J. Chem. Eng. Data **1994,** *39,* 679–684

Mutual Solubilities of Alkylbenzene + Water Systems at Temperatures from 303 to 373 K: Ethylbenzene, *p*-Xylene, 1,3,5-Trimethylbenzene, and Butylbenzene

Huaping Chen and Jan Wagner*

School of Chemical Engineering, Oklahoma State University, Stillwater, Oklahoma 74078

Mutual solubilities for *p*-xylene, 1,3,5-trimethylbenzene, ethylbenzene, and butylbenzene have been measured near the three-phase curve from 303 to 373 K. Calculated enthalpies of solution of hydrocarbons into water compare well with published calorimetric measurements. The estimated minimum solubility temperatures agree well with those estimated from calorimetric measurements. The results also provide insight into the mechanism of water dissolving into liquid hydrocarbons. The calculated enthalpies of solution of water into hydrocarbons are approximately equal to the molar hydrogen bonding energy of water. The entropy of mixing water into this series of alkylbenzenes can be considered constant in the range 303–373 K.

Introduction

Mutual solubility measurements have been reported previously for benzene + water (*1*) and toluene + water (*2*) over the temperature range of 303–373 K. In an effort to gain some insight into the effects of molecular size and structure, as well as temperature, and to provide guidance in the development and evaluation of equations of state and activity coefficient models for hydrocarbon + water systems, we have extended the experimental data base to other alkylbenzene-water mixtures. *p*-Xylene and 1,3,5-trimethylbenzene were selected to determine the effects of molecular size. Together with benzene, this series represents fairly symmetrical compounds of increasing molecular volume. Ethylbenzene and butylbenzene, together with toluene, form a homologous series of increasing length of the side chain on the substituted benzene structure. The length of the side chain should tend to make the molecule more asymmetrical and induce a larger dipole moment relative to a more symmetrical component of the same molecular weight, i.e., ethylbenzene compared to *p*-xylene.

In addition to representing a range of molecular size and structure, alkylbenzene + water systems are important in the chemical process industry. They also represent a class of environmentally important chemicals. Emissions of benzene are currently regulated (*3*), and other aromatic hydrocarbons are among the U.S. Environmental Protection Agency priority pollutants (*4*).

Experimental Section

The detailed design and operation of a continuous flow equilibrium apparatus for mutual solubility measurements have been described by Chen and Wagner (*1*). Temperatures are controlled to within ±0.2 K over the temperature range of 303–383 K. The hydrocarbon and water phases are sampled simultaneously. Sample preparation and analysis procedures described by Chen and Wagner (*2*) were followed. The solvents used as extractants and internal standards for each of the hydrocarbons dissolved in the aqueous samples are listed in Table 1, together with the type of column used in the gas chromatographic analyses.

Table 1. Cosolvents and GC Columns for Water-Phase Analyses

solute	solvent	GC column
ethylbenzene	methylene chloride	Porapac
butylbenzene	2,2,4-trimethylpentane	Gas Chrom
p-xylene	methylene chloride	Porapac
1,3,5-trimethylbenzene	2,2,4-trimethylpentane	Gas Chrom

The procedure described by Chen and Wagner (*2*) was modified to monitor solute left in the aqueous phase after solvent extraction. When methylene chloride serves as extractant and internal standard, the solubility of methylene chloride in water must be accounted for in the calibration procedure. To correct for the slight solubility of methylene chloride in water, the solubility at room temperature (1.9 mass %) is used to calculate the amount of methylene chloride remaining in the organic phase. This quantity of methylene chloride is subtracted from the amount added to the water-phase sample. The difference is the actual amount of the internal standard.

Ethanol was used as a cosolvent and an internal standard for all organic-phase samples. Water solubility in hydrocarbon was corrected for the concentration of water in the ethanol cosolvent following the method described by Chen and Wagner (*2*).

Materials. Ethylbenzene (99%), *p*-xylene (99.5+%, HPLC grade), 1,3,5-trimethylbenzene (98.5%), butylbenzene (99+%), 2,2,4-trimethylpentane (99+%), and methylene chloride (99.9%, HPLC grade) were used as received from Aldrich Chemical Co. Distilled/deionized water was used without further purification. Ethanol USP Absolute-200 Proof from AAPER Alcohol and Chemical Co. was dehydrated and stored over 4A molecular sieves from Fisher Chemical Co.

Results and Discussion

The mutual solubilities of *p*-xylene, 1,3,5-trimethylbenzene, ethylbenzene, and butylbenzene are presented in Table 2. Each measurement was replicated as shown, and the mean values are reported together with the standard deviations. The maximum correction for water content introduced by the ethanol cosolvent is about 15%, while the maximum correction introduced by the methylene chloride is about 18%. The maximum coefficient of variation is less than 6% for hydrocarbon solubility in water and less than 9% for water solubility in hydrocarbons.

0021-9568/94/1739-0679$04.50/0

Table 2. Mutual Solubilities of Alkylbenzene + Water[a]

		hydrocarbon solubility in water			water solubility in hydrocarbon		
T/K	P/bar	10^6x_1	$10^6\sigma$	N	10^3x_2	$10^3\sigma$	N
		Ethylbenzene (1) + Water (2)					
303.15	1.36	28.8	0.4	6	2.71	0.18	6
313.15	1.36	29.2	0.4	4	3.66	0.23	6
323.15	1.36	33.5	0.9	6	4.57	0.25	6
333.15	1.36	40.7	2.3	5	5.73	0.26	6
343.15	1.36	49.3	2.1	6	8.30	0.66	6
353.15	1.36	59.9	2.4	6	10.7	0.47	6
363.15	1.70	69.5	1.7	5	15.4	1.34	6
373.15	2.24	85.4	3.4	6	20.2	0.64	5
		p-Xylene (1) + Water (2)					
303.15	1.36	28.6	0.6	5	2.71	0.09	4
313.15	1.36	31.8	1.5	6	3.48	0.20	4
323.15	1.36	34.4	0.7	6	4.75	0.16	4
333.15	1.36	40.4	0.5	6	6.51	0.47	4
343.15	1.36	48.3	0.6	6	8.70	0.75	6
353.15	1.36	57.1	0.7	6	11.5	0.73	5
363.15	1.70	67.0	1.0	6	15.7	0.63	6
373.15	2.04	87.4	2.2	6	20.2	1.07	6
		1,3,5-Trimethylbenzene (1) + Water (2)					
303.15	1.36	9.58	0.53	6	2.47	0.09	6
313.15	1.36	10.0	0.5	6	3.50	0.19	6
323.15	1.36	11.1	0.6	5	4.88	0.18	6
333.15	1.36	13.6	0.7	7	6.09	0.17	6
343.15	1.36	16.6	1.2	6	7.97	0.28	6
353.15	1.36	20.9	0.6	6	10.6	0.3	6
363.15	2.04	24.5	0.6	6	14.0	0.7	6
373.15	2.38	29.1	0.6	4	19.0	0.4	5
		Butylbenzene (1) + Water (2)					
303.15	1.36	2.24	0.12	3	2.36	0.10	5
313.15	1.36	2.39	0.17	6	3.15	0.06	5
323.15	1.36	2.73	0.10	5	4.13	0.07	5
333.15	1.36	3.61	0.10	5	5.95	0.27	6
343.15	1.36	4.30	0.11	3	8.37	0.33	5
353.15	1.36	6.40	0.20	5	10.7	0.5	6
363.15	2.04	8.20	0.43	5	14.8	0.3	5
373.15	2.38	11.2	0.1	4	19.9	0.8	5

[a] σ = standard deviation. N = number of measurements.

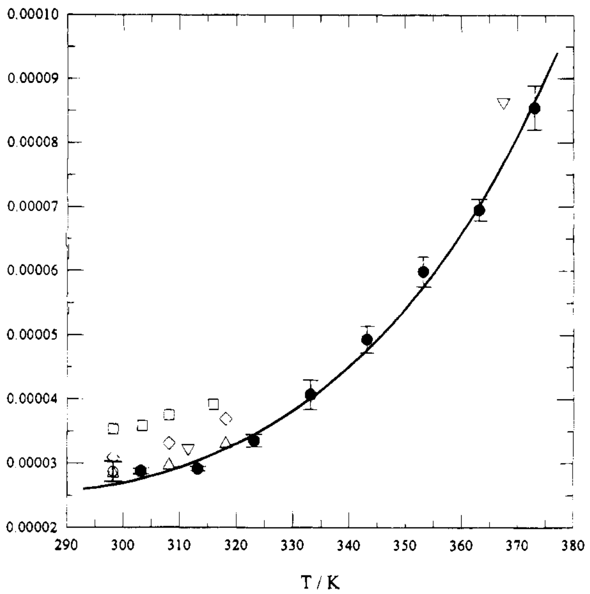

Figure 1. Solubility of ethylbenzene in water: (●) this work, (□) Bohon and Claussen (*17*), (▽) Heidman et al. (*18*), (◇) Sanemasa et al. (*14*), (△) Sanemasa et al. (*15*), (○) average of data at 298.15 K (Table 4).

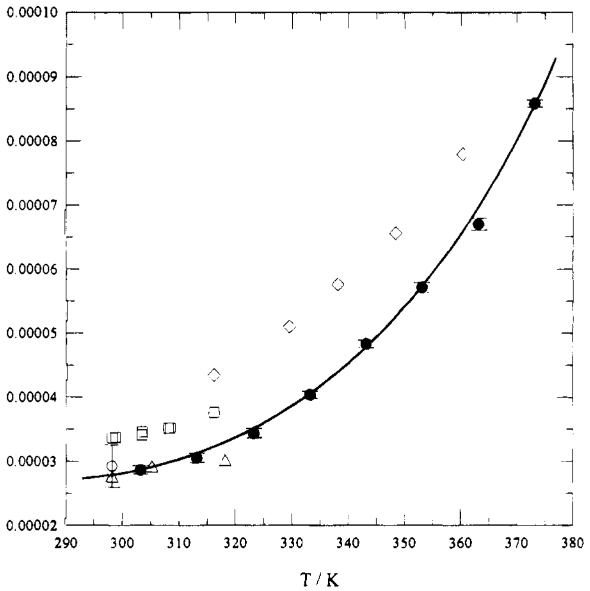

Figure 2. Solubility of p-xylene in water: (●) this work, (□) Bohon and Claussen (*17*), (◇) Pryor and Jentoft (*21*), (△) Sanemasa (*15*), (○) average of data at 298.15 K (Table 5).

Alkylbenzene Solubility in Water. The measured solubility data are correlated with the following empirical relation:

$$\ln x_i = A + BT_{r,i}^{-1} + CT_{r,i}^{-2} \qquad (1)$$

where x_i is the mole fraction of hydrocarbon i and $T_{r,i}$ is the reduced temperature of the hydrocarbon (system temperature divided by the critical temperature, $T_{c,i}$, of the hydrocarbon as reported by Reid et al. (*5*)). The coefficients of this equation for each of the systems, as well as those from previous studies on benzene (*1*) and toluene (*2*), are summarized in Table 3. These correlations are plotted as solid lines in Figures 1–4 for each of the systems discussed below.

Ethylbenzene Solubility in Water. Few data are available in the temperature range covered in this study. There are about 12 independent measurements at 298 K. These data are summarized in Table 4, with the average and standard deviations plotted in Figure 1. The data of Bohon and Claussen (*17*) are significantly higher than those from other studies (more than 4 standard deviations greater than the mean of other measurements at 298 K). There is fairly good agreement with the earlier data reported by Sanemasa et al. (*14*) and excellent agreement

Table 3. Aqueous Alkylbenzene Solubility Correlations and Derived Enthalpies of Solution

solute	coefficients in eq 1 A	B	C	min solubility temp/K (eq 3/ref 23)	ΔH_i/(kJ·mol^{-1}) at 298.15 K (eq 5/ref 23)	ΔC_{Pi}/(kJ·mol^{-1}·K^{-1}) at 298.15 K (eq 6/ref 23)
benzene	6.191	−14.03	3.511	281/288.9	3.69/2.08	207/225
toluene	12.21	−21.39	5.372	297/291.6	0.37/1.73	351/263
ethylbenzene	11.59	−20.52	4.750	285/292.0	4.38/2.02	338/318
p-xylene	11.79	−20.89	4.892	288/–	3.48/–	347/–
1,3,5-trimethylbenzene	11.33	−20.64	4.630	265/–	4.49/–	352/–
propylbenzene				–/292.3	–/2.3	–/391
butylbenzene	26.26	−35.26	7.905	296/–	1.29/–	645/–

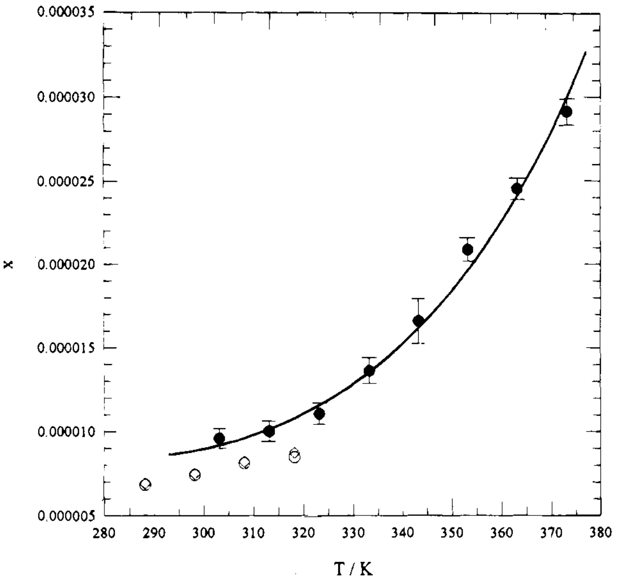

Figure 3. Solubility of 1,3,5-trimethylbenzene in water: (●) this work, (○) Sanemasa et al. (*15*), (◇) Sanemasa et al. (*16*).

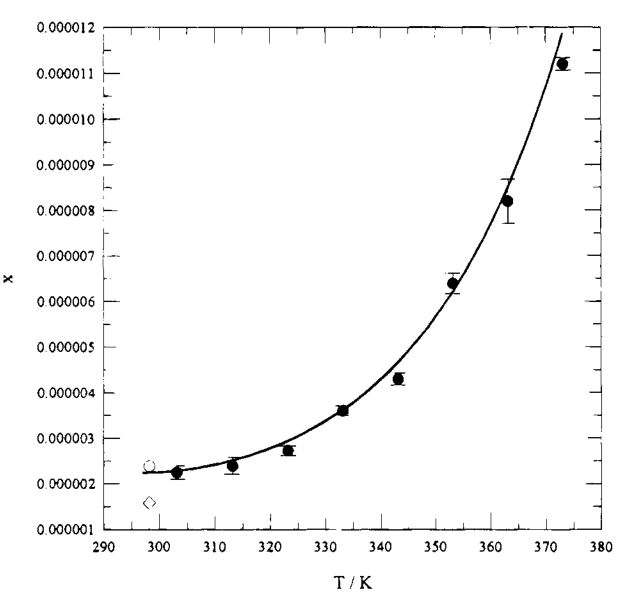

Figure 4. Solubility of *n*-butylbenzene in water: (●) this work, (○) Masaldi and King (*24*), (◇) Sutton and Calder (*12*).

Table 4. Solubility of Ethylbenzene (1) in Water (2) at 298.15 K

10^3x_1	ref
0.0285	Andrews and Keefer, 1950 (*6*)
0.0297	Klevans, 1950 (*7*)
0.0280	Morrison and Billett, 1952 (*8*)
0.0270	McAuliffe, 1963 (*9*)
0.0258	McAuliffe, 1966 (*10*)
0.0301	Polak and Lu, 1973 (*11*)
0.0273	Sutton and Calder, 1975 (*12*)
0.0306	Korenman and Aref'eva, 1978 (*13*)
0.0307	Sanemasa et al., 1981 (*14*)
0.0287	Sanemasa et al., 1982 (*15*)
0.0292	Sanemasa et al., 1984 (*16*)
0.0287	average
0.0016	standard deviation

with their later measurements (*15*). At higher temperatures, our measurements tend to be lower than those of Heidman et al. (*18*), but the difference is within the combined experimental errors.

***p*-Xylene Solubility in Water.** There are limited data published for this system. The measurements at 298 K are listed in Table 5, and the average and standard deviation (as an error bar) are plotted in Figure 2. The solubilities measured in this work are consistent with the published values at 298 K. The data of Bohon and Claussen (*17*) are more than 1 standard deviation above the average of the other data at 298 K, and are considered to be too high. The *p*-xylene solubility reported by Pryor and Jentoft (*21*) is higher than the value of Bohon and Claussen (*17*) at 316 K. Hefter (*22*) also concluded that none of the solubility data for *p*-xylene in water were very reliable.

Table 5. Solubility of *p*-Xylene (1) in Water (2) at 298.15 K

10^3x_1	ref
0.0340	Andrews and Keefer, 1949 (*19*)
0.0314	Polak and Lu, 1973 (*11*)
0.0265	Sutton and Calder, 1975 (*12*)
0.0267	Price, 1976 (*20*)
0.0277	Sanemasa et al., 1982 (*15*)
0.0293	average
0.0033	standard deviation

1,3,5-Trimethylbenzene Solubility in Water. The measurements for this system are summarized in Table 2 and plotted in Figure 3. The solubilities at 303, 313, and 323 K are approximately 20% higher than the values reported by Sanemasa et al. (*15, 16*). Gill et al. (*23*) have estimated the minimum solubility temperatures of other alkylbenzenes to be approximately 292 K on the basis of calorimetric measurements (Table 3). These independendent estimates indicate that the data of Sanemasa et al. (*15, 16*) do not exhibit the correct temperature dependence in the region 288−298 K. Comparisons of properties derived from solubility and calorimetric measurements are discussed in more detail below.

Butylbenzene Solubility in Water. There are four published measurements on butylbenzene solubility in water at 298 K by Andrews and Keefer (*6*), Klevens (*7*), Massaldi and King (*23*), and Sutton and Calder (*12*). Of these measurements, the value of Andrews and Keefer (*6*) has been judged as too low by Hefter (*22*), while the value of Klevens (*7*) is too high (*20*). As shown in Figure 4, the current measurements are in good agreement with the value of Massaldi and King (*24*). From the trend of the solubility measurements with temperature, the minimum solubility temperature should be near 290 K. Thus, the value of Sutton and Calder (*12*) may be low.

The alkylbenzene solubility measurements reported in this study and previously published data for benzene and toluene are cross-plotted as a function of the hydrocarbon molecular weight in Figure 5. The least-squares regression lines through the data are shown to indicate trends in the data, not to correlate solubility or to interpret physical solution processes. Figure 5 indicates a systematic decrease in solubility with increasing molecular weight (size) and decreasing temperature (down to the minimum solubility temperature) for this series of hydrocarbons. Sutton and Calder (*12*) and Sanemasa et al. (*15*) noted that the solubilites of these alkylbenzenes are primarily dependent upon the number of methyl groups, and the position of substitution on the ring is of secondary importance. This trend is also exhibited in Figure 5 which illustrates the overall consistency of this series of alkylbenzene solubility measurements.

Equation 1 can be used to estimate the enthalpy of solution of hydrocarbons in water. Assuming both the activity coefficient for water in the water phase and that for the hydrocarbon component in the hydrocarbon phase

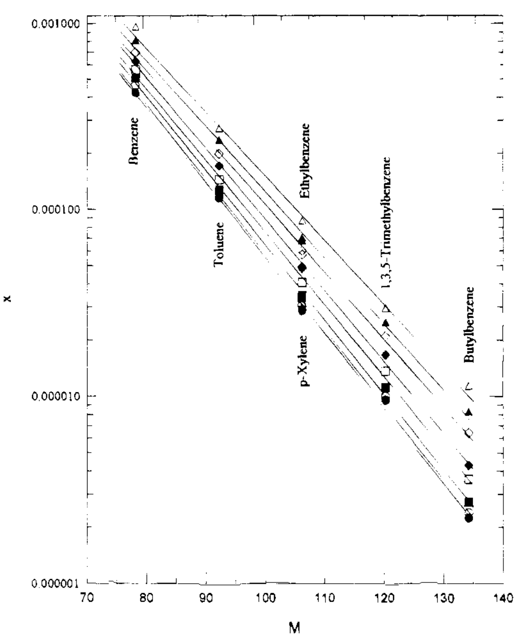

Figure 5. Solubility of alkylbenzenes as a function of hydrocarbon molecular weight: (●) 303 K, (○) 313 K, (■) 323 K, (□) 333 K, (◆) 343 K, (◇) 353 K, (▲) 363 K, (△) 373 K.

are equal to 1 and using the Gibbs–Duhem equation leads to

$$\left(\frac{\partial \ln x_i}{\partial T}\right)_P = \frac{\Delta H_i}{RT^2} \tag{2}$$

or

$$\Delta H_i = -RT\left[\frac{B}{T_{r,i}} + \frac{2C}{T_{r,i}^{\ 2}}\right] \tag{3}$$

where ΔH_i is the difference between the partial molar enthalpy of component i in solution and the molar enthalpy of pure i. The specific heat of solution, ΔC_{Pi}, is defined as

$$\Delta C_{Pi} = (\partial \Delta H_i/\partial T)_P \tag{4}$$

and from eq 2

$$\Delta C_{Pi} = \frac{R}{T}\left[\frac{B}{T_{r,i}} + \frac{4C}{T_{r,i}^{\ 2}}\right] \tag{5}$$

The minimum solubility temperature can be estimated from eq 1 as

$$T_{\min,i} = -(2C/B)T_{c,i} \tag{6}$$

which is the temperature where $\Delta H_i = 0$.

Enthalpies and specific heats of solution at 298.15 K calculated using eqs 3 and 5 and the minimum solubility temperature estimated using eq 6 are presented in Table 3. The calorimetric measurements of Gill et al. (*23*) are included for comparison. For this series of hydrocarbons, the minimum solubility temperatures are close to 298 K. The value of ΔH_i (a derivative property of the solubility measurements) evaluated at 298 K is very sensitive to the values of the coefficients of the empirical equation used to fit the experimental results. In addition, the nonlinear eq 1 must be extrapolated beyond the range of the experimantal data to evaluate these derivative properties at 298 K. Thus, some disagreement between enthalpies of solution estimated from solubility data and those obtained from calorimetric measurements is expected. Second derivative properties, ΔC_{Pi}, are extremely sensitive to parameters in the correlations near the minimum solubility temperature. Franks (*25*) also points out the pitfalls of differentiating solubility data, and the functional form of eq 1 may not represent the actual solution behavior of these apolar species in water. The comparisons of calculated and experimental enthalpies of solution and specific heats of solution presented in Table 3 are intended to provide a general indication of the quality of the solubility data, not to compare enthalpy effects from calorimetric and solubility measurements. In this context, calorimetric measurements tend to validate the magnitude and temperature dependence of the measured alkylbenzene solubilities in water.

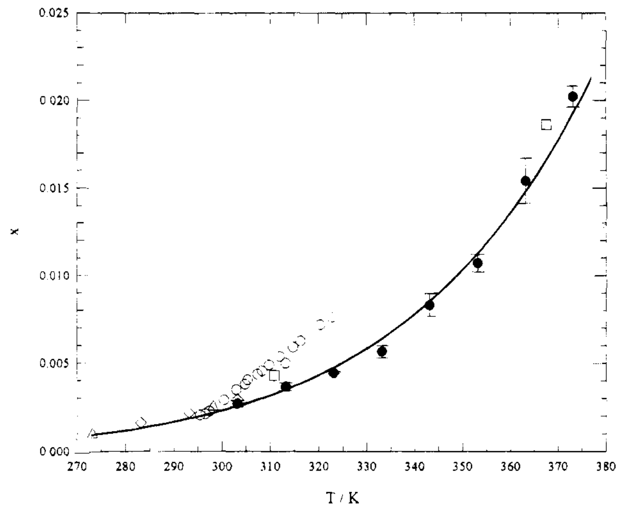

Figure 6. Solubility of water in ethylbenzene: (●) this work, (◇) Englin et al. (*27*), (○) Filipov and Furman (*26*), (□) Heidman et al. (*18*), (△) Polak and Lu (*11*).

Table 6. Water Solubility Correlations and Derived Enthalpies of Solution

solvent	coefficients in eq 7		ΔH_w/(kJ·mol^{-1}) at 298.15 K	ΔS_w/(kJ·mol^{-1}·K^{-1}) at 298.15 K
	A	*B*		
benzene	1.557	9.415	23.3	0.0782
toluene	1.483	9.647	23.9	0.0802
ethylbenzene	1.391	9.714	24.1	0.0808
p-xylene	1.512	9.844	24.4	0.0818
1,3,5-trimethylbenzene	1.265	9.556	23.7	0.0794
butylbenzene	1.775	10.370	25.7	0.0862

Water Solubility in Alkylbenzenes. The solubility of water in each of the alkylbenzene solvents was correlated with an equation of the form

$$\ln x_w = A + B \ln T_{r,w} \tag{7}$$

where x_w is the mole fraction of water and $T_{r,w}$ is the reduced temperature of water (system temperature divided by the critical temperature, $T_{c,w}$, of water, 647.3 K). The coefficients of eq 7 for each of the alkylbenzene + water systems appear in Table 6. The correlating equations are plotted as solid lines in Figures 6–9.

Water Solubility in Ethylbenzene. Four data sets have been published for water solubility in ethylbenzene. Most consist of measurements at two or three temperatures, except those by Filippov (*26*). Filippov's data (shown in Figure 6) exhibit a steep, linear temperature dependence as noted by Heidman (*18*). The linear temperature dependence is not consistent with water solubilities in the homologous series of alkylbenzenes. The data by Heidman (*18*) are slightly higher than our data and the measurements of Englin et al. (*27*), but probably within combined

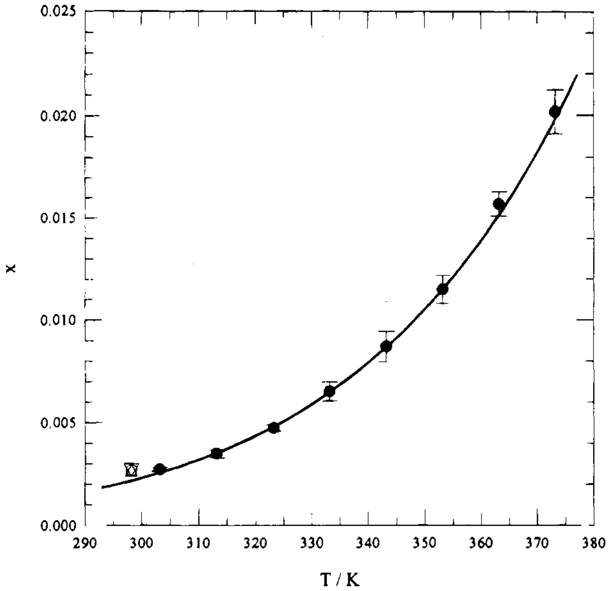

Figure 7. Solubility of water in *p*-xylene: (●) this work, (○) Kirchnerova and Cave (*28*), (△) Hoegfeldt and Bolander (*29*), (▽) Polak and Lu (*11*).

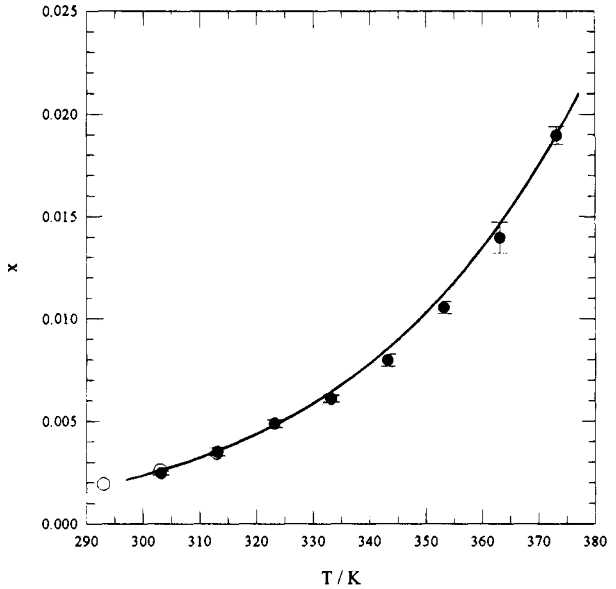

Figure 8. Solubility of water in 1,3,5-trimethylbenzene: (●) this work, (○) Englin et al. (*27*).

experimental errors. The new data are in good agreement with those of Polak and Lu (*11*) and Englin et al. (*27*).

Water Solubility in p-Xylene. There are only three measurements reported in the literature, all at 298.15 K. As shown in Figure 7, our extrapolated data appear slightly lower than these three measurements. The difference is probably within experimental error, and the temperature dependence is similar to that for ethylbenzene (Figure 6), as well as benzene (*1*) and toluene (*2*).

Water Solubility in 1,3,5-Trimethylbenzene. The solubility data for water in 1,3,5-trimethylbenzene summarized in Table 2 and plotted in Figure 8 are in excellent agreement with the three values reported by Englin et al. (*27*). The temperature dependence is similar to that of the other alkylbenzenes in this series of mixtures.

Water Solubility in Butylbenzene. Englin et al. reported values for the solubility of water in butylbenzene from 283 to 303 K, and the new measurements are almost 30% lower at 303 K. Hefter (*22*) notes that the data of Englin et al. (*27*) are generally reliable below 300 K, but tend to be too high at greater temperatures. No other data are available. Once again the temperature dependence shown in Figure 9 is reasonable. The consistency of the solubility measurements among the mixtures is discussed below.

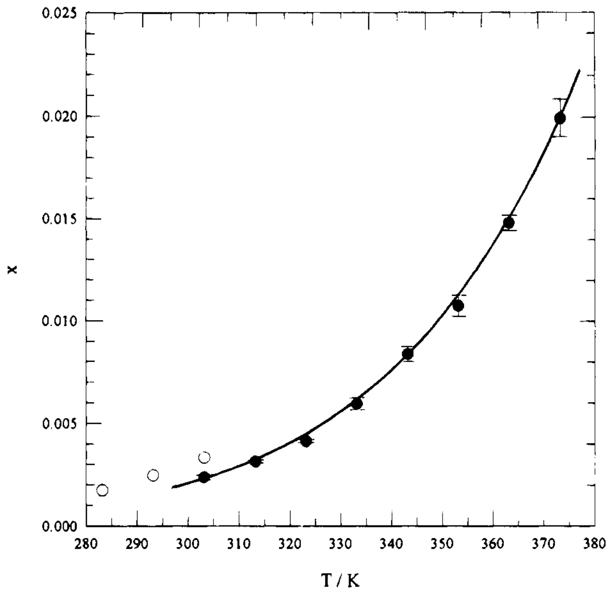

Figure 9. Solubility of water in butylbenzene: (●) this work, (○) Englin et al. (*27*).

The entropy of mixing for these dilute systems can be approximated as

$$\left(\frac{\partial \ln x_w}{\partial T}\right)_P = \frac{\Delta S_w}{RT} \tag{8}$$

or

$$\Delta S_w = RB \tag{9}$$

where ΔS_w is the difference between the partial molar entropy of component i in solution and molar entropy of pure i. Equation 7 is obtained by integrating eq 8, assuming the entropy of mixing for water dissolving in the hydrocarbon is constant. An analysis of variance to compare the slopes of the correlations for water solubility in each of the hydrocarbons indicates that, with respect to these data, the deviation removed by using individual least-squares lines for each hydrocarbon solvent over that removed using a pooled slope is only slightly significant (*30*). The approximately equal slopes for each system indicate that the enthalpy of solution is primarily dependent on the properties of water, with an average value of 24.2 kJ·mol^{-1} based on the pooled slope from Table 6. This result and other theoretical and experimental studies (*25*) support the argument that liquid water dissolving into a liquid hydrocarbon phase is essentially a process of breaking hydrogen bonds. The enthalpy of solution of water estimated from the solubility data as

$$\Delta H_w = RBT \tag{10}$$

compares well with typical hydrogen bonding energies of 21–29 kJ·mol^{-1} (*31*). Both the enthalpy and entropy of solution of water into these liquid hydrocarbons can be considered independent of the solvent in the temperature range of 303–373 K.

Summary

Mutual solubilities for binary aqueous mixtures of ethylbenzene, *p*-xylene, 1,3,5-trimethylbenzene, and butylbenzene were measured at temperatures from 303 to 373 K near the three phase locus. Together with previous measurements for benzene and toluene, these measurements provide liquid–liquid equilibrium data for a series of alkylbenzenes which cover a range of molecular size and structure. The new measurements compare well with the limited reliable data in the literature.

Enthalpies of mixing for the hydrocarbons dissolving in water estimated from solubility measurements compare favorably with published calorimetric measurements. For water dissolving in these liquid hydrocarbons, the enthalpy of mixing is essentially independent of the solvent and within the range of hydrogen bonding energies. These heat effects provide a general indication of consistency in the mutual solubility measurements for this series of alkylbenzene + water mixtures.

Acknowledgment

Comments and suggestions by Robert L. Robinson, Jr., are acknowledged.

Nomenclature

A, B, C	constants in solubility correlations
M	molecular weight
N	number of measurements
R	ideal gas constant (=8.3144 kJ·mol^{-1}·K)
$T_{c,w}$	critical temperature of water (=647.3 K)
$T_{r,i}$	reduced temperature of alkybenzene i ($=T/T_{c,i}$)
$T_{r,w}$	reduced temperature of water ($=T/T_{c,w}$)
x_i	mole fraction of alkylbenzene i
x_w	mole fraction of water
ΔH_i	enthalpy of mixing alkylbenzene i in water (kJ·mol^{-1})
ΔC_{Pi}	specific heat of mixing alkylbenzene i in water (kJ·mol^{-1}·K)
ΔS_w	entropy of mixing water in alkylbenzene (kJ·mol^{-1}·K)
σ	standard deviation

Literature Cited

(1) Chen, H.; Wagner, J. *J. Chem. Eng. Data* **1994**, *39*, 470–474.
(2) Chen, H.; Wagner, J. *J. Chem. Eng. Data* **1994**, *39*, 475–479.
(3) *Fed. Regist.* **1990**, *55* (45), 8292–8331.
(4) Code of Federal Regulations, Protection of Environment, Parts 100–149, revised as of July 1, 1990.
(5) Reid, R. C.; Prausnitz, J. M.; Poling, B. E. *The Properties of Gases & Liquids,* 4th ed.; McGraw-Hill: New York, 1987.
(6) Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.*, **1950**, *72*, 5034–5037.
(7) Klevens, H. B. *J. Phys. Chem.* **1950**, *54*, 283–298.
(8) Morrison, T. J.; Billett, F. *J. Chem. Soc.* **1952**, 3819–1822.
(9) McAuliffe, C. *Nature* **1963**, *200*, 1092–1093.
(10) McAuliffe, C. *J. Phys. Chem.* **1966**, *70*, 1267–1275.
(11) Polak, J.; Lu, B. C.-Y. *Can. J. Chem.* **1973,** *51*, 4018–4023.
(12) Sutton, C.; Calder J. A. *J. Chem. Eng. Data* **1975**, *20*, 320–322.
(13) Korenman, I. M.; Aref'eva, R. P. *Zh. Prikl. Khim.* **1978**, *51*, 957–958.
(14) Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Chem. Lett.* **1981**, 225–228.
(15) Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* **1982**, *55*, 1054–1062.
(16) Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. *Bull. Chem. Soc. Jpn.* **1984**, *57*, 1539–1544.
(17) Bohon, R. L., Claussen W. F. *J. Am. Chem. Soc.*, **1951**, *73*, 1571–1578.
(18) Heidman, J. L.; Tsonopoulos, C.; Brady, C. J.; Wilson, G. M. *AIChE J.* **1985**, *31*, 376.
(19) Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* **1949**, *71*, 3644–3647.
(20) Price, L. C. *Am. Assoc. Petrol. Geol. Bull.* **1976**, *60*, 213–244.
(21) Pryor, W. A.; Jentoft, R. E. *J. Chem. Eng. Data* **1961**, *6*, 36–37.
(22) Hefter, G. T. In *IUPAC Solubility Data Series;* Shaw, D. G., Ed.; Pergamon: Oxford, 1989; Vol. 37, pp 42–46.
(23) Gill, S. J., Nichols, N. F., Wadso. *J. Chem. Thermodyn.* **1976**, *8*, 445–452.
(24) Massaldi, H. A.; King, C. J. *J. Chem. Eng. Data* **1973**, *18*, 393–397.
(25) Franks, F. In *Water, a Comprehensive Treatise*; Franks, F., Ed.; Plenum: New York, 1979; Vol. 2.
(26) Filippov, T. S.; Furman, A. *Zh. Prikl. Khim.* **1952**, *25*, 895.
(27) Englin, B. A., Plate, A. F., Tugolukov, V. M., Pyranishnikova, M. A. *Khim. Tekhnol. Topl. Masel.* **1965**, *10*, 42.
(28) Kirchnerova, J.; Cave, G. C. B. *Can. J. Chem.* **1976**, *54*, 3909–3916.
(29) Hoegfeldt, E.; Bolander, B. *Ark. Kemi* **1964**, *21*, 161–186.
(30) Chen, H. Ph.D. Thesis, Oklahoma State University, May 1994.
(31) Tsonopoulos, C.; Wilson, G. M. *AIChE J.* **1983**, *29*, 990.

Received for review September 22, 1993. Revised April 28, 1994. Accepted May 12, 1994.[⊗] This work was supported in part by the Oklahoma Refiners Waste Control Council and the Oklahoma Center for the Advancement of Science and Technology.

[⊗] Abstract published in *Advance ACS Abstracts,* August 15, 1994.