

Supporting Information

**Interactions between haloperfluorobenzenes and fluoranthene in
luminescent cocrystals from π -hole $\cdots\pi$ to σ -hole $\cdots\pi$ bonds**

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Results and discussion (Supplementary)

1. Structures of cocrystals

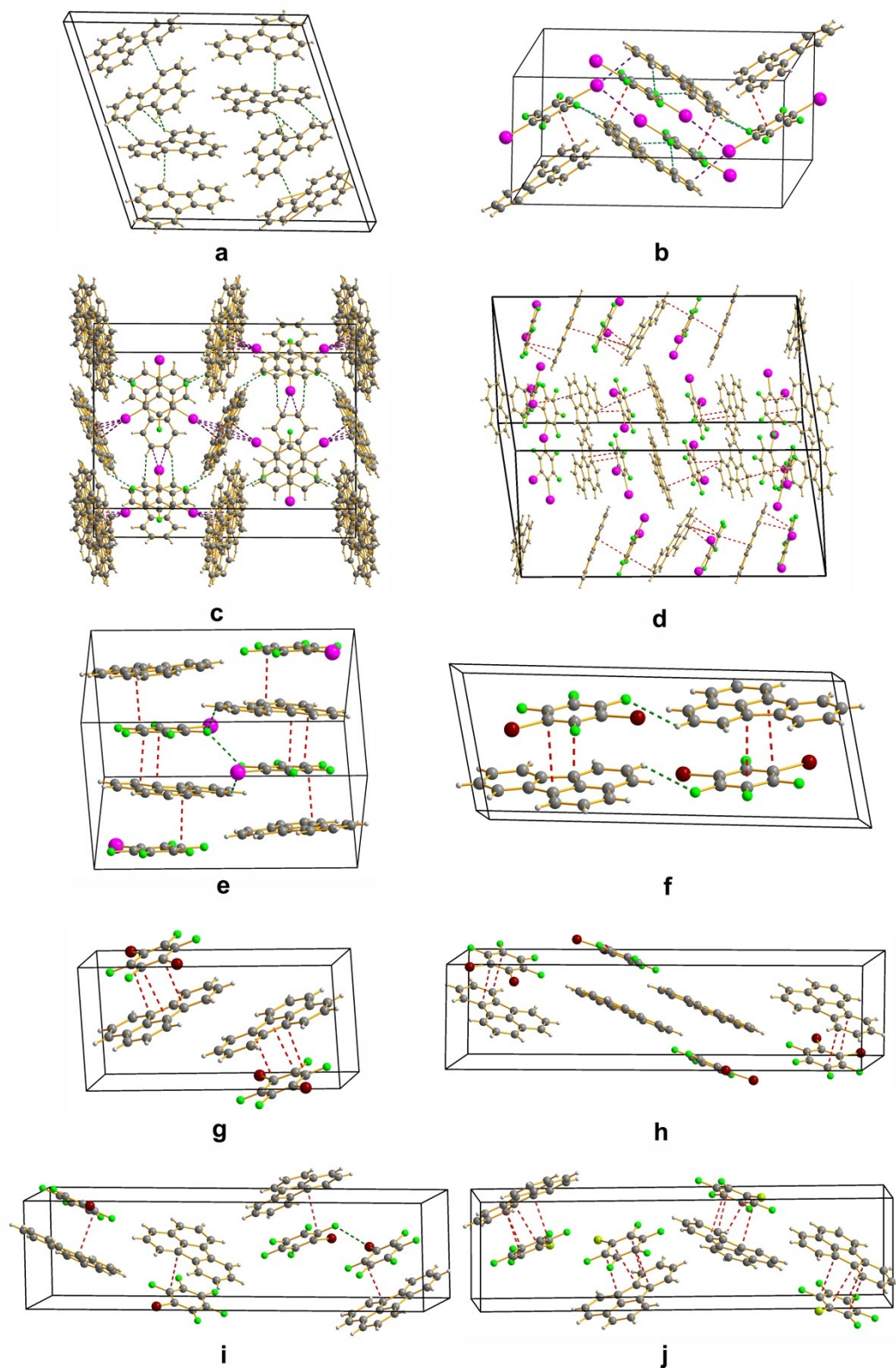


Figure S1 Crystal cell unit. (a) FA crystal. (b) 14DIPB-FA cocrystal. (c) 135TIPB-FA cocrystal. (d) 12DIPB-FA cocrystal. (e) 1IPB-FA cocrystal. (f) 13DBrPB-FA cocrystal. (g) 14DBrPB-FA cocrystal. (h) 12DBr-FA cocrystal. (i) 1BrPB-FA cocrystal. (j) 1ClPB-FA cocrystal.

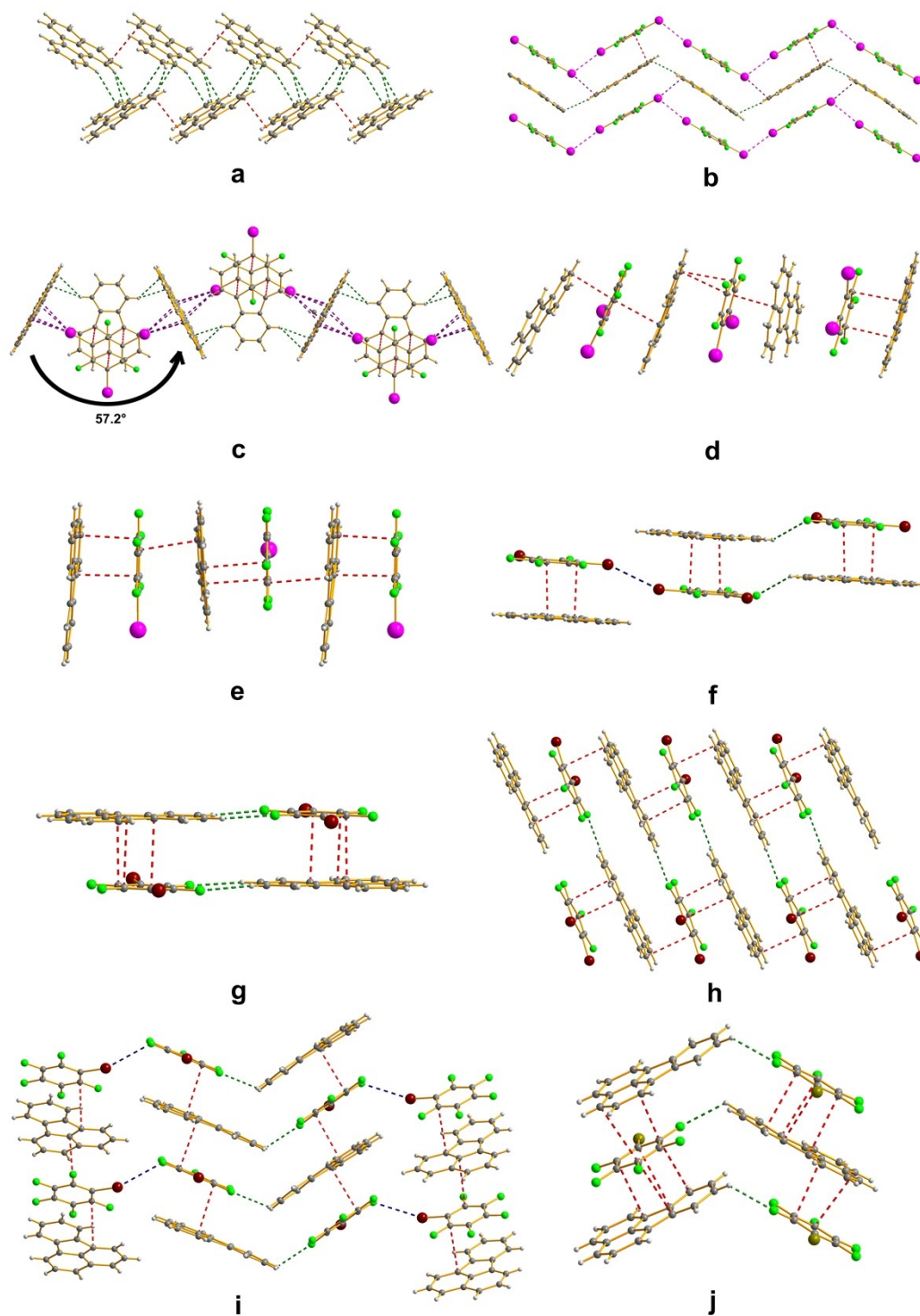


Figure S2 The local structure of FA and the corresponding cocrystals. The meanings of symbols **a** to **j** are same with **Figure S1**.

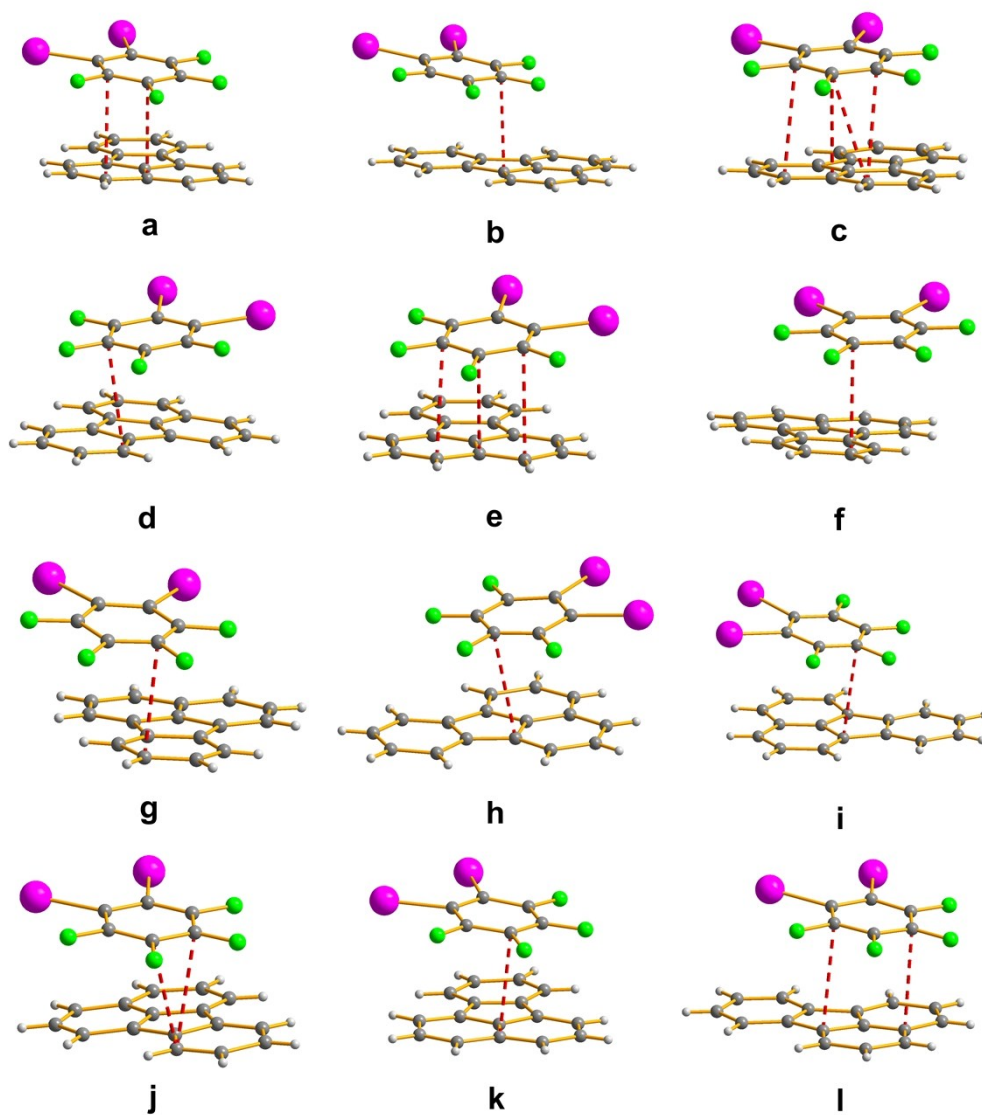


Figure S3 All the π -hole $\cdots\pi$ bonding units from 12DIPB-FA cocrystal

Table S1 The main bonding properties and geometrical parameters of 12DIPB–FA cocrystal.

Cocrystals	Interactions	$d/\text{\AA}$	θ°
FA–12DIPB	π –hole $\cdots\pi$ (a)	3.370, 3.239	7.037
	π –hole $\cdots\pi$ (b)	3.269	7.495
	π –hole $\cdots\pi$ (c)	3.328, 3.335, 3.371, 3.333	7.715
	π –hole $\cdots\pi$ (d)	3.334	9.045
	π –hole $\cdots\pi$ (e)	3.362, 3.346, 3.359	8.251
	π –hole $\cdots\pi$ (f)	3.316	9.619
	π –hole $\cdots\pi$ (g)	3.224	9.684
	π –hole $\cdots\pi$ (h)	3.239	6.847
	π –hole $\cdots\pi$ (i)	3.284	6.878
	π –hole $\cdots\pi$ (j)	3.388, 3.334	9.045
	π –hole $\cdots\pi$ (k)	3.278	7.124
	π –hole $\cdots\pi$ (l)	3.396, 3.217	7.111

2. Luminescence spectra and decays of cocrystals

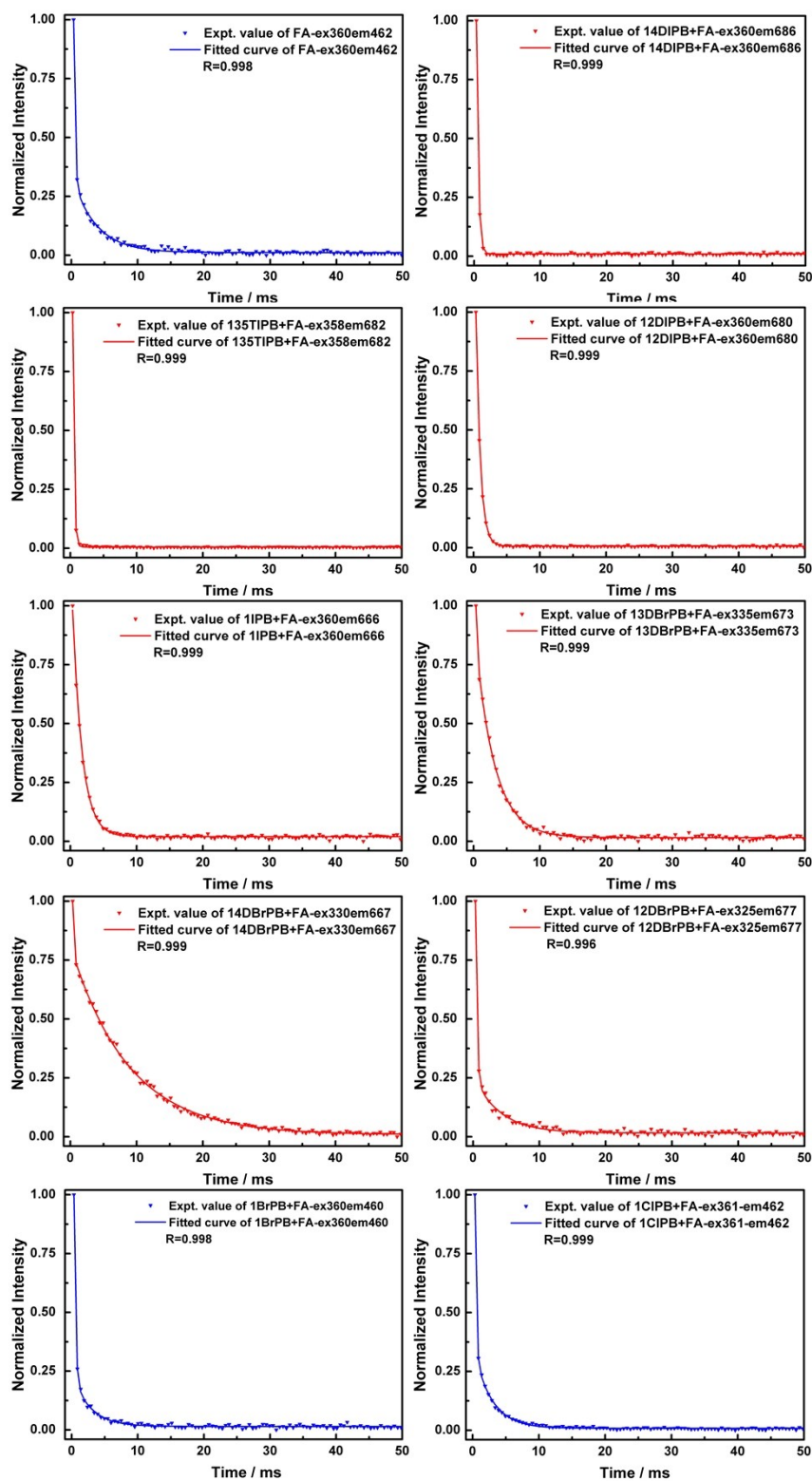
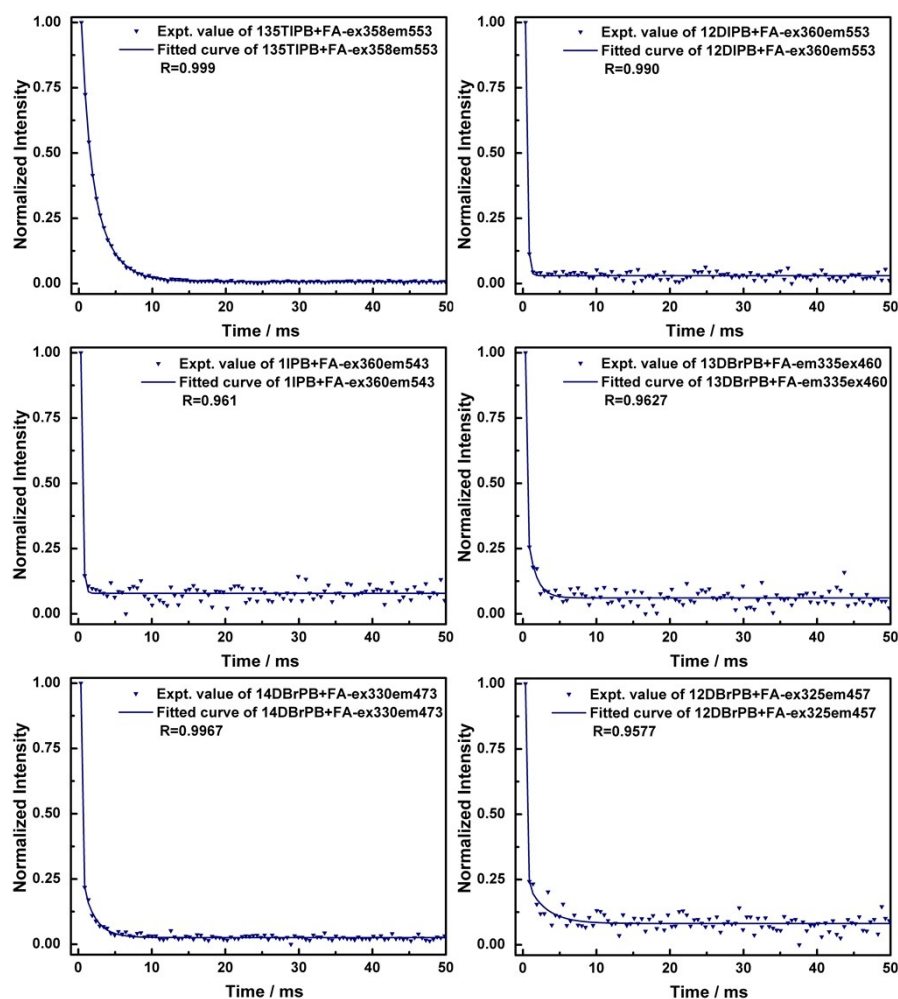


Figure S4 Phosphorescence and delayed fluorescence decays of the cocrystals.



Continuous **Figure S4** Phosphorescence and delayed fluorescence decays of the cocrystals.

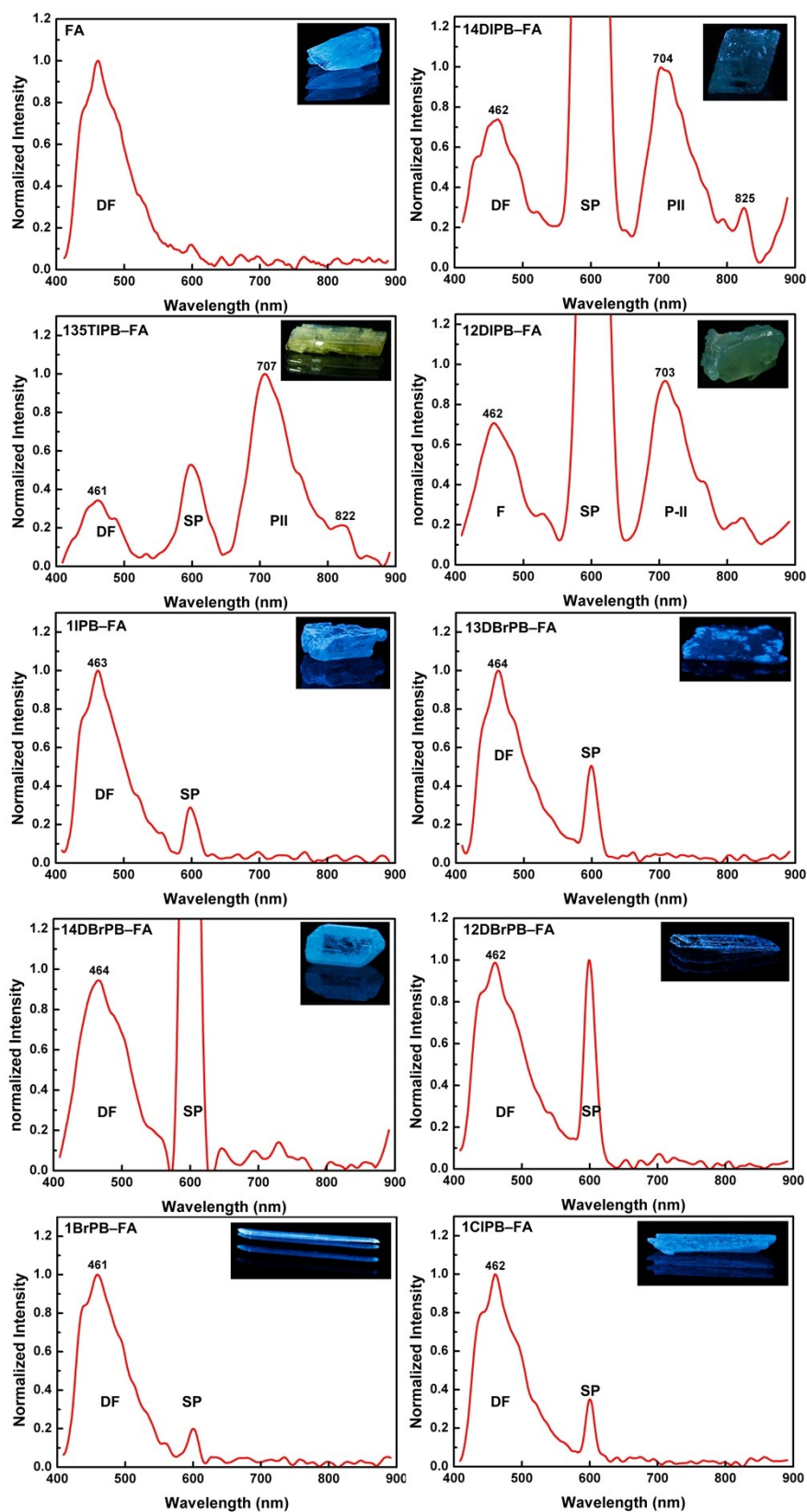


Figure S5 Total luminescence (fluorescence+phosphorescence) spectra of the cocrystals. Excitation at 300 nm. DF: delay fluorescence; PI and PII: phosphorescence band I and II; SP: scattering peak. The photographs of cocrystals are taken under UV-

365 nm irradiation.

Table S2 The 0–0 transition energy difference ΔE between $S_1 \rightarrow S_0$ and $T_1 \rightarrow S_0$ in cocrystals and the lifetime of DF, PI and PII.

	$\Delta E(\text{PII}-\text{DF})^a$			$\Delta E(\text{PII}-\text{PI})^b$			$\tau_{\text{-DF}}$	$\tau_{\text{-PI}}$	$\tau_{\text{-PII}}$
	in nm	in cm^{-1}	in kcal/mol	in nm	in cm^{-1}	in kcal/mol	in ms	in ms	in ms
135TIPB-FA	—	—	—	129	3420	9.78	—	2.304	0.195
12DIPB-FA	—	—	—	127	3380	9.66	—	0.209	0.654
1IPB-FA	—	—	—	123	3400	9.73	—	0.200	1.431
13DBrPB-FA	230	7710	22.1	—	—	—	0.075	—	2.751
14DBrPB-FA	224	7580	21.7	—	—	—	0.782	—	8.691
12DBrPB-FA	234	7800	22.3	—	—	—	0.154	—	2.741

^a $\Delta E(|\text{PII}-\text{DF}|)$ refers to 0–0 transition energy between PII and DF expressed by wavelength, wavenumber or kcal/mol, ^b $\Delta E(|\text{PII}-\text{PI}|)$ refers to the difference of the wavelength or wavenumber between PII and PI. “—” means that delayed fluorescence (DF) or phosphorescent (P) were not observed in FA or the corresponding cocrystals.

3. Quantum chemistry calculation

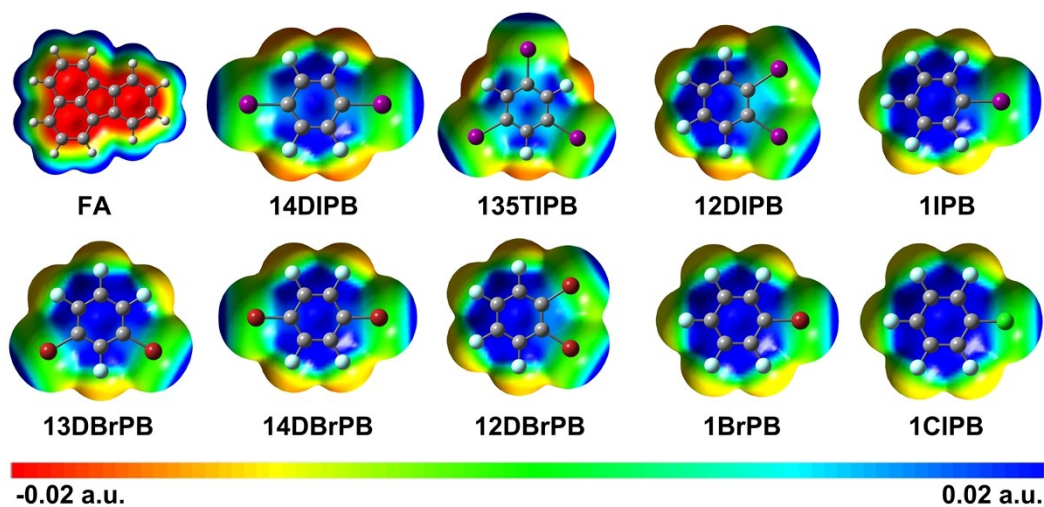


Figure S6 Map (electron density $0.001 \text{ e} \cdot \text{Bohr}^{-3}$) of electrostatic potential surfaces of

molecules involved herein calculated at M06–2X/6–311++G(d,p)/Lanl2dzd ECP level.

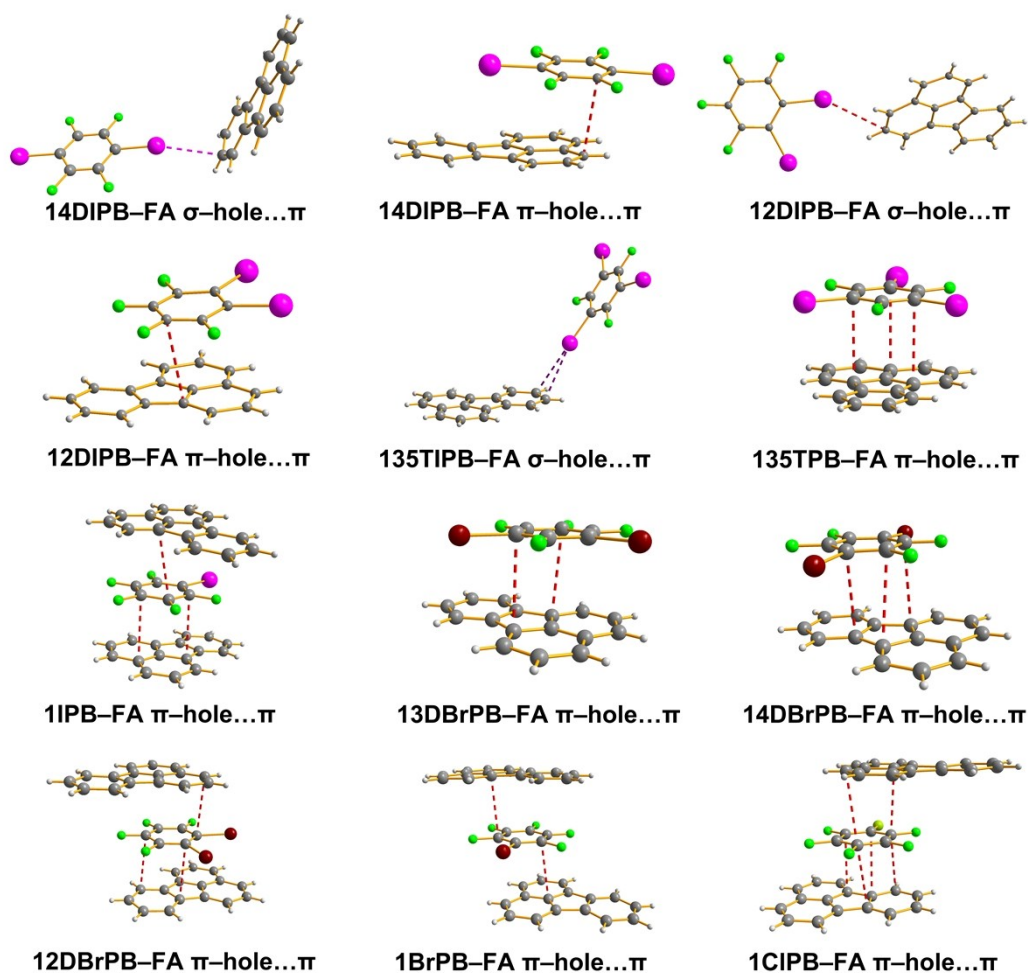


Figure S7 The σ -hole... π and π -hole... π bonding units from single cocrystal structure data for calculation of energies (M06–2X with the 6–311++ G(d,p) basis set for H, C, F atoms and 6–311 G(d,p) for I atom).

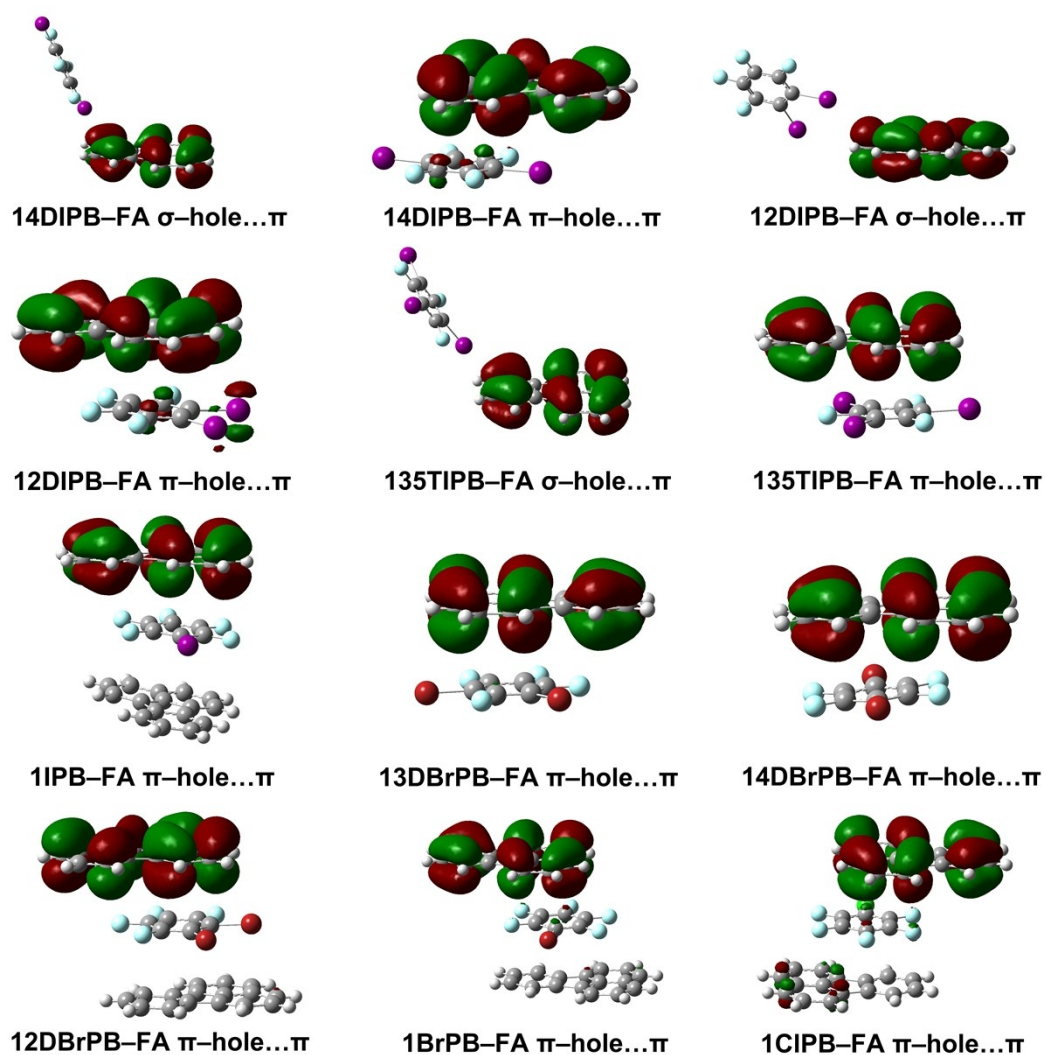
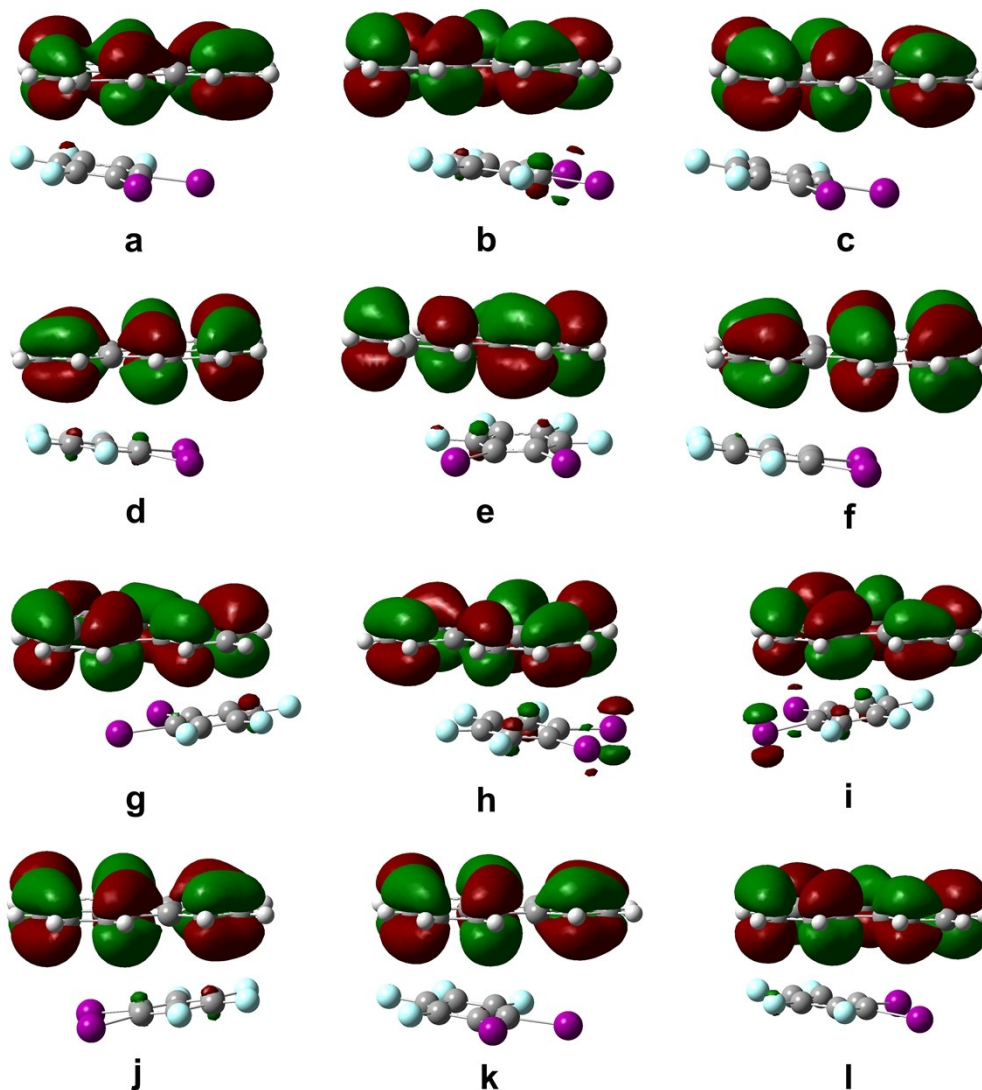


Figure S8 The highest occupied molecule orbital (HOMO) of π -hole and σ -hole bonding in cocrystals.



Continuous **Figure S8** The highest occupied molecule orbital (HOMO) of π -hole bonding in 12DIPB-FA cocrystal (the π -hole $\cdots\pi$ bonding units as same as shown in **Figure S3**)

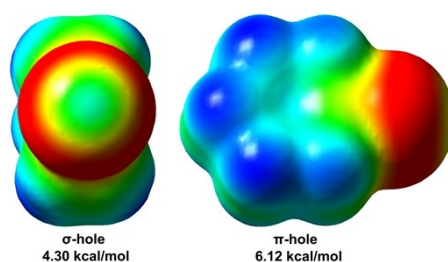


Figure S9 Electrostatic potential surfaces (electron density 0.001 e·Bohr⁻³) of Br-CH calculated at M06-2X/6-311++G(d,p) level.

Table S3 The charge donor-acceptor interactions, second-order perturbation stabilization energies E^2 (in kJ·mol⁻¹) and the amount of charge transfer Δq (in *a.u.*) in 14DIPB-FA, 135TIPB-FA, 12DIPB-FA and 1IPB-FA cocrystal by NBO analysis.

		Charge Donor	Charge Acceptor	E^2	E^2_{total}	Δq
14DIPB-FA	$\sigma\text{-hole} \cdots \pi$	BD(2)C3-C14	BD*(1)I1-C2	9.08	19.41	0.0100
		BD(1)C3-H15	BD*(1)I1-C2	0.71		
		BD*(2)C3-C14	BD*(1)I1-C2	9.62		
	$\sigma\text{-hole} \cdots \text{lep}$	LP(1)I5	BD*(1)I3-C4	2.72	16.86	0.0175
		LP(3)I5	BD*(1)I3-C4	14.14		
	$\pi\text{-hole} \cdots \pi$	BD(2)C13-C16	BD*(2)C2-C8	1.46	5.31	0.0046
		BD(2)C13-C16	BD*(2)C4-C12	1.51		
		BD(2)C13-C16	BD*(1)F7-C8	0.46		
		BD(2)C13-C16	BD*(1)F11-C12	0.29		
		BD(2)C15-C17	BD*(2)C4-C12	0.92		
		BD(2)C15-C17	BD*(2)C6-C10	0.38		
		BD(2)C18-C24	BD*(1)F5-C6	0.29		
135TIPB-FA	$\sigma\text{-hole} \cdots \pi$	BD(2)C29-C30	BD*(1)C1-I35	9.92	11.00	0.0094
		BD(1)C29-H31	BD*(1)C1-I35	0.54		
		BD(1)C30-H32	BD*(1)C1-I35	0.54		
	$\pi\text{-hole} \cdots \pi$	BD(2)C7-C21	BD*(2)C4-C6	1.92	7.32	0.0134
		BD(2)C8-C28	BD*(2)C3-C5	0.96		
		BD(2)C11-C15	BD*(2)C1-C2	0.84		
		BD(2)C11-C15	BD*(1)C2-F33	0.59		
		BD(2)C12-C16	BD*(2)C3-C5	1.51		
		BD(2)C12-C16	BD*(1)C3-F34	0.59		

12DIPB-FA	σ -hole $\cdots\pi$	BD(2)C19-C20	BD*(2)C1-C2	0.38	3.10	0.0029
		BD(2)C24-C26	BD*(2)C4-C6	0.54		
		BD(2)C10-C13	BD*(1)I27-C28	2.68		
		BD(1)C13-H21	BD*(1)I27-C28	0.42		
	σ -hole $\cdots$ lep	LP(1)I12	BD*(1)I13-C14	1.80	12.97	0.0131
		LP(2)I12	BD*(1)I13-C14	2.71		
		LP(3)I12	BD*(1)I13-C14	8.45		
	π -hole $\cdots\pi$	BD(2)C13-C15	BD*(2)C3-C5	0.46	6.28	0.0049
		BD(2)C14-C18	BD*(1)F1-C2	0.38		
		BD(2)C14-C18	BD*(2)C2-C4	0.25		
		BD(2)C22-C26	BD*(2)C2-C4	0.88		
		BD(2)C22-C26	BD*(1)C4-F6	0.42		
		BD(2)C23-C28	BD*(2)C3-C5	1.33		
		BD(2)C24-C29	BD*(2)C7-C8	0.42		
		BD(2)C24-C29	BD*(1)C8-F10	0.46		
		BD(2)C25-C30	BD*(2)C7-C8	1.13		
		BD(2)C25-C30	BD*(1)C7-C9	0.54		
1IPB-FA	π -hole $\cdots\pi$	BD(2)C10-C41	BD*(2)C2-C6	0.63	6.77	0.0045
		BD(2)C10-C41	BD*(1)C9-F11	0.59		
		BD(2)C10-C41	BD*(2)C9-C12	2.22		
		BD(2)C40-C43	BD*(1)C6-F8	0.25		
		BD(2)C42-C47	BD*(2)C1-C3	0.29		
		BD(2)C42-C47	BD*(2)C9-C12	0.29		
		BD(2)C46-C53	BD*(2)C9-C12	0.38		
		BD(2)C46-C53	BD*(1)C12-F14	0.46		
		BD(2)C48-C55	BD*(2)C1-C3	1.13		
		BD(2)C48-C55	BD*(2)C2-C6	0.54		

“LP” for 1-center valence lone pair, “BD” for 2-center bond and “BD*” for 2-center antibond.

Continuous **Table S3** The charge donor-acceptor interactions, second-order perturbation stabilization energies E^2 (in $\text{kJ}\cdot\text{mol}^{-1}$) and the amount of charge transfer Δq (in *a.u.*) in 13DBrPB-FA, 14DBrPB-FA, 12DBrPB-FA, 1BrPB-FA cocrystal and 1CIPB-FA by NBO analysis.

Charge Donor	Charge Acceptor	E^2	E^2_{total}	Δq
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13DBrPB-FA	π -hole $\cdots\pi$	BD(2)C13-C16	BD*(2)C2-C6	0.33	7.15	0.0043
		BD(2)C14-C19	BD*(2)C4-C8	0.25		
		BD(2)C14-C19	BD*(2)C10-C12	1.72		
		BD(2)C14-C19	BD*(1)F11-C12	0.59		
		BD(2)C15-C20	BD*(2)C4-C8	0.33		
		BD(2)C17-C23	BD*(2)C2-C6	0.29		
		BD(2)C17-C23	BD*(2)C10-C12	0.38		
		BD(2)C18-C24	BD*(1)F9-C10	0.29		
		BD(2)C18-C24	BD*(2)C10-C12	0.46		
		BD(2)C22-C27	BD*(2)C2-C6	0.79		
		BD(2)C22-C27	BD*(1)F5-C6	0.33		
		BD(2)C26-C28	BD*(2)C4-C8	0.84		
		BD(2)C26-C28	BD*(1)F7-C8	0.54		
14DBrPB-FA	π -hole $\cdots\pi$	BD(2)C13-C16	BD*(2)C4-C8	0.79	13.39	0.0074
		BD(2)C13-C16	BD*(1)F7-C8	0.50		
		BD(2)C14-C18	BD*(2)C4-C8	2.34		
		BD(2)C14-C18	BD*(2)C6-C12	1.55		
		BD(2)C15-C26	BD*(2)C2-C10	0.79		
		BD(2)C15-C26	BD*(1)F9-C10	0.50		
		BD(2)C17-C28	BD*(2)C2-C110	1.17		
		BD(2)C17-C28	BD*(2)C4-C8	1.17		
		BD(2)C19-C25	BD*(2)C2-C10	2.34		
		BD(2)C19-C25	BD*(2)C6-C12	1.55		
		BD(2)C23-C32	BD*(1)F5-C6	0.33		
		BD(2)C23-C32	BD*(1)F11-C12	0.33		
12DBrPB-FA	π -hole $\cdots\pi$	BD(2)C39-C41	BD*(2)C2-C5	1.00	13.13	0.0091
		BD(2)C39-C41	BD*(2)C4-C7	1.59		
		BD(2)C44-C47	BD*(1)C5-F14	0.21		
		BD(2)C45-C49	BD*(2)C4-C7	0.84		
		BD(2)C45-C49	BD*(1)C7-F8	0.21		
		BD(2)C45-C49	BD*(1)C9-F10	0.33		
		BD(2)C45-C49	BD*(2)C9-C11	1.05		
		BD(2)C51-C53	BD*(2)C9-C11	0.21		
		BD(2)C51-C53	BD*(1)C11-F12	0.25		
		BD(2)C13-C20	BD*(2)C2-C5	0.38		

		BD(2)C13–C20	BD*(2)C9–C11	1.80		
		BD(2)C13–C20	BD*(1)C11–F12	0.75		
		BD(2)C16–C18	BD*(2)C2–C5	0.54		
		BD(2)C16–C18	BD*(1)C5–F14	0.46		
		BD(2)C17–C34	BD*(2)C2–C5	0.25		
		BD(2)C17–C34	BD*(2)C4–C7	0.75		
		BD(2)C24–C25	BD*(2)C4–C7	1.63		
		BD(2)C24–C25	BD*(1)C7–F8	0.33		
		BD(2)C24–C25	BD*(2)C9–C11	0.54		
1BrPB–FA	π -hole $\cdots\pi$	BD(2)C12–C40	BD*(2)C7–C19	0.63	13.31	0.0070
		BD(2)C15–C33	BD*(1)F6–C19	0.50		
		BD(2)C15–C33	BD*(1)C7–C19	1.13		
		BD(2)C17–C27	BD*(2)C7–C19	0.25		
		BD(2)C23–C25	BD*(2)C8–C10	0.33		
		BD(2)C32–C36	BD*(1)F3–C18	0.59		
		BD(2)C32–C36	BD*(2)C14–C18	0.84		
		BD(2)C9–C38	BD*(1)F2–C10	0.50		
		BD(2)C9–C38	BD*(2)C8–C10	0.84		
		BD(2)C11–C20	BD*(2)C7–C19	1.21		
		BD(2)C11–C20	BD*(2)C8–C10	1.84		
		BD(2)C22–C28	BD*(2)C7–C19	1.59		
		BD(2)C22–C28	BD*(2)C14–C18	1.17		
		BD(2)C30–C35	BD*(1)F4–C7	0.33		
		BD(2)C39–C47	BD*(2)C8–C10	0.46		
		BD(2)C39–C47	BD*(2)C14–C18	1.09		
1CIPB–FA	π -hole $\cdots\pi$	BD(2)C38–C41	BD*(2)C2–C4	1.00	14.90	0.0045
		BD(2)C38–C41	BD*(2)C6–C8	0.54		
		BD(2)C39–C44	BD*(2)C6–C8	1.63		
		BD(2)C39–C44	BD*(1)F7–C8	0.67		
		BD(2)C39–C44	BD*(2)C10–C11	0.33		
		BD(2)C40–C46	BD*(1)F5–C6	0.59		
		BD(2)C40–C46	BD*(2)C6–C8	0.96		
		BD(2)C47–C54	BD*(2)C2–C4	1.42		
		BD(2)C47–C54	BD*(2)C10–C11	0.42		
		BD(2)C13–C19	BD*(2)C2–C4	0.42		

BD(2)C13–C19	BD*(1)F9–C10	0.50
BD(2)C13–C19	BD*(2)C10–C11	2.05
BD(2)C16–C22	BD*(2)C6–C8	0.75
BD(2)C16–C22	BD*(2)C10–C11	1.00
BD(2)C20–C24	BD*(2)C2–C4	1.26
BD(2)C20–C24	BD*(1)F3–C4	0.38
BD(2)C20–C24	BD*(1)F5–C6	0.25
BD(2)C20–C24	BD*(2)C6–C8	0.71

“LP” for 1–center valence lone pair, “BD” for 2–center bond and “BD*” for 2–center antibond.

Continuous **Table S3** The charge donor–acceptor interactions, second–order perturbation stabilization energies E^2 (in $\text{kJ}\cdot\text{mol}^{-1}$) and the amount of charge transfer Δq (in *a.u.*) in 12DIPB–FA cocrystal by NBO analysis.

		Charge Donor	Charge Acceptor	E^2	E^2_{total}	Δq
12DIPB–FA(a)	π –hole $\cdots\pi$	BD(2)C2–C4	BD*(2)C21–C23	1.46	8.08	0.0043
		BD(2)C2–C4	BD*(2)C23–F25	0.92		
		BD(2)C3–C6	BD*(2)C21–C23	0.33		
		BD(2)C3–C6	BD*(1)C21–F24	0.38		
		BD(2)C7–C10	BD*(2)C17–C20	0.84		
		BD(2)C7–C10	BD*(2)C21–C23	0.25		
		BD(2)C11–C28	BD*(1)C17–F19	0.96		
		BD(2)C11–C28	BD*(2)C17–C20	1.30		
		BD(2)C13–C30	BD*(2)C16–C18	0.29		
		BD(2)C14–C15	BD*(2)C16–C18	1.09		
12DIPB–FA(b)	π –hole $\cdots\pi$	BD(2)C3–C6	BD*(2)C27–C30	0.79	2.05	0.0061
		BD(2)C3–C6	BD*(1)C30–F33	0.59		
		BD(2)C17–C19	BD*(2)C29–C32	0.67		
12DIPB–FA(c)	π –hole $\cdots\pi$	BD(2)C2–C5	BD*(2)C33–C34	1.30	6.53	0.0046
		BD(2)C2–C5	BD*(1)C33–F35	0.92		
		BD(2)C6–C10	BD*(1)C26–F27	0.96		
		BD(2)C6–C10	BD*(2)C26–C29	0.92		
		BD(2)C8–C12	BD*(2)C33–C34	1.09		

		BD(2)C11–C15	BD*(1)C28–F30	0.38		
		BD(2)C11–C15	BD*(2)C28–C31	0.96		
12DIPB–FA(d)	π -hole $\cdots\pi$	BD(2)C10–C12	BD*(2)C29–C31	1.13	6.44	0.0044
		BD(2)C10–C12	BD*(1)C29–F33	0.21		
		BD(2)C13–C15	BD*(2)C29–C31	2.85		
		BD(2)C13–C15	BD*(2)C30–C32	1.13		
		BD(2)C13–C15	BD*(1)C31–F35	0.59		
		BD(2)C13–C15	BD*(1)C32–F36	0.29		
		BD(2)C14–C16	BD*(1)C31–F35	0.25		
12DIPB–FA(e)	π -hole $\cdots\pi$	BD(2)C13–C14	BD*(2)C–C3	0.33	6.74	0.0041
		BD(2)C13–C14	BD*(1)C1–F8	0.25		
		BD(2)C15–C19	BD*(2)C1–C3	1.76		
		BD(2)C15–C19	BD*(1)C3–F9	0.96		
		BD(2)C15–C19	BD*(1)C5–C6	0.42		
		BD(2)C18–C23	BD*(2)C5–C6	0.25		
		BD(2)C29–C35	BD*(1)C2–C4	0.46		
		BD(2)C29–C35	BD*(2)C5–C6	1.63		
		BD(2)C29–C35	BD*(2)C6–F10	0.67		
12DIPB–FA(f)	π -hole $\cdots\pi$	BD(2)C17–C20	BD*(2)C32–C33	1.05	3.60	0.0035
		BD(2)C17–C20	BD*(1)C33–C35	0.42		
		BD(2)C22–C24	BD*(2)C32–C33	1.13		
		BD(2)C22–C24	BD*(1)C32–F34	1.00		
12DIPB–FA(g)	π -hole $\cdots\pi$	BD(2)C15–C17	BD*(2)C1–C2	1.09	5.82	0.0041
		BD(2)C15–C17	BD*(2)C4–C10	1.17		
		BD(2)C19–C28	BD*(1)C4–F9	0.25		
		BD(2)C19–C28	BD*(1)C10–F12	0.25		
		BD(2)C20–C21	BD*(2)C3–C8	0.79		
		BD(2)C20–C21	BD*(2)C4–C10	1.34		
		BD(2)C20–C21	BD*(1)C10–F12	0.21		
		BD(2)C15–C17	BD*(1)C2–I6	0.21		
		BD(2)C19–C28	BD*(2)C10–F12	0.21		
		BD(2)C20–C21	BD*(1)C10–F12	0.29		
12DIPB–FA(h)	π -hole $\cdots\pi$	BD(2)C13–C15	BD*(2)C3–C5	0.46	6.28	0.0048
		BD(2)C14–C18	BD*(1)F1–C2	0.38		
		BD(2)C14–C18	BD*(2)C2–C4	0.25		

		BD(2)C22–C26	BD*(2)C2–C4	0.88		
		BD(2)C22–C26	BD*(1)C4–F6	0.42		
		BD(2)C23–C28	BD*(2)C3–C5	1.34		
		BD(2)C24–C29	BD*(2)C7–C8	0.42		
		BD(2)C24–C29	BD*(1)C8–F10	0.46		
		BD(2)C25–C30	BD*(2)C7–C8	1.13		
		BD(2)C25–C30	BD*(1)C7–F9	0.54		
12DIPB–FA(i)	π –hole $\cdots\pi$	BD(2)C3–C5	BD*(1)C29–F33	0.46	7.57	0.0038
		BD(2)C3–C5	BD*(2)C29–C34	0.75		
		BD(2)C6–C10	BD*(2)C27–C28	1.00		
		BD(2)C7–C12	BD*(2)C29–C34	2.05		
		BD(2)C7–C12	BD*(2)C30–C36	0.92		
		BD(2)C7–C12	BD*(1)C34–F37	0.33		
		BD(2)C15–C20	BD*(1)C30–F35	0.38		
		BD(2)C15–C20	BD*(1)C36–F38	0.21		
		BD(2)C21–C24	BD*(2)C27–C28	1.05		
		BD(2)C21–C24	BD*(2)C30–C36	0.42		
12DIPB–FA(j)	π –hole $\cdots\pi$	BD(2)C4–C8	BD*(1)F9–C10	0.29	6.44	0.0044
		BD(2)C4–C8	BD*(2)C10–C18	1.13		
		BD(2)C4–C8	BD*(1)C17–F25	0.59		
		BD(2)C4–C8	BD*(2)C17–C26	2.85		
		BD(2)C7–C14	BD*(2)C17–C26	1.13		
		BD(2)C7–C14	BD*(1)C26–F31	0.21		
		BD(2)C15–C22	BD*(1)C17–F25	0.25		
12DIPB–FA(k)	π –hole $\cdots\pi$	BD(2)C15–C18	BD*(1)F1–C2	0.38	7.11	0.0052
		BD(2)C15–C18	BD*(2)C2–C5	0.75		
		BD(2)C15–C18	BD*(1)C4–F6	0.29		
		BD(2)C15–C18	BD*(2)C4–C7	0.63		
		BD(2)C17–C21	BD*(2)C8–C10	0.46		
		BD(2)C19–C23	BD*(1)F1–C2	0.29		
		BD(2)C20–C24	BD*(2)C2–C5	0.50		
		BD(2)C22–C27	BD*(2)C4–C7	0.63		
		BD(2)C25–C31	BD*(2)C8–C10	1.00		
		BD(2)C26–C33	BD*(2)C4–C7	1.26		
		BD(2)C26–C33	BD*(1)C7–F9	0.67		

		BD(2)C22–C27	BD*(1)C4–F6	0.25		
12DIPB–FA(l)	π –hole $\cdots\pi$	BD(2)C2–C4	BD*(2)C29–C32	0.50	9.33	0.0013
		BD(2)C6–C9	BD*(2)C34–C35	0.63		
		BD(2)C8–C11	BD*(2)C27–C30	0.29		
		BD(2)C10–C13	BD*(2)C27–C30	0.46		
		BD(2)C10–C13	BD*(1)C29–F31	0.50		
		BD(2)C10–C13	BD*(2)C29–C32	1.84		
		BD(2)C12–C14	BD*(2)C27–C30	0.42		
		BD(2)C12–C14	BD*(2)C34–C35	2.05		
		BD(2)C12–C14	BD*(1)C34–F36	0.79		
		BD(2)C15–C16	BD*(1)C27–F28	0.88		
		BD(2)C15–C16	BD*(2)C27–C30	0.67		
		BD(2)C8–C11	BD*(1)C30–F33	0.29		

Table 4 The MEPs of the interaction site in **Figure 1** and **Figure 2** (kJ·mol^{−1})

14DI	C5			
	38.40			
135TI	C5	C3	C3	
	30.29	31.48	30.57	
12DI	C23			
	43.79			
11PB	C2	C3	C4	
	45.93	48.66	50.18	
13DBr	C16	C9		
	36.30	45.70		
14DBr	C4	C5	C6	
	42.79	43.06	37.72	
12DBr	C8	C7	C11	
	34.48	33.24	49.06	
1BrPB	C2	C6		
	49.25	48.05		
1CIPB	C2	C1	C6	C4
	49.75	43.75	50.96	55.08