Mutual Binary Solubilities: Water–Alcohols and Water–Esters

Richard Stephenson* and James Stuart

University of Connecticut, Storrs, Connecticut 06268

Mutual binary solubilities have been measured for partially miscible water–organic pairs at temperatures of 0–90 °C. Experimental data are given for 31 C_4 to C_{12} alcohols, 10 formate esters, 14 acetate esters, 7 propionate esters, and 38 other esters ranging from C_3 to C_{10}. In essentially all cases, solubility of water in the organic layer increases with temperature. For the esters, solubility of organic in the aqueous layer decreases with temperature; for the alcohols, solubility of organic in the aqueous layer first decreases with temperature, goes through a minimum at about 60 °C, and then increases at higher temperatures.

A previous paper (*1*) described our research on the solubility of water in organics and organics in water, and presented solubility data for 19 water–alcohol pairs. The present paper gives data for an additional 31 alcohols and 59 esters.

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 acetonitrile (sometimes propanol) was added and the ratio of the water to acetonitrile 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 acetonitrile added and the GC scale factors for water and acetonitrile as determined from GC analyses of known water and acetonitrile solutions. This calibration was done for each system using at least three standards covering the composition range of the unknown solutions.

Organic in the water layer was obtained in a similar way by using a higher boiling material as a standard. For example, cyclopentanol was measured with 1-hexanol as standard. As in the case of the organic layer, the calibration was done for each system studied using at least three standard solutions.

To check the accuracy of the method, our data were compared with the recommended values given by Sorensen and Arlt (*2*). Figures 1–4 give values for 1-butanol, 2-butanol, 2-methyl-1-propanol, and ethyl acetate. It can be seen that the agreement is very good.

Because of the sensitivity of GC analysis, the method was accurate for concentrations down to 0.1 wt % or less. In some instances samples phase separated, and had to be brought into solution by heating or by the addition of a solvent such as acetonitrile or dimethyl sulfoxide. All measurements were done at atmospheric pressure, and all organics were obtained from the usual laboratory supply houses in purities of normally 98% or better. In some cases such as 2-butanol and the methylcyclohexanols, the organics consisted of the usual mixture of stereoisomers.

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. Temperature of the thermostat was controlled by a Braun Thermomix-1441 having a temperature stability of 0.01 °C. Absolute temperature was measured by a calibrated thermometer accurate to better than 0.1 °C.

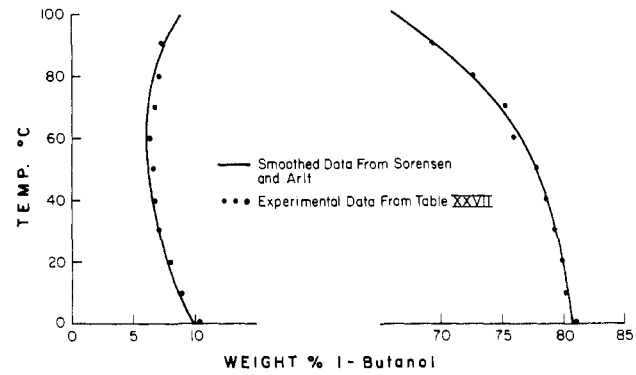

Figure 1. Mutual solubility of water and 1-butanol.

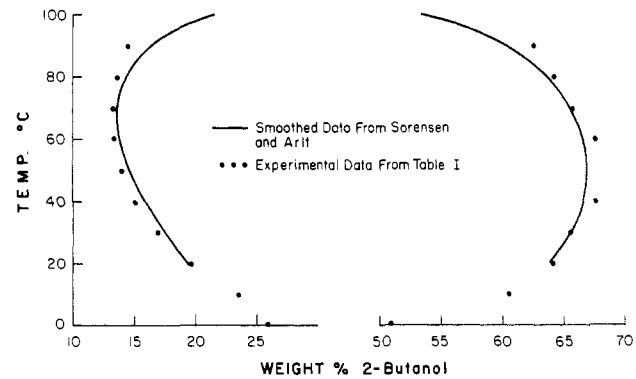

Figure 2. Mutual solubility of water and 2-butanol.

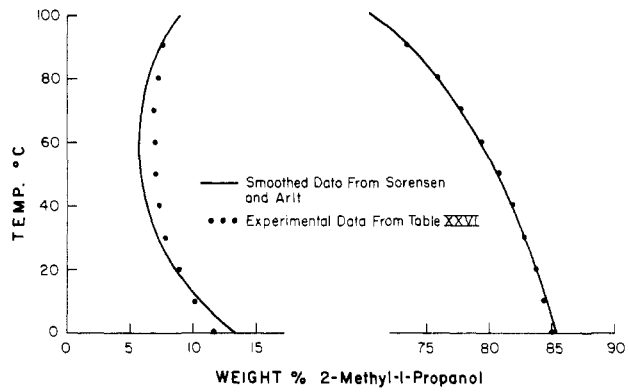

Figure 3. Mutual solubility of water and 2-methyl-1-propanol.

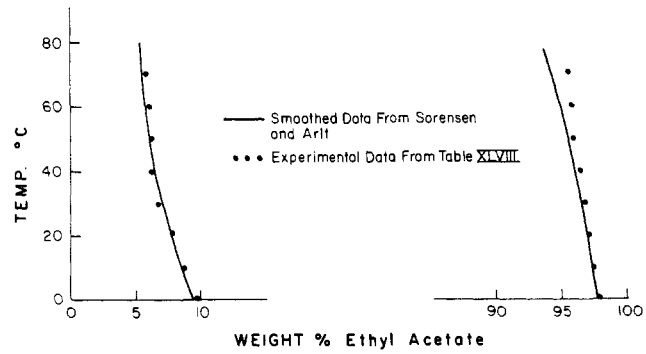

Figure 4. Mutual solubility of water and ethyl acetate.

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There are several interesting conclusions from studying the data. Solubility seems to depend primarily on the number of carbon atoms in the molecule. For example, the solubility of 3,5,5-trimethyl-1-hexanol in water is 0.05 wt % at 30 °C as compared to a value of 0.031 wt % for 1-nonanol at the same temperature. The solubility of water in the organic layer is 2.92 wt % at 30 °C for 3,5,5-trimethyl-1-hexanol as compared to a value of 3.92% for 1-nonanol. The solubility of methyl caproate in water is 0.167% at 30 °C as compared to an identical value for butyl propionate. The solubility of water in the organic layer is 0.60% for methyl caproate as compared to 0.86% for butyl propionate.

Cyclic alcohols show higher solubility than aliphatics having the same number of carbon atoms. For many systems, solubility of water in the organic layer remains quite high, even when the solubility of organic in water has become very low.

As can be seen from Figures 1–4, solubility of organic in water first shows a decreasing solubility with temperature. In the case of the alcohols, the solubility curve usually goes through a minimum at about 60 °C and then starts increasing. In the case of the esters, solubility of organic in water usually decreases continuously over the temperature range of zero–90 °C. For all systems studied, solubility of water in the organic layer increases with temperature. This complex solubility behavior is of some practical importance, because solubility equations often assume increasing solubility with temperature, and equations of this type will be in error for these systems.

Experimental data and mean deviations for all systems studied are given in Tables I–C.

Table I. Mutual Solubility of Water and 2-Butanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	26.0	49.1
10.0	23.5	39.5
20.0	19.6	35.9
29.9	17.0	34.5
40.0	15.1	32.4
50.0	14.0	
60.3	13.4	32.4
70.1	13.3	34.3
80.1	13.6	35.8
90.2	14.5	37.4
std devn	0.2	0.3

[a] A: 2-Butanol (99%). B: Water.

Table II. Mutual Solubility of Water and 2-Phenylethanol[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0		7.10
10.0	2.61	7.95
19.7	2.45	8.06
30.5	2.32	8.54
40.0	2.38	8.89
50.0	2.55	9.42
60.3	2.67	10.24
std devn	0.02	0.03

[a] Does not separate well at higher temperatures. [b] A: 2-Phenylethanol (98%). B: Water.

Table III. Mutual Solubility of Water and Cyclohexanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	6.77	11.9
9.3		12.0
9.5	5.40	
19.3		11.7
19.7	4.44	
30.6	3.74	11.7
40.0	3.63	12.0
50.0	3.49	12.4
60.3	3.37	13.0
70.1	3.44	13.6
80.2	3.60	14.3
90.3	3.75	15.3
std devn	0.02	0.15

[a] A: Cyclohexanol (99%). B: Water.

Table IV. Mutual Solubility of Water and Cyclohexylmethanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.14	4.8
9.5	1.06	4.6
19.8	0.84	5.0
29.9	0.83	5.2
39.8	0.76	5.6
50.2	0.74	6.0
60.0	0.74	6.4
70.0	0.77	6.9
80.0	0.84	7.6
90.2	0.92	8.0
std devn	0.01	0.1

[a] A: Cyclohexylmethanol (98%). B: Water.

Table V. Mutual Solubility of Water and Benzyl Alcohol[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	4.8	6.7
9.8	4.7	7.3
20.1	4.3	8.3
29.6	4.3	9.8
40.2	4.6	9.9
50.0	5.2	11.2
60.3		12.2
70.1		13.7
80.2		15.4
90.3		17.4
std devn	0.1	0.1

[a] Does not separate well above 50 °C. [b] A: Benzyl alcohol (98%). B: Water.

Table VI. Mutual Solubility of Water and 3,3-Dimethyl-2-butanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	3.80	6.81
10.0	2.77	7.09
19.8	2.41	7.08
30.5	2.03	7.44
39.9	1.80	7.28
50.0	1.64	7.45
60.0	1.54	7.50
69.8	1.50	7.86
79.9	1.49	7.69
90.2	1.34	8.38
std devn	0.01	0.07

[a] A: 3,3-Dimethyl-2-butanol (97%). B: Water.

Table VII. Mutual Solubility of Water and 3-Heptanol

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	0.87	
10.0	0.65	2.71
19.9	0.51	2.98
29.8	0.42	3.31
40.0	0.38	3.49
50.0	0.35	3.71
60.0	0.33	4.11
70.0	0.35	3.99
79.8	0.30	4.15
90.2	0.31	5.13
std devn	0.02	0.05

[a] A: 3-Heptanol (99%). B: Water.

Table VIII. Mutual Solubility of Water and 2-Octanol

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	0.221	
10.0	0.166	3.55
20.1	0.128	3.63
29.6	0.100	3.73
39.5	0.095	4.02
50.0	0.088	3.99
60.3	0.091	4.24
70.1	0.098	4.30
80.1	0.102	4.29
90.5	0.122	4.69
std devn	0.002	0.04

[a] A: 2-Octanol (98%). B: Water.

Table IX. Mutual Solubility of Water and 3-Octanol

temp, °C	solubility, wt % A in B[a]	B in A[a]
0		1.67
10.0	0.197	2.14
19.6	0.150	2.29
30.6	0.121	2.50
40.3	0.108	2.84
50.1	0.103	2.84
60.0	0.102	3.09
70.0	0.102	3.60
80.0	0.106	3.49
90.1	0.116	
std devn	0.008	0.03

[a] A: 3-Octanol (99+%). B: Water.

Table X. Mutual Solubility of Water and 1-Nonanol

temp, °C	solubility, wt % A in B[a]	B in A[a]
0		3.22
9.8	0.036	3.72
20.0	0.028	3.68
29.6	0.031	3.92
39.6	0.034	3.94
49.8	0.032	3.93
60.1	0.034	4.03
70.5	0.033	3.94
80.2	0.028	4.26
90.5	0.030	4.29
std devn	0.001	0.01

[a] A: 1-Nonanol (99%). B: Water.

Table XI. Mutual Solubility of Water and 2-Nonanol

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	0.063	3.04
9.9	0.053	2.89
19.8	0.039	3.14
30.0	0.033	3.28
40.0	0.022	3.32
50.0	0.019	3.49
60.1	0.021	3.49
70.2	0.025	3.93
80.3	0.022	4.02
90.5	0.028	4.10
std devn	0.001	0.06

[a] A: 2-Nonanol (99%). B: Water.

Table XII. Mutual Solubility of Water and 1-Decanol[a]

temp, °C	solubility, wt % A in B[b]	B in A[b]
19.8		3.68
29.6	0.021	3.35
40.3	0.026	3.48
50.0	0.026	3.59
60.3	0.028	3.58
70.2	0.022	3.58
80.2	0.024	3.67
90.4	0.023	3.82
std devn	0.001	0.03

[a] Freezes at 5 °C. [b] A: 1-Decanol (99+%). B: Water.

Table XIII. Mutual Solubility of Water and 2-Methylcyclohexanol

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	2.68	
10.0	2.24	6.1
20.1	1.77	6.4
30.6	1.54	6.6
39.8	1.30	6.6
50.0	1.19	6.9
60.1	1.18	6.9
70.2	1.12	7.5
80.1	1.20	7.7
90.2		8.0
std devn	0.08	0.2

[a] A: 2-Methylcyclohexanol (99%). B: Water.

Table XIV. Mutual Solubility of Water and 2-Ethyl-1-butanol

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	1.61	3.84
9.7	1.25	4.27
20.2	0.92	4.67
30.9	0.83	4.99
40.3	0.82	5.45
50.0	0.79	5.82
60.3	0.81	6.25
70.2	0.80	6.81
80.3	0.87	6.93
90.5	0.94	7.61
std devn	0.01	0.03

[a] A: 2-Ethyl-1-butanol (98%). B: Water.

Table XV. Mutual Solubility of Water and 3,3,5-Trimethyl-1-hexanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0		2.30
10.0		2.42
19.8		2.57
30.7	0.118	2.80
39.8	0.107	3.02
50.0	0.080	3.18
60.1	0.066	3.41
70.3	0.087	3.45
80.3	0.120	3.54
90.5	0.137	
std devn	0.005	0.01

[a] A: 3,3,5-Trimethyl-1-hexanol (98%). B: Water.

Table XVI. Mutual Solubility of Water and 3,5,5-Trimethyl-1-hexanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.06	2.31
10.1	0.05	2.47
19.9		2.66
29.7	0.05	2.92
39.7	0.05	3.02
50.0	0.06	3.17
60.1	0.08	3.18
70.5	0.05	3.72
80.3	0.07	3.81
90.5	0.08	4.22
std devn	0.01	0.05

[a] A: 3,5,5-Trimethyl-1-hexanol (98%). B: Water.

Table XVII. Mutual Solubility of Water and 2,6-Dimethyl-4-heptanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.094	0.92
9.8	0.107	1.01
20.1	0.066	1.01
30.6	0.053	1.18
40.0	0.043	1.36
50.0	0.052	1.53
60.4	0.031	1.68
70.3	0.038	2.04
80.4	0.032	2.21
90.5	0.036	2.26
std devn	0.005	0.01

[a] A: 2,6-Dimethyl-4-heptanol (99%). B: Water.

Table XVIII. Mutual Solubility of Water and 3-Methyl-1-pentanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.48	5.33
9.6	1.13	5.61
20.0	1.01	5.96
30.6	0.88	6.35
40.3	0.84	6.65
50.0	0.85	7.07
60.0	0.82	7.48
70.0	0.84	7.88
80.0	0.94	8.43
90.5	1.01	9.58
std devn	0.03	0.04

[a] A: 3-Methyl-1-pentanol (99%). B: Water.

Table XIX. Mutual Solubility of Water and 5-Methyl-2-hexanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.940	
9.0	0.675	4.25
20.0	0.525	4.43
30.7	0.462	4.76
40.2	0.434	4.85
50.0	0.380	5.24
60.3	0.383	5.55
70.3	0.394	5.80
80.2	0.414	6.10
90.3	0.427	6.47
std devn	0.004	0.01

[a] A: 5-Methyl-2-hexanol (99%). B: Water.

Table XX. Mutual Solubility of Water and Cyclopentanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	14.43	17.1
19.2	10.66	17.8
30.2	9.55	18.0
40.8	8.81	18.7
50.1	8.32	19.3
60.5	8.21	20.2
70.3	8.30	21.3
80.3	8.62	22.6
90.5	9.20	24.5
std devn	0.05	0.2

[a] A: Cyclopentanol (99%). B: Water.

Table XXI. Mutual Solubility of Water and 3-Methylcyclohexanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.97	6.67
9.7	1.65	6.60
20.0	1.46	6.94
30.5	1.23	7.27
40.0	1.09	7.51
49.8	1.06	7.80
60.2	1.07	8.21
70.5	1.09	8.48
80.5	1.18	8.94
90.7	1.25	9.75
std devn	0.03	0.04

[a] A: 3-Methylcyclohexanol (99%). B: Water.

Table XXII. Mutual Solubility of Water and 4-Methylcyclohexanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.86	8.65
9.5	1.55	8.47
20.3	1.29	8.50
30.5	1.14	8.62
40.1	1.06	8.88
50.0	1.02	8.95
60.4	0.89	9.15
70.2	0.91	9.48
80.3	1.10	9.93
90.5	1.16	10.18
std devn	0.02	0.05

[a] A: 4-Methylcyclohexanol (99%). B: Water.

Table XXIII. Mutual Solubility of Water and 2,6-Dimethylcyclohexanol

temp, °C	solubility, wt %: A in B[a]	B in A[a]
0	0.83	2.54
9.5	0.64	2.86
19.7	0.49	3.16
30.6	0.41	3.39
40.0	0.36	3.48
49.9	0.35	3.73
60.5	0.42	3.73
70.6	0.36	3.73
80.5	0.36	3.82
90.6	0.43	3.98
std devn	0.03	0.03

[a] A: 2,6-Dimethylcyclohexanol (mixed isomers, 99%). B: Water.

Table XXIV. Mutual Solubility of Water and Cycloheptanol

temp, °C	solubility, wt %: A in B[a]	B in A[a]
0	2.24	
9.5	1.88	7.2
20.0	1.59	7.4
30.7	1.43	7.6
39.3	1.20	7.8
50.3	1.17	8.1
60.4	1.26	8.4
70.5	1.25	8.8
80.4	1.28	9.2
90.6	1.46	9.6
std devn	0.06	0.1

[a] A: Cycloheptanol (99%). B: Water.

Table XXV. Mutual Solubility of Water and Cyclooctanol

temp, °C	solubility, wt %: A in B[a]	B in A[a]
10.0	0.80	
20.0	0.69	5.09
31.0	0.61	5.18
40.0	0.60	5.49
50.0	0.66	5.49
60.5	0.61	5.83
70.3	0.61	6.05
80.5	0.66	6.33
90.5	0.73	6.84
std devn	0.01	0.02

[a] A: Cyclooctanol (96%). B: Water.

Table XXVI. Mutual Solubility of Water and 2-Methyl-1-propanol

temp, °C	solubility, wt %: A in B[a]	B in A[a]
0	11.60	15.0
9.8	10.05	15.6
19.7	8.84	16.4
30.6	7.87	17.2
40.4	7.30	18.2
50.1	7.08	19.3
60.2	7.05	20.6
70.3	6.93	22.3
80.5	7.31	24.1
90.7	7.71	26.6
std devn	0.08	0.1

[a] A: 2-Methyl-1-propanol (99+%). B: Water.

Table XXVII. Mutual Solubility of Water and 1-Butanol

temp, °C	solubility, wt %: A in B[a]	B in A[a]
0	10.33	19.0
9.6	8.98	19.7
20.0	8.03	20.1
30.8	7.07	20.6
40.1	6.77	21.4
50.0	6.54	22.2
60.1	6.35	24.0
70.2	6.73	24.8
80.1	7.04	27.4
90.6	7.26	30.6
std devn	0.02	0.1

[a] A: 1-Butanol (99+%). B: Water.

Table XXVIII. Mutual Solubility of Water and 4-Heptanol

temp, °C	solubility, wt %: A in B[a]	B in A[a]
0	0.83	2.14
9.5	0.70	2.29
20.5	0.47	2.60
30.6	0.40	2.88
40.3	0.37	3.12
50.0	0.34	3.37
60.4	0.33	3.62
70.2	0.32	3.80
80.5	0.33	4.18
90.7	0.36	4.58
std devn	0.01	0.05

[a] A: 4-Heptanol (99%). B: Water.

Table XXIX. Mutual Solubility of Water and 1-Undecanol[a]

temp, °C	solubility, wt %: A in B[b]	B in A[b]
19.8	0.030	3.21
29.9	0.051	3.09
40.3	0.090	3.09
50.0	0.065	3.02
60.1		3.10
70.2	0.095	3.23
80.1	0.039	3.37
90.5	0.095	3.37
std devn	0.004	0.02

[a] Freezes at 14 °C. [b] A: 1-Undecanol (99%). B: Water.

Table XXX. Mutual Solubility of Water and 1-Dodecanol[a]

temp, °C	solubility, wt %: A in B[b]	B in A[b]
29.5	0.04	2.87
40.0	0.05	2.85
50.2	0.09	2.69
60.5	0.15	2.94
70.5	0.09	2.70
80.3	0.14	2.89
90.8	0.18	2.96
std devn	0.02	0.01

[a] Freezes at 24 °C. [b] A: 1-Dodecanol (98%). B: Water.

Table XXXI. Mutual Solubility of Water and 1-Phenyl-1-propanol

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
20.0	1.08	3.16
30.0	0.99	3.41
40.1	0.93	3.61
50.0	0.93	3.91
60.5	0.99	4.03
70.4	0.98	4.23
80.7	1.08	4.77
90.5	1.15	4.95
std devn	0.03	0.02

[a] A: 1-Phenyl-1-propanol (98%). B: Water.

Table XXXII. Mutual Solubility of Water and Octyl Formate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0		0.421
9.2	0.078	0.445
19.0	0.064	0.417
29.4	0.039	0.428
39.5	0.040	0.445
50.0	0.071	0.455
60.0	0.028	0.478
70.1	0.044	0.494
80.2	0.036	0.574
90.5	0.061	0.539
std devn	0.003	0.003

[a] A: Octyl formate (99%). B: Water.

Table XXXIII. Solubility of Water in Propyl Formate[a]

temp, °C	solubility, B in A,[b] wt %
0	1.07
9.5	1.32
20.3	1.58
31.0	1.91
40.3	2.27
50.1	3.01
61.0	3.74
70.6	5.25
std devn	0.02

[a] Data subject to error because of substantial hydrolysis in aqueous layer. [b] A: Propyl formate (96%). B: Water.

Table XXXIV. Solubility of Water in Isopropyl Formate[a]

temp, °C	solubility, B in A,[b] wt %
0	1.05
9.6	1.33
19.7	1.66
30.7	1.76
40.0	2.17
49.9	3.03
60.2	3.60
std devn	0.05

[a] Data subject to error because of substantial hydrolysis in aqueous layer. [b] A: Isopropyl formate (96%). B: Water.

Table XXXV. Solubility of Water in Butyl Formate[a]

temp, °C	solubility B in A,[b] wt %
0	0.80
9.5	1.05
20.2	1.14
30.8	1.04
40.0	1.21
50.2	1.37
60.5	1.55
70.3	1.54
80.1	1.66
90.6	1.93
std devn	0.02

[a] Data subject to error because of substantial hydrolysis in aqueous layer. [b] A: Butyl formate (97%). B: Water.

Table XXXVI. Mutual Solubility of Water and Isobutyl Formate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	1.14	
9.8	1.11	0.71
20.8	0.93	0.86
30.8	0.82	1.05
39.8	0.76	1.02
50.3	0.79	1.21
60.4	0.78	1.35
70.3	dec	1.39
80.2	dec	1.67
std devn	0.01	0.01

[a] Some hydrolysis at all temperatures. [b] A: Isobutyl formate (96%). B: Water.

Table XXXVII. Mutual Solubility of Water and Ethyl Benzoate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	0.108	1.19
9.5		0.82
19.6	0.085	0.99
30.5	0.081	0.92
40.0	0.106	0.98
50.0	0.108	1.12
60.1	0.117	1.03
70.5	0.121	
80.2	0.121	
90.3	0.143	
std devn	0.002	0.01

[a] Layers difficult to separate. [b] A: Ethyl benzoate (97%). B: Water.

Table XXXVIII. Mutual Solubility of Water and Isoamyl Formate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	0.198	0.76
9.3	0.151	1.09
19.6	0.108	1.08
31.0	0.116	1.20
39.6	0.111	1.34
50.0	0.135	1.49
60.4		1.75
70.5	0.115	1.92
80.3	0.082	2.07
90.5	0.131	2.36
std devn	0.005	0.02

[a] Some hydrolysis at all temperatures. [b] A: Isoamyl formate (96%). B: Water.

Table XXXIX. Mutual Solubility of Water and Hexyl Formate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0		0.526
8.7	0.17	0.525
19.7	0.15	0.508
29.7	0.13	0.599
39.6	0.13	0.660
49.8	0.11	0.654
60.2	0.11	0.719
70.3	0.12	
80.2	0.13	0.847
90.6	0.14	0.799
std devn	0.01	0.003

[a] Slight hydrolysis. [b] A: Hexyl formate (96%). B: Water.

Table XL. Mutual Solubility of Water and Heptyl Formate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0		0.68
9.1		0.63
19.5	0.162	0.68
29.7	0.142	
39.6	0.078	0.80
50.0	0.071	0.85
60.1	0.063	1.12
70.1	0.087	1.06
80.0	0.075	1.08
90.6	0.056	1.19
std devn	0.002	0.01

[a] A: Heptyl formate (97%). B: Water.

Table XLI. Mutual Solubility of Water and Dimethyl Carbonate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
9.8	12.5	2.16
20.5	12.7	2.61
29.7	12.4	3.21
40.1	13.2	4.10
50.0	13.5	4.66
60.4	14.3	6.81
70.1		7.76
79.5		8.33
std devn	0.1	0.06

[a] Freezes at 4 °C. Layers difficult to separate. [b] A: Dimethyl carbonate (99%). B: Water.

Table XLII. Mutual Solubility of Water and Diethyl Carbonate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	2.49	0.65
9.9	2.15	0.72
20.1	1.90	0.89
30.0	1.67	1.06
40.0	1.58	1.12
50.0	1.53	1.32
60.2	1.54	1.62
70.1	1.63	1.73
80.1	1.69	2.37
90.3	1.63	2.78
std devn	0.02	0.01

[a] A: Diethyl carbonate (99%). B: Water.

Table XLIII. Mutual Solubility of Water and Methyl Propionate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	7.80	1.51
10.0	6.89	1.77
20.2	6.24	2.54
30.9	5.71	2.40
40.3	5.35	2.78
50.3	5.10	2.81
60.1	5.05	3.09
70.2	4.79	3.24
std devn	0.03	0.01

[a] A: Methyl propionate (98%). B: Water.

Table XLIV. Mutual Solubility of Water and Ethyl Propionate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	3.26	0.89
9.7	2.59	1.04
19.5	2.23	1.24
29.7	1.93	1.50
39.5	1.75	1.70
50.0	1.66	1.86
60.1	1.61	1.92
70.2	1.58	1.98
80.3	1.59	2.20
90.5		2.39
std devn	0.01	0.02

[a] A: Ethyl propionate (97%). B: Water.

Table XLV. Mutual Solubility of Water and Propyl Propionate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.01	0.63
9.1	0.80	0.70
19.3	0.66	0.80
29.6	0.52	0.94
39.5	0.50	1.02
50.0	0.43	1.24
60.3	0.43	1.22
70.6	0.44	1.22
80.3	0.44	1.21
90.5	0.36	1.31
std devn	0.01	0.02

[a] A: Propyl propionate (98%). B: Water.

Table XLVI. Mutual Solubility of Water and Butyl Propionate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.298	0.48
9.4	0.230	0.53
19.8	0.197	0.62
30.6	0.167	0.86
40.2	0.144	0.85
50.0	0.146	0.85
59.9	0.142	0.89
70.1	0.140	0.92
80.2	0.147	0.93
90.4	0.142	1.00
std devn	0.003	0.01

[a] A: Butyl propionate (99%). B: Water.

Table XLVII. Mutual Solubility of Water and Hexyl Propionate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.029	0.39
9.7	0.022	0.34
20.0	0.024	0.34
29.6	0.012	0.45
39.8	0.012	0.48
50.0	0.014	0.46
60.0	0.016	0.50
70.3	0.018	0.49
80.3	0.017	0.51
90.6	0.018	0.83
std devn	0.001	0.02

[a] A: Hexyl propionate (99+%). B: Water.

Table XLVIII. Mutual Solubility of Water and Ethyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	9.71	2.13
9.8	8.62	2.48
20.2	7.79	2.88
29.7	6.81	3.26
39.5	6.28	3.64
50.0	6.20	4.04
59.9	6.06	4.23
70.5	5.88	4.44
std devn	0.05	0.02

[a] A: Ethyl acetate (99.9%). B: Water.

Table XLIX. Mutual Solubility of Water and Propyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	3.21	1.16
9.5	2.78	1.36
20.0	2.26	1.59
30.0	1.98	1.88
40.0	1.87	2.17
50.0	1.72	2.29
60.1	1.64	2.34
70.5	1.72	2.95
80.0	1.66	3.01
90.2	1.35	
std devn	0.02	0.04

[a] A: Propyl acetate (99%). B: Water.

Table L. Mutual Solubility of Water and Isopropyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	4.08	
9.0	3.46	1.34
19.9	2.79	1.58
29.7	2.44	1.75
39.8	2.19	2.20
50.0	2.07	2.23
62.2	1.92	2.38
74.6	1.80	2.50
std devn	0.02	0.01

[a] A: Isopropyl acetate (99%). B: Water.

Table LI. Mutual Solubility of Water and *sec*-Butyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.330	0.83
9.6	0.879	0.95
19.5	0.869	1.06
29.7	0.753	1.30
39.9	0.663	1.36
50.0	0.629	1.46
60.1	0.613	1.60
70.5	0.605	1.62
80.2	0.622	1.84
90.5	0.604	1.69
std devn	0.005	0.01

[a] A: *sec*-Butyl acetate (99%). B: Water.

Table LII. Mutual Solubility of Water and Isobutyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.03	0.72
10.0	0.83	0.82
19.7	0.66	0.95
29.9	0.61	1.12
39.7	0.54	1.21
50.0	0.49	1.26
60.5	0.57	1.29
70.1	0.53	1.36
80.2	0.55	1.65
90.2		1.49
std devn	0.02	0.01

[a] A: Isobutyl acetate (99%). B: Water.

Table LIII. Mutual Solubility of Water and Butyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.96	0.78
9.1	0.76	0.84
19.7	0.64	0.98
30.3	0.52	1.25
39.6	0.50	1.35
50.0	0.50	1.28
60.2	0.50	1.38
70.2	0.47	1.37
80.1	0.48	1.44
90.5	0.48	1.55
std devn	0.01	0.02

[a] A: Butyl acetate (99.9%). B: Water.

Table LIV. Mutual Solubility of Water and *tert*-Butyl Acetate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	1.170	0.83
9.2	1.000	0.97
19.2	0.803	1.13
29.6	0.703	1.30
40.0	0.620	1.32
50.0	0.573	1.35
60.5	0.526	1.47
70.5	0.538	1.71
80.5	0.499	1.69
88.0		1.66
std devn	0.004	0.02

[a] Slight hydrolysis in aqueous layer. [b] A: *tert*-Butyl acetate (99+%). B: Water.

Table LV. Mutual Solubility of Water and Pentyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.29	0.79
9.8		0.81
19.7	0.22	0.86
30.6	0.16	1.22
39.5	0.16	1.09
50.0	0.10	1.12
60.3	0.10	1.27
70.2	0.17	1.37
80.1	0.17	1.38
90.5		1.54
std devn	0.01	0.02

[a] A: Pentyl acetate (99%). B: Water.

Table LVI. Mutual Solubility of Water and Isopentyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.340	0.56
9.1	0.265	0.67
19.4	0.212	0.76
30.3	0.208	0.80
39.7	0.184	0.85
50.0	0.174	1.11
60.1	0.152	1.16
70.2	0.203	1.24
80.3	0.182	1.20
90.7	0.205	1.34
std devn	0.002	0.01

[a] A: Isopentyl acetate (99%). B: Water.

Table LVII. Mutual Solubility of Water and Hexyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.084	0.494
9.5	0.070	0.496
19.7	0.043	0.566
29.6	0.054	0.730
40.0	0.056	0.746
50.0	0.047	0.633
60.7	0.051	0.695
70.0	0.057	0.749
80.0	0.063	0.780
90.2	0.066	0.785
std devn	0.003	0.004

[a] A: Hexyl acetate (99%). B: Water.

Table LVIII. Mutual Solubility of Water and Cyclohexyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.393	0.67
9.4	0.317	0.65
19.8	0.304	0.71
29.7	0.260	0.79
39.6	0.251	0.90
49.8	0.229	0.99
60.1	0.218	1.05
70.0	0.224	1.07
80.1	0.257	1.15
90.3	0.286	1.36
std devn	0.002	0.01

[a] A: Cyclohexyl acetate (99%). B: Water.

Table LIX. Mutual Solubility of Water and Heptyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.023	0.34
9.2	0.018	0.38
19.6	0.020	0.45
30.6	0.023	0.48
40.3	0.021	0.59
50.0	0.020	0.59
60.2	0.019	0.63
70.2	0.017	0.65
80.4	0.015	0.67
90.6	0.019	0.67
std devn	0.001	0.01

[a] A: Heptyl acetate (98%). B: Water.

Table LX. Mutual Solubility of Water and Isononyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.018	0.334
9.2	0.023	0.313
19.4	0.020	0.292
29.6	0.018	0.372
39.8	0.021	0.392
49.8	0.021	0.371
60.3	0.013	0.369
70.2	0.018	0.387
80.3	0.026	0.363
90.5	0.021	0.402
std devn	0.002	0.003

[a] A: Isononyl acetate (98%). B: Water.

Table LXI. Mutual Solubility of Water and Benzyl Acetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.253	0.62
9.7	0.253	0.64
20.0	0.266	0.78
30.7	0.240	0.92
40.3	0.278	1.06
49.8	0.305	1.21
60.1	0.336	1.39
70.4	0.375	1.59
80.1	0.409	1.83
90.4	0.448	2.17
std devn	0.002	0.03

[a] A: Benzyl acetate (99%). B: Water.

Table LXII. Mutual Solubility of Water and Methyl Butyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	2.62	0.84
9.4	2.24	0.97
19.7	1.87	1.14
29.7	1.68	1.27
39.5	1.54	1.45
50.0	1.44	1.50
60.3	1.45	1.75
70.3	1.42	1.66
80.1	1.41	2.02
90.5	1.26	2.02
std devn	0.01	0.02

[a] A: Methyl butyrate (99%). B: Water.

Table LXIII. Mutual Solubility of Water and Ethyl Butyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.06	0.56
9.5	0.81	0.68
20.0	0.69	0.79
31.0	0.58	1.02
39.9	0.52	1.07
50.0	0.46	1.22
60.4	0.46	1.17
70.2	0.46	1.28
80.3	0.46	1.18
90.5	0.44	1.26
std devn	0.01	0.01

[a] A: Ethyl butyrate (99%). B: Water.

Table LXIV. Mutual Solubility of Water and Butyl Butyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.122	0.339
9.5	0.102	0.370
20.0	0.066	0.440
29.7	0.056	0.427
39.6	0.052	0.540
50.0	0.051	0.577
59.9	0.047	0.642
70.2	0.047	0.651
80.0	0.049	0.680
90.3	0.051	0.683
std devn	0.001	0.004

[a] A: Butyl butyrate (99%). B: Water.

Table LXV. Mutual Solubility of Water and Methyl Isobutyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	2.68	1.03
9.1	2.23	1.21
18.9	1.96	1.30
29.5	1.69	1.48
39.9	1.52	1.62
49.8	1.46	1.79
60.4	1.38	2.25
70.5	1.40	2.07
80.3	1.32	2.15
std devn	0.01	0.02

[a] A: Methyl isobutyrate (99%). B: Water.

Table LXVI. Mutual Solubility of Water and Ethyl Isobutyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.01	0.59
10.0	0.77	0.67
19.8	0.68	0.82
29.7	0.58	1.10
40.1	0.51	1.13
50.1	0.45	1.16
60.2	0.44	1.13
70.4	0.45	1.16
80.5	0.44	1.46
90.6	0.38	1.51
std devn	0.01	0.01

[a] A: Ethyl isobutyrate (99%). B: Water.

Table LXVII. Mutual Solubility of Water and Methyl Valerate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.80	0.56
9.2	0.64	0.63
19.5	0.53	0.75
29.5	0.45	1.02
39.8	0.47	1.05
50.0	0.46	1.05
60.1	0.44	1.10
70.2	0.46	1.12
80.3	0.46	1.33
90.5	0.45	1.57
std devn	0.01	0.02

[a] A: Methyl valerate (99%). B: Water.

Table LXVIII. Mutual Solubility of Water and Ethyl Isovalerate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.34	0.412
9.0	0.24	0.473
19.4	0.22	0.558
30.6	0.20	0.645
39.8	0.17	0.707
49.5	0.16	0.789
60.1	0.15	0.827
70.0	0.16	0.845
80.3	0.16	0.943
90.5	0.16	1.123
std devn	0.01	0.004

[a] A: Ethyl isovalerate (99%). B: Water.

Table LXIX. Mutual Solubility of Water and Methyl Trimethylacetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.81	0.49
9.7	0.66	0.57
19.7	0.56	0.66
29.7	0.51	0.80
40.0	0.45	0.93
50.1	0.43	1.03
60.5	0.42	1.01
70.4	0.39	1.10
80.5	0.41	1.18
90.5	0.33	1.15
std devn	0.02	0.02

[a] A: Methyl trimethylacetate (99%). B: Water.

Table LXX. Mutual Solubility of Water and Ethyl Trimethylacetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.304	0.35
9.5	0.298	0.43
20.0	0.183	0.51
30.7	0.168	0.61
40.1	0.135	0.67
50.0	0.152	0.71
60.2	0.126	0.76
70.3	0.120	0.78
80.4	0.124	0.82
90.4	0.112	0.81
std devn	0.004	0.01

[a] A: Ethyl trimethylacetate (98%). B: Water.

Table LXXI. Mutual Solubility of Water and Methyl Chloroacetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	5.44	0.71
9.8	5.18	0.85
19.8	5.16	1.03
29.8	5.09	1.31
39.5	5.31	1.42
50.2	5.34	1.84
60.0	5.79	2.12
70.2	5.79	2.56
80.1	6.70	3.04
90.1	7.00	3.91
std devn	0.08	0.03

[a] A: Methyl chloroacetate (99%). B: Water.

Table LXXII. Mutual Solubility of Water and Ethyl Chloroacetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	2.49	0.47
9.0	2.50	0.57
19.8	2.00	0.67
30.8	1.90	0.81
39.9	1.88	0.89
50.0	1.92	1.17
60.1	1.97	1.45
70.2	2.11	1.76
80.1	2.19	2.01
90.5	2.33	2.46
std devn	0.01	0.01

[a] A: Ethyl chloroacetate (99+%). B: Water.

Table LXXIII. Mutual Solubility of Water and Methyl Dichloroacetate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	1.09	0.22
9.6	0.86	0.27
20.1	0.33	0.32
29.6	0.33	0.37
39.5	0.35	0.48
50.0	0.37	0.51
60.0	0.36	0.60
70.3	0.37	0.73
79.9	0.46	1.40
90.2	0.44	1.80
std devn	0.04	0.01

[a] A: Methyl dichloroacetate (99%). B: Water.

Table LXXIV. Mutual Solubility of Water and Methyl Enanthate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.105	0.55
9.5	0.122	0.58
19.3	0.094	0.67
30.0	0.090	0.70
39.6	0.063	0.64
49.8		0.76
60.5	0.054	0.73
70.5	0.087	0.72
80.5	0.066	0.76
90.5	0.053	0.87
std devn	0.001	0.01

[a] A: Methyl enanthate (99%). B: Water.

Table LXXV. Mutual Solubility of Water and Methyl Caproate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.241	0.38
9.3	0.177	0.46
20.0	0.166	0.55
29.7	0.167	0.60
39.5	0.129	0.68
50.0	0.137	0.75
60.0	0.132	0.81
70.2	0.128	0.80
80.2	0.138	0.83
90.5	0.147	0.89
std devn	0.001	0.01

[a] A: Methyl caproate (99%). B: Water.

Table LXXVI. Mutual Solubility of Water and Ethyl Caproate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.107	0.36
9.6	0.102	0.39
19.7	0.083	0.47
29.6	0.075	0.51
39.8	0.070	0.56
50.0	0.060	0.58
60.6	0.049	0.62
70.5	0.055	0.66
80.4	0.055	0.71
90.6	0.059	0.74
std devn	0.007	0.01

[a] A: Ethyl caproate (99+%). B: Water.

Table LXXVII. Mutual Solubility of Water and Diethyl Oxalate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	5.47	0.60
9.5	4.45	0.77
19.7	3.82	1.08
30.9	3.71	1.20
39.8	3.17	1.35
49.7	2.74	1.70
60.0		2.08
70.2		2.52
80.4		3.32
90.7		3.88
std devn	0.09	0.03

[a] Difficult to separate layers and some decomposition at temperatures over 60 °C. [b] A: Diethyl oxalate (99%). B: Water.

Table LXXVIII. Mutual Solubility of Water and Diethyl Succinate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	2.86	1.28
10.0	2.67	1.51
20.7	2.13	1.78
29.7	1.99	2.08
39.8	1.79	2.42
50.0	1.79	2.87
60.3	1.74	3.24
70.0	1.79	3.60
80.1	1.84	3.97
90.7	2.09	4.23
std devn	0.05	0.07

[a] A: Diethyl succinate (99%). B: Water.

Table LXXIX. Mutual Solubility of Water and Dimethyl Glutarate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	7.1	2.30
9.4	6.3	2.63
20.0	6.1	3.28
29.6	5.9	3.56
39.5	5.8	4.12
49.8	5.8	4.64
60.3	6.1	5.31
70.2	6.4	7.11
80.0	6.6	7.14
90.5	8.1	8.23
std devn	0.10	0.03

[a] A: Dimethyl glutarate (98%). B: Water.

Table LXXX. Mutual Solubility of Water and Pentyl Formate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	0.36	0.99
9.1	0.31	0.97
19.9	0.27	1.07
30.9	0.26	1.11
39.6	0.26	1.25
50.0	0.27	1.34
60.1	0.24	1.37
70.2	0.27	1.49
80.0	0.29	1.49
90.5	0.26	2.41
std devn	0.01	0.02

[a] Some decomposition at all temperatures. [b] A: Pentyl formate (95%). B: Water.

Table LXXXI. Mutual Solubility of Water and Cyclohexyl Formate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0		1.10
9.3	1.70	1.42
19.0	0.65	1.56
29.6	0.39	1.37
39.5		1.39
49.9		1.64
69.9		1.90
80.0		2.13
90.3		2.50
std devn	0.01	0.02

[a] Substantial decomposition above 40 °C. [b] A: Cyclohexyl formate (95%). B: Water.

Table LXXXII. Mutual Solubility of Water and Methyl Trichloroacetate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0		0.26
9.5		0.21
20.0		0.19
29.6	0.09	
39.8	0.09	0.30
49.8	0.04	0.35
60.0	0.05	0.48
70.5	0.06	0.71
80.1	0.03	0.72
90.2	0.03	1.03
std devn	0.01	0.01

[a] Some decomposition above 40 °C. [b] A: Methyl trichloroacetate (99%). B: Water.

Table LXXXIII. Mutual Solubility of Water and Isopentyl Propionate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.097	0.43
9.3	0.100	0.43
19.3	0.065	0.48
29.7	0.056	0.54
40.0	0.063	0.60
49.8	0.045	0.53
60.0	0.056	0.60
70.0	0.075	
79.7	0.057	0.78
90.6	0.064	1.32
std devn	0.001	0.01

[a] A: Isopentyl propionate (99%). B: Water.

Table LXXXIV. Mutual Solubility of Water and Cyclohexyl Propionate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.109	0.83
9.5	0.096	0.71
20.2	0.079	0.79
30.6	0.073	0.94
39.6	0.065	0.82
50.0	0.061	0.68
60.1	0.073	0.72
70.2	0.066	0.94
80.2	0.080	1.09
90.6	0.075	1.22
std devn	0.001	0.05

[a] A: Cyclohexyl propionate (99%). B: Water.

Table LXXXV. Mutual Solubility of Water and Methyl 2-Chloropropionate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0		0.42
10.0	2.42	0.53
19.8	2.29	0.60
29.7	1.66	0.68
40.3	1.62	0.76
50.2	1.69	0.83
60.1	1.81	0.92
70.3	1.91	1.54
80.2	1.98	1.37
90.5	2.13	2.04
std devn	0.01	0.02

[a] A: Methyl 2-chloropropionate (97%). B: Water.

Table LXXXVI. Mutual Solubility of Water and Propyl Butyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.30	0.64
9.6	0.23	
20.1	0.19	0.63
29.6	0.15	0.64
39.5	0.14	0.66
49.8	0.17	0.84
60.1	0.21	1.48
70.1	0.15	
80.1	0.14	0.99
90.5	0.17	1.81
std devn	0.01	0.01

[a] A: Propyl butyrate (99%). B: Water.

Table LXXXVII. Mutual Solubility of Water and Isopropyl Butyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	3.12	1.71
9.7	3.08	1.87
19.5	2.65	1.82
30.8	2.75	2.10
39.5	2.57	2.09
49.7	2.49	2.30
60.2	2.49	2.61
70.1	2.70	2.82
80.0	2.84	3.07
90.2	2.98	3.15
std devn	0.02	0.02

[a] A: Isopropyl butyrate (98%). B: Water.

Table LXXXVIII. Mutual Solubility of Water and Pentyl Butyrate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	0.026	0.46
9.4	0.034	0.34
19.2	0.025	0.40
29.6	0.024	0.35
40.1	0.030	0.52
50.0	0.032	0.39
60.0	0.028	0.44
70.3		0.62
80.0	0.019	0.48
90.5	0.025	0.56
std devn	0.002	0.01

[a] Slight decomposition above 60 °C. [b] A: Pentyl butyrate (99%). B: Water.

Table LXXXIX. Mutual Solubility of Water and Isopentyl Butyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0		0.25
9.4	0.035	0.29
19.6	0.022	0.24
30.9	0.027	0.38
39.9	0.015	0.41
49.8	0.037	0.31
59.7	0.013	0.32
70.2	0.014	0.39
80.1	0.024	0.48
90.7	0.020	0.50
std devn	0.004	0.01

[a] A: Isopentyl butyrate (99%). B: Water.

Table XC. Mutual Solubility of Water and Methyl 4-Chlorobutyrate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	1.32	0.70
9.4	1.18	0.83
19.6	1.14	0.93
30.9	1.07	1.07
39.6	1.18	1.07
50.0	1.26	1.50
60.6	1.31	1.79
70.0	1.36	2.27
80.1	1.66	2.33
90.3	1.68	3.02
std devn	0.01	0.03

[a] Some decomposition at all temperatures. [b] A: Methyl 4-chlorobutyrate (98+%). B: Water.

Table XCI. Mutual Solubility of Water and Butyl Isobutyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.090	0.36
9.8	0.071	0.37
19.6	0.077	0.43
30.9	0.076	0.39
40.1	0.051	0.47
50.0	0.043	0.49
60.0	0.048	0.58
70.0	0.043	0.66
80.2	0.044	0.65
90.5	0.043	0.68
std devn	0.003	0.01

[a] A: Butyl isobutyrate (98%). B: Water.

Table XCII. Mutual Solubility of Water and Isobutyl Isobutyrate[a]

	solubility, wt %	
temp, °C	A in B[b]	B in A[b]
0	0.098	0.43
9.3		0.52
19.4	0.050	0.54
29.6	0.049	0.71
39.5	0.050	0.57
50.0	0.051	0.60
59.8	0.046	0.82
70.2	0.045	0.74
80.1	0.041	0.76
90.3	0.056	0.80
std devn	0.001	0.02

[a] Some decomposition at all temperatures. [b] A: Isobutyl isobutyrate (98%). B: Water.

Table XCIII. Mutual Solubility of Water and Hexyl Isobutyrate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0	0.0116	0.50
9.4	0.0061	0.31
19.5	0.0038	0.37
29.7		0.26
39.5	0.0032	
50.0	0.0076	0.44
59.8	0.0081	
70.1		0.40
80.0	0.0040	0.41
90.6	0.0087	0.42
std devn	0.0005	0.02

[a] A: Hexyl isobutyrate (98%). B: Water.

Table XCIV. Mutual Solubility of Water and Ethyl Caprylate

	solubility, wt %	
temp, °C	A in B[a]	B in A[a]
0		0.82
9.5	0.054	1.15
19.6	0.051	0.90
30.6	0.038	0.45
39.5		0.39
50.0	0.037	0.65
60.1	0.044	0.51
70.2	0.040	0.43
80.0	0.042	0.41
90.6		0.39
std devn	0.003	0.01

[a] A: Ethyl caprylate (99+%). B: Water.

Table XCV. Mutual Solubility of Water and Dimethyl Adipate[a]

temp, °C	solubility, wt % A in B[b]	B in A[b]
9.2	3.81	1.94
19.6	3.07	2.30
30.9	2.85	2.67
39.5	2.77	3.07
49.8	2.70	3.66
60.0	2.73	4.10
70.5	2.87	4.73
80.2	3.50	5.41
90.5	3.23	5.72
std devn	0.06	0.06

[a] Freezes at 8 °C. [b] A: Dimethyl adipate (98%). B: Water.

Table XCVI. Mutual Solubility of Water and Diethyl Adipate

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	1.07	1.08
9.8	1.26	1.11
20.5	0.69	
39.5	0.54	1.95
50.0	0.52	2.11
60.1	0.50	2.38
69.7	0.50	2.44
80.2	0.49	2.83
90.3	0.56	2.88
std devn	0.01	0.03

[a] A: Diethyl adipate (99%). B: Water.

Table XCVII. Mutual Solubility of Water and Methyl Salicylate

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	0.116	0.16
9.5	0.131	0.17
19.9	0.120	0.26
29.7	0.124	0.30
39.5	0.145	0.34
50.0	0.175	0.41
60.1		0.48
70.2	0.221	0.60
80.1	0.270	0.75
90.5	0.270	0.80
std devn	0.004	0.01

[a] A: Methyl salicylate (99+%). B: Water.

Table XCVIII. Mutual Solubility of Water and Ethyl Salicylate

temp, °C	solubility, wt % A in B[a]	B in A[a]
0		0.20
9.2	0.067	0.24
19.5	0.036	0.21
29.8	0.037	0.32
39.7	0.029	0.26
49.8	0.050	0.27
60.1	0.040	0.24
70.1	0.040	0.46
80.1	0.069	0.63
90.5	0.078	0.67
std devn	0.003	0.01

[a] A: Ethyl salicylate (97%). B: Water.

Table XCIX. Mutual Solubility of Water and Dimethyl Maleate

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	7.7	2.10
9.6	7.3	2.54
19.8	7.6	3.18
29.7	7.8	3.76
39.5	8.1	4.50
50.0	8.7	5.50
59.9	8.9	6.43
69.8	9.6	7.60
80.1	10.4	9.08
90.5	10.9	10.38
std devn	0.2	0.03

[a] A: Dimethyl maleate (99%). B: Water.

Table C. Mutual Solubility of Water and Methyl Benzoate

temp, °C	solubility, wt % A in B[a]	B in A[a]
0	0.221	0.46
9.7	0.221	0.54
20.1	0.213	0.65
29.6	0.282	0.73
40.2	0.247	0.84
49.8	0.258	0.98
60.1	0.286	1.24
70.2	0.325	1.38
80.3	0.358	1.56
90.5	0.408	2.04
std devn	0.002	0.02

[a] A: Methyl benzoate (99+%). B: Water.

Registry No. H_2O, 7732-18-5; 2-butanol, 78-92-2; 2-phenylethanol, 60-12-8; cyclohexanol, 108-93-0; cyclohexylmethanol, 100-49-2; benzyl alcohol, 100-51-6; 3,3-dimethyl-2-butanol, 464-07-3; 3-heptanol, 589-82-2; 2-octanol, 123-96-6; 3-octanol, 589-98-0; 1-nonanol, 143-08-8; 2-nonanol, 628-99-9; 1-decanol, 112-30-1; 2-methylcyclohexanol, 583-59-5; 2-ethyl-1-butanol, 97-95-0; 3,3,5-trimethyl-1-hexanol, 1484-87-3; 3,5,5-trimethyl-1-hexanol, 3452-97-9; 2,6-dimethyl-4-heptanol, 108-82-7; 3-methyl-1-pentanol, 589-35-5; 5-methyl-2-hexanol, 627-59-8; cyclopentanol, 96-41-3; 3-methylcyclohexanol, 591-23-1; 4-methylcyclohexanol, 589-91-3; 2,6-dimethylcyclohexanol, 5337-72-4; cycloheptanol, 502-41-0; cyclooctanol, 696-71-9; 2-methyl-1-propanol, 78-83-1; 1-butanol, 71-36-3; 4-heptanol, 589-55-9; 1-undecanol, 112-42-5; 1-dodecanol, 112-53-8; 1-phenyl-1-propanol, 93-54-9; octyl formate, 112-32-3; propyl formate, 110-74-7; isopropyl formate, 625-55-6; butyl formate, 592-84-7; isobutyl formate, 542-55-2; ethyl benzoate, 93-89-0; isoamyl formate, 110-45-2; hexyl formate, 629-33-4; heptyl formate, 112-23-2; dimethyl carbonate, 616-38-6; diethyl carbonate, 105-58-8; methyl propionate, 554-12-1; ethyl propionate, 105-37-3; propyl propionate, 106-36-5; butyl propionate, 590-01-2; hexyl propionate, 2445-76-3; ethyl acetate, 141-78-6; propyl acetate, 109-60-4; isopropyl acetate, 108-21-4; *sec*-butyl acetate, 105-46-4; isobutyl acetate, 110-19-0; butyl acetate, 123-86-4; *tert*-butyl acetate, 540-88-5; pentyl acetate, 628-83-7; isopentyl acetate, 123-92-2; hexyl acetate, 142-92-7; cyclohexyl acetate, 622-45-7; heptyl acetate, 112-06-1; isononyl acetate, 40379-24-6; benzyl acetate, 140-11-4; methyl butyrate, 623-42-7; ethyl butyrate, 105-54-4; butyl butyrate, 109-21-7; methyl isobutyrate, 547-63-7; ethyl isobutyrate, 97-62-1; methyl valerate, 624-24-8; ethyl isovalerate, 108-64-5; methyl trimethylacetate, 598-98-1; ethyl trimethylacetate, 3938-95-2; methyl chloroacetate, 96-34-4; ethyl chloroacetate, 105-39-5; methyl dichloroacetate, 116-54-1; methyl enanthate, 106-73-0; methyl caproate, 106-70-7; ethyl caproate, 123-66-0; diethyl oxalate, 95-92-1; diethyl succinate, 123-25-1; dimethyl glutarate, 1119-40-0; pentyl formate, 638-49-3; cyclohexyl formate, 4351-54-6; methyl trichloroacetate, 598-99-2; isopentyl propionate, 105-68-0; cyclohexyl propionate, 6222-35-1; methyl 2-chloropropionate, 17639-93-9; propyl butyrate, 105-66-8; isopropyl butyrate, 638-11-9; pentyl butyrate, 540-18-1; isopentyl butyrate, 106-27-4; methyl 4-chlorobutyrate, 3153-37-5; butyl isobutyrate,

97-87-0; isobutyl isobutyrate, 97-85-8; hexyl isobutyrate, 2349-07-7; ethyl caprylate, 106-32-1; dimethyl adipate, 627-93-0; diethyl adipate, 141-28-6; methyl salicylate, 119-36-8; ethyl salicylate, 118-61-6; dimethyl maleate, 624-48-6; methyl benzoate, 93-58-3.

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(2) Sorensen, J. M; Arit, W. "Liquid-Liquid Equilibrium Data Collection"; DECHEMA: Frankfurt/Main, Federal Republic of Germany, 1979; Vol. V, Part 1.

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Quaternary Liquid–Liquid Equilibrium. Acetonitrile–Cyclohexane–Acetone–Benzene

Isamu Nagata

Department of Chemical Engineering, Kanazawa University, Kanazawa, 920 Japan

Solubility and tie-line data are reported for the ternary system acetonitrile–acetone–cyclohexane at 298.15 K and for the quaternary system acetonitrile–cyclohexane–acetone–benzene at 298.15 and 318.15 K. The extended UNIQUAC equation is used to correlate the ternary liquid–liquid equilibrium data and to predict the quaternary liquid–liquid equilibrium data with good accuracy.

Introduction

As part of a program to study quaternary liquid–liquid equilibrium for nonelectrolyte mixtures, this paper reports the results of measurements on liquid–liquid equilibrium for the acetonitrile–acetone–cyclohexane system at 298.15 K and for the acetonitrile–cyclohexane–acetone–benzene system at 298.15 and 318.15 K. The experimental data are analyzed by the extended UNIQUAC equation (*1*). Ternary liquid–liquid equilibrium results had been published for the acetonitrile–acetone–cyclohexane system at 318.15 K (*2*) and for the acetonitrile–benzene–cyclohexane system at 298.15 and 318.15 K (*3*). Vapor–liquid equilibrium data for the five component binaries are available: acetonitrile–acetone at 318.15 K (*4*); acetonitrile–benzene at 298.15 and 318.15 K (*5*); acetone–benzene at 298.15 and 318.15 K (*4*); benzene–cyclohexane at 313.14 K (*6*).

Experimental Section

Materials. All special grade chemicals used for experimental work were purchased from Wako Pure Chemical Industries Ltd. Acetone was fractionally distilled in a 1-m glass column with McMahon packing after drying over anhydrous calcium sulfate. Cyclohexane was fractionated similarly. Benzene was recrystallized 3 times. Acetonitrile was used directly. Densities of substances, measured with an Anton Paar (DMA-40) densimeter at 298.15 K, agree well with literature values (*7*).

Methods. Solubility data for the ternary and quaternary systems were obtained by using the cloud-point method. Tie-line data were determined by intense stirring of a two-phase mixture in an equilibrium cell and allowing the mixture to settle for 3 h at a specified temperature ±0.01 K. After equilibrium was reached, sample solutions were taken from two phases

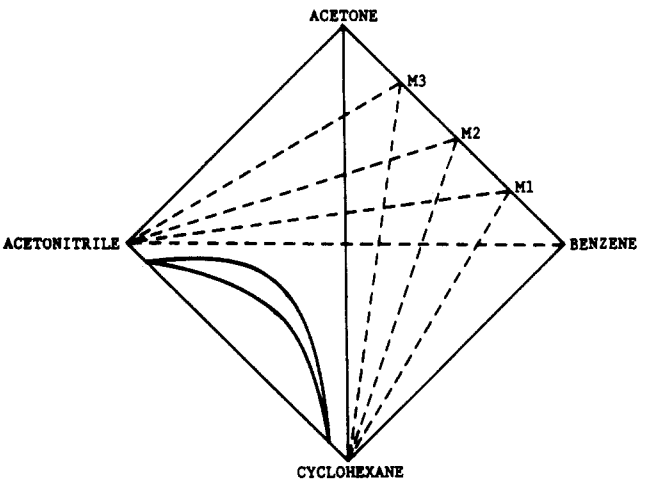

Figure 1. Schematic representation of liquid–liquid equilibrium to the quaternary system acetonitrile–cyclohexane–acetone–benzene: sectional planes.

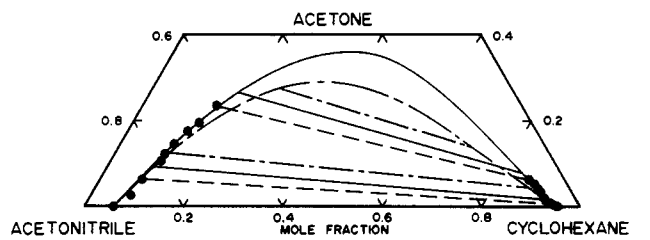

Figure 2. Liquid–liquid equilibrium for acetonitrile–acetone–cyclohexane at 298.15 K. Experimental tie-line (●–●); calculated (- - -), parameters were taken from Table VII; (—) parameters were taken from Table VIII.

Table I. Solubility Data for Acetonitrile (1)–Acetone (2)–Cyclohexane (3) at 298.15 K

x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2
0.9399	0.0000	0.6490	0.2136	0.3552	0.3236	0.1208	0.1585
0.8750	0.0447	0.5797	0.2570	0.2986	0.3050	0.0914	0.1117
0.8233	0.0855	0.5294	0.2832	0.2573	0.2795	0.0714	0.0755
0.7630	0.1331	0.4789	0.3050	0.2174	0.2538	0.0501	0.0234
0.7185	0.1657	0.4085	0.3225	0.1460	0.1934	0.0440	0.0000

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