

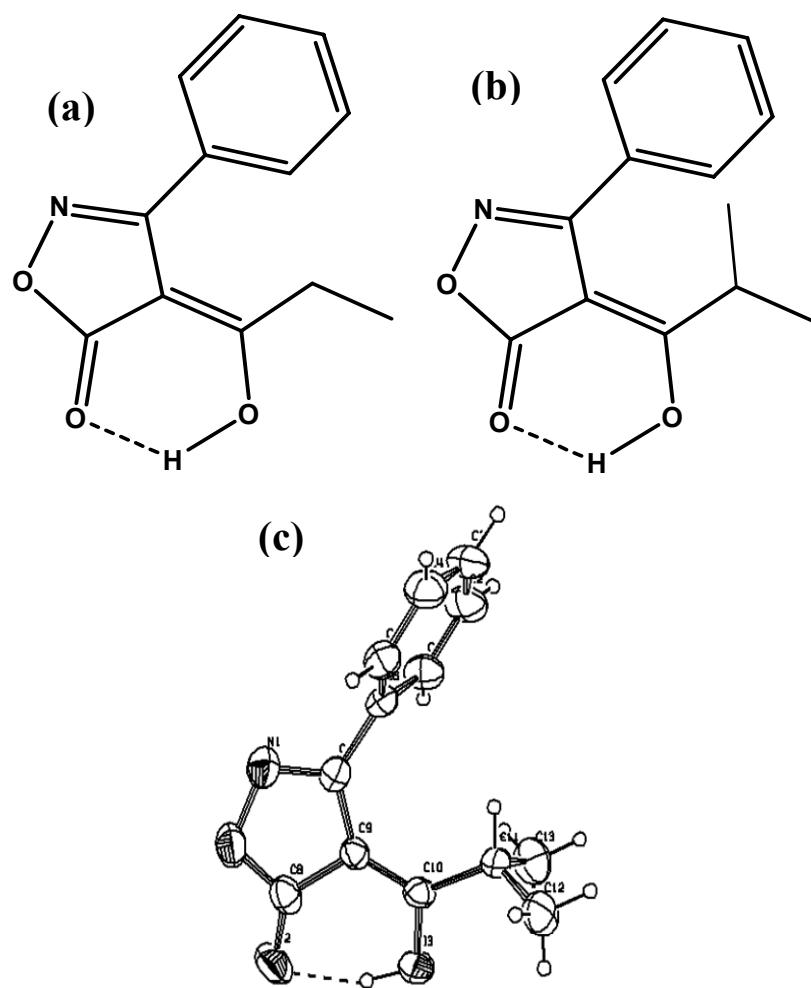
## **Supplementary Information**

### **3-Phenyl-4-acyl-5-isoxazolonate complex of Tb<sup>3+</sup> doped into poly-β-hydroxybutyrate matrix as a promising light-conversion molecular device**

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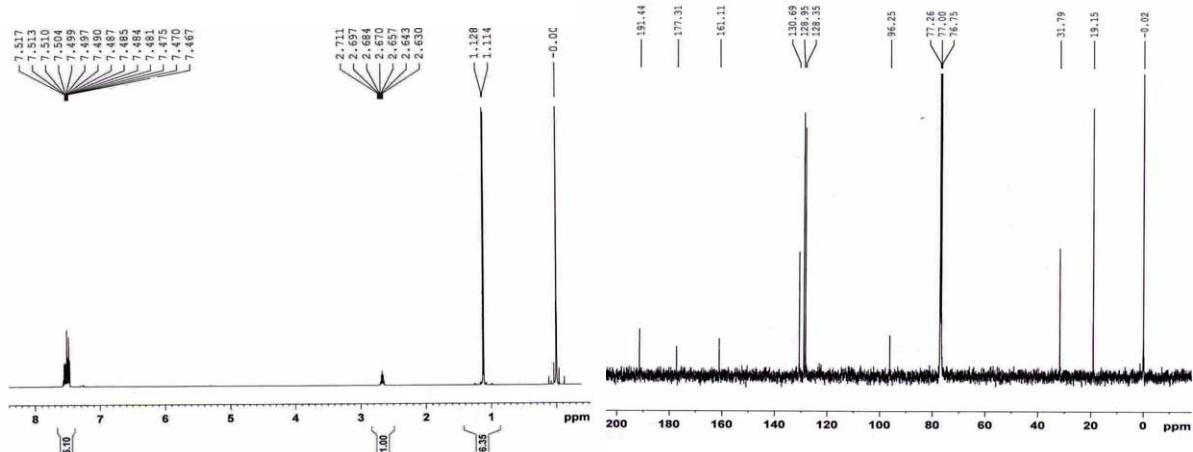
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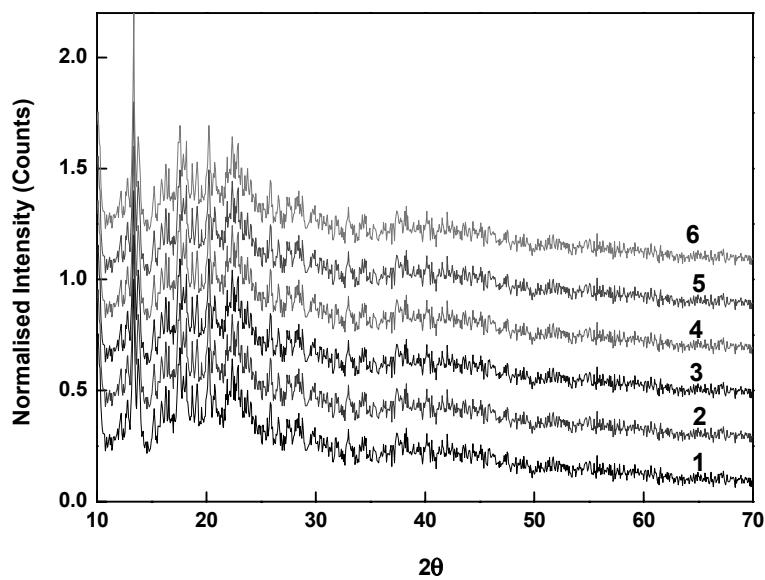


**Fig. S1** Structural formulas for the HPPI (a) and HIBPI (b) ligands. (c) X-ray structure of the HIBPI ligand. Thermal ellipsoids were drawn at the 30% probability level.

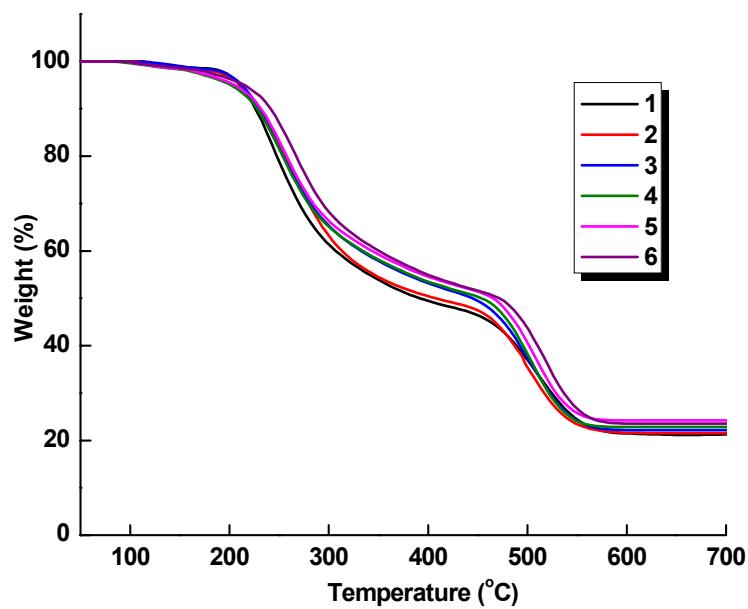
**Fig. S2** 500MHz  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the ligand HPPI.



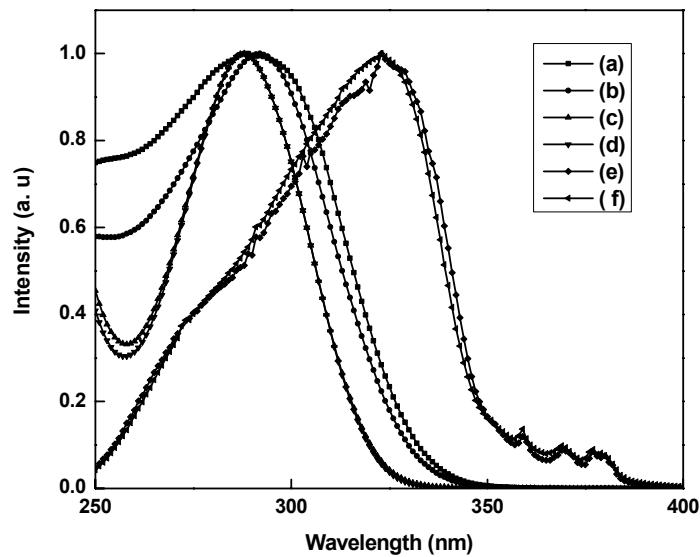
**Fig. S3** 500MHz  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the ligand HIBPI.



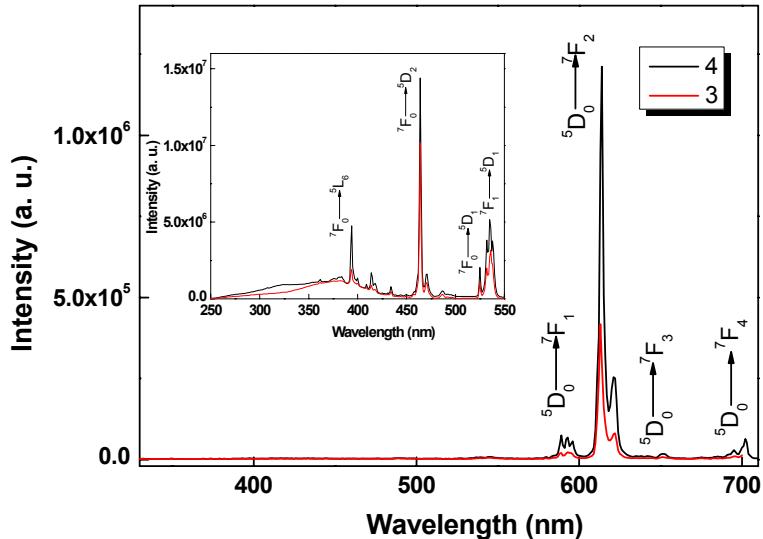
**Fig. S4** XRD patterns for complexes **1-6**.



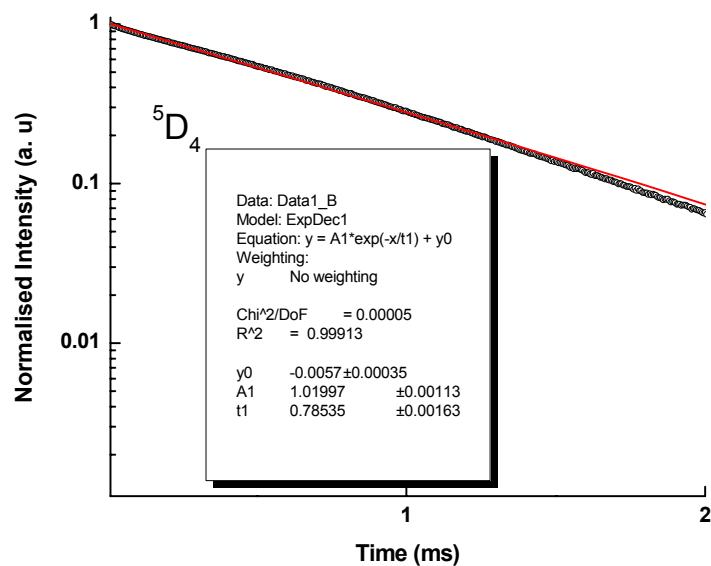
**Fig. S5** Thermogravimetric curves for the  $\text{Ln}^{3+}$  complexes **1-6**.



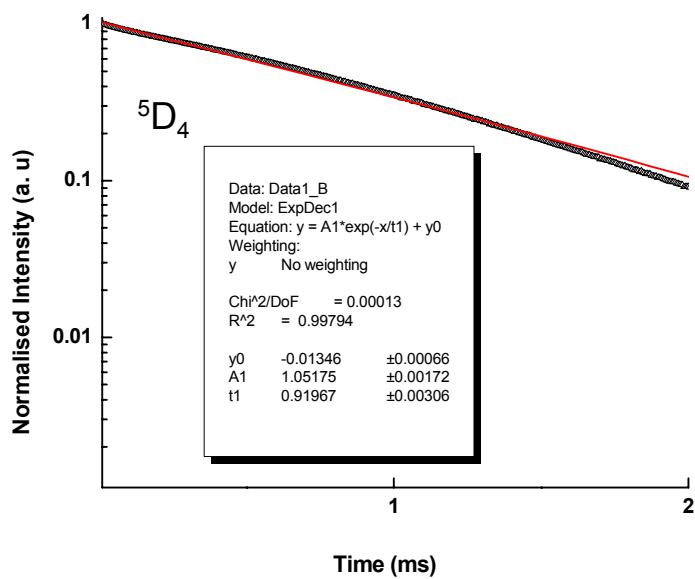
**Fig. S6** UV-vis absorption spectra of HPPI (a) and HIBPI (b); UV-vis absorption spectra of **1** (c) and **2** (d); and excitation spectra of complexes **1** (e) and **2** (f). The excitation spectra is recorded in solid state, and absorption spectra were in CH<sub>3</sub>CN (c = 2×10<sup>-5</sup> M ). All spectra are normalized to a constant intensity at the maximum.



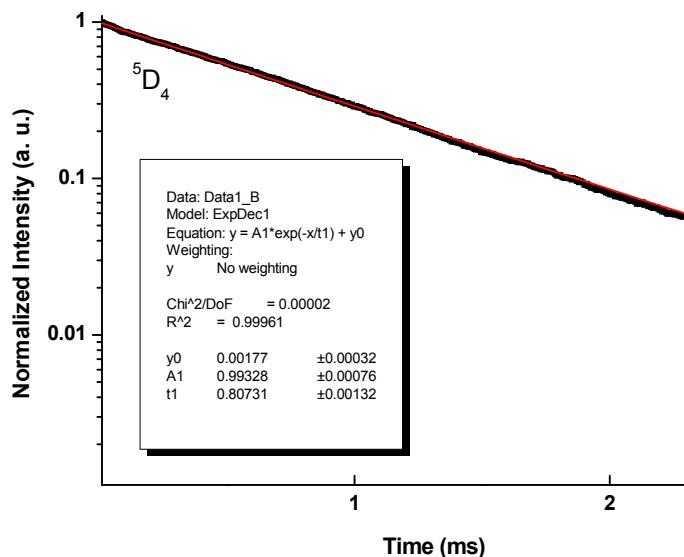
**Fig. S7** Solid state excitation (shown in inset) and emission spectra for complexes **3** and **4** at 298 K ( $\lambda_{\text{ex}} = 320$  nm and emission monitored around 614 nm).



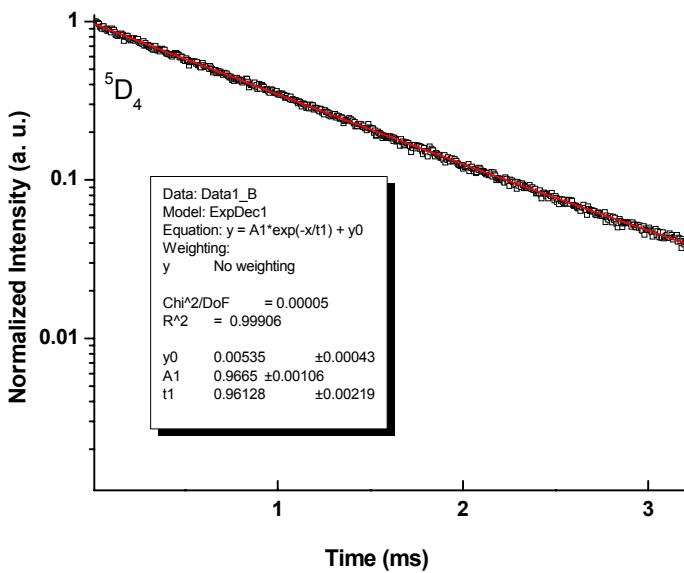
**Fig. S8** Experimental luminescence decay profiles for complex **1** at 298 K (in solid state) monitored around 545 nm and excited at 320 nm.



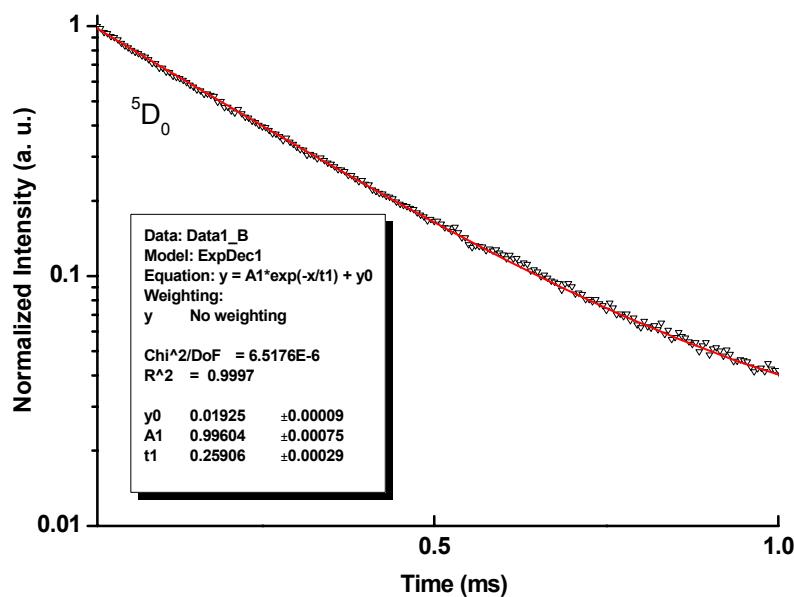
**Fig. S9** Experimental luminescence decay profiles for complex **2** at 298 K (in solid state) monitored around 545 nm and excited at 320 nm.



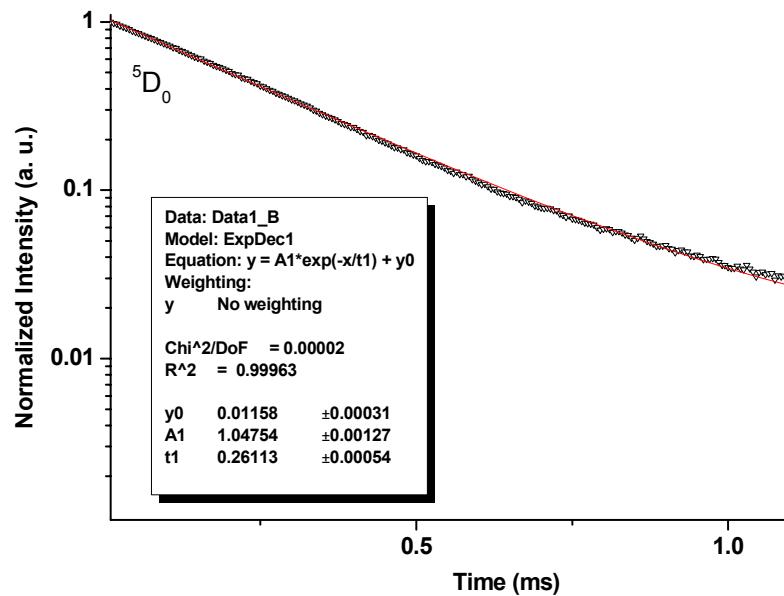
**Fig. S10** Experimental luminescence decay profiles of complex **1** at 77 K in  $\text{CDCl}_3$  monitored around 545 nm and excited at 320nm.



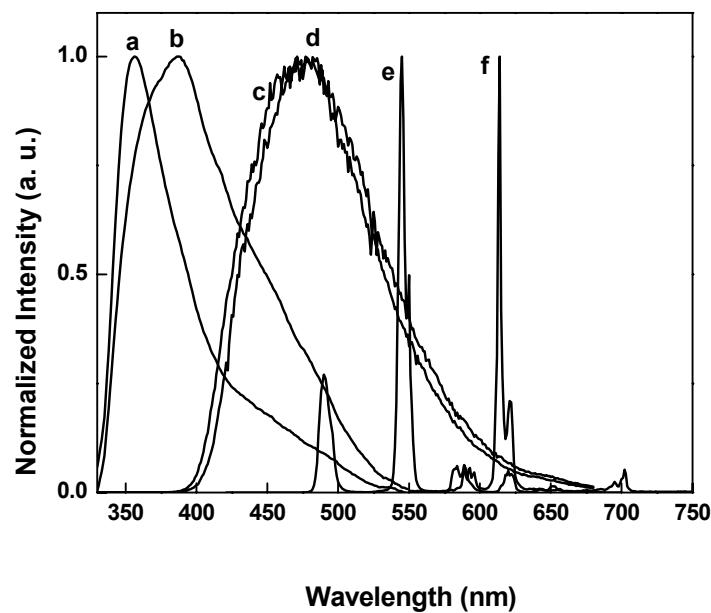
**Fig. S11** Experimental luminescence decay profiles of complex **2** at 77K in  $\text{CDCl}_3$  ( $c = 2 \times 10^{-5}$ ) monitored around 545 nm and excited at 320nm.



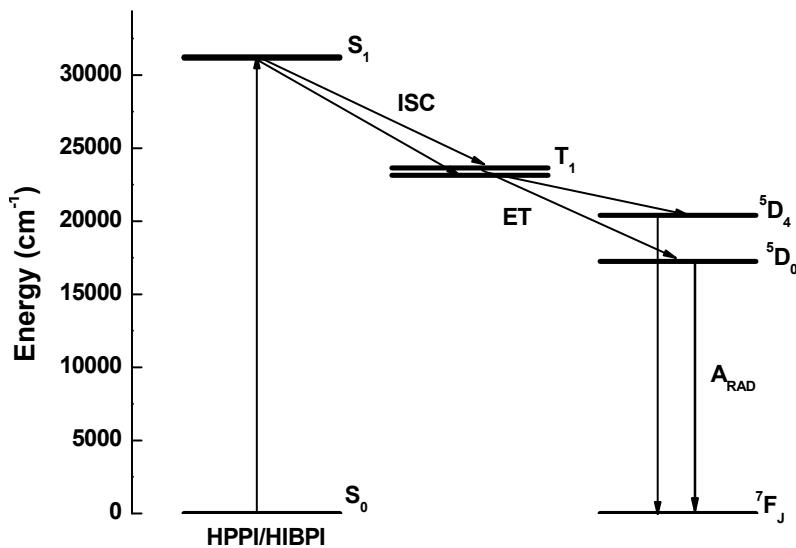
**Fig. S12** Experimental luminescence decay profiles for complex **3** at 298 K (in solid state) monitored around 614 nm and excited at 320 nm.



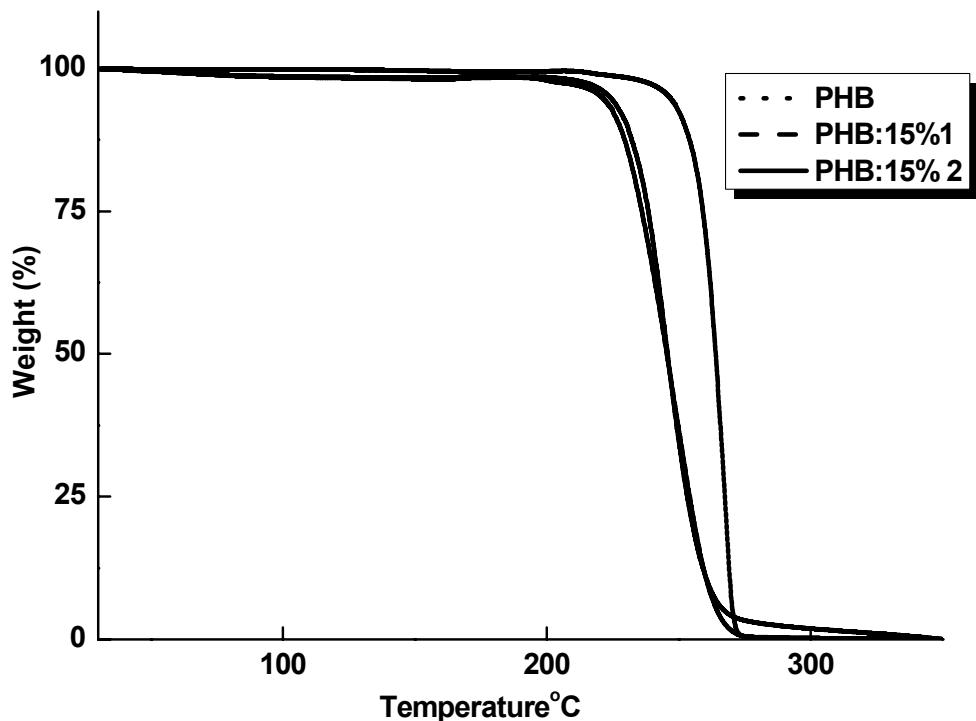
**Fig. S13** Experimental luminescence decay profiles for complex **4** at 298 K (in solid state) monitored around 614 nm and excited at 320 nm.



**Fig. S14** Room-temperature emission spectra of the ligands HPPI (a), HIBPI (b) and complexes **2** (e), **4** (f) and low-temperature (77K) phosphorescent spectra of complexes **5** (c) and **6** (d). in  $\text{CH}_3\text{CN}$  solution ( $c = 2 \times 10^{-5}$ ).



**Fig. S15** Schematic energy level diagram and energy transfer processes:  $S_1$ , first excited singlet state;  $T_1$ , first excited triplet state.



**Fig. S16** Thermogravimetric curves for the doped and undoped PHB polymer films.