

## Tuning Emissive Color of Trivalent Terbium Ion through Environmental Factors: Optoelectronic Insights from Theoretical, Spectral and Computational Studies

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### SUPPLEMENTARY INFORMATION

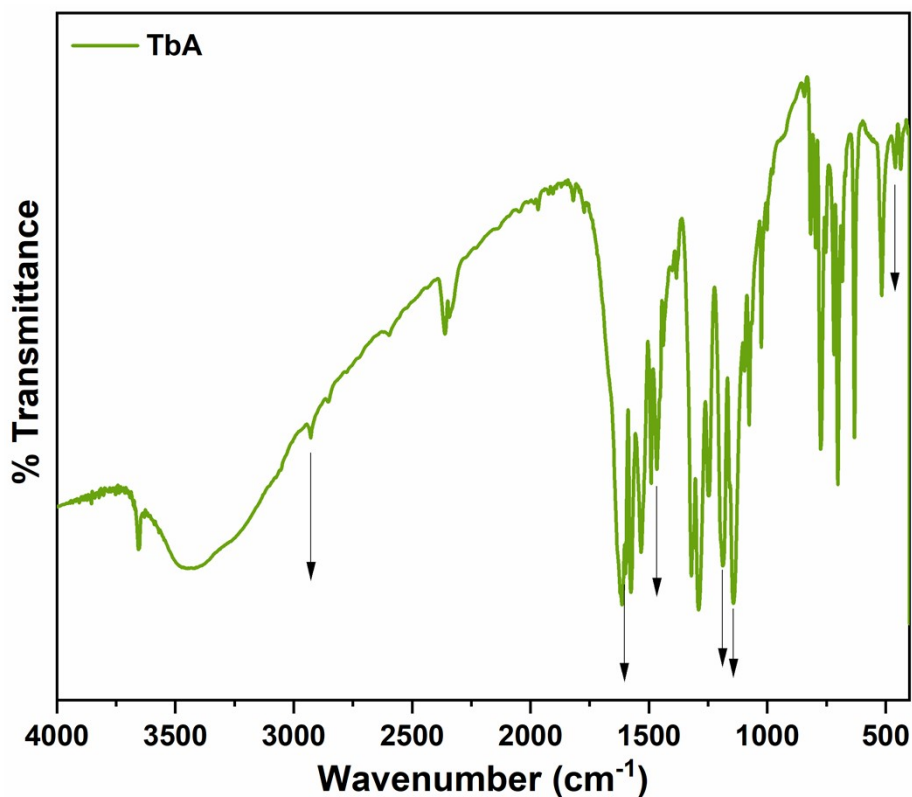


Fig. S1 IR profile of TbA

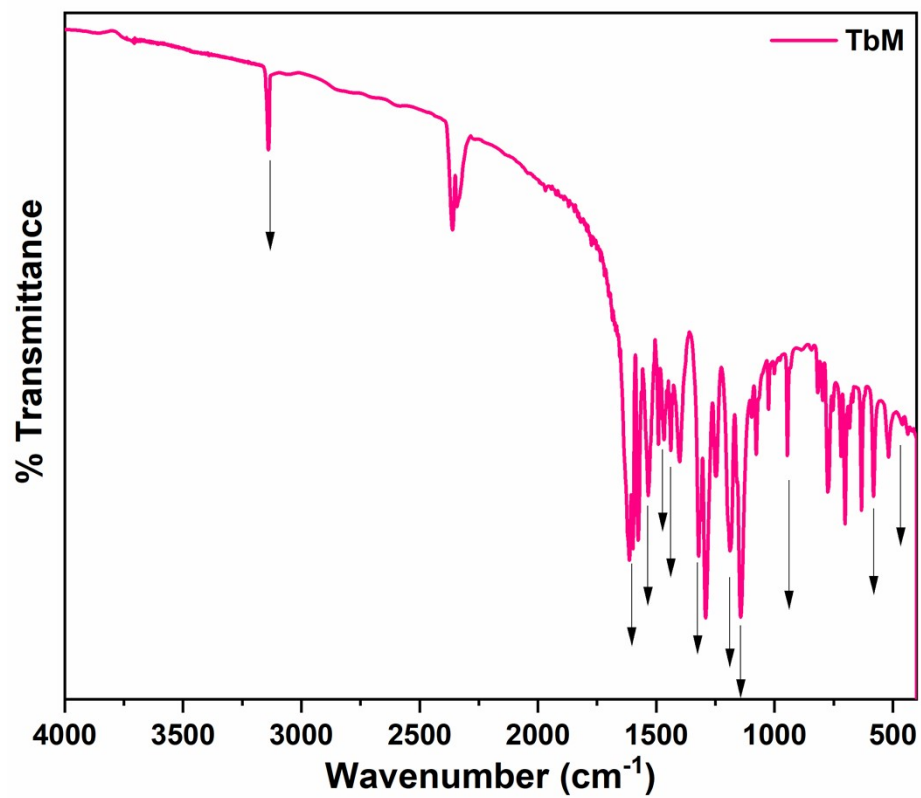


Fig. S2 IR profile of TbM

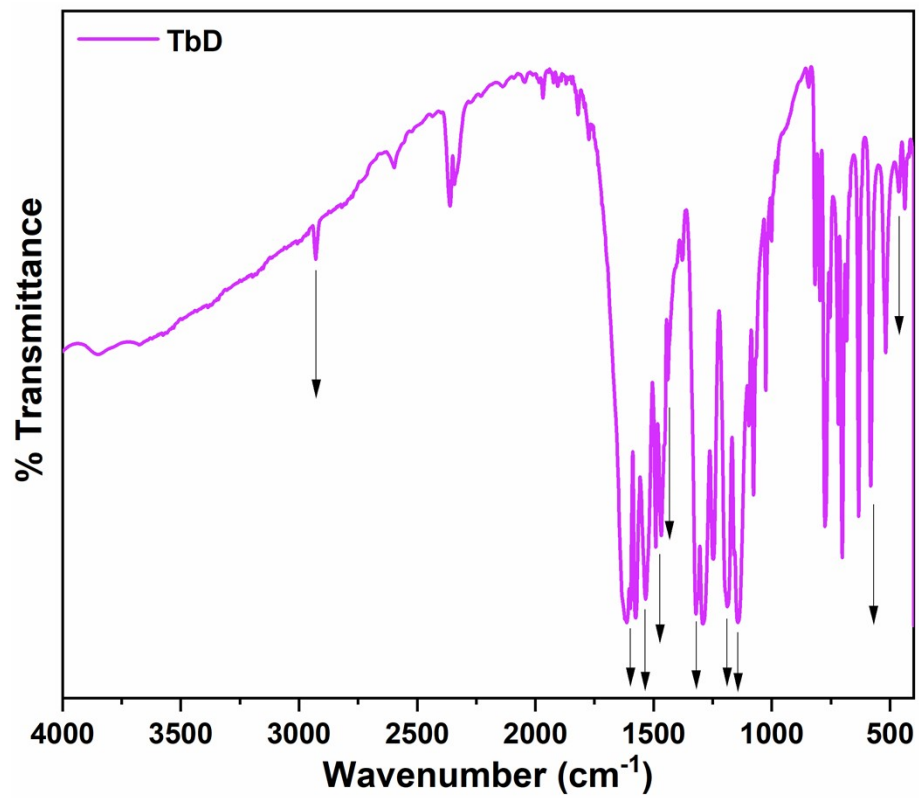
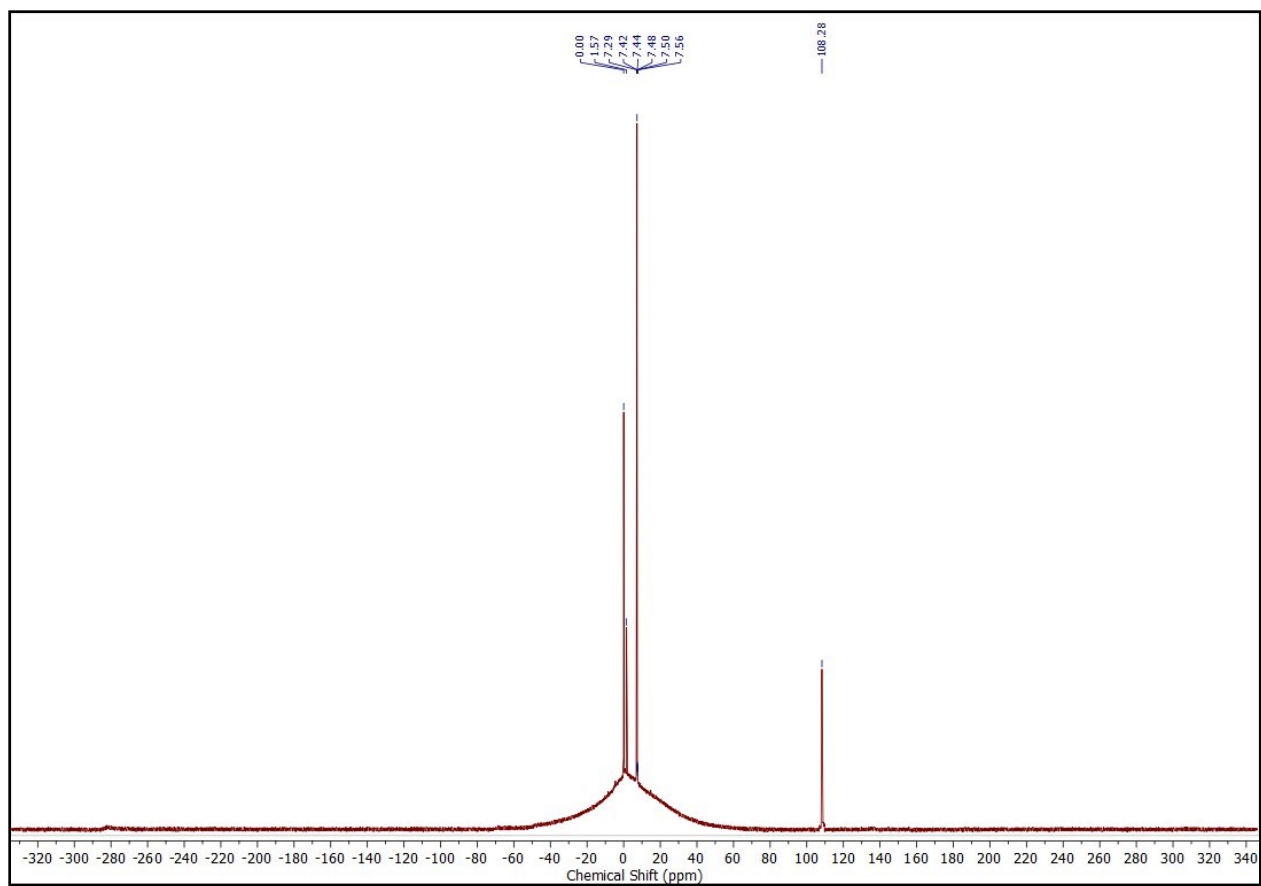
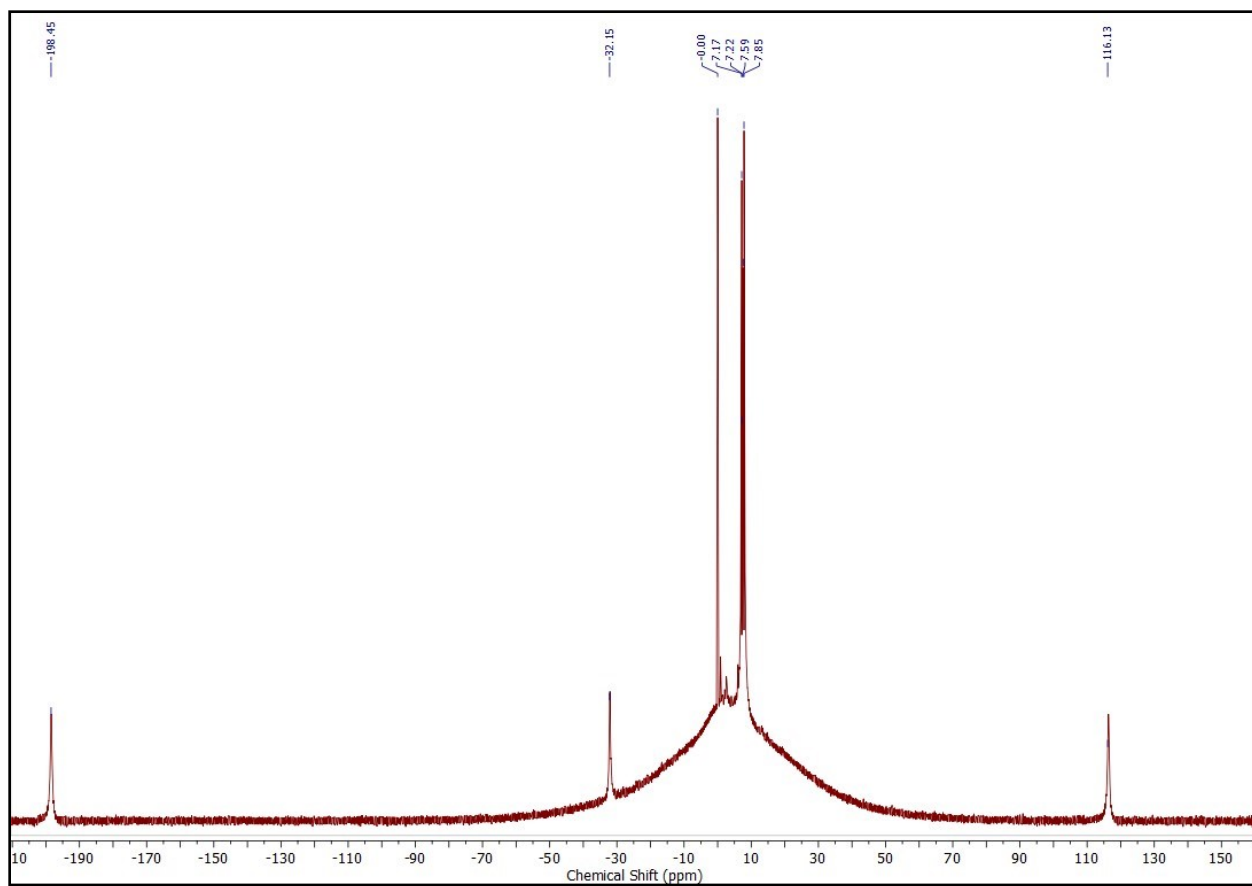


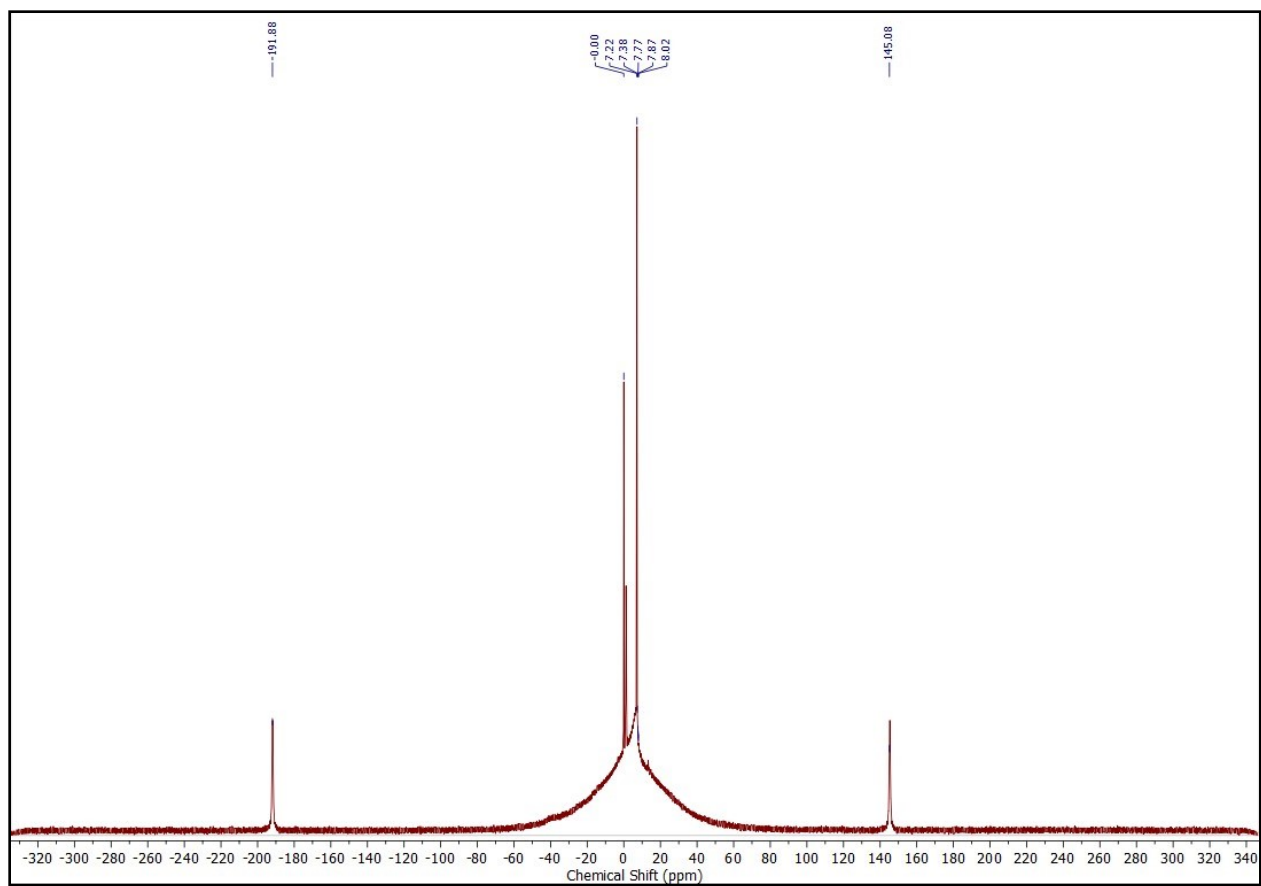
Fig. S3 IR profile of TbD



**Fig. S4** <sup>1</sup>H-NMR spectrum of TbA in CDCl<sub>3</sub>



**Fig. S5** <sup>1</sup>H-NMR spectrum of TbM in CDCl<sub>3</sub>



**Fig. S6**  $^1\text{H}$ -NMR spectrum of TbD in  $\text{CDCl}_3$

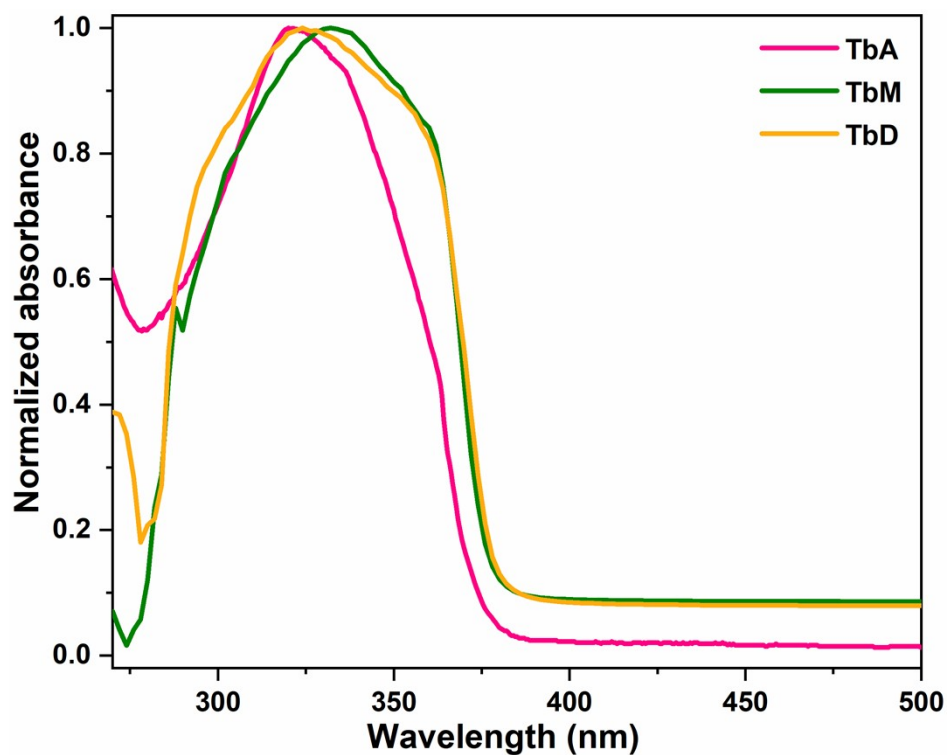


Fig. S7 UV-Absorption profiles of synthesised complexes in solid form

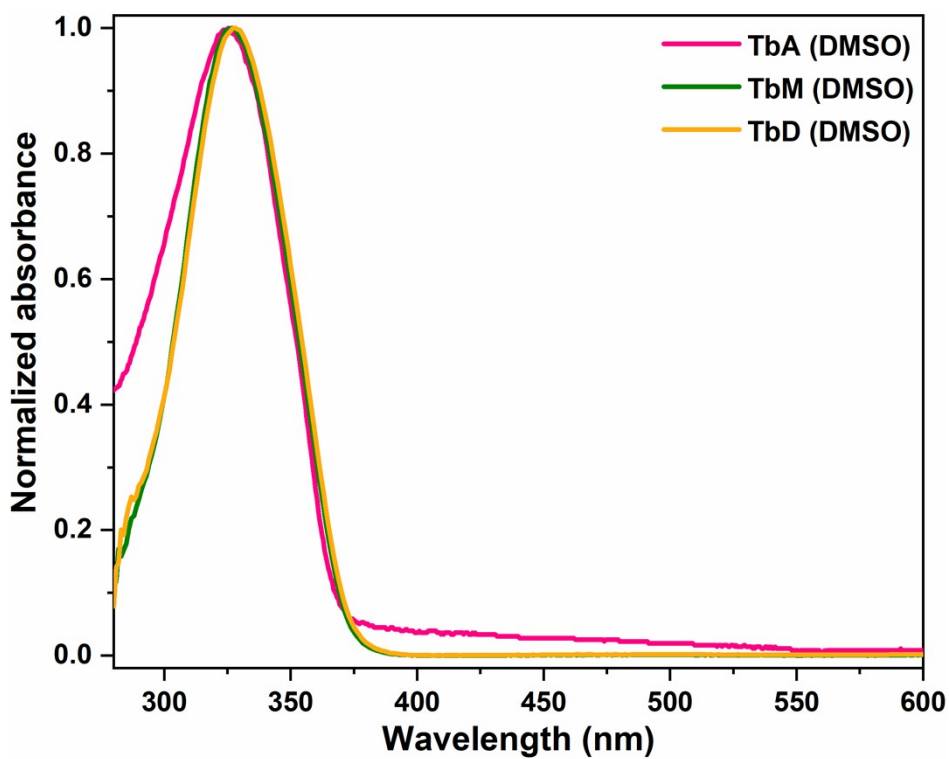


Fig. S8 UV-Absorption profiles of synthesised complexes in DMSO