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Solid−Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers

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Experimental data on the solid−liquid equilibria for dimethylnaphthalene (DMN) isomer systems (2,6-DMN + 2,3-DMN, 2,6-DMN + 2,7-DMN, 2,6-DMN + 1,5-DMN, 2,6-DMN + 1,8-DMN, 2,6-DMN + 1,4-DMN, 2,6-DMN + 1,6-DMN, 2,6-DMN-1-MN, 2,6-DMN-2-MN, 2,7-DMN-1-MN, 2,7-DMN-2-MN, 1,5-DMN-1-MN, and 1,5-DMN-2-MN) have been measured by the polythermal method. Experimental results found that all systems were simple eutectic systems.

Introduction

2,6-Dimethylnaphthalene (2,6-DMN) is an important material because it is the starting material for the manufacture of polyethylene naphthalate (PEN) and liquid crystal polymer (LCP). PEN has especially received much attention because it performs better than polyethylene terephthalate (PET) with respect to heat resistance, elasticity, chemical stability, and gas barrier. Such higher performance properties make it possible to be used in applications such as special films, fibers, reaction containers, and packings. Therefore, with the expansion of PEN applications, the need for 2,6-DMN will increase. To enhance the quality of PEN, a higher purity of 2,6-DMN is desired.[1]

DMN can be obtained by alkylation of naphthalene and monomethylnaphthalenes or by isomerization and disproportionation of monomethylnaphthalenes.[2,3] Both methods synthesize the byproducts including DMN isomers, which consist of 10 compounds. The conventional processes[4−6] such as distillation and adsorption have been applied to separation of 2,6-DMN from the isomer mixtures but have a limitation with regard to purity and yield of products because of the similar boiling point and chemical structure of its isomers. Extractive crystallization needs a proper solvent, which must be removed after crystallization.[7]

Melt crystallization is one possibility to separate isomers.[8] Our recent work presented that 2,6-DMN was separated by melt crystallization.[9] In melt crystallization, 2,6-DMN could be crystallized separately from the isomers by cooling the melt without using a solvent. Therefore, to understand separation by melt crystallization, solid−liquid equilibrium (SLE) for mixtures must be investigated first. For the design and optimization of crystallization processes, reliable phase diagrams are also required as a basis for the separation of isomers.

This work measured the SLE of binary mixtures for DMN isomers and the dimethylnaphthalene + methylnaphthalene (1-MN and 2-MN) system to grasp the adequate operating conditions of the separation of 2,6-DMN by melt crystallization.

Experimental Section

Materials. Reagent-grade 2,6-DMN (Aldrich Chemical Co., 99 %), 2,7-DMN (Aldrich Chemical Co., 99 %), 2,3-DMN (Aldrich Chemical Co., 98 %), 1,6-DMN (Aldrich Chemical Co., 99 %), 1,4-DMN (Aldrich Chemical Co., 95 %), 1,8-DMN (Aldrich Chemical Co., 95 %), and 1,5-DMN (Aldrich Chemical Co., 98 %) were used. Before use, DMN isomers were purified further by recrystallization in methanol. Gas chromatographic analysis indicated that their purities were more than 99.9 %, respectively. Reagent-grade 1-MN (Aldrich Chemical Co., 95 %) and 2-MN (Aldrich Chemical Co., 97 %) were used. Before use, 1-MN and 2-MN were purified further by recrystallization, and the purity was more than 99.5 % and 99.7 %, respectively. The materials were analyzed by FID DONAM GC 6200 gas chromatography (GC) equipped with capillary columns (Shinwa, GC-8A capillary column ULBON HR-1).

Table 1. Physical Properties of Pure Compounds

		T_{fus} /K		T_b/K	ρ/g·cm^{-3}		$\Delta_{fus}H$/kJ·mol^{-1}	
compd	CAS no.	lit.[b]	this work	lit.[b]	lit.[a]	this work	lit.[a]	this work
1-MN	90-12-0	242.64	242.20	517.84	1.016	−	6.945	−
2-MN	91-57-6	307.15	307.85	514.15	−	−	11.96	−
1,6-DMN	575-43-9	257.15	256.95	539.15	1.002	−	−	8.50
1,4-DMN	575-58-4	279.15	279.15	538.15	−	−	−	10.60
1,8-DMN	569-41-5	338.15	338.15	543.15	1.010	−	−	18.53
1,5-DMN	571-61-9	355.15	355.15	542.15	1.002	−	−	20.00
2,7-DMN	582-16-1	371.15	370.15	535.15	1.010	1.010	23.35	22.20
2,3-DMN	581-40-8	377.15	377.15	542.15	−	1.012	−	23.97
2,6-DMN	581-42-0	385.69	385.15	535.15	1.020	1.021	25.06	25.30

[a] Refs 19 and 20. [b]Refs 21 and 22.

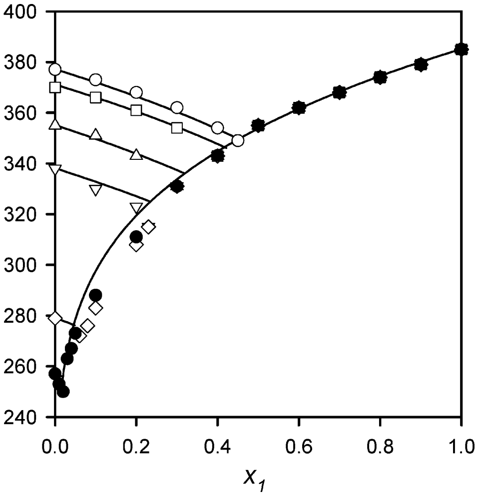

Figure 1. SLE of the 2,6-DMN (1) + DMN isomer (2) systems under atmospheric pressure: ○, 2,6-DMN + 2,3-DMN; □, 2,6-DMN + 2,7-DMN; △, 2,6-DMN + 1,5-DMN; ▽, 2,6-DMN + 1,8-DMN; ◇, 2,6-DMN + 1,4-DMN; ●, 2,6-DMN + 1,6-DMN; −, ideal line from eq 4.

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Table 2. Solid−Liquid Equilibria for 2,6-DMN (1) + DMN Isomer (2) Systems

x_1	T/K	δT/K	γ	x_1	T/K	δT/K	γ	x_1	T/K	δT/K	γ
2,6-DMN (1) + 2,3-DMN (2) System				2,6-DMN (1) + 2,7-DMN (2) System				2,6-DMN (1) + 1,5-DMN (2) System			
0.00	377.15	0	1.000	0.00	370.15	0	1.000	0.00	355.15	0	1.000
0.10	373.15	0.09	1.024	0.10	366.15	−0.28	1.027	0.10	351.05	1.81	1.027
0.20	368.15	−0.15	1.037	0.20	361.15	0.32	1.044	0.20	343.15	−1.01	0.986
0.30	362.15	0.12	1.041	0.30	354.15	−0.12	1.031	0.30	335.15	0.06	0.954
0.40	354.15	−0.11	1.014	0.40	343.15	0.01	0.945	0.40	343.25	−0.34	0.953
0.45	349.15	−0.03	0.984	0.50	355.15	−0.02	1.026	0.50	355.25	0.63	1.029
0.50	355.15	−0.2	1.026	0.60	362.15	0.06	1.009	0.60	362.15	−0.41	1.009
0.60	362.15	0.43	1.009	0.70	368.15	−0.08	0.992	0.70	368.05	−0.23	0.990
0.70	368.15	−0.31	0.992	0.80	374.15	0.07	0.991	0.80	374.15	0.52	0.991
0.80	374.15	0.43	0.991	0.90	379.15	−0.03	0.981	0.90	379.25	−0.3	0.983
0.90	379.15	−0.3	0.981	1.00	385.15	0	1.000	1.00	385.15	0	1.000
1.00	385.15	0	1.000								
2,6-DMN (1) + 1,8-DMN (2) System				2,6-DMN (1) + 1,4-DMN (2) System				2,6-DMN (1) + 1,6-DMN (2) System			
0.00	338.15	0	1.000	0.00	279.15	0	1.000	0.00	256.95	0	1.000
0.10	330.15	0	0.947	0.03	278.15	0	1.014	0.01	255.25	0	0.984
0.20	323.25	0.08	0.923	0.06	276.35	−0.2	0.743	0.02	250.15	−4.4	0.703
0.25	325.15	−0.38	1.024	0.08	280.75	0.24	0.662	0.03	263.15	2.71	0.855
0.30	331.15	0.53	0.919	0.10	285.15	0.12	0.626	0.04	267.15	1.33	0.763
0.40	343.25	−0.45	0.953	0.20	309.15	−0.56	0.717	0.05	273.15	2.41	0.784
0.50	355.15	0.33	1.026	0.30	331.15	1.01	0.919	0.10	288.35	−1.76	0.705
0.60	362.15	−0.11	1.009	0.40	343.35	−1.07	0.955	0.20	311.15	−1.76	0.764
0.70	368.15	−0.04	0.992	0.50	355.15	0.56	1.026	0.30	331.15	2.07	0.919
0.80	374.25	0.06	0.993	0.60	362.45	0.07	1.016	0.40	342.25	−0.18	0.929
0.90	379.25	−0.02	0.983	0.70	368.25	−0.33	0.994	0.50	355.15	−0.04	1.026
1.00	385.15	0	1.000	0.80	374.05	0.22	0.989	0.60	362.15	−0.94	1.009
0.90	379.15	−0.07	0.981	0.70	368.05	0.11	0.990				
1.00	385.15	0	1.000	0.80	374.15	1.17	0.991				
0.90	379.25	−0.92	0.983								
1.00	385.15	0	1.000								

Table 3. Solid−Liquid Equilibria for DMN (1) + MN (2) Systems

x_1	T/K	δT/K	γ	x_1	T/K	δT/K	γ	x_1	T/K	δT/K	γ
2,6-DMN (1) + 1-MN (2) System				2,6-DMN (1) + 2-MN (2) System				2,7-DMN (1) + 1-MN (2) System			
0.0012	241.95	−0.06	0.998	0.0521	305.85	−0.11	1.023	0.0037	241.45	−0.02	0.994
0.0037	241.25	0.05	0.991	0.0761	305.25	0.07	1.040	0.0093	240.35	0.01	0.984
0.0098	255.85	0.93	1.215	0.0990	306.05	−0.25	1.080	0.0166	239.95	0	0.985
0.0216	275.45	9.22	1.551	0.1207	310.05	0.25	1.176	0.0231	242.35	−0.66	1.027
0.0387	283.55	4.14	1.523	0.1415	313.15	0.18	1.149	0.0609	268.65	0.49	1.055
0.0589	289.95	−1	1.268	0.2155	323.15	−0.14	1.019	0.0831	280.15	1.92	1.163
0.0840	296.95	−3.82	1.139	0.2918	332.15	−0.51	0.971	0.1060	285.55	−0.42	1.092
0.1271	306.65	−3.69	1.041	0.3545	340.15	0.54	0.992	0.1441	292.75	−2.18	1.011
0.1616	314.15	−0.53	1.038	0.4071	345.25	0.31	0.986	0.2258	305.95	−0.32	0.956
0.2048	321.35	2.29	1.017	0.4517	348.95	−0.19	0.975	0.2608	311.65	1.42	0.971
0.2801	331.05	2.93	0.982	0.4901	352.45	−0.07	0.980	0.3400	320.05	0.46	0.933
0.3657	339.95	−0.76	0.956	0.5235	355.05	−0.23	0.978	0.3846	325.25	0.21	0.942
0.4459	348.25	−2.24	0.971	0.5528	357.15	−0.41	0.974	0.4345	329.55	−1.26	0.928
0.5266	355.95	0.01	0.993	0.5786	359.85	0.38	0.992	0.4664	333.85	−0.28	0.960
0.6239	363.15	2.08	0.993	0.6017	361.25	0.16	0.985	0.5322	340.25	0.51	0.978
0.6582	365.15	0.42	0.986	0.6223	362.55	0.08	0.982	0.6321	346.25	0.39	0.943
0.6887	368.15	−1.47	1.008	0.6872	366.35	−0.09	0.970	0.6932	349.65	−0.28	0.927
2,7-DMN (1) + 2-MN (2) System				1,5-DMN (1) + 1-MN (2) System				1,5-DMN (1) + 2-MN (2) System			
0.0054	306.65	0.79	0.987	0.0043	241.35	0.09	0.993	0.0054	305.15	−0.2	0.965
0.0109	305.35	0.12	0.973	0.0106	239.75	−0.06	0.976	0.0109	303.25	−1.43	0.942
0.0215	304.55	−0.65	0.972	0.0224	239.15	0.01	0.980	0.0215	302.65	−0.81	0.943
0.0521	302.65	−0.51	0.974	0.0403	244.75	−0.05	1.169	0.0521	300.75	0.19	0.945
0.0990	300.75	−0.08	0.994	0.0609	254.85	0.25	1.142	0.0990	298.05	0.73	0.952
0.1415	298.95	0.5	1.243	0.0831	262.75	−0.39	1.112	0.1415	295.35	0.27	0.956
0.1801	298.55	−0.06	0.965	0.1060	270.05	−0.2	1.116	0.1801	292.75	−0.41	0.958
0.2155	307.65	0.01	1.051	0.1441	280.55	0.98	1.146	0.2155	290.65	−0.59	1.032
0.2479	312.75	0.17	1.053	0.2258	292.75	−1.33	1.045	0.2479	289.65	0.46	0.872
0.2777	316.15	−0.35	1.030	0.2608	299.65	0.26	1.094	0.2777	294.25	−0.24	0.886
0.3053	319.75	0.02	1.030	0.3400	311.65	1.07	1.143	0.3053	298.55	0.51	0.907
0.3973	329.35	0.48	1.010	0.3846	315.75	−0.44	1.117	0.3973	307.65	−0.85	0.885
0.4678	334.65	−0.44	0.975	0.4345	322.05	0.39	1.147	0.4678	316.35	0.91	0.931
0.5687	343.65	0	0.989	0.4664	323.85	−0.76	1.114	0.5687	323.85	−0.38	0.914
0.6374	349.55	0.36	1.006	0.5322	329.55	0.06	1.110	0.6374	329.55	−0.16	0.927
0.6641	351.05	−0.17	0.997	0.6321	335.85	0.31	1.072	0.6641	331.95	0.18	0.938
0.6872	352.85	−0.06	1.002	0.6932	340.25	−0.16	1.072	0.6872	333.55	0.03	0.938

The injector and FID were set at 250 °C. Helium was used as the carrier gas at a constant flow rate of 1.0 mL·min^{-1}. The oven temperature was increased from 70 to 210 °C at a rate of 5 °C·min^{-1}.

Procedure. The mixtures were prepared by mass using a Mettler AG 204 balance with an accuracy of ± 0.0001 g. The estimated accuracy in the mass fraction is less than ± 2·10^{-4}. SLE temperatures were determined using a polythermal method described in detail previously.[10−16] The equilibrium cell, a cylindrical glass vessel (50 mm inside diameter, 120 mm long), was placed, by a ground-glass joint, in a triple-jacketed vessel. The outer jacket was evacuated, and either heated or cooled medium from a thermostated bath could be circulated through the middle jacket. The water + ethylene glycol solution used as medium was thermostated and controlled by a thermoelectric Eurotherm 808 PID controller with ± 0.1 K accuracy. The cell had a perforated rubber stopper, through which a thermocouple was inserted. The contents were stirred with a magnetic spin bar. The cell was tightly sealed to protect the system from dust and moisture condensation. Mixture was fed to the equilibrium cell and heated for melting. The melted solution was cooled until an abundant amount of crystal was formed and then heated very slowly at less than 0.001 K·min^{-1} near the equilibrium temperature. The crystal disappearance temperature, detected

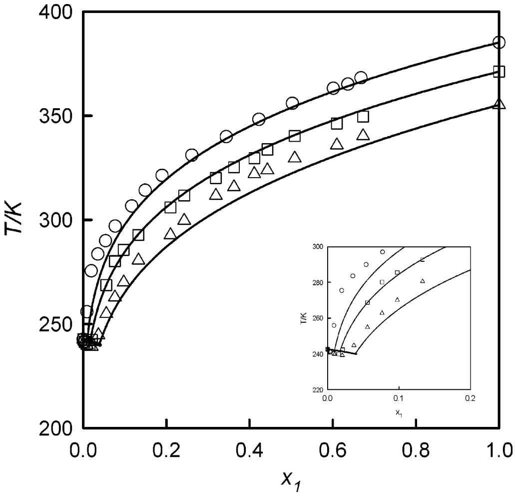

Figure 2. SLE of the DMN isomer + 1-MN systems under atmospheric pressure: ○, 1-MN + 2,6-DMN; □, 1-MN + 2,7-DMN; △, 1-MN + 1,5-DMN; −, ideal line from eq 4.

visually, was measured with a calibrated thermocouple connected to a recorder (Yokogawa, 180 micro R). The thermocouples were calibrated with a calibrated thermometer from Fisher Scientific (No. 15-078-7) with an accuracy of ± 0.05 K. The accuracy of the thermocouple measurements is believed to be ± 0.1 K. Some of the experiments were conducted in triplicate to check the reproducibility. The saturation temperature for a given mixture was reproducible within ± 0.1 K.

The enthalpy of fusion and the melting temperature of the pure materials were determined by a differential scanning calorimeter (DSC; TA Instruments, USA). For each measurement, a sample of about 10 mg was used, sealed in an aluminum pan, and heated to 400 K at a heating rate of 10 K·min^{-1}. The density of the compounds has been determined using a digital densimeter (Mettler Toledo).

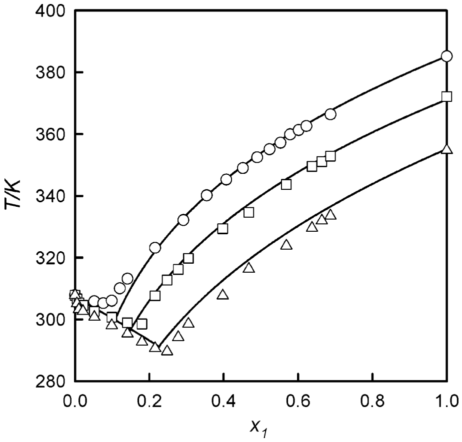

Figure 3. SLE of the DMN isomer + 2-MN systems under atmospheric pressure: ○, 2-MN + 2,6-DMN; □, 2-MN + 2,7-DMN; △, 2-MN + 1,5-DMN; −, ideal line from eq 4.

Results and Discussion

Enthalpy of fusion, density, and melting temperatures (T_{fus}) of the compounds investigated in this study are compared with the data cited in the literature in Table 1. The experimental melting and eutectic temperatures for the 2,6-DMN + DMN isomers and the DMN + MN mixtures were measured. The accuracy for experimental data of SLE was previously confirmed for the 2,6-DMN + 2,7-DMN system.[16] The experimental results

Table 4. Coefficients for Equation 1

$x_{1,\min}$	$x_{1,\max}$	x_1^*	T^*/K	a_1	a_2	a_3	a_4	a_5	a_6	a_7	Δ/K
					2,6-DMN (1) + 2,3-DMN (2) System						
0.0	0.446	0.0	377.15	1.0196	2.8521	2.7590	0.9266				0.03
0.446	1.0	1.0	385.15	0.1383	−0.1618	−0.7637	−1.0381				0.07
					2,6-DMN (1) + 2,7-DMN (2) System						
0.0	0.414	0.0	371.15	0.5341	1.0057	0.4719					0.05
0.414	1.0	1.0	385.15	0.2100	0.9016	4.3427	8.7613	6.4957			0.27
					2,6-DMN (1) + 1,5-DMN (2) System						
0.0	0.320	0.0	355.15	0.2024	0.2047						0.03
0.320	1.0	1.0	385.15	0.1202	−0.4899	−2.6099	−5.0929	−3.0428			0.31
					2,6-DMN (1) + 1,8-DMN (2) System						
0.0	0.235	0.0	338.15	0.3756	0.5009	0.1253					0.01
0.235	1.0	1.0	385.15	0.0963	−0.7559	−3.6062	−6.6062	3.8425			0.20
					2,6-DMN (1) + 1,4-DMN (2) System						
0.0	0.045	0.0	279.15	1.8931	3.7178	1.8247					0.01
0.045	1.0	1.0	385.15	0.1379	−0.4560	−4.2988	−16.0552	−28.9284	−25.9189	−9.0444	0.37
					2,6-DMN (1) + 1,6-DMN (2) System						
0.0	0.019	0.0	257.15	1.5712	1.5712						0.01
0.019	1.0	1.0	385.15	−0.0130	−2.4390	−12.3907	−27.3430	−26.8725	−9.8682		1.41
					2,6-DMN (1) + 1-MN (2) System						
0.0	0.0095	0.0	242.20	1.3624	1.3614						0.06
0.0095	1.0	1.0	385.15	−3.9660	−37.0398	−128.5450	−215.5186	−174.6778	−54.9975		2.68
					2,6-DMN (1) + 2-MN (2) System						
0.0	0.1056	0.0	307.85	0.1224	0.1223						0.09
0.1056	1.0	1.0	385.15	0.2439	0.6630	1.6466	1.5680	0.5931			0.25
					2,7-DMN (1) + 1-MN (2) System						
0.0	0.0169	0.0	242.20	−47.0581	−95.6043	−48.5461					0.01
0.0169	1.0	1.0	372.15	−0.9580	−11.6943	−45.6446	−84.8171	−75.2079	−25.7039		0.77
					2,7-DMN (1) + 2-MN (2) System						
0.0	0.1474	0.0	307.85	−0.4446	−1.2219	−0.7747					0.35
0.1474	1.0	1.0	372.15	0.2284	0.7725	2.9308	4.2300	2.2103			0.21
					1,5-DMN (1) + 1-MN (2) System						
0.0	0.0386	0.0	242.20	−38.2368	−78.0371	−39.8004					0.05
0.0386	1.0	1.0	354.75	−1.3523	−13.5478	−47.8308	−81.8875	−67.6694	−21.8002		0.48
					1,5-DMN (1) + 2-MN (2) System						
0.0	0.2260	0.0	307.85	2.8381	9.1351	10.2094	3.9066				0.69
0.2260	1.0	1.0	354.75	0.1650	−0.1293	−0.2185	−0.2409				0.41

are given in Tables 2 and 3 and shown in Figures 1, 2, and 3. For interpolation purposes, the liquidus lines were correlated with the empirical equation of Ott and Goates[17]

$$T/\mathrm{K} = T^*[1 + \sum_{j=1}^{M} a_j(x_1 - x_1^*)^j] \qquad (1)$$

where x_1^* and T^* are the mole fraction of DMN and the solid-disappearance temperature of the congruently melting compound or the pure substance, respectively. x_1 is the mole fraction of DMN. T is the solid-disappearance temperature of the sample, and a_j is the coefficient to be regressed to the experimental data.

Table 4 presents the best-fitted coefficients and the average absolute deviations (AAD; Δ) of the correlation for each mixture. The AAD is defined as

$$\Delta/\mathrm{K} = \left(\frac{1}{N}\right)\sum_{i=1}^{N} |T_{\mathrm{calcd},i} - T_{\mathrm{exptl},i}| \qquad (2)$$

where N is the number of experimental points. The subscripts calcd and exptl stand for the calculated values and the experimental values, respectively. The deviation of the calculated temperature from the experimental value at each measured temperature, δT, is listed in Tables 2 and 3.

If a solid−solid transition does not occur below the melting point of the pure component, the solid−liquid equilibrium can be expressed as[18]

$$\ln x_1^{\mathrm{L}}\gamma_1^{\mathrm{L}} = -\frac{\Delta_{\mathrm{fus}}H_1}{RT}\left(1 - \frac{T}{T_{\mathrm{fus},1}}\right) \qquad (3)$$

Because the activity coefficient γ_1^{L} depends not only on mole fraction but also on temperature, it must be calculated iteratively. If the real behavior of the mixture can be neglected, the activity coefficient is near unity ($\gamma_i^{\mathrm{L}} \approx 1$). Then eq 3 can be rewritten as

$$x_1^{\mathrm{L}} = \exp\left[-\frac{\Delta_{\mathrm{fus}}H_1}{RT}\left(1 - \frac{T}{T_{\mathrm{fus},1}}\right)\right] \qquad (4)$$

where x_1^{L} is the mole fraction in the liquid phase; γ_1^{L} is the activity coefficient in the liquid phase; $\Delta_{\mathrm{fus}}H_1$ is the mole enthalpy of fusion; $T_{\mathrm{fus},1}$ is the melting temperature; T is the absolute temperature of the mixture; and R is the universal gas constant.

The calculated results from eq 4 are shown in Figures 1, 2, and 3. As seen from figures, the calculated values are not in agreement with the experimental results. It means that the SLE of the binary mixture of DMN isomers presents deviation from ideal solution behavior due to interaction between compounds. To understand the deviation from ideal behavior, the activity coefficient can be calculated from eq 3 using the experimental data. In the higher concentration, the lower deviation from the ideal was found. As a result, a melt crystallization can be recommended for the separation of 2,6-DMN from the isomer mixture. Eutectic points were also found as a cooling limit for melt crystallization.

Literature Cited

(1) Smith, K.; Roberts, S. D. Regioselective dialkylation of naphthalene. *Catal. Today* **2000**, *60*, 227−233.

(2) Fraenkel, D.; Cherniavsky, M.; Ittah, B.; Ievy, M. Alkylation of Naphthalene and Methylnaphthalene with Methanol over H-ZSM-5 Zeolite Catalysts. *J. Catal.* **1986**, *101*, 273−276.

(3) Komatsu, T.; Araki, Y.; Namba, S.; Yashima, T. Selective Formation of 2,6-Dimethylnaphthalene from 2-Methylnaphthalene on ZSM-5 and Metallosilicates with MFI Structure. *Stud. Surf. Sci. Catal.* **1994**, *84*, 1821−1827.

(4) Pu, S. B.; Inui, T. Synthesis of 2,6-dimethylnaphthalene by methylation of methylnaphthalene on various medium and large-pore zeolite catalysts. *Appl. Catal. A: General* **1996**, *146*, 305−316.

(5) Pu, S. B.; Tananka, Y.; Inui, T. Adsorption and separation of β,β-dimethylnaphthalene isomers on various large-pore zeolites having 12-oxygen-member-ring structure. *Sep. Technol.* **1996**, *6*, 189−195.

(6) Inui, T.; Pu, S. B. Separation of 2,6-dimethylnaphthalene from a mixture of its isomers using lithium-incorporated zeolite Y synthesized by rapid crystallization method. *Sep. Technol.* **1995**, *5*, 229−237.

(7) Kim, K. J.; Cheon, Y. H.; Lee, J. M. Separation of 2,6-DMN by extractive crystallization. *BIWIC 2002*; Martin Luther Halle: Wittenberg, Germany 2002; pp 187−193.

(8) Ulrich, J. Melt crystallization. In: Myerson, A.S.(E.), Ed.; *Handbook of Industrial Crystallization*; Butterworth-Heinemann: Oxford, 1993.

(9) Cheon, Y. H.; Kim, K. J. Separation and purification of highly pure 2,6-diethylnaphthalene by melt crystallization. *Chem. Eng. Trans.* **2002**, *1*, 1503−1508.

(10) Kim, K. J.; Lee, C. H.; Ryu, S. K. Kinetic Study on Thiourea Adduction with Cyclohexanone−Methylcyclopentane System. 1. Equilibrium Study. *Ind. Eng. Chem. Res.* **1994**, *33*, 118−124.

(11) Kim, K. J.; Ryu, S. K. Nucleation of Thiourea Adduct Crystals with Cyclohexanone−Methylcyclopentane System. *Chem. Eng. Commun.* **1997**, *159*, 51−66.

(12) Kim, K. J.; Kim, M. J.; Lee, J. M.; Kim, S. H.; Kim, H. S.; Park, B. S. Experimental solubility and density for 3-nitro-1,2,4-triazol-5-one + C1 to C7 1-alkanols. *Fluid Phase Equilib.* **1998**, *146*, 261−268.

(13) Kim, K. J.; Kim, M. J.; Lee, J. M.; Kim, S. H.; Kim, H. S.; Park, B. S. Solubility, Density and Metastable Zone Width of the 3-Nitro-1,2,4-triazol-5-one + Water System. *J. Chem. Eng. Data* **1998**, *43* (1), 65−68.

(14) Kim, K. J.; Lee, C. H.; Ryu, S. K. Solubilities of Thiourea in n-C_1 C_6 Alcohols. *J. Chem. Eng. Data* **1994**, *39* (2), 228−239.

(15) Kim, K. J.; Cheon, Y. H. Solubility and Density of 2,6-Dimethylnaphthalene in C_1−C_7 1-Alkanols. *J. Chem. Eng. Data* **2004**, *49*, 992−996.

(16) Cheon, Y. H.; Kim, K. J.; Kim, J. W.; Kim, S. H. Solid−Liquid Equilibria of Binary and Ternary Mixtures for 2,6-Dimethylnaphthalene and 2,7-Dimethylnaphthalene with Ethanol or Methanol. *J. Chem. Eng. Data* **2005**, *50*, 863−867.

(17) Ott, J. B.; Goates, J. R. (Solid + liquid) phase equilibria in binary mixtures containing benzene, a cycloalkane, a *n*-alkane or tetrachloromethane. An equation for representing (solid−liquid) phase equilibria. *J. Chem. Thermodyn.* **1983**, *15*, 267−278.

(18) Gmehling, J.; Anderson, T. F.; Prausnitz, J. M. Solid−Liquid Equilibria Using UNIFAC. *Ind. Eng. Chem. Fundam.* **1978**, *17*, 269−273.

(19) Finke, H. L.; Messerly, J. F.; Lee, S. H.; Osborn, A. G.; Douslin, D. R. Comprehensive thermodynamic studies of seven aromatic hydrocarbons, *J. Chem. Thermodyn.* **1977**, *9*, 937−956.

(20) Domalski, E. S.; Hearing, E. D. Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. Vol. II. *J. Phys. Chem. Ref. Data* **1990**, *19*, 881−1041.

(21) Korean Thermophysical Porperties Data Bank, http://www.cheric.org.

(22) Riddick, J. A.; Bunger, W. B.; Sakano, T. K. *Organic Solvents*, 4th ed.; Wiley-Interscience: New York, 1986.

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