

Electronic Supplementary Material

Studying the Fluorescence Conversion in Organic Charge Transfer Cocrystals of Chalcone Derivatives and TCNB

Kun Zhao,[†] Mingliang Wang, ^{†*} Hao Sun, [†] Wen Tian, [†] Shanguang Yang, [†] Jingjing Liu, [†]
Jing Peng, [†] Huimin Wang, [†] and Chunxiang Xu ^{‡*}

[†] *School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, P. R. China*

[‡] *State Key Laboratory of Bioelectronics, Southeast University, Nanjing 210096, P. R. China*

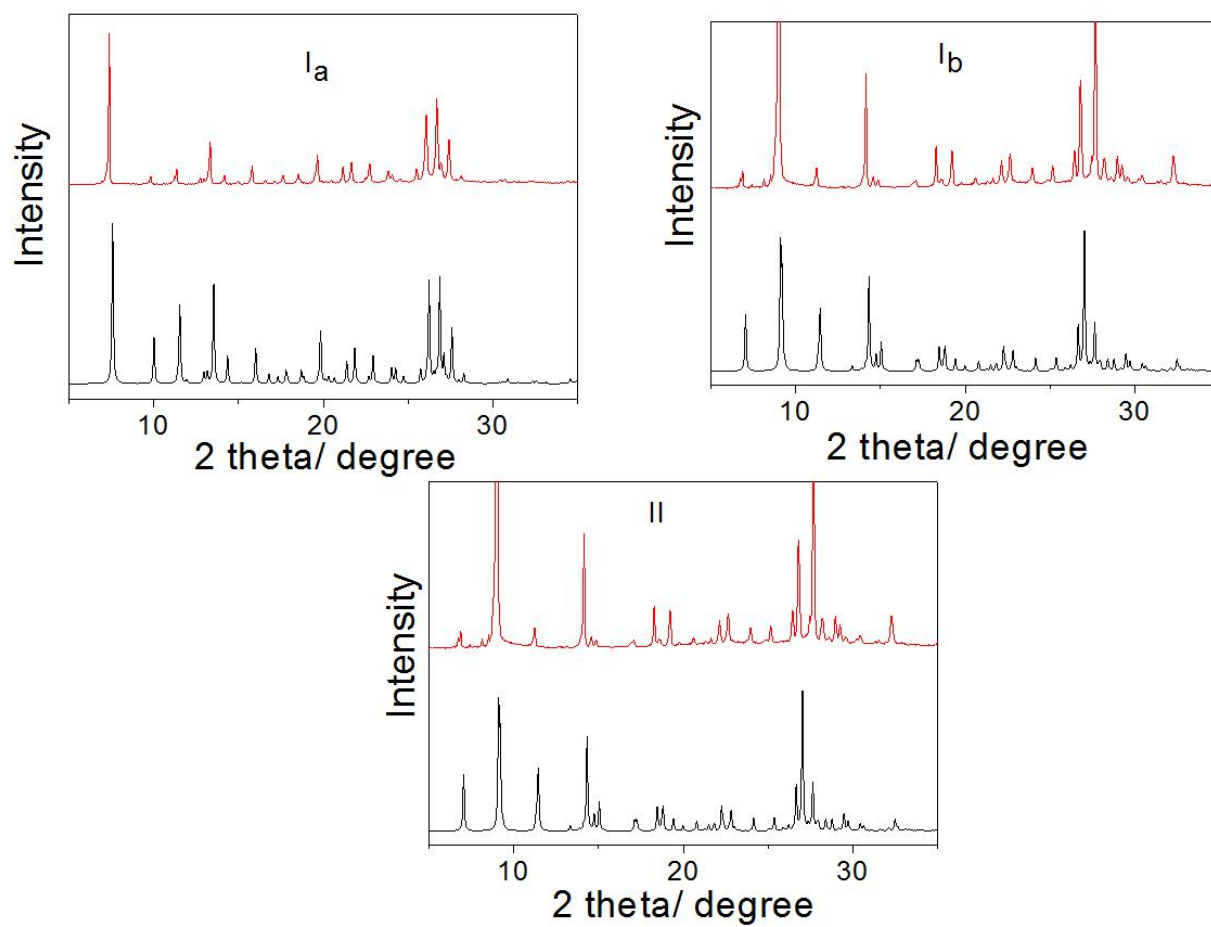


Fig. S1. Experimental (red) and simulated (black) PXRD patterns of I_a, I_b, II

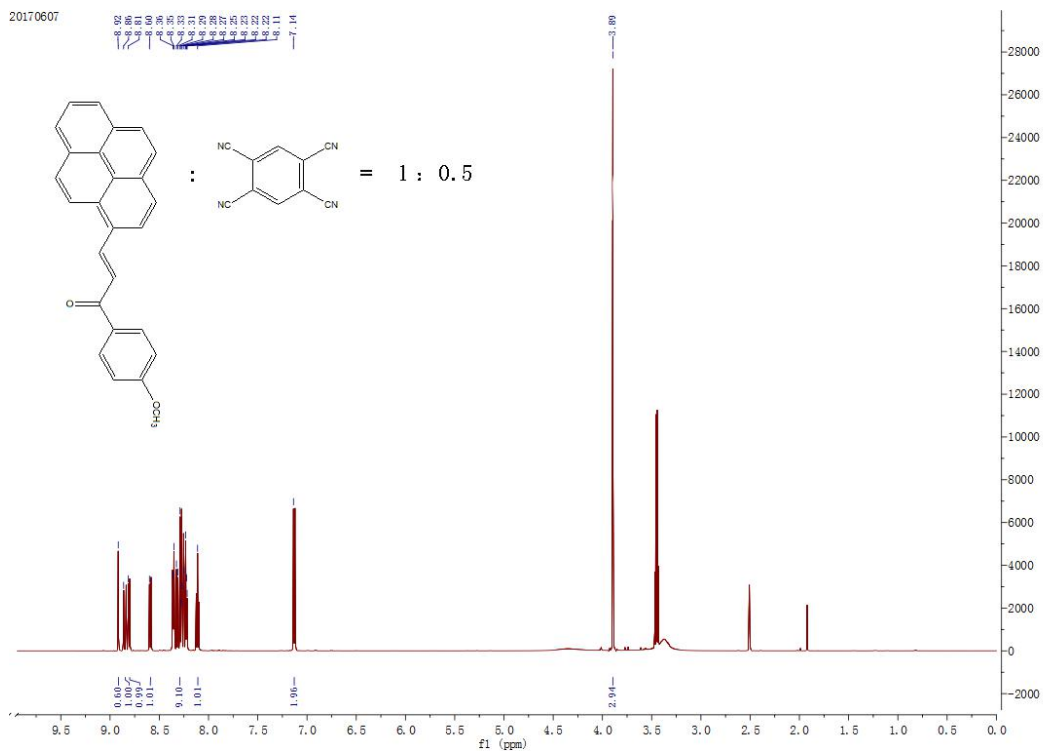


Fig. S2. ^1H NMR spectra of II

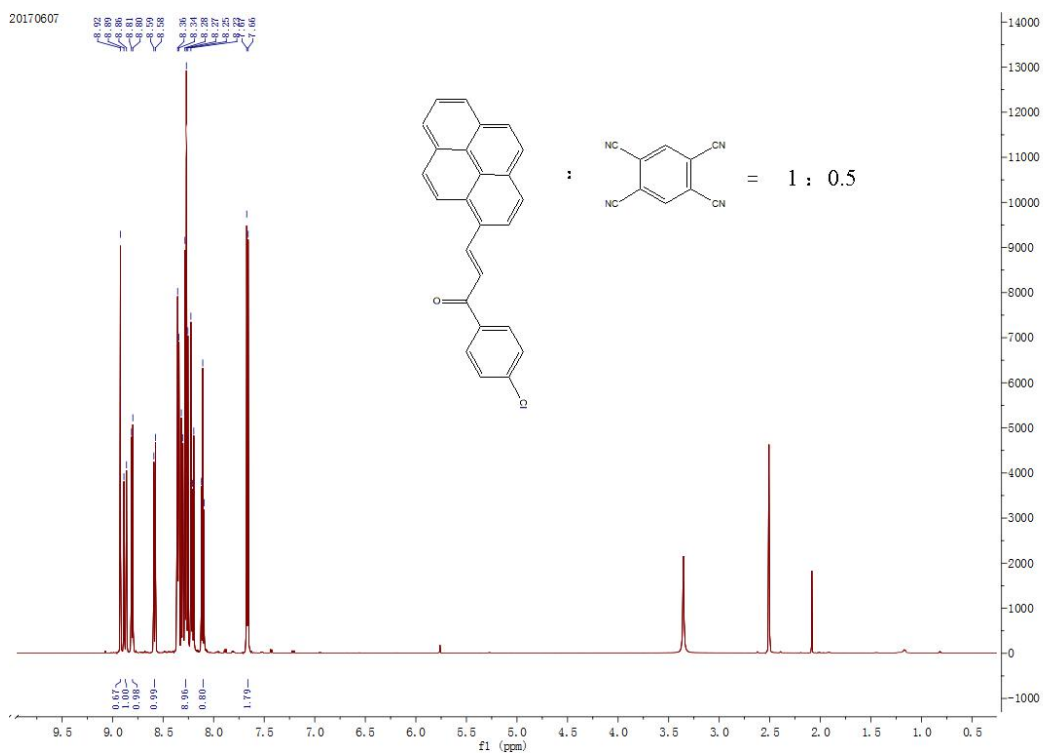


Fig. S3. ^1H NMR spectra of III

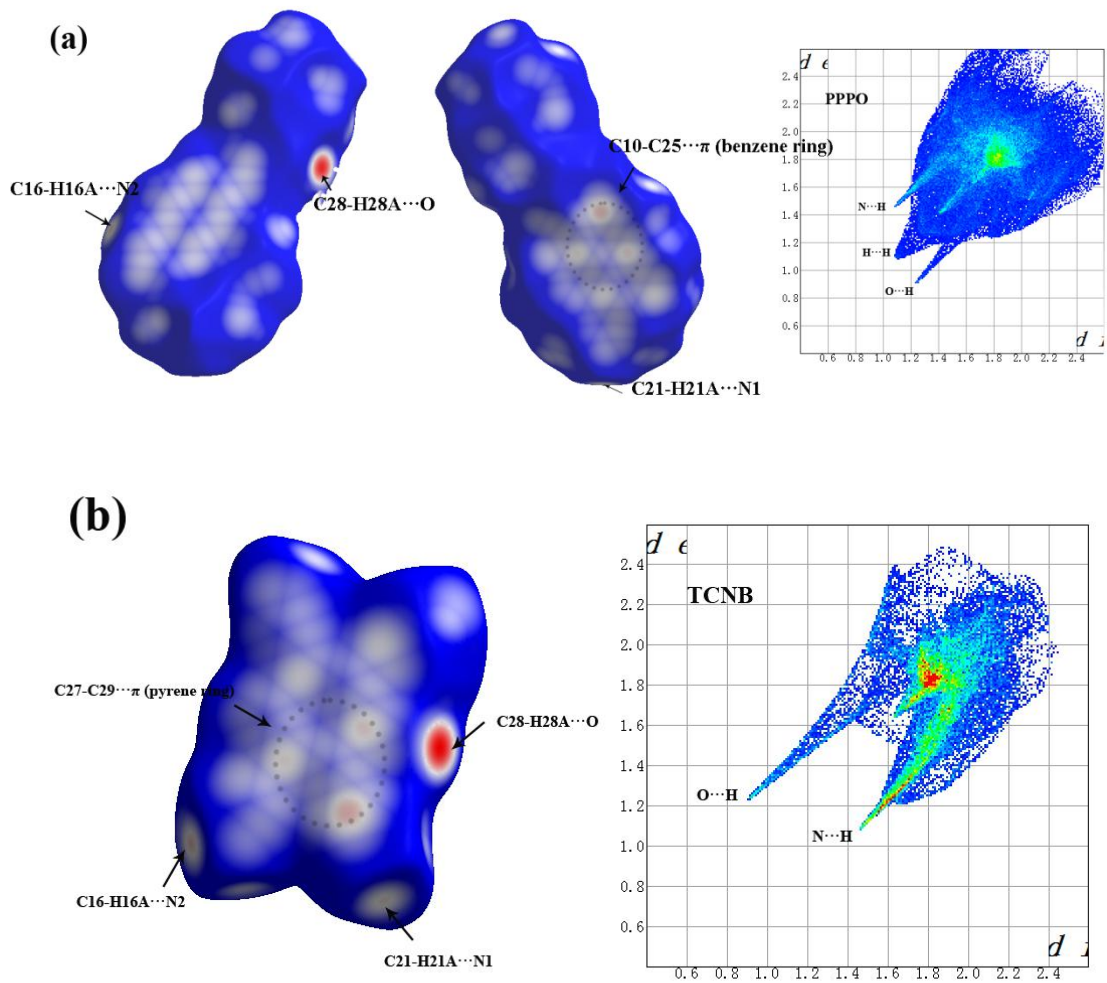


Fig. S4 Views of d_{norm} (from 0.5 Å (blue) to 0.5 Å (red)), mapped on the Hirshfeld surface of cocrystal I_a (seen from two angles) and corresponding fingerprint plot. (a) PPPO (the donor), (b) TCNB (the acceptor)

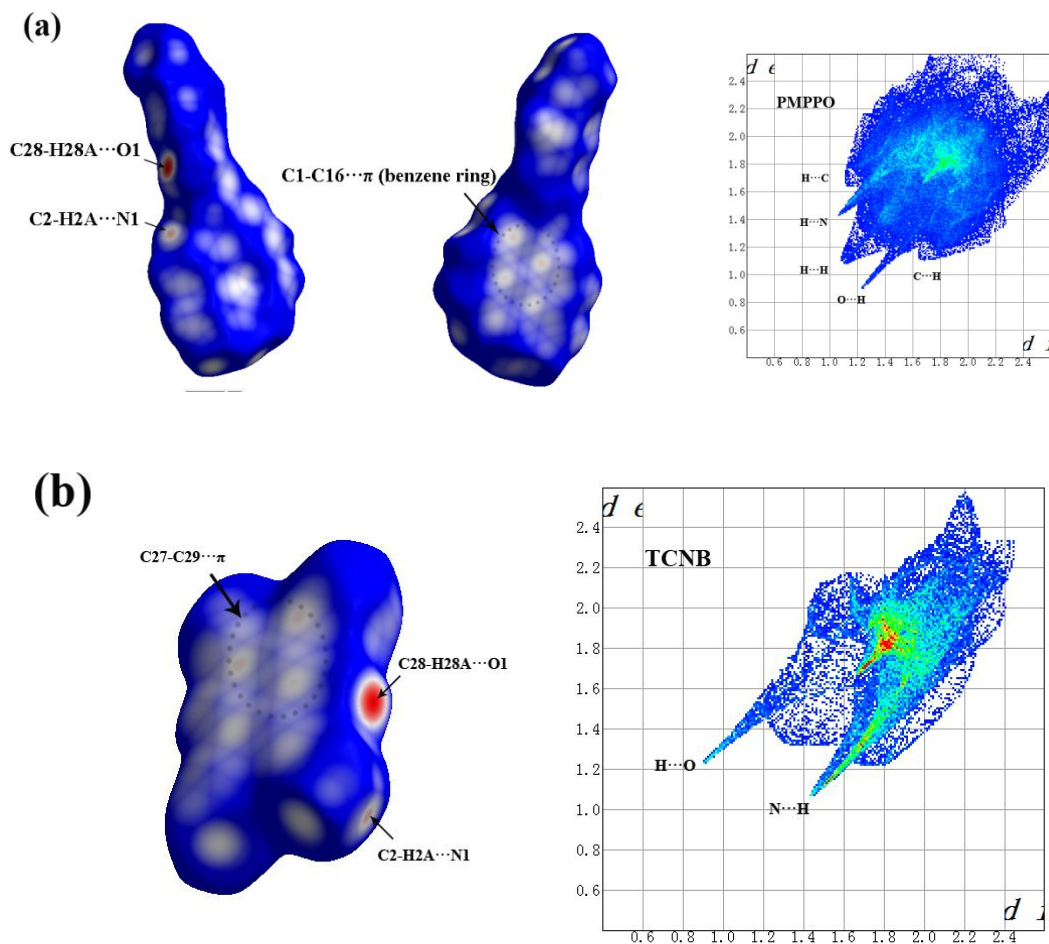


Fig. S5 Views of d_{norm} (from 0.5 Å (blue) to 0.5 Å (red)), mapped on the Hirshfeld surface of cocrystal II (seen from two angles) and corresponding fingerprint plot. (a) PPPO (the donor), (b) TCNB (the acceptor)

Table S1 charge transfer interactions in cocrystals

Crystal	Interaction	$d_{\pi-\pi}, d_{c-c}(\text{Å})$ [b]	Angle (°) [c]
I a	TCNB...pyrene	3.390,3.620(2)	1.87(17)
I b	TCNB(A)...pyrene	3.371 ,3.525(2)	1.71(18)
	TCNB(B)...pyrene	3.301, 3.514(18)	0.60(13)
II	TCNB...pyrene	3.373 , 3.621(2)	0.23(15)