

# Features of the Molecular Structure and Luminescence of Rare-Earth Metal Complexes with Perfluorinated (Benzothiazolyl)phenolate Ligands

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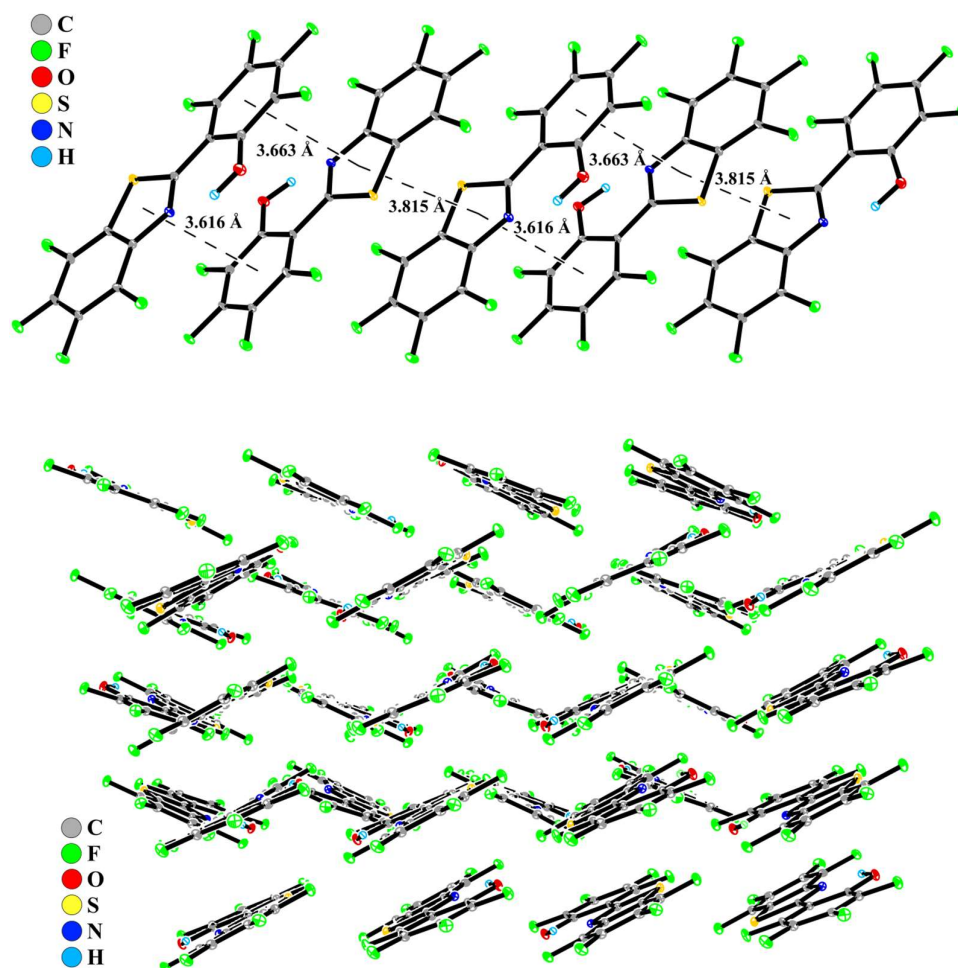


Figure S1. Packing motifs of H(SONF).

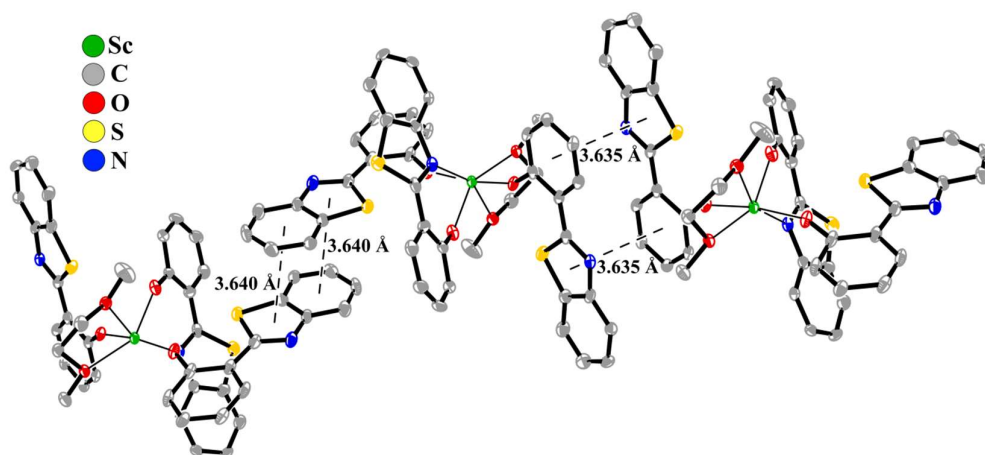


Figure S2. Fragment of crystal packing of 2. The F and H atoms are omitted for clarity.

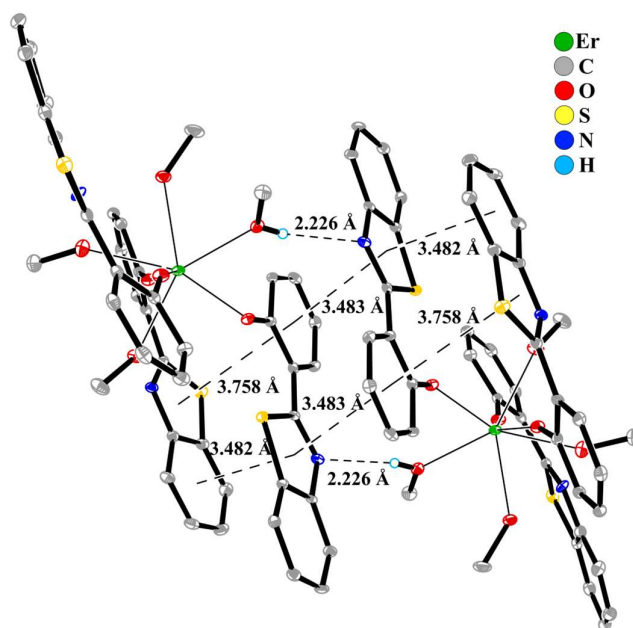


Figure S3. Fragment of crystal packing of 7. The F and H atoms are omitted for clarity.

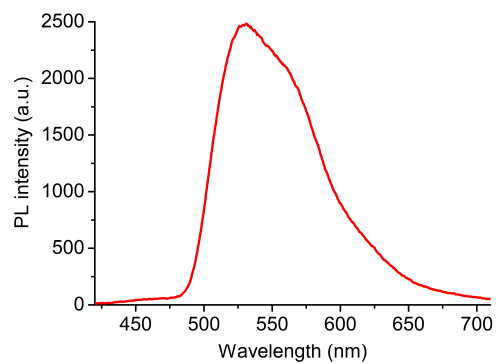
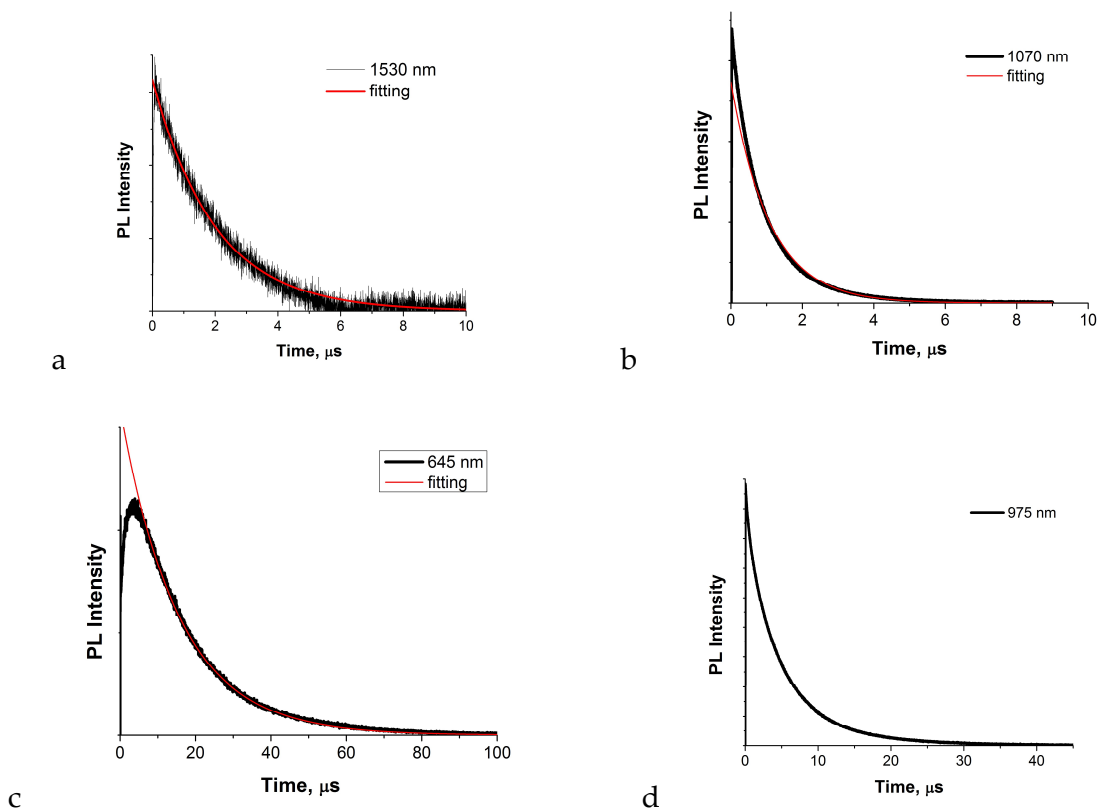
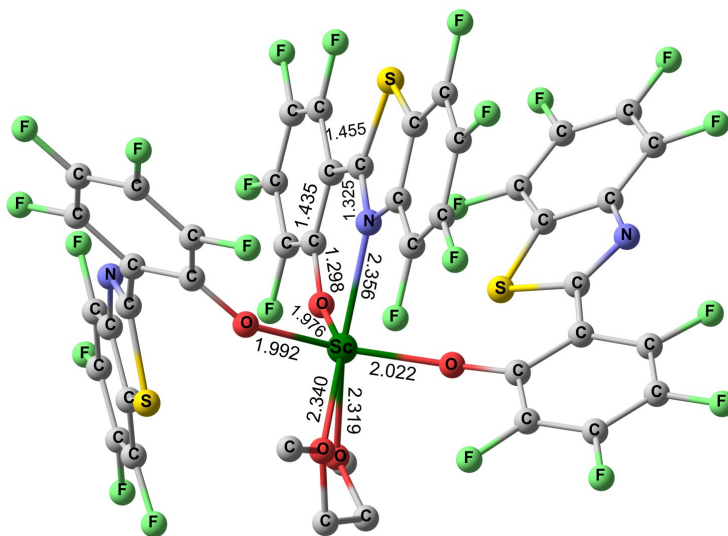


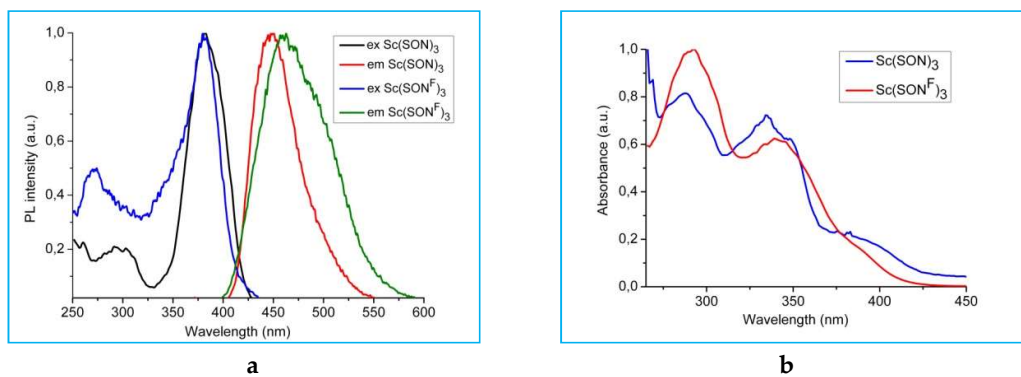
Figure S4. Photoluminescence spectrum of the gadolinium complex 1 at 77 K.



**Figure S5.** NIR PL kinetics of  $\text{Er}(\text{SO}_3\text{F})_3$  at 1530 (a),  $\text{Nd}(\text{SO}_3\text{F})_3$  at 1070 (b),  $\text{Sm}(\text{SO}_3\text{F})_3$  at 645 (c) and  $\text{Yb}(\text{SO}_3\text{F})_3$  at 975 nm (d). Excitation – Nd:YAG laser with  $\lambda$  355 nm (pulse duration  $\sim$  5 ns). Red lines are fitting curves.



**Figure S6.** The optimized geometry of **2**.



**Figure 7.** Normalized EPL, PL (**a**) and absorption (**b**) spectra of nonfluorinated and fluorinated scandium complexes in THF solution ( $\lambda_{exc} = 385 \text{ nm}$ ,  $10^{-5} \text{ M}$ ).