Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Effect of geometry factor on the priority of σ-hole···π and π-hole···π bond in phosphorescent cocrystals by pyrene or phenanthrene and trihaloperfluorobenzenes

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Results and discussion (Supplementary)

1. Structures of cocrystals

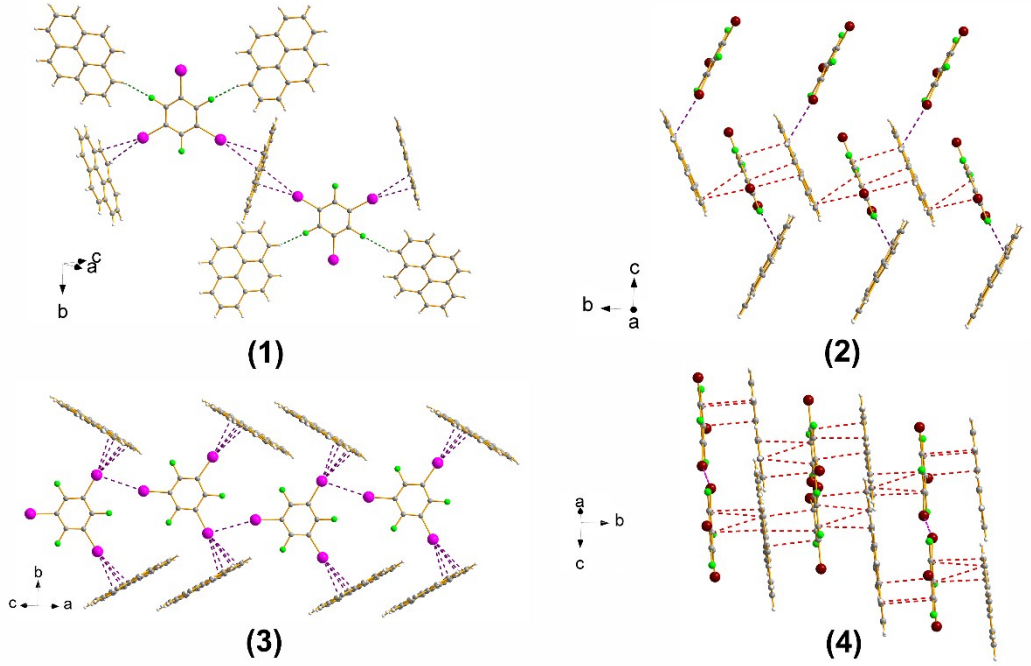


Fig S1 The 2D network structure unit of cocrystals. (1) TIPB–Py; (2) TBrPB–Py; (3) TIPB–Phe; (4) TBrPB–Phe.

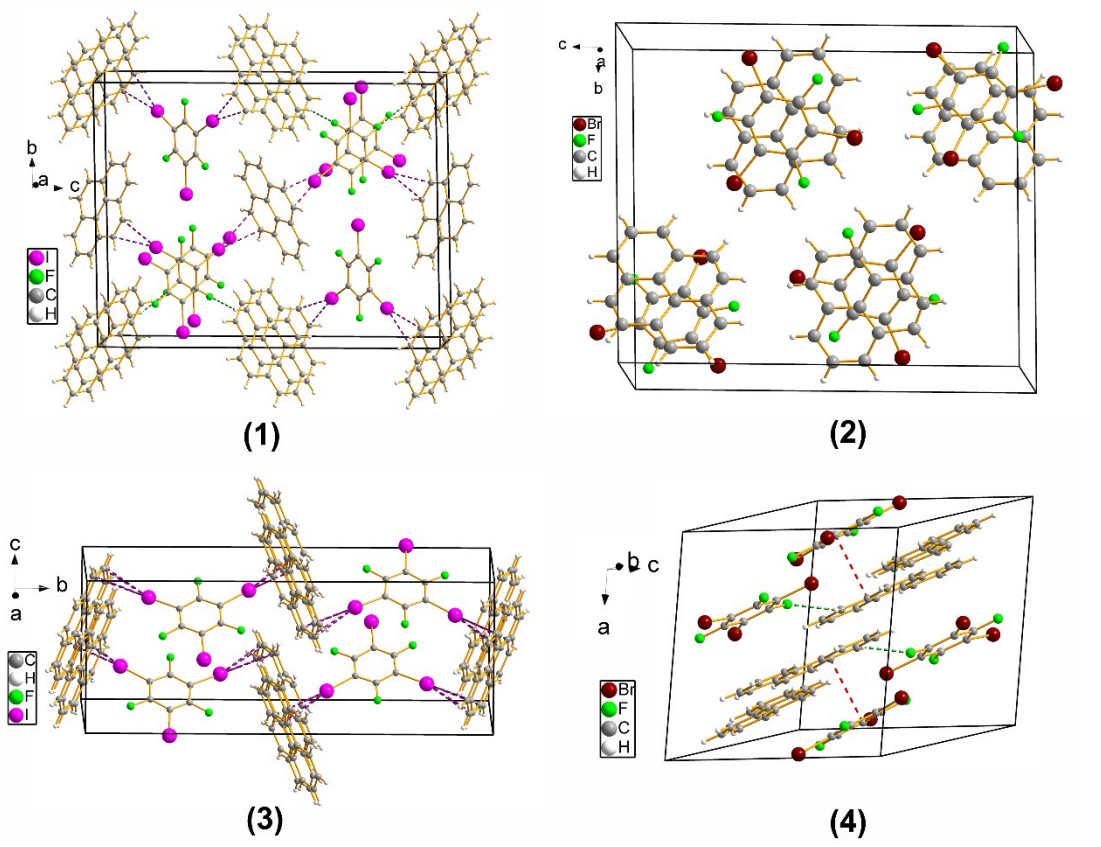
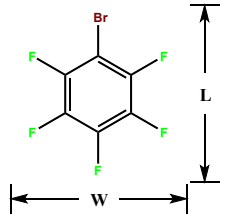
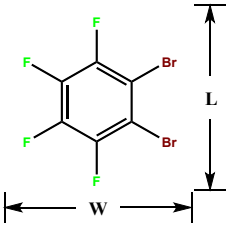
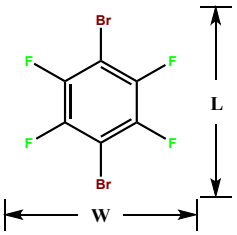
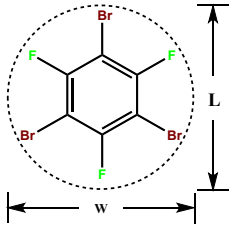
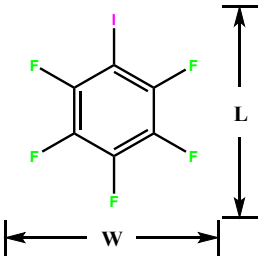
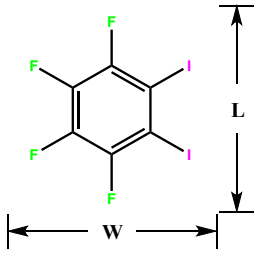
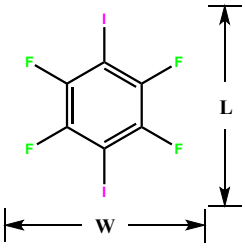
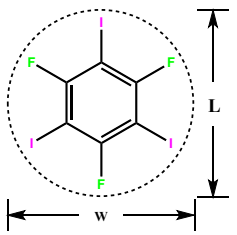


Fig S2 The unit cell of cocrystals. (1) TIPB–Py; (2) TBrPB–Py; (3) TIPB–Phe; (4) TBrPB–Phe.

Table S1 The length, width and thickness of molecules in Å.

	Length	Width	Thickness [a]
	6.0181	4.6209	3.70
	5.4911	5.2393	3.70

	6.5450	4.6209	3.70
	6.5450	6.5450	3.70
	6.2378	4.6209	3.96
	5.4911	5.4038	3.96
	6.9844	4.6209	3.96
	6.9844	6.9844	3.96

[a] *calculated by the double distance of the Van der Waals radius of Br and I.*

2. *Luminescence spectra of cocrystals*

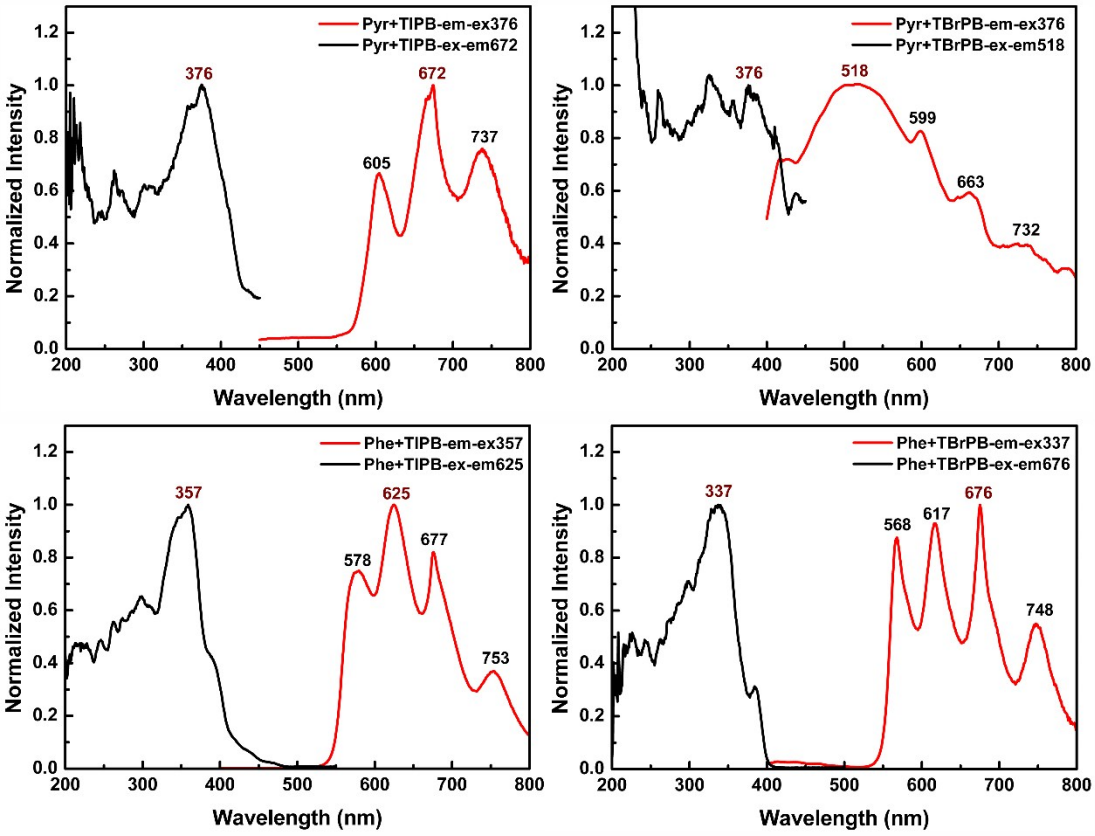


Fig S3 Phosphorescent spectra of the crystals measured under phosphorescent mode.

Table S2 Phosphorescent characteristics of cocrystals at room temperature.

	Spectra	
	λ_{ex}/nm	λ_{em} /nm
Pyr–TIPB	***376***[a]	605, ***672,*** 737
Pyr–TBrPB	***376***	***518***, 599, 663, 732
Phe–TIPB	***357***	578, ***625***, 677, 753
Phe–TBrPB	***330***	565, 615, ***677***, 751

In **Table 4**, the phosphorescence decays of the cocrystal **1**-**4** were measured under λ_{ex} (376)-λ_{em} (672), λ_{ex} (376)-λ_{em} (663), λ_{ex} (357)-λ_{em} (677), λ_{ex} (330)-λ_{em} (677), respectively.