values are recorded in Table II and have been plotted in Figures 3–6.

The lines in the figures are drawn to make the best fit of the calculated values. From Figures 3 to 6 it is evident that the plots of molar refraction against composition are not linear. There is a slight scatter of points from linear behavior.

Acknowledgments

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Vapor–Liquid Equilibria of the Binary and Ternary Systems Containing *n*-Hexane (1)–Benzene (2)–*tert*-Butyl Alcohol (3) at 760 mmHg Pressure

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Vapor–liquid equilibrium data at 760 mmHg pressure are reported for the binary systems *n*-hexane–*tert*-butyl alcohol and benzene–*tert*-butyl alcohol and for the ternary system *n*-hexane–benzene–*tert*-butyl alcohol. The binary and ternary vapor–liquid equilibrium data were tested by Herington's method and the Li and Lu method, respectively, for the thermodynamic consistency. While the binary data were correlated through the Wilson, NRTL, and Andiappan–McLean equations the ternary data were correlated through the Wilson and NRTL equations.

In continuation of the research program made by the authors to study the effect of alcohols on the separation of *n*-hexane–benzene mixtures, this is the fifth (*2–5*) and the last in the series dealing with the vapor–liquid equilibrium of the binary and ternary systems containing *n*-hexane–benzene and *tert*-butyl alcohol at 760 mmHg pressure. Of the three possible binary systems the vapor–liquid equilibrium data for the system *n*-hexane–benzene are available in literature (*9, 11, 14*). These authors also measured the data on this system. The vapor–liquid equilibrium data for the other binaries, *n*-hexane–*tert*-butyl alcohol and benzene–*tert*-butyl alcohol and the ternary *n*-hexane–benzene–*tert*-butyl alcohol are reported in this communication.

Experimental Section

"Analar" grade benzene supplied by B.D.H., India, and Guaranteed Reagent grade *n*-hexane, Japan make, were used after drying with sodium and distillation.

Laboratory grade *tert*-butyl alcohol supplied by B.D.H., India, was treated with burnt lime for about 2 days. Then it was distilled and the fraction boiling at 82.2–82.4 °C was collected for use. The physical properties of the liquids together with the literature values (*15*) are reported in Table I.

The experimental procedure for measuring the equilibrium data was the same as described in the previous communications (*2, 3*).

Density was used as the means of analyzing the binary mixtures while density and refractive index were used for analyzing the ternary mixtures. For the ternary system, curves of constant density and refractive index as functions of compositions were drawn. From these curves the composition of each unknown mixture was established. These curves are shown in Figure 1.

Table I. Physical Properties of Pure Components

Component	Density g cm^{-3} (35 °C) Obsd	Density g cm^{-3} (35 °C) Lit.	Refractive index (35 °C) Obsd	Refractive index (35 °C) Lit.	Bp, °C Obsd	Bp, °C Lit.
n-Hexane	0.6460	0.6470	1.3680	1.3670	68.70	68.70
Benzene	0.8630	0.8633	1.4915	1.4915	80.10	80.10
tert-Butyl alcohol	0.7703	0.7709	1.3800	1.3823 (25 °C)	82.30	82.41

Table II. Vapor–Pressure Constants of Pure Components

Component	C_1	C_2	C_3	C_4	C_5	C_6
n-Hexane	113.283	−7151.50	0.0	0.019 95	0.0	−17.00
Benzene	133.313	−8026.29	0.0	0.023 93	0.0	−20.29
tert-Butyl alcohol	12.3567	−3858.00	−43.15	0.00	0.0	0.0

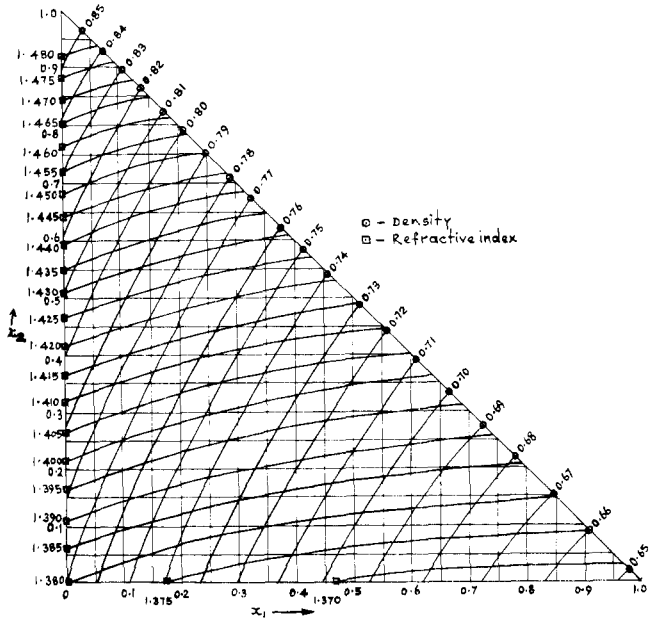

Figure 1. Refractive index and density curves at 35 °C for the system *n*-hexane (1)–benzene (2)–*tert*-butyl alcohol (3).

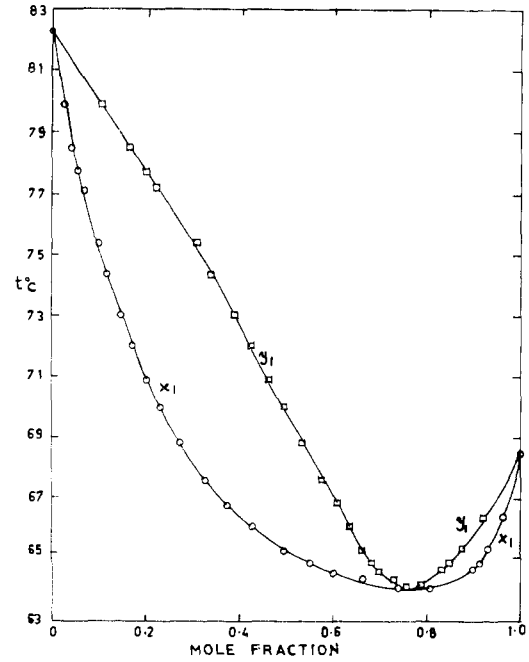

Figure 2. *t–x–y* diagram for *n*-hexane (1)–*tert*-butyl alcohol (3) at 760 mmHg pressure.

Vapor pressures of pure components were calculated using the equation

$$\ln p = C_1 + \frac{C_2}{C_3 + T} + C_4 T + C_5 T^2 + C_6 \ln T \qquad (1)$$

The vapor pressure constants, C_1, C_2, C_3, . . . C_n, for *n*-hexane and benzene were obtained from literature (*12*) and those for *tert*-butyl alcohol were estimated from the vapor pressure–temperature data given by Perry (*10*). The values of these constants for the pure components are given in Table II.

The activity coefficient was evaluated through the equation,

$$\gamma_i = \frac{\pi y_i}{p_1^0 x_i} \exp[(v_i - B_i)(p_i^0 - \pi)/RT] \qquad (2)$$

The second virial coefficient B_i was obtained by the method described by Hala (*6*).

The activity coefficients of the components in the binary system were computed through the Wilson (*16*), NRTL (*13*), and

Table III. Vapor–Liquid Equilibrium Data for *n*-Hexane (1)–*tert*-Butyl Alcohol (3) at 760 mmHg [a]

No.	Temp, °C	Liquid comp (x_1)	Vapor composition, y_1				g^E, cal g-mol^{-1}
			Exptl	Wilson	NRTL	Andiappan–McLean	
1	79.90	0.0240	0.1030	0.0978	0.0945	0.0845	22.80
2	78.50	0.0430	0.1675	0.1632	0.1590	0.1513	36.26
3	77.75	0.0565	0.2000	0.2040	0.1997	0.1938	46.10
4	77.20	0.0650	0.2180	0.2279	0.2237	0.2188	55.12
5	75.45	0.0950	0.3030	0.3018	0.2987	0.2951	66.85
6	74.35	0.1150	0.3400	0.3437	0.3416	0.3375	83.79
7	73.05	0.1425	0.3880	0.3933	0.3927	0.3869	101.50
8	72.00	0.1675	0.4215	0.4319	0.4327	0.4249	119.90
9	70.85	0.1990	0.4625	0.4734	0.4757	0.4654	137.30
10	70.00	0.2265	0.4950	0.5043	0.5077	0.4956	149.00
11	68.80	0.2740	0.5360	0.5488	0.5533	0.5392	170.90
12	67.60	0.3275	0.5750	0.5891	0.5943	0.5796	193.20
13	66.80	0.3700	0.6050	0.6155	0.6206	0.6069	205.40
14	66.10	0.4250	0.6360	0.6438	0.6480	0.6372	215.60
15	65.35	0.4950	0.6600	0.6736	0.6759	0.6710	229.30
16	64.90	0.5480	0.6825	0.6928	0.6932	0.6940	231.70
17	64.65	0.6000	0.6960	0.7096	0.7078	0.7151	229.20
18	64.40	0.6600	0.7240	0.7279	0.7235	0.7386	218.10
19	64.20	0.7390	0.7540	0.7521	0.7451	0.7695	199.00
20	64.25	0.8000	0.7850	0.7733	0.7658	0.7944	177.00
21	64.75	0.8950	0.8350	0.8232	0.8209	0.8406	113.30
22	64.95	0.9100	0.8475	0.8353	0.8347	0.8498	101.30
23	65.35	0.9300	0.8725	0.8550	0.8569	0.8635	86.16
24	66.40	0.9620	0.9200	0.9001	0.9056	0.8935	52.18
			ABSD:	0.0094	0.0108	0.0081	

[a] Binary energy parameters: Wilson, $\lambda_{13} - \lambda_{11} = -7.3445$, $\lambda_{31} - \lambda_{33} = 1313.1877$ cal g-mol^{-1}; NRTL, $g_{13} - g_{33} = 1130.68$, $g_{31} - g_{11} = 53.31$ cal g-mol^{-1}; Andiappan–McLean, $w_{13} = 494.262$, $w_{31} = 1770.380$ cal g-mol^{-1}.

Table IV. Vapor–Liquid Equilibrium Data for Benzene (2)–*tert*-Butyl Alcohol (3) at 760 mmHg [a]

No.	Temp, °C	Liquid comp x_2	Vapor composition, y_2 Exptl	Wilson	NRTL	Andiappan–McLean	g^E, cal g-mol^{-1}
1	80.85	0.0400	0.0820	0.0940	0.0935	0.0787	24.93
2	80.00	0.0600	0.1300	0.1348	0.1343	0.1163	38.15
3	79.45	0.0770	0.1600	0.1666	0.1662	0.1464	48.97
4	78.70	0.1010	0.1975	0.2076	0.2075	0.1861	65.07
5	76.95	0.1800	0.3050	0.3164	0.3173	0.2944	101.30
6	76.35	0.2150	0.3400	0.3550	0.3562	0.3338	116.30
7	75.35	0.2840	0.3960	0.4190	0.4204	0.4006	143.40
8	74.70	0.3375	0.4450	0.4602	0.4616	0.4453	157.10
9	73.95	0.4500	0.5280	0.5304	0.5305	0.5252	173.60
10	73.60	0.5350	0.5740	0.5748	0.5736	0.5787	179.70
11	73.50	0.5875	0.6050	0.6004	0.5983	0.6102	178.60
12	73.50	0.6680	0.6510	0.6395	0.6364	0.6582	174.60
13	73.80	0.7425	0.6940	0.6786	0.6752	0.7041	152.50
14	74.25	0.8040	0.7300	0.7167	0.7144	0.7456	129.10
15	75.90	0.9000	0.8250	0.8028	0.8040	0.8260	80.50
16	78.90	0.9800	0.9500	0.9418	0.9444	0.9438	17.64
			ABSD:	0.0110	0.0117	0.0073	

[a] Binary parameters: Wilson, $\lambda_{23} - \lambda_{22} = 210.556$, $\lambda_{32} - \lambda_{33} = 706.139$ cal g-mol^{-1}; NRTL, $g_{23} - g_{33} = 804.250$, $g_{32} - g_{22} = 50.910$ cal g-mol^{-1}; Andiappan–McLean; $w_{23} = 426.060$, $w_{32} = 929.323$ cal g-mol^{-1}.

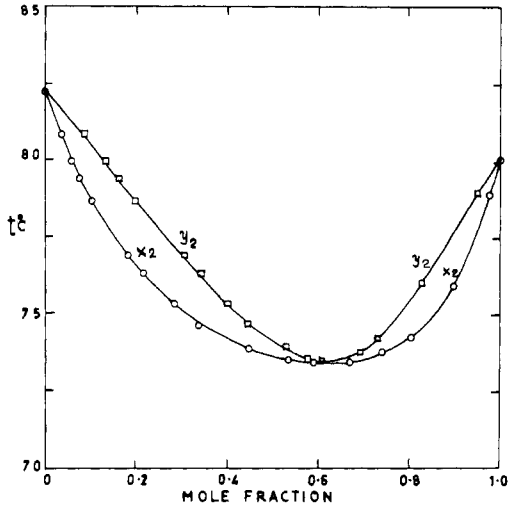

Figure 3. *t–x–y* diagram for benzene (2)–*tert*-butyl alcohol (3) at 760 mmHg pressure.

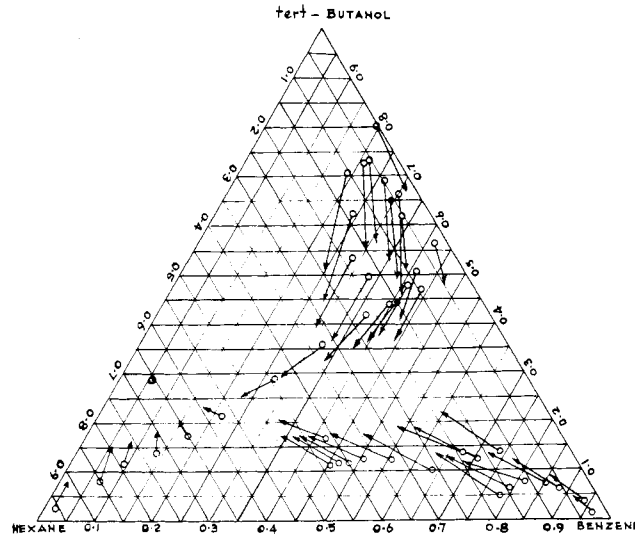

Figure 4. Vapor–liquid equilibrium tie-lines for the system *n*-hexane (1)–benzene (2)–*tert*-butyl alcohol (3) at 760 mmHg pressure.

Andiappan–McLean (*1*) equations which are given in Appendix I.

The correlation of activity coefficients and hence the prediction of boiling points and vapor phase compositions of the ternary system were done through the Wilson and NRTL equations which are presented in Appendix II.

Gibbs excess free energy, g^E, was calculated for the binary systems using the equation,

$$g^E = 2.303RT \sum_{i=1}^{N} x_i \log \gamma_i \qquad (3)$$

Results and Discussion

Binary System. The vapor–liquid equilibrium data at 760 mmHg pressure for the binary systems *n*-hexane–*tert*-butyl alcohol and benzene–*tert*-butyl alcohol are reported in Tables III and IV and shown graphically in Figures 2 and 3. From the tables and figures it may be observed that both systems form azeotropes. While the system *n*-hexane–*tert*-butyl alcohol forms the azeotrope at 0.7600 mole fraction of *n*-hexane boiling at 64.0 °C, the system benzene–*tert*-butyl alcohol forms the azeotrope at 0.6200 mole fraction of benzene with a boiling point of 73.45 °C. These values compare well with the values available in literature (*14*). The thermodynamic consistency of the binary data was tested using Herington's test (*7*). The values of $(D - J)$ for the systems *n*-hexane–*tert*-butyl alcohol and benzene–*tert*-butyl alcohol were found to be −4.370 and − 3.831, respectively. As these values were less than 10 as required by the test, the data were thermodynamically consistent. Using the *p–t–x* data alone the vapor phase compositions of these two binary systems were calculated through the Wilson, NRTL, and Andiappan–McLean equations. The calculated vapor compositions along with the average absolute deviations are also reported in Tables III and IV. It may be seen that all the three equations predict the vapor compositions of both the systems within the experimental error.

Tables III and IV also present the Gibbs excess free energy for the binary system. It is observed from these tables that both systems deviate positively from the ideal solution behavior. This is consistent with the formation of low boiling azeotropes in both cases.

Ternary System. The ternary vapor–liquid equilibrium data for the system *n*-hexane–benzene–*tert*-butyl alcohol are presented in Table V. The data were tested for thermodynamic consistency by the Li and Lu method (*8*). Figure 4 shows the vapor–liquid equilibrium tie-lines for this system, the circle representing the liquid composition and the tip of the arrow representing the vapor composition. From Figure 4 it may be seen that this system forms a ternary azeotrope with a 0.6600 mole fraction of *n*-hexane and a 0.0500 mole fraction of benzene. This was confirmed by preparing a ternary mixture of the above composition and distilling through a fractionating column. The boiling point of the ternary azeotrope was 64.90 °C.

Using the experimental p–x ternary data and the corresponding binary energy parameters, the vapor compositions and boiling points were predicted through the Wilson and NRTL equations. The predicted values along with the binary energy parameters used in the ternary prediction and the average absolute deviation in the vapor compositions and boiling points are reported in Table V. From these deviations it may be concluded that both Wilson and NRTL equations predict the ternary vapor composition and boiling points equally well.

Conclusion

The vapor–liquid equilibrium data for the binary systems of *tert*-butyl alcohol with *n*-hexane and benzene were azeotropic. While the system *n*-hexane–*tert*-butyl alcohol formed the azeotrope at 0.7600 mole fraction of *n*-hexane boiling at 64.0 °C, the system benzene–*tert*-butyl alcohol formed the azeotrope at 0.6200 mole fraction of benzene with a boiling point of 73.45 °C. The ternary equilibrium data of *n*-hexane–benzene–*tert*-butyl alcohol showed that there was a ternary azeotrope with 0.6600 mole fraction of *n*-hexane, 0.0500 mole fraction of benzene, and 0.285 mole fraction of *tert*-butyl alcohol boiling at 64.90 °C. The binary and ternary data were thermodynamically consistent. The binary data were correlated through the Wilson, NRTL, and Andiappan–McLean equations and the ternary boiling points and vapor compositions were predicted through the Wilson and NRTL equations.

Acknowledgment

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Appendix I

Binary Equations. Wilson.

$$\ln \gamma_i = -\ln (x_i + \Lambda_{ij}x_j) + x_j\left[\frac{\Lambda_{ij}}{x_i + \Lambda_{ij}x_j} - \frac{\Lambda_{ji}}{x_j + \Lambda_{ji}x_i}\right] \quad (1)$$

where

$$\Lambda_{ij} = \frac{v_j}{v_i}\exp\left[-\frac{\lambda_{ij} - \lambda_{ii}}{CRT}\right] \quad (2)$$

The binary interaction constant C was taken as equal to 1.

NRTL.

$$\ln \gamma_i = x_j^2\left[\frac{\tau_{ji}G_{ji}^2}{(x_i + x_jG_{ji})^2} + \frac{\tau_{ij}G_{ij}}{(x_j + x_iG_{ij})^2}\right] \quad (3)$$

where

$$\tau_{ij} = (g_{ij} - g_{jj})/RT \quad (4)$$

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij}) \quad (5)$$

α_{ij} = NRTL binary constant which may vary from 0.2 to 0.47 for nonelectrolyte mixtures. The value of the binary constant used in the present calculation was 0.3.

Andiappan–McLean.

$$\ln \gamma_i = \frac{Z}{2}[\ln A_{ij} + x_j\{(x_j - x_i)\xi + \Psi\}] \quad (6)$$

where

$$\xi = \xi_{ij} + \xi_{ji} \quad (7)$$

$$\xi_{ij} = (\beta_{ij} - 1)/\beta_{ij}(\beta_{ij} + x_i - x_j) \quad (8)$$

$$\Psi = \Psi_{ij} - \Psi_{ji} \quad (9)$$

$$\Psi_{ij} = 2x_i/(\beta_{ij} + x_i - x_j) \quad (10)$$

$$A_{ij} = (\beta_{ij} + x_i - x_j)/x_i(\beta_{ij} + 1) \quad (11)$$

$$\beta_{ij} = \{1 + 4x_ix_j(\eta_{ij}^2 - 1)\}^{1/2} \quad (12)$$

$$\eta_{ij} = \exp(w_{ij}/ZRT) \quad (13)$$

Z = the binary constant the value of which is 2 for miscible systems and greater than 2 for partially miscible systems. In the present work Z was taken to be equal to 2 as all the systems are completely miscible.

Appendix II

Ternary Equations. Wilson.

$$g^E/RT = -\sum_{i=1}^{3} x_i \ln\left(\sum_{j=1}^{3} x_j\Lambda_{ij}\right) \quad (14)$$

$$\ln \gamma_i = -\ln\left(\sum_{j=1}^{3} x_j\Lambda_{ij}\right) + 1 - \sum_{j=1}^{3}\frac{x_j\Lambda_{ji}}{\sum_{k=1}^{3} x_k\Lambda_{jk}} \quad (15)$$

NRTL.

$$g^E/RT = \sum_{i=1}^{3} x_i\frac{\sum_{j=1}^{3}\tau_{ji}G_{ji}x_j}{\sum_{k=1}^{3} G_{ki}x_k} \quad (16)$$

$$\ln \gamma_i = \frac{\sum_{j=1}^{3}\tau_{ji}G_{ji}x_j}{\sum_{k=1}^{3} G_{ki}x_k} + \sum_{j=1}^{3}\frac{G_{ij}x_j}{\sum_{k=1}^{3} G_{kj}x_k}\left(\tau_{ji} - \frac{\sum_{l=1}^{3}\tau_{lj}G_{lj}}{\sum_{k=1}^{3} G_{kj}x_k}x_l\right) \quad (17)$$

Glossary

B_i	second virial coefficient
$C_1, C_2, \ldots, C_6$	vapor pressure constants
g^E	excess Gibbs free energy
p_i^0	vapor pressure of the pure component i
T	absolute temperature
R	gas constant
v_i	average liquid molar volume of component i
x_i	liquid phase mole fraction of component i
y_i	Vapor phase mole fraction of component i
γ_i	activity coefficient of component d
π	total pressure of the system

Table V. Vapor–Liquid Equilibrium Data for *n*-Hexane (1)–Benzene (2)–*tert*-Butyl Alcohol (3) at 760 mmHg [a]

No.	Temp, °C	Liquid comp		Vapor comp (exptl)		Calcd values					
						Wilson			NRTL		
		x_1	x_2	y_1	y_2	T, °C	y_1	y_2	T, °C	y_1	y_2
1	76.10	0.0067	0.1900	0.0267	0.3100	76.88	0.0206	0.3209	76.19	0.0209	0.3242
2	75.45	0.0134	0.2184	0.0367	0.3350	76.02	0.0388	0.3452	75.41	0.0393	0.3485
3	74.60	0.0185	0.2600	0.0485	0.3716	75.17	0.0499	0.3797	74.63	0.0506	0.3829
4	75.60	0.0200	0.1917	0.0550	0.3035	76.08	0.0589	0.3118	75.48	0.0597	0.3147
5	75.05	0.0200	0.2150	0.0550	0.3200	75.71	0.0570	0.3362	75.13	0.0578	0.3392
6	75.05	0.0234	0.2134	0.0535	0.3134	75.58	0.0651	0.3321	75.02	0.0660	0.3350
7	75.15	0.0234	0.1985	0.0650	0.2950	75.78	0.0675	0.3164	75.21	0.0685	0.3192
8	74.80	0.0234	0.2200	0.0634	0.3217	75.46	0.0656	0.3384	74.91	0.0665	0.3413
9	74.10	0.0234	0.2890	0.0567	0.3985	74.62	0.0601	0.3995	74.13	0.0608	0.4024
10	73.05	0.0260	0.4134	0.0500	0.4695	73.59	0.0582	0.4821	73.17	0.0587	0.4838
11	74.55	0.0285	0.2350	0.0667	0.3285	75.00	0.0771	0.3485	74.49	0.0782	0.3513
12	74.05	0.0300	0.2550	0.0800	0.3550	74.68	0.0788	0.3653	74.20	0.0799	0.3681
13	73.60	0.0300	0.3200	0.0620	0.4095	74.04	0.0731	0.4172	73.60	0.0739	0.4197
14	72.85	0.0300	0.4050	0.0660	0.4750	73.48	0.0670	0.4734	73.09	0.0676	0.4750
15	73.00	0.0334	0.3700	0.0734	0.4435	73.54	0.0765	0.4485	73.15	0.0773	0.4504
16	73.60	0.0350	0.2750	0.0934	0.3717	74.24	0.0885	0.3781	73.79	0.0897	0.3806
17	74.35	0.0367	0.2117	0.1015	0.3909	74.90	0.1000	0.3196	74.41	0.1015	0.3220
18	74.00	0.0367	0.2318	0.1000	0.3167	74.64	0.0974	0.3390	74.18	0.0988	0.3414
19	72.95	0.0385	0.3000	0.1034	0.3900	73.85	0.0937	0.3949	73.45	0.0949	0.3972
20	73.95	0.0450	0.2168	0.1190	0.3145	74.44	0.1189	0.3185	74.00	0.1207	0.3206
21	72.55	0.0450	0.4168	0.0890	0.4700	72.90	0.0958	0.4671	72.58	0.0967	0.4680
22	73.05	0.0490	0.2610	0.1234	0.3500	73.77	0.1213	0.3553	73.38	0.1230	0.3573
23	72.25	0.0490	0.4085	0.1050	0.4836	72.77	0.1050	0.4584	72.47	0.1061	0.4592
24	72.15	0.0500	0.4236	0.1036	0.4700	72.70	0.1045	0.4668	72.41	0.1055	0.4675
25	72.20	0.0525	0.4330	0.1050	0.4785	72.60	0.1082	0.4702	72.31	0.1093	0.4706
26	72.75	0.0530	0.2930	0.1300	0.3800	73.32	0.1251	0.3779	72.97	0.1268	0.3796
27	72.30	0.0534	0.3250	0.1200	0.4117	73.08	0.1217	0.4012	72.75	0.1232	0.4027
28	72.35	0.0534	0.3380	0.1285	0.4050	72.99	0.1200	0.4102	72.67	0.1215	0.4117
29	73.55	0.0550	0.2167	0.1300	0.3084	73.98	0.1414	0.3113	73.59	0.1436	0.3130
30	72.10	0.0584	0.3305	0.1400	0.4000	72.86	0.1306	0.4011	72.55	0.1323	0.4024
31	73.10	0.0630	0.2100	0.1500	0.2968	73.71	0.1597	0.2994	73.35	0.1624	0.3009
32	71.70	0.0660	0.4170	0.1300	0.4485	72.22	0.1336	0.4502	71.99	0.1350	0.4503
33	71.70	0.0660	0.4268	0.1290	0.4580	72.20	0.1325	0.4558	71.96	0.1339	0.4558
34	71.60	0.0725	0.4190	0.1367	0.4485	72.03	0.1443	0.4464	72.81	0.1459	0.4462
35	72.50	0.0734	0.2334	0.1720	0.3095	73.04	0.1759	0.3142	72.73	0.1788	0.3153
36	72.85	0.0768	0.2017	0.1835	0.2800	73.21	0.1896	0.2828	72.90	0.1929	0.2838
37	72.70	0.0768	0.2034	0.1850	0.2768	73.20	0.1892	0.2844	72.89	0.1925	0.2854
38	71.25	0.0768	0.4100	0.1450	0.4367	71.92	0.1524	0.4380	71.72	0.1541	0.4378
39	72.45	0.0800	0.2218	0.1867	0.2968	72.88	0.1911	0.2997	72.59	0.1943	0.3006
40	71.00	0.0800	0.4320	0.1834	0.4450	71.79	0.1549	0.4483	71.60	0.1566	0.4477
41	70.70	0.0850	0.4117	0.1834	0.4334	71.69	0.1655	0.4330	71.51	0.1674	0.4325
42	70.90	0.0880	0.4100	0.1650	0.4314	71.61	0.1704	0.4299	71.44	0.1724	0.4293
43	72.00	0.0890	0.1768	0.2220	0.2400	73.00	0.2195	0.2510	72.70	0.2236	0.2516
44	71.85	0.0900	0.2000	0.2117	0.2634	72.71	0.2150	0.2735	72.45	0.2189	0.2740
45	71.70	0.0968	0.1985	0.2300	0.2568	72.47	0.2277	0.2683	72.21	0.2319	0.2687
46	70.40	0.0968	0.4360	0.1900	0.4385	71.34	0.1799	0.4390	71.21	0.1819	0.4377
47	71.50	0.1050	0.1890	0.2450	0.2485	72.25	0.2447	0.2549	72.02	0.2493	0.2550
48	70.40	0.1100	0.4067	0.2000	0.4215	71.04	0.2036	0.4134	70.93	0.2061	0.4121
49	70.65	0.1150	0.2134	0.2700	0.2684	71.69	0.2540	0.2724	71.50	0.2587	0.2722
50	70.20	0.1200	0.4067	0.2080	0.4115	70.80	0.2175	0.4073	70.71	0.2202	0.4056
51	70.50	0.1250	0.2260	0.2650	0.2716	71.28	0.2658	0.2783	71.13	0.2707	0.2778
52	70.05	0.1250	0.4067	0.2134	0.4085	70.68	0.2242	0.4043	70.61	0.2270	0.4025
53	69.85	0.1334	0.4035	0.2320	0.4067	70.50	0.2358	0.3976	70.44	0.2388	0.3956
54	69.95	0.1350	0.2460	0.2765	0.2834	70.87	0.2745	0.2898	70.75	0.2794	0.2889
55	69.90	0.1367	0.2500	0.2817	0.2867	70.80	0.2757	0.2921	70.69	0.2807	0.2912
56	70.05	0.1395	0.2395	0.2767	0.2767	70.77	0.2827	0.2823	70.66	0.2879	0.2814
57	69.60	0.1410	0.3730	0.2500	0.3750	70.34	0.2515	0.3750	70.30	0.2549	0.3731
58	69.40	0.1535	0.2600	0.2967	0.2860	70.30	0.2954	0.2918	70.24	0.3006	0.2903
59	69.75	0.1568	0.4050	0.2435	0.3933	70.01	0.2642	0.3858	69.99	0.2676	0.3832
60	69.10	0 1585	0.3334	0.2880	0.3417	70.00	0.2820	0.3409	69.98	0.2863	0.3388
61	69.25	0.1615	0.2700	0.3000	0.2916	70.07	0.3025	0.2956	70.03	0.3078	0.2938
62	69.20	0.1615	0.3950	0.2667	0.3800	69.91	0.2718	0.3775	69.91	0.2754	0.3748
63	69.05	0.1690	0.2760	0.3134	0.2967	69.87	0.3099	0.2966	69.85	0.3152	0.2946
64	68.85	0.1720	0.3334	0.2985	0.3317	69.71	0.2978	0.3345	69.72	0.3023	0.3320
65	68.75	0.1767	0.3415	0.3020	0.3317	69.61	0.3011	0.3375	69.63	0.3056	0.3348
66	68.85	0.1767	0.3868	0.2845	0.3680	69.62	0.2906	0.3654	69.65	0.2944	0.3623
67	68.95	0.1850	0.2834	0.3134	0.2910	69.51	0.3261	0.2949	69.52	0.3316	0.2924
68	68.65	0.1870	0.3800	0.2900	0.3500	69.43	0.3032	0.3566	69.47	0.3073	0.3534
69	68.70	0.1916	0.2900	0.3216	0.2934	69.36	0.3314	0.2968	69.38	0.3368	0.2941

Table V (continued)

No.	Temp, °C	Liquid comp x_1	Liquid comp x_2	Vapor comp (exptl) y_1	Vapor comp (exptl) y_2	Calcd values: Wilson T, °C	Wilson y_1	Wilson y_2	NRTL T, °C	NRTL y_1	NRTL y_2
70	68.15	0.2210	0.3667	0.3350	0.3380	68.85	0.3403	0.3345	68.95	0.3448	0.3306
71	67.25	0.2750	0.3350	0.3867	0.3000	68.05	0.3955	0.2965	68.22	0.4006	0.2918
72	66.60	0.3260	0.3130	0.4350	0.2768	67.43	0.4397	0.2687	67.65	0.4449	0.2636
73	66.10	0.3867	0.2968	0.4734	0.2533	66.87	0.4836	0.2455	67.14	0.4884	0.2400
74	65.60	0.4435	0.2700	0.5210	0.2275	66.41	0.5240	0.2189	66.72	0.5283	0.2134
75	65.10	0.5734	0.2140	0.5967	0.1750	65.71	0.6057	0.1683	66.09	0.6086	0.1636
76	64.95	0.6567	0.1725	0.6550	0.1467	65.45	0.6571	0.1354	65.85	0.6594	0.1316
77	64.95	0.7260	0.1360	0.7067	0.1167	65.34	0.7014	0.1076	65.75	0.7037	0.1048
78	65.25	0.7950	0.0884	0.7617	0.0800	65.21	0.7491	0.0711	65.66	0.7513	0.0693
79	65.60	0.8585	0.0634	0.8020	0.0534	65.57	0.7982	0.0525	65.04	0.8030	0.0514
80	66.85	0.9640	0.0167	0.9150	0.0117	67.34	0.9253	0.0154	67.65	0.9321	0.0151
81	78.30	0.0250	0.9633	0.0400	0.9130	79.00	0.0485	0.9166	78.02	0.0505	0.9168
82	77.30	0.0285	0.9333	0.0567	0.8633	77.42	0.0530	0.8498	76.68	0.0551	0.8521
83	76.45	0.0467	0.9200	0.0867	0.8233	77.09	0.0846	0.8300	76.38	0.0878	0.8311
84	75.40	0.0553	0.8834	0.1033	0.7767	75.70	0.0963	0.7688	75.17	0.0995	0.7702
85	74.30	0.0717	0.8516	0.1385	0.7250	74.77	0.1203	0.7246	74.35	0.1239	0.7253
86	73.60	0.1033	0.8185	0.1933	0.6885	73.95	0.1653	0.6819	73.61	0.1699	0.6818
87	71.60	0.1167	0.7233	0.1900	0.5916	72.35	0.1813	0.5902	71.95	0.1845	0.5882
88	71.80	0.1200	0.7400	0.1867	0.6033	72.33	0.1851	0.6019	72.14	0.1887	0.6004
89	71.90	0.1250	0.7515	0.1900	0.6067	72.48	0.1917	0.6109	72.28	0.1957	0.6089
90	72.80	0.1400	0.7933	0.2166	0.6500	73.46	0.2139	0.6522	73.17	0.2198	0.6515
91	71.80	0.1433	0.7467	0.2233	0.6067	72.35	0.2147	0.6020	72.17	0.2195	0.6008
92	72.70	0.1500	0.7867	0.2267	0.6367	73.35	0.2266	0.6451	73.07	0.2328	0.6442
93	71.75	0.1650	0.7385	0.2555	0.5916	72.20	0.2410	0.5916	72.03	0.2466	0.5903
94	70.80	0.1667	0.6933	0.2533	0.5600	71.39	0.2419	0.5519	71.31	0.2463	0.5498
95	72.10	0.1667	0.7133	0.2416	0.5685	71.71	0.2420	0.5683	71.60	0.2470	0.5665
96	71.20	0.1733	0.7200	0.2467	0.5700	71.82	0.2500	0.5733	71.70	0.2554	0.5717
97	71.30	0.1767	0.7267	0.2667	0.5733	71.96	0.2545	0.5793	71.84	0.2601	0.5779
98	71.20	0.1800	0.7167	0.2700	0.5633	71.76	0.2577	0.5696	71.65	0.2633	0.5680
99	70.50	0.1867	0.6750	0.2717	0.5333	71.05	0.2643	0.5332	71.01	0.2691	0.5309
100	70.50	0.1933	0.6767	0.2800	0.5267	71.06	0.2715	0.5333	71.02	0.2766	0.5311
101	70.70	0.1967	0.6967	0.2733	0.5450	71.40	0.2758	0.5498	71.33	0.2815	0.5480
102	69.80	0.2100	0.6367	0.3800	0.5133	70.45	0.2896	0.4996	70.46	0.2944	0.4967
103	70.30	0.2100	0.6616	0.2900	0.5200	70.79	0.2893	0.5185	70.77	0.2947	0.5161
104	69.80	0.2600	0.6400	0.3367	0.4900	70.50	0.3402	0.4964	70.52	0.3468	0.4942
105	68.40	0.3000	0.5933	0.3767	0.4600	69.78	0.3768	0.4558	69.87	0.3835	0.4532
106	68.85	0.3200	0.5600	0.3933	0.4300	69.29	0.3940	0.4282	69.42	0.4005	0.4252
107	68.70	0.3400	0.5485	0.4167	0.4216	69.18	0.4114	0.4186	69.31	0.4182	0.4158
108	68.30	0.3667	0.5100	0.4316	0.3985	68.66	0.4336	0.3879	68.84	0.4401	0.3847
109	68.25	0.3967	0.4850	0.4567	0.3767	68.38	0.4579	0.3683	68.60	0.4646	0.3651
110	67.20	0.4134	0.4200	0.4750	0.3250	67.59	0.4736	0.3205	67.85	0.4790	0.3162
111	67.90	0.4134	0.4685	0.4670	0.3633	68.20	0.4712	0.3556	68.43	0.4778	0.3523
112	67.80	0.4150	0.4616	0.4700	0.3516	68.11	0.4724	0.3503	68.34	0.4789	0.3469
113	67.65	0.4333	0.4533	0.4816	0.3485	68.07	0.4867	0.3441	68.31	0.4935	0.3408
114	67.60	0.4350	0.4490	0.4880	0.3433	68.01	0.4880	0.3408	68.25	0.4947	0.3374
115	67.40	0.4367	0.4385	0.4867	0.3385	67.86	0.4894	0.3327	68.12	0.4958	0.3292
116	67.50	0.4433	0.4333	0.4967	0.3333	67.81	0.4944	0.3288	68.07	0.5009	0.3253

[a] Binary parameters: Wilson, $\lambda_{12} - \lambda_{11} = 30.5670$, $\lambda_{21} - \lambda_{22} = 256.45$, $\lambda_{23} - \lambda_{22} = 210.556$, $\lambda_{32} - \lambda_{33} = 706.1389$, $\lambda_{31} - \lambda_{33} = 1313.188$, $\lambda_{13} - \lambda_{11} = -7.3445$ cal g-mol^{-1}; NRTL, $g_{12} - g_{22} = -115.16$, $g_{21} - g_{11} = 410.00$, $g_{23} - g_{33} = 804.25$, $g_{32} - g_{22} = 50.91$, $g_{31} - g_{11} = 53.31$, $g_{13} - g_{33} = 1130.68$ cal g-mol^{-1}. ABSD: Wilson, $\Delta T = 0.60$ °C, $\Delta y_1 = 0.0064$, $\Delta y_2 = 0.0061$, $\Delta y_3 = 0.0096$; NRTL, $\Delta T = 0.46$ °C, $\Delta y_1 = 0.0078$, $\Delta y_2 = 0.0072$, $\Delta y_3 = 0.0104$.

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