A Molecular Dynamics (MD) simulation of an aqueous TbCl₃ (~0.3 M) solution was performed using the GROMACS 3.3 package,¹,² and to study the effect of SO₄²⁻, an MD simulation of an aqueous solution containing ~0.3 M TbCl₃ and ~3.9 M (NH₄)₂SO₄ was done as well. The parameters used for these calculations are provided in Table S1.

According to these calculations, the first coordination shell of the Tb³⁺ ion is composed of 8 H₂O molecules in a pure aqueous TbCl₃ solution, while in a mixed aqueous TbCl₃ + (NH₄)₂SO₄ solution, it was composed of 4 H₂O molecules and 2 SO₄²⁻ ions. A possible structure for Tb(OH₂)₈³⁺ and Tb(SO₄)₂(OH₂)₄⁻, respectively, is shown in Figure S1. These results suggest that SO₄²⁻ anions replace some of the H₂O molecules in the first coordination shell, which reduces the quenching of the luminescence. However, it should be noted that the coordination number for the aquo complex (8)
determined by these calculations differs from the value (9) reported in the literature. Further studies are required to clarify this discrepancy.

Figure S1: One of the possible structures for Tb(OH$_2$)$_8^{3+}$ (left) and Tb(SO$_4$)$_2$(OH$_2$)$_4^{-}$ (right).

References:


