

МЕТОД ДИНАМИЧЕСКОЙ МАГНИТНОЙ ВОСПРИИМЧИВОСТИ В ИССЛЕДОВАНИИ КООРДИНАЦИОННЫХ СОЕДИНЕНИЙ

© 2024 г. Н. Н. Ефимов¹, *, К. А. Бабешкин¹, А. В. Ротов¹

¹Институт общей и неорганической химии им. Н.С. Курнакова РАН, Москва, Россия

*e-mail: nnefimov@narod.ru

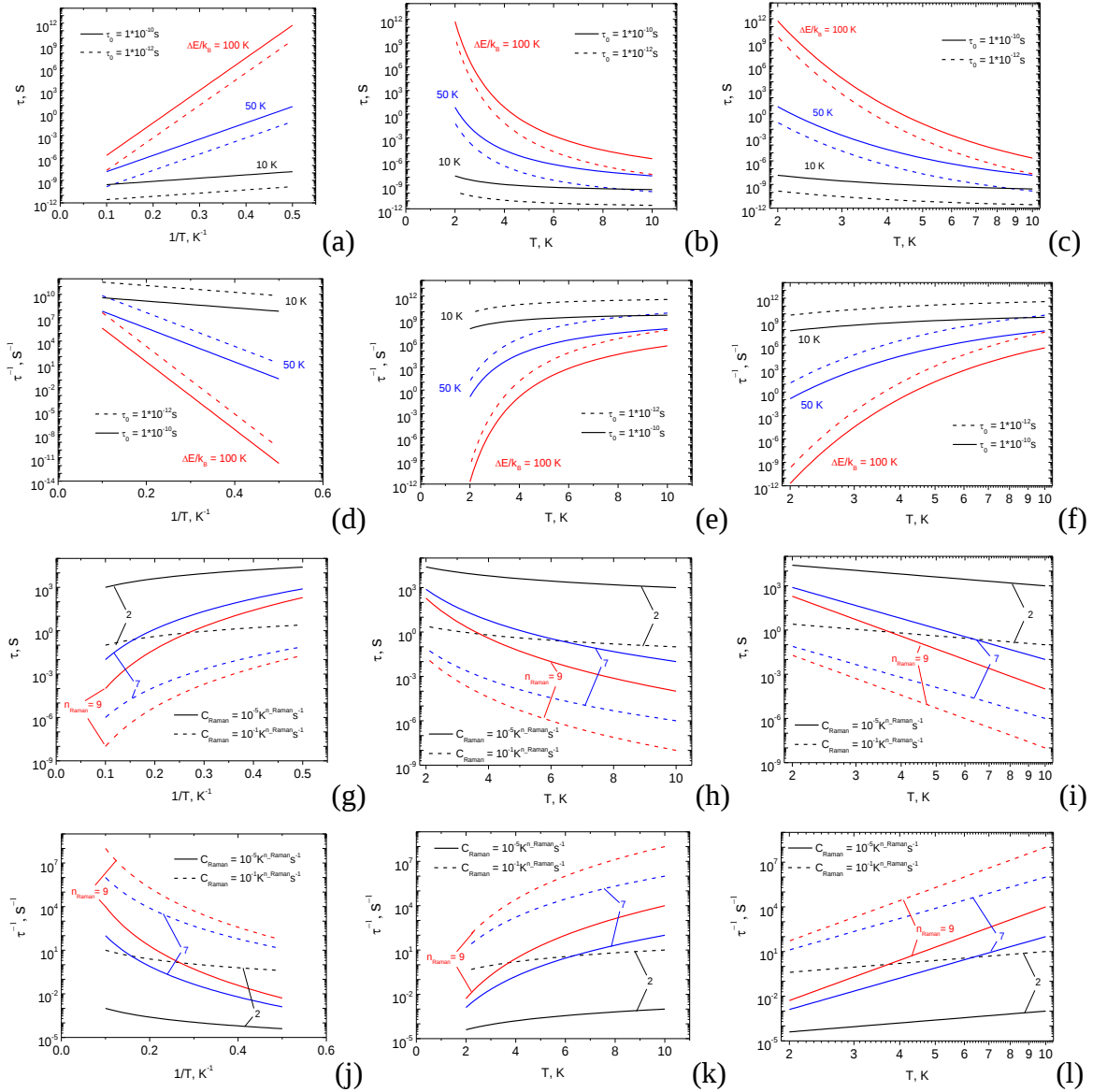


Fig. S1. Dependences of relaxation time(τ) vs. temperature (T) for different versions of coordinate axes for the Orbach (a-f) and Raman (g-l) mechanisms with the parameters presented on the graphs.

View of the generalized Debye model in the Origin program.

Part of the *.FDF file (Origin program) with the formula for approximating the dependence $\chi'(v)$ by the generalized Debye model.

[Fitting Parameters]

Names = Hi_inf,dHi,Tau,Alpha

[Independent Variables]

v =

[Dependent Variables]

Hi1 =

[Formula]

$$\text{Hi_inf} + ((d\text{Hi}) * (1 + (2 * \text{Pi} * v * \text{Tau})^{(1 - \text{Alpha})} * \sin(0.5 * \text{Alpha} * 3.1416))) / (1 + 2 * (2 * \text{Pi} * v * \text{Tau})^{(1 - \text{Alpha})} * \sin(0.5 * \text{Alpha} * 3.1416) + (2 * \text{Pi} * v * \text{Tau})^{(2 - 2 * \text{Alpha})})$$

Part of the *.FDF file (Origin program) with the formula for approximating the dependence $\chi''(\nu)$ by the generalized Debye model.

[Fitting Parameters]

Names = dHi,Tau,Alpha

[Independent Variables]

ν =

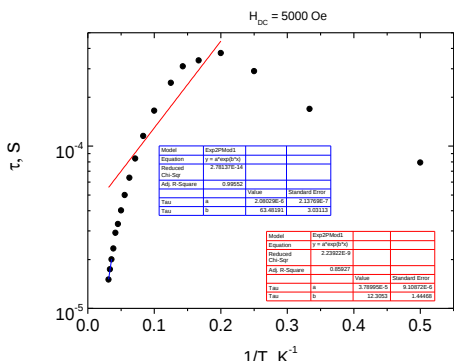
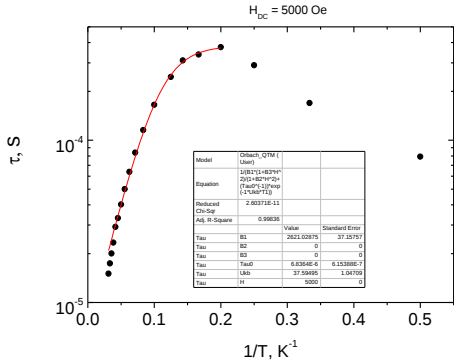
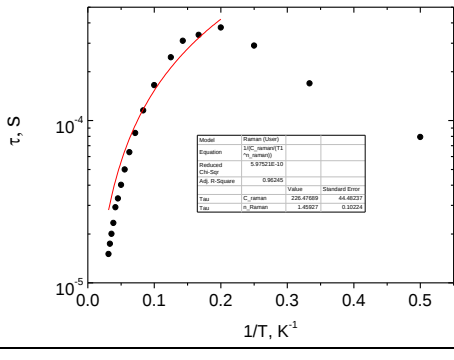
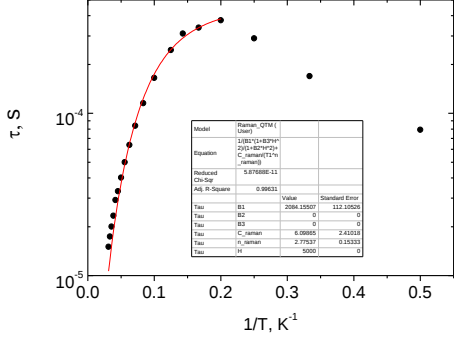
[Dependent Variables]

Hi2 =

[Formula]

$$\frac{((dHi)*(2*\pi*\nu*\tau)^{(1-\alpha)}*\cos(0.5*\alpha*3.1416))}{(1+2*(2*\pi*\nu*\tau)^{(1-\alpha)}*\sin(0.5*\alpha*3.1416)+(2*\pi*\nu*\tau)^{(2-2*\alpha)})}$$

Table S1. An example of enumerating relaxation mechanisms when interpreting measurement data for a complex **1** - $[\text{NaGd}(\text{VO})_2(\text{cbdc})_4(\text{H}_2\text{O})_{10}]_n$, where cbdc - cyclobutane-1,1-dicarboxylic acid anion. [Bazhina E.S., Korlyukov A.A., Voronina J.K. et al. // Magnetochemistry. 2021. V. 7]

Dependence of the relaxation time τ on the reciprocal temperature for complex 1 ($H = 5$ kOe, $T = 6\text{--}32$ K).	Fit function, temperature range, and the best-fit parameters with uncertainties.
	Orbach $\tau = \tau_0 \cdot \exp(\Delta E/kT)$ $T = 28\text{--}32$ K $\Delta E/k = 63 \pm 3$ K $\tau_0 = 2.1 \cdot 10^{-6} \pm 2 \cdot 10^{-7}$ s $R^2 = 0.99552$ (blue line) $T = 6\text{--}32$ K $\Delta E/k = 12 \pm 1$ K $\tau_0 = 3.8 \cdot 10^{-5} \pm 9 \cdot 10^{-6}$ s $R^2 = 0.85927$ (red line) Unsatisfactory fit
	Orbach+ QTM $\tau^{-1} = \tau_0^{-1} \cdot \exp(-\Delta E/kT) + B$ $T = 6\text{--}32$ K $\Delta E/k = 38 \pm 1$ K $\tau_0 = 6.8 \cdot 10^{-6} \pm 6 \cdot 10^{-7}$ s $B = 2621 \pm 37$ s^{-1} $R^2 = 0.99836$
	Raman $\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}}$ $T = 6\text{--}32$ K $C_{\text{Raman}} = 226 \pm 44$ s^{-1}K$^{-n_{\text{Raman}}}$ $n_{\text{Raman}} = 1.5 \pm 0.1$ $R^2 = 0.96245$
	Raman+ QTM $\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}} + B$ $T = 6\text{--}32$ K $C_{\text{Raman}} = 6 \pm 2$ s^{-1}K$^{-n_{\text{Raman}}}$ $n_{\text{Raman}} = 2.8 \pm 0.2$ $B = 2084 \pm 112$ s^{-1} $R^2 = 0.99631$

