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Supporting information for article:

**Color-tunable phosphorescence of 1,10-phenanthrolines by
4,7-methyl/-diphenyl/-dichloro-substituents in cocrystals
assembled *via* bifurcated C—I...N halogen bonds using 1,4-
diiodotetrafluorobenzene as a bonding donor**

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As show in **Figure S1**, the total luminescence (fluorescence + phosphorescence) spectrum of cocrystal **3** goes from 350 to 650 nm at the excitation wavelength of 335 nm. Among them, the band between 350 and 430 nm belongs to fluorescence, while the weak band between 450 and 650 nm is phosphorescence.

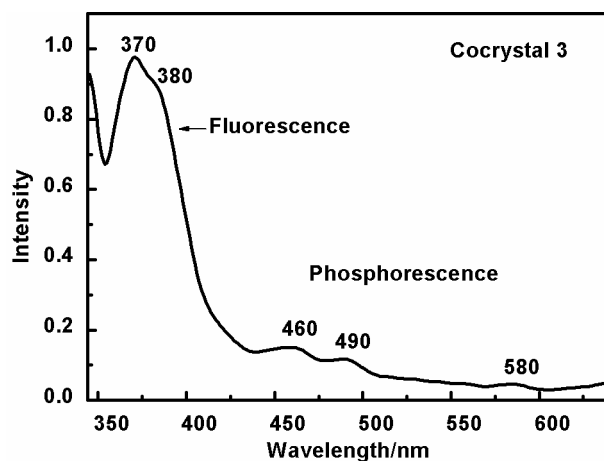


Figure S1 The normalized total luminescence (fluorescence + phosphorescence) spectra of cocrystals **3** at the excitation wavelength of 335nm.

Herein, one strategy was adopted to obtain the phosphorescence emitted from isolated free monomers using the hydrophobic cavity of γ -cyclodextrin (γ -CD) as a compartmentation medium and an external heavy atom species to form an inclusion complex in which the phosphorescence can be induced by the pure physically extrinsic heavy-atom effect. As shown in **Fig.S2**, the phosphorescent peak positions of DMPhe (510 nm), DPPhe (520 nm) and DCIPhe (520 nm) in the γ -CD aqueous solutions induced by bromo-cyclohexane (Br-CH₂, as the extrinsic heavy-atom perturber) display difference at room temperature.

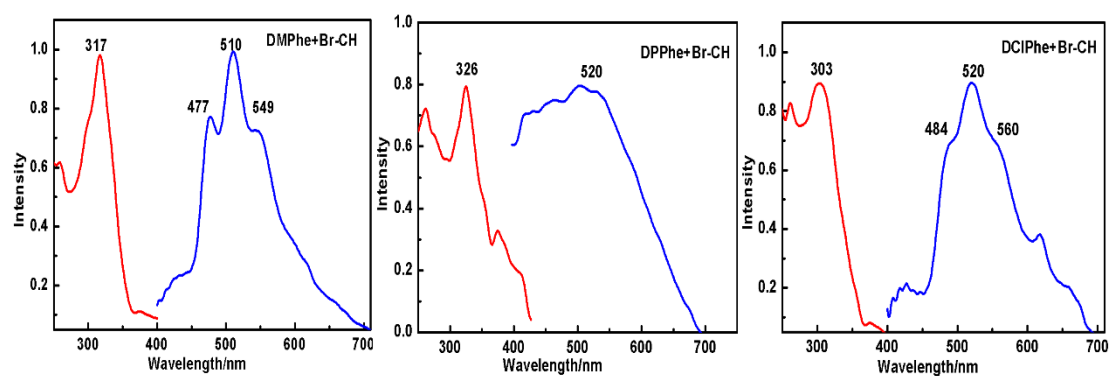


Figure S2 The normalized phosphorescence excitation (red line) and emission (blue line) spectra of DMPhe, DPPhe and DCIPhe induced by bromo-cyclohexane (Br-CH) in γ -CD aqueous solution. Conditions: DMPhe, DPPhe and DCIPhe, $5 \times 10^{-5} \text{ mol L}^{-1}$; [γ -CD], $8 \times 10^{-3} \text{ mol L}^{-1}$; [Br-CH], $2 \times 10^{-5} \text{ mol L}^{-1}$. Excitation wavelengths are 317 nm, 326 nm and 303 nm, respectively. The ex/em slits 20/20 nm.