

Supporting Information

Formation of Solid Solution and Ternary Phase Diagrams of Anthracene and Phenanthrene in Different Organic Solvents

Suping Ding[†], Qiuxiang Yin^{†,‡}, Wei Du[†], Xiaowei Sun[†], Baohong Hou^{†,‡}, Meijing Zhang^{†,‡},
Zhao Wang^{†,‡,*}

[†]School of Chemical Engineering and Technology, State Key Laboratory of Chemical Engineering, Tianjin University, and [‡] Collaborative Innovation Center of Chemical Science and Chemical Engineering (Tianjin), Tianjin 300072, People's Republic of China

Caption of Figures

Figure 1. DSC thermograms of pure ANT and PHE.

Figure 2. PXRD patterns of pure ANT and PHE; the identification of crystal faces of (0 0 1) and (1 0 0) referenced PDF cards 39-1848 and 47-2498.

Table 1. Phase equilibrium data of the ANT-PHE-toluene ternary phase diagrams at 308.15K

Table 2. Phase equilibrium data of ANT-PHE-xylene ternary phase diagram at 308.15K

Table 3. Phase equilibrium data of ANT-PHE-DMF ternary phase diagram at 308.15K

Figure 1.

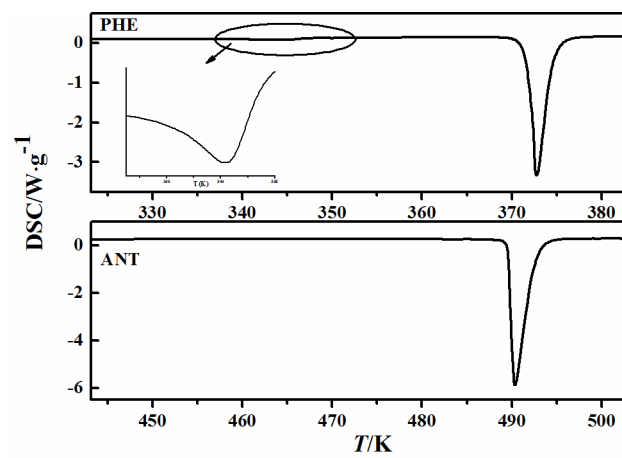


Figure 2.

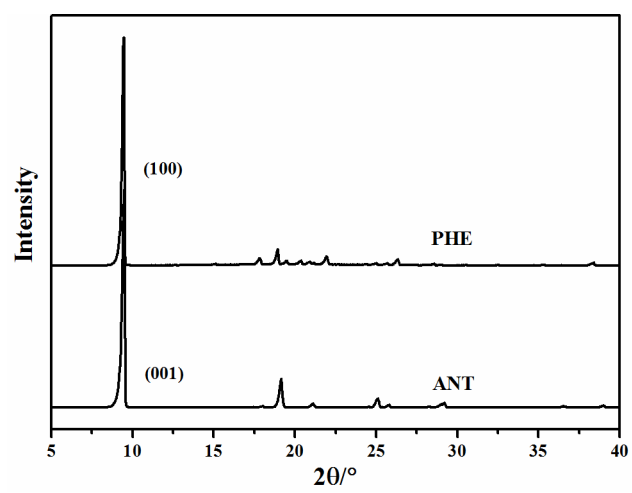


Table 1. Phase equilibrium data of ANT-PHE-toluene ternary phase diagram at 308.15K.^{a,b}

Composition of liquid phase/%			Equilibrium solid phase	Composition of solid phase/%	
x_{PHE}	x_{ANT}	x_{toluene}		x_{PHE}	x_{ANT}
0.00	1.73	98.27	ANT	0	100
6.01	1.96	92.03	β	1.50	98.50
10.91	1.97	87.13	β	3.74	96.26
16.78	2.26	80.96	β	7.16	92.84
21.90	1.92	76.18	β	11.51	88.49
27.74	2.10	70.16	β	22.87	77.13
28.14	2.22	69.64	$\alpha+\beta$	48.10	51.90
28.49	2.18	69.33	$\alpha+\beta$	72.88	27.12
34.46	1.46	64.09	α	81.37	18.63
39.89	0.00	60.11	PHE	100	0

a. The composition is shown by mass fraction x .

b. The relative standard uncertainty of mass fraction x is $u_r(x) = 0.05$, and that of temperature is $u(T) = 0.1\text{K}$.

Table2. Phase equilibrium data of ANT-PHE-xylene ternary phase diagram at 308.15K.^{a,b}

Composition of liquid phase/%			Equilibrium solid phase	Composition of solid phase/%	
x_{PHE}	x_{ANT}	x_{xylene}		x_{PHE}	x_{ANT}
0	1.72	98.28	ANT	0	100
3.52	1.71	94.78	β	0.91	99.09
7.07	1.72	91.20	β	1.62	98.38
13.41	1.93	84.66	β	2.84	97.16
18.29	1.69	80.02	β	4.69	95.31
22.55	1.95	75.50	β	5.39	94.61
25.68	2.00	72.32	$\alpha+\beta$	10.24	89.76
25.51	1.95	72.54	$\alpha+\beta$	59.43	40.57
25.78	1.97	72.26	$\alpha+\beta$	69.03	30.97
28.10	1.74	70.16	α	75.04	24.96
30.68	1.15	68.17	α	76.09	23.91
33.25	0	66.75	PHE	100	0

a. The composition is shown by mass fraction x .

b. The relative standard uncertainty of mass fraction x is $u_r(x) = 0.05$, and that of temperature is $u(T) = 0.1\text{K}$.

Table 3. Phase equilibrium data of ANT-PHE-DMF ternary phase diagram at 308.15K.^{a,b}

Composition of liquid phase/%			Equilibrium solid phase	Composition of solid phase/%	
x_{PHE}	x_{ANT}	x_{DMF}		x_{PHE}	x_{ANT}
0	2.78	97.22	ANT	0	100
3.72	2.76	93.52	β	0.72	99.28
6.99	2.87	90.14	β	1.44	98.56
9.98	2.87	87.15	β	3.07	96.93
15.19	2.95	81.86	β	3.20	96.80
22.62	3.02	74.36	β	6.66	93.34
28.24	3.01	68.75	β	9.99	90.01
35.80	3.06	61.14	β	10.99	89.01
38.41	2.89	58.71	$\alpha+\beta$	13.27	86.73
38.42	2.94	58.64	$\alpha+\beta$	12.44	87.56
38.46	2.70	58.84	$\alpha+\beta$	39.47	60.53
40.60	2.41	56.99	α	76.43	23.57
42.87	2.20	54.93	α	84.37	15.63
45.42	2.07	52.51	α	88.70	11.30
49.12	1.61	49.27	α	89.39	10.61
49.04	0.73	50.23	PHE	100	0
48.79	0	51.21	PHE	100	0

a. The composition is shown by mass fraction x .

b. The relative standard uncertainty of mass fraction x is $u_r(x) = 0.05$, and that of temperature is $u(T) = 0.1\text{K}$