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Modeling Lifetimes of Excited States in Mixed Coordination Compounds of Eu^{3+} and Tb^{3+}

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In this study, we applied two models, recently proposed by our group, for modeling lifetimes of excited states in mixed complexes of Eu^{3+} and Tb^{3+}[1]. Both models consider a statistical distribution of Eu^{3+} and Tb^{3+} ions in the crystal lattice to calculate ion-ion energy transfer rates, following literature procedures. In Model 1, n sets of rate equations are solved for the n shortest Eu^{3+}-Tb^{3+} distances, where ion-ion energy transfer rates are non-zero. Using the fourth-order Runge-Kutta method and the Malta et al. model [2] for ligand-to-metal energy transfer rates and LMCT states, the simulated luminescence decay curve is obtained as a superposition of fitted exponentials, weighted by the distribution coefficients for the n distances. In Model 2, the average ion-ion transfer rate is initially calculated, considering the statistical distribution of Eu^{3+}-Tb^{3+} distances in the crystal lattice. Then, a single set of rate equations is solved using the fourth-order Runge-Kutta method, also considering the Malta et al. model [2]. An example is shown in Figure 1 for modeling the lifetime of the $^5D_4$ level of the Tb^{3+} ion in the compound $(Hphen)_2[EuTb(2\text{-}OHBz)_8(H_2O)_2]\cdot 2H_2O$ [1]. Model 1 has proven more satisfactory than Model 2 and also more effective than a widely used methodology in the literature [3], which resulted in a lifetime 39% shorter than the experimental value for the example below.

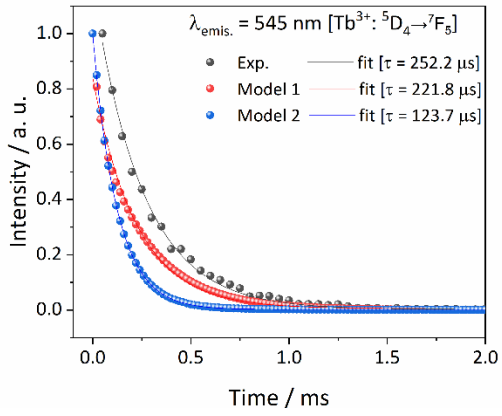

Figure 1: Decay Curves for the $^5D_4 \rightarrow {}^7F_5$ Transition of Tb^{3+} in $(Hphen)_2[EuTb(2\text{-}OHBz)_8(H_2O)_2]\cdot 2H_2O$.

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References

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