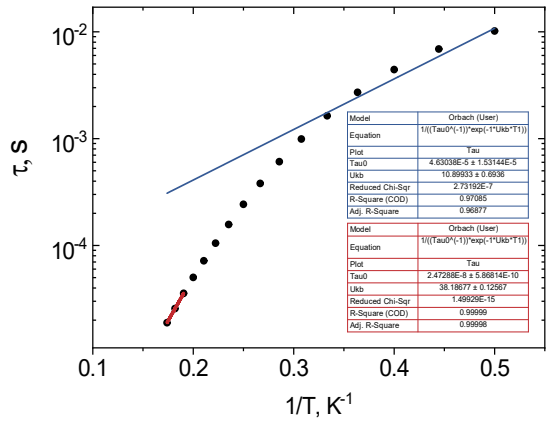
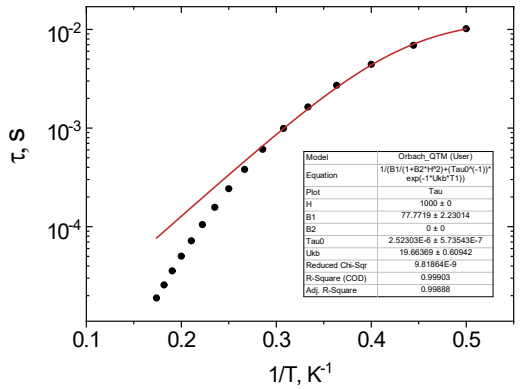
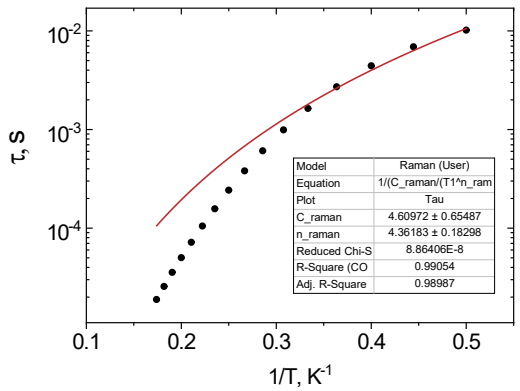
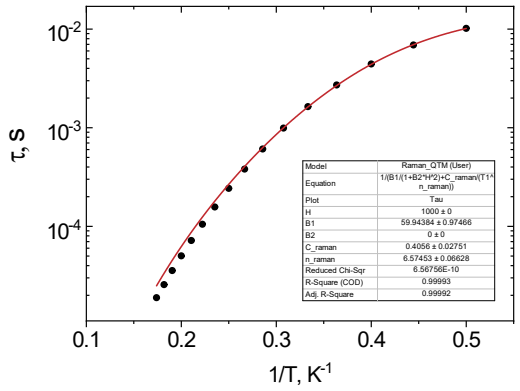



**Fig. S2.** Frequency dependencies of the real χ' (left) and imaginary χ'' (right) parts of the ac-magnetic susceptibility for complex **2** in dc-magnetic fields up to 5000 Oe at 2 K.

**Table S2.** Fitting of the $\tau$ *vs.* $T$ dependences for **2**.

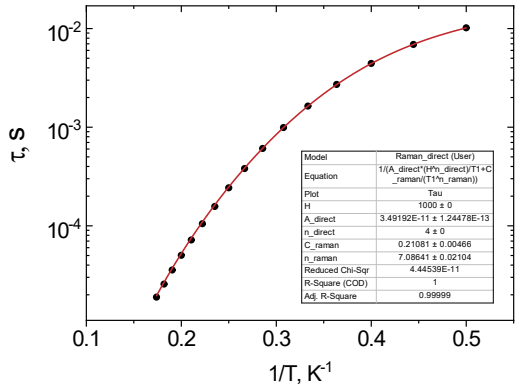
| Dependence of the relaxation time τ on the reciprocal temperature for complex **2** ($H$ = 1.0 kOe, $T$ = 2.00-5.75 K). | Fit function, temperature range, and the best-fit parameters with uncertainties. |
|---|---|
|  | **Orbach**<br>$\tau = \tau_0 \cdot \exp(\Delta E/kT)$<br><br>$T$ = 5.25-5.75 K<br>$\Delta E/k$ = 38.2 ± 0.1 K<br>$\tau_0 = 2.47 \cdot 10^{-8} \pm 0.06 \cdot 10^{-8}$ s<br>$R^2$ = 0.99999 (red line)<br><br>$T$ = 2.00-5.75 K<br>$\Delta E/k$ =10.9 ± 0.7 K<br>$\tau_0 = 5 \cdot 10^{-5} \pm 2 \cdot 10^{-5}$ s<br>$R^2$ = 0.97085 (blue line)<br>*Unsatisfactory fit* |
|  | **Orbach+ QTM**<br>$\tau^{-1} = \tau_0^{-1} \cdot \exp(-\Delta E/kT) + B$<br><br>$\Delta E/k$ = 19.7 ± 0.6 K<br>$\tau_0 = 2.5 \cdot 10^{-6} \pm 0.6 \cdot 10^{-6}$ s<br>B= 78 ± 2 $s^{-1}$<br>$R^2$ = 0.99903<br>*Unsatisfactory fit* |
|  | **Raman**<br>$\tau^{-1} = C_{Raman} T^{n\_Raman}$<br><br>$C_{Raman}$=4.6 ± 0.7 $s^{-1}K^{-nRaman}$<br>$n_{Raman}$=4.4 ± 0.2<br>$R^2$ = 0.99054<br>*Unsatisfactory fit* |




**Raman+ QTM**

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

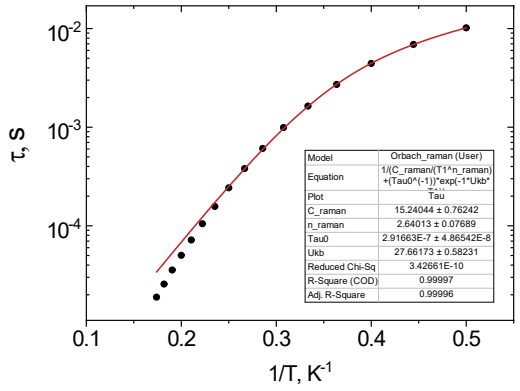
$C_{\text{Raman}} = 0.41 \pm 0.03\ \text{s}^{-1}\text{K}^{-\text{nRaman}}$
$\text{n}_{\text{Raman}} = 6.57 \pm 0.07$
$\text{B} = 59.9 \pm 1.0\ \text{s}^{-1}$
$R^2 = 0.99993$
*Unsatisfactory fit*




**Raman+Direct**

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

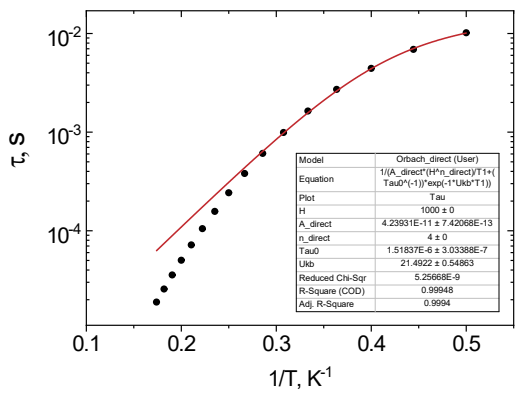
$C_{\text{Raman}} = 0.211 \pm 0.005\ \text{s}^{-1}\text{K}^{-\text{nRaman}}$
$\text{n}_{\text{Raman}} = 7.09 \pm 0.02$
$A_{direct} = 3.49 \cdot 10^{-11} \pm 0.01 \cdot 10^{-11}\ \text{K}^{-1}\text{Oe}^{-4}\text{s}^{-1}$
$R^2 = 1$




**Orbach+Raman**

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

$\Delta E/k = 27.7 \pm 0.6\ \text{K}$
$\tau_0 = 2.9 \cdot 10^{-7} \pm 0.5 \cdot 10^{-7}\ \text{s}$
$C_{\text{Raman}} = 15.2 \pm 0.8\ \text{s}^{-1}\text{K}^{-\text{nRaman}}$
$\text{n}_{\text{Raman}} = 2.64 \pm 0.08$
$R^2 = 0.99997$
*Unsatisfactory fit*




**Orbach+Direct**

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

$\Delta E/k = 21.5 \pm 0.5\ \text{K}$
$\tau_0 = 1.5 \cdot 10^{-6} \pm 0.3 \cdot 10^{-6}\text{s}$
$A_{direct} = 4.24 \cdot 10^{-11} \pm 0.07 \cdot 10^{-11}\ \text{K}^{-1}\text{Oe}^{-4}\text{s}^{-1}$
$R^2 = 0.99948$
*Unsatisfactory fit*

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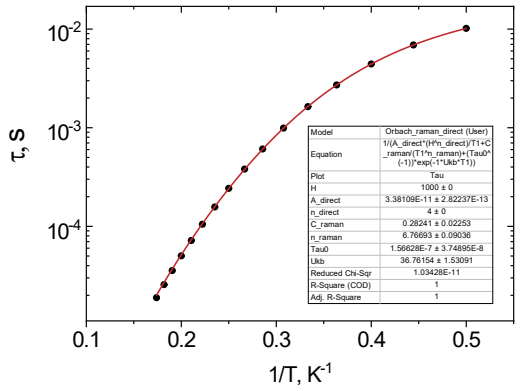
<td> 
</td>
<td>Orbach+Raman+Direct<br>$\tau^{-1} = \tau_0^{-1} \cdot \exp(-\Delta E/kT) + C_{\text{Raman}} T^{\text{nRaman}} + A_{direct} T H^4$<br><br>$\Delta E/k = 37 \pm 2$ K<br>$\tau_0 = 1.6 \cdot 10^{-7} \pm 0.4 \cdot 10^{-7}$ s<br>$C_{\text{Raman}} = 0.28 \pm 0.02$ s$^{-1}$K$^{-\text{nRaman}}$<br>$n_{\text{Raman}} = 6.77 \pm 0.09$<br>$A_{direct} = 3.38 \cdot 10^{-11} \pm 0.03 \cdot 10^{-11}$ K$^{-1}$Oe$^{-4}$s$^{-1}$<br>$R^2 = 1$</td>
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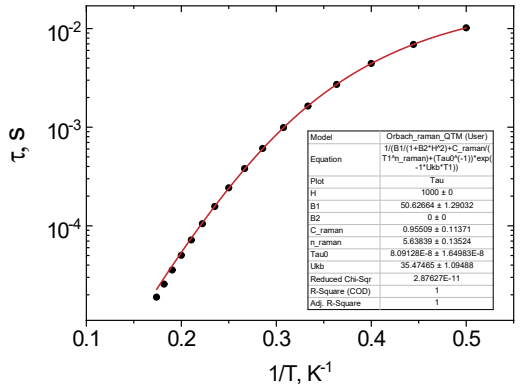
<td> 
</td>
<td>Orbach+Raman+QTM<br>$\tau^{-1} = \tau_0^{-1} \cdot \exp(-\Delta E/kT) + C_{\text{Raman}} T^{\text{nRaman}} + B$<br><br>$\Delta E/k = 35 \pm 1$ K<br>$\tau_0 = 8 \cdot 10^{-8} \pm 2 \cdot 10^{-8}$ s<br>$C_{\text{Raman}} = 0.96 \pm 0.11$ s$^{-1}$K$^{-\text{nRaman}}$<br>$n_{\text{Raman}} = 5.6 \pm 0.1$<br>$B = 51 \pm 1$ s$^{-1}$<br>$R^2 = 1$</td>
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