

## Supporting Information for

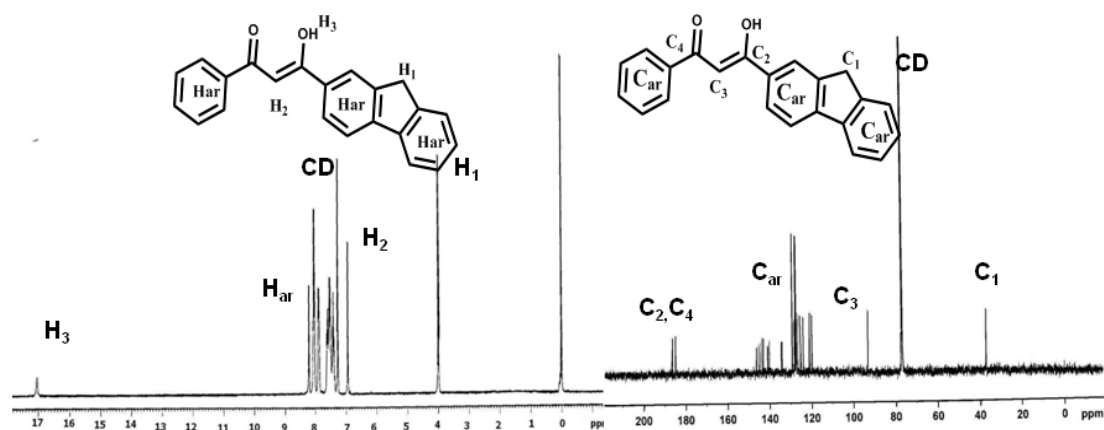
### **Tuning of the Excitation Wavelength from UV to Visible Region in Eu<sup>3+</sup>- $\beta$ -Diketonate Complexes: Comparison of Theoretical and Experimental Photophysical Properties**

**V. Divya<sup>a</sup>, M. L. P. Reddy\*<sup>a</sup> and Ricardo O. Freire<sup>b</sup>**

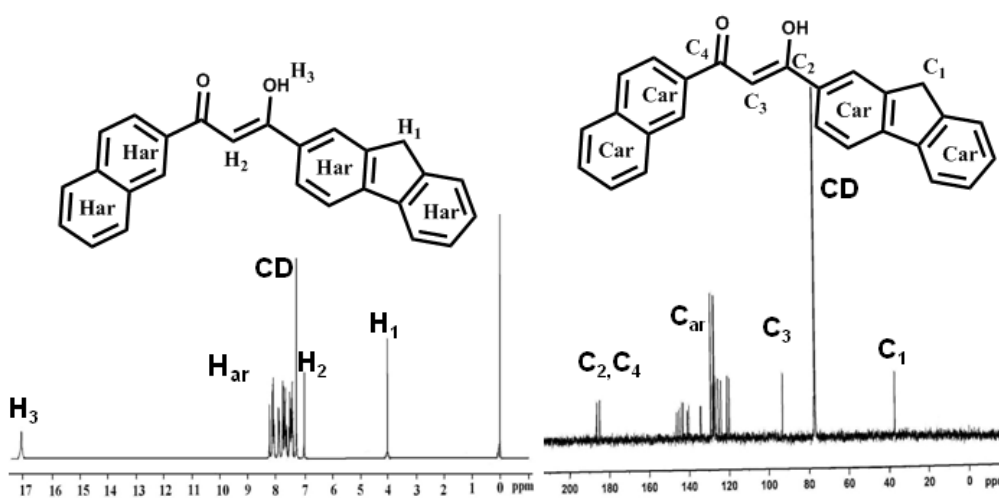
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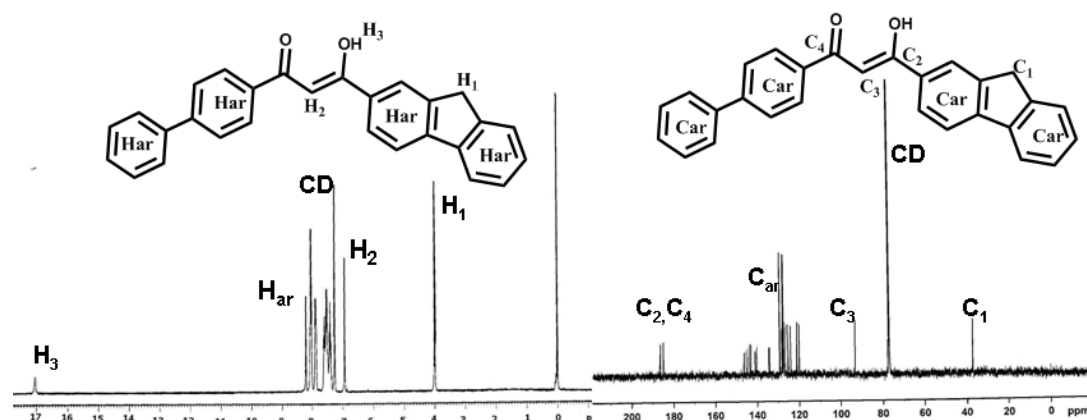
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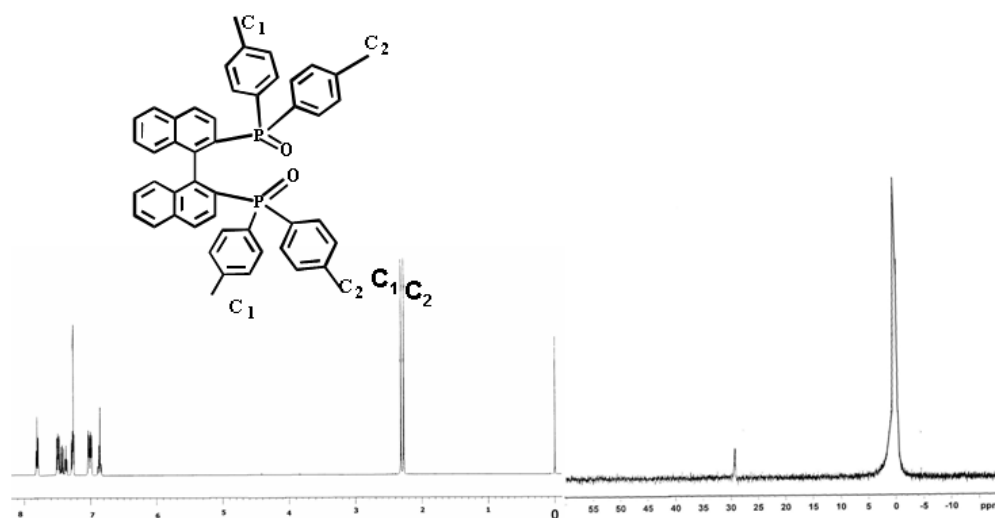
**Fig. S1**  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectrum of the ligand HBFPD.



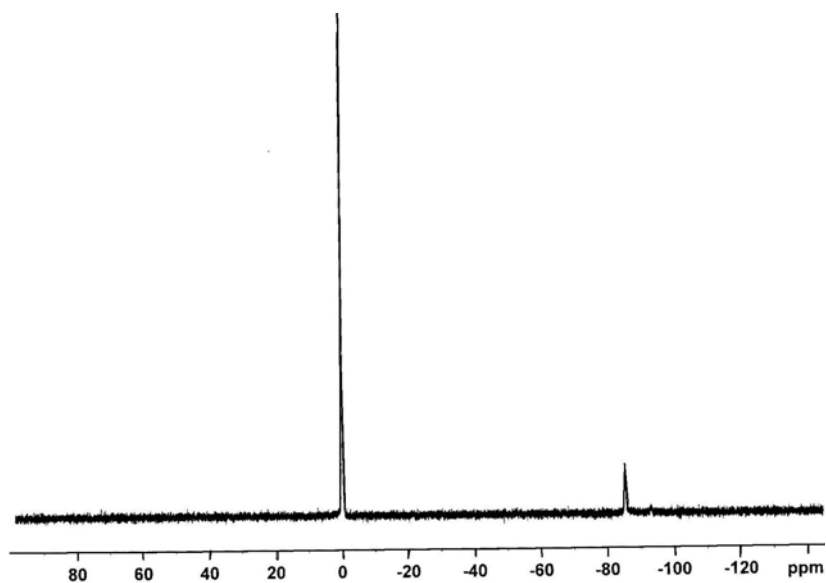
**Fig. S2**  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectrum of the ligand HNFPD.



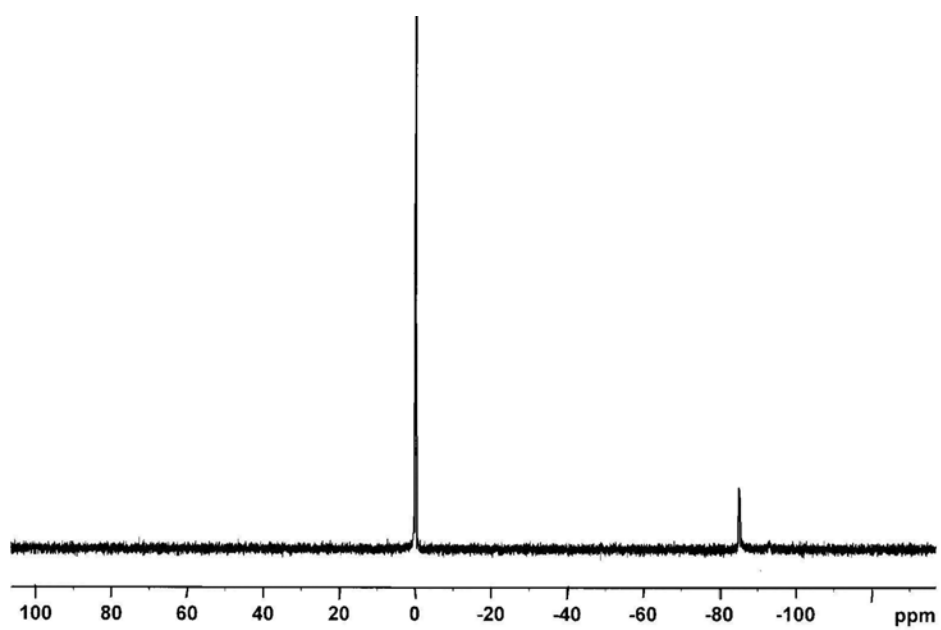
**Fig. S3**  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectrum of the ligand HBPFDP.



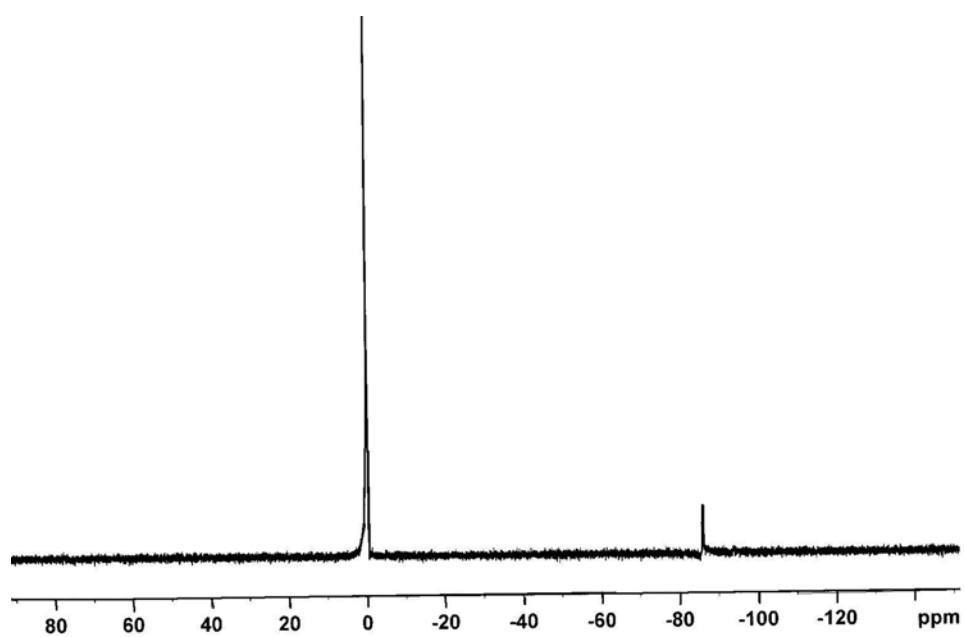
**Fig. S4**  $^1\text{H}$  NMR and  $^{31}\text{P}$  NMR spectrum of the ligand TBNPO.



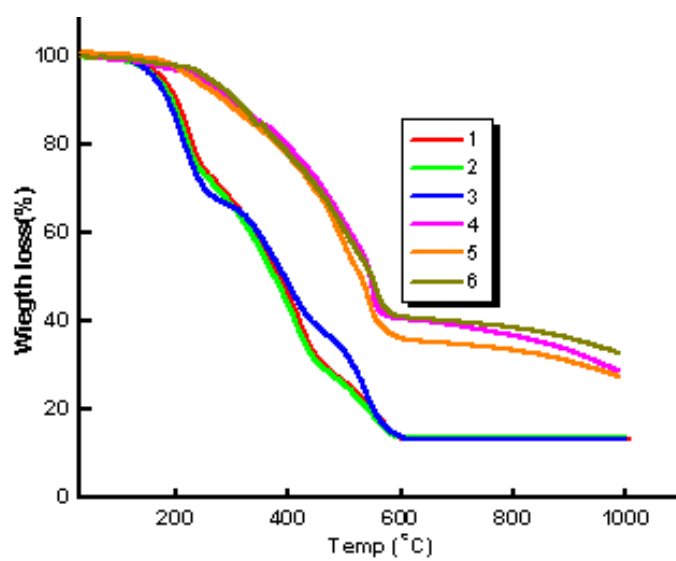
**Fig. S5**  $^{31}\text{P}$  NMR spectrum of the complex **4**



**Fig. S6**  $^{31}\text{P}$  NMR spectrum of the complex **5**



**Fig. S7**  $^{31}\text{P}$  NMR spectrum of the complex **6**



**Fig. S8** TG curve for the complexes **1-6**

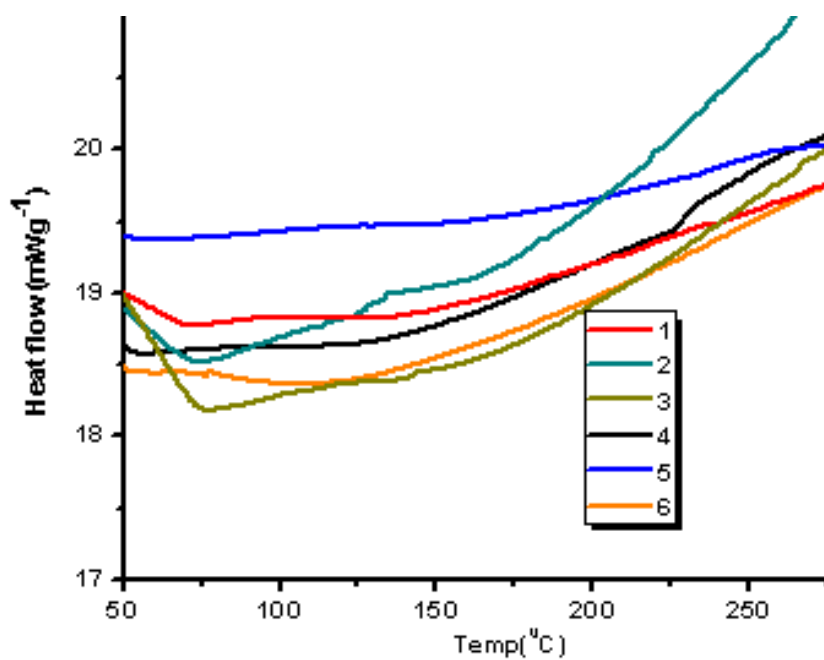


Fig. S9 DSC curve for the complexes 1-6

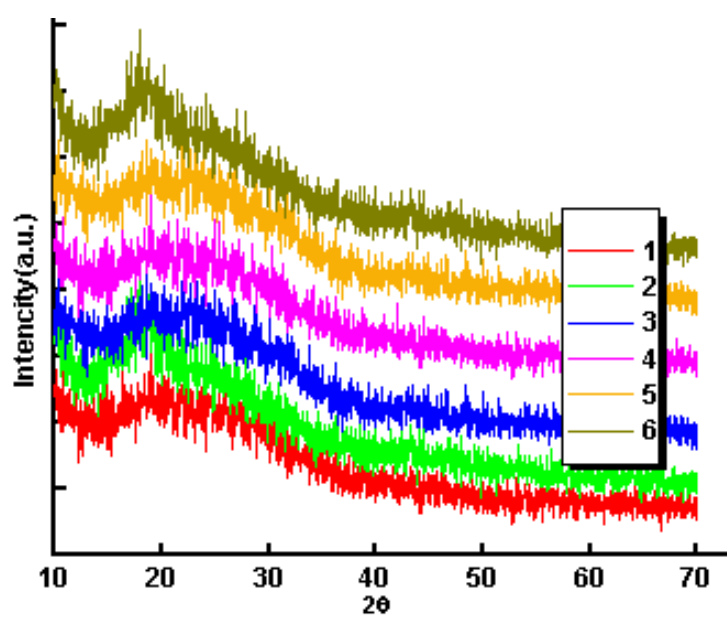
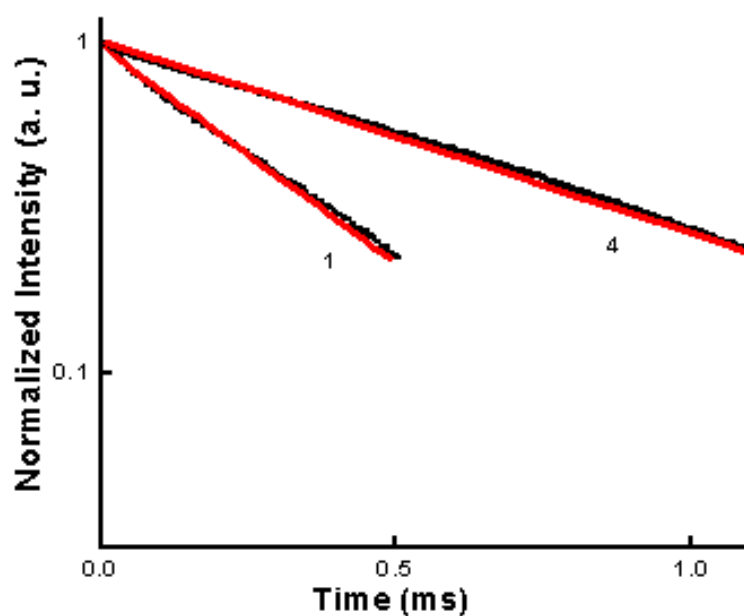
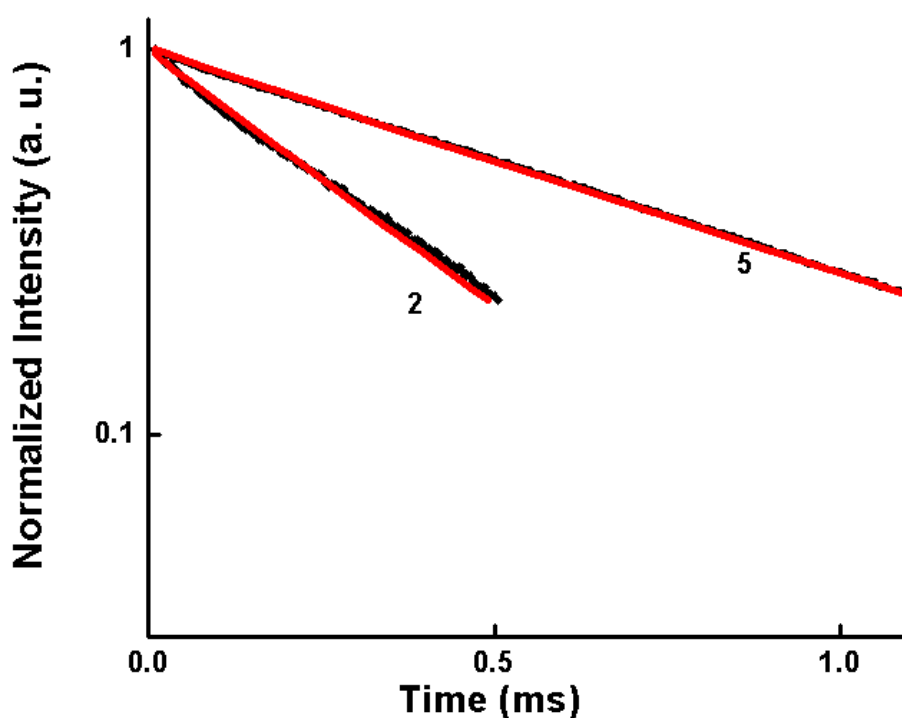


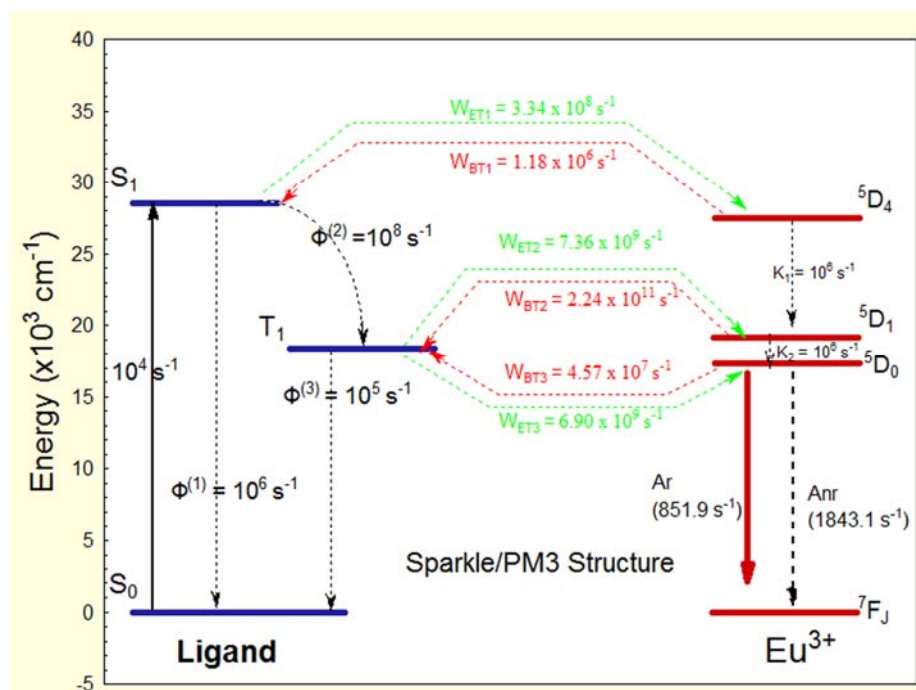
Fig. S10 XRD patterns for for the complexes 1-6



**Fig. S11**  $^5D_0$  decay profiles for complexes **1** and **4** (solid-state) excited at 400 nm and emission monitored around 612 nm. The straight lines are the best fits ( $r^2 = 0.99$ ) considering single-exponential behaviour.



**Fig. S12**  $^5D_0$  decay profiles for complexes **2** and **5** (solid-state) excited at 430 nm and emission monitored around 612 nm. The straight lines are the best fits ( $r^2 = 0.99$ ) considering single-exponential behaviour.



**Fig. S13** Energy level diagram for complex **3** showing the most probable channels for the intramolecular energy transfer process.