

Supplementary Materials:

Additive-assisted crystallization of 9,10-diphenylanthracene

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Table S1. Crystal data, data collection, and structure refinement parameters for PYR-DPA co-crystal.

Chemical formula	C ₂₆ H ₁₈ ·C ₁₆ H ₁₀	Crystal size (mm)	0.845; 0.719; 0.03
<i>M_r</i>	532.64	Crystal color	colorless
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	<i>μ</i> (mm⁻¹)	0.07
<i>a</i>, <i>b</i>, <i>c</i> (Å)	16.4311 (10), 8.0300 (3), 11.2057 (7)	No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	14194, 3143, 2160
<i>β</i> (°)	104.651 (2)	<i>R</i>_{int}	0.047
<i>V</i> (Å³)	1430.42 (14)	<i>R</i>[<i>F</i>² > 2σ(<i>F</i>²)], <i>wR</i>(<i>F</i>²), <i>S</i>	0.051, 0.143, 1.02
<i>Z</i>/<i>Z</i>'	2/0.5	Δ<i>Q</i>_{max}, Δ<i>Q</i>_{min} (e Å⁻³)	0.21, −0.17
<i>D</i>_{calcd} (g cm⁻³)	1.237		

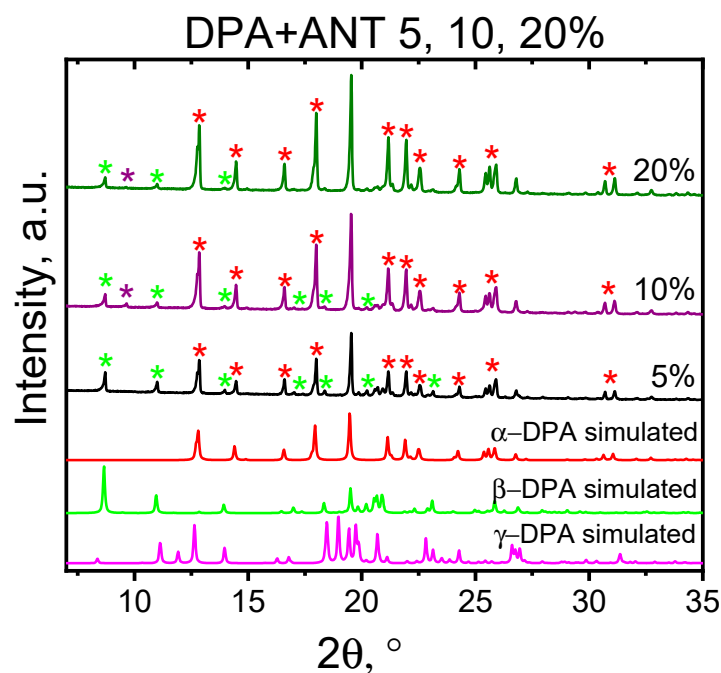


Figure S1. Powder X-ray diffraction patterns of DPA+ANT samples crystallized with different ANT concentrations in comparison with that of DPA polymorphs simulated from single crystal X-ray diffraction data of α-form (red), β-form (green) and γ-form (magenta). Asterisks with matching colors demonstrate the peaks related to α-(red), β-DPA (green) and anthracene peak (purple).

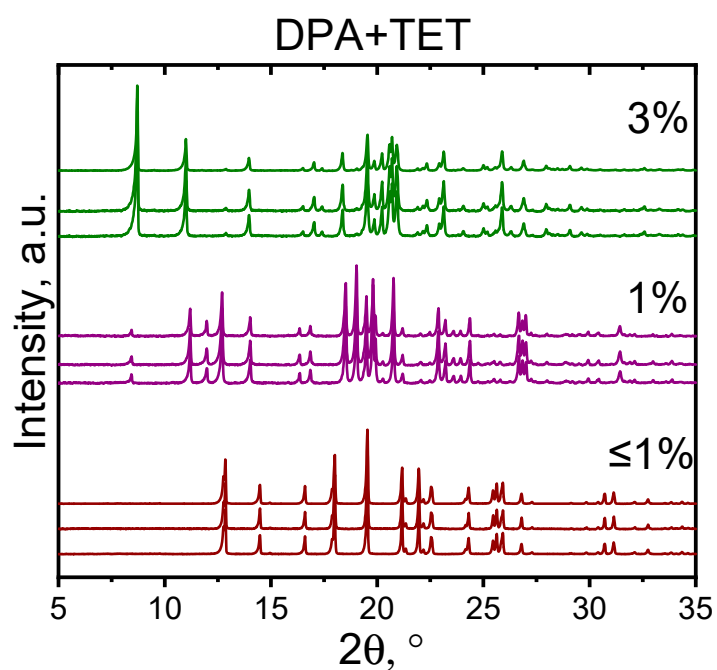


Figure S2. A series of powder X-ray diffraction patterns of DPA+TET samples with variable TET concentrations.

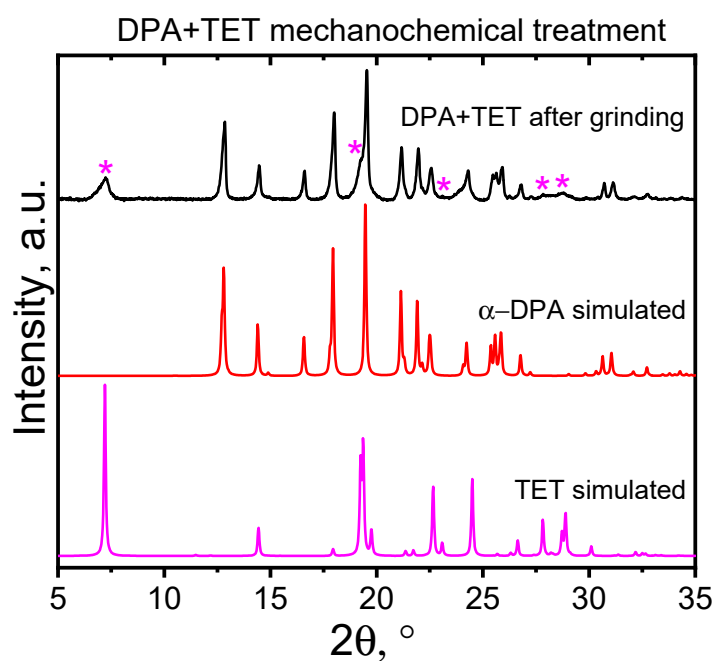


Figure S3. Powder X-ray diffraction patterns of DPA+TET mixture after mechanochemical treatment in comparison with that of α -DPA (red) and TET (magenta) simulated from single crystal X-ray diffraction data. Asterisks with magenta color demonstrate the peaks related to TET.

Table S2. Noncovalent interactions in PYR-DPA co-crystal at 296 K.

	Interactions	H...Cg (Å)	D _{pln} (Å)	C-H...Cg (°)
DPA-DPA	C ₄ -H...Cg ²	2.72	2.68	150
	C ₅ -H...Cg ¹	3.06	2.88	136
DPA-PYR	C ₁₀ -H...Cg ⁵	2.92	2.86	143
	C ₁₁ -H...Cg ⁶	3.00	2.93	150