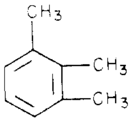
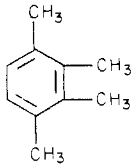
Encouraged by these results, we estimated the solubilities of iodine in 1,2,3-trimethylbenzene and 1,2,3,4-tetramethylbenzene.



$$S = S_T + 2[2I_{op} + I_m]/3 + 2I_{st}$$
$$= 0.0711 + 2[(2)(0.0135) + 0.0204]/3 + (2)(0.0030)$$
$$= 0.1087$$



$$S = S_T + 3[4I_{op} + 2I_m]/6 + 3I_{st}$$
$$= 0.0711 + 3[(4)(0.0135) + (2)(0.0204)]/6 + (3)(0.0030)$$
$$= 0.1275$$

To test the accuracy of these predicted values, we measured the solubility of iodine in these solvents at various temperatures. As the data in Table II (in parentheses) prove, the agreement is very good.

The application of the regular solution theory to solubility of iodine in mixed solvents is the subject of our next paper.

Acknowledgment

We thank Professor Paul Haberfield for his interest in this work.

Registry No. I_2, 7553-56-2; benzene, 71-43-2; toluene, 108-88-3; *o*-xylene, 95-47-6; *p*-xylene, 106-42-3; *m*-xylene, 108-38-3; 1,2,3-trimethylbenzene, 526-73-8; 1,2,4-trimethylbenzene, 95-63-6; 1,3,5-trimethylbenzene, 108-67-8; 1,2,3,4-tetramethylbenzene, 488-23-3; ethylbenzene, 100-41-4; *n*-propylbenzene, 103-65-1; cumene, 98-82-8; *n*-butylbenzene, 104-51-8; isobutylbenzene, 538-93-2; *tert*-butylbenzene, 98-06-6; chlorobenzene, 108-90-7; bromobenzene, 108-86-1; trifluoromethylbenzene, 98-08-8.

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Solubility of Iodine in Mixed Solvents

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The solubility of iodine in 10 two-component and 2 three-component solvent mixtures is measured at 30 °C. A method is suggested for predicting the solubilities in multicomponent solvents from known solubilities in single-component solvents. The agreement between the measured and predicted solubilities is very good.

Introduction

There have been several methods proposed for predicting solubilities in mixed solvents from known solubilities in single-component solvents (*1*–*12*). The methods based upon the solubility parameter theory were introduced by Hildebrand (*1*, *2*), the methods using the Margules equation by Prausnitz et al. (*3*), and the methods employing the concept of local volume fractions by Hildebrand et al. (*2*) and by Walkley et al. (*5*). Methods based on other concepts were employed by Bertrand (*8*, *11*), Nitta (*6*, *7*), and Kehiaian (*12*). The reliability of the individual methods and the accuracy of their prediction depend on the physical and chemical nature of the solute and solvent under investigation. Usually, the accuracy varies from good to satisfactory for systems in which the solute is a gas; it is, however, less satisfactory for systems in which the solute is a solid. The discrepancy is larger for systems with high solubilities and for solutions whose behavior is determined by specific interactions (hydrogen-bond and charge-transfer interactions).

In this study, we made some adjustments in the Hildebrand regular solution theory, so that it can cope better with solutions whose behavior is determined by specific interactions. The theory, in its modified version, is also able with better accuracy to predict the solubility of a solute in multicomponent solvents from known solubilities in single-component solvents. The reasons for employing iodine as a solute and the aromatic hydrocarbons as solvents have been given in our previous study (*13*).

Experimental Section

The purification of the employed chemicals as well as the method for measuring the solubility, its reproducibility, and accuracy were described previously (*13*). The accuracy of the measurement in multicomponent solvents is, however, not as good as in single-component solvents. The solvent components are usually of different volatilities—have different vapor pressures at the temperature of the experiment—and, consequently, exhibit different rates of evaporation. This leads to composition changes in the mixed solvent during the process of sampling. We estimated this composition change from Raoult's law and concluded that the error due to the different volatilities is about ±0.1%. This increases the overall error in the measurement to about ±0.5% (*13*).

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Table I. Solubility[a] of Iodine in Two-Component Solvent Mixtures at 30 °C

exptl		solubilities obtained from eq 3 with δ_m evaluated from		
x_1	S	eq 5	eq 6 and 7	eq 6 and 8
CCl_4 (1)-Cyclohexane (3)				
0.0000	0.01066			
0.2488	0.01152	0.01125	0.01126	0.01129
0.3484	0.01174	0.01143	0.01145	0.01144
0.5048	0.01221	0.01181	0.01187	0.01182
0.6496	0.01246	0.01217	0.01219	0.01218
0.9002	0.01295	0.01256	0.01285	0.01286
1.0000	0.01313			
Benzene (1)-CCl_4 (3)				
0.0000	0.01313			
0.0133[b]	0.01332			
0.1749[b]	0.01926	0.01718	0.01956	0.01819
0.2489	0.02110	0.0191	0.0227	0.0207
0.2907[b]	0.02322	0.02037	0.02344	0.02207
0.3399[b]	0.02431	0.02185	0.02630	0.02383
0.4925[b]	0.03011	0.02726	0.03287	0.02988
0.4987	0.0312	0.0277	0.0334	0.0304
0.5539[b]	0.03317	0.02981	0.03562	0.03279
0.6120[b]	0.03532	0.03237	0.03816	0.03519
0.6783[b]	0.03878	0.03555	0.04093	0.03832
0.7154[b]	0.04109	0.03757	0.04288	0.04025
0.7517	0.0424	0.0398	0.0447	0.0423
0.8064[b]	0.04467	0.04261	0.04689	0.04483
0.8874[b]	0.04957	0.04775	0.05063	0.04928
1.0000	0.0551			
Toluene (1)-CCl_4 (3)				
0.0000	0.01313			
0.2463	0.0245	0.0220	0.0291	0.0252
0.5094	0.0390	0.0320	0.0456	0.0405
0.7555	0.0538	0.0513	0.0591	0.0556
1.0000	0.0711			
Toluene (1)-Benzene (3)				
0.0000	0.0551			
0.2323	0.0585	0.0591	0.0592	0.0593
0.5854	0.0642	0.0646	0.0650	0.0649
0.7759	0.0670	0.0674	0.0678	0.0676
1.0000	0.0711			
p-Xylene (1)-Toluene (3)				
0.0000	0.0711			
0.2948	0.0749	0.0749	0.0754	0.0753
0.4891	0.0776	0.0776	0.0781	0.0779
0.7515	0.0816	0.0812	0.0815	0.0814
1.0000	0.0846			
p-Xylene (1)-Benzene (3)				
0.0000	0.0551			
0.3496	0.0674	0.0669	0.0688	0.0682
0.4957	0.0715	0.0712	0.0732	0.0726
0.6379	0.0761	0.0761	0.0778	0.0772
1.0000	0.0846			
p-Xylene (1)-Ethylbenzene (3)				
0.0000	0.0655			
0.2515	0.0696	0.0698	0.0704	0.0702
0.5005	0.0757	0.0746	0.0754	0.0751
0.6844	0.0798	0.0782	0.0789	0.0786
1.0000	0.0846			
p-Xylene (1)-Cumene (3)				
0.0000	0.0628			
0.2184	0.0644	0.0665	0.0669	0.0667
0.3246	0.0663	0.0684	0.0692	0.0687
0.5644	0.0731	0.0735	0.0745	0.0742
0.7694	0.0779	0.0783	0.0796	0.0788
1.0000	0.0846			
0.0000	0.0628			
0.2291	0.0664	0.0676	0.0687	0.0683
0.5419	0.0751	0.0759	0.0775	0.0769
0.7590	0.822	0.0824	0.0836	0.0832
1.0000	0.0905			
m-Xylene (1)-Toluene (3)				
0.0000	0.0711			
0.2119	0.0751	0.0751	0.0756	0.0755
0.4175	0.0793	0.0793	0.0799	0.0799
0.6921	0.0844	0.0846	0.0850	0.0853
1.0000	0.0905			
n-Hexadecane (1)-*n*-Heptane (3)[b]				
0.0000	0.006912			
0.0815	0.00762	0.00779	0.00789	0.00776
0.1429	0.00809	0.00823	0.00850	0.00831
0.1668	0.00816	0.00853	0.00884	0.00862
0.3267	0.00958	0.00993	0.01034	0.01006
0.6164	0.01174	0.01205	0.01238	0.01216
1.0000	0.01428			
n-Hexadecane (1)-isooctane (3)[c]				
0.0000	0.005923			
0.1015	0.00681	0.00690	0.00716	0.00697
0.1563	0.00735	0.00743	0.00779	0.00753
0.2169	0.00778	0.00800	0.00849	0.00826
0.3554	0.00896	0.00926	0.00980	0.00942
0.5800	0.01086	0.01116	0.1165	0.01131
1.0000	0.01428			

[a] The solubility is expressed in mole fraction. [b] Data taken from the literature (*14*). [c] Data taken from the literature (*9*).

Results and Discussion

The experimentally obtained solubility data of iodine in 10 two-component solvents and 2 three-component solvents at 30°C are listed in the second column of Table I and the third column of Table II. The last two systems in Table I are taken from the literature (*9*).

In our first attempt to correlate the solubility of iodine, S, in mixed solvents with the solubilities of iodine in single-component solvents, S_1 and S_3, respectively, we employed the two-parameter Margules equation (*4*)

$$\log S = x_1 \log S_1 + x_3 \log S_3 + x_1x_3[A_{13} + B_{13}(x_1 - x_3)] \quad (1)$$

where x_1 and x_3 designate the mole fractions of the two-solvent components ($x_1 + x_3 = 1$). In this work, iodine will always be designated as component 2. The constants, A_{13} and B_{13}, for the 10 two-component solvent systems, evaluated from the solubilities listed in Table I with the help of eq 1, are listed in Table III. The two-parameter Margules equation correlates the solubility with the solvent composition, for all 10 systems, very well. Some systems exhibit relatively low B_{13} values. Obviously, such systems can be treated well by a one-parameter Margules expression. The iodine-benzene-toluene system is the only system that obeys the ideal solubility law ($A_{13} \approx B_{13} \approx 0$). This might indicate that the deviations of a system from the ideal solubility law are more influenced by the solvent-solvent interactions than by the solvent-solute interactions. Preliminary investigations show that there might be some kind of a relationship between the constants A_{13} and B_{13} evaluated from solubility data and similar constants obtained from vapor-liquid equilibrium measurements.

For a three-component solvent system, we extended eq 1 by a ternary term. Thus

$$\log S = x_1 \log S_1 + x_3 \log S_3 + x_4 \log S_4 + x_1x_3[A_{13} + B_{13}(x_1 - x_3)] + x_1x_4[A_{14} + B_{14}(x_1 - x_4)] + x_3x_4[A_{34} + B_{34}(x_3 - x_4)] + A_{134}x_1x_3x_4 \quad (2)$$

Table II. Solubility of Iodine in Three-Component Solvent Mixtures at 30 °C

exptl			solubilities obtained from eq 3 with δ_m evaluated from		
x_1	x_3	S	eq 5	eq 6 and 7	eq 6 and 8
Toluene (1)–Benzene (3)–CCl_4 (4)					
1.0000	0.0000	0.0711			
0.0000	1.0000	0.0551			
0.0000	0.000	0.01313			
0.1228	0.7817	0.0521	0.0507	0.0536	0.0522
0.7894	0.1147	0.0624	0.0608	0.0658	0.0632
0.4981	0.2974	0.0534	0.0499	0.0559	0.0535
0.2908	0.2992	0.0409	0.0359	0.0443	0.0402
0.2029	0.2007	0.0303	0.0267	0.0344	0.0303
0.0907	0.1067	0.0212	0.0188	0.0231	0.0218
p-Xylene (3)–Toluene (3)–Benzene (4)					
1.0000	0.0000	0.0864			
0.0000	1.0000	0.0711			
0.0000	0.0000	0.0551			
0.1528	0.1477	0.0621	0.0627	0.0643	0.0636
0.2524	0.2509	0.0678	0.0675	0.0691	0.0685
0.3047	0.2948	0.0714	0.0690	0.0705	0.0700
0.4146	0.2915	0.0727	0.0728	0.0741	0.0737
0.5011	0.2465	0.0751	0.0744	0.0758	0.0753
0.7038	0.1486	0.0797	0.0788	0.0798	0.0795

Table III. *A* and *B* Constants in Eq 1

solvent	A_{13}	B_{13}
CCl_4 (1)–cyclohexane (3)	0.047 45	−0.017 61
benzene (1)–CCl_4 (3)	0.250 00	−0.050 71
toluene (1)–CCl_4 (3)	0.400 00	−0.162 89
toluene (1)–benzene (3)	0.005 09	−0.003 99
toluene (1)–*p*-xylene (3)	0.006 79	−0.018 23
benzene (1)–*p*-xylene (3)	0.039 64	0.005 39
p-xylene (1)–ethylbenzene (3)	0.014 14	−0.001 13
p-xylene (1)–cumene (3)	−0.057 87	0.067 50
m-xylene (1)–cumene (3)	0.028 93	0.003 77
toluene (1)–*m*-xylene (3)	0.010 47	0.000 53

where the A_{13}, B_{13}, A_{14}, B_{14}, A_{34}, and B_{34} constants characterize the three involved two-component solvent systems and the A_{134} constant is characteristic of the three-component solvent system itself. With the constants listed in Table III and with the A_{134} values of 0.4106 for the toluene (1)–benzene (3)–CCl_4 (4) system and 0.1262 for the toluene (1)–benzene (3)–*p*-xylene (4) system, eq 2 predicts the solubility of iodine in the two three-component solvent systems with high accuracy. The ternary term, however, contributes very little to the predicted solubilities for both three-component solvent systems and can be ignored. The ideal solubility law is not obeyed by either of the two three-component solvents systems. The toluene–benzene–*p*-xylene solvent system deviates, however, less from the ideal solubility law than the system containing CCl_4. This might again indicate that it is the solvent–solvent interaction rather than the solvent–solute interaction that determines whether the ideal solubility law is obeyed by a system or not.

In our second attempt, we tried to modify the regular solution theory so that it can deal more successfully with the solubility of iodine in electron-donating mixed solvents. We begin our treatment with the regular solution theory expression

$$\ln a_2 = \ln S + (\Phi_m^2 V_2/RT)(\delta_2 - \delta_m)^2 \qquad (3)$$

where a_2 (=0.258) is the activity of iodine in a saturated solution, V_2 (=59 cm^3/mol) is the molar volume of supercooled liquid iodine, and δ_2 (=$(cal/cm^3)^{1/2}$) is the solubility parameter of iodine. Its value is not affected by the composition of the solvent. All these values apply at 25 °C; however, we combined them with our solubility data measured at 30 °C. δ_m is the solubility parameter of the mixed solvent. Φ_m is the volume fraction of the solvent and is equal to $1 - \Phi_2$, where Φ_2, the volume fraction of iodine, was determined from the masses and densities of the individual solvent components and from the results of titration.

The success of eq 3 in predicting solubilities depends on the method of evaluating δ_m and Φ_m, respectively. It is well established by now that, for the great majority of systems, the average value of δ_m taken over the δ_i values of the individual solvent components

$$\delta_m = \sum_i \Phi_i \delta_i \qquad (4)$$

does not provide satisfactory results. The prediction of the solubility from eq 3 improves, however, if the δ_i's for the individual solvent components, obtained from enthalpy of vaporization and molar volume data ($\delta_i = ([\Delta H_{vap} - RT]/V)^{1/2}$], are replaced by the so-called effective solubility parameter values, δ_i^*, evaluated from direct solubility data (*13*)

$$\delta_m = \sum_i \Phi_i \delta_i^* \qquad (5)$$

Here again, the summation is taken over the δ_i^* values of the individual solvent components.

With the exception of the solvent components in the last two systems in Table I, values of δ_i ad δ_i^* are compared for all solvent components in the previous paper (*13*). For most solvents, there is no agreement: $\delta_i \neq \delta_i^*$. The few systems for which agreement is found obey the original regular solution theory reasonably well. For example, the iodine–CCl_4, iodine–cyclohexane, and iodine–chlorobenzene systems can be considered as regular solutions. Because of the very low solubilities (*9*), the iodine–*n*-hexadecane, iodine–*n*-heptane, and iodine–isooctane systems obey the regular solution theory in spite of $\delta_i \neq \delta_i^*$. For those systems for which values of δ_i and δ_i^* differ substantially, an improvement is achieved by using δ_i^* values. The solubilities obtained from eq 3 in connection with eq 5 are given in Table I for the two-component solvent systems and in Table II for the three-component solvent systems. The agreement is excellent for systems with low solubilities and for systems containing solvent components of practically equal abilities to complex.

The agreement is, however, unacceptable for systems containing solvent components of very different abilities to complex. For example, in the iodine–benzene–CCl_4 and iodine–toluene–CCl_4 systems, benzene and toluene complex well, while CCl_4 does not complex with iodine at all. Because of the preferential complexation shown by one of the solvent components, the immediate solute environment is different from the bulk solvent mixture composition. Thus, it seems to be desirable to replace the volume fractions in eq 5 by local volume fractions, Φ_i^*.

$$\delta_m = \sum_i \Phi_i^* \delta_i^* \qquad (6)$$

Purkayastha and Walkley (*5*) used Hildebrand's approach (*2*) based on the quasi-lattice theory to find an expression for the local volume fraction

$$\Phi_1^*/\Phi_3^* = K'\Phi_1/\Phi_3 \qquad (7)$$

where

$$K' \equiv (\delta_2 - \delta_3^*)^2/(\delta_2 - \delta_1^*)^2$$

$$\Phi_1^* + \Phi_3^* = 1$$

This modification of the regular solution theory leads perhaps to some improvement; for some systems, however, it overestimates the solubilities in solvents containing components largely differing in their abilities to complex (see Tables I and II).

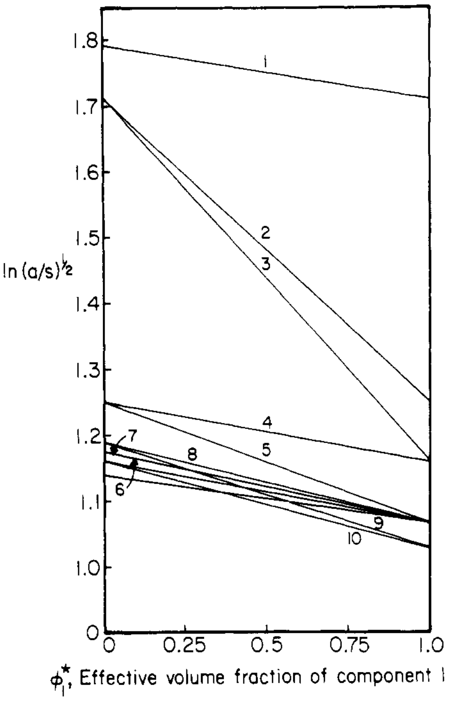

Figure 1. Test of accuracy of the new proposed method. ln $(a/S)^{1/2}$ as a function of effective volume fraction of component *l*, Φ^*: (1) CCl_4 (1)–cyclohexane (3); (2) benzene (1)–CCl_4 (3); (3) toluene (1)–CCl_4 (3); (4) toluene (1)–benzene (3); (5) *p*-xylene (1)–benzene (3); (6) *p*-xylene (1)–toluene (3); (7) *p*-xylene (1)–ethylbenzene (3); (8) *p*-xylene (1)–cumene (3); (9) *m*-xylene (1)–toluene (3); (10) *m*-xylene (1)–cumene (3).

To further improve the theory, we employed the pseudo-two-fluid theory for the evaluation of the local volume fraction. This approach resulted in

$$\Phi_1^*/\Phi_3^* = K'K''\Phi_1/\Phi_3 \qquad (8)$$

where K' is the Purkayastha and Walkley constant and $K'' = \delta_3^{*2}/\delta_1^{*2}$. Again, $\Phi_1^* + \Phi_3^* = 1$. With such local volume fractions, we were able to obtain good predictions even in such solvents as benzene–CCl_4 and toluene–CCl_4.

Using eq 8 to define Φ_1^* and using eq 6 to evaluate δ_m, one can easily show that eq 3 can be reformulated to require a linear relationship to exist between $[\ln (a_2/S)]^{1/2}$ and Φ_1^*. In Figure 1, such a linearity is seen to exist for each of the 10 systems considered.

The method can be easily extended to any multicomponent solvent system. For each pair of the solvent components in the mixed solvent, we write an equation similar to eq 8

$$\Phi_i^*/\Phi_j^* = K'_{ij}K''_{ij}\Phi_i/\Phi_j$$

The set of equations in combination with the requirement $\sum_k \Phi_k^* = 1$ (the summation is taken only over the solvent compounds) enable us to evaluate the local volume fraction for each solvent component. These values define then δ_m (see eq 6), which in turn, when substituted into eq 3, yields the solubility of the solute in a solvent of any composition.

The method was employed for two three-component solvent systems (Table II). The three procedures used in the evaluation, the one based on eq 5 and the other two on eq 6 in combination with eq 7 and 8, respectively, yield equally good results for the *p*-xylene–benzene–toluene mixed solvent system. The three procedures, however, provide different results for the toluene–benzene–CCl_4 system. Only the local volume fractions defined by eq 8 give results in agreement with experiment. The different behavior of the two three-component solvent systems is due to the fact that the first system contains solvent components of practically equal abilities to complex while, in the other system, CCl_4 does not complex at all.

The modified procedure has also been tested for naphthalene in various solvents. The results are equally good if not better than for iodine.

Registry No. I_2, 7553-56-2; CCl_4, 56-23-5; cyclohexane, 110-82-7; benzene, 71-43-2; toluene, 108-88-3; *p*-xylene, 106-42-3; ethylbenzene, 100-41-4; cumene, 98-82-8; *m*-xylene, 108-38-3; *n*-hexadecane, 544-76-3; *n*-heptane, 142-82-5; isooctane, 26635-64-3.

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Solubility of Trioxane in Some Common Solvents

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Solubility of trioxane in 11 solvents was measured at different temperatures; dichloromethane was found to be the best solvent. These solubility curves were compared with the ideal solubility curve deduced purely from thermodynamical calculations. The deviation between these two may be due to solute–solvent interaction. The heats of solution were calculated and reported.

Extraction of trioxane by a solvent, immiscible in water, is an important step for the production of trioxane. Information available on the solubility of trioxane in different solvents is scanty. Walker (*1*) reported the solubility in solvents like acetic acid, benzene, toluene, and trichloroethylene. Lyobomilow et al. (*2*) determined the solubility in methylene chloride, *n*-heptane, benzene, 31.9% formaldehyde solution, and water at various temperatures. But the solubility data of trioxane in

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