Supporting Information

Controllable Fabrication of Organic Cocrystals with Interior Hollow Structure Based on Donor-Acceptor Charge Transfer Molecules

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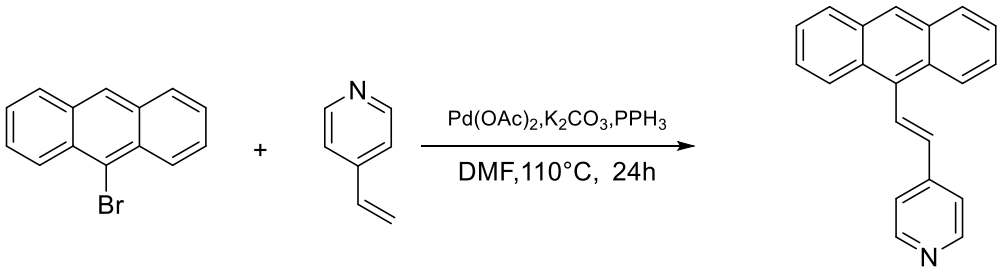

Figure S1. Pathway of synthesis of APE.

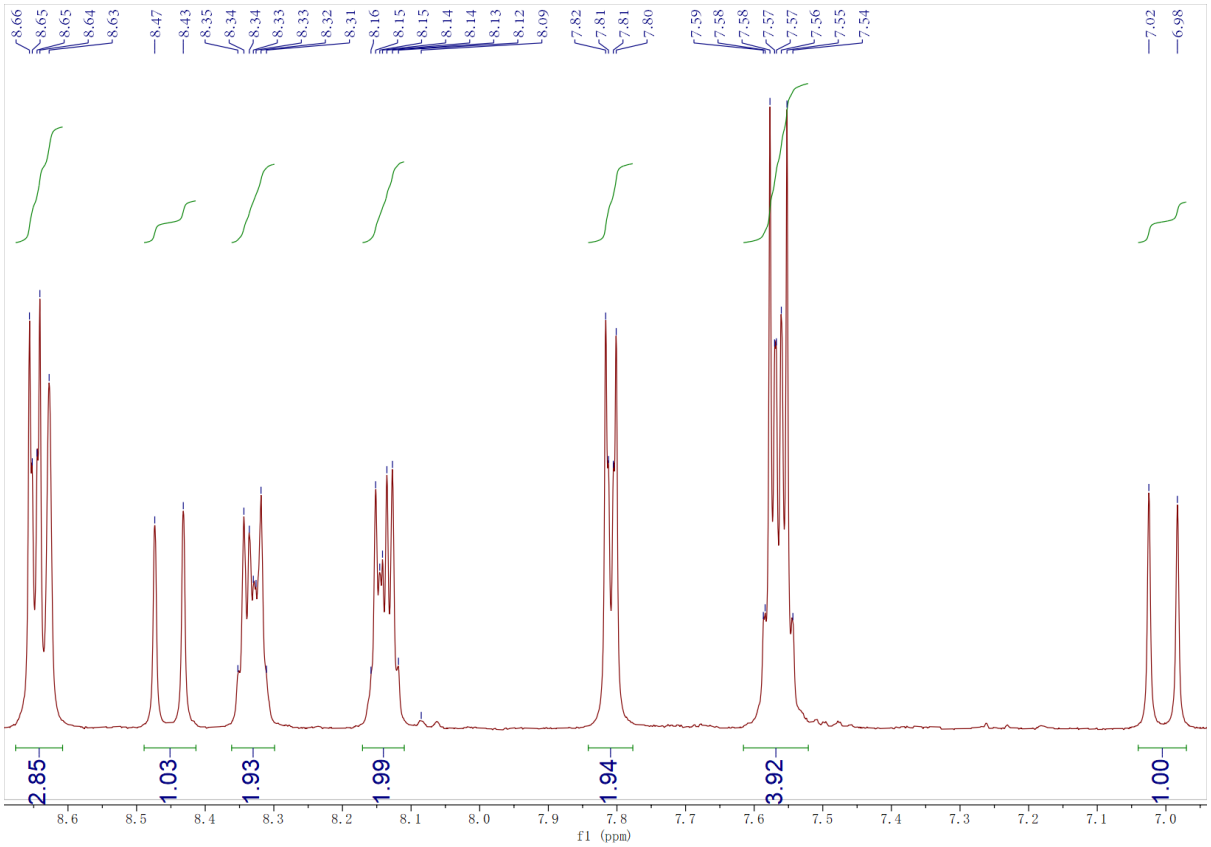

Figure S2. ^{1}H NMR spectrum of APE (DMSO-d_6 as deuterated solvent).

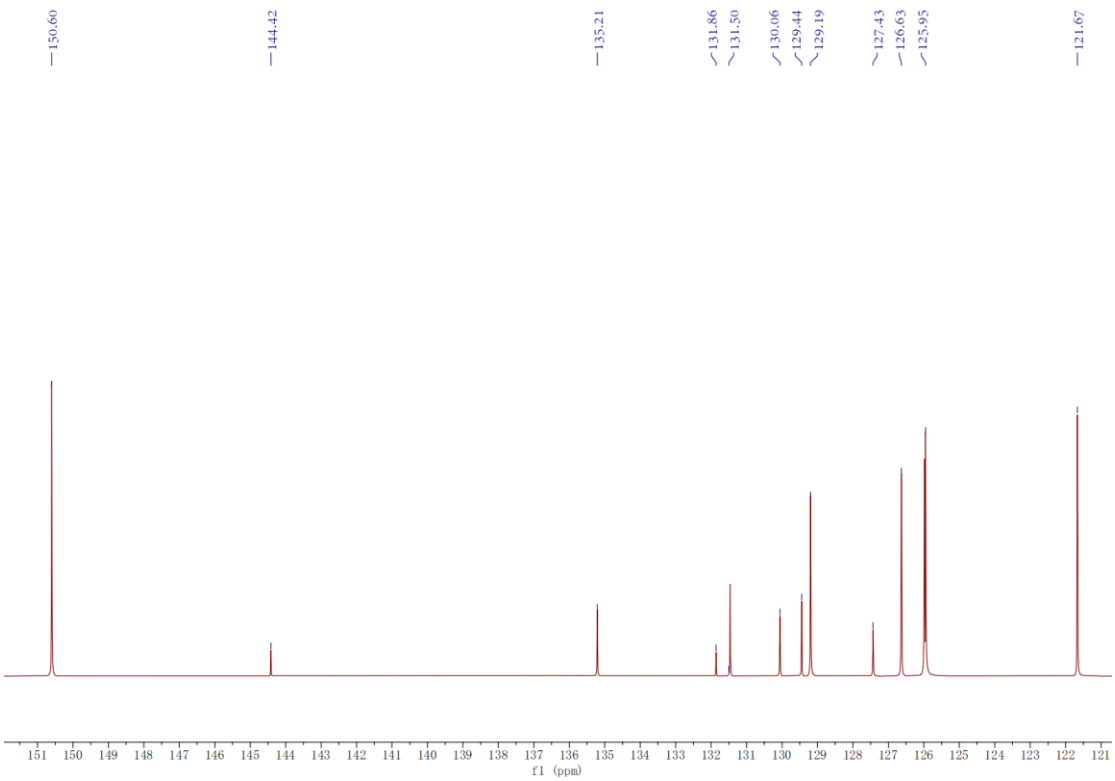

Figure S3. ^{13}C NMR spectrum of APE.

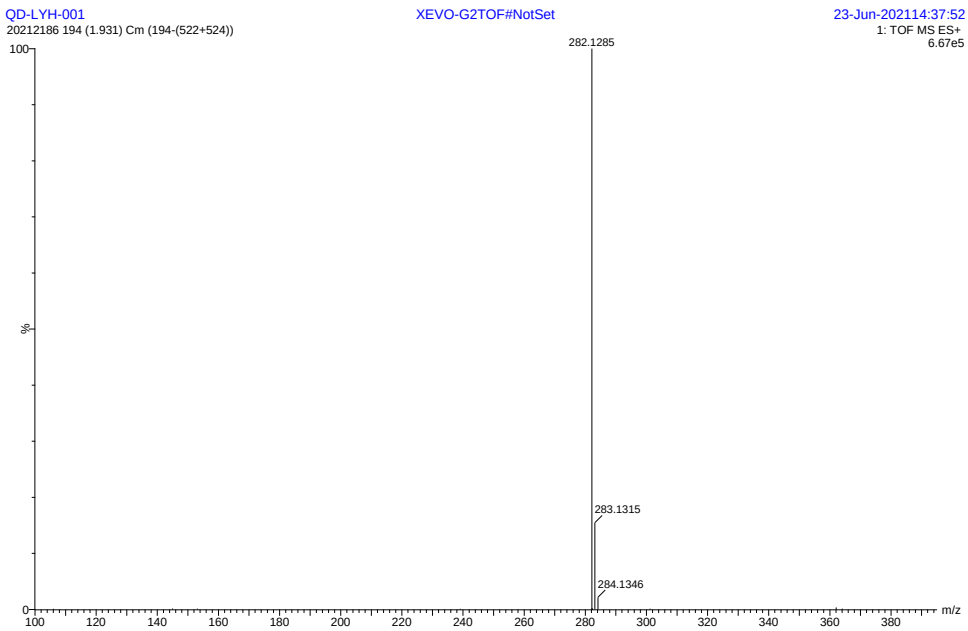

Figure S4.HR-MS(ESI) spectrum of APE.

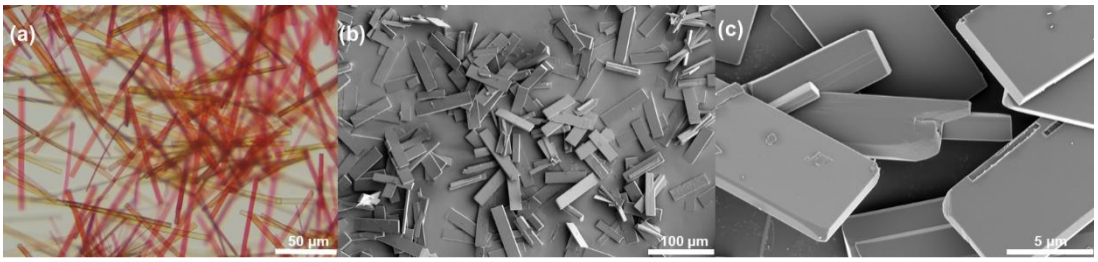

Figure S5. (a) Optical microscopy image of APE-TCNB solid cocrystals grown in SDS. (b) The SEM image of APE-TCNB solid cocrystals. (d) The SEM image of a fractured APE-TCNB solid cocrystal shows the interior structure.

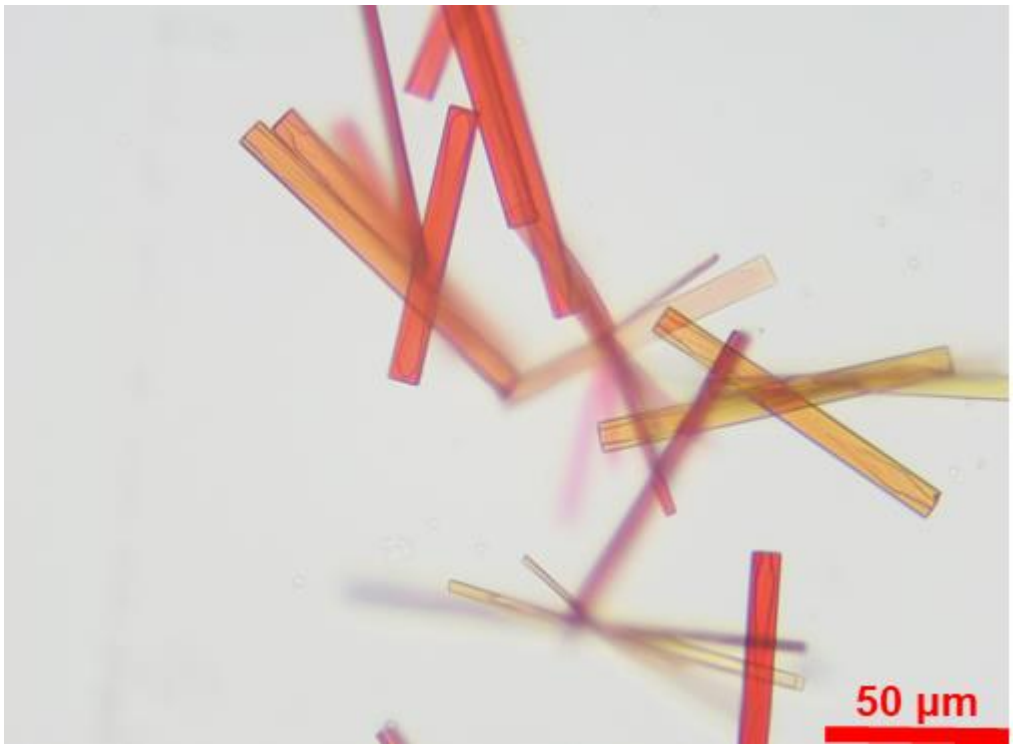

Figure S6. Optical microscopy image of APE-TCNB hollow cocrystals after 15 min intense sonication.

Table S1. Crystal data and structure refinement for mo_d8v211043_0m.

Identification code	mo_d8v211043_0m	
Empirical formula	$C_{31}H_{17}N_5$	
Formula weight	459.49	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.4656(12) Å	a= 90.960(4)°.
	b = 9.1294(15) Å	b= 92.040(4)°.
	c = 34.520(6) Å	g = 91.918(4)°.
Volume	2349.6(7) $Å^3$	
Z	4	
Density (calculated)	1.299 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	952	
Crystal size	0.190 x 0.120 x 0.060 mm^3	
Theta range for data collection	1.771 to 24.999°.	
Index ranges	-8<=h<=8, -10<=k<=10, -41<=l<=41	
Reflections collected	40360	
Independent reflections	8237 [R(int) = 0.0803]	
Completeness to theta = 25.242°	97.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6183	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints / parameters	8237 / 0 / 650	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0763, wR2 = 0.1812	
R indices (all data)	R1 = 0.1539, wR2 = 0.2379	
Extinction coefficient	0.014(2)	
Largest diff. peak and hole	0.536 and -0.357 $e.Å^{-3}$	