

## Electronic Supplementary Information

### Photoluminescence properties of a novel cyclometalated iridium(III) complex with coumarin-boronate and its recognition to hydrogen peroxide

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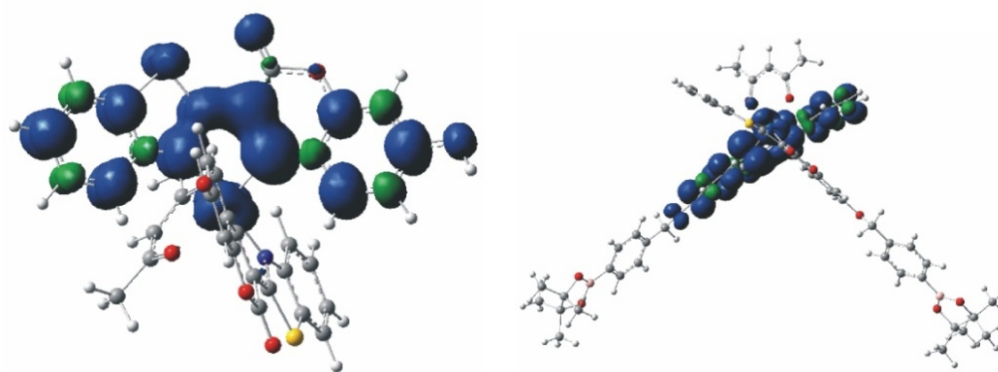


Figure S1 Countour plots of the spin density of the lowest-lying triplet state geometry of complex **Ir-2** (isovalue 0.002).

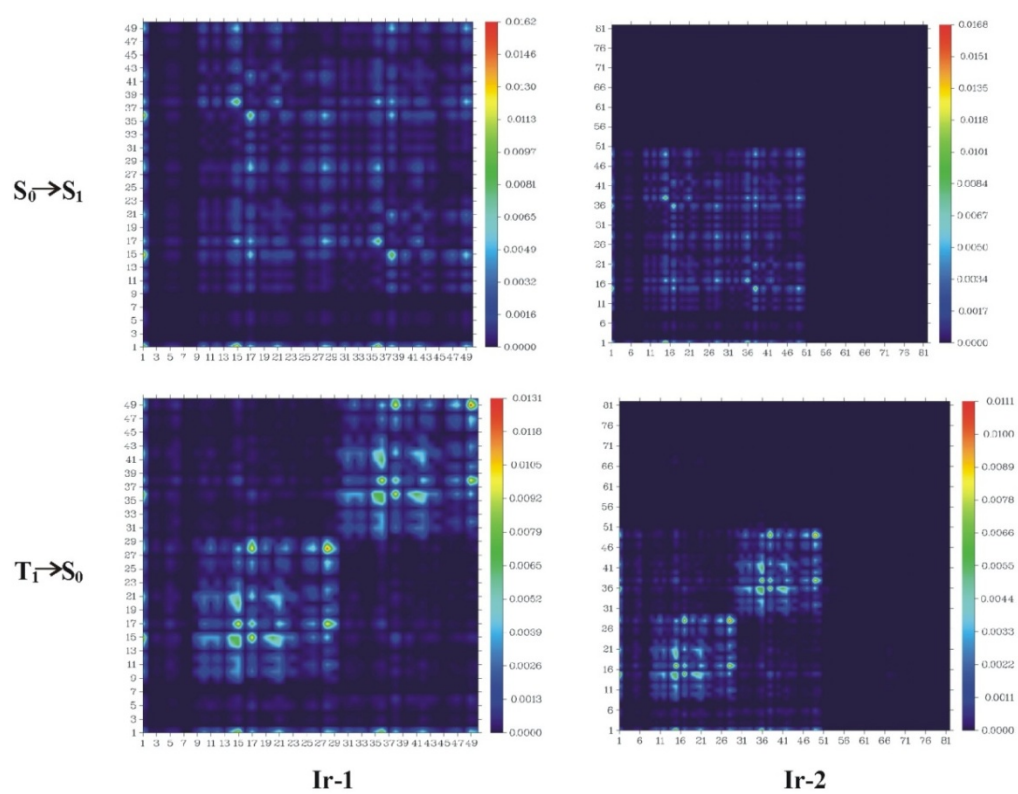


Figure S2. Contour plots of transition density matrices upon the  $S_0 \rightarrow S_1$  and  $T_1 \rightarrow S_0$  transition for **Ir-1** and **Ir-2**.

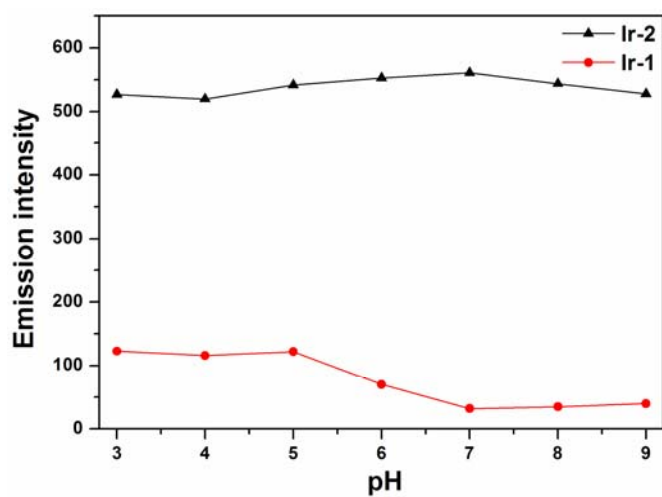


Figure S3. Effect of pH on emission spectra of **Ir-1** and **Ir-2** in CH<sub>3</sub>CN-PBS (20 mM, v/v = 1:4)

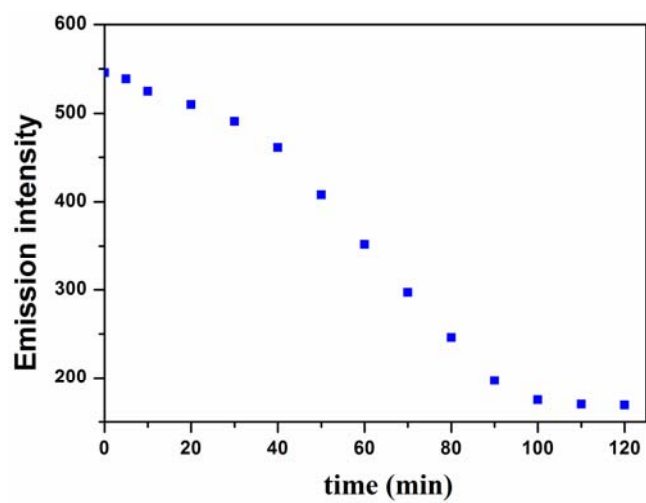
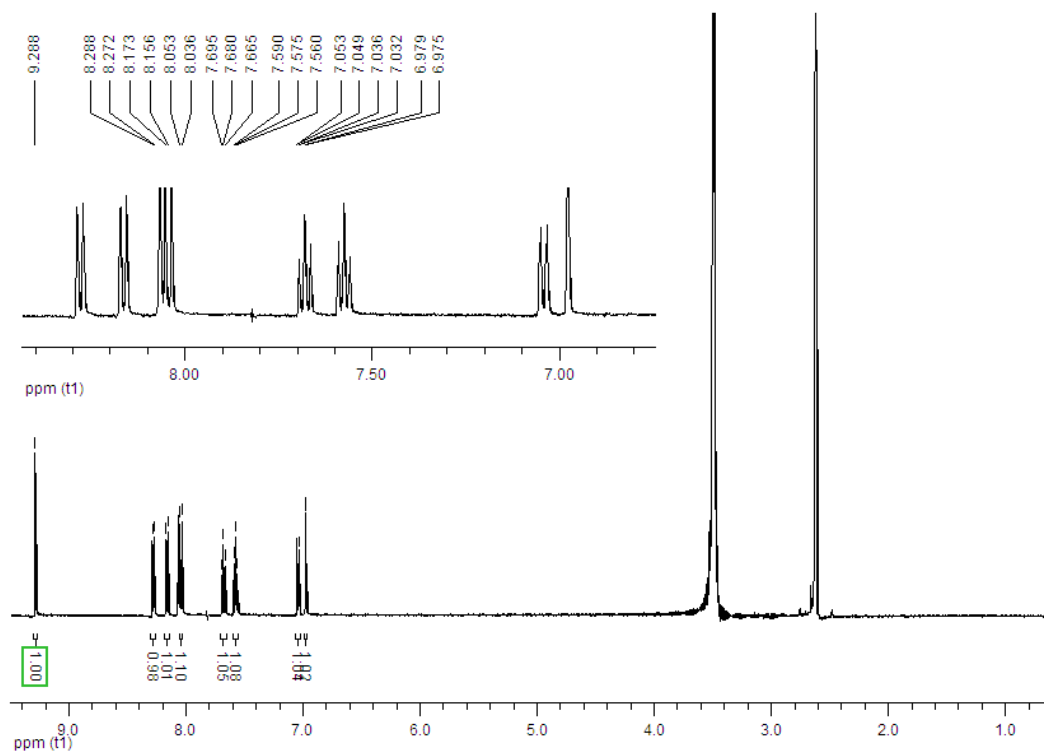
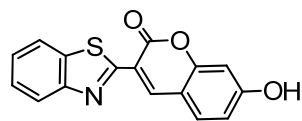
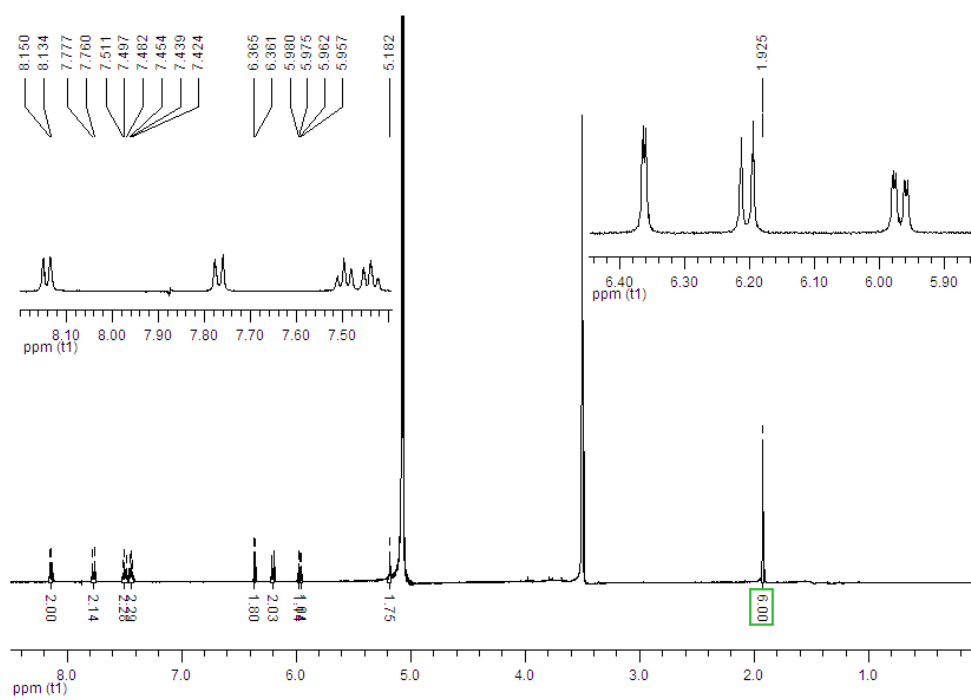
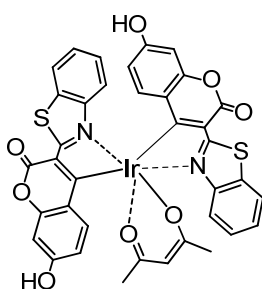


Figure S4. Time course of the reaction between the probe and H<sub>2</sub>O<sub>2</sub>

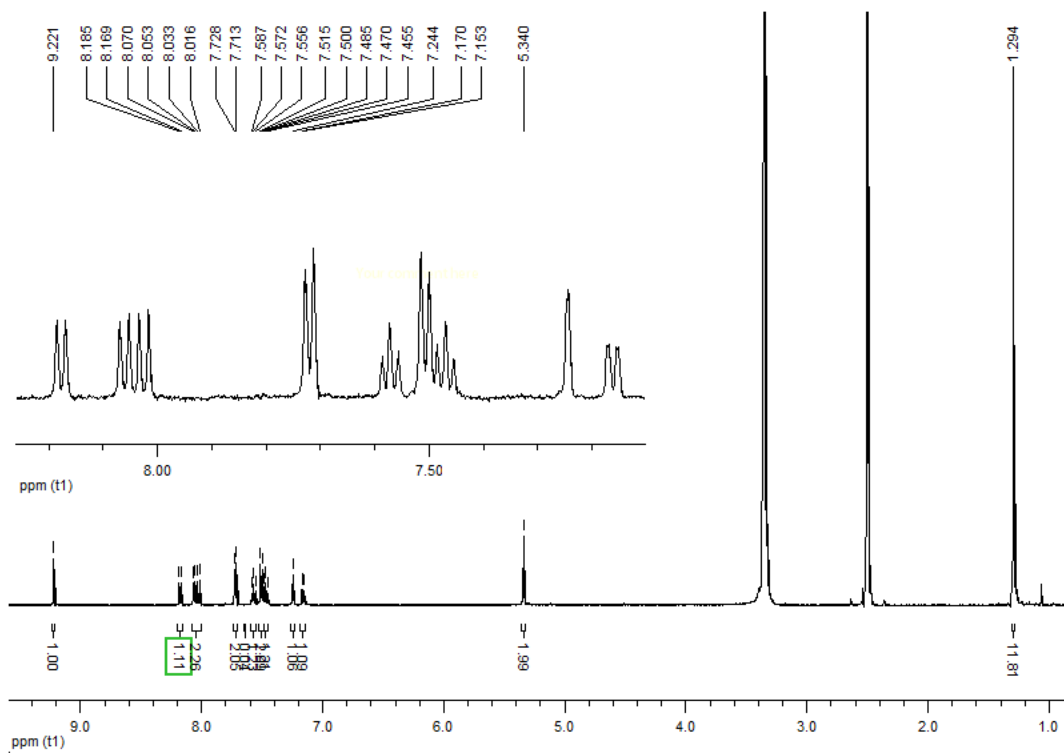
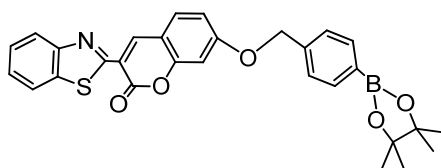
### $^1\text{H}$ NMR of Bthc



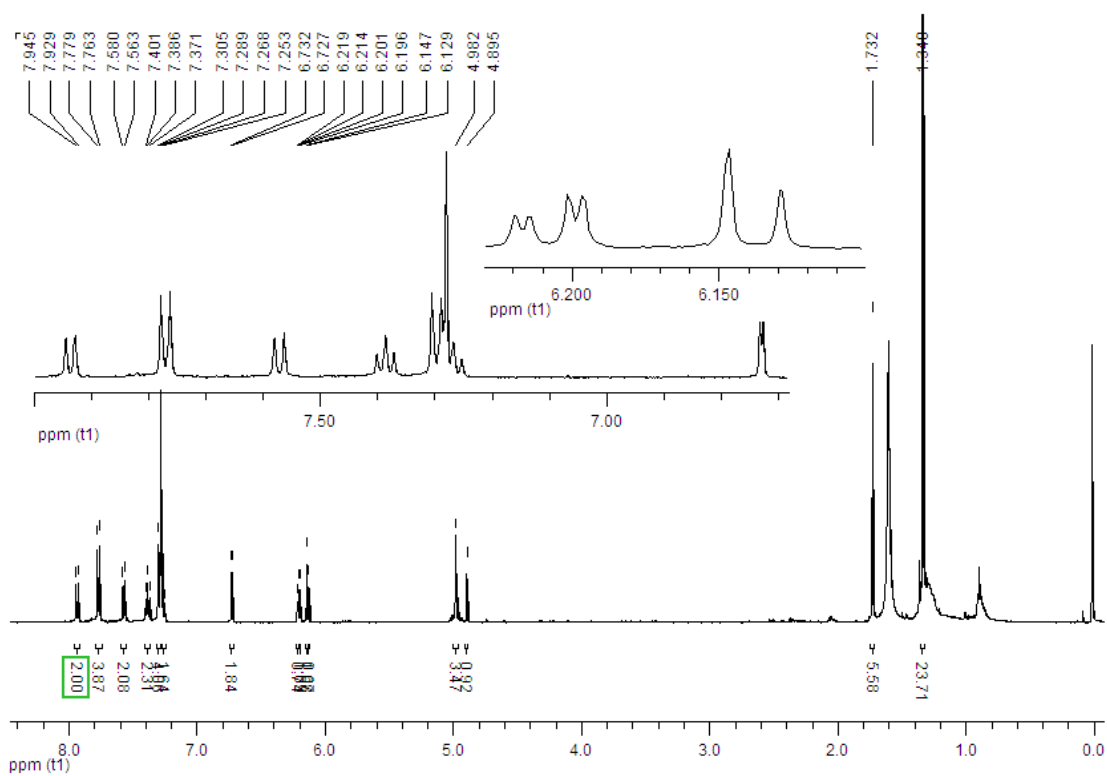
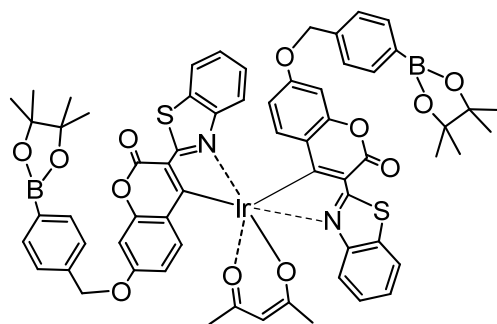
### $^1\text{H}$ NMR of Ir-1



### <sup>1</sup>H NMR of Bthc-bpe



### $^1\text{H}$ NMR of Ir-2



### $^{13}\text{C}$ NMR of Ir-2

