Mutual Solubilities: Water–Ketones, Water–Ethers, and Water–Gasoline–Alcohols

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Mutual binary solubilites have been measured for partially miscible water–organic pairs at temperatures of 0–90 °C. Experimental data are given for 37 ketones, 16 ethers, 14 esters, 10 chloroparaffins, and 4 nitroparaffins. Data are also given for 18 ternary systems, including several gasoline systems of environmental interest. In essentially all cases, the solubility of water in the organic layer increases with temperature. The solubility of the organic species in the water layer usually decreases with temperature, often going through a minimum at about 60 °C and then increasing at higher temperatures. Ternary systems involving water–gasoline–alcohols show that methanol distributes almost entirely in the aqueous layer, but the distribution shifts more to the organic layer as the molecular weight of the alcohol increases. Lower alcohols increase the solubility of aromatics in the aqueous layer; for higher alcohols such as pentanol and hexanol, aromatic solubility in the aqueous layer first increases with alcohol content, goes through a maximum, and then decreases.

Early solubility literature is summarized in books by Sorensen and Arlt (*1*) and the *Solubility Data Series* of the International Union of Pure and Applied Chemistry (*2*). Two previous papers (*3*) described our research on the solubility of water in organics and organics in water and gave data for 119 water–alcohol and water–ester pairs. The present paper gives experimental data for an additional 83 water–organic pairs in addition to 18 ternary systems.

As before, the method of standard additions was used. Water and organic were brought into equilibrium at a given temperature in a thermostat, and samples of each layer were removed with a syringe for analysis. To determine the amount of water in the organic layer sample, a weighed quantity of ethanol (sometimes methanol or acetonitrile) was added and the ratio of the water to ethanol peak was measured with a Gow-Mac Series 550 thermal conductivity GC, Chromosorb 101 packing, and a Hewlett-Packard 3390A recorder–integrator. The percentage of water in the sample could then be immediately calculated from the weight of ethanol added and the GC scale factors for water and ethanol, as determined from GC analyses of known water and ethanol solutions. This calibration was done for each system using at least three standards covering the composition range of the unknown solutions.

The amount of an organic in the water layer was obtained in a similar way by using a higher boiling material as standard. For example, cyclopentanone was determined using 2-pentanone as standard. As in the case of the organic layer, the calibration was done for each system using at least three standard solutions.

To check the accuracy of the experiments, data were compared with the values recommended by Sorensen and Arlt (*1*). Figures 1 and 2 give values for cyclohexanone and methyl ethyl ketone. It can be seen that the agreement is very good.

All experimental measurements were done at atmospheric pressure. Most organics came from Aldrich Chemical in purities of normally 98% or better. A few came from other laboratory

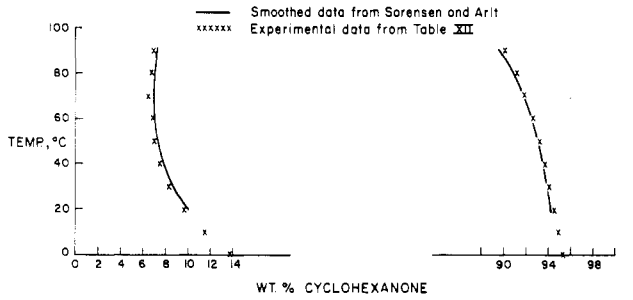

Figure 1. Mutual solubility of water and cyclohexanone.

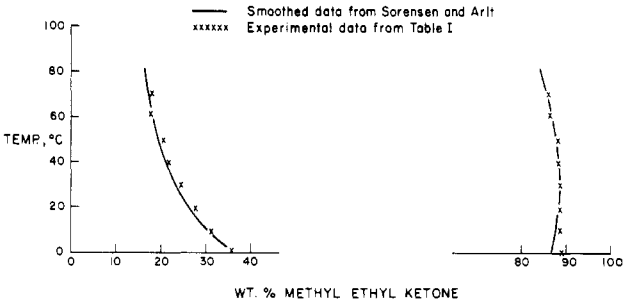

Figure 2. Mutual solubility of water and methyl ethyl ketone.

supply houses. In some instances samples phase separated and had to be brought into solution by heating or by the addition of a solvent such as ethanol or acetonitrile. For each system studied, 3–5 measurements of standard solutions were made to determine GC scale factors. From these, composition standard deviations are calculated and listed in the tables of data. The temperature of the thermostat was controlled by a Braun Thermomix-1441 having a stability of ±0.01 °C. Absolute temperature was measured by a calibrated thermometer accurate to 0.1 °C.

When this work was started several years ago, the primary interest was in obtaining data for use in the design of solvent extraction columns and decanters in distillation systems. Today the question of liquid–liquid solubility has become important in cleaning up hazardous wastes, since it is usually the easiest way to determine activity coefficients needed for the design of organic strippers. Suppose we have two partially miscible liquids in equilibrium with each other and with a vapor phase at some temperature. For each component we can write

$$y_1 P = \gamma_1^a x_1^a P_1^{sat.} = \gamma_1^b x_1^b P_1^{sat.} \quad (1)$$

where x_1 and y_1 are the mole fractions of one component in the liquid and vapor phases, P is the total pressure, $P_1^{sat.}$ is the saturation vapor pressure of the first component, and a and b refer to the two liquid phases. Thus

$$\gamma_1^a/\gamma_1^b = x_1^b/x_1^a \quad (2)$$

But if the two liquids have very low mutual solubility, $x_1^b \approx 1.0$, $\gamma_1^b \approx 1.0$, and $\gamma_1^a \approx 1/x_1^a$.

It is also, of course, possible to fit an activity parameter equation to the experimental values of solubility and determine

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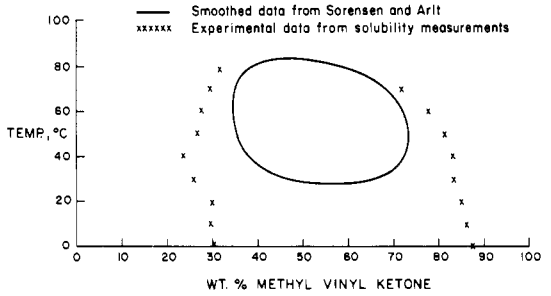

Figure 3. Mutual solubility of water and methyl vinyl ketone.

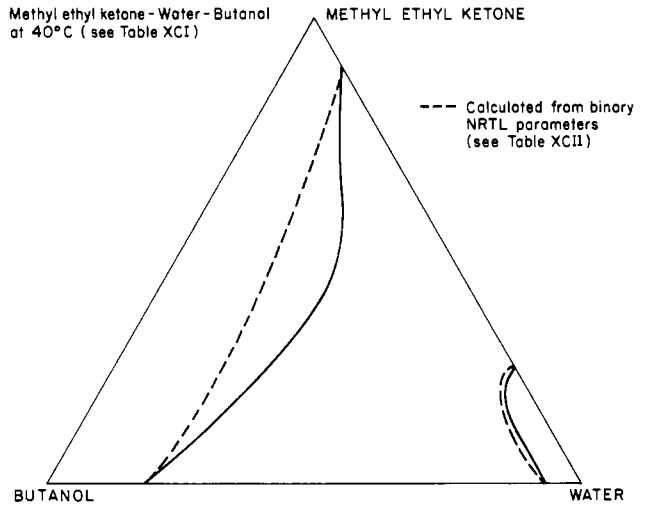

Figure 4. Mutual solubility of water, butanol, and methyl ethyl ketone at 40 °C.

activity coefficients directly from this. For details, see Sorensen and Arlt (*1*).

When working with systems of very low solubility, it is essential to remember that each component is exhibiting essentially its pure-component vapor pressure at the temperature in question. Under these conditions, the vapor lost in the head space of the sample bottle may represent an appreciable fraction of the dissolved material, and there also may be losses in transferring from sample bottle to syringe to detector. This can be minimized by completely filling the sample bottles and by taking care not to open them after the samples are taken. In several cases, such as the chloroform–water system, withdrawn samples were injected directly into cold ethanol to reduce the back-pressure of the dissolved component. The ethanol had no effect on the subsequent GC analysis, since it eluted well before the chloroform peak appeared.

As in the case of data previously reported for alcohols and esters, almost all systems showed an increasing solubility of water in organic with temperature. In most cases, the solubility of organic in water decreased from zero to 90 °C, although sometimes the solubility went through a minimum at 30–60 °C and then started to increase. Cyclic and polyfunctional compounds showed higher solubilities than the corresponding straight chains. In general, ketones and ethers showed higher solubility in water than alcohols with the same number of carbon atoms. Substitution of hydrogen by chloride reduced solubility, and the chlorocarbons all showed very low solubilities in water.

To illustrate some of the uncertainties which frequently occur in solubility work, Figure 3 gives experimental data for the system water–methyl vinyl ketone together with smoothed data from Sorensen and Arlt. There is no agreement at all in this case. It is well-known that impurities can strongly affect solubility, and there is the obvious question as to the purity of the materials used. Methyl vinyl ketone can polymerize to form a less soluble polymer and can react with water to form a very soluble hydroxy ketone. Thus solubility data may not mean much in the case of reactive materials such as this.

Table I. Mutual Solubility *S* of Water (B) and Methyl Ethyl Ketone[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	35.7	10.9
	9.6	31.0	11.1
	19.3	27.6	11.2
	29.7	24.5	11.3
	39.6	22.0	11.7
	49.7	20.6	11.9
	60.6	18.0	13.4
	70.2	18.2	13.7
std dev		0.2	0.15

[a] Purity: 99+ mass %.

Table II. Mutual Solubility *S* of Water (B) and 2-Pentanone[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	8.7	2.57
	9.7	6.9	2.92
	19.7	5.9	3.19
	31.0	5.0	3.48
	39.6	4.6	4.13
	49.8	4.2	4.17
	60.1	4.0	5.13
	70.2	4.0	4.86
	80.0	3.8	4.72
	90.5	3.4	5.28
std dev		0.1	0.05

[a] Purity: 97 mass %.

Table III. Mutual Solubility *S* of Water (B) and 3-Pentanone[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	7.68	1.57
	9.7	6.25	1.77
	19.3	5.30	2.00
	30.6	4.24	2.51
	40.3	3.86	2.49
	50.0	3.62	2.81
	60.1	3.43	2.98
	70.1	3.30	2.99
	80.2	3.16	3.69
	90.5		4.10
std dev		0.05	0.05

[a] Purity: 99 mass %.

Ternary Solutions

Most practical cases of solubility encountered in industry involve solutions of two or more solvents in water. To illustrate ternary solubilities, we give data for 18 different systems, including several of environmental interest.

When more than two components are present in a multicomponent mixture, it is standard practice to calculate the composition using binary solubility parameters. Figure 4 and Tables XCI and XCII give data for the ternary system water–butanol–methyl ethyl ketone, showing both experimental values and values calculated by Dr. Jean Leinroth from binary NRTL parameters. The conclusions are extremely interesting. At the low-solubility region of the diagram, the calculated values agree very closely with experimental values. However at the high solubility region of the diagram, the experimental values for solubility are appreciably higher than calculated values, showing

Table IV. Mutual Solubility S of Water (B) and 2,4-Dimethyl-3-pentanone[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.77	0.56
	9.3	0.56	0.60
	20.0	0.52	0.75
	29.7	0.41	0.88
	39.6	0.36	0.95
	50.5	0.35	1.09
	60.6	0.33	1.17
	70.2	0.32	1.37
	80.2	0.32	1.49
	90.3	0.30	1.68
std dev		0.01	0.02

[a] Purity: 98 mass %.

Table V. Mutual Solubility S of Water (B) and Cyclohexyl Butyrate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.10	
	9.8	0.18	0.39
	19.7	0.11	0.45
	29.8	0.19	0.51
	39.8	0.23	0.56
	50.1	0.14	0.63
	60.2	0.11	0.72
	70.4	0.13	0.75
	80.3	0.08	0.84
	90.5	0.09	0.90
std dev		0.01	0.01

[a] Purity: 98 mass %.

Table VI. Mutual Solubility S of Water (B) and Hexyl Butyrate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0		0.22
	11.9	0.011	0.29
	20.0		0.30
	29.0	0.021	0.37
	40.0	0.045	0.38
	50.4	0.042	0.37
	60.1	0.032	0.41
	70.3	0.047	0.52
	80.0		0.48
	90.2		0.54
std dev		0.005	0.01

[a] Purity: 98 mass %.

Table VII. Mutual Solubility S of Water (B) and Heptyl Butyrate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0		0.21
	10.3	0.026	0.32
	19.8	0.028	0.32
	29.8	0.036	0.31
	39.7	0.025	0.36
	49.9	0.021	0.39
	60.2	0.028	0.42
	70.3	0.022	0.46
	80.1	0.020	0.50
	90.5	0.013	0.50
std dev		0.005	0.01

[a] Purity: 99 mass %.

Table VIII. Mutual Solubility S of Water (B) and Benzyl Formate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	1.22	0.71
	9.8	1.19	0.96
	19.6	1.07	1.04
	29.8	1.09	1.26
	39.7	0.97	1.33
	49.7	1.05	1.36
	60.0	1.10	1.45
	70.3	1.24	2.12
	80.1	1.43	3.04
	90.5	2.79	3.14
std dev		0.05	0.05

[a] Purity: 98 mass %.

Table IX. Mutual Solubility S of Water (B) and Nonyl Formate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.023	0.30
	9.5	0.012	0.30
	19.8		0.31
	30.7	0.006	0.35
	40.1	0.007	0.37
	49.8		0.44
	60.1	0.029	0.39
	70.2	0.027	0.51
	80.1	0.031	0.54
	90.3	0.039	0.57
std dev		0.003	0.02

[a] Purity: 98 mass %.

Table X. Mutual Solubility S of Water (B) and 2-Methyltetrahydrofuran[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	21.0	4.0
	9.5	17.8	4.1
	19.3	14.4	4.1
	29.5	11.4	4.3
	39.6	9.2	4.5
	50.1	7.8	4.5
	60.7	6.6	4.5
	70.6	6.0	5.0
std dev		0.2	0.2

[a] Purity: 99 mass %.

Table XI. Mutual Solubility S of Water (B) and Cyclopentanone[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	37.7	13.0
	10.0	34.4	13.8
	20.1	31.0	14.4
	30.0	27.9	15.0
	40.2	25.7	15.7
	50.0	24.4	16.9
	60.6	23.6	18.3
	70.5	23.7	20.3
	80.0	24.8	22.4
	90.7	26.1	26.5
std dev		0.2	0.1

[a] Purity: 99+ mass %.

Table XII. Mutual Solubility S of Water (B) and Cyclohexanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	13.7	4.69
9.8	11.5	5.05
19.5	9.7	5.35
29.8	8.2	5.93
40.1	7.5	6.28
50.2	7.0	6.81
60.5	6.7	7.34
71.1	6.5	8.15
80.2	6.8	8.84
90.7	6.9	9.82
std dev	0.1	0.05

[a] Purity: 99.8 mass %.

Table XIII. Mutual Solubility S of Water (B) and 3-Methyl-2-butanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	10.0	2.7
9.5	8.0	2.9
18.3	6.7	3.3
30.8	5.8	3.6
39.6	5.0	4.0
50.0	4.8	4.4
60.8	4.4	4.3
69.8	4.2	5.0
80.0	3.9	5.0
89.0	3.6	5.3
std dev	0.05	0.2

[a] Purity: 99 mass %.

Table XIV. Mutual Solubility S of Water (B) and 3,3-Dimethyl-2-butanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	2.97	1.08
9.5	2.39	1.18
19.2	1.97	1.36
31.0	1.69	1.52
39.5	1.56	1.70
50.2	1.49	1.81
59.8	1.38	1.84
70.4	1.38	1.98
80.1	1.32	1.87
90.2	1.14	2.08
std dev	0.03	0.06

[a] Purity: 97 mass %.

Table XV. Mutual Solubility S of Water (B) and 4-Methyl-2-pentanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	2.92	1.7
9.5	2.21	1.9
19.4	1.92	2.6
30.8	1.66	2.5
39.6	1.47	2.5
50.1	1.38	2.9
60.4	1.29	2.9
70.2	1.24	3.3
80.1	1.18	3.3
90.4	1.22	3.8
std dev	0.05	0.2

[a] Purity: 99.5 mass %.

Table XVI. Mutual Solubility S of Water (B) and 5-Methyl-2-hexanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.800	0.98
9.0	0.655	1.05
19.1	0.537	1.23
29.7	0.452	1.54
39.5	0.427	1.41
49.8	0.404	1.59
59.5	0.406	1.64
70.0	0.410	1.71
79.9	0.443	1.74
89.7	0.417	2.17
std dev	0.005	0.03

[a] Purity: 99 mass %.

Table XVII. Mutual Solubility S of Water (B) and 2-Heptanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.649	0.952
9.7	0.535	1.060
19.8	0.436	1.237
30.7	0.358	1.400
39.7	0.343	1.477
49.8	0.336	1.539
60.2	0.333	1.691
70.1	0.314	1.740
80.2	0.348	1.871
90.5	0.353	1.990
std dev	0.005	0.005

[a] Purity: 98 mass %.

Table XVIII. Mutual Solubility S of Water (B) and 3-Heptanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.717	0.561
9.3	0.586	0.634
20.5	0.479	0.778
30.7	0.431	0.897
39.6	0.385	0.949
50.0	0.333	1.058
59.8	0.309	1.182
70.2	0.366	1.237
79.9	0.310	1.322
90.1	0.309	1.383
std dev	0.005	0.005

[a] Purity: 98 mass %.

Table XIX. Mutual Solubility S of Water (B) and 4-Heptanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.707	0.52
9.6	0.537	0.62
19.5	0.457	0.69
29.7	0.448	0.81
39.7	0.347	0.86
50.0	0.379	0.90
60.6	0.320	1.12
70.3	0.302	1.23
80.9	0.319	1.20
90.2	0.316	1.17
std dev	0.005	0.02

[a] Purity: 98 mass %.

Table XX. Mutual Solubility S of Water (B) and 2,4-Pentanedione[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	14.1	1.7
9.6	14.9	2.1
19.8	16.1	2.8
29.8	17.6	3.5
39.7	18.9	4.4
50.1	21.0	5.8
60.6	24.4	7.8
70.5	27.0	10.0
80.3	32.2	13.5
90.5	40.3	19.9
std dev	0.8	0.2

[a] Purity: 99+ mass %.

Table XXI. Mutual Solubility S of Water (B) and Octyl Acetate[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.021	0.37
9.5		0.42
19.2	0.020	0.44
29.7	0.018	0.51
40.0	0.018	0.54
50.5	0.016	0.57
61.0		0.59
71.2	0.017	0.64
80.6	0.014	0.71
92.1	0.012	0.71
std dev	0.001	0.01

[a] Purity: 99 mass %.

Table XXII. Mutual Solubility S of Water (B) and Diethyl Malonate[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	3.09	1.09
9.1	2.80	1.28
20.0	2.26	1.60
31.0	2.10	1.92
39.6	2.09	2.16
49.9	2.05	2.62
60.2	2.12	2.91
70.5	2.18	3.63
81.0	2.33	4.02
90.6	2.47	4.30
std dev	0.10	0.03

[A] Purity: 99 mass %.

Table XXIII. Mutual Solubility S of Water (B) and Dichloromethane[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	2.03	0.082
9.2	1.92	0.106
17.3	1.80	0.135
26.8	1.72	0.186
35.7	1.77	0.218
std dev	0.03	0.003

[a] Purity: 99.9 mass %.

Table XXIV. Mutual Solubility S of Water (B) and 2-Chloroethyl Ether[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	1.14	0.57
9.6	1.09	0.54
20.0	1.04	0.68
31.0	1.03	0.78
40.0	1.05	0.86
50.1	1.11	1.02
60.7	1.11	1.13
70.6	1.28	1.24
80.9	1.36	1.55
91.7	1.51	1.75
std dev	0.03	0.03

[a] Purity: 99 mass %.

Table XXV. Mutual Solubility S of Water (B) and Dichloroisopropyl Ether[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0		0.44
9.5	0.409	0.43
19.1	0.245	0.37
31.0	0.237	0.38
40.3	0.218	
51.1	0.182	0.52
60.6	0.209	0.55
80.7	0.265	0.71
91.4	0.241	0.87
std dev	0.002	0.02

[a] Purity: 95 mass %.

Table XXVI. Mutual Solubility S of Water (B) and 2-Chloroethyl Methyl Ether[a] (A)

	S/(mass %)	
t/°C	A in B[b]	B in A[b]
0	9.71	1.13
9.8	8.43	1.04
20.2	7.79	1.30
29.7	7.46	1.40
39.7	6.89	1.60
50.0	6.26	
70.2	6.31	2.42
80.8	6.18	2.78
88.4		2.58
std dev	0.05	0.03

[a] Purity: 98 mass %. [b] Above 60 °C, organic on top; below 60 °C, organic on bottom.

Table XXVII. Mutual Solubility S of Water (B) and 1,2-Dichloroethane[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.82	0.106
9.3	0.77	0.133
19.7	0.72	0.176
29.7	0.81	0.230
39.4	0.98	0.276
50.3	1.06	0.349
61.0	1.08	0.412
70.6	1.13	
80.7	1.06	0.492
std dev	0.02	0.005

[a] Purity: 99.8 mass %.

Table XXVIII. Mutual Solubility S of Water (B) and 4-Decanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.0394	0.49
9.2	0.0300	0.40
19.7	0.0238	0.43
30.2	0.0180	0.51
39.6	0.0158	0.55
50.2	0.0098	0.62
60.6		0.68
70.6	0.0087	0.69
80.2	0.0064	0.68
91.5	0.0125	0.76
std dev	0.0005	0.01

[a] Purity: 99 mass %.

Table XXIX. Mutual Solubility S of Water (B) and Veratrole[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
19.9	0.716	1.30
31.0	0.706	1.42
41.1	0.723	1.57
50.6	0.758	1.73
60.2	0.794	1.92
70.6	0.877	2.08
80.7	0.970	2.35
91.8	1.073	2.61
std dev	0.002	0.02

[a] Purity: 99 mass %.

Table XXX. Mutual Solubility S of Water (B) and 2-Nonanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.053	0.75
9.8	0.043	0.68
20.2	0.038	0.81
30.3	0.032	0.82
39.8	0.034	0.90
50.0	0.025	1.02
60.0	0.031	0.97
70.4	0.034	1.14
81.2	0.027	1.11
91.2	0.038	1.24
std dev	0.001	0.01

[a] Purity: 99+ mass %.

Table XXXI. Mutual Solubility S of Water (B) and Anisole[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0		0.119
10.2	0.237	0.160
20.0	0.203	0.175
29.7	0.186	0.209
39.9	0.184	0.238
50.2	0.199	0.257
60.2	0.255	0.299
70.2	0.253	0.321
81.2	0.294	0.364
90.7	0.352	0.477
std dev	0.005	0.002

[a] Purity: 99 mass %.

Table XXXII. Mutual Solubility S of Water (B) and Tetrachloroethylene[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.0273	0.0045
9.5	0.0270	0.0054
19.5	0.0286	0.0075
31.1	0.0221	0.0091
40.0	0.0213	0.0104
50.1	0.0273	0.0117
61.3	0.0304	0.0142
71.0	0.0377	0.0205
80.2	0.0380	0.0214
91.8	0.0523	0.0245
std dev	0.0003	0.0003

[a] Purity: 99.99 mass %.

Table XXXIII. Mutual Solubility S of Water (B) and Butyl Ethyl Ether[a] (A)

	S/(mass %)	
t/°C	A in B[b]	B in A[b]
0	1.09	0.72
9.3	0.83	0.75
20.0	0.65	0.81
31.2	0.53	0.92
39.7	0.58	0.96
50.8	0.46	1.06
60.2	0.51	1.17
70.2	0.39	1.16
80.2	0.43	1.24
90.7	0.40	1.32
std dev	0.02	0.03

[a] Purity: 98 mass %. [b] Some decomposition in both layers.

Table XXXIV. Mutual Solubility S of Water (B) and Chloroform[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	1.02	0.0365
9.5	0.93	0.0527
19.6	0.82	0.0661
29.5	0.79	0.0841
39.3	0.74	0.1108
49.2	0.77	0.1353
59.2	0.79	0.1672
std dev	0.02	0.0005

[a] Purity: 99.9 mass %.

Table XXXV. Mutual Solubility S of Water (B) and Carbon Tetrachloride[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.089	0.0086
10.0	0.063	0.0102
20.5	0.060	0.0124
31.0	0.072	0.0156
41.3	0.068	0.0194
52.5	0.078	0.0263
64.0	0.096	0.0284
75.0	0.115	0.0304
std dev	0.002	0.0002

[a] Purity: 99.9 mass %.

Table XXXVI. Mutual Solubility S of Water (B) and 1,2-Dichloropropane[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.29	0.075
9.5	0.28	0.112
20.0	0.30	0.149
29.7	0.29	0.173
40.3	0.30	0.190
49.8	0.32	0.263
60.0	0.35	0.294
70.5	0.39	0.300
80.2	0.47	0.355
90.4		0.330
std dev	0.01	0.005

[a] Purity: 99 mass %.

Table XXXVII. Mutual Solubility S of Water (B) and 1,1,2,2-Tetrachloroethane[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.317	0.074
9.5	0.290	0.078
20.0	0.291	0.116
29.7	0.292	0.127
39.6	0.301	0.154
50.1	0.316	0.186
61.0	0.357	0.200
70.5	0.385	0.230
80.6	0.425	0.236
90.8	0.474	0.263
std dev	0.004	0.004

[a] Purity: 98 mass %.

Table XXXVIII. Mutual Solubility S of Water (B) and 3-Chloro-2-butanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	3.30	0.71
9.7	2.91	0.92
19.1	2.80	1.05
31.0		1.27
41.1	2.66	1.52
51.1	2.63	1.76
61.1	2.71	2.10
71.5	2.88	2.44
81.2		2.89
91.8	3.38	3.33
std dev	0.04	0.05

[a] Purity: 95 mass %.

Table XXXIX. Mutual Solubility S of Water (B) and 5-Chloro-2-pentanone[a] (A)

	S/(mass %)	
t/°C	A in B[b]	B in A[b]
0	9.3	3.0
22.3	4.7	3.2
30.8	4.1	3.2
40.2		6.1
50.1	4.4	7.6
60.7	6.8	
70.7	13.5	
91.0		10.2
std dev	0.6	0.2

[a] Purity: 97 mass %. [b] Below 80 °C, organic layer on bottom; above 80 °C, organic layer on top. Layers hard to separate.

Table XL. Mutual Solubility S of Water (B) and Cycloheptanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	5.24	3.3
9.5	4.38	3.0
19.8	3.61	
31.0	3.12	3.7
39.8	2.70	3.9
50.2	2.69	4.1
60.8	2.68	4.6
70.7	2.64	4.8
81.3	2.73	5.5
91.9	2.82	5.6
std dev	0.05	0.1

[a] Purity: 97 mass %.

Table XLI. Mutual Solubility S of Water (B) and 2-Methylcyclohexanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	2.94	1.51
9.0	2.41	1.63
19.5	1.98	1.94
31.0	1.68	2.10
40.8	1.56	2.32
50.2	1.47	2.54
60.3	1.45	2.88
71.0	1.47	3.32
81.3	1.46	3.55
90.3	1.54	4.02
std dev	0.01	0.02

[a] Purity: 98 mass %.

Table XLII. Mutual Solubility S of Water (B) and 4-Methylcyclohexanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	3.54	2.53
9.6	2.84	2.75
20.1	2.43	2.92
29.7	2.15	3.28
40.3	1.95	3.53
50.1	1.90	3.88
61.0	1.84	4.25
72.0	1.89	4.76
80.5	1.95	5.24
91.8	2.02	5.69
std dev	0.01	0.03

[a] Purity: 99 mass %.

Table XLIII. Mutual Solubility S of Water (B) and 2-Hexanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	2.46	1.7
9.6	1.91	1.9
19.8	1.51	2.1
29.7	1.37	2.4
39.6	1.24	2.6
50.0	1.16	2.8
60.5	1.12	3.1
70.3	1.12	3.2
80.7	1.15	3.3
91.5	1.19	3.8
std dev	0.01	0.1

[a] Purity: 98 mass %.

Table XLIV. Mutual Solubility S of Water (B) and 5-Methyl-3-hexanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.78	0.83
9.5	0.60	0.85
19.6	0.47	0.91
31.0	0.40	1.08
39.6	0.36	1.18
50.5	0.34	1.39
61.3	0.33	1.55
70.6	0.33	1.73
81.2	0.32	1.93
91.4	0.32	2.09
std dev	0.01	0.06

[a] Purity: 97 mass %.

Table XLV. Mutual Solubility S of Water (B) and 2,6-Dimethyl-4-heptanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.069	0.28
9.2	0.058	0.30
20.6	0.045	0.38
30.8	0.040	0.44
40.5	0.032	0.51
50.0	0.032	0.58
60.7	0.031	0.62
70.5	0.034	0.71
80.8	0.035	0.62
90.7	0.037	0.58
std dev	0.002	0.02

[a] Purity: 97 mass %.

Table XLVI. Mutual Solubility S of Water (B) and 5-Methyl-3-heptanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.275	1.0
9.3	0.227	1.1
19.9	0.192	1.1
30.9	0.151	1.5
40.8	0.151	1.6
50.2	0.142	1.8
59.8	0.124	2.0
70.5	0.132	2.0
80.2	0.128	1.9
90.5	0.131	2.1
std dev	0.003	0.2

[a] Purity: 99 mass %.

Table XLVII. Mutual Solubility S of Water (B) and 2-Octanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.227	1.29
9.7	0.211	1.39
19.2	0.172	1.20
29.7	0.101	1.28
40.4	0.102	1.38
50.0	0.112	1.29
60.4	0.107	1.56
70.2		1.46
80.6	0.103	1.34
91.0	0.094	1.29
std dev	0.007	0.03

[a] Purity: 95 mass %.

Table XLVIII. Mutual Solubility S of Water (B) and 3-Octanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.182	
9.7		0.55
20.1	0.137	0.62
29.7	0.135	0.68
39.6	0.119	0.75
50.0	0.110	0.77
60.0	0.098	0.77
70.5	0.100	0.78
80.3	0.117	0.92
91.0	0.106	0.90
std dev	0.003	0.04

[a] Purity: 99 mass %.

Table XLIX. Mutual Solubility S of Water (B) and 1,2-Dichlorobenzene[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.005	0.061
9.6		0.045
19.5	0.0031	0.047
31.1		0.056
40.0	0.0017	0.063
50.0	0.0024	0.076
60.5	0.0054	0.097
70.7	0.0055	0.107
80.0	0.0091	0.134
90.5	0.0083	0.138
std dev	0.0008	0.002

[a] Purity: 98.5 mass %.

Table L. Mutual Solubility S of Water (B) and 3-Nonanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.049	0.67
9.5	0.046	0.69
19.4		0.80
29.7	0.056	0.93
39.8	0.045	1.05
50.0	0.054	1.17
60.6	0.058	1.23
70.5		1.30
80.2	0.046	1.27
90.8		1.35
std dev	0.002	0.02

[a] Purity: 99 mass %.

Table LI. Mutual Solubility S of Water (B) and 5-Nonanone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.072	0.32
9.5	0.064	0.45
19.8	0.054	0.44
30.1	0.048	0.54
40.8	0.040	0.57
50.0	0.029	0.62
60.6	0.035	0.59
70.3	0.031	0.63
80.0	0.029	0.86
90.6	0.038	0.77
std dev	0.002	0.01

[a] Purity: 98 mass %.

Table LII. Mutual Solubility S of Water (B) and 2,6,8-Trimethyl-4-nonanone[a] (A)

		S/(mass %)	
	t/°C	A in B[b]	B in A[b]
	0		0.17
	9.6	0.012	0.22
	20.0		0.25
	29.5		0.29
	39.7	0.012	0.32
	50.1	0.014	0.31
	60.8	0.017	0.32
	70.3		0.35
	80.0	0.014	0.31
	90.5		0.31
std dev		0.001	0.01

[a] Purity: 98 mass %. [b] Analysis of aqueous layer uncertain because of impurities.

Table LIII. Mutual Solubility S of Water (B) and Dibutyl Ether[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.040	0.15
	9.3	0.032	0.19
	19.9	0.023	0.27
	30.9	0.023	0.25
	40.3	0.020	0.28
	50.5	0.022	0.31
	61.3	0.012	0.36
	70.5	0.015	0.40
	80.7	0.009	0.47
	90.5	0.010	0.52
std dev		0.001	0.03

[a] Purity: 99+ mass %.

Table LIV. Mutual Solubility S of Water (B) and *tert*-Butyl Methyl Ether[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	8.3	1.14
	9.7	5.1	1.24
	19.8	4.2	1.27
	29.6	3.1	1.36
	39.3	2.5	1.47
	48.6	1.9	1.58
std dev		0.2	0.06

[a] Purity: 99.5 mass %.

Table LV. Mutual Solubility S of Water (B) and Isopropyl Ether[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	2.28	0.40
	9.7	1.02	0.42
	20.0	0.79	0.48
	31.0	0.54	0.52
	40.8	0.41	0.57
	50.7	0.28	0.65
	61.0	0.22	0.72
std dev		0.02	0.02

[a] Purity: 99 mass %.

Table LVI. Mutual Solubility S of Water (B) and Tetrahydropyran[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	12.90	2.08
	9.4	10.03	2.35
	19.9	8.57	2.50
	31.0	6.88	2.63
	39.6	6.04	2.99
	50.5	5.16	3.20
	60.7	4.62	3.64
	71.3	4.50	3.98
	81.3	4.29	4.21
std dev		0.02	0.02

[a] Purity: 99+ mass %.

Table LVII. Mutual Solubility S of Water (B) and 3-Methyltetrahydropyran[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	3.60	1.1
	9.7	2.76	1.3
	19.7	2.13	1.4
	29.8	1.84	1.6
	40.8	1.56	1.8
	50.3	1.42	1.9
	60.5	1.30	2.2
	70.5	1.24	2.4
	81.6	1.21	2.7
	92.0	1.05	2.6
std dev		0.01	0.1

[a] Purity: 98 mass %.

Table LVIII. Mutual Solubility S of Water (B) and 3,4-Dihydropyran[a] (A)

		S/(mass %)	
	t/°C	A in B[b]	B in A[b]
	0	0.98	0.33
	9.5	1.17	0.39
	19.7	1.04	
	31.2	1.02	0.52
	41.1	1.02	0.60
	51.1	1.23	0.66
	61.9	1.33	0.84
	71.5	1.51	1.02
	81.6	2.26	1.55
std dev		0.03	0.02

[a] Purity: 97 mass %. [b] Some decomposition in aqueous layer.

Table LIX. Mutual Solubility S of Water (B) and 2,5-Dimethyltetrahydrofuran[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	10.72	1.80
	9.2	7.99	1.84
	19.5	5.64	1.98
	31.0	4.10	2.10
	40.8	3.17	2.25
	50.7	2.57	2.33
	61.5	2.19	3.03
	71.8	1.93	2.67
	83.0	1.54	2.66
std dev		0.03	0.07

[a] Purity: cis + trans, 99 mass %.

Table LX. Mutual Solubility S of Water (B) and 2,5-Dimethoxytetrahydrofuran[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	35	2.03
	9.3	33	2.40
	21.0	32	2.98
	31.0	30	
	40.7	27	3.94
	50.1	25	4.50
	61.1	23	4.95
	71.3	21	5.93
	81.0	20	6.48
	90.2	19	7.26
std dev		1.0	0.05

[a] Purity: 97+ mass %.

Table LXI. Mutual Solubility S of Water (B) and Isobutyl Propionate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.312	0.54
	9.3	0.292	0.61
	19.4	0.225	0.68
	31.1	0.185	0.79
	40.3	0.177	0.90
	51.1	0.163	1.00
	61.0	0.154	1.19
	71.0	0.149	1.31
	81.3	0.151	1.47
	91.3	0.142	1.65
std dev		0.002	0.02

[a] Purity: 98 mass %.

Table LXII. Mutual Solubility S of Water (B) and Ethyl 2-Methylbutyrate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.404	0.54
	9.0	0.319	0.60
	18.7	0.257	0.70
	31.1	0.211	0.86
	40.7	0.189	0.95
	50.5	0.178	1.07
	60.8	0.159	1.25
	70.0	0.166	1.35
	79.7	0.162	1.57
	91.3	0.151	1.89
std dev		0.005	0.07

[a] Purity: 99 mass %.

Table LXIII. Mutual Solubility S of Water (B) and Phenyl Acetate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.62	0.33
	9.7	0.61	
	20.0	0.59	0.62
	29.7	0.56	0.71
	40.0	0.62	0.81
	51.0	0.59	0.87
	60.7	0.72	0.95
	70.5	0.70	0.99
	80.2	0.80	1.13
	90.8	0.91	1.00
std dev		0.02	0.02

[a] Purity: 97 mass %.

Table LXIV. Mutual Solubility S of Water (B) and Dimethyl Succinate[a] (A)

		S/(mass %)	
	t/°C	A in B[b]	B in A[b]
	20.6	12.4	4.50
	30.1	12.3	5.38
	39.6	13.0	6.30
	50.0	13.1	7.57
	60.8	13.7	8.53
	70.5	14.3	10.53
	80.0	15.3	12.96
	91.6	17.1	16.60
std dev		0.16	0.04

[a] Purity: 98 mass %. [b] Melting point 19 °C.

Table LXV. Mutual Solubility S of Water (B) and Nitromethane[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	9.0	1.10
	9.5	9.7	1.44
	19.7	10.4	1.91
	31.0	11.7	2.50
	40.4	12.8	3.65
	50.0	14.8	6.13
	60.5	15.1	7.92
	70.5	17.1	8.18
	80.2	19.6	10.42
	89.8	20.8	
std dev		0.2	0.05

[a] Purity: 99+ mass %.

Table LXVI. Mutual Solubility S of Water (B) and Nitroethane[a] (A)

		S/(mass %)	
	t/°C	A in B[b]	B in A[b]
	0	4.32	0.62
	9.2	4.22	0.75
	19.6	4.38	0.99
	31.0	4.44	1.31
	40.6	4.60	1.58
	50.5	5.19	1.90
	60.8	5.40	3.31
	70.4	5.82	4.76
	80.4	6.27	6.17
	90.1	6.55	7.07
std dev		0.01	0.03

[a] Purity: 96 mass %. [b] Below 70 °C, organic on bottom; above 70 °C, organic on top.

Table LXVII. Mutual Solubility S of Water (B) and 2-Nitropropane[a] (A)

		S/(mass %)	
	t/°C	A in B[b]	B in A[b]
	0	3.07	0.34
	19.7	1.80	0.49
	30.9	1.70	0.65
	40.0	1.78	0.70
	50.5	1.79	0.93
	61.1	2.07	1.27
	70.6	2.09	1.45
	81.0	2.26	1.91
	90.2	2.36	2.23
std dev		0.03	0.03

[a] Purity: 96 mass %. [b] Below 10 °C, organic on bottom; above 10 °C, organic on top.

Table LXVIII. Mutual Solubility S of Water (B) and 2,3-Butanedione[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	34.2	3.65
	9.2	33.5	4.36
	19.6	31.7	4.80
	31.0	29.5	5.53
	40.0	28.8	6.62
	50.7	25.8	7.30
	61.1	24.2	8.23
	70.3	22.6	9.47
	80.3	21.8	10.35
std dev		0.1	0.15

[a] Purity: 99 mass %.

Table LXIX. Mutual Solubility S of Water (B) and Isophorone[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	2.40	3.9
	9.3	1.80	3.9
	19.8	1.57	3.8
	30.9	1.32	4.1
	40.5	1.24	4.4
	50.4	1.19	4.7
	60.2	1.18	5.0
	70.0	1.14	5.5
	80.5	1.27	5.9
	91.1	1.35	6.2
std dev		0.02	0.2

[a] Purity: 97 mass %.

Table LXX. Mutual Solubility S of Water (B) and Fluorobenzene[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.162	0.082
	9.5	0.166	0.077
	19.2	0.170	0.103
	29.7	0.155	0.132
	39.6	0.153	0.186
	47.7	0.173	0.172
	60.1	0.190	0.226
	70.0	0.191	0.256
	80.0	0.188	0.313
std dev		0.004	0.002

[a] Purity: 99 mass %.

Table LXXI. Mutual Solubility S of Water (B) and Diethyl Maleate[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	1.93	1.05
	9.1	1.79	1.20
	19.5	1.56	1.43
	29.5	1.42	1.70
	40.8	1.40	1.99
	50.5	1.41	2.33
	60.7	1.49	2.50
	71.1	1.57	2.99
	80.8	1.68	3.10
	90.9	1.75	3.97
std dev		0.03	0.05

[a] Purity: 97 mass %.

Table LXXII. Mutual Solubility S of Water (B) and Dibromomethane[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	1.17	
	9.7	1.13	0.040
	19.3	1.28	0.056
	29.5	1.14	0.069
	39.5	1.20	0.091
	49.5	1.27	0.120
	59.9	1.36	0.164
	69.9	1.36	0.155
	79.8	1.61	0.153
	90.1	1.51	0.200
std dev		0.005	0.002

[a] Purity: 99 mass %.

Table LXXIII. Mutual Solubility S of Water (B) and 1,2-Dibromoethane[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	10.1	0.395	0.035
	19.5	0.412	0.043
	30.7	0.431	0.063
	39.6	0.444	0.080
	50.0	0.493	0.085
	59.9	0.489	0.120
	70.2	0.542	0.148
	80.3	0.572	0.181
	90.6	0.658	0.260
std dev		0.007	0.004

[a] Purity: 99 mass %.

Table LXXIV. Mutual Solubility S of Water (B) and 1,1,2-Trichloroethane[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.464	0.070
	9.2	0.439	0.098
	19.7		0.122
	31.3	0.458	0.157
	41.0	0.483	0.181
	50.6	0.518	0.221
	60.5	0.497	0.267
	71.0	0.555	0.310
	81.7	0.658	0.352
	90.8	0.703	0.418
std dev		0.008	0.006

[a] Purity: 98 mass %.

Table LXXV. Mutual Solubility S of Water (B) and 1,1,1-Trichloroethane[a] (A)

		S/(mass %)	
	t/°C	A in B	B in A
	0	0.147	0.027
	9.5		0.029
	20.2	0.070	0.035
	31.6	0.076	0.034
	41.1	0.101	
	51.3	0.106	0.065
	61.5	0.103	0.088
	71.5	0.114	
std dev		0.005	0.002

[a] Purity: 99+ mass %.

Table LXXVI. Mutual Solubility S of Water (B) and 1-Nitropropane[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	1.78	0.40
9.5	1.65	0.49
20.0	1.58	
31.0	1.70	
41.0	1.73	0.95
50.2	1.78	1.13
60.2	1.91	1.36
70.1	2.05	1.87
81.2	2.17	1.86
90.5	2.29	2.05
std dev	0.05	0.05

[a] Purity: 98 mass %.

Table LXXVII. Mutual Solubility S of Water (B) and Dimethyl Malonate[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	13.7	2.65
9.2	14.3	3.36
19.4	14.9	4.31
29.7	15.3	5.32
39.5	16.1	6.50
50.2	17.7	8.25
61.0	19.8	9.33
70.3	23.4	10.34
79.8	23.6	12.20
90.2	29.8	18.85
std dev	0.3	0.03

[a] Purity: 99+ mass %.

Table LXXVIII. Mutual Solubility S of Water (B) and Diethyl Glutarate[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	1.54	1.20
9.1	1.23	1.34
20.3	1.01	1.67
29.7	1.20	1.88
39.7	1.27	2.18
49.9	0.94	2.40
60.7		2.70
70.6	0.84	3.16
80.7	0.91	3.31
90.6	0.91	3.51
std dev	0.05	0.02

[a] Purity: 99+ mass %.

Table LXXIX. Mutual Solubility S of Water (B) and Acetophenone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
19.9	0.652	1.84
29.5	0.710	1.95
39.5	0.833	2.21
49.8	0.814	2.14
60.1	0.888	2.44
70.2	0.992	3.33
80.2	1.204	3.44
91.7		3.55
std dev	0.005	0.02

[a] Purity: 99 mass %.

Table LXXX. Mutual Solubility S of Water (B) and Propiophenone[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
19.4	0.32	0.70
30.9		0.67
40.8	0.30	0.94
50.7		1.09
60.3	0.20	1.31
71.2	0.29	1.46
80.2	0.24	1.52
90.5	0.32	1.52
std dev	0.01	0.02

[a] Purity: 99 mass %.

Table LXXXI. Mutual Solubility S of Water (B) and Toluene[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.12	0.042
9.5	0.09	0.057
19.8	0.08	0.087
29.7	0.08	0.092
39.6	0.10	0.110
50.0	0.09	0.140
60.1	0.10	0.151
70.4	0.09	0.206
81.0	0.13	0.247
90.2	0.12	0.281
std dev	0.01	0.005

[a] Purity: 99.9 mass %.

Table LXXXII. Mutual Solubility S of Water (B) and Hexyl Ether[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	0.020	0.067
9.5		0.078
20.0	0.019	0.087
29.7		0.108
39.4	0.019	0.108
49.8		0.119
60.0		0.123
70.3	0.014	0.139
80.2	0.014	0.142
90.3	0.019	0.156
std dev	0.002	0.002

[a] Purity: 98 mass %.

Table LXXXIII. Mutual Solubility S of Water (B) and *tert*-Amyl Methyl Ether[a] (A)

	S/(mass %)	
t/°C	A in B	B in A
0	2.48	0.57
9.7	1.59	0.57
19.9	1.10	0.66
31.0	0.85	0.75
40.3	0.64	0.77
48.8	0.57	0.82
59.2	0.47	0.88
69.2	0.45	0.93
79.2	0.36	0.95
std dev	0.02	0.02

[a] Purity: 98 mass %.

Table LXXXIV. Mutual Solubility S of Water (A), Cyclohexane (C), and Ethanol (B) at 40 °C[a]

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
100.0	0	0	0.006	0	99.994
85.77	14.23	0	0.018	0.19	99.79
71.08	28.92	trace	0.030	0.78	99.19
56.61	42.99	0.40	0.052	1.24	98.71
41.52	56.14	2.34	0.09	2.17	97.74
28.83	65.02	6.15	0.14	3.46	96.4
18.70	67.90	13.40	0.24	5.44	94.32
14.40	65.35	20.25	0.39	7.51	92.10
8.93	58.77	32.30	0.72	12.26	87.02
2.6	32.6	64.8	2.6	32.6	64.8

[a] Purities: ethanol, 99.8 mass %; cyclohexane, 99+ mass %.

Table LXXXV. Mutual Solubility S of Water (C), Benzene (B), and *tert*-Butyl Methyl Ether (A) at 25 °C[a]

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
0	0.193	99.807	0	99.91	0.09
trace	0.170	99.83	2.72	97.16	0.12
trace	0.160	99.84	6.18	93.65	0.17
trace	0.153	99.847	14.69	85.11	0.20
0.98	0.138	98.882	29.24	70.54	0.22
1.34	0.124	98.536	40.64	59.04	0.32
0.85	0.122	99.028	30.3	69.41	0.29
0.98	0.117	98.903	40.7	58.95	0.35
1.48	0.106	98.414	52.5	47.05	0.45
1.59	0.098	98.312	54.71	44.87	0.42
1.90	0.074	98.026	56.85	42.41	0.74
2.00	0.056	97.944	68.51	30.92	0.57
3.61	0.033	96.357	84.00	14.86	1.14
4.17	trace	95.83	91.91	6.72	1.37
3.90	trace	96.10	94.72	3.86	1.42

[a] Purities: *tert*-butyl methyl ether, 99+ mass %; benzene, 99.9+ mass %.

Table LXXXVI. Mutual Solubility S of Water (A), Benzene (C), and Hexanol (B) at 25 °C[a]

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
99.843	0	0.157	0.067	0	99.933
99.784	0.055	0.161	0.098	2.13	97.772
99.739	0.096	0.165	0.14	5.03	94.83
99.654	0.177	0.169	0.49	18.18	81.33
99.627	0.232	0.141	1.11	32.66	66.23
99.635	0.228	0.137	1.81	47.37	50.82
99.577	0.297	0.126	2.20	47.63	50.17
99.585	0.289	0.126	2.55	54.95	42.50
99.558	0.321	0.121	3.17	61.87	34.96
99.503	0.410	0.087	4.69	76.50	18.81
99.48	0.520	0	7.31	92.69	0

[a] Purities: hexanol, 98 mass %; benzene, 99.9+ mass %.

Table LXXXVII. Mutual Solubility S of Water (A), Pentanol (B), and Benzene (C) at 25 °C[a]

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
99.842	0	0.158	0.076	0	99.924
99.436	0.40	0.164	0.137	2.24	97.623
99.128	0.70	0.172	0.231	5.88	93.889
98.954	0.90	0.146	0.628	14.85	84.522
98.697	1.17	0.133	2.14	38.12	59.74
98.414	1.46	0.126	3.95	52.73	43.32
98.274	1.63	0.096	5.95	68.26	25.79
98.11	1.89	0	11.01	88.99	0
97.926	2.05	0.024	9.64	84.86	5.50
98.232	1.71	0.058	7.79	78.33	13.88
98.303	1.61	0.087	6.52	69.52	23.96
98.362	1.53	0.108	4.99	62.07	32.94
98.555	1.33	0.115	3.81	53.09	43.10
98.603	1.27	0.127	2.95	47.03	50.02
98.73	1.14	0.130	2.21	38.80	58.99

[a] Purities: pentanol, 99+ mass %; benzene, 99.9+ mass %.

Table LXXXVIII. Mutual Solubility S of Water (A), Isobutyl Alcohol (B), and Benzene (C) at 25 °C[a]

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
99.8	0	0.2	0.2	0	99.8
99.1	0.7	0.2	0.15	trace	99.85
97.6	2.2	0.2	0.25	2.6	97.15
95.9	3.9	0.2	0.7	12.7	86.6
95.4	4.4	0.2	1.7	25.0	73.3
95.0	4.8	0.2	3.1	36.8	61.1
94.6	5.2	0.2	4.7	46.8	48.5
94.4	5.4	0.2	6.6	60.0	33.4
91.8	8.2	0	19.0	81.0	0
92.5	7.5	trace	15.7	78.9	5.4
93.5	6.5	trace	11.6	73.0	15.4
94.2	5.6	0.2	7.2	57.0	35.8
94.7	5.1	0.2	4.6	47.2	48.2

[a] Purities: isobutyl alcohol, 99.9+ mass %; benzene, 99.9+ mass %.

Table LXXXIX. Mutual Solubility S of Water (A), Methanol (C), and Toluene (B) at 40 °C[a]

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
99.94	0.06	0	0.11	99.89	0
95.03	0.06	4.91	0.16	99.75	0.09
89.05	0.06	10.89	0.16	99.62	0.22
80.57	0.12	19.31	0.20	99.38	0.42
71.25	0.21	28.54	0.28	98.98	0.74
60.95	0.48	38.57	0.27	98.61	1.12
57.14	0.67	42.19	0.19	98.50	1.31
52.39	1.05	46.56	0.22	98.26	1.52
47.44	1.29	51.27	0.35	97.84	1.81
41.92	2.55	55.53	0.23	97.83	1.94
39.86	2.43	57.71	0.28	97.36	2.36
28.32	7.34	64.34	0.39	95.92	3.69
17.48	17.92	64.60	0.76	91.47	7.77
3.60	64.57	31.83	3.60	64.57	31.83

[a] Purities: toluene, 99.9+ mass %; methanol, 99.9+ mass %.

Table XC. Mutual Solubility S of Water (A), Isobutyl Alcohol (B), and Toluene (C) at 25 °C[a]

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
99.947	0	0.053	0.060	0	99.940
99.101	0.84	0.059	0.105	0.739	99.156
97.492	2.45	0.058	0.14	3.09	96.77
96.379	3.56	0.061	0.29	7.12	92.59
95.388	4.55	0.062	0.85	17.19	81.96
94.919	5.02	0.061	1.74	27.82	70.44
94.622	5.32	0.058	2.90	37.61	59.49
94.529	5.41	0.061	2.79	38.89	58.32
94.264	5.68	0.056	4.44	49.72	45.84
94.227	5.71	0.063	4.14	48.85	47.01
94.018	5.93	0.052	5.28	55.50	39.22
93.761	6.19	0.049	7.53	60.74	31.73
92.737	7.23	0.033	12.16	75.00	12.84
92.088	7.90	0.012	15.79	80.38	3.83
91.54	8.46	0	17.56	82.44	0

[a] Purities: isobutyl alcohol, 99.9+ mass %; toluene, 99.9+ mass %.

as much as a 50% higher solubility than calculated values. This is perhaps not surprising, and does tend to show that multicomponent calculations are fairly reliable when solubilities are low, but cannot be relied on for systems showing high solubilities.

Several of the ternary systems studied involved the use of gasoline as one of the components. This immediately created problems because the large number of different components in gasoline caused a very high background whenever GC analysis was used. To eliminate this problem, we developed a "synthetic gasoline" containing hexane, methylcyclopentane,

Table XCI. Mutual Solubility *S* of Water (C), Butanol (B), and Methyl Ethyl Ketone (A) at 40 °C[a]

S(aqueous layer)/(mass %)			*S*(organic layer)/(mass %)		
A	B	C	A	B	C
23.24	1.36	75.40	77.84	6.21	15.95
21.59	3.19	75.22	64.30	13.10	22.60
18.94	4.93	76.13	50.88	19.31	29.81
15.66	6.02	78.32	42.89	25.41	31.70
13.77	6.29	79.94	39.81	29.11	31.08
11.13	6.56	82.31	34.01	35.17	30.82
9.10	6.60	84.30	29.87	40.92	29.21
7.69	6.58	85.73	26.35	45.03	28.62
6.16	6.57	87.27	22.07	50.24	27.69
5.34	6.58	88.08	19.21	54.15	26.64
3.71	6.54	89.75	14.53	62.63	22.84
0	6.70	93.30	0	81.23	18.77
1.89	6.74	91.37	7.45	71.83	20.72
3.59	6.56	89.85	14.15	62.88	22.97
5.63	6.62	87.75	20.75	54.78	24.47
8.09	6.62	85.29	27.11	43.78	29.11
10.62	6.58	82.80	33.12	36.15	30.73

[a] Purities: methyl ethyl ketone, 99+ mass %; butanol, 99.9 mass %.

Table XCII. Mutual Solubility *S* of Water (C), Butanol (B), and Methyl Ethyl Ketone (A) at 40 °C[a]

S(aqueous layer)/(mass %)			*S*(organic layer)/(mass %)		
A	B	C	A	B	C
24.80	1.72	73.48	79.91	6.71	13.38
22.65	3.43	73.92	70.24	14.67	15.09
20.04	4.95	75.01	59.56	23.58	16.86
17.46	6.03	76.51	49.92	31.88	18.20
5.46	8.01	86.53	13.14	66.53	20.33
10.46	7.61	81.92	27.06	52.95	19.99

[a] Values calculated by Dr. Jean Leinroth from binary NRTL parameters.

Table XCIII. Mutual Solubility *S* of Water (A), Methanol[a] (B), and Synthetic Gasoline[b] (C) at 25 °C

S(aqueous layer)/(mass %)			*S*(organic layer)/(mass %)		
A	B	C	A	B	C
99.86	0	0.14	0.045	0	99.955
96.85	3.00	0.15	0.051	0.019	99.930
93.13	6.70	0.17	0.058	0.054	99.888
86.14	13.55	0.31	0.047	0.105	99.848
78.93	20.70	0.37	0.048	0.146	99.806
66.57	32.41	1.02	0.045	0.271	99.684
56.25	42.30	1.45	0.043	0.379	99.578
47.78	50.34	1.88	0.064	0.501	99.435
20.57	59.0	20.43	0.080	1.425	98.495
13.59	55.1	31.31	0.090	2.246	97.664
6.65	44.2	49.16	0.136	4.468	95.396
5.88	15.2	78.92	0.169	5.541	94.290
3.61	37.7	58.69	0.174	6.864	92.962
2.68	16.6	80.72	0.282	10.603	89.115
1.47	17.9	80.63	0.519	18.532	80.949

[a] Purity: 99.9 mass %. [b] Composition: 24 vol % hexane, 10 vol % methylcyclopentane, 32 vol % 2,2,4-trimethylpentane, 3 vol % benzene, 7 vol % toluene, 24 vol % *m*-xylene.

Table XCIV. Mutual Solubility *S* of Water (A), *tert*-Butanol[a] (B), and Synthetic Gasoline[b] (C) at 25 °C

S(aqueous layer)/(mass %)			*S*(organic layer)/(mass %)		
A	B	C	A	B	C
100.00	0	trace	0.046	0	99.954
98.61	1.39	trace	0.086	0	99.914
96.95	3.05	trace	0.23	trace	99.77
93.41	6.59	trace	0.24	trace	99.76
89.79	10.21	trace	0.56	1.91	97.53
85.30	14.70	trace	0.89	13.32	85.79
81.76	18.24	trace	2.58	28.4	69.02
80.51	19.46	0.03	5.61	42.2	52.19
78.41	21.54	0.05	9.7	52.8	37.5
76.76	23.16	0.08	15.7	59.6	24.7
74.95	24.92	0.13	22.3	63.3	14.4
72.93	26.88	0.19	25.4	62.4	12.2
69.37	30.28	0.35	33.7	58.9	7.4
69.41	30.25	0.34	33.6	58.8	7.6
64.44	34.85	0.71	42.0	53.6	4.4

[a] Purity: 99+ mass %. [b] Composition: 24 vol % hexane, 10 vol % methylcyclopentane, 32 vol % 2,2,4-trimethylpentane, 3 vol % benzene, 7 vol % toluene, 24 vol % *m*-xylene.

Table XCV. Mutual Solubility *S* of Water (A), Methyl *tert*-Butyl Ether[a] (B), and Synthetic Gasoline[b] (C) at 25 °C

S(aqueous layer)/(mass %)			*S*(organic layer)/(mass %)		
A	B	C	A	B	C
100.00	0	0	0.040	0	99.960
100.00	0	0	0.072	8.7	91.228
100.00	trace	0	0.090	13.2	86.710
99.42	0.58	trace	0.094	12.9	87.006
99.03	0.97	trace	0.287	30.4	69.313
98.69	1.31	trace	0.220	33.2	66.580
98.17	1.83	trace	0.218	38.2	61.582
97.47	2.53	trace	0.298	45.7	54.002
96.21	3.79	trace	0.377	45.3	54.323
95.88	4.12	trace	0.448	52.9	46.652
95.41	4.59	trace	0.549	50.1	49.351

[a] Purity: 99+ mass %. [b] Composition: 24 vol % hexane, 10 vol % methylcyclopentane, 32 vol % 2,2,4-trimethylpentane, 3 vol % benzene, 7 vol % toluene, 24 vol % *m*-xylene.

Table XCVI. Mutual Solubility *S* of Water (A), Ethyl Acetate[a] (B) and Synthetic Gasoline[b] (C) at 25 °C

S(aqueous layer)/(mass %)			*S*(organic layer)/(mass %)		
A	B	C	A	B	C
99.62	0.38	trace	0.05	3.0	96.95
99.36	0.64	trace	0.06	6.0	93.94
98.47	1.53	trace	0.10	15.0	84.90
97.79	2.21	trace	0.17	19.2	80.63
96.69	3.31	trace	0.24	28.3	71.46
95.86	4.14	trace	0.39	41.4	58.21
95.10	4.90	trace	0.63	51.37	38.00
94.51	5.49	trace	0.89	65.21	33.90
94.05	5.95	trace	1.31	73.69	25.00
92.45	7.55	0	3.07	96.93	0
93.25	6.75	trace	1.95	86.6	11.45
94.88	5.12	trace	0.73	61.3	37.97

[a] Purity: 99.5+ mass %. [b] Composition: 24 vol % hexane, 10 vol % methylcyclopentane, 32 vol % 2,2,4-trimethylpentane, 3 vol % benzene, 7 vol % toluene, 24 vol % *m*-xylene.

isooctane, benzene, toluene, and *m*-xylene which had a solubility identical with that of commercial unleaded gasoline. The use of this synthetic gasoline greatly simplified future experimental work.

It is interesting to note the solubility behavior of alcohols added to gasoline–water mixtures. Methanol (Table XCIII) distributes almost entirely in the water layer, and the plait point is very close to the gasoline apex. Ethanol (Table XCVIII) is more soluble then methanol in the gasoline layer, and the plait point moves away from the gasoline apex. Isopropyl alcohol (Table XCVII) is still more soluble in the gasoline layer, and *tert*-butanol (Table XCIV) first distributes largely in the water layer but above about 15% starts to distribute almost entirely in the gasoline layer.

Today there is much talk about the possibility of requiring the use of methanol–gasoline blends to reduce pollution in areas such as Southern California. There are many problems associated with the use of methanol in addition, of course, to the

Table XCVII. Mutual Solubility S of Water (A), Isopropyl Alcohol[a] (B), and Synthetic Gasoline[b] (C) at 25 °C

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
91.98	8.02	trace	0.057	0.634	99.309
84.08	15.92	trace	0.107	1.341	98.552
73.91	26.09	trace	0.369	6.809	92.822
74.18	25.82	trace	0.384	7.161	92.455
71.01	28.99	trace	0.567	9.107	90.326
67.70	32.21	0.09	0.915	13.41	85.675
66.08	33.81	0.11	1.039	14.40	84.561
63.52	36.21	0.27	1.294	17.35	81.356
60.36	39.24	0.40	1.781	19.40	78.819
58.16	41.26	0.58	2.072	21.98	75.948
55.96	43.29	0.75	2.487	22.82	74.693
51.03	47.74	1.23	3.310	26.70	69.99
50.25	48.39	1.36	3.546	28.00	68.454
50.04	48.57	1.39	3.578	27.89	68.532
55.57	43.60	0.83	2.54	25.03	72.43
50.42	48.31	1.27	3.38	27.14	69.48
45.70	52.20	2.10	4.58	31.17	64.25
42.03	53.57	4.40	5.54	33.81	60.65
37.19	54.96	7.85	6.55	36.29	57.16
35.29	55.72	8.99	7.21	38.05	54.74
21.00	52.37	26.63	15.55	49.12	35.33

[a] Purity: 99+ mass %. [b] Composition: 24 vol % hexane, 10 vol %, methylcyclopentane, 32 vol % 2,2,4-trimethylpentane, 3 vol % benzene, 7 vol % toluene, 24 vol % m-xylene.

Table XCVIII. Mutual Solubility S of Water (A), Ethanol[a] (B), and Synthetic Gasoline[b] (C) at 25 °C

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
100.00	0	trace	0.026	0	99.974
96.59	3.41	trace	0.029	0.10	99.871
93.30	6.70	trace	0.032	0.21	99.758
86.12	13.88	trace	0.037	0.414	99.549
79.02	20.98	trace	0.036	0.444	99.520
66.575	33.36	0.065	0.074	0.907	99.019
54.387	45.19	0.423	0.075	1.57	98.355
38.265	60.85	0.885	0.107	2.13	97.763
35.426	61.22	3.354	0.192	3.46	96.348
25.648	67.97	6.382	0.305	5.02	94.675
17.094	70.55	12.356	0.489	7.55	91.961
13.003	69.70	17.297	0.705	10.12	89.175
9.717	59.42	30.863	1.09	13.73	85.18

[a] Purity: 99.8 mass %. [b] Composition: 24 vol % hexane, 10 vol % methylcyclopentane, 32 vol % 2,2,4-trimethylpentane, 3 vol % benzene, 7 vol % toluene, 24 vol % m-xylene.

Table XCIX. Mutual Solubility S of Water (A) Methanol[a] (B), and Gasoline[b] (C) at 25 °C

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
100.00	0	trace	trace	0	100.00
96.98	3.02	trace	trace	0.003	99.997
93.185	6.76	0.055	trace	0.10	99.90
86.149	13.81	0.041	trace	0.28	99.72
79.189	20.73	0.081	0.22	0.40	99.38
66.538	33.3	0.162	0.22	1.01	98.77
47.095	52.6	0.305	0.18	0.94	98.88
0.82	70.5	28.68	0.26	4.21	95.53
2.84	76.8	20.36	0.36	2.69	96.95
20.20	75.7	4.10	0.21	1.78	98.01
32.50	64.9	2.60	0.20	1.11	98.69
46.57	52.4	1.03	0.20	0.98	98.82
56.17	43.0	0.83	0.18	0.85	98.97

[a] Purity: 99.9 mass %. [b] Commercial regular unleaded gasoline.

question of cost and availability. Methanol forms nonideal solutions with many of the components of gasoline, with negative deviations from Raoult's law. Thus the vapor pressure of a

Table C. Mutual Solubility S of Water (A), Methanol[a] (B), and Gasoline[b] (C) at 10 °C

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
100.00	0	trace	0.084	0	99.916
96.02	3.22	0.76	0.084	0.035	99.881
92.64	6.59	0.77	0.081	0.075	99.844
78.82	20.38	0.80	0.081	0.290	99.629
66.80	32.08	1.12	0.088	0.525	99.387
57.75	40.70	1.55	0.103	0.816	99.081
25.53	67.67	6.80	0.239	4.349	95.412
26.54	67.30	6.16	0.171	2.672	97.157
37.40	58.92	3.68	0.133	1.576	98.291
49.90	47.71	2.39	0.127	1.104	98.769
57.54	41.14	1.32	0.094	0.705	99.201
65.38	33.61	1.01	0.106	0.575	99.319
71.80	27.33	0.87	0.082	0.348	99.570

[a] Purity: 99.9 mass %. [b] Commercial regular unleaded gasoline.

Table CI. Mutual Solubility S of Water (A), Benzene (C), and Methyl Ethyl Ketone (B) at 25 °C[a]

S(aqueous layer)/(mass %)			S(organic layer)/(mass %)		
A	B	C	A	B	C
99.84	0	0.16	0.092	0	99.908
99.817	0.033	0.15	0.134	1.346	98.52
99.18	0.66	0.16	0.14	3.06	96.80
98.44	1.40	0.16	0.21	7.53	92.26
97.51	2.30	0.16	0.25	11.94	87.81
96.00	3.85	0.15	0.36	17.57	82.07
94.99	4.85	0.16	0.55	26.89	72.56
94.24	5.63	0.13	0.76	32.92	66.32
93.46	6.39	0.15	0.85	36.49	62.66
92.90	6.98	0.12	1.05	40.88	58.07
91.68	8.18	0.14	1.18	45.44	53.38
90.90	8.97	0.13	1.58	51.21	47.21
90.17	9.69	0.14	1.67	53.42	44.91
87.20	12.69	0.11	2.91	67.96	29.13
74.61	25.39	0	11.82	88.19	0

[a] Purities: methyl ethyl ketone, 99+ mass %; benzene, 99.9+ mass %.

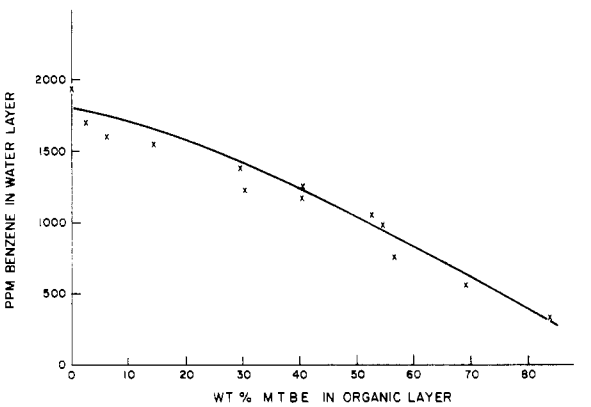

Figure 5. Mutual solubility of water, benzene, and *tert*-butyl methyl ether at 25 °C.

blend increases more than would be predicted from the methanol content, which causes problems for the refiners who must meet standard volatility requirements. Higher methanol concentrations cause problems of corrosion of storage tanks and various automobile components. The methanol–gasoline system has a very low tolerance for water up to about 20% methanol, and since it is impossible to completely keep water out of gasoline storage tanks, there is always the possibility of separation into two layers. For these reasons, many refiners

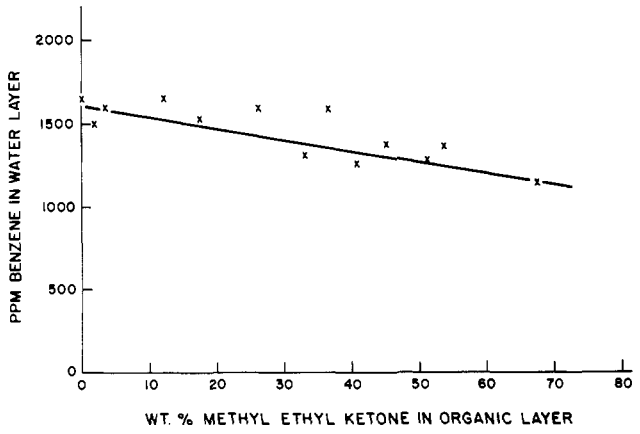

Figure 6. Mutual solubility of water, benzene, and methyl ethyl ketone at 25 °C.

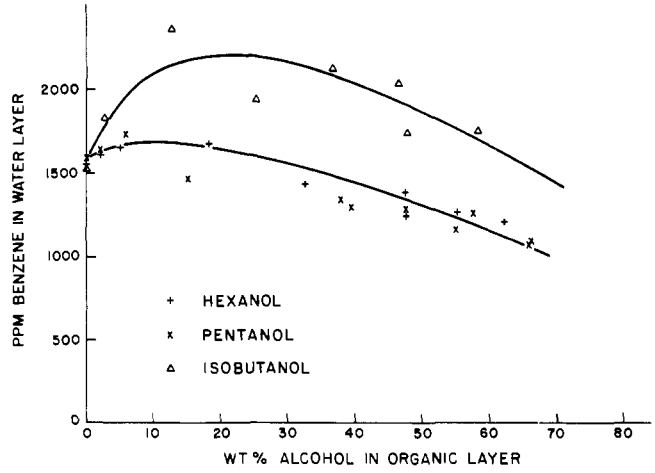

Figure 7. Mutual solubility of water, benzene, and alcohols at 25 °C.

are considering the possible use of mixtures of alcohols rather than using pure methanol as a blending agent.

Today the most common blending agent for gasoline is methyl *tert*-butyl ether (MTBE), which reduces pollution and increases the octane number of a gasoline. From Table XCV, it can be seen that MTBE distributes almost entirely in the gasoline layer, perhaps indicating that MTBE is a better blending agent than the lower alcohols.

Solubility of Aromatics in Water. When refiners were forced to eliminate the use of lead in gasoline, they had to find other ways to improve the octane number. This is done by the addition of blending agents such as MTBE and by increasing the amounts of benzene, toluene, and the other aromatics in gasoline. But unfortunately the aromatics are the most toxic constituents of gasoline—as well as the most soluble in water. Thus for any oxygenated additive to gasoline, there is always the question, "In case of a spill, what is the effect of the added material on the solubility of aromatics in ground water?"

In the case of methanol, ethanol, and isopropyl alcohol, the alcohol always acts to increase the solubility of all aromatics in water. This is a significant disadvantage of these systems. In the case of MTBE (see Table LXXXV and Figure 5), the solubility of benzene in water decreases with addition of MTBE. A similar effect occurs with the addition of methyl ethyl ketone (see Figure 6).

A very interesting effect is noted in the case of higher alcohols, such as isobutyl alcohol, pentanol, and hexanol (see Tables LXXXVII and LXXXVIII and Figure 7). Here the solubility of benzene in the water layer first increases with alcohol addition, goes through a maximum, and then decreases. This is a significant environmental hazard for these systems, since it increases the solubility of benzene in case of a spill.

Acknowledgment

I thank Dr. Jean Leinroth for making solubility calculations for the water–butanol–methyl ethyl ketone system. Andrew Graham assisted with some of the gasoline measurements.

Registry No. 2-Pentanone, 107-87-9; 3-pentanone, 96-22-0; 2,4-dimethyl-3-pentanone, 565-80-0; cyclohexyl butyrate, 1551-44-6; hexyl butyrate, 2639-63-6; heptyl butyrate, 5870-93-9; benzyl formate, 104-57-4; nonyl formate, 5451-92-3; 2-methyltetrahydrofuran, 96-47-9; cyclopentanone, 120-92-3; cyclohexanone, 108-94-1; 3-methyl-2-butanone, 563-80-4; 3,3-dimethyl-2-butanone, 75-97-8; 4-methyl-2-pentanone, 108-10-1; 5-methyl-2-hexanone, 110-12-3; 2-heptanone, 110-43-0; 3-heptanone, 106-35-4; 4-heptanone, 123-19-3; 2,4-pentanedione, 123-54-6; octyl acetate, 112-14-1; diethyl malonate, 105-53-3; dichloromethane, 75-09-2; 2-chloroethyl ether, 111-44-4; dichloroisopropyl ether, 63283-80-7; 2-chloroethyl methyl ether, 627-42-9; 1,2-dichloroethane, 107-06-2; 4-decanone, 624-16-8; veratrole, 91-16-7; 2-nonanone, 821-55-6; anisole, 100-66-3; tetrachloroethylene, 127-18-4; butyl ethyl ether, 628-81-9; chloroform, 67-66-3; carbon tetrachloride, 56-23-5; 1,2-dichloropropane, 78-87-5; 1,1,2,2-tetrachloroethane, 79-34-5; 3-chloro-2-butanone, 4091-39-8; 5-chloro-2-pentanone, 5891-21-4; cycloheptanone, 291-64-5; 2-methylcyclohexanone, 583-60-8; 4-methylcyclohexanone, 589-92-4; 2-hexanone, 591-78-6; 5-methyl-3-hexanone, 623-56-3; 2,6-dimethyl-4-heptanone, 108-83-8; 5-methyl-3-heptanone, 541-85-5; 2-octanone, 111-13-7; 3-octanone, 106-68-3; 1,2-dichlorobenzene, 95-50-1; 3-nonanone, 925-78-0; 5-nonanone, 502-56-7; 2,6,8-trimethyl-4-nonanone, 123-18-2; dibutyl ether, 142-96-1; *tert*-butyl methyl ether, 1634-04-4; isopropyl ether, 108-20-3; tetrahydropyran, 142-68-7; 3-methyltetrahydropyran, 26093-63-0; 3,4-dihydropyran, 110-87-2; 2,5-dimethyltetrahydrofuran, 1003-38-9; 2,5-dimethoxytetrahydrofuran, 696-59-3; isobutyl propionate, 540-42-1; ethyl 2-methylbutyrate, 7452-79-1; phenyl acetate, 122-79-2; dimethyl succinate, 106-65-0; nitromethane, 75-52-5; nitroethane, 79-24-3; 2-nitropropane, 79-46-9; 2,3-butanedione, 431-03-8; isophorone, 78-59-1; fluorobenzene, 462-06-6; diethyl maleate, 141-05-9; dibromomethane, 74-95-3; 1,2-dibromoethane, 106-93-4; 1,1,2-trichloroethane, 79-00-5; 1,1,1-trichloroethane, 71-55-6; 1-nitropropane, 108-03-2; dimethyl malonate, 108-59-8; diethyl glutarate, 818-38-2; acetophenone, 98-86-2; propiophenone, 93-55-0; toluene, 108-88-3; hexyl ether, 112-58-3; *tert*-amyl methyl ether, 994-05-8; cyclohexane, 110-82-7; benzene, 71-43-2; ethanol, 64-17-5; hexanol, 111-27-3; isobutyl alcohol, 78-83-1; methanol, 67-56-1; butanol, 71-36-3; *tert*-butyl alcohol, 75-65-0; ethyl acetate, 141-78-6; isopropyl alcohol, 67-63-0.

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