Cocrystals assembled by pyrene and 1,2- or 1,4-diiodotetrafluorobenzenes and their phosphorescent behaviors modulated by local molecular environment

Qian Jin Shen, Hong Qing Wei, Wen Sheng Zou, Hao-Ling Sun*, Wei Jun Jin*

College of Chemistry, Beijing Normal University, Beijing 100875, P. R. China

Email: wjjin@bnu.edu.cn (W. J. Jin) and haolingsun@bnu.edu.cn (H. L. Sun);

Fax: +86 58802146; Tel: +86 58802146

Supporting Information

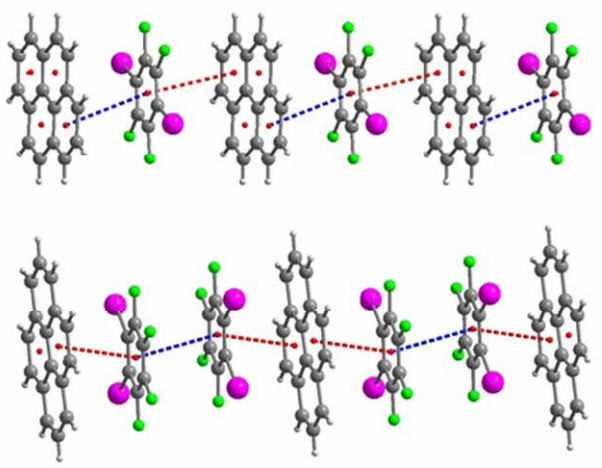

Fig. S1 The π-π stacking arrangements of cocrystal **1** (top) and **2** (bottom).

Table S1 The details of C-H···F-C contacts in **1** and **2**.

Crystals	No.	C-H	A	$d_{(H\cdots F)}$, Å	$\theta_{C\text{-}H\cdots F}$, °
1	1	C1-H1	F3 [-x+2, -y+1, -z+1]	2.862	146.8
	2	C13-H13	F3 [-x+2, -y+1, -z+1]	2.697	152.7
	3	C6-H6	F4 [x-1, -y+1.5, z-0.5]	2.875	151.1
	4	C8-H8	F4 [x-1, -y+1.5, z-0.5]	2.826	152.4
	5	C11-H11	F2 [-x+1, -y+1, -z]	2.567	144.6
	6	C9-H9	F2 [-x+1, -y+1, -z]	2.845	137.0
2	1	C13H13A	F4 [-x+1 y-0.5, -z+0.5]	2.872	152.3
	2	C13-H13A	F3 [-x+1 y-0.5, -z+0.5]	2.729	144.1
	3	C7-H7A	F2 [-x+1, y-1.5, -z+0.5]	2.602	153.2

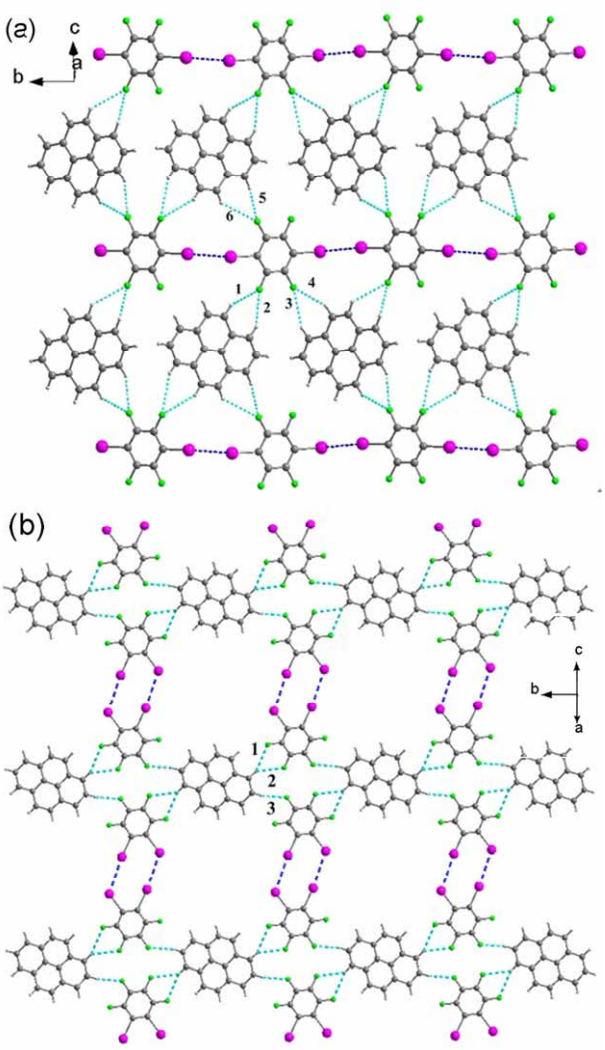

Fig. S2 Diagram of C-H···F-C contacts and C-I···I-C interactions of **1** (a) and **2** (b).

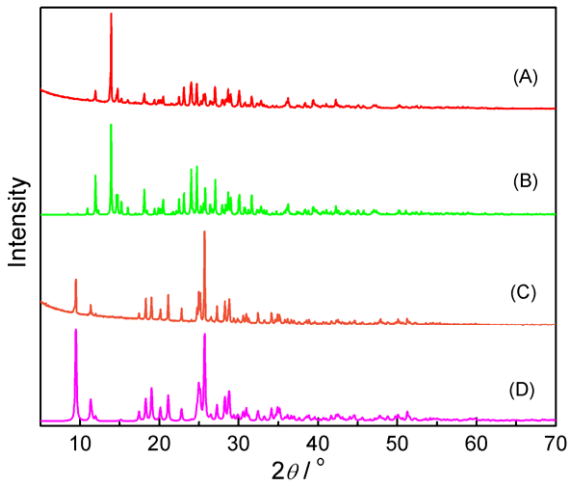

Fig. S3 The whole XRPD patterns (5-70°) of cocrystal **1** and **2.** (A), (B): experimental and simulated patterns of **1**, (C), (D): experimental and simulated patterns of **2**.

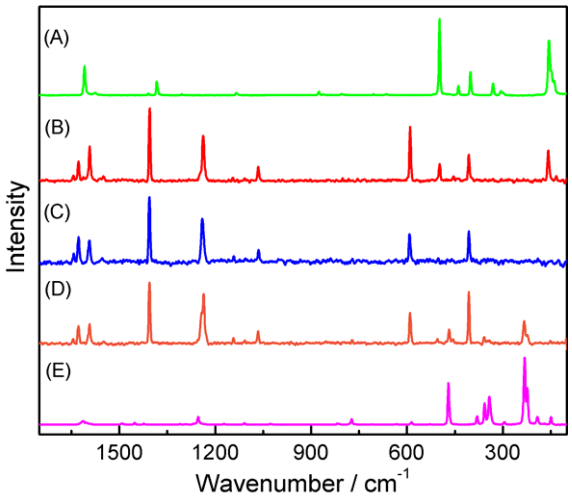

Fig. S4 Raman spectra of monomers and cocrystals. (A): pure 1,4-DITFB; (B): cocrystal **1**; (C): pure pyrene; (D): cosrystal **2**; (E): pure 1,2-DITFB.

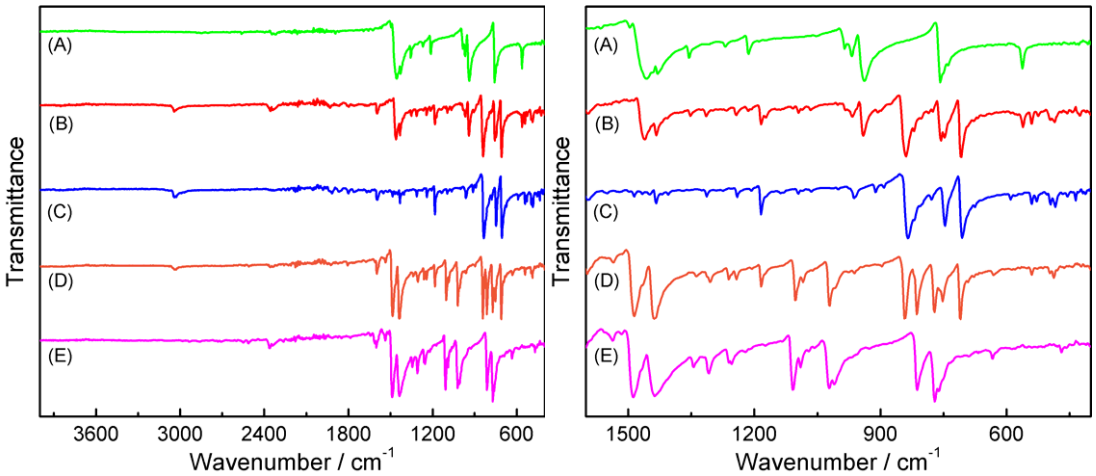

Fig. S5 ATR IR spectra of monomers and cocrystals in the whole range (4000-400 cm^{-1}, left) and selected range (1600-400 cm^{-1}, right). (A): pure 1,4-DITFB; (B): cocrystal **1**; (C): pure pyrene; (D): cosrystal **2**; (E): pure 1,2-DITFB.