Supplementary Materials

Phase Diagrams of Ternary π-Conjugated Polymer Solutions for Organic Photovoltaics

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Calculation Methods for the CB/P3HT/$PC_{61}BM$ System

- **Flory-Huggins interaction parameter**: χ_{12}, χ_{13}, and χ_{23}

CB: $\delta_1 = 9.5$ (cal/cm^3)$^{1/2}$; MW_1 =112.56 g/mol; ρ_1=1.11 g/cm^3; $v_1 = \frac{MW_1}{\rho_1} = 101.41 \text{cm}^3/\text{mol}$

P3HT: $\delta_2 = 8.7$ (cal/cm^3)$^{1/2}$; $MW_2 = M_n$ =22,000 g/mol; ρ_2=1.1 g/cm^3.

$PC_{61}BM$: $\delta_3 = 11.3$ (cal/cm^3)$^{1/2}$; MW_3 = 910 g/mol; ρ_3=1.5 g/cm^3.

$R = 1.987 \text{ cal/K} \cdot \text{mol}$

$$\chi_{12} = \frac{\frac{MW_1}{\rho_1}}{R \cdot T}\left(\delta_1 - \delta_2\right)^2 + 0.34 = \frac{\frac{112.56 \text{ g/mol}}{1.11 \text{ g/cm}^3}}{1.987 \text{ cal/K} \cdot \text{mol}} \frac{1}{T \text{ K}} \cdot \left(9.5\left(\text{cal/cm}^2\right)^{1/2} - 8.7 \left(\text{cal/cm}^2\right)^{1/2}\right)^2 + 0.34$$
$$= \frac{32.7\text{K}}{T} + 0.34$$

$$\chi_{13} == \frac{\frac{MW_1}{\rho_1}}{R \cdot T}\left(\delta_1 - \delta_3\right)^2 + 0.34 = \frac{\frac{112.56 \text{ g/mol}}{1.11 \text{ g/cm}^3}}{1.987 \text{ cal/K} \cdot \text{mol}} \frac{1}{T \text{ K}} \cdot \left(9.5\left(\text{cal/cm}^2\right)^{1/2} - 11.3 \left(\text{cal/cm}^2\right)^{1/2}\right)^2 + 0.34$$
$$= \frac{165.4\text{K}}{T} + 0.34$$

$$\chi_{23} == \frac{\frac{MW_1}{\rho_1}}{R \cdot T}\left(\delta_2 - \delta_3\right)^2 + 0.34 = \frac{\frac{112.56 \text{ g/mol}}{1.11 \text{ g/cm}^3}}{1.987 \text{ cal/K} \cdot \text{mol}} \frac{1}{T \text{ K}} \cdot \left(8.7\left(\text{cal/cm}^2\right)^{1/2} - 11.3 \left(\text{cal/cm}^2\right)^{1/2}\right)^2 + 0.34$$
$$= \frac{345.0\text{K}}{T} + 0.34$$

- **Relative molar volume: *s* and *r***

CB: $v_1 = \frac{MW_1}{\rho_1} = \frac{112.56 \text{ g/mol}}{1.11 \text{ g/cm}^3} = 101.41 \text{ cm}^3/\text{mol}$

P3HT: $v_2 = \frac{MW_2}{\rho_2} = \frac{22,000 \text{ g/mol}}{1.1 \text{ g/cm}^3} = 20,000 \text{ cm}^3/\text{mol}$

$PC_{61}BM$: $v_3 = \frac{MW_3}{\rho_3} = \frac{910 \text{ g/mol}}{1.5 \text{ g/cm}^3} = 607 \text{ cm}^3/\text{mol}$

$s = \frac{v_1}{v_2} = \frac{101.41 \text{ cm}^3/\text{mol}}{20,000 \text{ cm}^3/\text{mol}} = 0.005071$ and $r = \frac{v_1}{v_3} = \frac{101.41 \text{ cm}^3/\text{mol}}{607 \text{ cm}^3/\text{mol}} = 0.167068$

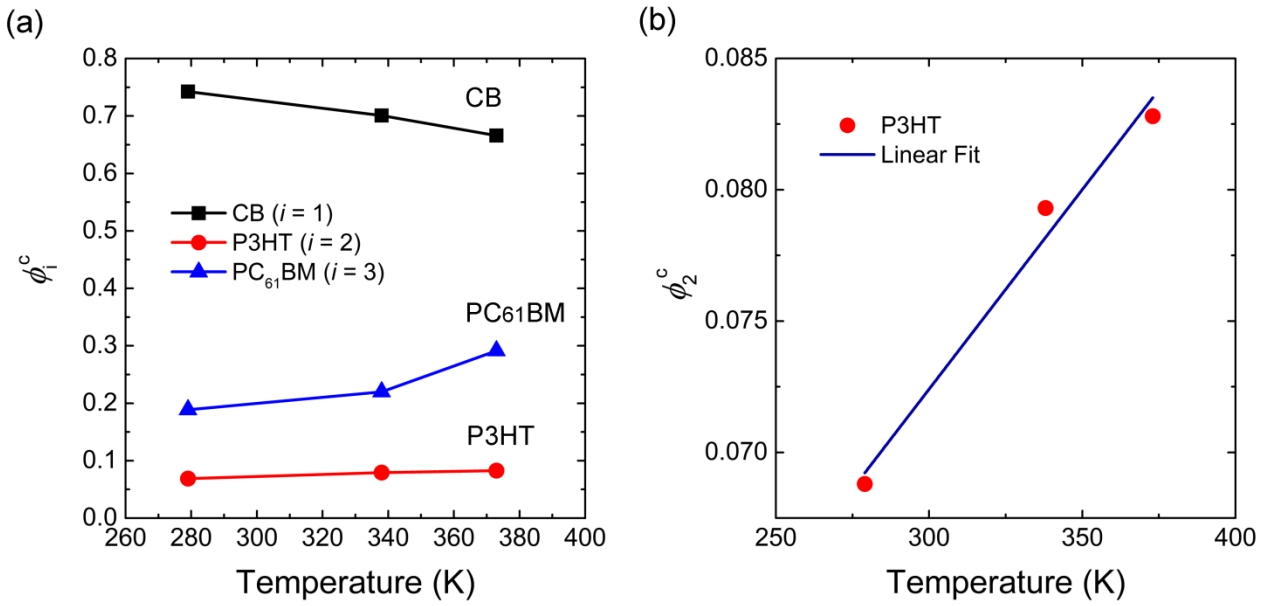

Figure S1. (a) Critical point ($\phi_1^c, \phi_2^c, \phi_3^c$) of the ternary CB-P3HT-$PC_{61}BM$ system as a function of temperature. (b) Linear fit for the plot of ϕ_2^c (P3HT) vs. temperature: $\phi_2^c = 1.51972\times10^{-4}\cdot T + 0.02682$.

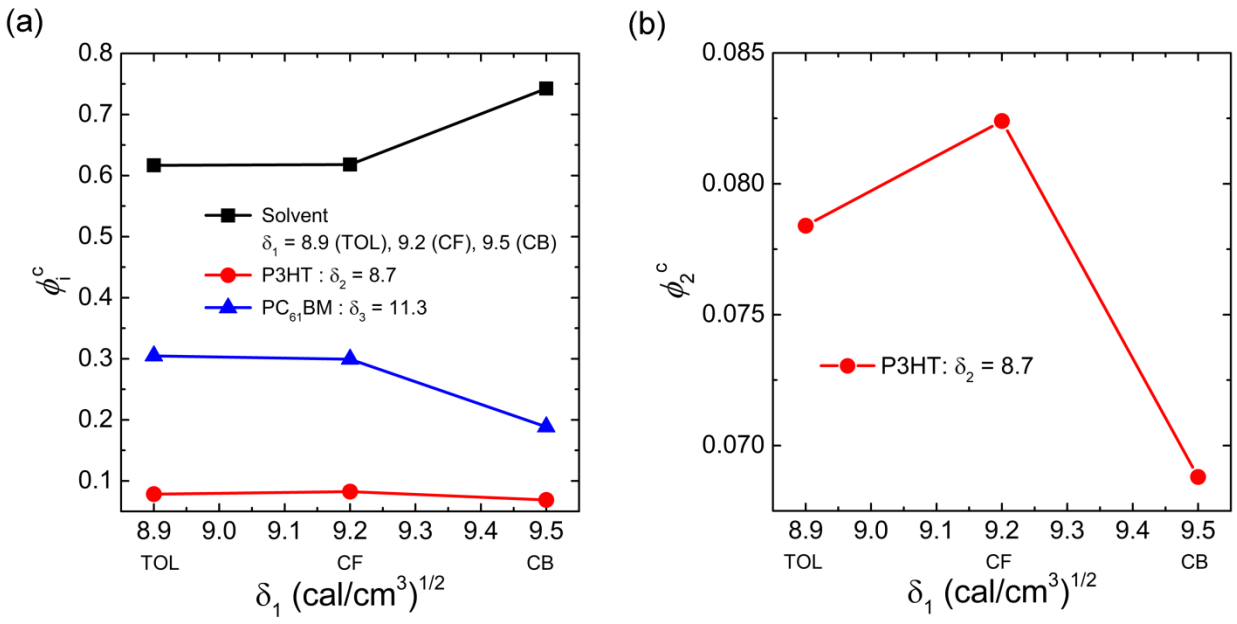

Figure S2. (a) Critical point (ϕ_1^c, ϕ_2^c, ϕ_3^c) of the ternary Solvent/P3HT/$PC_{61}BM$ system as a function of solvent species (CB, CF and TOL). CB, CF, and TOL stand for chlorobenzene, chloroform, and toluene, respectively. (b) The plot of ϕ_2^c vs. δ_1 for clarifying the indistinguishable data shown in Fig S2(a).