Phase Behavior of Pyrene and Vinyl Polymers with Aromatic Side Groups

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Supporting Information

Supplementary Figures

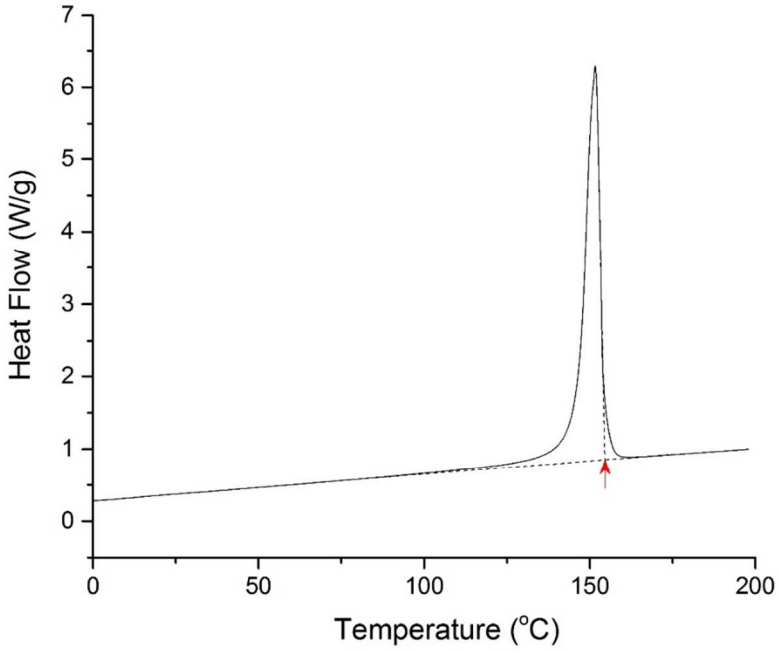

Figure S1. DSC thermogram (endo-up) obtained by heating a pyrene crystal sample, previously annealed at 85 °C for 5 hours, at 10 °C/min. The upward arrow indicates the melting point of pyrene.

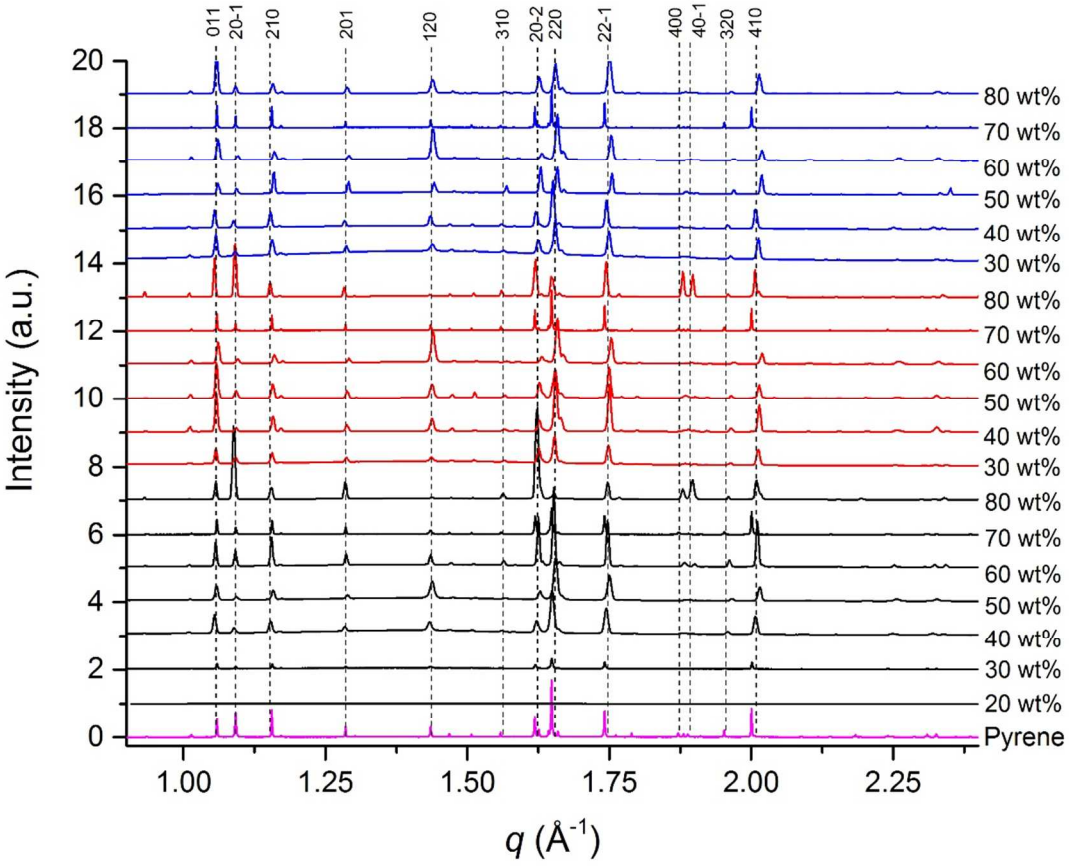

Figure S2. Wide-angle X-ray scattering profiles of pyrene crystals mixed with the model polymers. The black, red, and blue profiles are the scattering patterns of pyrene crystals mixed with polystyrene, poly(2-vinylpyridine) and poly(3-vinylanisole), respectively. The weight percentages listed on the right are that of pyrene in the mixtures. The dashed lines indicate the positions of the Bragg peaks of the pyrene crystals corresponding to the *hkl* planes noted. These profiles were collected at different beamlines of the Advanced Photon Source (11-BM, 12-ID-B, 5-ID) at different times, and the peak locations are slightly different due to variabilities in calibration.

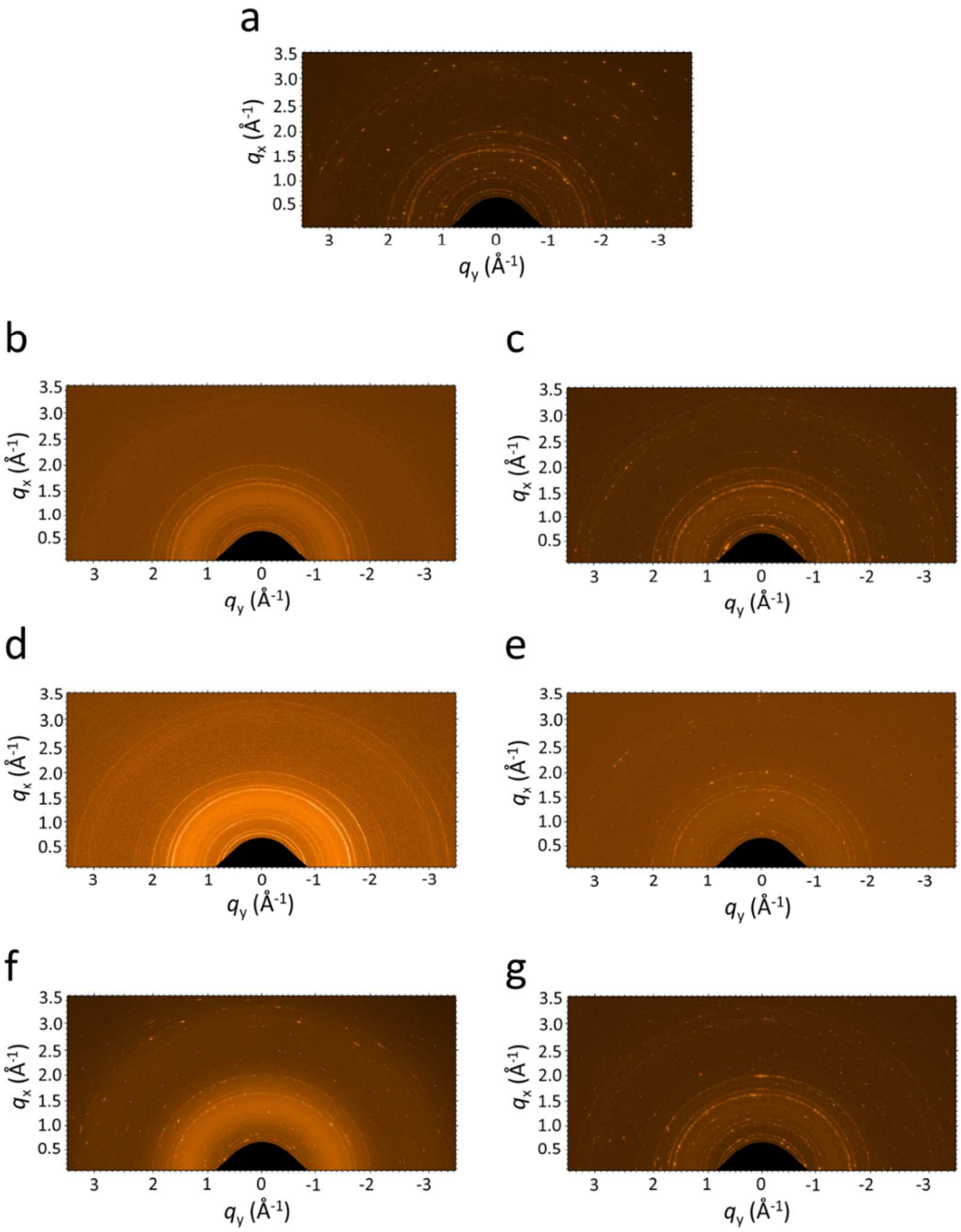

Figure S3. The 2D WAXS patterns of (a) pure pyrene, (b) 30 wt.% and (c) 70 wt.% pyrene blended with polystyrene, (d) 30 wt.% and (e) 70 wt.% pyrene blended with poly(2-vinylpyridine), and (f) 30 wt.% and (g) 70 wt.% pyrene blended with poly(3-vinylanisole). The 30 wt.% pyrene blends showed patterns similar to those of powder samples.

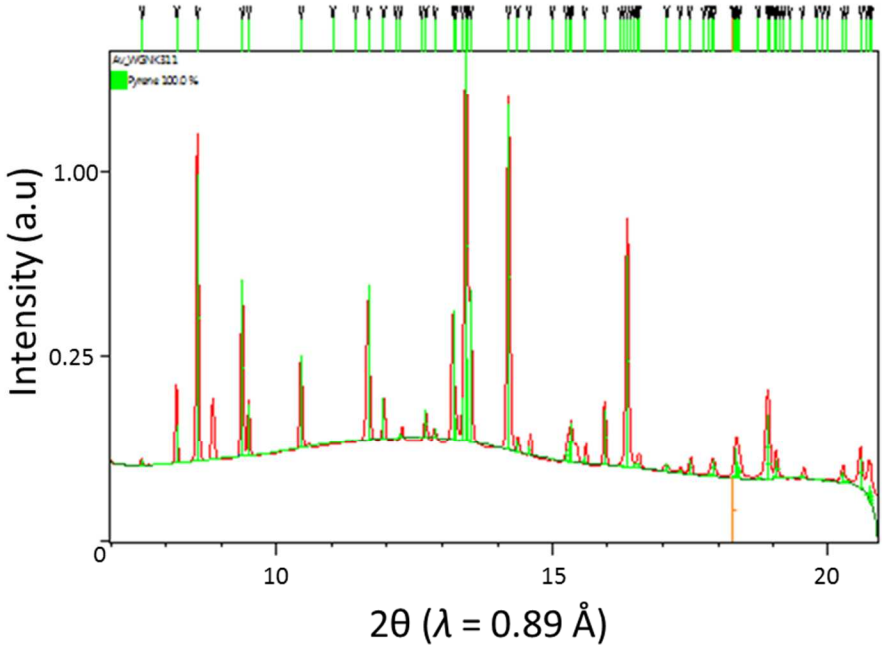

Figure S4. Rietveld analysis of a powdered pyrene sample. The red line indicates the X-ray diffraction profile of a mixture of poly(2-vinylpyridine) and pyrene (40 wt.%). The green line indicates the Rietveld simulated pattern for the unit cell parameters and atomic coordinates of pyrene. The green lines at the top correspond to the peak positions generated by the X'Pert High Score software from the unit cell parameters for pyrene (a = 13.5 Å, b = 9.16 Å, c = 8.36 Å, β = 100.4°) obtained from the literature[1, 2] and by indexing using the ab initio method.[3]

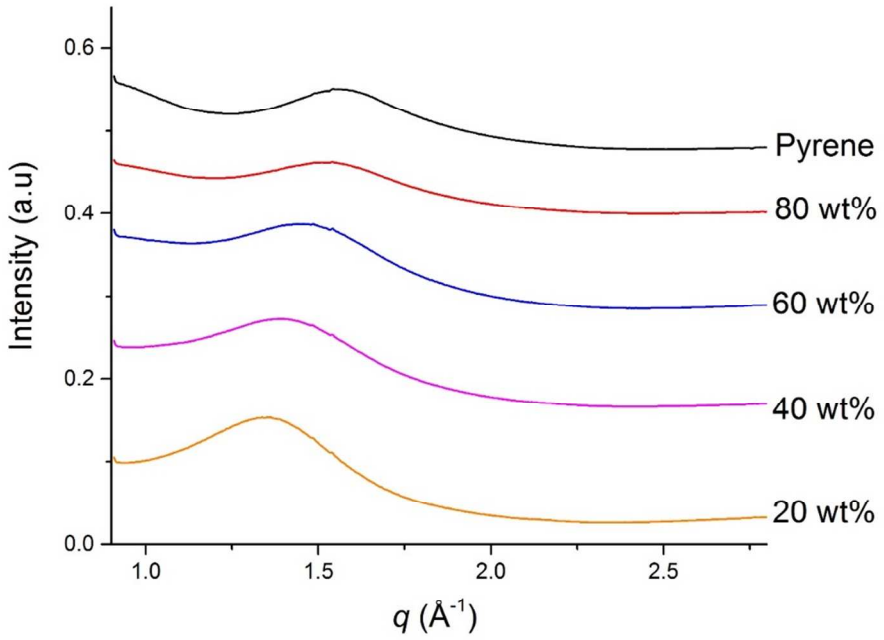

Figure S5. Wide-angle X-ray scattering profiles of pyrene blended with polystyrene at 175 °C.

References:

1. Robertson, J. M.; White, J. G. The Crystal Structure of Pyrene. A Quantitative X-Ray Investigation. *Journal of the Chemical Society (Resumed)* **1947**, 358-368.
2. Cameraman, A.; Trotter, J. The Crystal and Molecular Structure of Pyrene. *Acta Crystallographica* **1965,** 18, 636-643.
3. Favre-Nicolin, V.; Cerny, R. FOX, `free objects for crystallography': a modular approach to ab initio structure determination from powder diffraction. *Journal of Applied Crystallography* **2002,** 35 (6), 734-743.