

## Supplementary information

# The Competitive Role of C-H $\cdots$ X (X=F, O) and $\pi$ - $\pi$ Interaction in Contributing to the Charge Transfer Degree in Organic Cocrystals: A Case Study of Heteroatoms-free Donors with *p*-Fluoranil (FA)

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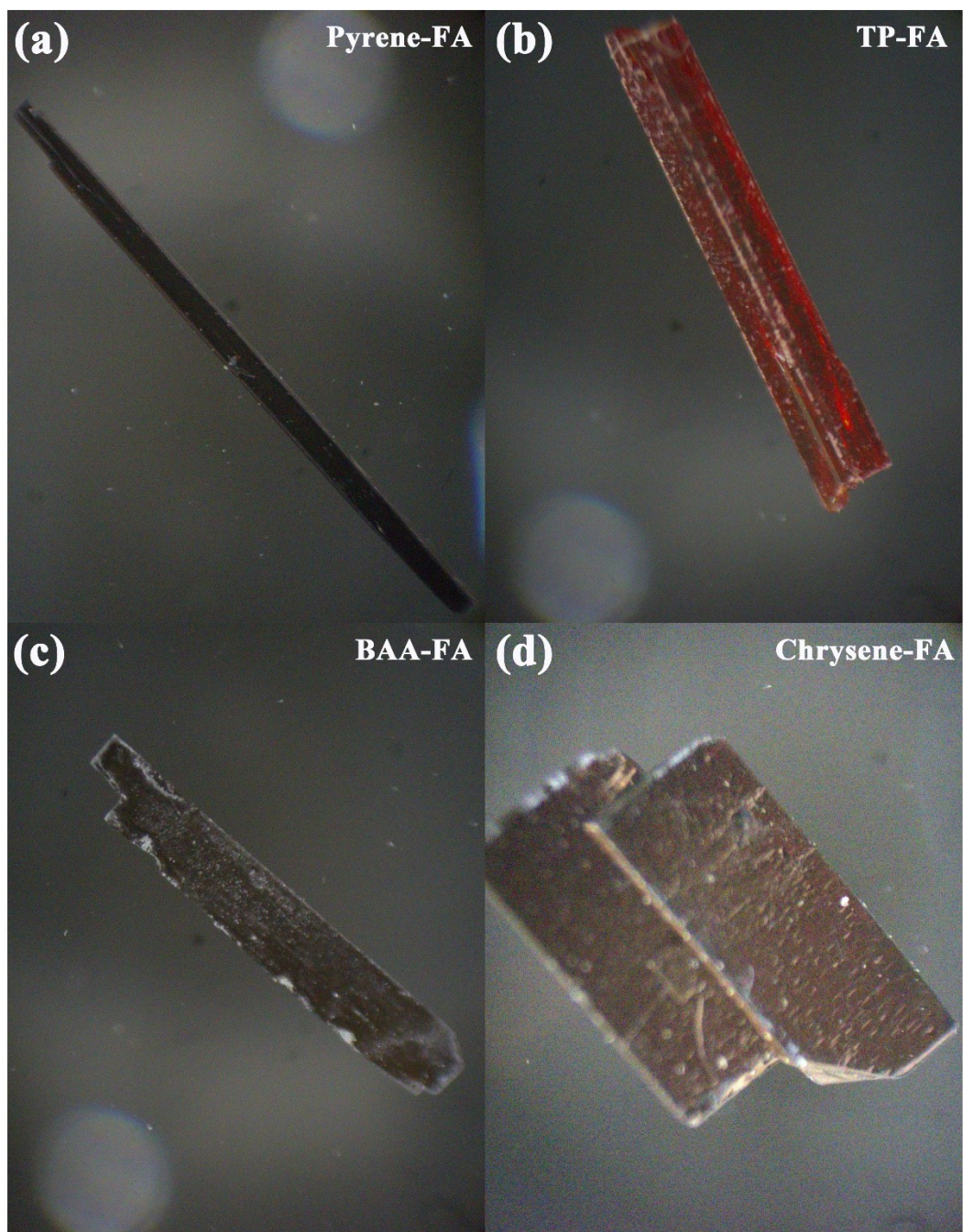


Figure S1. The optical images of the four charge transfer cocrystals in transmission mode.

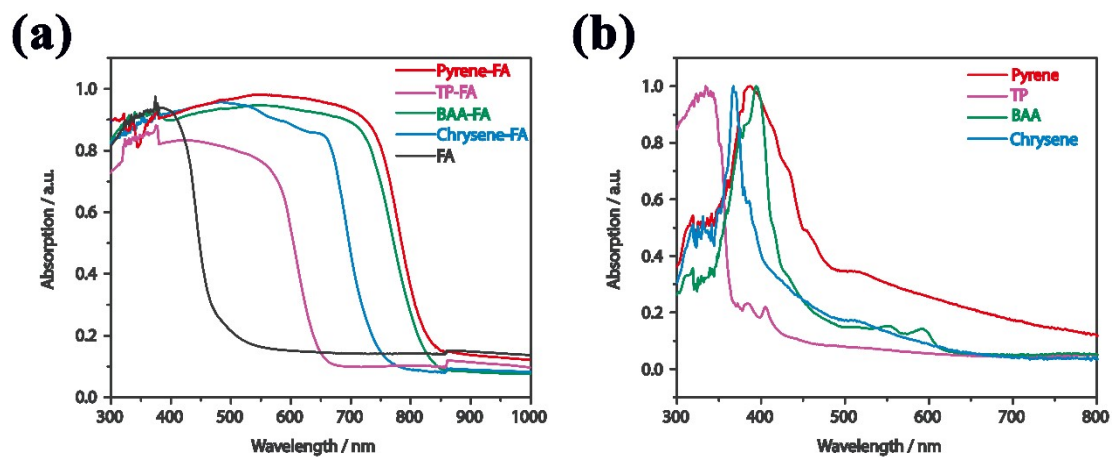


Figure S2. Solid state UV-vis-NIR diffuse reflectance spectra of (a) FA, pyrene-FA, TP-FA, BAA-FA and chrysene-FA (b) pyrene, TP, BAA and chrysene.

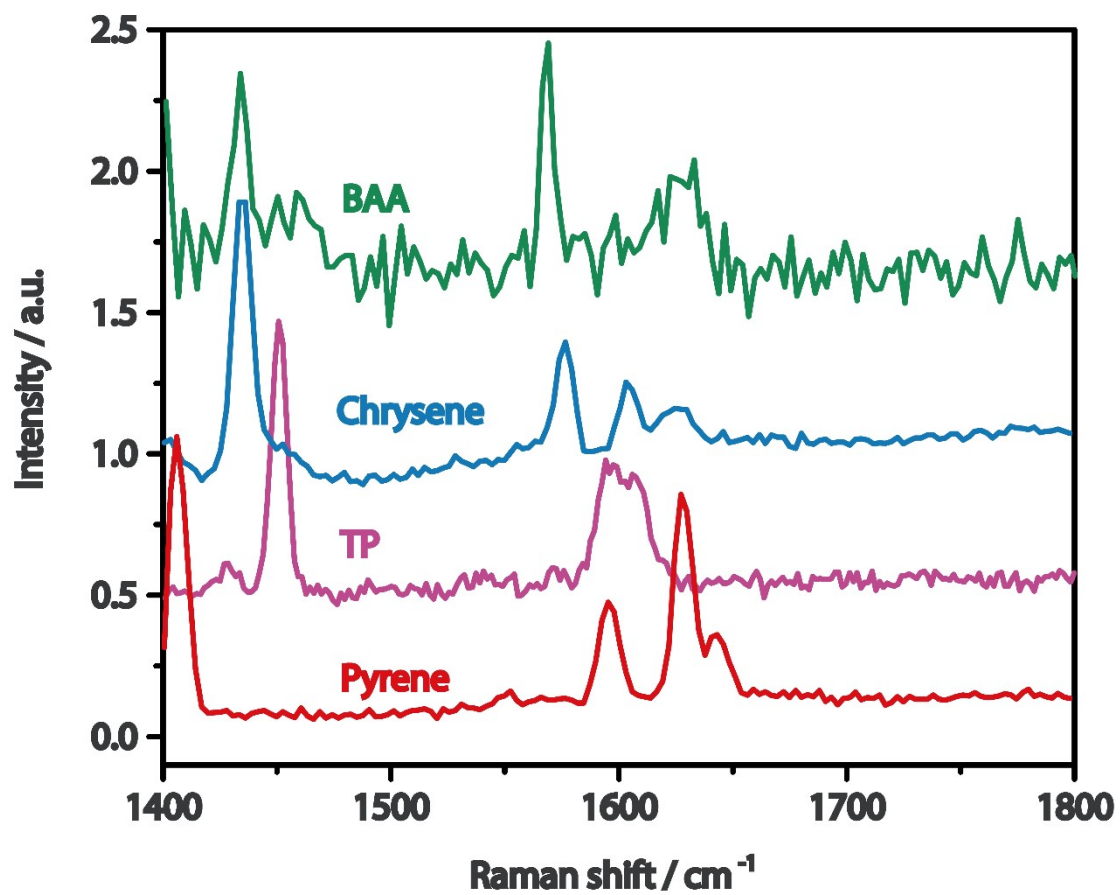


Figure S3. Raman spectra pristine pyrene, TP, BAA and chrysene.

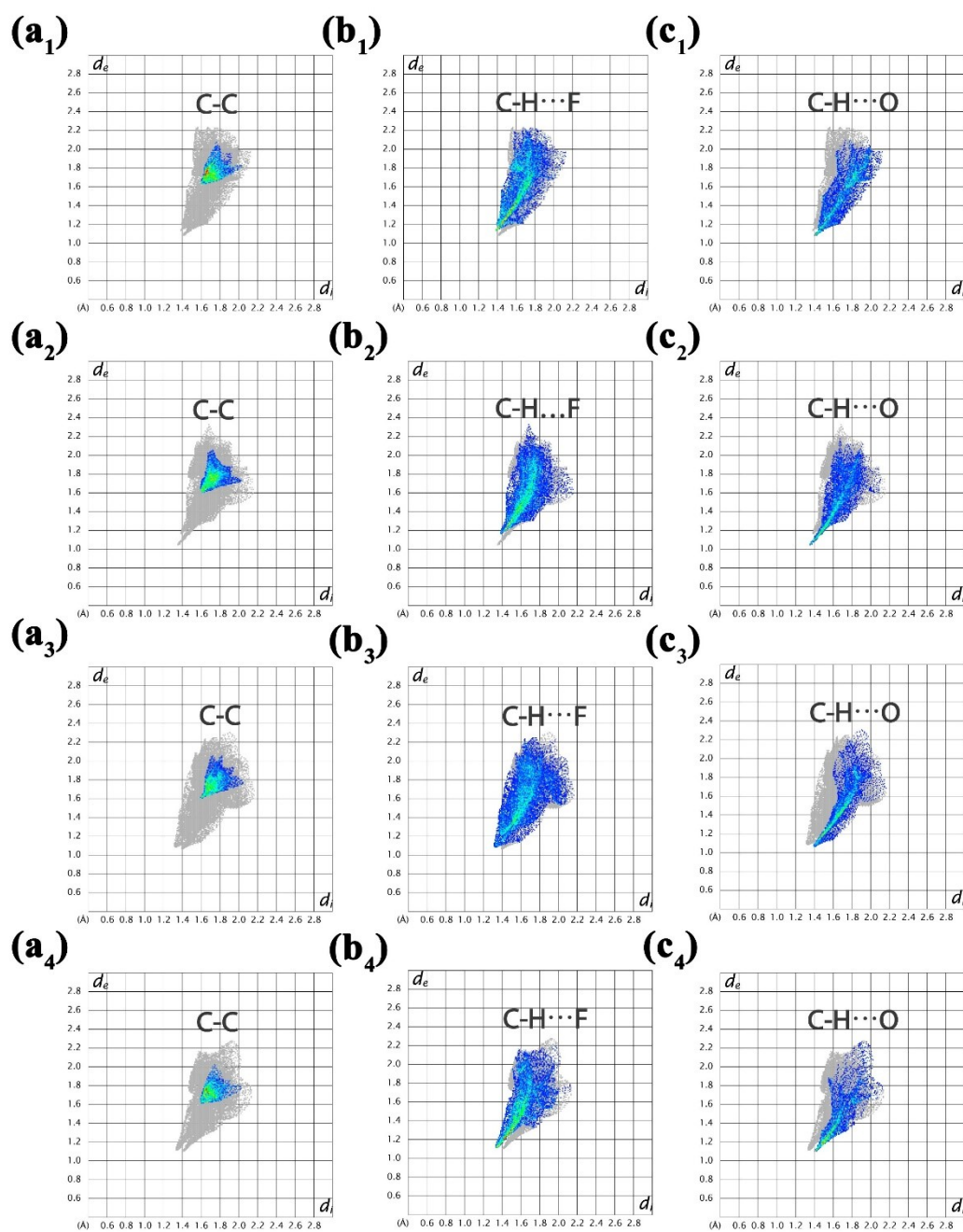


Figure S4. Fingerprint plots visualizing  $d_e$  and  $d_i$  for C-C contact, C-H...F contact and C-H...O contact for generated for FA in (a<sub>1</sub>, b<sub>1</sub>, c<sub>1</sub>) pyrene-FA cocrystal, (a<sub>2</sub>, b<sub>2</sub>, c<sub>2</sub>) TP-FA cocrystal, (a<sub>3</sub>, b<sub>3</sub>, c<sub>3</sub>) BAA-FA cocrystal, (a<sub>4</sub>, b<sub>4</sub>, c<sub>4</sub>) chrysene-FA cocrystal.



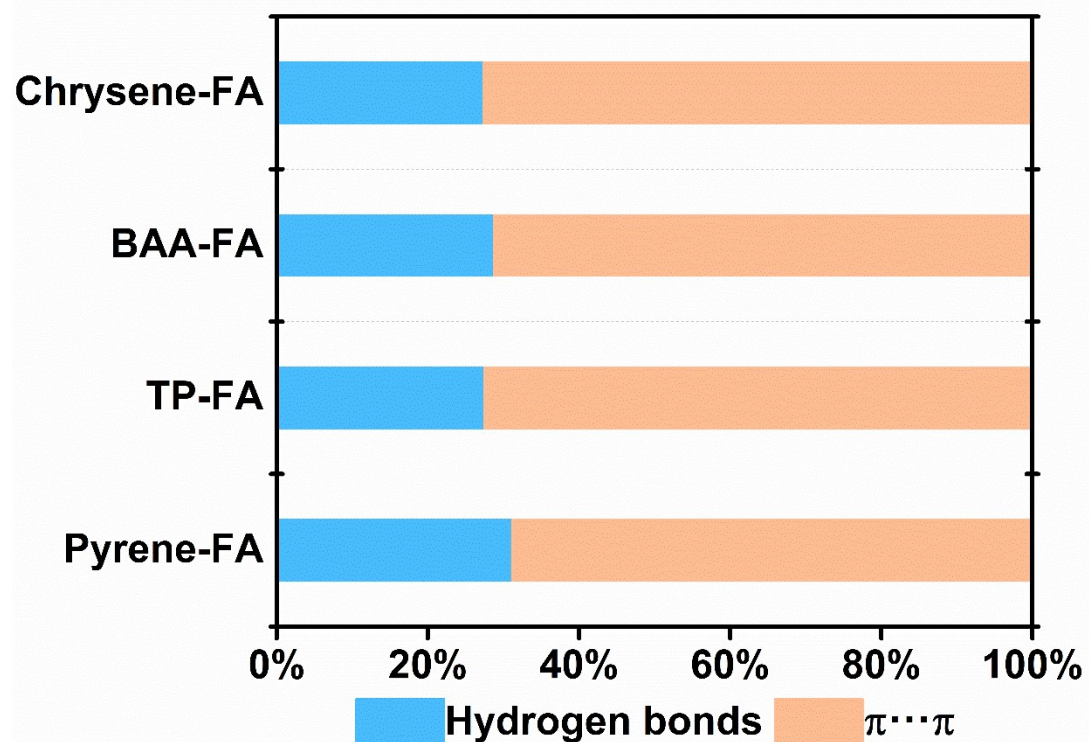


Figure S5. Percentage contributions to the Hirshfeld surface for the various intermolecular contacts for pyrene-FA, TP-FA, BAA-FA and chrysene-FA.