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SOLUBILITY DATA SERIES

Volume 48

ESTERS WITH WATER
PART I: ESTERS 2-C TO 6-C

SOLUBILITY DATA SERIES

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
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A complete list of volumes published in the Solubility Data Series will be found on p. 357.

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Volume 48

ESTERS WITH WATER PART I: ESTERS 2-C TO 6-C

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FOREWORD

> *If the knowledge is*
> *undigested or simply wrong,*
> *more is not better.*

The Solubility Data Series is a project of Commission V.8 (Solubility Data) of the International Union of Pure and Applied Chemistry (IUPAC). The project had its origins in 1973, when the Analytical Chemistry Division of IUPAC set up a Subcommission on Solubility Data under the chairmanship of the late Prof. A. S. Kertes. When publication of the *Solubility Data Series* began in 1979, the Committee became a full commission of IUPAC, again under the chairmanship of Prof. Kertes, who also became Editor-in-Chief of the Series. The Series has as its goal the preparation of a comprehensive and critical compilation of data on solubilities in all physical systems, including gases, liquids and solids.

The motivation for the Series arose from the realization that, while solubility data are of importance in a wide range of fields in science and technology, the existing data had not been summarized in a form that was at the same time comprehensive and complete. Existing compilations of solubility data indeed existed, but they contained many errors, were in general uncritical, and were seriously out-of-date.

It was also realized that a new series of compilations of data gave educational opportunities, in that careful compilations of existing data could be used to demonstrate what constitutes data of high and lasting quality. As well, if the data were summarized in a sufficiently complete form, any individual could prepare his or her own evaluation, independently of the published evaluation. Thus, a special format was established for each volume, consisting of individual data sheets for each separate publication, and critical evaluations for each separate system, provided sufficient data from different sources were available for comparison. The compilations and, especially, the evaluation were to be prepared by active scientists who were either involved in producing new data, or were interested in using data of high quality. With minor modifications in format, this strategy has continued throughout the Series.

In the standard arrangement of each volume, the Critical Evaluation gives the following information:

(i) A text which discusses the numerical solubility information which has been abstracted from the primary sources in the form of compilation sheets. The text concerns primarily the quality of the data, after consideration of the purity of the materials and their characterization, the experimental method used, the uncertainties in the experimental values, the reproducibility, the agreement with accepted test values, and finally, the fitting of the data to suitable functions, along with statistical tests of the fitted data.

(ii) A set of recommended data, whenever possible, including weighted averages and estimated standard deviations. If applicable, one or more smoothing equations which have been computed or verified by the evaluator are also given.

(iii) A graphical plot of the recommended data, in the form of phase diagrams where appropriate.

The Compilation part consists of data sheets which summarize the experimental data from the primary literature. Here much effort is put into obtaining complete coverage; many good data have appeared in publications from the late nineteenth and early twentieth centuries, or in obscure journals. Data of demonstrably low precision are not compiled, but are mentioned in the Critical Evaluation. Similarly, graphical data, given the uncertainty of accurate conversion to numerical values, are compiled only where no better data are available. The documentation of data of low precision can serve to alert researchers to areas where more work is needed.

A typical data sheet contains the following information:

(i) list of components: names, formulas, Chemical Abstracts Registry Numbers;
(ii) primary source of the data;
(iii) experimental variables;
(iv) compiler's name;
(v) experimental values as they appear in the primary source, in modern units with explanations if appropriate;
(vi) experimental methods used;
(vii) apparatus and procedure used;
(viii) source and purity of materials used;
(ix) estimated error, either from the primary source or estimated by the compiler;
(x) references relevant to the generation of the data cited in the primary source.

Each volume also contains a general introduction to the particular type of system, such as solubility of gases, of solids in liquids, etc., which contains a discussion of the nomenclature used, the principle of accurate determination of solubilities, and related thermodynamic principles. This general introduction is followed by a specific introduction to the subject matter of the volume itself.

The Series embodies a new approach to the presentation of numerical data, and the details continue to be influenced strongly by the perceived needs of prospective users. The approach used will, it is hoped, encourage attention to the quality of new published work, as authors become more aware that their work will attain permanence only if it meets the standards set out in these volumes. If the Series succeeds in this respect, even partially, the Solubility Data Commission will have justified the labour expended by many scientists throughout the world in its production.

January, 1989

J. W. Lorimer,
London, Canada

PREFACE

This volume, one of a pair in the Solubility Data Series devoted to esters in water, includes solubility data for binary systems containing an ester and water published up through the end of 1988. The first volume contains the esters having two through six carbon atoms with water and the second volume contains esters having seven or more carbon atoms with water. With only rare exceptions, the compiled data and evaluations involve measurements made at constant pressure over rather restricted ranges of temperature. The limited ranges of pressure and temperature involved are to be expected in view of the liquid-liquid condition prescribed for the systems.

For the most part, the data presented show general patterns of behavior expected for the topic systems. While rather extensive data have been reported for many of the systems under consideration, no effort was made to attempt any detailed correlations of behavior or descriptions of trends beyond those presented by the evaluator in the evaluation sections.

The critical evaluations were all prepared by one author and an introductory section has been included to elaborate the philosophy and methodology followed in the evaluations. No attempts were made to extract thermodynamic parameters such as activity coefficients, enthalpies of solution, and the like from the reported data although much of the published work is sufficiently precise for such activities.

Every attempt was made to include all published data for the subject systems through the end of 1988. The editors would be grateful for any information concerning material which was overlooked in the preparation of this work.

The editors would like to express their appreciation to all those who have provided assistance in the volume preparation, especially to fellow members of the IUPAC Commission on Solubility Data and to those who have served as reviewers of this work.

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November 1991.

LIQUID-LIQUID SOLUBILITY: EVALUATION PHILOSOPHY AND METHODOLOGY

G.T. HEFTER

INTRODUCTION

Because of the differing ways in which it is possible to critically evaluate published solubility data it is worthwhile to present a coherent statement on the philosophy and procedures which have been used in this volume. Although this is a personal statement concerning the present volume, many of the ideas have been developed by myself as an evaluator for previous liquid-liquid volumes in the Solubility Data Series [1-3] and are shared, to some degree, by other evaluators.

EVALUATION PHILOSOPHY

The critical evaluation of data is, at least in part, a subjective process. Some physical scientists are uncomfortable with this notion but the history of science shows us it is undeniable. Because some subjective judgements are inevitably involved, it is vital that the evaluator's procedure should be as visible as possible. In this way, if the user does not agree with the evaluator's judgement or arguments or if new data become available it is possible, with a minimum of effort, to derive a new set of preferred or "best" values. For this reason the Critical Evaluations in this and those previous volumes to which I have contributed [1-3] have been, in essence, written like research papers with enough information provided for users to repeat or change the evaluation should they so desire.

The starting point for each Critical Evaluation is that the data compilation is complete, i.e., the data sheets include all the available data. This is an important premise because the addition of extra data may change the evaluation considerably. This is especially true of liquid-liquid systems since very few have been adequately studied over a wide temperature range and disagreements often exist between independent investigations.

In general, a "democracy of observers" is followed. That is, the data of all investigators are given equal weight irrespective of their reputation or location. This is justifiable in scientific terms because experience shows that real "errors" in liquid-liquid solubility data are much greater than individual authors' reported precisions. Thus, the benzene-water system, which is relatively simple and probably the most widely studied of all liquid-liquid systems [2], has solubilities which are known to an accuracy of about ± 2% (relative). The same estimated error is obtained regardless of whether a simple average of the available data is taken or whether a complex weighting procedure is used. This suggests that, at the present stage of development of liquid-liquid solubility determinations, equal weighting for all data is the most appropriate course of action. The exceptions to this rule are discussed below.

REJECTION OF DATA

The statement that all data are given equal weight must be qualified: some data are assigned zero weight, i.e., they are rejected. Data rejection is potentially dangerous, especially when few data are available. Nevertheless, since a critical evaluation is required, it has to be considered. The most important reasons for rejecting data are as follows.

1. The data disagree "significantly" from most other studies (especially if these are numerous). Significance is subjective but a criterion of

   $$| s_{obs} - s_{av} | > 3\sigma_n$$

   where s_{obs} is the reported solubility datum being considered for rejection

   s_{av} is the arithmetic average (mean) of all other studies at the same temperature and pressure

   σ_n is the standard deviation from the mean of these studies

   has been generally, but not rigidly, applied [1-3].

It should be noted that this procedure can be invoked only once. That is, having rejected some points in a particular data set it is not statistically valid to recalculate a new value of σ_n and then reject further points. Strictly speaking this means that outlying data should be included in the original calculation of σ_n. However, the amount of available data does not always make this approach realistic and common sense must be applied.

2. Approximate data (one significant figure) are rejected when a reasonable amount of more precise data is available.

3. Data which are grossly inconsistent with chemical systematics or thermodynamic expectations are also rejected.

4. In keeping with the practice adopted in previous liquid-liquid solubility values, data originally presented in graphical form or in volume ratio units are also excluded. In the latter case, data are retained if appropriate density data are readily available to permit conversion to mass units. As density measurements are usually far more reliable than solubility data, the choice of density values is usually not critical.

It is appropriate to add here that data for a particular system coming from the same authors or the same laboratories have generally not been regarded as independent measurements and have therefore been subsumed into a single result (at each temperature).

THE EVALUATION FORMAT

The Critical Evaluations in this volume follow the format evolved in previous liquid-liquid solubility volumes [1-3]. In essence each Evaluation is divided into three parts. In the first part Table 1 lists all the available publications containing quantitative solubility data for the particular system. Broad experimental details such as temperature range, type of solubility measured ((1) in (2), (2) in (1) or mutual) and the method used are also included in Table 1. After mention of any other special features such as critical points, or any special types of investigation, further discussion is usually divided into two parts: the solubility of the organic in the aqueous phase, and that of water in the organic-rich phase. Since these two sections are handled in the same way they will be discussed together.

After listing rejected data, anomalies and caveats, all the available data (usually expressed as g/100g sln) are collected into Tables (usually Tables 2 & 3). To facilitate comparisons, data are interpolated (if necessary) to specific temperatures at 5K intervals near 298K, then 10 or 20K intervals. These temperatures are exact, i.e. 298.15, 303.15 ... K but for convenience are written 298, 303, ... K in the text. The nature of most liquid-liquid solubility data makes graphical interpolation the most appropriate approach [4]. Interpolated values are always designated with an asterisk (*). Very occasionally data are extrapolated but only over a short range (<5K) and only if the solubility curve is not changing sharply.

All the retained values at each temperature are then averaged and the mean and σ_n recorded in the Tables. Few of the systems in this volume have sufficient data to permit meaningful statistical analysis. The value of σ_n is therefore included only as a convenient measure of the spread of the experimental data.

"BEST" VALUES

The word "best", almost always in inverted commas (quotation marks), is used throughout the Critical Evaluations in this and previous liquid-liquid solubility volumes [1-3] in a specific way: to mean "best available estimate". It follows from what has been said above that "best" values are simply the arithmetic average (mean) of all the accepted data, including those obtained by interpolation and excluding rejected data. "Best" values are given in both g/100g sln and mole fraction units (x).

RECOMMENDED VALUES

Solubilities are recommended only if two or more independent studies (including rejected data) agree to within ± 5%(relative), i.e.,

$$| 100\sigma_n/s_{av} | \leq 5$$

and there are no other obvious problems. Recommended data are designated by (*R*) immediately following the numerical value.

For sparingly soluble systems this criterion may be too harsh and

$$| 100\sigma_n/s_{av} | \leq 10 \text{ or } 20$$

may be more appropriate [3]. Very few high molecular weight esters have been sufficiently well characterized to enable even these less restrictive criteria to be applied.

Data which are not "Recommended" are regarded as "Tentative". The likely accuracy of these data varies from system to system and from temperature to temperature but may be inferred from

1. σ_n
2. $100\sigma_n/s_{av}$
3. n (the number of independent measurements).

Occasionally there are definite reasons to suspect the available data are not reliable. Such data are labelled "Doubtful" and the detailed reasons for this classification given. Considerable care should be exercised in the use of such data.

Note that the mole fraction "best" solubilities in each table should be regarded as having the same status ("Recommended", "Tentative" or "Doubtful") and the same (relative) percentage uncertainties (where given) as the corresponding mass % solubilities.

GRAPHICS

In systems for which a reasonable amount of data exists, selected results are plotted graphically over the studied temperature range. Appropriate comments on the plots are made in the figure caption or in the text.

FITTING EQUATIONS

The use of fitting equations to smooth solubility data as a function of temperature is controversial and a topic in its own right which will not be discussed here. As in previous liquid-liquid solubility volumes [1-3], fitting equations are not generally given in the printed version of this volume. There are several reasons for this.

1. There is no single equation form which can be used for all systems.
2. The data for some systems are too scattered or poorly defined for realistic curve fitting.
3. Without special care empirical fitting equations may give misleading results (spurious extrema, etc.) when interpolating and can almost never be reliably used for extrapolation.

For certain systems where reliable data appear evident, fitting equations have been provided. Such equations come directly from the original works or from the efforts of the compilers in the course of their examination of reported data and preparation of smoothed value tables.

Users who wish to derive their own fitting equations are advised to do so with caution. It is suggested that the "best" values be used for this purpose, but it should be noted that this may create anomalies because of the way in which the "best" values are derived (see above). Where fitting equations are given in this volume they should be used only over the stated range.

THERMODYNAMIC CONSISTENCY

Using standard relationships from thermodynamics it can be shown that:

$$\Delta_{sln}G = -RT \ln a_{sat}$$

$$\frac{\partial(\Delta_{sln}G/T)}{\partial T} = -\frac{\Delta_{sln}H}{RT^2}$$

and $$\frac{\partial^2(\Delta_{sln}G/T)}{\partial T^2} = \frac{\partial(\Delta_{sln}H)}{\partial T} = \Delta_{sln}C_p$$

where $\Delta_{sln}G$, $\Delta_{sln}H$ and $\Delta_{sln}C_p$ are respectively the Gibbs energy, enthalpy and heat capacity (at constant pressure) changes corresponding to the dissolution of the solute in the solvent and a_{sat} is the activity of the saturated solute in the solvent. If the solute is only sparingly soluble the thermodynamic parameters may be equated with their standard state values, and it should be noted that $\Delta_{sln}C_p$ may itself be temperature dependent.

Both $\Delta_{sln}H$ and $\Delta_{sln}C_p$, at least in principle, can be measured directly by separate calorimetric procedures [5,6] and therefore can serve as an independent check on the temperature dependence of published solubility data. This approach has been used with significant effect in evaluating hydrocarbon solubilities in water [2-3]. However, very few calorimetric data have been reported for ester-water systems and so this approach has not been utilized in the present volume.

REFERENCES

1. G.T. Hefter, in A.F.M. Barton, Ed., *Solubility Data Series, Vol. 15, Alcohols with Water* (Pergamon Press, Oxford, 1984).
2. G.T. Hefter, in D.G. Shaw, Ed., *Solubility Data Series, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C5 to C7* (Pergamon Press, Oxford, 1989).
3. G.T. Hefter, in D.G. Shaw, Ed., *Solubility Data Series, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C8 to C36* (Pergamon Press, Oxford, 1989).
4. G.T. Hefter, unpublished paper presented at 1st Intl. *Symp. Soly. Phenom.*, London, Canada, August, 1984.
5. S.O. Nilsson and I. Wadso, *J. Chem. Thermodyn.* 1984, 16, 317.
6. P. Picker, P.A. Leduc, P.R. Philip and J.E. Desnoyers, *J. Chem. Thermodyn.* 7, 3, 641.

COMPONENTS:

(1) Formic acid methyl ester (*methyl formate*); $C_2H_4O_2$; [107-31-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rayman, J.

Thesis, Budapest, 1906.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of formic acid methyl ester in water

$t/^{\circ}C$	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	26.79	21.13	0.0744
10.	28.60	22.24	0.0790
20.	30.36	23.29	0.0835
30.	32.51	24.53	0.0888

These data have also been published in (ref 2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, *55*, 360.
2. Hill, A.E. *International Critical Tables* (Washburn, E.W., Ed.) McGraw Hill, New York, 1928, Vol. 3, 387-98.

COMPONENTS:

(1) Acetic acid, trichloro-, methyl ester (*methyl trichloroacetate*); $C_3H_3Cl_3O_2$; [598-99-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 363

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of trichloroacetic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	-	99.74	-	0.9750
9.5	-	99.79	-	0.9797
20.0	-	99.81	-	0.9816
29.6	0.09	-	0.00009	-
39.8	0.09	99.70	0.00009	0.9712
49.8	0.04	99.65	0.00004	0.9665
60.0	0.05	99.52	0.00005	0.9546
70.5	0.06	99.29	0.00006	0.9342
80.1	0.03	99.28	0.00003	0.9333
90.2	0.03	98.97	0.00003	0.9070
std. dev.	0.01	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid, dichloro-, methyl ester (*methyl dichloroacetate*); $C_3H_4Cl_2O_2$; [116-54-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

$T/K = 273 - 363$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of dichloroacetic acid methyl ester and water

$t/°C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.09	99.78	0.00139	0.9828
9.6	0.86	99.73	0.00109	0.9790
20.1	0.33	99.68	0.00042	0.9751
29.6	0.33	99.63	0.00042	0.9714
39.5	0.35	99.52	0.00044	0.9631
50.0	0.37	99.49	0.00047	0.9609
60.0	0.36	99.40	0.00045	0.9543
70.3	0.37	99.27	0.00047	0.9448
79.9	0.46	98.60	0.00058	0.8987
90.2	0.44	98.20	0.00056	0.8730
std. dev.	0.04	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid, chloro-, methyl ester (*methyl chloroacetate*); $C_3H_5ClO_2$; [96-34-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 363

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of chloroacetic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	5.44	99.29	0.00946	0.9587
9.8	5.18	99.15	0.00898	0.9509
19.8	5.16	98.97	0.00895	0.9410
29.8	5.09	98.69	0.00882	0.9259
39.5	5.31	98.58	0.00922	0.9201
50.2	5.34	98.16	0.00928	0.8985
60.0	5.79	97.88	0.01010	0.8846
70.2	5.79	97.44	0.01010	0.8633
80.1	6.70	96.96	0.01178	0.8411
90.1	7.00	96.09	0.01234	0.8031
std. dev.	0.08	0.03		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A., Australia
January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the Acetic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid methyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Fuehner (ref 3)	293	(1) in (2)	titration
Hill (ref 4)	267-381	mutual	synthetic
Kendall and Harrison (ref 5)	278-357	(1) in (2)	synthetic
Murti *et al.* (ref 6)	303	mutual	titration
Venkataratnam *et al.* (ref 7)	303	mutual	titration
Lutugina and Kalyuzhnyi (ref 8)	293,330	mutual	titration
Beregovykh *et al.* (ref 9)	293-377	mutual	titration
Filip and Maciejewski (ref 10)	293	mutual	titration
Skrzecz (ref 11)	295-357	mutual	synthetic
Richon and Viallard (ref 12)	298	mutual	calorimetric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID METHYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid methyl ester (1) in water (2) are summarized in Table 2 with the following exceptions. The approximate value of Traube (ref 1) at 293 K is excluded because more precise information is readily available (ref 3,5,8,9,11). The data of Rayman (ref 2), Murti *et al.* (ref 6) and Venkataratnam *et al.* (ref 7), all at 303 K, and of Lutugina and Kalyuzhnyi (ref 8) at 330 K are substantially higher ($> 3\sigma_n$) than all other studies and are rejected. The data of Filip and Maciejewski (ref 10) at 293 K and Richon and Viallard (ref 12) at 298 K are substantially lower ($> 3\sigma_n$) than all other values at these temperatures The data of Hill (ref 4) which are composite values and are also rejected.

(continued next page)

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A., Australia
January, 1989

CRITICAL EVALUATION: (continued)

based on published and unpublished data are also in disagreement with most other studies over most of the temperature range and are rejected.

The remaining data (Table 2) are in excellent agreement over a wide range of temperature enabling many of the average "Best" values to be Recommended. Selected data are plotted in Figure 1.

TABLE 2: Recommended (*R*) and Tentative Solubilities of Acetic acid methyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^2x_1
273	24.95 (ref 2)	25.0	7.48
278	24.7* (ref 2), 22.6 (ref 5)	23.7 ± 1.1	7.02
283	24.49 (ref 2), 22.6* (ref 5)	23.5 ± 1.1	6.95
293	24.18 (ref 2), 24.35 (ref 3), 22.8* (ref 5), 24.49 (ref 8), 24.0* (ref 11), 23.35 (ref 9)	23.9 ± 0.6 (*R*)	7.10
298	22.9* (ref 5), 23.35* (ref 9), 23.05* (ref 11)	23.1 ± 0.2 (*R*)	6.81
303	23.0* (ref 5), 23.4* (ref 9), 22.32* (ref 11)	22.9 ± 0.4 (*R*)	6.74
313	23.2* (ref 5), 23.4 (ref 9), 21.58* (ref 11)	22.7 ± 0.8 (*R*)	6.67
323	23.3* (ref 5), 23.5* (ref 9), 21.78* (ref 11)	22.9 ± 0.8 (*R*)	6.74
333	23.8* (ref 5), 23.9* (ref 9), 22.93* (ref 11)	23.5 ± 0.4 (*R*)	6.95
343	25.2* (ref 5), 25.3* (ref 9), 25.01* (ref 11)	25.2 ± 0.2 (*R*)	7.57
353	27.7* (ref 5), 27.9* (ref 9), 28.03* (ref 11)	27.9 ± 0.1 (*R*)	8.60
363	32.2* (ref 9)	32.2	10.36
373	36.5* (ref 9)	36.5	12.27

[a] Obtained by averaging where appropriate.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

In Table 2, σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

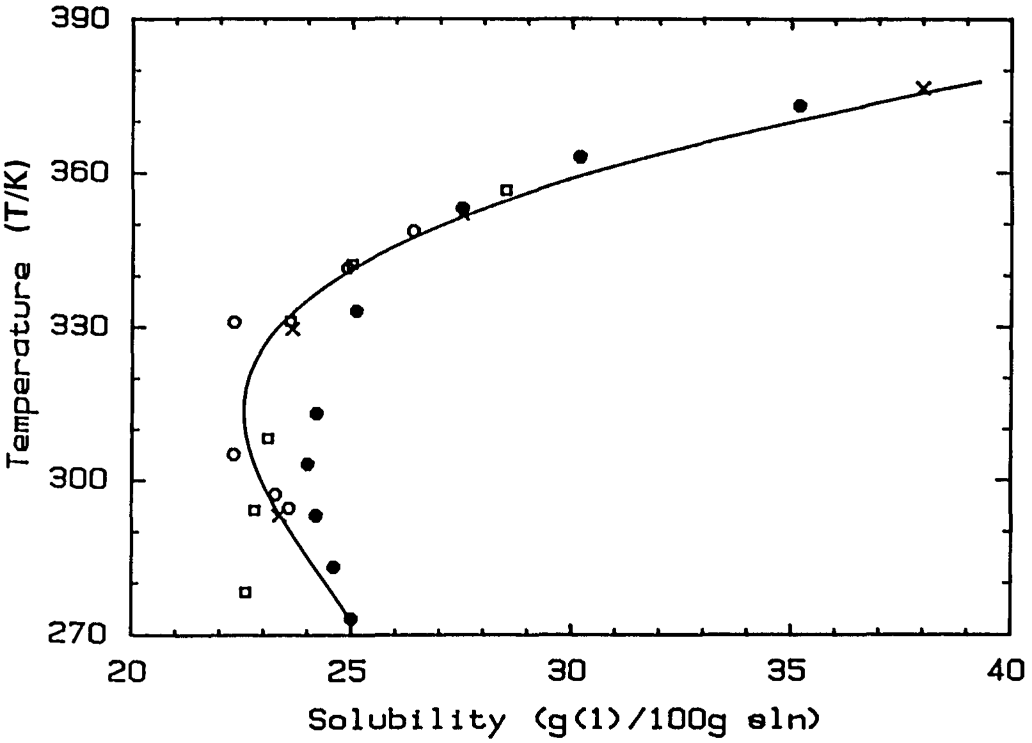

FIGURE 1. Selected data for the solubility of acetic acid methyl ester (1) in water (2): ref 4 (●); ref 5 (□); ref 9 (X); ref 11 (O). Solid line is drawn through the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID METHYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid methyl ester (1) are summarized in Table 3 with the following exceptions. The data of Murti *et al.* (ref 6) and Venkataratnam *et al.* (ref 7) at 303 K and Lutugina and Kalyuzhnyi (ref 8) at 330 K are substantially higher than all other studies and are rejected.

The remaining data, mainly due to Hill (ref 4), Beregovykh *et al.* (ref 9) and Skrzecz (ref 11) are generally in reasonable agreement, especially the values given in ref 4 and 11. At low (T < 293 K) and high (T > 373 K)

(continued next page)

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A., Australia
January, 1989

CRITICAL EVALUATION: (continued)

temperatures only the data of Hill (ref 4) are available and must be considered tentative. Hill also reports the upper critical solution temperature of methyl acetate and water to be at 108 °C (381.2 K) at a composition of 52.5 g (1)/100 g sln (x_1 = 0.212).

Selected data for the solubility of water in methyl acetate are plotted in Figure 2.

TABLE 3: Recommended (*R*) and Tentative Solubilities of Water (2) in Acetic acid methyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values ($\pm\sigma_n$)[a]	
	g(2)/100g sln	g(2)/100g sln	x_2
268	6.2* (ref 4)	6.2	0.214
273	6.4* (ref 4)	6.4	0.219
283	6.8* (ref 4)	6.8	0.231
293	7.5* (ref 4), 7.41 (ref 8), 8.16 (ref 9), 7.77 (ref 10), 7.38 (ref 11)	7.6 ± 0.3 (*R*)	0.253
298	8.0* (ref 4), 8.15* (ref 9), 8.03 (ref 11), 8.33 (ref 12)	8.1 ± 0.1 (*R*)	0.266
303	8.7* (ref 4), 8.20* (ref 9), 8.73 (ref 11)	8.5 ± 0.2 (*R*)	0.276
313	10.3* (ref 4), 8.5* (ref 9), 10.30* (ref 11)	9.7 ± 0.8	0.306
323	12.1* (ref 4), 9.2* (ref 9), 12.10* (ref 11)	11.1 ± 1.4	0.339
333	14.2* (ref 4), 11.1* (ref 9), 14.12* (ref 11)	13.1 ± 1.4	0.382
343	16.6* (ref 4), 14.6* (ref 9), 16.35* (ref 11)	15.9 ± 0.9	0.437
353	19.4* (ref 4), 19.0* (ref 9), 18.81* (ref 11)	19.1 ± 0.2 (*R*)	0.493
363	22.7* (ref 4), 24.5* (ref 9)	23.6 ± 0.9 (*R*)	0.560
373	28.2* (ref 4), 29.5* (ref 9)	28.9 ± 0.7 (*R*)	0.626

[a] Obtained by averaging where appropriate.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

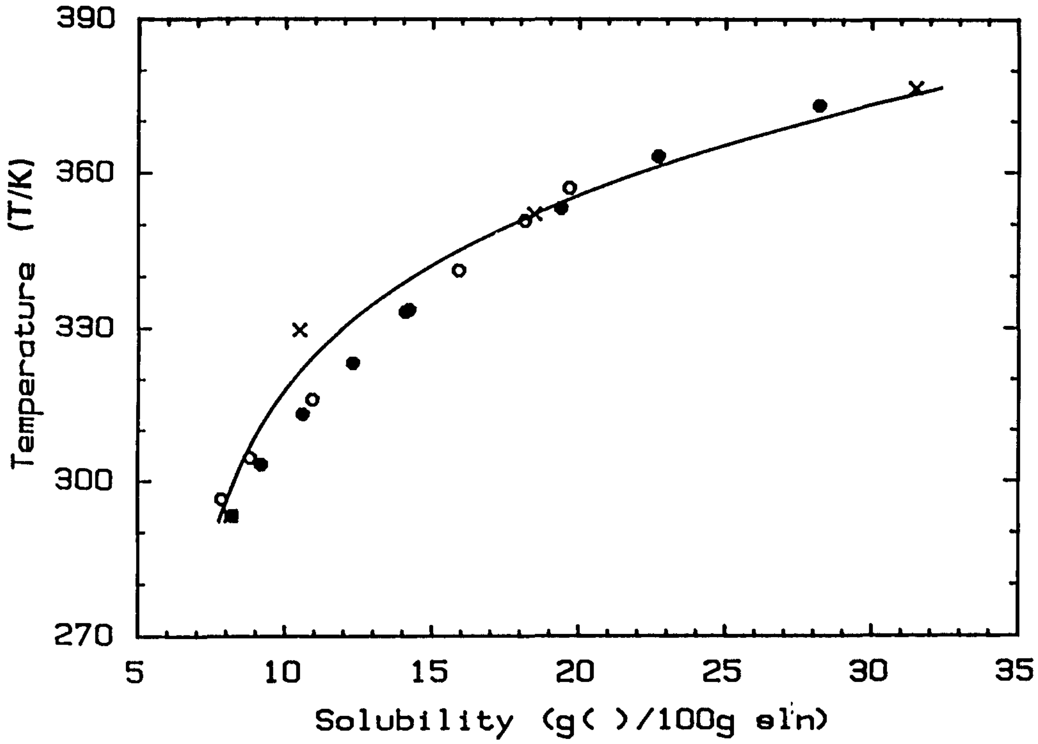

FIGURE 2. Selected data for the solubility of water (2) in acetic acid methyl ester (1): ref 4 (●); ref 9 (X); ref 11 (O). Solid line is drawn through the "Best" values from Table 3.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.

2. Rayman, J. *Thesis*, Budapest 1906.

3. Fuehner, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-5.

4. Hill, A. E. *International Critical Tables* (Washburn, E. W., Ed.), McGraw-Hill, New York, 1928, Vol. 3, 387-98.

5. Kendall, J.; Harrison, E. *Trans. Faraday Soc.* 1928, *24*, 588-96.

6. Murti, P. S.; Venkataratnam, A.; Rao, C. V. *J. Sci. Ind. Res.* 1954, *13B*, 392-6.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid methyl ester; *(methyl acetate)*; $C_3H_6O_2$; [79-20-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

7. Venkataratnam, A.; Rao, J. R.; Rao, C. V. *Chem. Eng. Sci.* 1957, *7*, 102-10.
8. Lutugina, N. V.; Kalyuzhnyi, V. M. *Zh. Prikl. Khim.* 1959, *32*, 2626-33.
9. Beregovykh, V. V.; Grishunin, A. V.; Balashov, M. I.; Serafimov, L. A. *Fiz. Khim. Osn. Rektifikatsii* 1970, 103-12.
10. Filip, S.; Maciejewski, Z. *Chem. Stosow.* 1972, *16*, 445-51.
11. Skrzecz, A. *Pol. J. Chem.* 1980, *54*, 1101-4; see also Skrzecz, A. *Thesis, I. Ch. F. PAN,* Warszawa, 1979.
12. Richon, D.; Viallard, A. *Fluid Phase Equil.* 1985, *21*, 279-93.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Acetic acid methyl ester; *(methyl acetate)*; $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Traube, J.

Ber. Dtsch. Chem. Ges. 1884, *17*, 2294-316.

VARIABLES:

T/K = 295

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid methyl ester in water at 22°C was reported to be 1 part of methyl acetate in 3 parts of water. The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 25 g(1)/100g sln and 0.075.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±1.5 g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid methyl ester (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rayman, J.

Thesis, Budapest, 1906.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of acetic acid methyl ester in water

$t/°C$	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	33.24	24.95	0.0748
10.	32.43	24.49	0.0731
20.	31.89	24.18	0.0720
30.	31.73	24.09	0.0717

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, *55*, 360.

COMPONENTS:

(1) Acetic acid methyl ester; *(methyl acetate)*; $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Fuehner, H.

Ber. Dtsch. Chem. Ges. 1924, *57*, 510-5.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid methyl ester in water at 20°C was reported to be 25.37 vol%, 24.35 g(1)/100g sln. and 3.290 mol(1)/L sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.07259.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.5 g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid methyl ester; *(methyl acetate)*; $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hill, A. E.

International Critical Tables (Washburn, E.W., Ed.) McGraw-Hill, New York, 1928, Vol. 3, 387-98.

VARIABLES:

T/K = 267 - 381

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
-6.55	25.5	93.8	0.0769	0.786
0.0	25.0	93.6	0.0750	0.781
10.	24.6	93.0	0.0735	0.764
20.	24.2	91.8	0.0721	0.756
25.	24.1	91.3	0.0717	0.743
30.	24.0	90.8	0.0713	0.729
40.	24.2	89.4	0.0721	0.672
50.	24.6	87.7	0.0735	0.634
60.	25.1	85.9	0.0754	0.597
80.	27.5	80.6	0.0845	0.503
90.	30.2	77.3	0.0952	0.453
100.	35.2	71.8	0.117	0.382
105.	40.3	66.0	0.141	0.321
108. (UCST)	52.5	-	0.212	-

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The data appear to be that of Hill and Morrow (unpublished) and were probably obtained by the synthetic method although no specific details were given in the article.

SOURCE AND PURITY OF MATERIALS:

Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Kendall, J.; Harrison, L.E.

Trans. Faraday Soc. 1928, *24*, 588-96.

VARIABLES:

T/K = 278 - 357

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of acetic acid methyl ester in water

$t/°C$	x_1	g(1)/100g sln (compiler)
5.0	0.0662	22.6
21.0	0.0670	22.8
35.0	0.0679	23.1
58.0	0.0700	23.6
58.9	0.0703	23.7
60.1	0.0706	23.8
61.7	0.0711	23.9
69.1	0.0751	25.0
70.5	0.0766	25.4
71.9	0.0773	25.6
83.5	0.0883	28.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method was used. The sealed tube method (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±1 g(1)/100g sln (compiler).

REFERENCES:

1. Smith, A.; Eastlack, H.E. *J. Am. Chem. Soc.* 1916, *38*, 1269.

COMPONENTS:

(1) Acetic acid methyl ester; *(methyl acetate)*; $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Murti, P.S.; Venkataratnam, A.; Rao, C.V.

J. Sci. Ind. Res. 1954, *13B*, 392-6.

VARIABLES:

T/K = 303 [a]

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid methyl ester in water at 30°C[a] was reported to be 26.1 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0791.

The solubility of water in acetic acid methyl ester at 30°C[a] was reported to be 9.7 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.31.

[a] Presumably the measurments were made at 30°C; the temperature was not reported in the paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Determinations were made either from the production of turbidity or from its disappearance.
The data were reported together with the ternary system methyl acetate-water-acetic acid.
No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House, laboratory reagent grade; distilled; b.p. 57.3°C, d 0.9274, n_D^{30} 1.3570.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±3.6 g(1)/100g sln and ±0.9 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Venkataratnam, A.; Rao, J.R.; Rao, C.V.

Chem. Eng. Sci. 1957, *7*, 102-10.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid methyl ester in water at 30°C was reported to be 25.4 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0765.

The solubility of water in acetic acid methyl ester at 30°C was reported to be 11.4 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.346.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described in Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system methyl acetate-water-acetone.
No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House Ltd., laboratory reagent grade; distilled; b.p. 57.3°C, d^{30} 0.9234, n^{30} 1.3570.

(2) Distilled; free of CO_2.

ESTIMATED ERROR:

Soly. about ±2.9 g(1)/100g sln and ±2.6 g(2)/100g sln (compiler).

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Lutugina, N.V.; Kalyuzhnyi, V.M.

Zh. Prikl. Khim. 1959, *32*, 2526-33.

VARIABLES:

T/K = 293 and 330

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid methyl ester and water

$t/^{\circ}C$	x_1		g(1)/100g sln (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20.0	0.0731	0.7525	24.49[b]	92.59[c]
56.8[a]	0.104	0.544	32.30[d]	83.10[e]

[a] Boiling temperature at 760 mm Hg.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Bottles with both narrow and long necks were used at room temperature. The apparatus with dephlegmator was used at the boiling temperature. The mixture was stirred by the boiling liquid. The data were reported together with the ternary system methyl acetate-water-chloroform.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized in laboratory; washed with Na_2CO_3(aq) and water, dried with $CaCl_2$, distilled three times; b.p. 56.8°C, n_D^{30} 1.3614.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.6[b], ±0.1[c], ±10.[d] and ±3.6[e] g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Beregovykh, V.V.; Grishunin, A.V.; Balashov, M.I.; Serafimov, L.A.

Fiz. Khim. Osn. Rektifikatsii 1970, 103-12.

VARIABLES:

$T/K = 293 - 377$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20.0[a]	23.35[b]	91.84[c]	0.06897	0.7324
56.5	23.65[d]	89.5[e]	0.07005	0.6746
78.9	27.50[f]	81.5[g]	0.08445	0.5172
103.4	38.00	68.50	0.12972	0.3459

[a] Data at 20°C taken from Balashov (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The mutual solubility was observed visually during titration in a ebulliometer. The exact values were obtained from a graph of the boiling temperature vs. concentration. (The results of the vapor-liquid equilibrium measurements were presented in the paper.) No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purified; n_D^{20} 1.3619, b.p. 56.3°C.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.4[b], ±0.7[c], ±1.3[d], ±0.4[e], ±0.4[f] and ±0.1[g] g(1) /100g sln (compiler).

REFERENCES:

1. Balashov, M.I. *Thesis*, M.I.Kh.T., Moskva, 1967.

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Filip, S.; Maciejewski, Z.

Chem. Stosow. 1972, *16*, 445-51.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid methyl ester in water at 20°C was reported to be 13.65 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0370.

The solubility of water in acetic acid methyl ester at 20°C was reported to be 7.77 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.257.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. To determine the solubility, weighed amounts of one component (ca. 50g) were titrated with the second component in a constant temperature bath. Titrations were performed using a burette graduated in 0.1-mL divisions. The samples were stirred vigorously.

SOURCE AND PURITY OF MATERIALS:

(1) FOCH Gliwice; chemically pure grade; used as received.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±10. g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skrzecz, A.

Pol. J. Chem. 1980, *54*, 1101-4.

Skrzecz, A.

Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

VARIABLES:

T/K = 295 - 357

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid methyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
294.6	0.0698	-	23.58	-
295.1	0.0697	-	23.55	-
296.5	-	0.7407	-	92.15
297.3	0.0687	-	23.27	-
304.5	-	0.7155	-	91.18
305.1	0.0653	-	22.32	-
316.1	-	0.6646	-	89.07
322.7	-	0.6417	-	88.05
331.0	0.0653	-	22.32	-
332.5	0.0660	-	22.51	-
333.6	-	0.5944	-	85.77
335.4	0.0687	-	23.27	-
336.3	0.0698	-	23.58	-

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew was used.
An ampoule with the solution of fixed concentration was placed into a glass tube connected with a thermostat filled completely with distilled water. During the measurements the temperature of the bath was changed continuously and the appearance and disappearance of turbidity within the ampoule was observed visually. The amount of water in pure ester was taken into account.

SOURCE AND PURITY OF MATERIALS:

(1) International Enzymes Limited, pure grade; distilled; purity 99.99% by glc, 0.07 wt% water by the Karl Fischer method.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.2-0.6)°C.
Soly. see above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9] (2) Water; H_2O; [7732-18-5]	Skrzecz, A. *Pol. J. Chem.* 1980, *54*, 1101-4. Skrzecz, A. *Thesis*, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid methyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
337.1	0.0710	-	23.91	-
341.2	-	0.5624	-	84.09
341.6	0.0746	-	24.90	-
345.5	0.0775	-	25.68	-
348.7	0.0802	-	26.39	-
350.8	-	0.5227	-	81.83
357.1	-	0.4980	-	80.31

Author's smoothing equations:

$x_1 = 0.093868 - 1.4651\text{x}10^{-3}\ (T/K - 273.15) + 1.708\text{x}10^{-5}\ (T/K - 273.15)^2$

st. dev. = 7.87×10^{-4} (2)-rich phase

$x_2 = 0.168783 + 3.6860\text{x}10^{-3}\ (T/K - 273.15) + 3.54\text{x}10^{-6}\ (T/K - 273.15)^2$

st. dev. = 2.40×10^{-3} (1)-rich phase

COMPONENTS:

(1) Acetic acid methyl ester; (*methyl acetate*); $C_3H_6O_2$; [79-20-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid methyl ester in water at 298.1 K was reported to be x_1 = 0.0545. The corresponding mass per cent value calculated by the compiler is 19.16 g(1)/100g sln.

The solubility of water in acetic acid methyl ester at 298.1 K was reported to be x_2 = 0.272. The corresponding mass per cent value calculated by the compiler is 8.33 g(2)/100g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The calorimetric method was used. The method was described by Richon (ref 1) and by Richon and Villard (ref 2).
No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Carlo Erba (for analysis); purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±4g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.
2. Richon, D.; Villard, A. *Can. J. Chem.* 1976, *54*, 2584.

COMPONENTS:	EVALUATOR:
(1) Formic acid ethyl ester (*ethyl formate*); $C_3H_6O_2$; [109-94-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the formic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Formic acid ethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Rayman (ref 1)	273-303	(1) in (2)	volumetric
Kendall and Harrison (ref 2)	278-349	(1) in (2)	synthetic
Batmanova *et al.* (ref 3)	293,326	mutual	titration, analytical

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF FORMIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of formic acid ethyl ester (1) in water (2) are summarized in Table 2 except for the 293 K datum of Batmanova *et al.* (ref 3) which is significantly lower (> $3\sigma_n$) than the other available values (ref 1,2).

Over the temperature range $273 \le T \le 303$ K where independent data are available, the solubilities of Rayman (ref 1) and Kendall and Harrison (ref 2) are in good agreement. However, the average solubilities derived from these two studies have not been Recommended because they show a totally contradictory dependence of solubility on temperature (Figure 1). Thus although some reliance may be placed on the average "Best" values further studies are clearly necessary. These should include detailed consideration of the possibility of ester hydrolysis.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid ethyl ester (*ethyl formate*); $C_3H_6O_2$; [109-94-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Solubilities
of Formic acid ethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values [a]	
	g(1)/100g sln	g(1)/100g sln	10^2x_1
273	9.34 (ref 1), 7.4* (ref 2)	8.4 ± 1.0	2.2
283	9.07 (ref 1), 7.78* (ref 2)	8.4 ± 0.6	2.18
293	8.58 (ref 1), 8.04* (ref 2)	8.3 ± 0.3	2.15
298	8.06* (ref 1), 8.16* (ref 2)	8.1 ± 0.1	2.10
303	7.34 (ref 1), 8.29* (ref 2)	7.8 ± 0.5	2.01
313	8.63* (ref 2)	8.6	2.2
323	9.16* (ref 2), 10[b] (ref 3)	9.2	2.4
333	9.95* (ref 2)	10	2.6
343	11.12* (ref 2)	11	2.9

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] 325.8 K; not included in "Best" value.

2. SOLUBILITY OF WATER (2) IN FORMIC ACID ETHYL ESTER (1)

Only the data of Batmanova *et al.* (ref 3) are available for the solubility of water in formic acid ethyl ester and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubilities although the comments in Part 1 above should be noted.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid ethyl ester (*ethyl formate*); $C_3H_6O_2$; [109-94-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

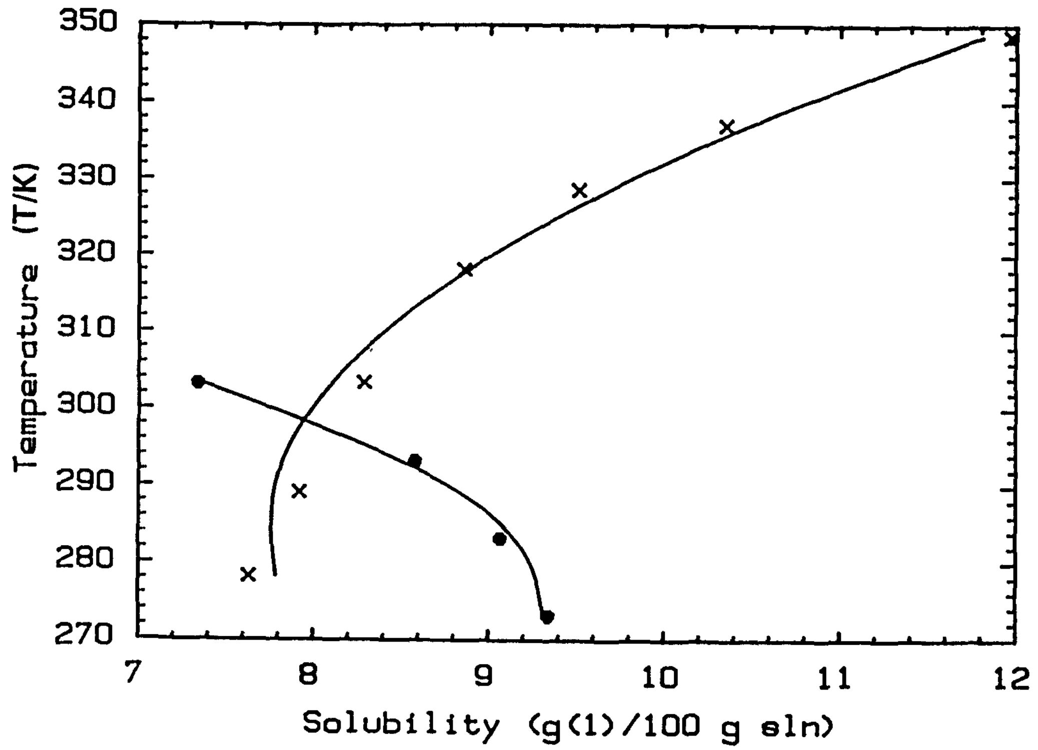

FIGURE 1. Data for the solubility of Formic acid ethyl ester (1) in water (2): ref 1 (●); ref 2 (X). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

REFERENCES

1. Rayman, J. *Thesis*, Budapest, 1906; see also Hill, A. E. *International Critical Tables* (Washburn, E. W., Ed.), McGraw-Hill, New York, 1928, Vol. 3, 387-98.

2. Kendall, J.; Harrison, E. *Trans. Faraday Soc.* 1928, *24*, 588-96.

3. Batmanova, G.A.; Balashov, M.I.; Grishunin, A.V.; Savinskaya, I.G.; Serafimov, L.A. *Gidroliz. Lesokhim. Prom.* 1971, *24*(8), 11-12.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Formic acid ethyl ester (*ethyl formate*); $C_3H_6O_2$; [109-94-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rayman, J.

Thesis, Budapest, 1906.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of formic acid ethyl ester in water

$t/^\circ C$	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	10.30	9.34	0.0244
10.	9.97	9.07	0.0237
20.	9.39	8.58	0.0223
30.	9.00	7.34	0.0189

These data have also been published in (ref 2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, *55*, 360.
2. Hill, A.E. *International Critical Tables* (Washburn, E.W., Ed.) McGraw-Hill, New York, 1928, Vol. 3, 387-98.

COMPONENTS:

(1) Formic acid ethyl ester (*ethyl formate*); $C_3H_6O_2$; [109-94-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Kendall, J.; Harrison, L.E.

Trans. Faraday Soc. 1928, *24*, 588-96.

VARIABLES:

$T/K = 278 - 349$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of formic acid ethyl ester in water

$t/^{\circ}C$	x_1	g(1)/100g sln (compiler)
5.0	0.0197	7.63
15.9	0.0205	7.92
30.2	0.0215	8.29
38.0	0.0223	8.57
45.1	0.0231	8.86
50.0	0.0241	9.22
55.5	0.0249	9.51
63.9	0.0273	10.35
70.0	0.0295	11.11
75.5	0.0320	11.97

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method was used. The sealed tube method (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.1-0.2)°C.

REFERENCES:

1. Smith, A.; Eastlack, H.E. *J. Am. Chem. Soc.* 1916, *38*, 1269.

COMPONENTS:

(1) Formic acid ethyl ester (*ethyl formate*); $C_3H_6O_2$; [109-94-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Batmanova, G.A.; Balashov, M.I.; Grishunin, A.V.; Savinskaya, I.G.; Serafimov, L.A.

Gidroliz. Lesokhim. Prom. 1971, *24(8)*, 11-2.

VARIABLES:

T/K = 293 and 326

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of formic acid ethyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20^a	6.1	97.1	0.0156	0.891
$52.6^{b,c}$	7.0	96.0	0.0180	0.854
$52.6^{a,c}$	13.9	95.5	0.0378	0.838

[a] Titration method.

[b] Analytical method.

[c] Numerical value of boiling temperature at 760 mm Hg is not reported in the paper; boiling temperature of two-phase mixture equal to 52.6°C was taken from Horsley (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration and analytical methods were used. In the titration method, the titrations were carried out in thermostated bottles using a magnetic stirrer at 20°C and in a heated flask with a magnetic stirrer and reflux condenser at the boiling temperature. In the analytical procedure, a two-phase mixture was placed into a heated flask attached to a reflux condenser, mixed for 1/2 h. at the boiling temperature, separated and analyzed by glc. A small amount of water was also determined by the Karl Fischer method.
The data and methods were reported together with the ternary systems ethyl formate-water-ethyl acetate and ethyl formate-water-ethanol.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled, dried with $CaCl_2$ and redistilled; b.p. 54.13°C, n_D^{20} 1.3605.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Horsley, L.E. *Azeotropic Data III*, Advances in Chemistry Series 116, American Chemical Society, Washington, 1973.

COMPONENTS:

(1) Carbonic acid dimethyl ester (*dimethyl carbonate*); $C_3H_6O_3$; [616-38-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 353

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of carbonic acid dimethyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
9.8	12.5	97.84	0.0278	0.9006
20.5	12.7	97.39	0.0283	0.8818
29.7	12.4	96.79	0.0275	0.8577
40.1	13.2	95.90	0.0295	0.8239
50.0	13.5	95.34	0.0303	0.8036
60.4	14.3	93.19	0.0323	0.7324
70.1	-	92.24	-	0.7039
79.5	-	91.67	-	0.6876
std. dev.	0.1	0.06		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Phosphorothioic acid O,O,O-trimethyl ester (*trimethyl thiophosphate*); $C_3H_9O_3PS$; [152-18-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Apelblat, A.

J. Chem. Soc. B 1969, 175-7.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of water in phosphorothioic acid O,O,O-trimethyl ester[a] at 25°C was reported to be 0.49 mol(2)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 8.8 g(2)/L sln.

The density of the ester-phase was reported to be d_4^{25} 1.1904.

[a] The structure of the molecule was not specified. The C.A. number, [152-18-1], is that for the O,O,O,-trimethyl phosphorothioic acid ester.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture was equilibrated by vigorous stirring for 30 min. and settling for 12 h. The organic phase was analyzed with the Karl Fischer reagent.
Preliminary experiments showed that stirring and settling times were sufficient.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co.; purified by method described in Alcock, Grimley, *et al.* (ref 1); d_4^{25} 1.1919, n_D^{25} 1.4535.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.

REFERENCES:

1. Alcock, K.; Grimley, S.S.; Healy, T.V.; Kennedy, J.; McKay, H.A.C. *Trans. Faraday Soc.* 1956, *52*, 39.

COMPONENTS:

(1) Acetic acid ethenyl ester (*vinyl acetate*); $C_4H_6O_2$; [108-05-4]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid ethenyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid ethenyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Smith (ref 1)	298	mutual	titration
Pratt and Glover (ref 2)	293	mutual	titration
Nakamura (ref 3)	293	mutual	analytical
Tikhonova *et al*. (ref 4)	293,339	mutual	analytical
Richon and Viallard (ref 5)	298	(1) in (2)	refractometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID ETHENYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid ethenyl ester (1) in water (2) are summarized in Table 2 except for the value reported by Pratt and Glover (ref 2) at 293 K which is much lower than other studies (ref 3,4) and is rejected.

The remaining data, mainly at 293 and 298 K, are in reasonable agreement although further studies are required before any values can be Recommended.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethenyl ester (*vinyl acetate*); $C_4H_6O_2$; [108-05-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Solubilities of Acetic acid ethenyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
293	2.3 (ref 3), 2.0 (ref 4)	2.15 ± 0.15	4.9
298	2.5 (ref 1), 2.67 (ref 5)	2.58 ± 0.09	5.5
339	1.2 (ref 4)	1.2^b	2.5

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] Value should be regarded as very Tentative.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID ETHENYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid ethenyl ester (1) are summarized in Table 3. The data are in very poor agreement and further studies will be necessary before even Tentative values can be nominated.

TABLE 3: Reported Solubilities of Water (2) in Acetic acid ethenyl ester (1)

T/K	Reported solubilities	
	g(2)/100g sln	10^2x_2
293	1.08 (ref 2), 1.1 (ref 3), 0.1 (ref 4)	5.0 (ref 2), 5.0 (ref 3) 0.5 (ref 4)
298	0.1 (ref 1)	0.5 (ref 1)
339	12.3 (ref 4)	40 (ref 4)

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethenyl ester (*vinyl acetate*); $C_4H_6O_2$; [108-05-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

REFERENCES

1. Smith, J. C. *J. Phys. Chem.* 1942, *46*, 229-32.
2. Pratt, H. R. C.; Glover, S. T. *Trans. Inst. Chem. Eng.* 1946, *24*, 54-65.
3. Nakamura, A. *Kogyo Kagaku Zosshi* 1968, *71*, 319-21.
4. Tikhonova, N. K.; Timofeev, V. S.; Serafimov, L. A.; Tolkacheva, N. L. *Izv. Vyssh. Ucheb. Zaved Khim. Khim. Tekhnol.* 1970, *13*, 175-7.
5. Richon, D.; Viallard, A. *Fluid Phase Equil.* 1985, *21*, 279-93.

COMPONENTS:

(1) Acetic acid ethenyl ester (*vinyl acetate*); $C_4H_6O_2$; [108-05-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Smith, J.C.

J. Phys. Chem. 1942, *46*, 229-32.

VARIABLES:

$T/K = 298$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid ethenyl ester in water at 25°C was reported to be 2.5 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0053.

The solubility of water in acetic acid ethenyl ester at 25°C was reported to be 0.1 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.005.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration method was used. The data and method were reported together with the ternary system acetic acid ethenyl ester-water-2-propanone (*vinyl acetate-water-acetone*).

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethenyl ester (*vinyl acetate*); $C_4H_6O_2$; [108-05-4] (2) Water; H_2O; [7732-18-5]	Pratt, H.R.C.; Glover, S.T. *Trans. Inst. Chem. Eng.* 1946, *24*, 54-65.
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethenyl ester in water at 20°C was reported to be 1.14 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00241.

The solubility of water in acetic acid ethenyl ester at 20°C was reported to be 1.08 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0496.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method was used. The data and methods were reported together with the ternary system acetic acid ethenyl ester-water-2-propanone (*vinyl acetate-water-acetone*).	(1) Source not specified; commercial product; distilled; stabilized with 0.1% hydroquinone. (2) Distilled.
	ESTIMATED ERROR:
	Temp. ±0.1°C.
	REFERENCES:

COMPONENTS:

(1) Acetic acid ethenyl ester (*vinyl acetate*); $C_4H_6O_2$; [108-05-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Nakamura, A.

Kogyo Kagaku Zasshi 1968, *71*, 319-21.

VARIABLES:

T/K = 293

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethenyl ester in water at 20°C was reported to be 2.3 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0049.

The solubility of water in acetic acid ethenyl ester at 20°C was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.050.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture was placed in a 1 L flask and stirred for 1 h. which was sufficient for equilibrium. Then, after 1/2 h. separation, samples of both phases were analysed. Acetic acid ethenyl ester was titrated with 1.4 mole% Br_2 in acetic acid. Water was determinated by the Karl Fischer method. Both volumetric and analytical methods gave similar results. The method and data were reported together with the ternary system acetic acid ethenyl ester-water-methanol.

SOURCE AND PURITY OF MATERIALS:

(1) Commercial product; distilled; impurities (wt%): ethanol 0.009, acids 0.001, non-volatile 0.001, water 0.005; d 0.934 g/cm^3.

(2) Purified on ion-exchange material; resistivity >4×10^6 ohm.

ESTIMATED ERROR:

Temp. ±0.2°C.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethenyl ester (*vinyl acetate*); $C_4H_6O_2$; [108-05-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tikhonova, N.K.; Timofeev, V.S.; Serafimov, L.A.; Tolkacheva, N.L.

Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. 1970, *13*, 175-7.

VARIABLES:

T/K = 293 and 339

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethenyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	2.0	99.9	0.0043	0.995
66.0[a]	1.2	87.7	0.0025	0.599

[a] Boiling temperature at atmospheric pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Two-phases mixtures were placed in a thermostated apparatus with a mechanical stirrer, mixed and after separation the samples of both equilibrium phases were analyzed. Water was determined by the Karl Fischer method. The boiling temperature was measured in a Swietoslawski ebulliometer. Only the measurements for the ternary system were described. The data were reported together with the ternary system acetic acid ethenyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purified; b.p. 72.5°C, physico-chemical properties were in agreement with literature data.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethenyl ester *(vinyl acetate)*; $C_4H_6O_2$; [108-05-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethenyl ester in water at 298.1 K was reported to be 0.0319 mol(1)/100g(2) and 2.74 g(1)/100g(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 2.67 g(1)/100g sln and 0.00570.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) Merck (for synthesis); purified by preparation gas chromatographic method, the purity >99.5%; water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.

COMPONENTS:

(1) 2-Propenoic acid methyl ester (*methyl acrylate*); $C_4H_6O_2$; [96-33-3]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A., Australia
March, 1990

CRITICAL EVALUATION:

Quantitative solubility data for the 2-propenoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2-Propenoic acid methyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Chubarov *et al.* (ref 1)	293	mutual	analytical
Filip and Maciejewski (ref 2)	288	mutual	titration
Dabrowski (ref 3)	288,298	(1) in (2)	turbidimetric
Richon and Viallard (ref 4)	298	(1) in (2)	refractometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 2-PROPENOIC ACID METHYL ESTER (1) IN WATER (2)

All the available solubility data for 2-propenoic acid methyl ester (1) in water (2) are summarized in Table 2. The data are in good agreement and the average values are Recommended although the temperature dependence of the averaged "Best" values is probably dubious.

TABLE 2: Recommended (*R*) Solubilities of 2-Propenoic acid methyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^2x_1
288	5.29 (ref 2), 4.96 (ref 3)	5.1 ± 0.2 (*R*)	1.11
293	5.4 (ref 1), 4.96* (ref 3)	5.2 ± 0.2 (*R*)	1.13
298	4.96 (ref 3), 5.47 (ref 4)	5.2 ± 0.3 (*R*)	1.13

[a] Obtained by averaging where appropriate.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Propenoic acid methyl ester (*methyl acrylate*); $C_4H_6O_2$; [96-33-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia March, 1990

CRITICAL EVALUATION: (continued)

In Table 2, σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN 2-PROPENOIC ACID METHYL ESTER (1)

All the available data for the solubility of water (2) in 2-propenoic acid methyl ester (1) are summarized in Table 3. The data of Chubarov *et al.* (ref 1) and of Filip and Maciejewski (ref 2) although at slightly different temperatures, are in broad agreement, giving some confidence in the values reported which are regarded as Tentative.

TABLE 3: Tentative Solubilities of Water (2) in 2-Propenoic acid methyl ester (1)

T/K	Reported Solubilities	
	g(2)/100g sln	x_2
288	2.05 (ref 2)	0.091
293	2.3 (ref 1)	0.101

REFERENCES

1. Chubarov, G. A.; Danov, S. M.; Logutov, V. I.; Brovkina, G. V. *Zh. Prikl. Khim.* 1979, *52*, 1082-5.
2. Filip, S.; Maciejewski, Z. *Chem. Stosow.* 1972, *16*, 445-51.
3. Dabrowski, L. *Thesis*, I. Ch. F. PAN, Warszawa, 1984.
4. Richon, D.; Viallard, A. *Fluid Phase Equil.* 1985, *21*, 279-93.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Propenoic acid methyl ester (*methyl acrylate*); $C_4H_6O_2$; [96-33-3] (2) Water; H_2O; [7732-18-5]	Chubarov, G.A.; Danov, S.M.; Logutov, V.I. *Zh. Prikl. Khim.* 1982, *55*, 1032-4.
VARIABLES:	**PREPARED BY:**
T/K = 293	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 2-propenoic acid methyl ester in water at 20°C was reported to be 5.4 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0118.

The solubility of water in 2-propenoic acid methyl ester at 20°C was reported to be 2.3 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.101.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The sample was vigorously mixed for 3 min and analysed after separation. Water was determined using the Karl Fischer reagent. The concentration of 2-propenoic acid methyl ester was determined by the bromate method. The data and method were reported together with the ternary system 2-propenoic acid methyl ester-water-sulphuric acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; used as received; n_D^{20} 1.3984.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.5°C.

REFERENCES:

COMPONENTS:

(1) 2-Propenoic acid methyl ester (*methyl acrylate*); $C_4H_6O_2$; [96-33-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Filip, S.; Maciejewski, Z.

Chem. Stosow. 1972, *16*, 445-51.

VARIABLES:

T/K = 288

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 2-propenoic acid methyl ester in water at 15°C was reported to be 5.29 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.01155.

The solubility of water in 2-propenoic acid methyl ester at 15°C was reported to be 2.05 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0909.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. To determine the solubility, weighed amounts of one component (ca. 50g) were titrated with the second component in a constant temperature bath. Titrations were performed using a burette graduated in 0.1-mL divisions. The samples were stirred vigorously.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; d_4^{20} 0.956, n_D^{20} 1.3984.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 2-Propenoic acid methyl ester (*methyl acrylate*); $C_4H_6O_2$; [96-33-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Dabrowski, L.

Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1984.

VARIABLES:

T/K = 288 and 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Solubility of 2-propenoic acid methyl ester in water

T/K	g(1)/100g sln	x_1
288.15	4.96	0.0108
298.15	4.96	0.0108

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The modified Othmer-White-Trueger method was used.
The samples of known composition were slowly cooled to obtain the temperature of turbidity which was a little below the desired temperature. After addition of a small amount of one component the procedure was repeated.
The solubility at the desired temperature was obtained by an interpolation. All measurements were made in a thermostated vessel of 50 cm^3 in the range ±3°C of the needed temperature. Temperatures of the samples were measured with a mercury-in-glass thermometer.
A magnetic stirrer was used. The water included in ester was taken into account. The data and method were reported together with the ternary system 2-propenoic acid methyl ester-water-2-propenoic acid (*methyl acrylate- water-acrylic acid*).

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized by esterification; distilled on a 70 TP column, washed with 20 % KOH and several times with distilled water, 0.1 % of hydroquinone was added to protect polymerization.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.05°C.
Soly. ±0.02 g(1)/100g sln.

REFERENCES:

COMPONENTS:

(1) 2-Propenoic acid methyl ester (*methyl acrylate*); $C_4H_6O_2$; [96-33-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 2-Propenoic acid methyl ester in water at 298.1 K was reported to be 0.0672 mol(1)/100g(2) and 5.79 g(1)/100g(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 5.47 g(1)/100g sln and 0.01197.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) Merck (for synthesis); purified by preparation gas chromatographic method, the purity >99.5%; water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.

COMPONENTS:

(1) 1,3-Dioxolan-2-one, 4-methyl- (*propylene carbonate*); $C_4H_6O_3$; [108-32-7]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
March, 1990

CRITICAL EVALUATION:

Quantitative solubility data for the 4-methyl-1,3-dioxolan-2-one (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 4-Methyl-1,3-dioxolan-2-one (1) - Water (2) System

Reference	T/K	Solubility	Method
Catherall and Williamson (ref 1)	243-334	mutual	synthetic
Hong *et al*. (ref 2)	223-344	mutual	titration

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 4-METHYL-1,3-DIOXOLAN-2-ONE (1) IN WATER (2)

All the available data for the solubility of 4-methyl-1,3-dioxolan-2-one (1) in water (2) are summarized in Table 2. Whilst agreement between the two studies (ref 1,2) in the middle temperature range is good and the average values are Recommended, they differ at more extreme temperatures, see Figure 1.

TABLE 2: Recommended (R) and Tentative Solubilities of 4-Methyl-1,3-dioxolan-2-one (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^2x_1
278	13* (ref 1), 6* (ref 2)	10 ± 4	1.9
283	15* (ref 1), 10* (ref 2)	13 ± 3	2.6
293	17* (ref 1), 16* (ref 2)	16.5 ± 0.5 (R)	3.4
298	17.5* (ref 1), 17.8* (ref 2)	17.7 ± 0.2 (R)	3.7

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1,3-Dioxolan-2-one, 4-methyl- (*propylene carbonate*); $C_4H_6O_3$; [108-32-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia March, 1990

CRITICAL EVALUATION: (continued)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^2x_1
303	19.5* (ref 1), 20.5* (ref 2)	20.0 ± 0.5 (*R*)	4.2
313	26* (ref 1), 25* (ref 2)	25.5 ± 0.5 (*R*)	5.7
323	34* (ref 1), 30* (ref 2)	32 ± 2	7.7
333	48* (ref 1), 36* (ref 2)	42 ± 6	11
343	43* (ref 2)	43	12

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

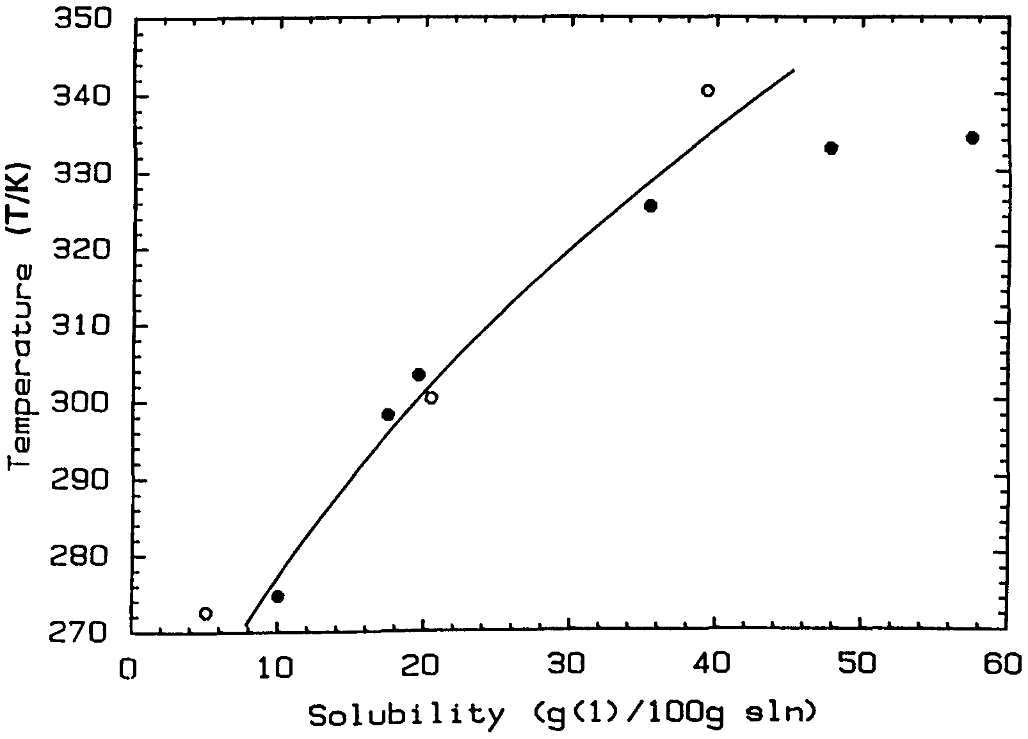

FIGURE 1. Data for the solubility of 4-methyl-1,3-dioxolan-2-one (1) in water (2): ref 1 (●); ref 2 (O). Solid line is drawn through the "Best" values from Table 2.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1,3-Dioxolan-2-one, 4-methyl- (*propylene carbonate*); $C_4H_6O_3$; [108-32-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia March, 1990

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 4-METHYL-1,3-DIOXOLAN-2-ONE (1)

All the available data for the solubility of water (2) in 4-methyl-1,3-dioxolan-2-one (1) are summarized in Table 3. In general the data are in only fair agreement and show a very different dependence on temperature. Further studies are required before any of the average "Best" values can be Recommended. The data are also plotted in Figure 2.

TABLE 3: Tentative Solubilities of Water (2) in 4-Methyl-1,3-dioxolan-2-one (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	x_2
243^b	1.0* (ref 1), 1.2* (ref 2)	1.1 ± 0.1	0.06
253^b	2.0* (ref 1), 2.2* (ref 2)	2.1 ± 0.1	0.11
263^b	2.8* (ref 1), 3.3* (ref 2)	3.1 ± 0.3	0.15
273	3.3* (ref 1), 4.3* (ref 2)	3.8 ± 0.5	0.18
283	4.0* (ref 1), 5.2* (ref 2)	4.6 ± 0.6	0.21
293	5.4* (ref 1), 6.1* (ref 2)	5.8 ± 0.4	0.26
298	7.0 (ref 1), 6.9 (ref 2)	7.0 ± 0.1	0.30
303	9.2* (ref 1), 8.0* (ref 2)	8.6 ± 0.6	0.35
313	14.1* (ref 1), 10.6* (ref 2)	12 ± 2	0.44
323	21.1* (ref 1), 13.8* (ref 2)	17 ± 4	0.54
333	18.4* (ref 2)	18	0.55
343	36.0* (ref 2)	36	0.76

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] Solid-liquid equilibrium.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1,3-Dioxolan-2-one, 4-methyl- (*propylene carbonate*); $C_4H_6O_3$; [108-32-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia March, 1990

CRITICAL EVALUATION: (continued)

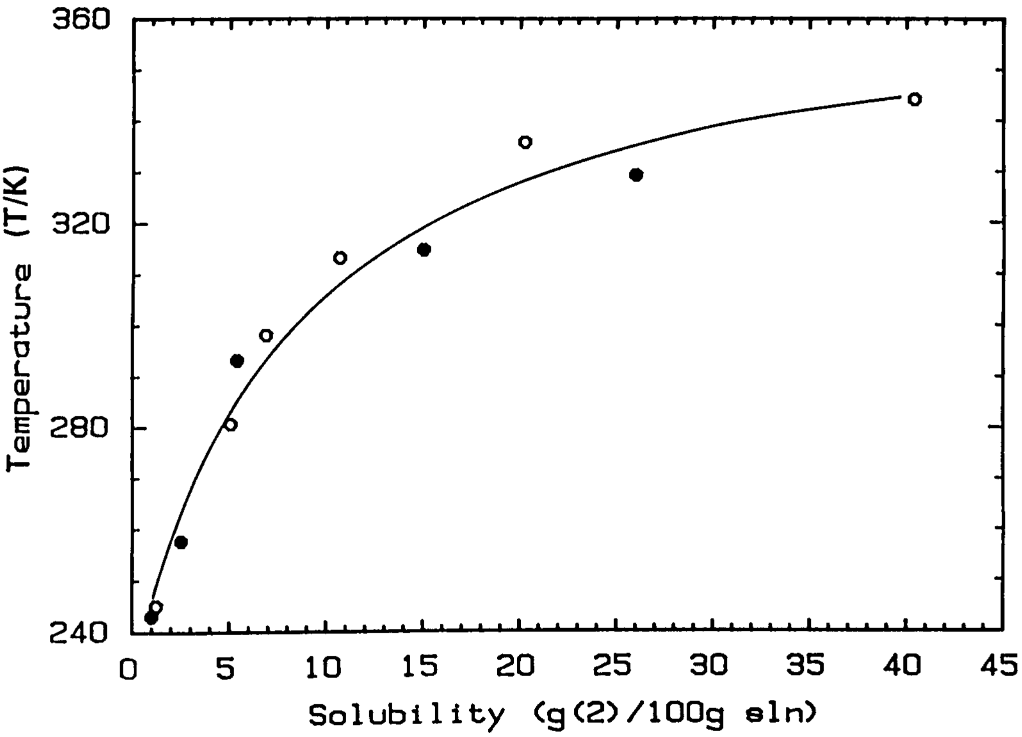

FIGURE 2. Data for the solubility of water (2) in 4-methyl-1,3-dioxolan-2-one (1): ref 1 (●); ref 2 (O). Solid line is drawn through the "Best" values from Table 3.

REFERENCES

1. Catherall, N. F.; Williamson, A. G. *J. Chem. Eng. Data* 1971, *16*, 335-6.

2. Hong, C. S.; Waksiak, R.; Finston, H.; Fried, V. *J. Chem. Eng. Data* 1982, *27*, 146-8.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dioxolan-2-one, 4-methyl- (*propylene carbonate*); $C_4H_6O_3$; [108-32-7] (2) Water; H_2O; [7732-18-5]	Catherall, N.F.; Williamson, A.G. *J. Chem. Eng. Data* 1971, *16*, 335-6.
VARIABLES:	PREPARED BY:
T/K = 243 - 334	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of 4-methyl-1,3-dioxolan-2-one and water

t/°C	g(1)/100g sln		x_1	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
-30.1[a]	-	99.0	-	0.9854
-15.5[a]	-	97.5	-	0.8732
-0.6[a]	5.0	-	0.0092	-
0.	0.	-	0.	-
1.5	10.0	-	0.0192	-
20.1	-	94.6	-	0.7556
25.0	17.5	93.0	0.0361	0.7010
30.1	19.6	-	0.0412	-
41.6	-	85.0	-	0.5000
52.1	35.4	-	0.0882	-
56.1	-	74.0	-	0.3343
59.7	47.8	-	0.1391	-
61.1	57.5	-	0.1926	-

[a] Solid-liquid equilibrium.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The cloud-point method at temperatures above 0°C and the cooling curves method at low temperature were used. For the cloud-point method, mixtures of known composition, sealed in 5-mm pyrex tubes, were immersed in a water bath at a temperature above the unmixing temperature and cooled at about 0.5°C/min. The cloud point temperatures were measured with a mercury-in-glass thermometer and the means of several observations were presented.
In the cooling curves procedure, Cooling curves were measured on mixtures prepared by weight in 25 cm^3 test tubes and cooled slowly in a dry ice-acetone bath. Temperatures were measured with a thallium amalgam thermometer.

SOURCE AND PURITY OF MATERIALS:

(1) Koch Light "puriss"-grade; purity >99%; dried over a Linde molecular sieve, grade 5A.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C[b] and ±0.2°C[c].

[b] Cloud-point method.
[c] Cooling curves method.

REFERENCES:

COMPONENTS:

(1) 1,3-Dioxolan-2-one, 4-methyl- (*propylene carbonate*); $C_4H_6O_3$; [108-32-7]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hong, C.S.; Waksiak, R.; Finston, H.; Fried, V.

J. Chem. Eng. Data 1982, *27*, 146-8.

VARIABLES:

T/K = 223 - 344

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of 4-methyl-1,3-dioxolan-2-one and water

$t/°C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
-50.2[a]	-	100.00	-	1.0000
-28.1[a]	-	98.76	-	0.9336
-1.8[a]	10.11	-	0.01946	-
-0.9[a]	5.13	-	0.00945	-
0.0	0.00	-	0.00000	-
7.5	-	94.94	-	0.7680
25.0	17.8	93.1	0.03681	0.7042
27.1	20.46	-	0.04342	-
40.1	-	89.34	-	0.5966
62.6	-	79.76	-	0.4102
67.2	39.41	-	0.10296	-
71.0	-	59.58	-	0.2064

[a] Solid-liquid equilibrium.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The water samples were titrated with 4-methyl-1,3-dioxolan-2-one and 4-methyl-1,3-dioxolan-2-one samples were titrated with water at various temperatures. The turbidity point was found to be reproducible within one very small drop (0.015 cm^3). No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Jefferson Chemical Co., Inc.; purified by repeated low-pressure distillation; b.p 241.9°C, m.p. -50°C, d_4^{25} 1.2004.

(2) Not specified; d_4^{25} 0.9986.

ESTIMATED ERROR:

Soly. <±0.3 g(1)/100g sln (accuracy).

REFERENCES:

COMPONENTS:

(1) Ethanedioic acid dimethyl ester (*dimethyl oxalate*); $C_4H_6O_4$; [553-90-2]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A., Australia
January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the ethanedioic acid dimethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Ethanedioic acid dimethyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Skrabal (ref 1)	273-327	mutual	thermal
Dehn (ref 2)	R.T.[a]	(1) in (2)	gravimetric
Kendall and Harrison (ref 3)	273-369	(1) in (2)	synthetic

[a] R.T. - room temperature (*sic*).

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ETHANEDIOIC ACID DIMETHYL ESTER (1) IN WATER (2)

All the available solubility data for ethanedioic acid dimethyl ester (1) in water (2) are summarized in Table 2. As can be seen, the independent studies are not in good agreement. The data of Kendall and Harrison (ref 3) have been chosen as the best available because solubilities reported by these authors in well characterized systems are generally reliable. Nevertheless, it should be noted that the experimental results of Kendall and Harrison (ref 3) for this system are rather scattered.

(continue next page)

COMPONENTS:	EVALUATOR:
(1) Ethanedioic acid dimethyl ester (*dimethyl oxalate*); $C_4H_6O_4$; [553-90-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Solubilities of Ethanedioic acid dimethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values [a]	
	g(1)/100g sln	g(1)/100g sln	10^2x_1
273	4[b] (ref 1), 2.60* (ref 3)	3	0.5
283	7.13* (ref 3)	7	1.1
293	5.82[c] (ref 2), 12.4* (ref 3)	12	2.0
298	15.3* (ref 3)	15	2.6
303	18.1* (ref 3)	18	3.2
313	23.9* (ref 3)	24	4.6
323	16[d] (ref 1), 29.4* (ref 3)	29	5.9
333	34.3* (ref 3)	34	7.3
343	38.3* (ref 3)	38	8.5
353	40.9* (ref 3)	41	9.6

[a] Rounded values of ref 3.

[b] 272.7 K.

[c] Room temperature.

[d] 321 K.

2. SOLUBILITY OF WATER (2) IN ETHANEDIOIC ACID DIMETHYL ESTER (1)

The only datum available for the solubility of water (2) in ethanedioic acid dimethyl ester (1) is that of Skrabal (ref 1) and so no Critical Evaluation is possible. The interested reader is referred to the relevant Data Sheet for the experimental solubility.

REFERENCES

1. Skrabal, A. *Monatsch. Chem.* 1917, *38*, 25-9.
2. Dehn, W. M. *J. Am. Chem. Soc.* 1917, *39*, 1399-404.
3. Kendall, J.; Harrison, E. *Trans. Faraday Soc.* 1928, *24*, 588-96.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethanedioic acid dimethyl ester (*dimethyl oxalate*); $C_4H_6O_4$; [553-90-2] (2) Water; H_2O; [7732-18-5]	Skrabal, A. *Monatsch. Chem.* 1917, *38*, 25-9.
VARIABLES:	PREPARED BY:
T/K = 273 - 327	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of ethanedioic acid dimethyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
-0.5[a]	4	-	0.006	-
48[b]	16	94	0.028	0.71
53.5[c]	-	100	-	1.00

[a] Eutectic point.

[b] Synthetic point.

[c] Pure solid.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The thermal analysis method was used. No details were reported in the paper.	(1) Not specified. (2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS: (1) Ethanedioic acid dimethyl ester (*dimethyl oxalate*); $C_4H_6O_4$; [553-90-2] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Dehn, W.M. *J. Am. Chem. Soc.* 1917, *39*, 1399-1404.
VARIABLES: T/K = room temperature	PREPARED BY: A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of ethanedioic acid dimethyl ester in water at room temperature[a] was reported to be 6.18 g(1)/100g(2). The corresponding mass percentage and mole fraction, x_1, values calculated by the compiler are 5.82 g(1)/100g sln and 0.00934.

[a] room temperature was reported to be 20-25°C.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Excess of the substance and 5 mL of water were enclosed in small vials, which when stoppered were shaken or let stand until equilibria were established. The solution was then filtered into weighed crucibles and reweighed. After drying in a vacuum desiccator or on a water bath, the crucibles were again weighed and the loss of solvent calculated.	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS:

(1) Ethanedioic acid dimethyl ester (*dimethyl oxalate*); $C_4H_6O_4$; [553-90-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Kendall, J.; Harrison, L.E.

Trans. Faraday Soc. 1928, *24*, 588-96.

VARIABLES:

T/K = 273 - 369

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of ethanedioic acid dimethyl ester in water

t/°C	x_1	g(1)/100g sln (compiler)
0.1	0.00541	3.44
11.1	0.01242	7.62
19.5	0.01853	11.01
27.1	0.0268	15.3
31.9	0.0336	18.6
44.4	0.0536	27.1
49.2	0.0607	29.8
51.0	0.0646	31.2
53.0	0.0691	32.7
75.0	0.0861	38.2
79.3	0.0889	39.0
96.1	0.1022	42.7

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method was used. The sealed tube method (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C, m.p. 54.35°C.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.1-0.2)°C.

REFERENCES:

1. Smith, A.; Eastlack, H.E. *J. Am. Chem. Soc.* 1916, *38*, 1269.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-bromoethyl ester *(2-bromoethyl acetate)*; $C_4H_7BrO_2$; [927-68-4] (2) Water; H_2O; [7732-18-5]	Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E. *J. Chem. Eng. Data* 1982, *27*, 451-4.
VARIABLES:	**PREPARED BY:**
$T/K = 298$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-bromoethyl ester in water at 25°C was reported to be 0.212 mol(1)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 25.9 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of water reservoir using compressed air at 5 psi. The solute concentration in the aqueous phase was analyzed by a high-pressure liquid chromatographic technique described in DeVoe, Miller and Wasik (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purity >99% by glc.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. ±1.0%.

REFERENCES:

1. DeVoe, H.; Miller, M.M.; Wasik, S.P. *J. Res. Nat. Bur. Stand.* 1981, *86*, 361.

COMPONENTS:

(1) Acetic acid, chloro-, ethyl ester (*ethyl chloroacetate*); $C_4H_7ClO_2$; [105-39-5]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 364

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of chloroacetic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	2.49	99.53	0.00374	0.9689
9.0	2.50	99.43	0.00375	0.9625
19.8	2.00	99.33	0.00299	0.9561
30.8	1.90	99.19	0.00284	0.9474
39.9	1.88	99.11	0.00281	0.9424
50.0	1.92	98.83	0.00287	0.9254
60.1	1.97	98.55	0.00294	0.9090
70.2	2.11	98.24	0.00316	0.8913
80.1	2.19	97.99	0.00328	0.8775
90.5	2.33	97.54	0.00349	0.8535
std. dev.	0.01	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Propanoic acid, 2-chloro-, methyl ester (*methyl 2-chloropropionate*); $C_4H_7ClO_2$; [17639-93-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 364

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of 2-chloropropanoic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	-	99.58	-	0.9721
10.0	2.42	99.47	0.00363	0.9650
19.8	2.29	99.40	0.00343	0.9606
29.7	1.66	99.32	0.00247	0.9555
40.3	1.62	99.24	0.00241	0.9505
50.2	1.69	99.17	0.00252	0.9461
60.1	1.81	99.08	0.00270	0.9406
70.3	1.91	98.46	0.00285	0.9038
80.2	1.98	98.63	0.00296	0.9137
90.5	2.13	97.96	0.00319	0.8759
std. dev.	0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 97%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid ethyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Mohr (ref 1)	RT[a]	(1) in (2)	titration
Marsson (ref 2)	291	mutual	cloud point
Traube (ref 3)	295	(1) in (2)	unspecified
Bancroft (ref 4)	293	mutual	titration
Euler (ref 5)	301	(1) in (2)	analytical
Rayman (ref 6)	273-303	(1) in (2)	volumetric
Bonner (ref 7)	273	mutual	titration?
Seidell (ref 8)	283-313	mutual	titration
Merriman (ref 9)	273-333	mutual	synthetic, analytical
Euler and Svanberg (ref 10)	291	(1) in (2)	unspecified
Fuehner (ref 11)	293	(1) in (2)	titration
Glasstone and Pound (ref 12)	273-323	(1) in (2)	analytical
Kendall and Harrison (ref 13)	273-323	(1) in (2)	synthetic
Jones (ref 14)	293	mutual	synthetic?
Schlesinger and Kubasowa (ref 15)	288-323	(1) in (2)	synthetic
Mion (ref 16)	273-303	mutual	turbidimetric
Park and Hofmann (ref 17)	298	mutual	unspecified
Doolittle (ref 18)	293	mutual	unspecified
Lloyd *et al.* (ref 19)	298	mutual	titration
Beech and Glasstone (ref 20)	273-313	mutual	synthetic?
Shanley and Greenspan (ref 21)	RT[a]	(2) in (1)	unspecified
Griswold *et al.* (ref 22)	290-344	mutual	synthetic
Sohoni and Warhadpande (ref 23)	303	mutual	synthetic

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

Reference	*T*/K	Solubility	Method
Altshuller and Everson (ref 24)	292-313	(1) in (2)	synthetic
Garner and Ellis (ref 25)	303	(1) in (2)	titration
Gayler and Pratt (ref 26)	288-303	mutual	titration, analytical
Jones and McCants (ref 27)	311	mutual	titration
Rao and Rao (ref 28)	303	mutual	titration
Venkataratnam *et al.* (ref 29)	303	mutual	titration
Rao *et al.* (ref 30)	308	mutual	titration
Akita and Yoshida (ref 31)	298,343	mutual	titration, analyical
Zheleznyak and Brounshtein (ref 32)	298,323	mutual	analytical
Pai and Sane (ref 33)	273,303	mutual	turbidimetric
Nakamura (ref 34)	303	mutual	analytical
Batmanova *et al.* (ref 35)	293,344	mutual	titration, analytical
Iguchi and Fuse (ref 36)	298	mutual	titration
Krupatkin and Shcherbakova (ref 37)	298	mutual	titration
Utkin *et al.* (ref 38)	298,313	mutual	titration
Aleksandrova *et al.* (ref 39)	293	mutual	titration
Filip and Maciejewski (ref 40)	293	mutual	titration
Mertl (ref 41)	293-343	mutual	titration
Sadovnikova *et al.* (ref 42)	293	mutual	unspecified
Woycicka *et al.* (ref 43)			
Van Zandijcke and Verhoeye (ref 44)	343	mutual	GLC
Tare *et al.* (ref 45)	303	(1) in (2)	titration
Sugi and Katayama (ref 46)	333	mutual	cloud point
Alvarez and Neila (ref 47)	298	mutual	titration?

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

Reference	*T*/K	Solubility	Method
Skrzecz and Maczynski (ref 48)	286-364	mutual	synthetic
Tewari *et al.* (ref 49)	298	(1) in (2)	GLC
Ouyang *et al.* (ref 50)	323	mutual	GLC
Richon and Viallard (ref 51)	298,318	mutual	calorimetric, refractometric
Stephenson and Stuart (ref 52)	273-344	mutual	GLC

[a] RT - room temperature.

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Data available in the article by Hill (ref 53), which are composite values based on published and unpublished data, have been omitted because of the ready availability of other good quality data. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid ethyl ester (1) in water (2) are summarized in Table 2 with the following exceptions.

The data of Marsson (ref 2), Traube (ref 3), Euler (ref 5), Fuehner (ref 11) and Doolittle (ref 18) at *ca.* 293 K, Iguchi and Fuse (ref 36) at 298 K, and Garner and Ellis (ref 25) at 303 K are all substantially lower ($> 3\sigma_n$) than other studies and have therefore been rejected. Similarly, the data of Van Zandijcke and Verhoeye (ref 44) at 343 K and Ouyang *et al.* (ref 50) are substantially higher ($> 3\sigma_n$) than other studies and have also been rejected. The data of Mohr (ref 1, unspecified temperature), Bancroft (ref 4, v/v units), Euler and Svanberg (ref 10), and Tewari *et al.* (ref 49, w/v units) have been excluded from consideration because of the abundance of other good quality data.

The remaining data, the most substantial set for any ester-water system, are generally in good agreement enabling the average "Best" values to be Recommended over a wide range. Selected data for the solubility of acetic acid ethyl ester in water are plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubilities of Acetic acid ethyl ester (1) in Water (2)

T/K	Solubilities Reported values g(1)/100g sln	"Best" values ($\pm\sigma_n$)[a] g(1)/100g sln	 10^2x_1
273	9.86 (ref 6), 9.80 (ref 7), 10.08 (ref 9), 10.40 (ref 12), 9.41 (ref 13), 10 (ref 16), 9.67 (ref 20), 9.29 (ref 33), 9.71 (ref 52)	9.8 ± 0.3 (*R*)	2.17
283	8.84 (ref 6), 9.15 (ref 8), 8.81 (ref 9), 8.96 (ref 12), 8.19 (ref 13), 8.8* (ref 16), 8.61 (ref 20), 8.2* (ref 48), 8.60* (ref 52)	8.7 ± 0.3 (*R*)	1.91
293	7.94 (ref 6), 8.27 (ref 8), 7.86 (ref 9), 7.85 (ref 12), 7.28 (ref 13), 8.53 (ref 14), 7.77 (ref 15), 7.8* (ref 16), 7.75 (ref 20), 7.68* (ref 22), 7.77 (ref 24), 7.74*[b] (ref 26), 8.51 (ref 32), 7.86 (ref 35), 8.70 (ref 39), 8.22 (ref 40), 7.31 (ref 41), 8.9 (ref 42), 8.1* (ref 48), 7.70* (ref 52)	8.0 ± 0.4 (*R*)	1.74
298	7.59* (ref 6), 7.90 (ref 8), 7.48 (ref 9), 7.39 (ref 12), 6.84 (ref 13), 7.43 (ref 15), 7.4* (ref 16), 7.9 (ref 17), 7.56 (ref 19), 7.42* (ref 20), 7.30* (ref 22), 7.42 (ref 24), 7.48*[b] (ref 26), 7.47 (ref 37), 6.9 (ref 38), 6.99 (ref 41), 7.48 (ref 43), 7.3 (ref 47), 8.0* (ref 48), 7.50 (ref 51), 7.21* (ref 52)	7.4 ± 0.3 (*R*)	1.61
303[c]	7.23 (ref 6), 7.61 (ref 8), 7.15 (ref 9), 7.06 (ref 12), 6.58 (ref 13), 7.14 (ref 15), 7.1 (ref 16), 7.10* (ref 20), 7.1* (ref 22), 7.10 (ref 23), 7.15 (ref 24), 7.22*[b] (ref 26), 7.22 (ref 28), 7.4 (ref 29), 7.5 (ref 31), 6.70 (ref 33), 6.7 (ref 34), 6.5* (ref 38), 6.68* (ref 41), 7.56* (ref 45), 7.5* (ref 48), 7.20* (ref 51), 6.76* (ref 52)	7.1 ± 0.3 (*R*)	1.54

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities		
	Reported values	"Best" values ($\pm\sigma_n$)[a]	
	g(1)/100g sln	g(1)/100g sln	$10^2 x_1$
313[d]	7.17 (ref 8), 6.63 (ref 9), 6.50 (ref 12), 6.10 (ref 13), 6.70 (ref 15), 6.52 (ref 20), 6.8* (ref 22), 6.65 (ref 24), 5.8 (ref 38), 5.95* (ref 41), 6.7* (ref 48), 6.70* (ref 51), 6.34* (ref 52)	6.5 ± 0.4	1.40
323	6.04 (ref 12), 5.65 (ref 13), 6.43 (ref 15), 6.6* (ref 22), 6.93 (ref 32), 5.72* (ref 41), 6.0* (ref 48), 6.18* (ref 52)	6.2 ± 0.4	1.33
333	6.4* (ref 22), 5.40* (ref 41), 5.52 (ref 46), 5.8* (ref 48), 6.04 (ref 52)	5.8 ± 0.4	1,24
343	6.3* (ref 22), 6.2* (ref 31), 6.3[e] (ref 35), 5.14* (ref 41), 6.1* (ref 48), 5.89* (ref 52)	6.0 ± 0.4	1.29
353	6.5* (ref 48)	6.5	1.40
363	8.4* (ref 48)	8.4	1.84

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] Average of results from two separate methods.

[c] Data from ref 5 at 301 K omitted for representational convenience.

[d] Data from ref 27 at 311 K omitted for representational convenience.

[e] 343.6 K.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

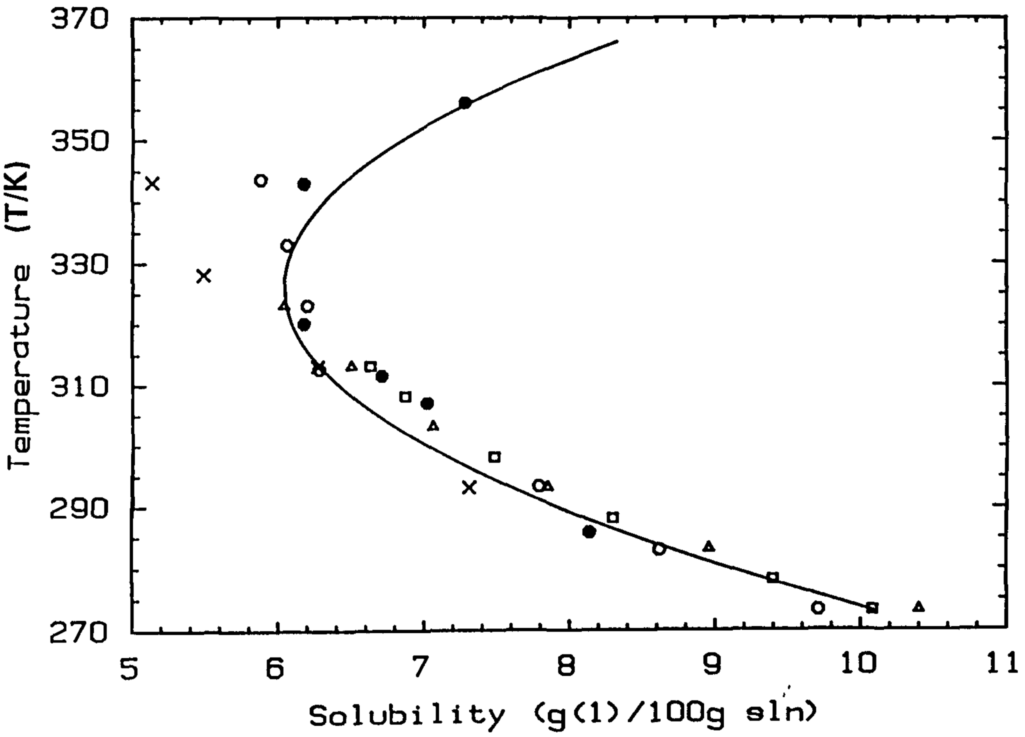

FIGURE 1. Selected data for the solubility of acetic acid ethyl ester (1) in water (2): ref 9 (□); ref 13 (△); ref 41 (X); ref 48 (●); ref 52 (○). Solid line is drawn through the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID ETHYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid ethyl ester (1) are summarized in Table 3 with the following exceptions.

The data of Bonner (ref 7), Doolittle (ref 18), Jones and McCants (ref 27), Zheleznyak and Brounshtein (ref 32), Filip and Maciejewski (ref 40), mainly at 293 K, are significantly higher (> $3\sigma_n$) than all other studies and are rejected. Similarly, the data of Akita and Yoshida (ref 31), Aleksandrova *et al.* (ref 39), Sadovnikova *et al.* (ref 42), and Woycicka *et al.* (ref 43) are significantly lower (> $3\sigma_n$) than other studies and are also rejected. The data of Bancroft (ref 4, in v/v units) and Shanley and Greenspan (ref 21, at "room temperature") are omitted in view of the ready availability of other good quality data.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

The remaining data are generally in good agreement enabling the averaged "Best" values to be Recommended over quite a range. Selected data are plotted in Figure 2.

TABLE 3: Recommended (*R*) and Tentative Solubilities of Water (2) in Acetic acid ethyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	x_2
273	2.28 (ref 9), 2.26' (ref 16), 2.3 (ref 20), 2.38 (ref 33), 2.13 (ref 52)	2.27 ± 0.08 (*R*)	0.102
283	2.61 (ref 9), 2.60* (ref 16), 2.49 (ref 52)	2.57 ± 0.05 (*R*)	0.114
293	2.98 (ref 9), 3.07 (ref 14), 3.05 (ref 16), 2.8 (ref 20), 3.1* (ref 22), 3.02^{b} (ref 26), 3.0 (ref 35), 2.96 (ref 41), 2.87* (ref 52)	2.98 ± 0.09 (*R*)	0.130
298	3.19 (ref 9), 3.28* (ref 16), 3.0 (ref 17), 3.24 (ref 19), 3.2* (ref 22), 3.22^{b} (ref 26), 3.1 (ref 38), 3.17* (ref 48), 3.08* (ref 52)	3.16 ± 0.08 (*R*)	0.138
303	3.42 (ref 9), 3.52 (ref 16), 3.5* (ref 22), 3.50 (ref 23), 3.47^{b} (ref 26), 3.47 (ref 28), 3.5 (ref 29), 3.25 (ref 33), 3.7 (ref 34), 3.4* (ref 38), 3.40 (ref 41), 3.60* (ref 48), 3.28* (ref 52)	3.46 ± 0.11 (*R*)	0.149
313	3.98 (ref 9), 4.0* (ref 22), 3.9 (ref 38), 3.88 (ref 41), 3.98 (ref 48), 3.68* (ref 52)	3.90 ± 0.11 (*R*)	0.166
323	4.46 (ref 9), 4.5* (ref 22), 4.40 (ref 41), 4.54* (ref 48), 4.23 (ref 50), 4.03* (ref 52)	4.36 ± 0.18 (*R*)	0.195
333	5.02 (ref 9), 5.1* (ref 22), 5.00* (ref 41), 4.985 (ref 46), 5.24* (ref 48)	5.07 ± 0.09 (*R*)	0.207

[a] Obtained by averaging where appropriate.

[b] Average of two independent determinations.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities: Reported values g(2)/100g sln	"Best" values ($\pm\sigma_n$)[a] g(2)/100g sln	x_2
343	5.8* (ref 22), 6.0 (ref 31), 5.8[c] (ref 35), 5.61 (ref 41), 6.38[d] (ref 44), 6.02 (ref 48)	5.9 ± 0.2 (*R*)	0.235
353	6.82* (ref 48)	6.8	0.263
363	7.59* (ref 48)	7.6	0.286

[c] 343.6 K.

[d] 343.4 K.

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

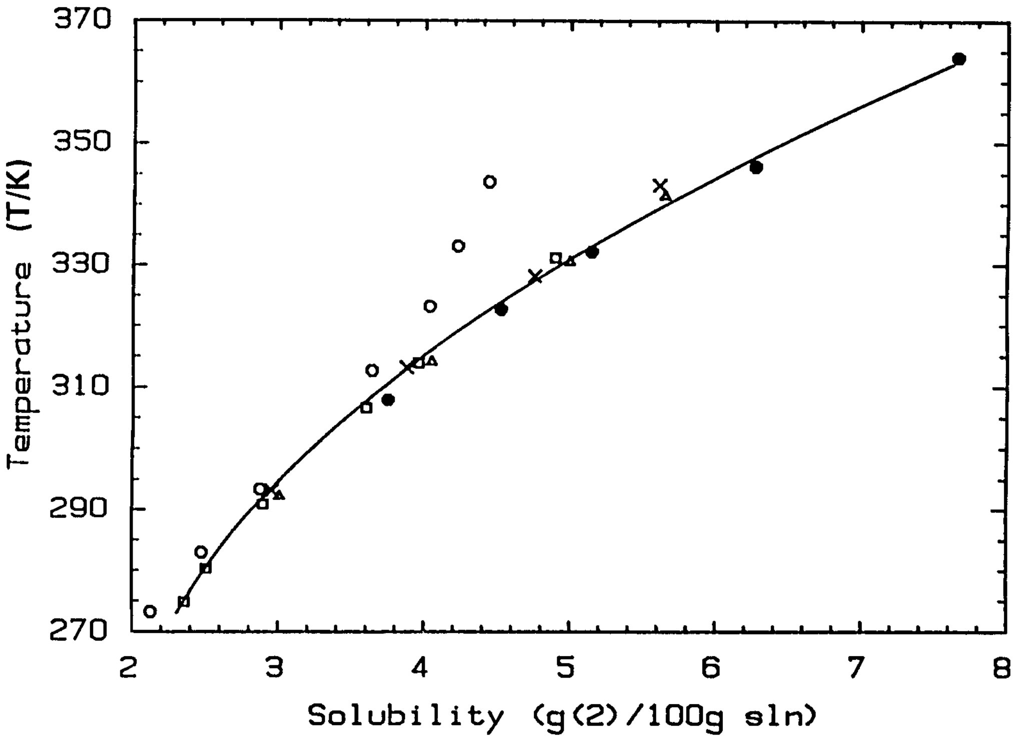

FIGURE 2. Selected data for the solubility of water (2) in acetic acid ethyl ester (1): ref 9 (□); ref 22 (△); ref 41 (X); ref 48 (●); ref 52 (O). Solid line is drawn through the "Best" values from Table 3.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

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COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

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(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

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ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Mohr

Arch. Pharm. 1851, *65*, 1-16.

VARIABLES:

T/K = room temperature [a]

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water was reported to be 3 g(1)/34.2 g(2) and 2.655 g(1)/31.045 g(2)[a]. The corresponding mass percentage and mole fraction, x_1, values calculated by the compiler are 8.06 g(1)/100g sln, 7.878 g(1)/100g sln and 0.01762, 0.01719 respectively.

[a] No information about temperature; probably below room temperature.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. A known mass of ester was titrated with water until the mixture became homogeneous.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; d_4^{20} 0.8889.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Marsson, T.

Arch. Pharm. 1853, *74*, 290-6.

VARIABLES:

$T/K = 290.5$

PREPARED BY:

A. Szafranski and G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 17.5°C was reported to be 7.86 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 1.72×10^{-2}.

The solubility of water in acetic acid ethyl ester at 17.5°C was reported to be 2.835 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 1.25×10^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The cloud point method was used. No further details were provided.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized (details not provided) and distilled; middle fraction shaken with water, dried over $CaCl_2$, redistilled; b.p. range 78.0-78.5°C.

(2) Distilled (no details given).

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. ±1.4% rel., (1) in (2).
±0.5% rel., (2) in (1).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.
VARIABLES:	PREPARED BY:
$T/K = 295$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 22°C was reported to be 1 part of ethyl acetate in 17-20 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 5.2 g(1)/100g sln and 0.011.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Not specified. (2) Not specified.
	ESTIMATED ERROR:
	Soly. ±0.4 g(1)/100g sln.
	REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bancroft, W.D.

Phys. Rev. 1895, *3*, 114-36.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 0.926 mL(1)/10mL(2). The solubility of water in ethyl acetate at 20°C was reported to be 0.294 mL(2)/10mL(1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. 10 mL of solvent in a test tube was titrated with the second component until the solution became cloudy.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; dried over $CaCl_2$, distilled.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±0.01 mL.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Euler, H.

Z. Phys. Chem. 1899, *31*, 360-69.

VARIABLES:

T/K = 301

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 28°C was reported to be 0.825 mol(1)/L(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 6.80 g(1)/100g sln and 0.0147.

Density of water d_4^{28} = 0.9962 (ref 1) was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture of 15 mL of (1) with 30-40 mL of (2) was shaken for 8 h. in a thermostated vessel. After separation, the water-rich phase was analyzed by saponification with a known excess of alkali solution which was then back titrated with standard acid.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.5 g(1)/100g sln (compiler).

REFERENCES:

1. *Selected Values of Properties of Hydrocarbons and Related Compounds*, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, 1973.

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rayman, J.

Thesis, Budapest, 1906.

VARIABLES:

T/K = 273 - 303

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of acetic acid ethyl ester in water

t/°C	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	10.94	9.86	0.0219
10.	9.70	8.84	0.0194
20.	8.63	7.94	0.0173
30.	7.79	7.23	0.0157

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, *55*, 360.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Bonner, W.D. *J. Phys. Chem.* 1910, *14*, 738-89.
VARIABLES:	PREPARED BY:
$T/K = 273$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 0°C was reported to be 1.086 g(1)/10g(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 9.80 g(1)/100g sln and 0.0217.

The solubility of water in acetic acid ethyl ester at 0°C was reported to be 0.301 g(2)/10g(1). The corresponding mass per cent and mole fraction, x_2, values calculated by the compiler are 2.92 g(2)/100g sln and 0.128.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method was used. Only the measurements for the ternary systems were described.	(1) Not specified. (2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.8 g(1)/100g sln and ±0.6 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Seidell, A.

Hygienic Lab. Bull. 1910, No. 67, 98 pp. (US Govt. Printing Office, Washington, DC).

VARIABLES:

T/K = 283 - 313

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of acetic acid ethyl ester in water

t/°C	g(1)/100g sln	x_1 (compiler)
10.	9.15	0.0202
15.	8.71	0.0191
20.	8.27	0.0181
25.	7.90	0.0172
30.	7.61	0.0166
35.	7.39	0.0161
40.	7.17	0.0156

Extrapolated data down to 0°C and up to 55°C are given also.
The solubility of water in acetic acid ethyl ester at 25°C was reported to be 4.8 cm^3(2)/100cm^3(1) and 5.38 g(2)/100g(1) giving 5.10 g(2)/100g sln. and a mole fraction, x_2, value of 0.208 as calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Portions of distilled water (50cm^3) at approximately the desired temperature were titrated to opalescence with (1). The exact temperature of the mixture was noted immediately after the saturation point was reached. The solubility of (2) in (1) appears to have been obtained by an analogous procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum, dried for 24h. over $CaCl_2$, filtered, and distilled; b.p. 75-76°C, d_{25}^{25} 0.8915 g/cm^3.

(2) Distilled; no other details given.

ESTIMATED ERROR:

soly. not stated.
temp. not stated.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Merriman, R.W.

J. Chem. Soc. 1913, *103*, 1774-89.

VARIABLES:

T/K = 273 - 333

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0[a]	10.08	97.72	0.02241	0.8976
1.6	-	97.64	-	0.8943
5[a]	9.40	97.56	0.02077	0.8910
7.1	-	97.49	-	0.8882
10[a]	8.81	97.39	0.01937	0.8841
13.3	-	97.29	-	0.8801
15[a]	8.30	97.21	0.01817	0.8769
17.7	-	97.10	-	0.8726
20[a]	7.86	97.02	0.01714	0.8694
20.0	-	97.04	-	0.8702
25[a]	7.48	96.81	0.01626	0.8612
25.9	-	96.74	-	0.8585
30[a]	7.15	96.58	0.01550	0.8524

[a] Author's smoothed results.

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic and analytical methods were used. The (2)-rich phase was determined by the cloud point method. A mixture of 100g of (1) and a required amount of (2) was warmed until clearness; then, it was allowed to cooled to produce a turbidity. The reported temperature was the mean of the two observations. Each experiment was repeated several times. The (1)-rich phase was determined at constant temperature in a sealed bulb of 75 mL capacity. Samples of known composition were shaken until constant volume of the layers was reached (<2 h.) and then the phase composition was calculated using mass balance, density and phase volume.

SOURCE AND PURITY OF MATERIALS:

(1) Prepared and purified in laboratory; purity not specified.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C (author).
Soly. about ±(0.05-0.1) g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Merriman, R.W.

J. Chem. Soc. 1913, *103*, 1774-89.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
33.4	-	96.40	-	0.8456
35[a]	6.87	96.34	0.01486	0.8433
36.7	-	96.28	-	0.8411
39.6	-	96.10	-	0.8344
40[a]	6.63	96.08	0.01431	0.8337
40.7	-	96.04	-	0.8322
45[a]	-	95.81	-	0.8238
46.0	-	95.78	-	0.8227
50[a]	-	95.54	-	0.8141
53.1	-	95.38	-	0.8085
55[a]	-	95.26	-	0.8043
58.0	-	95.10	-	0.7987
60[a]	-	94.98	-	0.7946

[a] Author's smoothed results.

COMPONENTS:

(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Euler, H.; Svanberg, O.

Ark. Kem. Mineral. Geol. 1917, *6*(14), 1-14.

VARIABLES:

$T/K = 291$

PREPARED BY:

A. Szafranski and G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 25°C was reported to be 7.3 g(1)/100g(2). The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 6.8 g(1)/100g sln and 0.0147.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental procedure was as described in (ref 1). The satura-composition was approached from both sides and the excess of (1) was kept to a minimum. No further details were provided.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Euler, H. *Z. Phys. Chem.* 1899, *31*, 360-9.

COMPONENTS:

(1) Acetic acid ethyl ester
(ethyl acetate); $C_4H_8O_2$;
[141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Fuehner, H.

Ber. Dtsch. Chem. Ges. 1924,
57, 510-5.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 7.00 vol%, 6.44 g(1)/100g sln and 0.731 mol(1)/L sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.01388.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±1.3 g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Glasstone, S.; Pound, A.

J. Chem. Soc. 1925, *127*, 2660-7.

VARIABLES:

T/K = 273 - 323

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Solubility of acetic acid ethyl ester in water

t/°C	g(1)/100g(2)	mol(2)/mol(1)	g(1)/100g sln (compiler)	x_1 (compiler)
0	10.40	-	9.42	0.02082
10	8.96	-	8.22	0.01779
20[a]	7.85	-	7.28	0.01580
25	7.39	-	6.88	0.01488
25[b]	-	66.15	6.88	0.01489
30[a]	7.06	-	6.59	0.01423
37	6.65	-	6.24	0.01341
40[a]	6.50	-	6.10	0.01312
50	6.04	-	5.70	0.01220
50[b]	-	80.98	5.70	0.01220

[a] Authors' graphically interpolated data.

[b] The method was not specified.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The water with a slight excess of ester was shaken at a temperature below the one measured and placed into a thermostat bath. The mixture was saturated in the course of one to two hours at the measured temperature. The saturated solution (3 to 8 g) was transferred to a stoppered bottle, weighed and hydrolyzed with standard NaOH. The residue was always tested to make sure that no acetic acid remained.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized as described in Roberts (ref 1); distilled over $CaCl_2$ and then several times over P_2O_5.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±(0.4-0.6) g(1)/100g sln (compiler).

REFERENCES:

1. Roberts, *J. Soc. Chem. Ind.* 1924, *43*, 295T.

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Kendall, J.; Harrison, L.E.

Trans. Faraday Soc. 1928, *24*, 588-96.

VARIABLES:

$T/K = 273 - 323$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of acetic acid ethyl ester in water

$t/°C$	x_1	g(1)/100g sln (compiler)
0.0	0.0208	9.41
10.0	0.0179	8.19
20.0	0.0158	7.28
25.0	0.0148	6.84
30.0	0.0142	6.58
37.0	0.0134	6.23
40.0	0.0131	6.10
50.0	0.0121	5.65

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method was used. The sealed tube method of Smith and Eastlack (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.1-0.2)°C (authors).
Soly. about ±0.5 g(1)/100g sln (compiler).

REFERENCES:

1. Smith, A.; Eastlack, H.E. *J. Am. Chem. Soc.* 1916, *38*, 1269.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Jones, D.C. *J. Chem. Soc.* 1929, 799-813.
VARIABLES:	PREPARED BY:
$T/K = 293$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 8.53 g(1)/100g sln and $x_1 = 0.016$.

The solubility of water in acetic acid ethyl ester at 20°C was reported to be 3.07 g(2)/100g sln and $x_2 = 0.152$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the synthetic method was used as described in Jones and Betts (ref 1). No further details were reported in the paper.	(1) Not specified. (2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.7 g(1)/100g sln and ±0.07 g(2)/100g sln (compiler).
	REFERENCES:
	1. Jones, D.C.; Betts, H.F. *J. Chem. Soc.* 1928, 1177.

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schlesinger, N.; Kubasowa, W.

Z. Phys. Chem. 1929, *142A*, 25-36.

VARIABLES:

$T/K = 288 - 323$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Solubility of acetic acid ethyl ester in water
authors' smoothed data

$t/^{o}C$	g(1)/100g(2)	g(1)/100g sln (compiler)	x_1 (compiler)
15	8.864	8.14	0.01780
20	8.420	7.77	0.01696
25	8.030	7.43	0.01615
30	7.692	7.14	0.01548
35	7.408	6.90	0.01492
40	7.177	6.70	0.01446
45	7.000	6.54	0.01411
50	6.875	6.43	0.01386

Authors' smoothing equation:

$$g(1)/100g(2) = 10.515 - 0.12605\ (t/°C) + 0.001065\ (t/°C)^2$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method described by Alexejev (ref 1) was used. Measurements were carried out in ampoules containing water and 0.10-0.15g of ester. The measurements were repeated several times.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; b.p. range 76.6-77.1°C at 753 mm Hg.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. ±0.01 g(1)/100g sln (compiler).

REFERENCES:

1. Alexejew, W. *Wied. Ann. Phys.* 1886, *28*, 306.

COMPONENTS:

(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Mion, M.

Compt. Rend. 1931, *193*, 1330-3.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

$t/^\circ C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	10.[a]	97.74[b]	0.0222	0.8984
15	8.3[b]	97.18[b]	0.0182	0.8757
30	7.1[b]	96.48[c]	0.0154	0.8486

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The turbidity method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-ethanol. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; used as received; d_4^{20} 0.9244.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±1.[a], ±0.1[b] and ±0.02[c] g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Park, J.G.; Hofmann, H.E.

Ind. Eng. Chem. 1932, *24* 132-4.

VARIABLES:

$T/K = 298$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 25°C was reported to be 7.9 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0172.

The solubility of water in acetic acid ethyl ester at 25°C was reported to be 3.0 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.131.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Nothing was specified in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, CP reagent grade; containing no alcohol; used as received.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.4 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester
(ethyl acetate); $C_4H_8O_2$;
[141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Doolittle, A.K.

Ind. End. Chem. 1935, *27*, 1169-79.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 6.92 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0150.

The solubility of water in acetic acid ethyl ester at 20°C was reported to be 11.01 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.377.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; purity 85%, b.p. range 70-80°C, d_4^{20} 0.886.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.9 g(1)/100g sln and
±7 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Lloyd, B.A.; Thompson, S.O.; Ferguson, J.B.

Can. J. Res. 1937, *15B*, 98-102.

VARIABLES:

T/K = 298

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 25°C was reported to be 7.56 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 1.64×10^{-2}.

The solubility of water in acetic acid ethyl ester at 25°C was reported to be 3.24 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 1.41×10^{-1}.

Note: The values are the same as those given in (ref 1) but apparently were confirmed experimentally by the authors.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. A two component sample was placed in a long tube with a small stoppered side-arm in a thermometer. The system was rotated so that the vapor phase moved from end-to-end and so stirred the liquid. One component was then added from a small weight burette to adjust the composition.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; CP grade washed with H_2O and distilled; d_4^{20} = 0.9006.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. Not stated.

REFERENCES:

1. Hill, A.E. *International Critical Tables* (Washburn, E.W., Ed.) McGraw Hill, New York, 1928, Vol. 3, 387-98.

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Beech, D.G.; Glasstone, S.

J. Chem. Soc. 1938, 67-73.

VARIABLES:

$T/K = 273 - 313$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

$t/^{\circ}C$	g(1)/100g(2)	g(1)/100g sln		x_1 (compiler)	
		(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
$0^{a,b,c}$	10.70 ± 0.05	9.67^d	-	0.0214	-
0^c	-	9.6	97.7	0.0213	0.897
$20^{a,b,c}$	8.40 ± 0.04	7.75^d	-	0.0169	-
20^c	-	7.8	97.2	0.0170	0.877
$40^{a,b,c}$	6.97 ± 0.04	6.52^d	-	0.0141	-

[d] Calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the synthetic method was used. Only the measurements for the ternary system were described.

SOURCE AND PURITY OF MATERIALS:

(1) [a] Synthesized; dried over K_2CO_3, refluxed with P_2O_5, distilled; b.p. range 77.0-77.2°C.
[b] Source not specified; kept over $CaCl_2$, distilled, fraction boiling at 74-76°C refluxed with P_2O_5 and distilled.
[c] Source not specified; washed three times with NaCl aq. and twice with H_2O, kept over $CaCl_2$, distilled.

(2) Not specified.

ESTIMATED ERROR:

Soly. see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Shanley, E.S.; Greenspan, F.P.

Ind. Eng. Chem. 1947, *39*, 1536-43.

VARIABLES:

T/K = room temperature

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of water in acetic acid ethyl ester at room temperature was reported to be 3.5 g(2)/100g(1). The corresponding mass per cent mole fraction, x_2, values calculated by the compiler are 3.4 g(2)/100g sln and 0.146.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester
(*ethyl acetate*); $C_4H_8O_2$;
[141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Griswold, J.; Chu, P.L.;
Winsauer, W.O.

Ind. Eng. Chem. 1949, *41*, 2352-8.

VARIABLES:

$T/K = 290 - 344$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

$t/^{\circ}C$	g(1)/100g sln (2)-rich phase	 (1)-rich phase	x_1 (compiler) (2)-rich phase	 (1)-rich phase
17.0	7.92	-	0.01728	-
19.0	-	96.99	-	0.8682
27.0	7.23	-	0.01569	-
27.5	7.18	-	0.01557	-
40.9	-	95.95	-	0.8289
57.3	-	95.00	-	0.7953
68.2	-	94.35	-	0.7735
70.4	6.3	-	0.0136	-

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method was used. A rotating cage containing the glass ampoule (ca. 10 mL) with a sample was warmed and cooled in a water bath until the cloud point appeared and disappeared over a 0.2°C temperature range. The average temperature was taken.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, anhydrous reagent grade; distilled; d_4^{25} 0.89428, n_D^{25} 1.37012.

(2) Distilled; d_4^{25} 0.99707.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. better than ±0.1 g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sohoni, V.R.; Warhadpande, U.R.

Ind. Eng. Chem. 1952, *44*, 1428-9.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 30°C was reported to be 7.10 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.01539.

The solubility of water in acetic acid ethyl ester at 30°C was reported to be 3.50 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.1507.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method described by Taylor (ref 1) was used. The data and method were reported together with the ternary system acetic acid ethyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, analytical reagent grade; d^{30} 0.8939, n_D^{30} 1.3700.

(2) Distilled; d_4^{30} 0.9957, n_D^{30} 1.3320.

ESTIMATED ERROR:

Soly. about ±0.1 g(1)/100g sln and ±0.02 g(2)/100g sln (compiler).

REFERENCES:

1. Taylor, S.F. *J. Phys. Chem.* 1897, *1*, 461.

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Altshuller, A.P.; Everson, H.E.

J. Am. Chem. Soc. 1953, *75*, 1727.

VARIABLES:

$T/K = 292 - 313$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of acetic acid ethyl ester in water

$t/°C$	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
19.2	8.34	7.70	0.01677
20.4	8.31	7.67	0.01670
20.5	8.29	7.66	0.01667
21.3	8.26	7.63	0.01661
22.0	8.22	7.60	0.01653
22.6	8.14	7.53	0.01637
22.7	8.12	7.51	0.01633
23.0	8.11	7.50	0.01631
23.4	8.10	7.49	0.01629
24.7	8.05	7.42	0.01612
25.1	8.03	7.41	0.01611
25.4	8.02	7.41	0.01611
25.4	8.03	7.41	0.01611

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method as described in Weissberger (ref 1) was used. The solubilities of acetic acid ethyl ester agreed to within ±0.1°C when determined by heating and then by cooling. (The appearance of turbidity may be detected within about 0.2°C range usually.) Temperature was measured with a 0.05°C, thermometer which gave agreement to within 0.01°C with the sodium sulphate transition point. Each solubility value was determined twice or thrice.

SOURCE AND PURITY OF MATERIALS:

(1) Mallinckrodt reagent analytical grade; 0.06% water asdetermined by Karl Fischer reagent; redistilled from a column of 24 theoretical plates; n_D^{24} 1.3697.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±(0.05-0.1) g(1)/100g sln (compiler).

REFERENCES:

1. Weissberger, A. *Physical Methods of Organic Chemistry*, Vol.1, Part I, Interscience Publishers, Inc., New York, 1939, p.319.

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Altshuller, A.P.; Everson, H.E. *J. Am. Chem. Soc.* 1953, *75*, 1727.

EXPERIMENTAL VALUES: (continued)

Solubility of acetic acid ethyl ester in water

t/°C	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
25.4	8.00	7.41	0.01609
25.9	7.93	7.35	0.01596
26.0	7.93	7.35	0.01596
26.3	7.94	7.36	0.01598
27.0	7.89	7.31	0.01588
28.0	7.80	7.24	0.01570
28.1	7.81	7.24	0.01572
28.4	7.82	7.25	0.01574
28.7	7.81	7.24	0.01572
29.7	7.71	7.16	0.01552
29.9	7.71	7.16	0.01552
30.0	7.72	7.17	0.01554
30.0	7.69	7.14	0.01548
30.1	7.69	7.14	0.01548
31.2	7.60	7.06	0.01530
31.8	7.58	7.05	0.01526
31.9	7.58	7.05	0.01526
31.9	7.57	7.04	0.01524
32.0	7.51	6.99	0.01512
32.8	7.49	6.97	0.01508
33.0	7.46	6.94	0.01502
33.8	7.40	6.89	0.01491
34.0	7.38	6.87	0.01487
36.8	7.32	6.82	0.01475
37.8	7.25	6.76	0.01461
39.9	7.15	6.67	0.01441
39.9	7.15	6.67	0.01441

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Altshuller, A.P.; Everson, H.E. *J. Am. Chem. Soc.* 1953, *75*, 1727.

EXPERIMENTAL VALUES: (continued)

The smoothed solubility of acetic acid ethyl ester in water

$t/°C$	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
20	8.42	7.77	0.01693
25	8.04	7.42	0.01612
30	7.70	7.15	0.01550
35	7.39	6.88	0.01489
40	7.12	6.65	0.01435

Authors' smoothing equation:

$$g(1)/100g(2) = (9.522 \pm 0.018) - (0.0618 \pm 0.0006)\ t/°C$$

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Garner, F.H.; Ellis, S.R.M.

Chem. Eng. Sci. 1953, *2*, 282-6.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 30°C was reported to be 1.7 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0035.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described in Garner, Ellis and Roy (ref 1) was used. The weighed amount of miscible mixture was placed into the test tube and titrated to turbidity. The apparatus was a thin-walled glass tube with a glass stirrer and thermometer inside, placed in a thermostat. Only the measurements for the ternary systems were described.
The data were reported together with the ternary system acetic acid ethyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, analytical grade; distilled; b.p. 77.1°C, n_D^{20} 1.3700.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±5 g(1)/100g sln (compiler).

REFERENCES:

1. Garner, F.H.; Ellis, S.R.M.; Roy, U.N.G. *Chem. Eng. Sci.* 1953, *2*, 14.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Gayler, R.; Pratt, H.R.C. *Trans. Inst. Chem. Eng.* 1953, *31*, 78-93.
VARIABLES:	**PREPARED BY:**
$T/K = 288 - 303$	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

$t/^\circ C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
15[a]	8.22	97.04	0.01798	0.8702
15[b]	8.05	97.26	0.01759	0.8789
20[a]	7.86	96.87	0.01714	0.8635
20[b]	7.62	97.10	0.01659	0.8726
25[a]	7.58	96.69	0.01649	0.8566
25[b]	7.38	96.87	0.01603	0.8635
30[a]	7.32	96.40	0.01589	0.8456
30[b]	7.11	96.65	0.01541	0.8551

[a] Titration method.

[b] Analytical method.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration and analytical methods were used. In the titration method, the component (1) or (2) was added in stages from a finely calibrated 5 mL burette to a thermostated 100 mL sample of the second component and shaken. The procedure was continued until a faint cloudiness persisted in the sample.
In the analytical procedure, the (2) in the ester phase was determined by the Karl Fischer iodometric titration. The (1) in the water phase was determined by hydrolysis of duplicate samples of 5 g each with 0.2N alcoholic KOH for 2 h. Also, a third blank sample was refluxed at the same time. The samples were titrated with 0.2N HCl using phenolphthalein as an indicator.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; distilled and dried; purity not specified.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C[a].
Soly. ±0.01 mL (reproducibility)[a].

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Jones, J.H.; McCants, J.F. *Ind. Eng. Chem.* 1954, *46*, 1956-62.
VARIABLES:	**PREPARED BY:**
T/K = 311	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 100°F was reported to be 7.0 g(1)/100g sln. The corresponding values of temperature Kelvin and mole fraction, x_1, calculated by the compiler are 311 K and 0.015.

The solubility of water in acetic acid ethyl ester at 100°F was reported to be 4.6 g(2)/100g sln. The corresponding values of temperature Kelvin and mole fraction, x_2, calculated by the compiler are 311 K and 0.19.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The organic-rich phase composition was obtained by adding water (first rapidly and then dropwise) to the glass-stoppered flask and agitated. The cloud point was assumed to be reached when the cloud persisted for 5 minutes. The water-rich phase was obtained by titration. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Commercial Solvents, 99% undenatured, n_D^{20} 1.3717; used as received.

(2) Distilled; n_D^{20} 1.3330.

ESTIMATED ERROR:

Temp. ±0.2°F (authors).
Soly. about ±0.2 g(1)/100g sln and ±0.7 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Rao, G.J.R.; Rao, C.V. *J. Sci. Ind. Res.* 1955, *14B*, 444-8.
VARIABLES:	PREPARED BY:
T/K = 303	Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 30°C was reported to be 7.22 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.01566.

The solubility of water in acetic acid ethyl ester at 30°C was reported to be 3.47 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.1495.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-propanoic acid. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Merck; b.p. 77.1°C, d^{30} 0.8885; used as received.

(2) Distilled and boiled; free from CO_2.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±0.3 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Venkataratnam, A.; Rao, J.R.; Rao, C.V.

Chem. Eng. Sci. 1957, *7*, 102-10.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 30°C was reported to be 7.4 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0161.

The solubility of water in acetic acid ethyl ester at 30°C was reported to be 3.5 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.151.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system acetic acid ethyl ester-water-2-propanone (*ethyl acetate-water-acetone*).

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House Ltd., analytical grade; used as received; b.p. 77.1°C, d^{30} 0.8885, n^{30} 1.3680.

(2) Distilled; free of CO_2.

ESTIMATED ERROR:

Soly. about ±0.1 g(1)/100g sln and ±0.05 g(2)/100g sln (compiler).

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS: (1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Rao, M.V.R.; Rao, K.S.; Rao, C.V. *J. Sci. Ind. Res.* 1961, *20B*, 379-81.
VARIABLES: T/K = 308	PREPARED BY: Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 35°C was reported to be 8.9 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0196.

The solubility of water in acetic acid ethyl ester at 35°C was reported to be 3.5 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.151.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-formic acid. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) BDH, laboratory reagent grade; used as received.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±1.9 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Akita, K.; Yoshida, F.

J. Chem. Eng. Data 1963, *8*, 484-90.

VARIABLES:

T/K = 298 and 343
p/kPa = 101.325 (1 atm)

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility in the system of acetic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
25	7.5^a	97.8^b	0.016	0.899
70	6.2^a	94.0^a	0.013	0.762

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method was used at 25°C. The analytical method was used at 70°C. The data were reported together with the ternary system acetic acid ethyl ester-water-methanol. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, special reagent grade; distilled with column 150 cm in height, with McMahlon packing; d_4^{25} 0.8945, n_D^{25} 1.3697, b.p. 77.1°C.

(2) Not specified.

ESTIMATED ERROR:

Soly. about $\pm 0.05^a$ and $\pm 1.0^b$ g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Zheleznyak, A.S.; Brounshtein, B.I.

Zh. Prikl. Khim. 1965, *38*, 694-6.

VARIABLES:

T/K = 298 and 323

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	8.51	96.70	0.01866	0.8570
50	6.93	96.08	0.01500	0.8336

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The samples were thermostated for 2.5 h. and then both phases were analyzed. Water was determined by the Karl Fischer method. The method of ester analysis was not reported. The data and method were reported with the ternary system acetic acid ethyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, analytical grade; used as received.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. better than ±0.7 g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Pai, M.U.; Sane, A.G.

Indian J. Technol. 1966, *4*, 373-5.

VARIABLES:

T/K = 273 and 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	9.29	97.62	0.0205	0.8935
30	6.70	96.75	0.0145	0.8589

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The turbidity method described in Othmer, White and Trueger (ref 1) was used. Mutual solubilities were determined in a 25 mL glass stoppered flask placed in a thermostat. The data were reported together with the ternary system acetic acid ethyl ester-water-ethylacetoacetate.

SOURCE AND PURITY OF MATERIALS:

(1) Union Carbide, technical grade; treated with anhydrous K_2CO_3, distilled; purity 99.8%, b.p. 77.0°C, d^{20} 0.9001.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±0.5 g(1)/100g sln (compiler).

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Acetic acid ethyl ester
(*ethyl acetate*); $C_4H_8O_2$;
[141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Nakamura, A.

Kogyo Kagaku Zasshi 1968, *71(10)*,
1577-80.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 30°C was reported to be 6.7 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0145.

The solubility of water in acetic acid ethyl ester at 30°C was reported to be 3.7 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.158.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture was placed in a 1 L flask and stirred for 1 h. which was sufficient for equilibrium. Then, after 1/2 h. separation, samples of both phases were analysed. The ester was analysed by saponification with 2N NaOH and reverse titration with 2N HCl. Water was determined by the Karl Fischer method. The method and data were reported together with the ternary system acetic acid ethyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; distilled; purity 99.20% wt, impurities: 0.63% water, 0.08% ethyl alcohol, 0.06% vinyl acetate, 0.02% toluene, 0.01% unknown.

(2) Purified on ion-exchange material; resistivity $>4\times10^6$ ohm.

ESTIMATED ERROR:

Temp. ±0.3°C (author).
Soly. about <3% (relative error of (1) author), ±0.5 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Batmanova, G.A.; Balashov, M.I.; Grishunin, A.V.; Savinskaya, I.G.; Serafimov, L.A.

Gidroliz. Lesokhim. Prom. 1971, *24(8)*, 11-2.

VARIABLES:

T/K = 293 and 344

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20[a]	7.86[d]	97.0[d]	0.01714	0.869
70.40[b,c]	6.3[d]	94.2[e]	0.0136	0.769

[a] Titration method.

[b] Analytical method.

[c] Numerical value of boiling temperature at 760 mm Hg is not reported in the paper; boiling temperature of two-phase mixture equal to 70.40°C was taken from Skrzecz and Maczynska (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration and analytical methods were used. In the titration method, the titrations were carried out in thermostated bottles using a magnetic stirrer at 20°C and in a heated flask with a magnetic stirrer and reflux condenser at the boiling temperature. In the analytical procedure, a two-phase mixture was placed into a heated flask attached to a reflux condenser, mixed for 1/2 h. at the boiling temperature, separated and analyzed by glc. A small amount of water was also determined by the Karl Fischer method.
The data and methods were reported together with the ternary system formic acid ethyl ester-water-acetic acid ethyl ester.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, chemically pure grade; used as received.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.05[d] and ±0.2[e] g(1)/100g sln (compiler).

REFERENCES:

1. Skrzecz, A.; Maczynska, Z. *Pol. J. Chem.* 1980, *54*, 2383.

COMPONENTS:

(1) Acetic acid ethyl ester
(ethyl acetate); $C_4H_8O_2$;
[141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Iguchi, A.; Fuse, K.

Kagaku Kogaku 1971, *35(9)*, 1035-7.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 25°C was reported to be 6.11 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.01313.

The solubility of water in acetic acid ethyl ester at 25°C was reported to be 2.54 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.1131.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used.
The samples were titrated with the second component to obtain turbidity. The method and data were rereported together with the ternary system acetic acid ethyl ester-water-acetic acid.
No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial grade of high purity, used as received.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. about ±1.4 g(1)/100g sln and
±1.0 g(2)/100g sln
(compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester
(*ethyl acetate*); $C_4H_8O_2$;
[141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Krupatkin, I.L.; Shcherbakova, T.A.

Zh. Prikl. Khim. 1971, *44*, 307-11.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 25°C was reported to be 7.47 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.01623.

The solubility of water in acetic acid ethyl ester at 25°C was reported to be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.1537.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Only the measurements for the ternary systems were described. The amount of water in the pure ester was taken into account. The data were reported together with the ternary system acetic acid ethyl ester-water-phosphoric acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, chemical reagent; d_4^{20} 0.9020.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±0.05 g(1)/100g sln
and ±0.3 g(2)/100g sln
(compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Utkin, G.K.; Zamyatina, V.K.; Andronnikov, N.V.; Golikov, L.V.

Gidroliz. Lesokhim. Prom. 1971, *24(8)*, 9-10.

VARIABLES:

$T/K = 298$ and 313

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
25	6.9^a	96.9^b	0.0149	0.865
40	5.8^a	96.1^b	0.0124	0.834

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. One-phase mixture was titrated and mixed in a thermostated apparatus with a reflux condenser for 1 h. until an opalescence appeared. Only the measurements for the ternary systems were described. The data were reported together with the ternary system acetic acid ethyl ester-water-propionic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, pure for analysis; distilled, fraction boiling at 77.0-77.5°C was used; purity 99.5%, dry residue 0.001%, without ashes, d^{20} 0.9002.

(2) Distilled; without CO_2.

ESTIMATED ERROR:

Soly. about $\pm 0.7^a$ and $\pm 0.1^b$ g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Aleksandrova, M.V.; Sadovnikova, L.V.; Martynov, V.V.
Sb. Nauch. Tr. Ivanov. Energ. Inst. 1972, *14*, 146-54.

Sadovnikova, L.V.; Aleksandrova, M.V.; Serafimov, L.A.
Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. 1972, *15*, 1183-5.

VARIABLES:

T/K = 293

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 8.70 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.01911.

The solubility of water in acetic acid ethyl ester at 20°C was reported to be 2.25 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.1012.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-acetic acid. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purified; n_D^{20} 13724.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±0.9 g(1)/100g sln and ±0.7 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester
(ethyl acetate); $C_4H_8O_2$;
[141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Filip, S.; Maciejewski, Z.

Chem. Stosow. 1972, *16*, 445-51.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 8.22 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0180.

The solubility of water in acetic acid ethyl ester at 20°C was reported to be 4.9 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.20.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. To determine the solubility, weighed amounts of one component (ca. 50g) were titrated with the second component in a constant temperature bath. Titrations were performed using a burette graduated in 0.1-mL divisions. The samples were stirred vigorously.

SOURCE AND PURITY OF MATERIALS:

(1) FOCH Gliwice; chemically pure grade; used as received.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.4 g(1)/100g sln and
±1.9 g(2)/100g sln
(compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Mertl, I. *Collect. Czech. Chem. Commun.* 1972, *37*, 366-74.
VARIABLES:	**PREPARED BY:**
T/K = 293 - 343	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20[a]	7.31	97.04	0.01587	0.8702
40	6.27	96.12	0.01349	0.8351
55	5.49	95.24	0.01174	0.8036
70[b]	5.14	94.39	0.01096	0.7748

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. To determine the solubilities, the selected component was added from a burette to the weighed sample in a vessel with a magnetic stirrer until a slight turbidity appeared and disappeared. The jacket of the vessel was connected by an insulated tube with a thermostat. A reflux condenser prevented the solution from evaporating. The observation was facilitated by shielding the vessel and by using intense illumination.

SOURCE AND PURITY OF MATERIALS:

(1) Lachema Brno, laboratory grade; triple distilled with acetic anhydride in a 40 plate bubble-cap glass column; b.p. 77.06°C, d_4^{20} 0.90057, n_D^{20} 1.37242.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.01°C[a] and ±0.05°C[b] (author).
Soly. about ±(0.1-1.0) g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sadovnikova, L.V.; Komarova, V.F.; Aleksandrova, M.V.; Serafimov, L.A.

Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. 1972, *15(12)*,

VARIABLES:

T/K = 293

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 8.9 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0196.

The solubility of water in acetic acid ethyl ester at 20°C was reported to be 2.25 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.1012.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified. The data were reported together with the ternary system acetic acid ethyl ester-water-2-methylpropanoic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±1.1 g(1)/100g sln and ±0.8 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Woycicka, M.; Richon, D.; Viallard, A.

C.R. Acad. Sci. (Paris) Ser. C 1973, *276*, 983-6.

VARIABLES:

T/K = 298

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The mole fraction, x_1, solubility of acetic acid ethyl ester in water at 25°C was reported to be 0.0162_5. The corresponding mass percent value calculated by the compiler is 7.475 g(1)/100g sln.

The mole fraction, x_2, solubility of water in acetic acid ethyl ester at 25°C was reported to be 0.145. The corresponding mass percent value calculated by the compiler is 2.66 g(2)/100g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A calorimetric method was used. Mutual solubility was determined from plots of excess enthalpy (H^E) against composition. The H^E values were derived from heats of mixing measurements made in a Seteram "CRMT" microcalorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purified by preparative gas chromatography.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Van Zandijcke, F.; Verhoeye, L. *J. Appl. Chem. Biotechnol.* 1974, *24*, 709-29.
VARIABLES:	**PREPARED BY:**
$T/K = 343$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 70.25°C was reported to be $x_1 = 0.025$. The corresponding mass per cent value calculated by the compiler is 11.1 g(1)/100g sln.

The solubility of water in acetic acid ethyl ester at 70.25°C was reported to be $x_2 = 0.250$. The corresponding mass per cent value calculated by the compiler is 6.38 g(2)/100g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The boiling liquid, in equilibrium with its vapor, was delivered into a thermostated vessel where the phase separation occurred at the boiling point. Samples of the two phases were taken for glc analysis. The temperature of the vessel was controlled automatically and was equal to the boiling temperature.	(1) Source not specified; b.p. 77.15°C, d_4^{25} 0.8945, n_D^{25} 1.3698. (2) Not specified.
	ESTIMATED ERROR:
	Temp. ±0.05°C (authors). Soly. about ±4.8 g(1)/100g sln and ±0.4 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tare, J.P.; Puranik, S.A.; Kher, M.G.

Indian Chem. Eng. 1976, *18(4)*, 27-30.

VARIABLES:

$T/K = 303$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 30°C was reported to be 7.56 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0164.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method as described by Othmur, White and Trueger (ref 1) was used. The data were reported together with the ternary system acetic acid ethyl ester-water-furfural. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) B.D.H., analar grade; distilled; purity not specified.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.5°C (authors),
Soly. about ±0.3 g(1)/100g sln (compiler).

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sugi, H.; Katayama, T.

J. Chem. Eng. Jpn. 1978, *11*, 167-72.

VARIABLES:

T/K = 333

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 60°C was reported to be x_1 = 0.0118. The corresponding mass per cent value calculated by the compiler is 5.52 g(1)/100g sln.

The solubility of water in acetic acid ethyl ester at 60°C was reported to be x_2 = 0.2042. The corresponding mass per cent value calculated by the compiler is 4.985 g(2)/100g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The cloud-point method as described by Sugi, Nitta and Katayama (ref 1) was used. The data were reported together with the ternary system acetic acid ethyl ester-water-acetonitrile.

SOURCE AND PURITY OF MATERIALS:

(1) Merck Uvasol, spectrograde; purity 99.7%, d^{25} 0.89453; used as received.

(2) Deionized, distilled.

ESTIMATED ERROR:

Temp. ±0.01°C (authors).
Soly. about ±0.1 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).

REFERENCES:

1. Sugi, H.; Nitta, T.; Katayama, T. *J. Chem. Eng. Jpn.* 1976, *9*, 12.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Alvarez, J.R.; Neila, J.J. *An. Quim.* 1978, *74*, 326-32.
VARIABLES:	PREPARED BY:
$T/K = 298$	Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 25°C was reported to be 7.3 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0159.

The solubility of water in acetic acid ethyl ester at 25°C was reported to be 3.6 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.154.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-phenol. No further details were reported in the paper.	(1) Source not specified, commercial product; used as received; $d_4^{21.8}$ 0.8943, n_D^{20} 1.3724. (2) Twice distilled over $KMnO_4$.
	ESTIMATED ERROR:
	Soly. about ±0.2 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester
(*ethyl acetate*); $C_4H_8O_2$;
[141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skrzecz, A.; Maczynski, A.

Pol. J. Chem. 1979, 53, 715-8.

Skrzecz, A.

Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

VARIABLES:

T/K = 286 - 364

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
285.8	0.0178	-	8.14	-
299.2	0.0176	-	8.06	-
307.1	0.0152	-	7.02	-
307.9	-	0.8401	-	96.25
311.6	0.0145	-	6.71	-
318.6	0.0136	-	6.32	-
320.2	0.0133	-	6.18	-
322.7	-	0.8116	-	95.47
327.7	0.0124	-	5.79	-
332.2	-	0.7902	-	94.85
343.0	0.0133	-	6.18	-
344.7	-	0.7575	-	93.86
346.2	-	0.7536	-	93.73

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew was used. An ampoule with the solution of fixed concentration was placed into a glass tube connected with a thermostat filled completely with distilled water. The temperature of the bath was changed continuously during the measurements and the appearance and disappearance of turbidity within the ampoule was observed visually. The amount of water in pure ester was taken into account.

SOURCE AND PURITY OF MATERIALS:

(1) Lachema Chemapol, pure for analysis grade; distilled; purity 99.99% by glc, 0.07 wt% water by the Karl Fischer method.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.2-0.6)°C.
Soly. see above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6] (2) Water; H_2O; [7732-18-5]	Skrzecz, A.; Maczynski, A. *Pol. J. Chem.* 1979, *53*, 715-8. Skrzecz, A. *Thesis*, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid ethyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
349.4	0.0145	-	6.71	-
356.1	0.0158	-	7.28	-
364.1	-	0.7114	-	92.34

Author's smoothing equations:

$$x_1 = 0.02175 - 3.081\times10^{-4} (T/K - 273.15) + 2.784\times10^{-6} (T/K - 273.15)^2$$

st. dev. = 5.5×10^{-4} (2)-rich phase

$$x_2 = 0.09360 + 1.6981\times10^{-3} (T/K - 273.15) + 5.0221\times10^{-6} (T/K - 273.15)^2$$

st. dev. = 2.19×10^{-3} (1)-rich phase

COMPONENTS:

(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E.

J. Chem. Eng. Data 1982, *27*, 451-4.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at 25°C was reported to be 0.726 mol(1)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 64.0 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of a water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible-with-water solution and then analyzed by a gas chromatographic technique.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purity >99% by glc.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. ±1.0%.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester *(ethyl acetate)*; $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Ouyang, F.; Wang, G.; Gao, W.

Hua Kung Hsueh Pao 1985, *(1)*, 110-18.

VARIABLES:

$T/K = 323$

PREPARED BY:

J. Fu

EXPERIMENTAL VALUES:

The proportion of acetic acid ethyl ester in the water-rich phase equilibrium at 50°C was reported to be 7.58 g(1)/100 g sln. The corresponding mole fraction solubility, x_1, is 0.0165.

The proportion of water in the ester-rich phase at 50°C was reported to be 4.23 g(2)/100 g sln. The corresponding mole fraction solubility, x_2, is 0.1778.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An analytical method was used. Sample mixtures in an equilibrium cell immersed in a constant temperature water bath were stirred with a magnetic agitator to be emulsified. Then, the mixture was settled for 4 h. and samples withdrawn from the upper and lower layers were analyzed by gas chromatograph.

SOURCE AND PURITY OF MATERIALS:

(1) CP reagent; fractionated before use and no other impurity peaks except that of ethyl acetate in chromatogram.

(2) Twice distilled; b.p. 100.00°C.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

T/K = 298 and 318

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

T/K	mol(1)/ 100g(2)	g(1)/ 100g(2)	x_1		g(1)/100g sln (compiler)	
			(2)-r. ph.	(1)-r. ph.	(2)-r. ph.	(1)-r. ph.
298.1[a]	-	-	0.01625	0.885	7.475[d]	97.41[e]
298.1[b]	0.0923	-	0.01636[c]	-	7.521[d]	-
298.1	-	8.13	0.01635[c]	-	7.519[d]	-
318.1[b]	0.0789	-	0.01401[c]	-	6.500[f]	-

[a] Calorimetric method.

[b] Refractometric method.

[c] Compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The calorimetric and differential refractometric methods were used. The calorimetric method was described in the thesis of Richon (ref 1) and by Richon and Villard (ref 2). For the refractometric measurements, a Phoenix model 1-2000T differential refractometer from Texas Instruments was used, and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) Merck (for analysis); purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.03[d], ±0.6[e] and ±0.1[f] g(1)/100g sln (compiler).

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.
2. Richon, D.; Villard, A. *Can. J. Chem.* 1976, *54*, 2584.

COMPONENTS:

(1) Acetic acid ethyl ester (*ethyl acetate*); $C_4H_8O_2$; [141-78-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

$T/K = 273 - 344$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid ethyl ester and water

$t/^\circ C$	g(1)/100g sln		x1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	9.71	97.87	0.0215	0.9038
9.8	8.62	97.52	0.0189	0.8894
20.2	7.79	97.12	0.0170	0.8733
29.7	6.81	96.74	0.0147	0.8585
39.5	6.28	96.36	0.0135	0.8440
50.0	6.20	95.96	0.0133	0.8292
59.9	6.06	95.77	0.0130	0.8223
70.5	5.88	95.56	0.0126	0.8148
std. dev.	0.05	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99.9%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Formic acid 1-methylethyl ester (*isopropyl formate*); $C_4H_8O_2$; [625-55-8]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 333

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in formic acid 1-methylethyl ester

$t/^\circ C$	g(1)/100g sln	x_1 (compiler)
0	98.95	0.9506
9.6	98.67	0.9381
19.7	98.34	0.9237
30.7	98.24	0.9194
40.0	97.83	0.9021
49.9	96.97	0.8674
60.2	96.40	0.8455

std. dev. 0.05

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 96%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the formic acid propyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Formic acid propyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Kendall and Harrison (ref 3)	272-318	(1) in (2)	synthetic
Rius and Alfonso (ref 4)	273-333	mutual	analytical, Karl Fischer
Stephenson and Stuart (ref 5)	273-343	(2) in (1)	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF FORMIC ACID PROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of formic acid propyl ester (1) in water (2) are summarized in Table 2 with the exception of the datum of Traube (ref 1) which is significantly lower (> $3\sigma_n$) than all other studies and is therefore rejected. The remaining studies, especially those of Rayman (ref 2) and Kendall and Harrison (ref 3) are in good agreement and a number of values are Recommended. Selected data are plotted in Figure 1. However, it is pertinent to note that Stephenson and Stuart (ref 5) who usually report mutual solubility data were unable to do so for this system because of substantial hydrolysis of the ester in the aqueous phase. Other authors do not appear to have experienced similar problems.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubilities of Formic acid propyl ester (1) in Water (2)

T/K	Solubilities Reported values g(1)/100g sln	"Best" values ($\pm\sigma_n$)[a] g(1)/100g sln	 10^3x_1
273	3.39 (ref 2), 3.54* (ref 3), 3.09 (ref 4)	3.3 ± 0.2 (*R*)	6.9
283	3.00 (ref 2), 3.04* (ref 3), 2.80* (ref 4)	2.95 ± 0.10 (*R*)	6.18
293	2.79 (ref 2), 2.82* (ref 3), 2.63* (ref 4)	2.75 ± 0.08 (*R*)	5.75
298	2.75 (ref 2), 2.76* (ref 3), 2.56 (ref 4)	2.69 ± 0.09 (*R*)	5.62
303	2.70 (ref 2), 2.71* (ref 3), 2.50* (ref 4)	2.64 ± 0.10 (*R*)	5.52
313	2.61* (ref 3), 2.44 (ref 4)	2.52 ± 0.09 (*R*)	5.26
323	2.49* (ref 4)	2.5	5.2
333	2.70 (ref 4)	2.7	5.6

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN FORMIC ACID PROPYL ESTER (1)

All the available data for the solubility of water (2) in formic acid propyl ester (1) are summarized in Table 3. Only two independent studies are available (ref 4,5) and the data are not in good agreement (see Figure 2) especially at higher temperatures. Consequently, no values have been Recommended and further investigation of this system is clearly justified with particular attention being given to the possibilities of ester hydrolysis.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

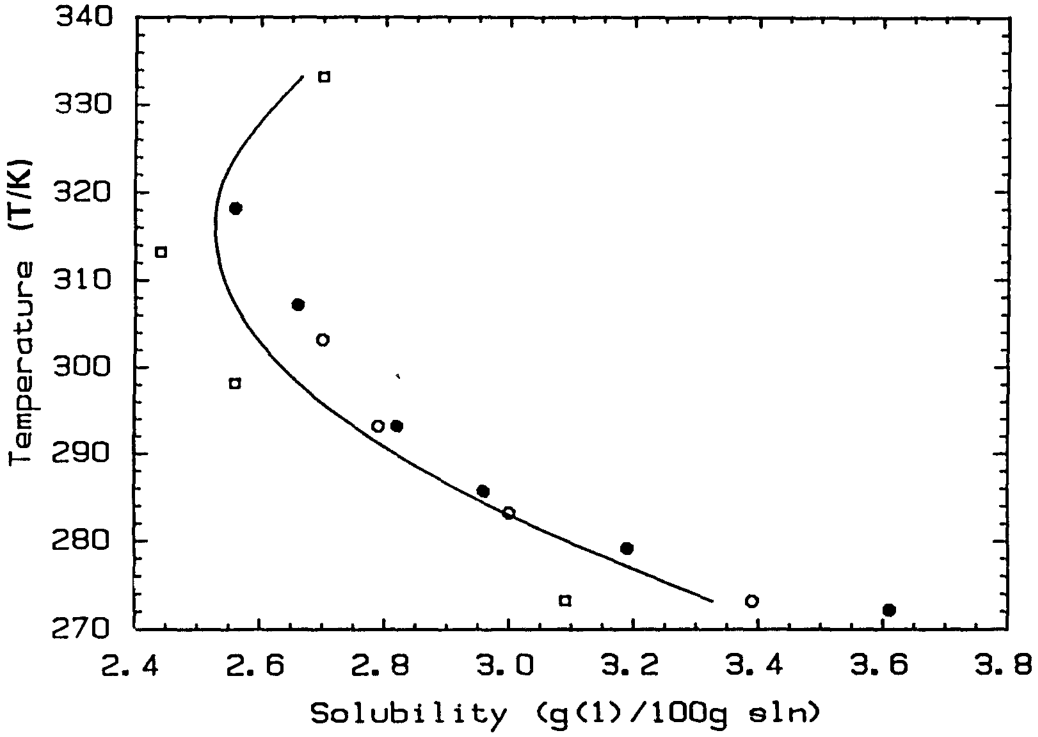

FIGURE 1. Selected data for the solubility of formic acid propyl ester (1) in water (2): ref 2 (○); ref 3 (●); ref 4 (□). Solid line is drawn through the "Best" values from Table 2.

TABLE 3: Tentative Solubilities of Water (2) in Formic acid propyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
273	0.82 (ref 4), 1.07 (ref 5)	0.9 ± 0.1	4.3
283	1.00^* (ref 4), 1.34^* (ref 5)	1.2 ± 0.2	5.6
293	1.17^* (ref 4), 1.58 (ref 5)	1.4 ± 0.2	6.5
298	1.26 (ref 4), 1.72^* (ref 5)	1.5 ± 0.2	6.9
303	1.35^* (ref 4), 1.88^* (ref 5)	1.6 ± 0.3	7.4

[a] Obtained by averaging where appropriate.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
313	1.54 (ref 4), 2.30* (ref 5)	1.9 ± 0.4	8.7
323	1.80* (ref 4), 2.90* (ref 5)	2.4 ± 0.6	11
333	2.17 (ref 4), 3.66* (ref 5)	2.9 ± 0.7	13
343	5.20* (ref 5)	- [b]	- [b]

[b] No average value calculated because of uncertainty in available data, see text.

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

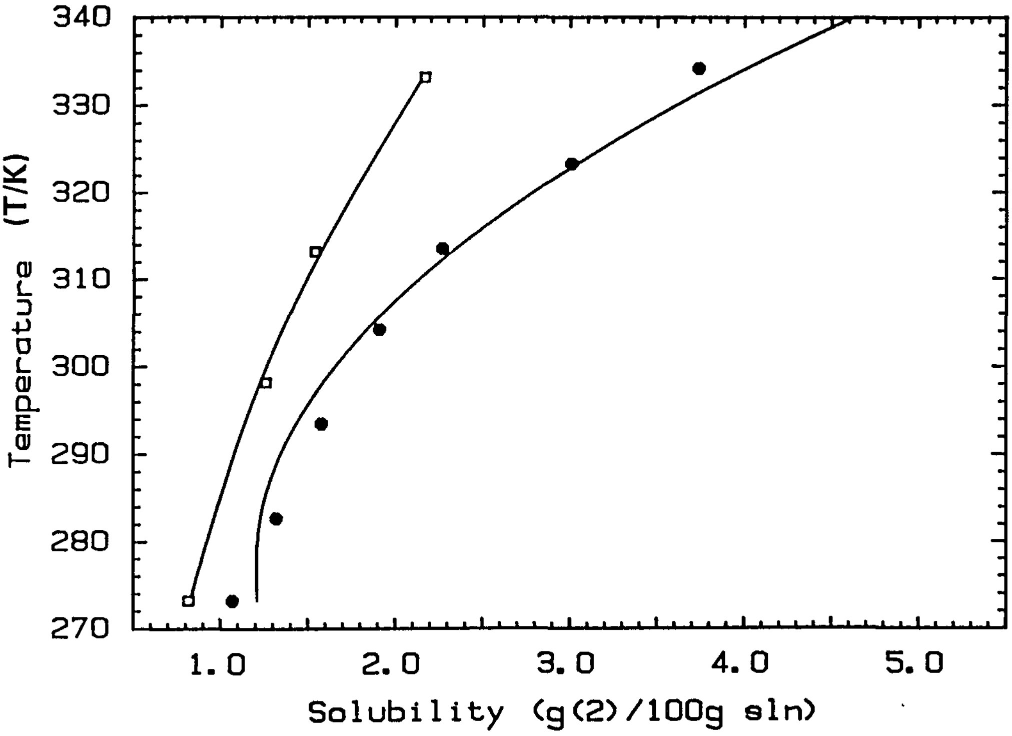

FIGURE 2. Data for the solubility of water (2) in formic acid propyl ester (1): ref 4 (□); ref 5 (●). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.
2. Rayman, J. *Thesis*. Budapest, 1906.
3. Kendall, J.; Harrison, E. *Trans. Faraday Soc.* 1928, *24*, 588-96.
4. Rius, A.; Alfonso, C. *An. Fis. Quim. Ser. B.* 1955, *51*, 649-58.
5. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.
VARIABLES:	PREPARED BY:
$T/K = 295$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of formic acid propyl ester in water at 22°C was reported to be 1 part of formic acid propyl ester in 46 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 2.13 g(1)/100g sln and 0.0044.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	Rayman, J. *Thesis*, Budapest, 1906.
VARIABLES:	PREPARED BY:
T/K = 273 - 303	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of formic acid propyl ester in water

t/°C	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	3.51	3.39	0.00712
10.	3.08	3.00	0.00629
20.	2.87	2.79	0.00584
30.	2.77	2.70	0.00564

These data have also been published in (ref 2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, 55, 360.
2. Hill, A.E. *International Critical Tables* (Washburn, E.W., Ed.) McGraw Hill, New York, 1928, Vol. 3, 387-98.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	Kendall, J.; Harrison, L.E. *Trans. Faraday Soc.* 1928, *24*, 588-96.
VARIABLES:	**PREPARED BY:**
$T/K = 272 - 318$	Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of formic acid propyl ester in water

$t/^{\circ}C$	x_1	g(1)/100g sln (compiler)
-1.0	0.00760	3.61
4.0	0.00695	3.31
6.0	0.00670	3.19
12.5	0.00620	2.96
20.0	0.00589	2.82
30.0	0.00569	2.72
34.0	0.00555	2.66
45.0	0.00535	2.56

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method was used. The sealed tube method (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.1-0.2)°C.

REFERENCES:

1. Smith, A.; Eastlack, H.E. *J. Am. Chem. Soc.* 1916, *38*, 1269.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7] (2) Water; H_2O; [7732-18-5]	Rius, A.; Alfonso, C. *An. Fis. Quim. Ser B.* 1955, *51*, 649-58.
VARIABLES:	**PREPARED BY:**
T/K = 273 - 333	G.T. Hefter

EXPERIMENTAL VALUES:

Mutual solubility of formic acid propyl ester and water

$t/^{\circ}C$	g(1)/100g sln	x_1	g(2)/100g sln	x_2
0.	3.09	0.00650	0.82	0.0387
25.	2.56	0.00535	1.26	0.0586
40.	2.44	0.00510	1.54	0.0709
60.	2.70	0.00565	2.17	0.0978

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Appropriate quantities of components (1) and (2) were thermostatted separately to avoid ester hydrolysis. Then, they were combined and shaken in a separatory funnel and the two layers were analyzed. The ester was determined by a micro-saponification technique using 2M NaOH in a 50% methanol/water solution. The water was determined by Karl Fischer titrations using electrometric end-point detection.

SOURCE AND PURITY OF MATERIALS:

(1) Prepared from formic acid (85%, CP, Probus) and 1-propanol; free acid < 0.1%; water content < 0.1%.

(2) Distilled from $KMnO_4$.

ESTIMATED ERROR:

Temp. ±0.02°C (25°C) - ±0.1°C (60°C)
Soly. ±0.5% rel., (1).
±0.4% rel., (2).

REFERENCES:

COMPONENTS:

(1) Formic acid propyl ester (*propyl formate*); $C_4H_8O_2$; [110-74-7]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

$T/K = 273 - 344$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in formic acid propyl ester

$t/^{\circ}C$	g(1)/100g sln	x_1 (compiler)
0	98.93	0.9497
9.5	98.68	0.9386
20.3	98.42	0.9272
31.0	98.09	0.9130
40.3	97.73	0.8980
50.1	96.99	0.8682
61.0	96.26	0.8403
70.6	94.75	0.7867

std. dev. 0.02

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 96%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988

CRITICAL EVALUATION:

Quantitative solubility data for the propanoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Propanoic acid methyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Kendall and Harrison (ref 3)	271-316	(1) in (2)	synthetic
Bomshtein *et al*. (ref 4)	293-343	mutual	titration
Richon and Viallard (ref 5)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 6)	273-343	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF PROPANOIC ACID METHYL ESTER (1) IN WATER (2)

All the available data for the solubility of propanoic acid methyl ester (1) in water (2) are summarized in Table 2 with the exception of the datum of Traube (ref 1) which is much lower ($>3\sigma_n$) than all other values (ref 2-6) and is therefore rejected.

The remaining data (ref 2-6) are generally in good agreement, enabling the average values to be Recommended over most of the temperature range studied, even though the temperature dependence of individual studies varies markedly. Selected data are plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubilities of Propanoic acid methyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^2x_1
273	8.46 (ref 2), 8.48* (ref 3), 7.80 (ref 6)	8.3 ± 0.4 (*R*)	1.81
283	7.30 (ref 2), 7.38* (ref 3), 6.89 (ref 6)	7.2 ± 0.2 (*R*)	1.56
293	6.50 (ref 2), 6.77* (ref 3), 6.18 (ref 4), 6.25 (ref 6)	6.4 ± 0.2 (*R*)	1.38
298	6.22* (ref 2), 6.59* (ref 3), 5.6* (ref 4), 5.98 (ref 5), 5.98* (ref 6)	6.1 ± 0.3 (*R*)	1.31
303	5.93 (ref 2), 6.46* (ref 3), 5.29 (ref 4), 5.72* (ref 6)	5.9 ± 0.5	1.26
313	6.24* (ref 3), 5.16 (ref 4), 5.36* (ref 6)	5.6 ± 0.5	1.20
323	5.07 (ref 4), 5.11 (ref 6)	5.1 ± 0.1 (*R*)	1.09
333	5.02 (ref 4), 4.96 (ref 6)	5.0 ± 0.1 (*R*)	1.06
343	4.98 (ref 4), 4.90 (ref 6)	4.9 ± 0.1 (*R*)	1.04

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN PROPANOIC ACID METHYL ESTER (1)

Only Bomshtein *et al.* (ref 3) and Stephenson and Stuart (ref 5) have reported the solubility of water (2) in propanoic acid methyl ester (1). Their data are summarized in Table 3 and plotted in Figure 2. In general the agreement between the two studies is poor and the solubilities show quite different temperature dependences. Further study of this system is clearly warranted and the "Best" values must be regarded as very Tentative.

(continued next page)

COMPONENTS: (1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1] (2) Water; H_2O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988

CRITICAL EVALUATION: (continued)

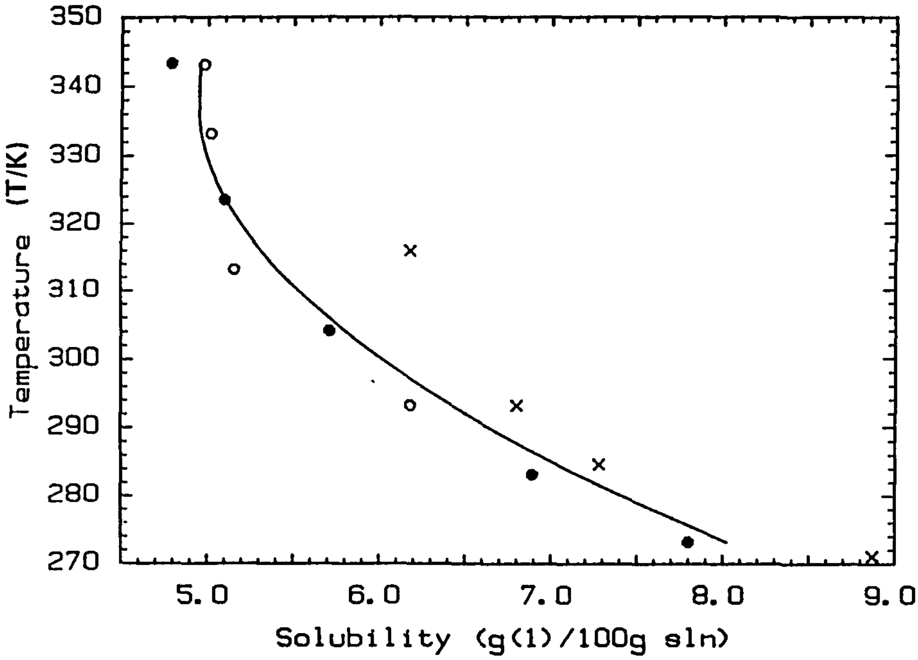

FIGURE 1. Selected data for the solubility of propanoic acid methyl ester (1) in water (2): ref 3 (X); ref 4 (O); ref 6 (●). Solid line is drawn through the "Best" values from Table 2.

TABLE 3: Tentative Solubilities of Water (2) in Propanoic acid methyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	$10x_2$
273	1.51 (ref 5)	1.5	0.7
283	1.9^* (ref 5)	1.9	0.9
293	1.00 (ref 3), 2.3^* (ref 5)	1.7 ± 0.7	0.8
298	1.70^* (ref 3), 2.4^* (ref 5)	2.1 ± 0.4	1.0
303	2.40 (ref 3), 2.5^* (ref 5)	2.5 ± 0.1	1.1
313	3.30 (ref 3), 2.7^* (ref 5)	3.0 ± 0.3	1.3
323	4.00 (ref 3), 2.9^* (ref 5)	3.5 ± 0.6	1.5
333	4.80 (ref 3), 3.1^* (ref 5)	4.0 ± 0.9	1.7
343	5.50 (ref 3), 3.2^* (ref 5)	4.4 ± 1.2	1.8

[a] Obtained by averaging where appropriate.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propanoic acid methyl ester *(methyl propionate)*; $C_4H_8O_2$; [554-12-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia December, 1988

CRITICAL EVALUATION: (continued)

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

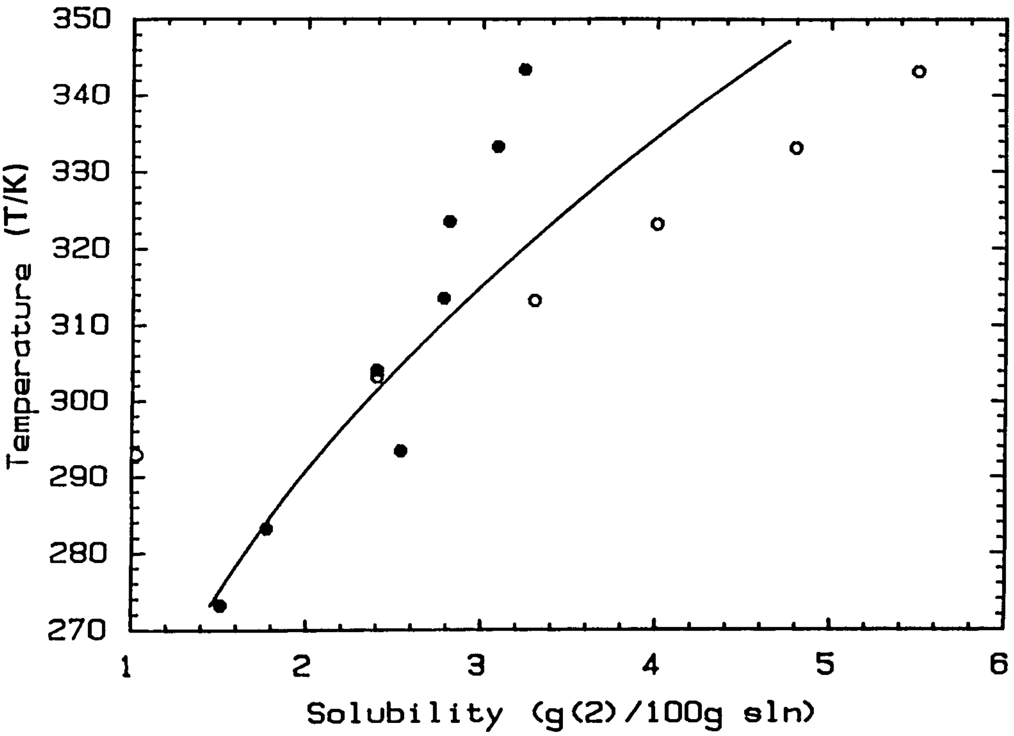

FIGURE 2. Selected data for the solubility of water (2) in propanoic acid methyl ester (1): ref 4 (O); ref 6 (●). Solid line is drawn through the "Best" values from Table 3.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.
2. Rayman, J. *Thesis*, Budapest, 1906; see also Hill, A. E. *International Critical Tables* (Washburn, E. W., Ed.) McGraw-Hill, New York, 1928, Vol. 3, 387-98.
3. Kendall, J.; Harrison, E. *Trans. Faraday Soc.* 1928, *24*, 588-96.
4. Bomshtein, A. L.; Trofimov, A. N.; Serafimov, L. A. *Zh. Prikl. Khim.* 1978, *51*, 1280-2.
5. Richon, D.; Viallard, A. *Fluid Phase Equil.* 1985, *21*, 279-93.
6. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Traube, J.

Ber. Dtsch. Chem. Ges. 1884, *17*, 2294-316.

VARIABLES:

$T/K = 295$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid methyl ester in water at 22°C was reported to be 1 part of propanoic acid methyl ester in 17-20 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 5.2 g(1)/100g sln and 0.011.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±0.4 g(1)/100g sln.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1] (2) Water; H_2O; [7732-18-5]	Rayman, J. *Thesis*, Budapest, 1906.
VARIABLES:	PREPARED BY:
$T/K = 273 - 303$	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of propanoic acid methyl ester in water

$t/^\circ C$	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	8.46	7.80	0.0170
10.	7.30	6.80	0.0147
20.	6.50	6.10	0.0131
30.	5.93	5.60	0.0119

These data have also been published in (ref 2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, *55*, 360.
2. Hill, A.E. *International Critical Tables* (Washburn, E.W., Ed.) McGraw Hill, New York, 1928, Vol. 3, 387-98.

COMPONENTS:

(1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Kendall, J.; Harrison, L.E.

Trans. Faraday Soc. 1928, *24*, 588-96.

VARIABLES:

$T/K = 271 - 316$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of propanoic acid methyl ester in water

$t/^\circ C$	x_1	g(1)/100g sln (compiler)
-2.1	0.0195	8.87
1.0	0.0180	8.23
11.5	0.0158	7.28
14.9	0.0153	7.06
20.0	0.0147	6.80
27.1	0.0140	6.49
32.5	0.0138	6.41
42.7	0.0133	6.18

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method was used. The sealed tube method (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C.

(2) Distilled.

ESTIMATED ERROR:

Temp. $\pm(0.1-0.2)^\circ C$.

REFERENCES:

1. Smith, A.; Eastlack, H.E. *J. Am. Chem. Soc.* 1916, *38*, 1269.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1] (2) Water; H_2O; [7732-18-5]	Bomshtein, A.L.; Trofimov, A.N.; Serafimov, L.A. *Zh. Prikl. Khim.* 1978, *51*, 1280-2.
VARIABLES:	PREPARED BY:
T/K = 293 - 343	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of propanoic acid methyl ester and water

$t/^\circ C$	x_1		g(1)/100g sln (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	0.0133	0.9529	6.18	99.00
30	0.0113	0.8927	5.29	97.60
40	0.0110	0.8571	5.16	96.70
50	0.0108	0.8308	5.07	96.00
60	0.0107	0.8023	5.02	95.20
70	0.0106	0.7785	4.98	94.50

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used at constant temperature.
No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; without impurities by glc, b.p. 79.8°C, n_D^{20} 1.376.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1] (2) Water; H_2O; [7732-18-5]	Richon, D.; Viallard, A. *Fluid Phase Equilib.* 1985, *21*, 279-93.
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid methyl ester in water at 298.1 K was reported to be 0.0722 mol(1)/100g(2) and 6.36 g(1)/100g(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 5.98 g(1)/100g sln and 0.01284.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) BDH: purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid methyl ester (*methyl propionate*); $C_4H_8O_2$; [554-12-1] (2) Water; H_2O; [7732-18-5]	Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.
VARIABLES:	PREPARED BY:
$T/K = 273 - 343$	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of propanoic acid methyl ester and water

$t/°C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	7.80	98.49	0.0170	0.9302
10.0	6.89	98.23	0.0149	0.9190
20.2	6.24	97.46	0.0134	0.8869
30.9	5.71	97.60	0.0122	0.8926
40.3	5.35	97.22	0.0114	0.8773
50.3	5.10	97.19	0.0109	0.8761
60.1	5.05	96.91	0.0108	0.8651
70.2	4.79	96.76	0.0102	0.8593
std. dev.	0.03	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 98%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Hypochlorous acid 1,1-dimethylethyl ester (*tert-butyl hypochlorite*); C_4H_9ClO; [507-40-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Westwater, J.W.; Audrieth, L.F.

Ind. Eng. Chem. 1954, *46*, 1281-4.

VARIABLES:

T/K = 273 and 293

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of Hypochlorous acid 1,1-dimethylethyl ester and water

$t/^\circ C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0^a	0.15	99.86	0.0002	0.9916
20^b	0.32	99.73	0.00053	0.9839

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Samples of 10-20g size, placed in a glass-stoppered bottle, were titrated and shook manually. The cloud point was assumed to be reached when the cloud persisted for 2 minutes during shaking.
The method and data were reported together with the ternary system Hypochlorous acid 1,1-dimethylethyl ester-water-1,1-dimethylethanol (*tert-butyl hypochlorite-water-tert-butyl alcohol*).

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized from 1,1-dimethyl ethanol (*tert-butyl alcohol*) by the method reported by Teeter, Bachman, Bell and Cowan (ref 1); washed six timed with Na_2CO_3(aq) and water, vacuum-distilled, the middle cut boiling at 31-33°C at 68-70 mm Hg was used without further purification; purity 94.4% by active chlorine analysis; d^{20} 0.9599, n^{20} 1.40354.

(2) Deionized; n_D^{20} 1.33292.

ESTIMATED ERROR:

[a] Temp. +0.6°C.
[b] Temp. ±0.1°C.

REFERENCES:

1. Teeter, H.M.; Bachman, R.C.; Bell, E.W.; Cowan, J.C. *Ind. Eng. Chem.* 1949, *41*, 849.

COMPONENTS: (1) Propanoic acid ethenyl ester (*vinyl propionate*); $C_5H_8O_2$; [105-38-4] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Tikhonova, N.K.; Timofeev, V.S.; Kozhukhova, N.I.; Serafimov, L.A. *Fiz. Khim. Osn. Rektifikatsii* 1970, 79-88.
VARIABLES: $T/K = 293$	PREPARED BY: A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethenyl ester in water at 20°C was reported to be 0.3 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 5.4×10^{-4}.

The solubility of water in propanoic acid ethenyl ester at 20°C was reported to be 0.5 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.027.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Two-phases mixtures were placed in a thermostated apparatus with a mechanical stirrer and mixed. After separation, the samples of both equilibrium phases were analyzed. Water was determined by the Karl Fischer method. No further details were reported in the paper. The data and method were reported together with the ternary system propanoic acid ethenyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; used as received; b.p. 94.7°C, n_D^{20} 1.4048.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2-Propenoic acid ethyl ester (*ethyl acrylate*); $C_5H_8O_2$; [140-88-5] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the 2-propenoic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2-Propenoic acid ethyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Frolov *et al.* (ref 1,2)	293	mutual	titration
Dabrowski (ref 3)	288,298	mutual	synthetic

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 2-PROPENOIC ACID ETHYL ESTER (1) IN WATER (2)

The available data for the solubility of 2-propenoic acid ethyl ester (1) in water (2) are summarized in Table 2. At 293 K, the only temperature where comparison is possible, the data of Frolov *et al.* (ref 1,2) and Dabrowski are in good agreement and the average value is Recommended. At other temperatures, only the values of Dabrowski are available and these data must be classified as Tentative pending further studies.

TABLE 2: Recommended (*R*) and Tentative Solubilities of 2-Propenoic acid ethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
288	2.27 (ref 3)	2.3	4.2
293	2.02 (ref 1,2), 2.20* (ref 3)	2.11 ± 0.09 (*R*)	3.86
298	2.13 (ref 3)	2.1	3.9

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Propenoic acid ethyl ester (*ethyl acrylate*); $C_5H_8O_2$; [140-88-5] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 2-PROPENOIC ACID ETHYL ESTER (1)

The available data for the solubility of water (2) in 2-propenoic acid ethyl ester (1) are summarized in Table 3. At 293 K, the only temperature where comparison is possible, the data of Frolov *et al*. (ref 1,2) and Dabrowski (ref 3) are only in fair agreement. Consequently, all data must be classified as Tentative pending further studies.

TABLE 3: Tentative Solubilities of Water (2) in 2-Propenoic acid ethyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values [a]	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
288	1.27 (ref 3)	1.3	6.8
293	0.956 (ref 1,2), 1.38* (ref 3)	1.4	7.3
298	1.49 (ref 3)	1.5	7.8

[a] Rounded values of ref 3.

REFERENCES

1. Frolov, A. F.; Loginova, M. A.; Pantukh, B. I.; Ustavshchikov, B. F. *Zh. Fiz. Khim.* 1966, *40*. 100-1.
2. Loginova, M. A.; Frolov, A. F.; Pantukh, B. I. *Khim. Prom.* 1966, *42*, 674-7.
3. Dabrowski, L. *Thesis, I. Ch. F. PAN*, Warszawa, 1984.

COMPONENTS:

(1) 2-Propenoic acid ethyl ester (*ethyl acrylate*); $C_5H_8O_2$; [140-88-5]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Frolov, A.F.; Loginova, M.A.; Pantukh, B.I.; Ustavshchikov, B.F.

Zh. Fiz. Khim. 1966, *40*, 100-1.

Loginova, M.A.; Frolov, A.F.; Pantukh, B.I.

Khim. Prom. 1966, *42*, 674-7.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 2-propenoic acid ethyl ester in water at 20°C was reported to be 2.02 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00370.

The solubility of water in 2-propenoic acid ethyl ester at 20°C was reported to be 0.956 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.00509.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Both a direct titration of the sample and a reverse titration up to turbidity were made. The data were reported together with the ternary system 2-propenoic acid ethyl ester-water-ethanol.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; technical grade; vacuum-distilled; purity 99.5%, b.p. 99.5°C, d_4^{20} 0.924, n_D^{20} 1.4075.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Propenoic acid ethyl ester (*ethyl acrylate*); $C_5H_8O_2$; [140-88-5] (2) Water; H_2O; [7732-18-5]	Dabrowski, L. *Thesis*, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1984.
VARIABLES:	**PREPARED BY:**
T/K = 288 and 298	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of 2-propenoic acid ethyl ester and water

T/K	g(1)/100g sln		x_1	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
288.15	2.27	98.73	0.0042	0.9333
298.15	2.13	98.51	0.0039	0.9225

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The modified Othmer-White-Trueger method was used. The samples of known composition were slowly cooled to obtain the temperature of turbidity which was a little below the desired temperature. After addition of a small amount of one component the procedure was repeated. The solubility at the desired temperature was obtained by an interpolation. All measurements were made in a thermostated vessel of 50 cm^3 in the range ±3°C of the needed temperature. Temperatures of the samples were measured with a mercury-in-glass thermometer. A magnetic stirrer was used. The water included in ester was taken into account. The data and method were reported together with the ternary system 2-propenoic acid ethyl ester-water-2-propenoic acid (*ethyl acrylate-water-acrylic acid*).

SOURCE AND PURITY OF MATERIALS:

(1) ICSO Blachownia Slaska; used as received; contained 0.24% water; n_D^{25} 1.40449.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.05°C.
Soly. ±0.02 g(1)/100g sln.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the 2-methyl-2-propenoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2-Methyl-2-propenoic acid methyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Shanley and Greenspan (ref 1)	R.T.[a]	(2) in (1)	unspecified
Schildknecht (ref 2)	273-353	(1) in (2)	unspecified
Frolov (ref 3)	293	mutual	unspecified
Frolov *et al.* (ref 4)	293	mutual	GLC, analytical
Arutyunyan *et al.* (ref 5)	303	(1) in (2)	volumetric
Chubarov *et al.* (ref 6)	293-363	(2) in (1)	unspecified
Fu *et al.* (ref 7)	298-333	mutual	synthetic ?

[a] R.T. - room temperature

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 2-METHYL-2-PROPENOIC ACID METHYL ESTER (1) IN WATER (2)

The available data for the solubility of 2-methyl-2-propenoic acid methyl ester (1) in water (2) are summarized in Table 2. The value reported by Frolov (ref 3) at 293 K has been rejected as it is lower than all other values and it has therefore been excluded from Table 2. The value reported by Shanley and Greenspan (ref 1) at an unspecified temperature has been similarly excluded from Table 2. All other data are in excellent agreement enabling the average "Best" values to be Recommended over a wide temperature range. Selected data are plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubilities of 2-Methyl-2-propenoic acid methyl ester (1) in Water (2)

T/K	Solubilities			
	Reported values	"Best" values $(\pm\sigma_n)^a$		
	g(1)/100g sln	g(1)/100g sln		10^3x_1
273	1.85 (ref 2)	1.9		3.5
283	1.71* (ref 2)	1.7		3.1
293	1.59 (ref 2), 1.55 (ref 4)	1.57 ± 0.02	(*R*)	2.86
298	1.54* (ref 2), 1.54 (ref 7)	1.54	(*R*)	2.80
303	1.50* (ref 2), 1.50 (ref 5) 1.49* (ref 7)	1.50	(*R*)	2.73
313	1.43 (ref 2), 1.43* (ref 7)	1.43	(*R*)	2.60
323	1.43* (ref 2), 1.47* (ref 7)	1.45 ± 0.02	(*R*)	2.64
333	1.49 (ref 2), 1.59 (ref 7)	1.54 ± 0.05	(*R*)	2.80
343	1.61* (ref 2)	1.6		2.9
353	1.80 (ref 2)	1.8		3.3

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN 2-METHYL-2-PROPENOIC ACID METHYL ESTER (1)

The available data for the solubility of water (2) in 2-methyl-2-propenoic acid methyl ester (1) are summarized in Table 3. The data of Chubarov *et al.* (ref 6) and Fu *et al.* (ref 7) are in excellent agreement enabling the average "Best" values to be recommended over a wide range of temperature. Selected data are plotted in Figure 2.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Propenoic acid, 2-methyl-, methyl ester *(methyl methacrylate)*; $C_5H_8O_2$; [80-62-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

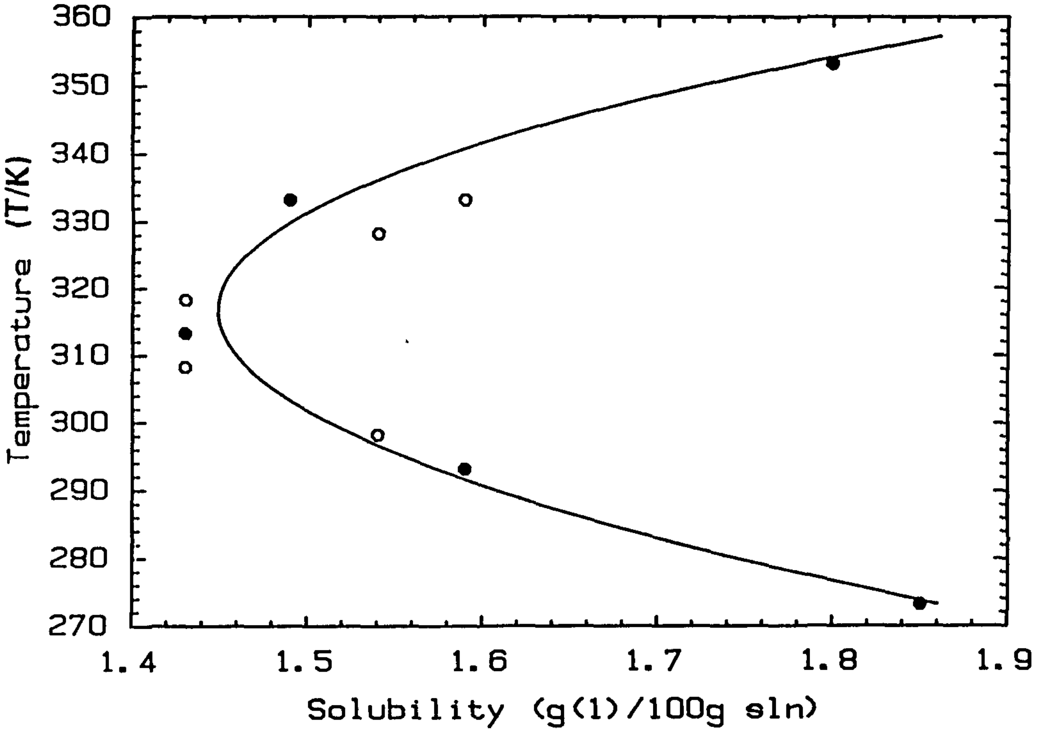

FIGURE 1. Selected data for the solubility of 2-methyl-2-propenoic acid methyl ester (1) in water (2): ref 2 (●); ref 7 (○). Solid line is drawn through the "Best" values from Table 2.

TABLE 3: Recommended (*R*) and Tentative Solubilities of Water (2) in 2-Methyl-2-propenoic acid methyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	$10x_2$
293	0.73 (ref 3), 1.2 (ref 4), 1.08 (ref 6)	1.0 ± 0.2	0.5
298	1.19 (ref 6), 1.20 (ref 7)	1.20 (*R*)	0.63
303	1.30^* (ref 6), 1.31 (ref 7)	1.31 (*R*)	0.69
313	1.54 (ref 6), 1.54^* (ref 7)	1.54 (*R*)	0.80
323	1.81^* (ref 6), 1.81^* (ref 7)	1.81 (*R*)	0.93

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Propenoic acid, 2-methyl-, methyl ester *(methyl methacrylate)*; $C_5H_8O_2$; [80-62-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	$10x_2$
333	2.09 (ref 6), 2.10 (ref 7)	2.10 (*R*)	1.07
343	2.43* (ref 6)	2.4	1.2
353	2.75 (ref 6)	2.8	1.4
363	3.17 (ref 6)	3.2	1.6

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

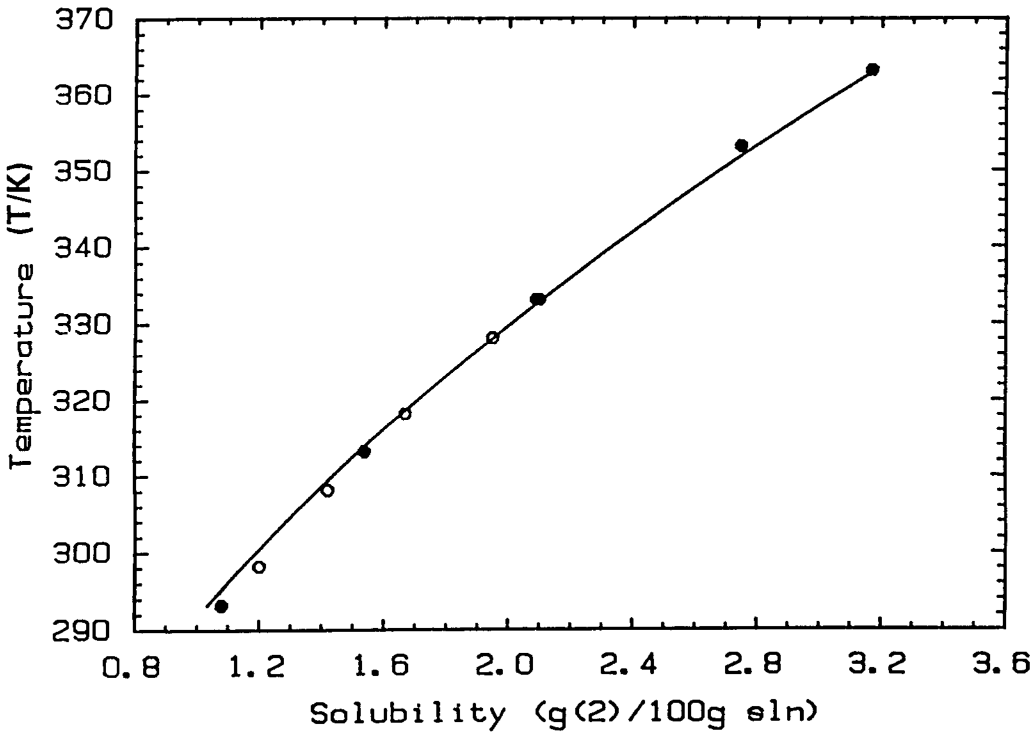

FIGURE 2. Selected data for the solubility of water (2) in 2-methyl-2-propenoic acid methyl ester (1): ref 2 (●); ref 7 (o). Solid line is drawn through the "Best" values from Table 3.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

REFERENCES

1. Shanley, E. S.; Greenspan, F. P. *Ind. Eng. Chem.* 1947, *39*, 1536-43.
2. Schildknecht, C. E. *Vinyl and Related Polymers*, J. Wiley, New York, 1952, p.185.
3. Frolov, A. F. *Zh. Fiz. Khim.* 1965, *39*, 2877-83.
4. Frolov, A. F.; Yarovikova, M. M.; Ustavshchikov, B. F.; Nikitina, N. S. *Izv. Vyssh. Ucheb. Zaved. Khim. Khim. Tekhnol.* 1965, *8*, 570-3.
5. Arutyunyan, R. S.; Atanasyan, E. N.; Beileryan, N. M. *Kolloid. Zh.* 1979, *41*, 968-72.
6. Chubarov, G. A.; Danov, S. M.; Logutov, V. I.; Brovkina, G. V. *Zh. Prikl. Khim.* 1979, *52*, 1082-5.
7. Fu, J. Y.; Wang, K.; Hu, Y. *Hua Kung Hsueh Pao* 1988, 64-76.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Shanley, E.S.; Greenspan, F.P.

Ind. Eng. Chem. 1947, *39*, 1536-43.

VARIABLES:

T/K = room temperature

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of water in 2-methyl-2-propenoic acid methyl ester at room temperature was reported to be 1.0 g(2)/100g(1). The corresponding mass per cent and mole fraction, x_2, values calculated by the compiler are 0.99 g(2)/100g sln and 0.053.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schildknecht, C.E.

Vinyl and Related Polymers, J. Wiley, New York, 1952, p 185.

VARIABLES:

$T/K = 273 - 353$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Solubility of 2-methyl-2-propenoic acid methyl ester in water

$t/°C$	g(1)/100g sln	x_1 (compiler)
0	1.85	0.0034
20	1.59	0.0029
40	1.43	0.0026
60	1.49	0.0027
80	1.80	0.0033

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified. Presumably data were taken from *The Monomeric Acrylic Esters* (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified presumably containing 0.006% hydroquinone.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. *The Monomeric Acrylic Esters*, booklet, Rohm and Haas Co., 1949.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6] (2) Water; H_2O; [7732-18-5]	Frolov, A.F. *Zh. Fiz. Khim.* 1965, *39*, 2877-83.
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 2-methyl-2-propenoic acid methyl ester in water at 20°C was reported to be 1.39 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00253.

The solubility of water in 2-methyl-2-propenoic acid methyl ester at 20°C was reported to be 0.73 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.039.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified. The data were reported together with the quaternary system 2-methyl-2-propenoic acid methyl ester-water-2-methyl-2-propenoic acid-methanol (*methyl methacrylate-water-methacrylic acid-methanol*).	(1) Not specified. (2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:

(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Frolov, A.F.; Yarovikova, M.M.; Ustavshchikov, B.F.; Nikitina, N.S.

Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. 1965, *8*, 570-3.

VARIABLES:

T/K = 293

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 2-methyl-2-propenoic acid methyl ester in water at 20°C was reported to be 1.55 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00283.

The solubility of water in 2-methyl-2-propenoic acid methyl ester at 20°C was reported to be 1.2 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.063.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture was thermostated in 100 mL flask and stirred for 1/2 h. Then, after separation (more than 20 min), the phases were analyzed. The glc method for water and the ester and the bromide-bromate method for the 2-methyl-2-propenoic acid methyl ester were used. The data were reported together with the ternary system 2-methyl-2-propenoic acid methyl ester-water-methanol.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, pure grade; distilled; purity 98.52% by bromide-bromate method, b.p. 100°C, d_4^{20} 0.940, n_D^{20} 1.4150.

(2) Not specified.

ESTIMATED ERROR:

Soly. <±3.0% (relative error).

REFERENCES:

COMPONENTS:

(1) 2-Propenoic acid, 2-methyl-, methyl ester
(methyl methacrylate);
$C_5H_8O_2$; [80-62-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Arutyunyan, R.S.; Atanasyan, E.N.; Beileryan, N.M.

Kolloid. Zh. 1979, *41*, 968-72.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 2-methyl-2-propenoic acid methyl ester in water at 30°C was reported to be 0.1500 mol(1)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 15.02 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method of Shaginyan, Aibazyan and Melkonyan (ref 1) was used. The volume of insoluble organic phase was measured. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purified.

(2) Not specified.

ESTIMATED ERROR:

Soly. <±1% (relative error).

REFERENCES:

1. Shaginyan, A.A.; Aibazyan, O.M.; Melkonyan, L.G. *Arm. Khim. Zh.* 1974, *27*, 904.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6] (2) Water; H_2O; [7732-18-5]	Chubarov, G.A.; Danov, S.M.; Logutov, V.I.; Brovkina, G.V. *Zh. Prikl. Khim.* 1979, *52*, 1082-5.
VARIABLES:	**PREPARED BY:**
T/K = 293 - 363	A. Skrzecz

EXPERIMENTAL VALUES:

Solubility of water in 2-methyl-2-propenoic acid methyl ester

$t/^\circ C$	g(2)/100g sln	x_2 (compiler)
20	1.08	0.0572
25	1.19	0.0627
40	1.54	0.0800
60	2.09	0.1060
80	2.75	0.1358
90	3.17	0.1539

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was as described in *Praktikum po Fizicheskoi Khimii* (ref 1). The data were reported together with the ternary system 2-methyl-2-propenoic acid methyl ester-water-2-propanone (*methyl methacrylate-water-acetone*).

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; b.p. 100.4°C, d_4^{20} 0.936, n_D^{25} 1.4118.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Vorob'lev, N.K.(ed.) *Praktikum po Fizicheskoi Khimii*, Izd. Khimiya, Moskva, 1975.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Propenoic acid, 2-methyl-, methyl ester (*methyl methacrylate*); $C_5H_8O_2$; [80-62-6] (2) Water; H_2O; [7732-18-5]	Fu, Jinyan Y.; Wang, Kun; Hu, Ying *Hua Kung Hsueh Pao* 1988, (1), 64-76.
VARIABLES:	**PREPARED BY:**
$T/K = 298 - 333$ $p/kPa = 7 - 42$	J. Fu

EXPERIMENTAL VALUES:

Mutual solubility of 2-methyl-2-propenoic acid methyl ester and water

		x_1		g(1)/100g sln (compiler)	
$t/^\circ C$	p/kPa	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
25	7.71	0.0028	0.9369	1.536	98.80
35	12.95	0.0026	0.9259	1.428	98.58
45	21.00	0.0026	0.9139	1.428	98.33
55	33.16	0.0028	0.9006	1.536	98.05
60	41.26	0.0029	0.8934	1.590	97.90

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Mutual solubilities were determined by a static method using a liquid solution, vapor pressure measuring apparatus having a sample cell, a mercury manometer, a degassing vessel, and a high vacuum manifold as described in (ref 1). The solutions (in a 50 ml vessel) were degassed with liquid N_2 and transferred into the sample cell. The free space was about 24 ml (giving a negligible error, by calculation). Paradioxybenzene was added to prevent polymerization of (1). Thus, (1) could be kept for 40 days with a vapor pressure change less than 0.1 kPa at 60°C.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; 99.8-99.9% wt. pure; n_D^{25} 1.3265, b.p. 337.8K.

(2) Deionized and distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Hu, Yin; Wang, Kun; Lu, Ruidong *Hua Kung Hsueh Pao* 1980, (4), 352.

COMPONENTS:

(1) Butanoic acid, 4-chloro-, methyl ester (*methyl 4-chlorobutyrate*); $C_5H_9ClO_2$; [3153-37-5]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 363

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of 4-chlorobutanoic acid methyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.32	99.30	0.00176	0.9493
9.4	1.18	99.17	0.00157	0.9403
19.6	1.14	99.07	0.00152	0.9335
30.9	1.07	98.93	0.00142	0.9242
39.6	1.18	98.93	0.00157	0.9242
50.0	1.26	98.50	0.00168	0.8965
60.6	1.31	98.21	0.00175	0.8786
70.0	1.36	97.73	0.00181	0.8503
80.1	1.66	97.67	0.00222	0.8468
90.3	1.68	96.98	0.00225	0.8090
std. dev.	0.01	0.03		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 98%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 1-methylethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid 1-methylethyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Fuehner (ref 1)	293	(1) in (2)	titration
Doolittle (ref 2)	293	mutual	unspecified
Hlavaty and Linek (ref 3)	298	mutual	titration
Skrzecz (ref 4)	291-357	mutual	synthetic, Karl Fischer
Stephenson and Stuart (ref 5)	273-348	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID 1-METHYLETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid 1-methylethyl ester (1) in water (2) are summarized in Table 2 with the following exclusions. The datum of Doolittle (ref 2) is rejected because the purity of the ester was low; the reported solubility is also rather lower than other determinations (ref 1,5). The approximate value of Hlavaty and Linek (ref 3) is also rejected because it is significantly lower than other studies (ref 4,5).

The remaining data, mainly due to Skrzecz (ref 4) and Stephenson and Stuart (ref 5), are in excellent agreement enabling the averaged "Best" values to be Recommended over a wide temperature range. Selected data are plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubilities of Acetic acid 1-methylethyl ester (1) in Water (2)

T/K	Solubilities: Reported values g(1)/100g sln	Solubilities: "Best" values $(\pm\sigma_n)^a$ g(1)/100g sln	"Best" values 10^3x_1
273	4.08 (ref 5)	4.1	7.5
283	3.40* (ref 5)	3.4	6.2
293	3.09 (ref 1), 2.78* (ref 5)	2.9 ± 0.2	5.2
298	2.67* (ref 4), 2.59* (ref 5)	2.63 ± 0.04 (*R*)	4.74
303	2.52* (ref 4), 2.42* (ref 5)	2.47 ± 0.05 (*R*)	4.44
313	2.30* (ref 4), 2.19* (ref 5)	2.25 ± 0.06 (*R*)	4.04
323	2.17* (ref 4), 2.06* (ref 5)	2.12 ± 0.06 (*R*)	3.80
333	2.13* (ref 4), 1.94* (ref 5)	2.04 ± 0.10 (*R*)	3.67
343	2.15* (ref 4), 1.84* (ref 5)	2.0 ± 0.2	3.6
353	2.21* (ref 4), 1.75* (ref 5)	2.0 ± 0.2	3.6

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID 1-METHYLETHYL ESTER (1)

All the available solubility data for water (2) in acetic acid 1-methylethyl ester (1) are summarized in Table 3 with the following exceptions. The datum of Doolittle (ref 2) is rejected because of the low ester purity; the reported solubility, also much higher than other determinations (ref 4,5). The approximate value of Hlavaty and Linek (ref 3) is also rejected as it is much higher than other data (ref 4,5).

The remaining data, due to Skrzecz (ref 4) and Stephenson and Stuart (ref 5) are in excellent agreement at $T \leq 313$ but differ increasingly at higher temperatures. The data are plotted in Figure 2.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

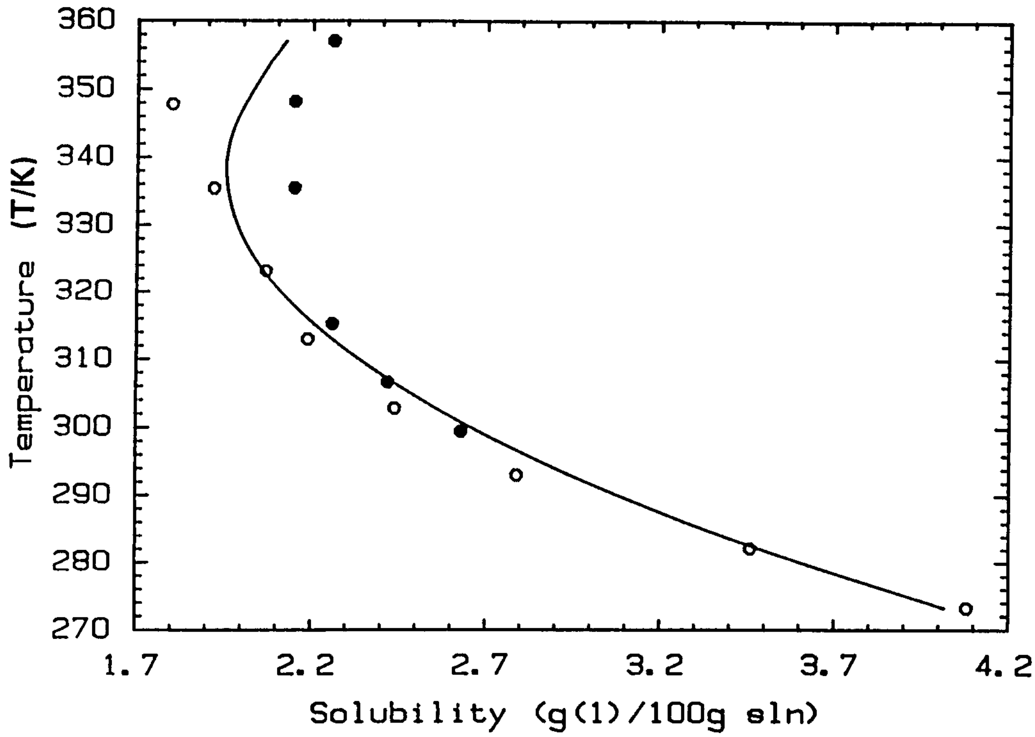

FIGURE 1. Selected data for the solubility of acetic acid 1-methylethyl ester (1) in water (2): ref 4 (●); ref 5 (O). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

TABLE 3: Recommended (*R*) and Tentative Solubilities of Water (2) in Acetic acid 1-methylethyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	$10x_2$
283	1.37^* (ref 5)	1.4	0.7
293	1.68^* (ref 4), 1.62^* (ref 5)	1.65 ± 0.03 (*R*)	0.87
298	1.82^* (ref 4), 1.72^* (ref 5)	1.77 ± 0.05 (*R*)	0.93
303	1.97^* (ref 4), 1.83^* (ref 5)	1.90 ± 0.07 (*R*)	1.07

[a] Obtained by averaging where appropriate.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities			
	Reported values	"Best" values ($\pm\sigma_n$)^a		
	g(2)/100g sln	g(2)/100g sln		$10x_2$
313	2.32^* (ref 4), 2.05^* (ref 5)	2.2 ± 0.1	(*R*)	1.13
323	2.71^* (ref 4), 2.23 (ref 5)	2.5 ± 0.2		1.3
333	3.15^* (ref 4), 2.37^* (ref 5)	2.8 ± 0.4		1.4
343	3.64^* (ref 4), 2.46^* (ref 5)	3.1 ± 0.6		1.5
353	4.17^* (ref 4), 2.55^* (ref 5)	3.4 ± 0.8		1.7

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

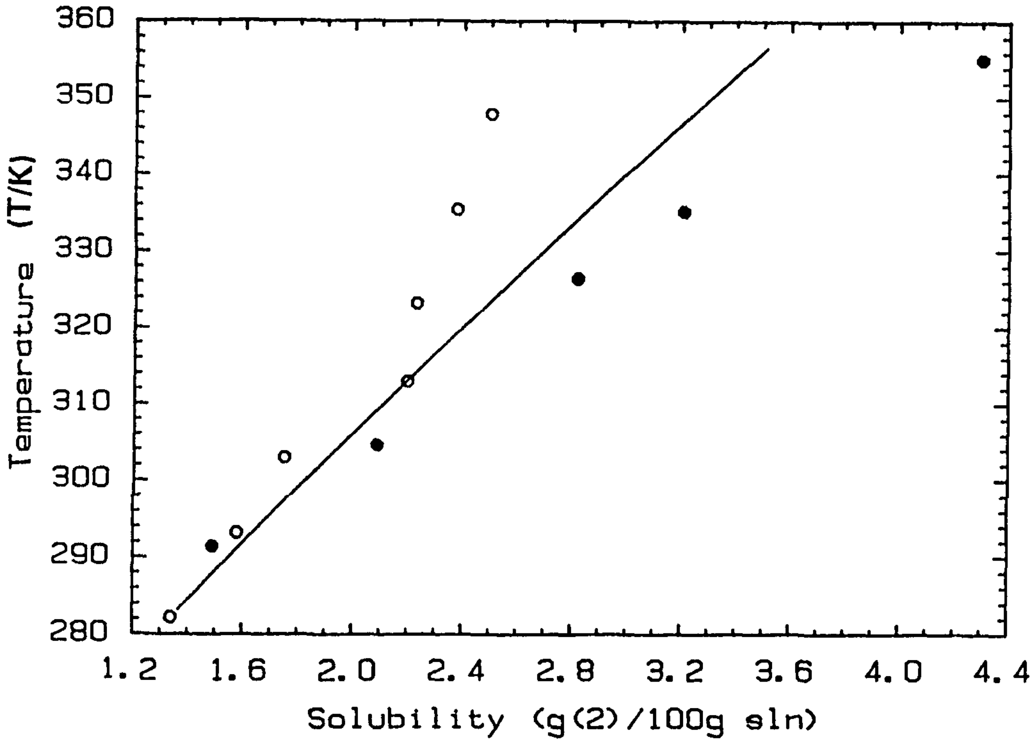

FIGURE 2. Selected data for the solubility of water (2) in acetic acid 1-methylethyl ester (1): ref 4 (●); ref 5 (○). Solid line is a least square polynomial fitted to the "Best" values from Table 3.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

REFERENCES

1. Fuehner, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-5.
2. Doolittle, A. K. *Ind. Eng. Chem.* 1935, *27*, 1169-79.
3. Hlavaty, K.; Linek, J. *Collect. Czech. Chem. Commun.* 1973, *38*, 374-8.
4. Skrzecz, A. *Pol. J. Chem.* 1981, *55*, 1177-80; see also Skrzecz, A. *Thesis*, *I. Ch. F. PAN*, Warszawa, 1979.
5. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Fuehner, H.

Ber. Dtsch. Chem. Ges. 1924, *57*, 510-5.

VARIABLES:

T/K = 293

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 1-methylethyl ester in water at 20°C was reported to be 3.40 vol%, 3.09 g(1)/100g sln and 0.303 mol(1)/L sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00559.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The ester was added from a pipette to a flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.3 g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Doolittle, A.K.

Ind. End. Chem. 1935, *27*, 1169-79.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 1-methylethyl ester in water at 20°C was reported to be 2.58 g(1)/100g sln^a and 2.78 g(1)/100g sln^b. The corresponding mole fraction, x_1, values calculated by the compiler are 0.00465^a and 0.00502^b respectively.

The solubility of water in acetic acid 1-methylethyl ester at 20°C was reported to be 2.86 g(2)/100g sln^a and 5.58 g(2)/100g sln^b. The corresponding mole fraction, x_2, values calculated by the compiler are 0.143^a and 0.251^b respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified.
  ^{a} Commercial product; purity 95%, b.p. range 84-94°C, d_4^{20} 0.870.
  ^{b} Commercial product; purity 85%, b.p. range 82-90°C, d_4^{20} 0.857.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hlavaty, K.; Linek, J.

Collect. Czech. Chem. Commun. 1973, *38*, 374-8.

VARIABLES:

$T/K = 298$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid 1-methylethyl ester in water at 24.6°C was reported to be 2.2 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0040.

The solubility of water in acetic acid 1-methylethyl ester at 24.6°C was reported to be 2.2 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.113.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The measurements were performed according to Mertl (ref 1), in a titration vessel which could be thermostated during the titration. Both the vessel and the burette were thermostated to 24.6 ±0.1°C. The mixture was agitated vigorously by a magnetic stirrer during the titration.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. better than ±0.3 wt%.

REFERENCES:

1. Mertl, I. *Thesis*, Inst. Chem. Process Fundam., Czechoslovak Academy of Sciences, Prague, 1969.

COMPONENTS:

(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skrzecz, A.

Pol. J. Chem. 1981, 55, 1177-80.

Skrzecz, A.

Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

VARIABLES:

T/K = 291 - 357

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 1-methylethyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
291.3[a]	-	0.9210	-	98.510
292.3	-	0.9078	-	98.240
299.5	0.00474	-	2.629	-
304.6	-	0.8921	-	97.911
306.7	0.00436	-	2.422	-
315.3	0.00406	-	2.259	-
326.4	-	0.8587	-	97.179
335.1	-	0.8417	-	96.789
335.5	0.00386	-	2.150	-

[a] By the Karl Fischer method.

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew and the analytical method were used. An ampoule with the solution of fixed concentration was placed in a glass tube connected with a thermostat filled completely with distilled water. During the measurements the temperature of the bath was changed continuously and the appearance and disappearance of turbidity within the ampoule was observed visually. For the analytical method, The amount of water in the saturated organic phase was determined using a Karl Fischer titration procedure. The amount of water in the pure ester was taken into account.

SOURCE AND PURITY OF MATERIALS:

(1) POCH Gliwice, pure grade; distilled; purity 99.99% by glc, 0.28 wt% water by the Karl Fischer method.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.2-0.6)°C.
Soly. see above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4] (2) Water; H_2O; [7732-18-5]	Skrzecz, A. *Pol. J. Chem.* 1981, *55*, 1177-80. Skrzecz, A. *Thesis*, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid 1-methylethyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
348.2	0.00386	-	2.150	-
355.1	-	0.7970	-	95.700
357.1	0.00406	-	2.259	-

Author's smoothing equations:

$x_1 = 6.4295\text{x}10^{-3} - 8.23\text{x}10^{-5}\ (T/K - 273.15) + 6.45\text{x}10^{-7}\ (T/K - 273.15)^2$

st. dev. = 4.91×10^{-5} (2)-rich phase

$x_2 = 0.076113 + 6.427\text{x}10^{-4}\ (T/K - 273.15) + 1.102\text{x}10^{-5}\ (T/K - 273.15)^2$

st. dev. = 5.56×10^{-4} (1)-rich phase

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 1-methylethyl ester (*isopropyl acetate*); $C_5H_{10}O_2$; [108-21-4] (2) Water; H_2O; [7732-18-5]	Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 348	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 1-methylethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	4.08	-	0.00745	-
9.0	3.46	98.66	0.00628	0.9285
19.9	2.79	98.42	0.00504	0.9166
29.7	2.44	98.25	0.00439	0.9083
39.8	2.19	97.80	0.00393	0.8869
50.0	2.07	97.77	0.00371	0.8855
62.2	1.92	97.62	0.00344	0.8786
74.6	1.80	97.50	0.00322	0.8731
std. dev.	0.02	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid propyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid propyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Fuehner (ref 3)	293	(1) in (2)	titration
Smith and Bonner (ref 4)	293,308	mutual	analytical
Murti *et al.* (ref 5)	303	mutual	titration
Venkataratnam *et al.* (ref 6)	303	mutual	titration
Pick *et al.* (ref 7)	357	mutual	unspecified
Rao and Rao (ref 8)	303	mutual	titration
Schuberth (ref 9)	293,318	mutual	titration, analytical
Smirnova *et al.* (ref 10)	323-356	mutual	analytical
Rao *et al.* (ref 11)	308	mutual	titration
Shakhud *et al.* (ref 12)	293-333	mutual	titration, analytical
Skrzecz (ref 13)	291-363	mutual	synthetic, Karl Fischer
Tewari *et al.* (ref 14)	298	(1) in (2)	GLC
Richon and Viallard (ref 15)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 16)	273-363	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H_2O; [7732-18-5]	January, 1989

CRITICAL EVALUATION: (continued)

1. SOLUBILITY OF ACETIC ACID PROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid propyl ester (1) in water (2) are summarized in Table 2 with the following exceptions. The data of Traube (ref 1) and Fuehner (ref 3) at *ca.* 293 K are significantly lower, and those of Pick *et al.* (ref 7) at 357 K and Shakhud *et al.* (ref 12) at T > 298 K significantly higher, than other studies and are therefore rejected. The results of Rao and co-workers (ref 5,6,8) at 303 K have been taken as one datum.

The remaining data are generally in good agreement (Table 2) enabling the averaged "Best" values to be Recommended over a wide range. Selected data are plotted in Figure 1.

TABLE 2: Recommended (*R*) and Tentative Solubilities of Acetic acid propyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
273	3.35 (ref 2), 3.21 (ref 16)	3.28 ± 0.07 (*R*)	5.95
283	2.57 (ref 2), 2.75* (ref 16)	2.66 ± 0.09 (*R*)	4.80
293	2.30 (ref 2), 2.2 (ref 4), 2.2 (ref 9), 2.2 (ref 12), 2.26 (ref 16)	2.23 ± 0.04 (*R*)	4.01
298	2.18* (ref 2), 2.2* (ref 12), 2.18* (ref 13), 2.19 (ref 15), 2.10* (ref 16)	2.17 ± 0.04 (*R*)	3.90
303	2.05 (ref 2), 1.8 (ref 5,6,8), 2.06* (ref 13), 1.98 (ref 16)	1.97 ± 0.10 (*R*)	3.53
313	1.81^b (ref 9), 1.89* (ref 13), 1.87 (ref 16)	1.86 ± 0.03 (*R*)	3.33
323	1.70^b (ref 9), 1.80 (ref 10), 1.80* (ref 13), 1.72 (ref 16)	1.76 ± 0.05 (*R*)	3.15
333	1.63^b (ref 9), 1.80* (ref 10), 1.79* (ref 13), 1.64* (ref 16)	1.72 ± 0.08 (*R*)	3.08
343	1.62^b (ref 9), 1.82* (ref 13), 1.72* (ref 16)	1.72 ± 0.08 (*R*)	3.08
353	1.86 (ref 10), 1.88* (ref 13), 1.66 (ref 16)	1.80 ± 0.10	3.22

[a] Obtained by averaging where appropriate.

[b] Calculated using the author's original fitting equation.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

In Table 2, σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

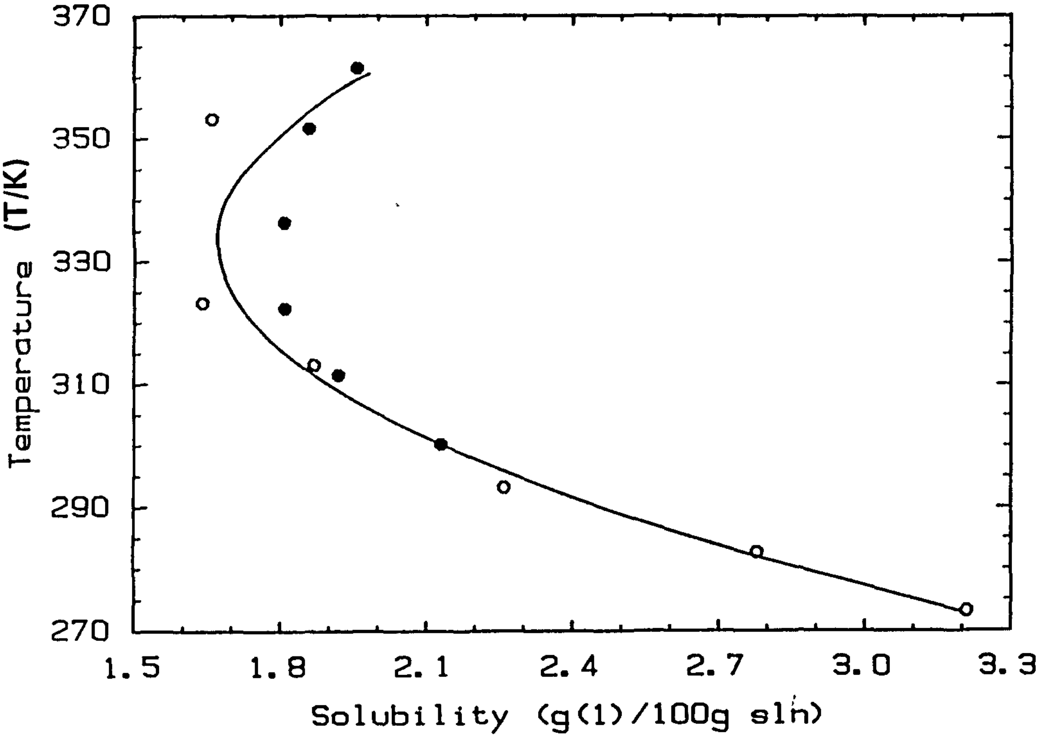

FIGURE 1. Selected data for the solubility of acetic acid propyl ester (1) in water (2): ref 13 (●); ref 16 (○). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID PROPYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid propyl ester (1) are summarized in Table 3 with the following exceptions. The data of Murti *et al.* (ref 5) and of Schuberth (ref 9) and Shakhud *et al.* (ref 12) are, respectively, much lower and higher than other studies and are rejected. The data of Rao and co-workers (ref 6,8) at 303 K have been taken as one value.

The remaining data (Table 3) are generally only in fair agreement enabling only some of the averaged "Best" values to be Recommended. Selected data are plotted in Figure 2.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 3: Recommended (*R*) and Tentative Solubilities of Water (2) in Acetic acid propyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
273	1.16 (ref 16)	1.2	6.4
283	1.37* (ref 16)	1.4	5.9
293	1.7 (ref 4), 1.7 (ref 9), 1.58* (ref 13), 1.59 (ref 16)	1.64 ± 0.06 (*R*)	7.5
298	1.72* (ref 13), 1.72* (ref 16)	1.72 (*R*)	9.0
303	1.6 (ref 6,8), 1.87* (ref 13), 1.88 (ref 16)	1.78 ± 0.13	9.3
313	2.21* (ref 13), 2.17 (ref 16)	2.19 ± 0.02 (*R*)	11.3
323	2.0 (ref 10), 2.59* (ref 13), 2.29 (ref 16)	2.3 ± 0.2	12
333	2.5* (ref 10), 3.01* (ref 13), 2.34* (ref 16)	2.6 ± 0.3	13
343	3.1* (ref 10), 3.48* (ref 13), 2.93* (ref 16)	3.2 ± 0.2	16
353	3.8 (ref 10), 3.98* (ref 13), 3.01 (ref 16)	3.6 ± 0.4	17
363	4.52* (ref 13)	4.5	21

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

(continued next page)

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical
and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
January, 1989

CRITICAL EVALUATION: (continued)

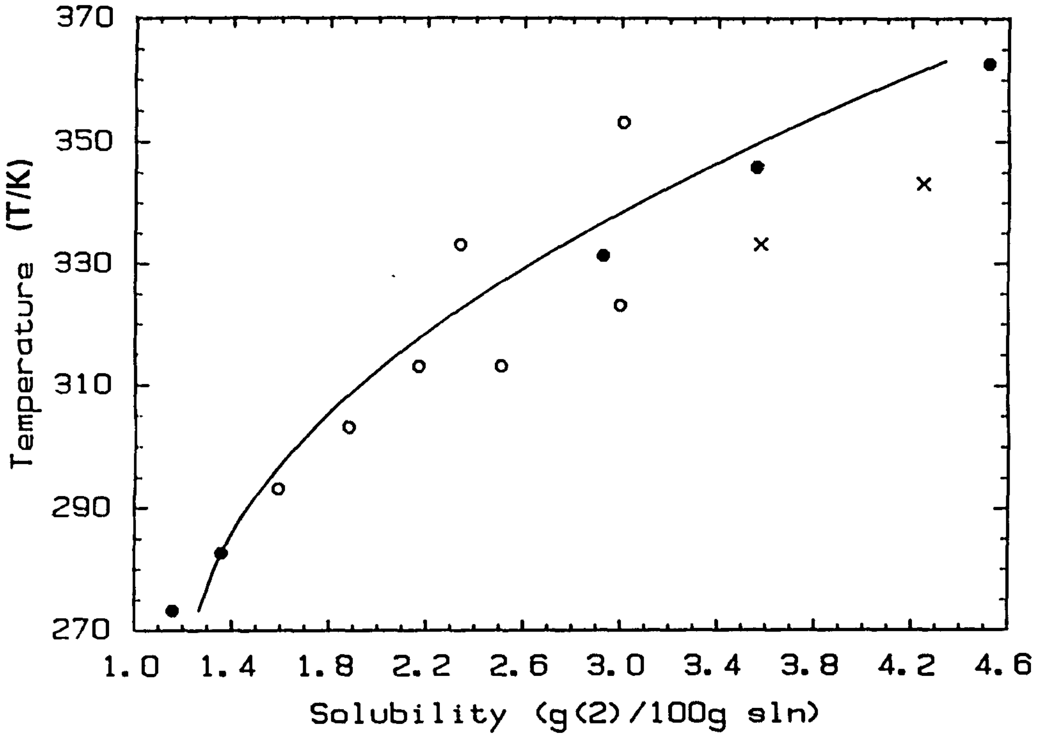

FIGURE 2. Selected data for the solubility of water (2) in acetic acid propyl ester (1): ref 13 (●); ref 16 (O); ref 9, rejected data, (X). Solid line is a least square polynomial fitted to the "Best" values from Table 3.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.
2. Rayman, J. *Thesis*, Budapest, 1906.
3. Fuehner, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-5.
4. Smith, T. E.; Bonner, R. F. *Ind. Eng. Chem.* 1950, *42*, 896-8.
5. Murti, P. S.; Venkataratnam, A.; Rao, C. V. *J. Sci. Ind. Res.* 1954, *13B*, 392-6.
6. Venkataratnam, A.; Rao, J. R.; Rao, C. V. *Chem. Eng. Sci.* 1957, *7*, 102-10.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

REFERENCES

7. Pick, J.; Hala, E.; Fried, V. *Chem. Listy* 1958, 561-6.

8. Rao, J. R.; Rao, C. V. *J. Appl. Chem.* 1959, *9*, 69-73.

9. Schuberth, H. *Abh. Deut. Akad. Wiss. Berlin Kl. Chem. Geol. Biol.* 1960, *3*, 1-82.

10. Smirnova, N. A.; Morachevskii, A. G. *Zh. Fiz. Khim.* 1960, *34*, 2546-53; see also Smirnova, N. A.; Morachevskii, A. G.; Storonkin, A. V. *Vestn. Leningr. Univ. Ser. Fiz. Khim.* 1959, *14(22)*, 70-80.

11. Rao, M. V. R.; Rao, K. S.; Rao, C. V. *J. Sci. Ind. Res.* 1961, *20B*, 379-81.

12. Shakhud, Zh. N.; Markusin, N. P.; Storonkin, A. V. *Vestn. Leningr. Univ. Ser. Fiz. Khim.* 1972, *(10)*, 89-92.

13. Skrzecz, A. *Pol. J. Chem.* 1980, *54*, 1101-4; see also Skrzecz, A. *Thesis, I. Ch. F. PAN,* Warszawa, 1979.

14. Tewari, Y. B.; Miller, M. M.; Wasik, S. P.; Martire, D. E. *J. Chem. Eng. Data* 1982, *27*, 451-4.

15. Richon, D.; Viallard, A. *Fluid Phase Equil.* 1985, *21*, 279-93.

16. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Traube, J.

Ber. Dtsch. Chem. Ges. <u>1884</u>, *17*, 2294-316.

VARIABLES:

T/K = 295

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 22°C was reported to be 1 part of propyl acetate in 55-65 parts of water.

The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 1.65 g(1)/100g sln and 0.0030.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±0.15 g(1)/100g sln.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	Rayman, J. *Thesis*, Budapest, 1906.
VARIABLES:	**PREPARED BY:**
$T/K = 273 - 303$	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of acetic acid propyl ester in water

$t/^{\circ}C$	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	3.47	3.35	0.00608
10.	2.83	2.57	0.00463
20.	2.36	2.30	0.00414
30.	2.09	2.05	0.00368

These data have also been published in (ref 2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, *55*, 360.
2. Hill, A.E. *International Critical Tables* (Washburn, E.W., Ed.) McGraw Hill, New York, 1928, Vol. 3, 387-98.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	Fuehner, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-5.
VARIABLES:	PREPARED BY:
$T/K = 293$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 20°C was reported to be 2.10 vol%, 1.89 g(1)/100g sln and 0.185 mol(1)/L sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00339.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.4 g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Smith, T.E.; Bonner, R.F.

Ind. Eng. Chem. 1950, *42*, 896-8.

VARIABLES:

T/K = 293 - 308

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid propyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	2.2[a]	98.3[b]	0.0040	0.911
35	1.8[a]	97.8[b]	0.0032	0.887

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture was stirred for about 1 h. and then separated and allowed to stand until each layer was visually perfectly clear (1-16 h.). Then, the layers were sampled and analyzed. Ester analyses were made by saponifying in an excess of 1N alcoholic KOH and back-titrating the unreacted alkali with 0.5N H_2SO_4 using phenolphthalein as the indicator. Water was determined by titration with the Karl Fischer reagent. The data were reported together with the ternary system acetic acid propyl ester-water-1-propanol.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; purity 99.2-99.8 wt%, 0.02 wt% water, 0.053 g/100 mL free acid, n_D^{20} 1.3850.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.1[a] and ±0.05[b] g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Murti, P.S.; Venkataratnam, A.; Rao, C.V.

J. Sci. Ind. Res. 1954, *13B*, 392-6.

VARIABLES:

T/K = 303 [a]

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 30°C[a] was reported to be 1.8 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0032.

The solubility of water in acetic acid propyl ester at 30°C[a] was reported to be 1.4 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.074.

[a] Persumably the measurments were made at 30°C; the temperature was not reported in the paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Determinations were made either from the production of turbidity or from its disappearance. The data were reported together with the ternary system acetic acid propyl ester-water-acetic acid. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House, laboratory reagent grade; distilled; 101.5°C, *d* 0.8830, n_D^{30} 1.3802.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.2 g(1)/100g sln and ±0.5 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Venkataratnam, A.; Rao, J.R.; Rao, C.V.

Chem. Eng. Sci. 1957, *7*, 102-10.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 30°C was reported to be 1.8 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0032.

The solubility of water in acetic acid propyl ester at 30°C was reported to be 1.6 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.084.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system acetic acid propyl ester-water-2-propanone (*propyl acetate-water-acetone*).

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House Ltd., laboratory reagent grade; distilled; b.p. 101.6°C, d^{30} 0.8773, n^{30} 1.3800.

(2) Distilled; free of CO_2.

ESTIMATED ERROR:

Soly. about ±0.2 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Pick, J.; Hala, E.; Fried,V.

Chem. Listy 1958, *52*, 561-6.

VARIABLES:

T/K = 357

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 84.0°C was reported to be x_1 = 0.005. The corresponding mass per cent value calculated by the compiler is 2.8 g(1)/100g sln.

The solubility of water in acetic acid propyl ester at 84.0°C was reported to be x_2 = 0.219. The corresponding mass per cent value calculated by the compiler is 4.71 g(2)/100g sln.

Pressure was reported to be 760 mm Hg.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not described. The ternary solubility at the boiling temperature was measured in a modified Washburn ebulliometer (ref 1,2). The temperature was measured with a calibrated Anschutz thermometer. The data were reported together with the ternary system acetic acid propyl ester-water-propanol.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; b.p. 101.4°C, d_4^{20} 0.88827 ±0.00006, n_D^{20} 1.3841 ±0.0001.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.9 g(1)/100g sln and ±0.5 g(2)/100g sln (compiler).

REFERENCES:

1. Washburn, E. *J. Am. Chem. Soc.* 1919, *41*, 729.
2. Pick, J.; Fried, V.; Hala, E.; Vilim, O. *Chem. Listy* 1955, *49*, 1112.

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rao, R.J.; Rao, C.V.

J. Appl. Chem. 1959, *9*, 69-73.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 30°C was reported to be 1.8 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0032.

The solubility of water in acetic acid propyl ester at 30°C was reported to be 1.6 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.084.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration method described by Rao and Rao (ref 1) was used. The data were reported together with the ternary system acetic acid propyl ester-water-1-propanol.

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House; distilled; b.p. 101.6°C, d^{30} 0.8773, n_D^{30} 1.3800.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.2 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).

REFERENCES:

1. Rao, R.J.; Rao, C.V. *J. Appl. Chem.* 1957, *7*, 435.

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schuberth, H.

Abh. Deut. Akad. Wiss. Berlin, Kl. Chem. Geol. Biol. 1960, *3*, 1-82.

VARIABLES:

T/K = 293 and 318

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid propyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20.0	2.2	98.3	0.0040	0.911
44.4	1.75	97.3	0.0031	0.864

Author's smoothed equations for mutual solubilities presented grahically at 308-341 K:

x_1 = $0.4876\times10^{-6}\ (T/K)^2 - 3.3144\times10^{-4}\ (T/K) + 5.9219\times10^{-2}$ (2)-rich phase

x_1 = $-12.965\times10^{-6}\ (T/K)^2 + 60.338\times10^{-4}\ (T/K) + 25.594\times10^{-2}$ (1)-rich phase

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration and analytical methods were used. The data and method were reported together with the ternary system acetic acid propyl ester-water-acetic acid butyl ester (*propyl acetate-water-butyl acetate*).

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized; dried over $CuSO_4$, distilled; b.p. 101.6°C, d^{20} 0.8879, n_D^{20} 1.3844.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.01°C.
Soly. ±0.05 g(1)/100g sln.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	Smirnova, N.A.; Morachevskii, A.G. *Zh. Fiz. Khim.* 1960, *34*, 2546-53. Smirnova, N.A.; Morachevskii, A.G.; Storonkin, A.V. *Vest. Leningrad. Univ., Fiz., Khim.* 1959, *14(22)*, 70-80.
VARIABLES:	PREPARED BY:
$T/K = 323 - 356$	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid propyl ester and water

$t/°C$	$g(1)/100g$ sln		x_1	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
50	1.80	98.0	0.0032	0.896
50.45[a]	1.80	98.0	0.0032	0.896
65	1.80	97.2	0.0032	0.860
66.30[a]	1.80	97.1	0.0032	0.856
76.50[a]	1.84	96.5	0.0033	0.828
80	1.86	96.2	0.0033	0.817
82.76[a]	1.86	96.0	0.0033	0.810

[a] Interpolated data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture of (1) and (2) was placed into a thermostated flask with a stirrer for 2 h. After separation, the ester was determined by saponification with 0.5N KOH and titration of the excess of KOH.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized and purified in the laboratory; b.p. 101.56°C, d_4^{20} 0.8884, n_D^{20} 1.3844.

(2) Not specified.

ESTIMATED ERROR:

Temp. $<\pm 0.5$°C.
Soly. $\pm 0.1\%$ (error of analysis).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	Rao, M.V.R.; Rao, K.S.; Rao, C.V. *J. Sci. Ind. Res.* 1961, *20B*, 379-81.
VARIABLES:	**PREPARED BY:**
$T/K = 308$	Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 35°C was reported to be 2.1 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0038.

The solubility of water in acetic acid propyl ester at 35°C was reported to be 2.0 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.104.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system acetic acid propyl ester-water-formic acid. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) BDH, laboratory reagent grade; used as received.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.15 g(1)/100g sln and ±0.1 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	Shakhud, Zh.N.; Markuzin, N.P.; Storonkin, A.V. *Vestn. Leningrad. Univ., Fiz., Khim.* 1972, *(10)*, 89-92.
VARIABLES:	**PREPARED BY:**
$T/K = 293 - 333$	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid propyl ester and water

$t/°C$	x_1		g(1)/100g sln (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	0.004	0.886	2.2	97.8
40	0.004	0.860	2.2	97.2
60	0.004	0.838	2.2	96.7

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical and titration methods as described by Shakhud, Markuzin and Storonkin (ref 1) were used. The two-phase mixture was stirred in a thermostated flask for 1 h. and then separated. The analysis of ester was made by saponification with 0.4N KOH in ethanol and then with titration using 0.1N HCl. The solubility of water in ester was established by the titration method in a flask with a mercury valve.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized; three times distilled; d_4^{20} 0.8879, n_D^{20} 1.3845.

(2) Twice distilled; n_D^{20} 1.3332.

ESTIMATED ERROR:

Temp. ±0.02°C.
Soly. ±1% (max. dev.).

REFERENCES:

1. Shakhud, Zh.N.; Markuzin, N.P.; Storonkin, A.V. *Vestn. Leningrad. Univ., Fiz., Khim.* 1972, *(10)*, 85.

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skrzecz, A.

Pol. J. Chem. 1980, *54*, 1101-4.

Skrzecz, A.

Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

VARIABLES:

T/K = 291 - 363

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid propyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
291.3	-	0.9253[a]	-	98.596
294.0	-	0.9093	-	98.271
300.2	0.00382	-	2.128	-
307.9	0.00351	-	1.958	-
310.3	-	0.8902	-	97.871
311.5	0.00344	-	1.919	-
314.2	0.00333	-	1.859	-
322.4	0.00324	-	1.809	-
331.3	-	0.8539	-	97.070
336.4	0.00324	-	1.809	-
345.6	0.00328	-	1.831	-
345.9	-	0.8269	-	96.439
351.6	0.00333	-	1.859	-

[a] By the Karl Fischer method.

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew and the analytical method were used. An ampoule with the solution of fixed concentration was placed into a glass tube connected with a thermostat filled completely with distilled water. The temperature of the bath was changed continuously during the measurements and the appearance and disappearance of turbidity within the ampoule was observed visually. For the analytical method, The amount of water in the saturated organic-phase was determined using a Karl Fischer titration procedure. The amount of water in the pure ester was taken into account.

SOURCE AND PURITY OF MATERIALS:

(1) POCH Gliwice, pure grade; distilled; purity 99.99% by glc, 0.15 wt% water by the Karl Fischer method.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.2-0.6)°C.
Soly. see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skrzecz, A.

Pol. J. Chem. 1980, *54*, 1101-4.

Skrzecz, A.

Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid propyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
355.6	0.00340	-	1.897	-
357.8	0.00344	-	1.919	-
361.5	0.00351	-	1.958	-
362.7	-	0.7884	-	95.480

Author's smoothing equations:

$$x_2 = 0.071291 + 7.085\text{x}10^{-4}\ (T/K - 273.15) + 9.57\text{x}10^{-6}\ (T/K - 273.15)^2$$

st. dev. = 1.21×10^{-3} (1)-rich phase

$$x_1 = 5.0250\text{x}10^{-3} - 5.97\text{x}10^{-5}\ (T/K - 273.15) + 4.85\text{x}10^{-7}\ (T/K - 273.15)^2$$

st. dev. = 3.96×10^{-5} (2)-rich phase

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E.

J. Chem. Eng. Data 1982, *27*, 451-4.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 25°C was reported to be 0.200 mol(1)/L sln.

The corresponding value on a mass/volume basis calculated by the compiler is 20.4 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of a water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible-with-water solution and then analyzed by a gas chromatographic technique.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purity >99% by glc.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. ±1.0%.

REFERENCES:

COMPONENTS:

(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 298.1K was reported to be 0.0219 mol(1)/100g(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 2.19 g(1)/100g sln and 0.00393.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) BDH: purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.02 g(1)/100g sln (compiler).

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid propyl ester (*propyl acetate*); $C_5H_{10}O_2$; [109-60-4] (2) Water; H_2O; [7732-18-5]	Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.
VARIABLES:	**PREPARED BY:**
T/K = 273 - 363	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid propyl ester and water

$t/^\circ C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	3.21	98.84	0.00581	0.9376
9.5	2.78	98.64	0.00503	0.9275
20.0	2.26	98.41	0.00406	0.9161
30.0	1.98	98.12	0.00355	0.9020
40.0	1.87	97.83	0.00335	0.8883
50.0	1.72	97.71	0.00308	0.8827
60.1	1.64	97.66	0.00293	0.8804
70.5	1.72	97.05	0.00308	0.8530
80.0	1.66	96.99	0.00297	0.8504
90.2	1.35	-	0.00241	-
std. dev.	0.02	0.04		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Butanoic acid methyl ester (*methyl butyrate*); $C_5H_{10}O_2$; [623-42-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the butanoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Butanoic acid methyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Hemptinne (ref 2)	298	(1) in (2)	analytical
Fuehner (ref 3)	294	(1) in (2)	titration
Stephenson and Stuart (ref 4)	273-364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF BUTANOIC ACID METHYL ESTER (1) IN WATER (2)

All the available data for the solubility of butanoic acid methyl ester (1) in water (2) are summarized in Table 2 with the exception of the datum of Hemptinne (ref 2) which is reported in w/v units and hence is excluded from this Evaluation.

At *ca*. 294 K, the only temperature where comparison is possible, the independent studies (ref 1,3,4) are in reasonable agreement suggesting that the data of Stephenson and Stuart (ref 4) at other temperatures should also be reliable. However, pending further studies, the data of Stephenson and Stuart must be considered Tentative.

TABLE 2: Tentative Solubilities Butanoic acid methyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values [a]	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
273	2.62 (ref 4)	2.6	4.7

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Butanoic acid methyl ester (*methyl butyrate*); $C_5H_{10}O_2$; [623-42-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities		
	Reported values	"Best" values [a]	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
283	2.21* (ref 4)	2.2	4.0
293	1.65[b] (ref 1), 1.56[c] (ref 3), 1.86* (ref 4)	1.9	3.3
298	1.76* (ref 4)	1.8	3.0
303	1.67* (ref 4)	1.7	2.8
313	1.53* (ref 4)	1.5	2.6
323	1.44 (ref 4)	1.4	2.5
333	1.42* (ref 4)	1.4	2.5
343	1.42* (ref 4)	1.4	2.5
353	1.41* (ref 4)	1.4	2.5
363	1.27* (ref 4)	1.3	2.3

[a] Rounded values from ref 4, see text.

[b] 295 K, not included in "Best" value at 293 K.

[c] 294 K, not included in "Best" value at 293 K.

2. SOLUBILITY OF WATER (2) IN BUTANOIC ACID METHYL ESTER (1)

The only data available for the solubility of water (2) in butanoic acid methyl ester (1) are those due to Stephenson and Stuart (ref 4) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubilities.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.
2. Hemptinne, A. *Z. Phys. Chem.* 1894, *13*, 561-9.
3. Fuehner, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-5.
4. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

COMPONENTS:

(1) Butanoic acid methyl ester (*methyl butyrate*); $C_5H_{10}O_2$; [623-42-7]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Traube, J.

Ber. Dtsch. Chem. Ges. 1884, *17*, 2294-316.

VARIABLES:

$T/K = 295$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid methyl ester in water at 22°C was reported to be 1 part of methyl butyrate in 55-65 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 1.65 g(1)/100g sln and 0.0030.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±0.15 g(1)/100g sln.

REFERENCES:

COMPONENTS:

(1) Butanoic acid methyl ester (*methyl butyrate*); $C_5H_{10}O_2$; [623-42-7]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hemptinne, A.

Z. Phys. Chem. 1894, *13*, 561-9.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid methyl ester in water at 25°C was reported to be 10.726 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture of water with excess ester was heated for some time in a water bath and the ester phase was filtered. A sample of known volume was then transferred to a smaller flask, heated with the known amount of baryta until complete saponification was obtained and then titrated. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS: (1) Butanoic acid methyl ester (*methyl butyrate*); $C_5H_{10}O_2$; [623-42-7] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Fuehner, H. *Ber. Dtsch. Chem. Ges.* <u>1924</u>, *57*, 510-5.
VARIABLES: T/K = 294	PREPARED BY: A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid methyl ester in water at 21°C was reported to be 1.792 vol%, 1.559 g(1)/100g sln and 0.1528 mol(1)/L sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.002786.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commercial product. (2) Not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:

(1) Butanoic acid methyl ester (*methyl butyrate*); $C_5H_{10}O_2$; [623-42-7]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

$T/K = 273 - 364$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of butanoic acid methyl ester and water

$t/°C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	2.62	99.16	0.00472	0.9542
9.4	2.24	99.03	0.00402	0.9474
19.7	1.87	98.86	0.00335	0.9386
29.7	1.68	98.73	0.00300	0.9320
39.5	1.54	98.55	0.00275	0.9230
50.0	1.44	98.50	0.00257	0.9205
60.3	1.45	98.25	0.00259	0.9083
70.3	1.42	98.34	0.00253	0.9127
80.1	1.41	97.98	0.00252	0.8953
90.5	1.26	97.98	0.00225	0.8953
std. dev.	0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Formic acid butyl ester *(butyl formate)*; $C_5H_{10}O_2$; [592-84-7] (2) Water; H_2O; [7732-18-5]	Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 364	Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in formic acid butyl ester

$t/^\circ C$	g(1)/100g sln	x_1 (compiler)
0	99.20	0.9563
9.5	98.95	0.9432
20.2	98.86	0.9386
30.8	98.96	0.9438
40.0	98.79	0.9350
50.2	98.63	0.9270
60.5	98.45	0.9180
70.3	98.46	0.9185
80.1	98.34	0.9126
90.6	98.07	0.8996

std. dev. 0.02

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 97%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Formic acid 2-methylpropyl ester (*isobutyl formate*); $C_5H_{10}O_2$; [542-55-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the formic acid 2-methylpropyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Formic acid 2-methylpropyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Stephenson and Stuart (ref 2)	273-353	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

As can be seen from Table 1 the only comparison possible is for the solubility of (1) in (2) at 295 K. The reported values of 1 (ref 1) and 0.90 (ref 2) g(1)/100g sln are in good agreement suggesting that the values of Stephenson and Stuart (ref 2) are probably reliable. However, in the absence of confirmatory studies, all of these data (ref 2) must be regarded as Tentative. The interested user is referred to the relevant Data Sheet for the experimental solubilities of Stephenson and Stuart.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-2316.
2. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

COMPONENTS:

(1) Formic acid 2-methylpropyl ester (*isobutyl formate*); $C_5H_{10}O_2$; [542-55-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Traube, J.

Ber. Dtsch. Chem. Ges. 1884, *17*, 2294-316.

VARIABLES:

$T/K = 295$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of formic acid 2-methylpropyl ester in water at 22°C was reported to be 1 part of isobutyl formate in 99 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 1 g(1)/100g sln and 0.0002.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Formic acid 2-methylpropyl ester (*isobutyl formate*); $C_5H_{10}O_2$; [542-55-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 353

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of formic acid 2-methylpropyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.14	-	0.00159	-
9.8	1.11	99.29	0.00155	0.9509
20.8	0.93	99.14	0.00130	0.9410
30.8	0.82	98.95	0.00114	0.9288
39.8	0.76	98.98	0.00106	0.9307
50.3	0.79	98.79	0.00110	0.9187
60.4	0.78	98.65	0.00109	0.9100
70.3	-	98.61	-	0.9075
80.2	-	98.33	-	0.8907
std. dev.	0.01	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 96%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the propanoic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Propanoic acid ethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Doolittle (ref 3)	293	mutual	unspecified
Rao and Rao (ref 4)	301,303	mutual	titration
Rao and Rao (ref 5)	303	mutual	titration
Venkataratnam *et al.* (ref 6)	303	mutual	titration
Rao and Rao (ref 7)	303	mutual	titration?
Bomshtein *et al.* (ref 8)	293-353	mutual	titration
Tewari *et al.* (ref 9)	298	(1) in (2)	GLC
Richon and Viallard (ref 10)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 11)	273-364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF PROPANOIC ACID ETHYL ESTER (1) IN WATER (2)

The available data for the solubility of propanoic acid ethyl ester (1) in water (2) are summarized in Table 2 with the following exceptions. The data of Traube (ref 1), Bomshtein *et al.* (ref 8, at $T < 313$ K) and Richon and Viallard (ref 10) have been rejected as they are considerably lower ($> 3\sigma_n$) than other reported values (ref 2,3,11). The datum of Venkataratnam *et al.* (ref 6) at 303 K has also been rejected as it is much higher than other values at this temperature (ref 2,4,5,7,11).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

At higher temperatures, the data of Bomshtein *et al*. (ref 8) and Stephenson and Stuart (ref 11) are in serious disagreement, showing an opposite trend in solubility with temperature. It should be noted that in general ester solubilities in water decrease with temperature up to *ca*. 333 K, i.e., opposite to the trend reported by Bomshtein *et al*. (ref 8). However, although the data of Stephenson and Stuart (ref 10) have been preferred in deriving the "Best" values, in the absence of independent studies, it is not possible at this stage to reject either data set. Further studies of this system are clearly warranted. Selected data are plotted in Figure 1.

TABLE 2: Recommended (*R*) and Tentative Solubilities of Propanoic acid ethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
273	3.41 (ref 2), 3.26 (ref 11)	3.34 ± 0.08 (*R*)	6.0
283	2.78 (ref 2), 2.58* (ref 11)	2.68 ± 0.10 (*R*)	4.8
293	2.32 (ref 2), 1.92 (ref 3), 2.21* (ref 11)	2.2 ± 0.2	4.0
298	2.17* (ref 2), 2.06* (ref 11)	2.12 ± 0.06 (*R*)	3.81
303	2.02 (ref 2), 2.01 (ref 4), 2.2 (ref 5), 2.2 (ref 7), 1.92* (ref 11)	2.07 ± 0.11 (*R*)	3.72
313	2.12 (ref 8), 1.74* (ref 11)	1.7[b]	3.0
323	2.28 (ref 8), 1.66 (ref 11)	1.7[b]	3.0
333	2.50 (ref 8), 1.61* (ref 11)	1.6[b]	2.9
343	2.88 (ref 8), 1.58* (ref 11)	1.6[b]	2.9
353	3.63 (ref 8), 1.59* (ref 11)	1.6[b]	2.9

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] Rounded value of ref 11; see text.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

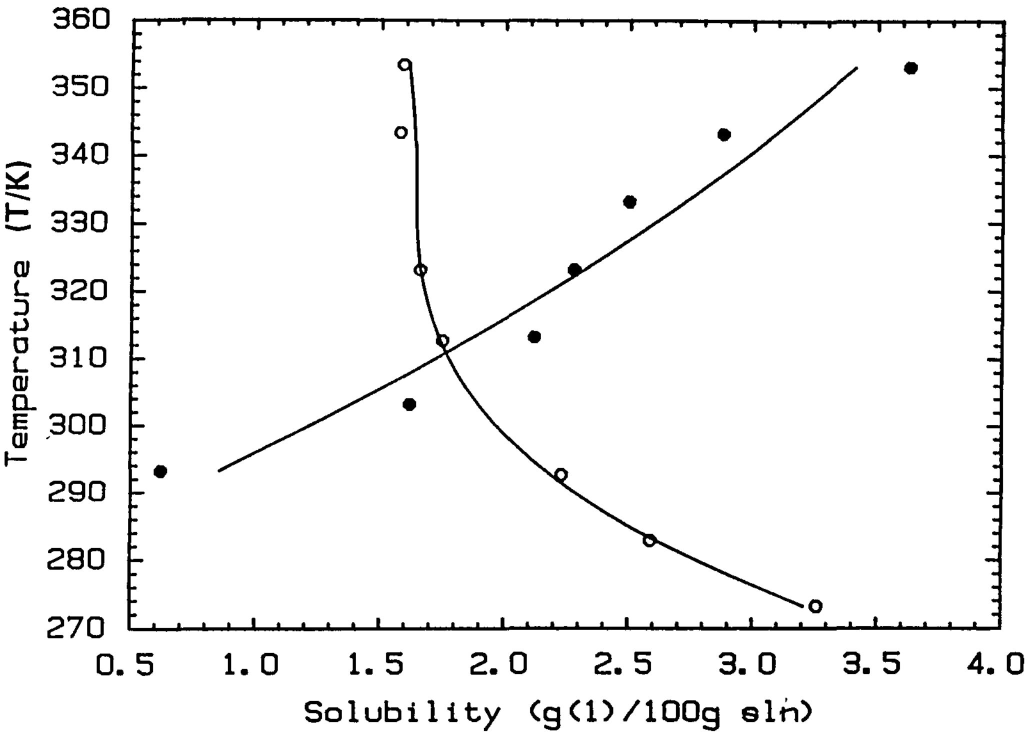

FIGURE 1. Selected data for the solubility of propanoic acid ethyl ester (1) in water (2): ref 8 (●); ref 11 (O). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

2. SOLUBILITY OF WATER (2) IN PROPANOIC ACID ETHYL ESTER (1)

All the available data for the solubility of water (2) in propanoic acid ethyl ester (1) are summarized in Table 3 except for the data at 303 K of Rao and Rao (ref 7) which appear to be self-contradictory and are rejected.

The remaining data are in general in reasonable agreement and the solubility values of Bomshtein *et al.* (ref 8) and Stephenson and Stuart (ref 11), although somewhat divergent, at least show the same trend with temperature (*cf.* the water-rich phase above). Selected data are plotted in Figure 2. In the absence of confirmatory studies it is not possible, at this stage, to prefer either data set.

(continued next page)

COMPONENTS:

(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
January, 1989

CRITICAL EVALUATION: (continued)

TABLE 3: Recommended (*R*) and Tentative Solubilities of Water (2) in Propanoic acid ethyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
273	0.89 (ref 10)	0.9	4.9
283	1.05* (ref 10)	1.1	5.9
293	1.22 (ref 2), 1.40 (ref 7), 1.24 (ref 10)	1.28 ± 0.08 (*R*)	6.9
298	1.55* (ref 7), 1.38* (ref 10)	1.47 ± 0.09 (*R*)	7.8
303	2.00 (ref 3), 1.4 (ref 4), 1.8 (ref 5), 1.70 (ref 7), 1.51* (ref 10)	1.7 ± 0.2	8.9
313	2.10 (ref 7), 1.71* (ref 10)	1.9 ± 0.2	9.9
323	2.50 (ref 7), 1.86 (ref 10)	2.2 ± 0.3	11
333	3.00 (ref 7), 1.92* (ref 10)	2.5 ± 0.5	13
343	3.50 (ref 7), 1.98* (ref 10)	2.7 ± 0.8	14
353	4.00 (ref 7), 2.19* (ref 10)	3 ± 1	15
363	2.38 (ref 10)	-	

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

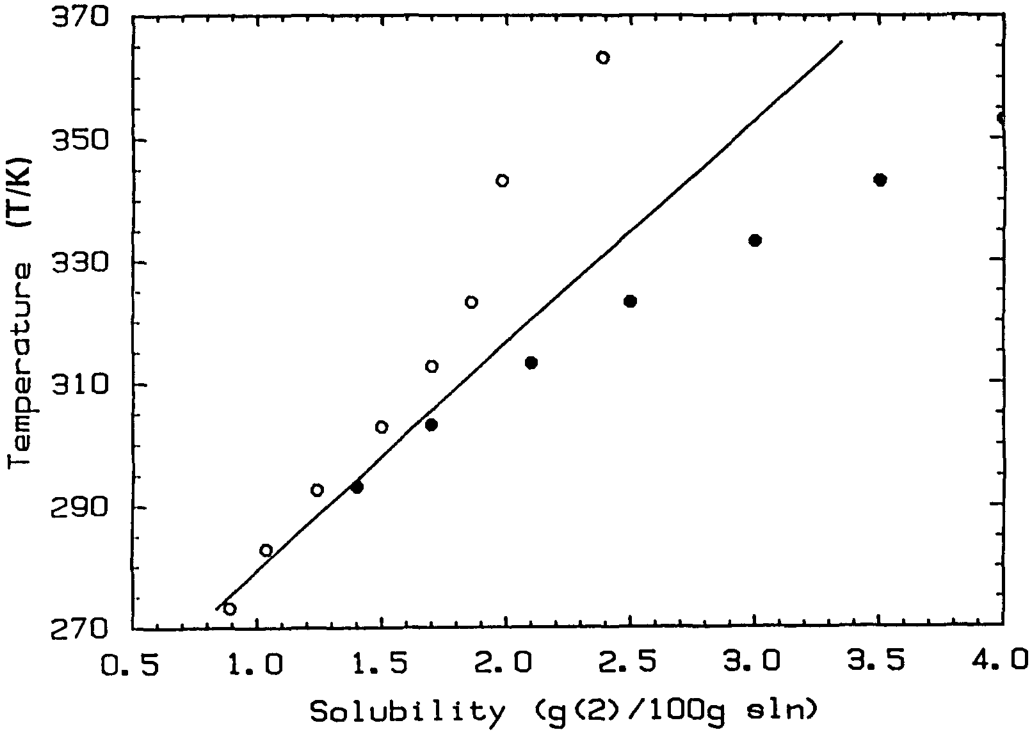

FIGURE 2. Selected data for the solubility of water (2) in propanoic acid ethyl ester (1): ref 8 (●); ref 11 (○). Solid line is drawn through the "Best" values from Table 3.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.

2. Rayman, J. *Thesis*, Budapest 1906.

3. Doolittle, A. K. *Ind. Eng. Chem.* 1935, *27*, 1169-79.

4. Rao, G. J. R.; Rao, C. V. *J. Sci. Ind. Res.* 1955, *14B*, 444-8.

5. Rao, J. R.; Rao, C. V. *J. Appl. Chem.* 1957, *7*, 435-9.

6. Venkataratnam, A.; Rao, J. R.; Rao, C. V. *Chem. Eng. Sci.* 1957, *7*, 102-10.

7. Rao, J. R.; Rao, C. V. *J. Appl. Chem.* 1959, *9*, 69-73.

8. Bomshtein, A. L.; Trofimov, A. N.; Serafimov, L. A. *Zh. Prikl. Khim.* 1978, *51*, 1280-2.

9. Tewari, Y. B.; Miller, M. M.; Wasik, S. P.; Martire, D. E. *J. Chem. Eng. Data* 1982, *27*, 451-4.

10. Richon, D.; Viallard, A. *Fluid Phase Equil.* 1985, *21*, 279-93.

11. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

COMPONENTS:

(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Traube, J.

Ber. Dtsch. Chem. Ges. 1884, *17*, 2294-316.

VARIABLES:

$T/K = 295$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethyl ester in water at 22°C was reported to be 1 part of ethyl propionate in 55-65 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 1.65 g(1)/100g sln and 0.0030.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±0.15 g(1)/100g sln.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3] (2) Water; H_2O; [7732-18-5]	Rayman, J. *Thesis*, Budapest, 1906.
VARIABLES:	**PREPARED BY:**
T/K = 273-303	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of propanoic acid ethyl ester in water

t/°C	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	3.54	3.44	0.00619
10.	2.86	2.78	0.00502
20.	2.38	2.32	0.00417
30.	2.06	2.02	0.00363

These data have also been published in (ref 2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, *55*, 360.
2. Hill, A.E. *International Critical Tables* (Washburn, E.W., Ed.) McGraw Hill, New York, 1928, Vol. 3, 387-98.

COMPONENTS:

(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Doolittle, A.K.

Ind. End. Chem. 1935, *27*, 1169-79.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethyl ester in water at 20°C was reported to be 1.92 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00344.

The solubility of water in propanoic acid ethyl ester at 20°C was reported to be 1.22 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0654.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; purity 96%, b.p. range 90-118°C, d_4^{20} 0.891.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3] (2) Water; H_2O; [7732-18-5]	Rao, G.J.R.; Rao, C.V. *J. Sci. Ind. Res.* 1955, *14B*, 444-8.
VARIABLES:	PREPARED BY:
T/K = 301 and 303	Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethyl ester in water at 28 and 30°C was reported to be 2.01 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00361.

The solubility of water in propanoic acid ethyl ester at 28 and 30°C was reported to be 2.00 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.104.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. The data were reported together with the ternary system propanoic acid ethyl ester-water-propionic acid. No further details were reported in the paper.	(1) Naarden; b.p. 99.1°C, d^{30} 0.8792; used as received. (2) Distilled and boiled; free from CO_2.
	ESTIMATED ERROR:
	Temp. ±0.1°C.
	REFERENCES:

COMPONENTS:

(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rao, J.R.; Rao, C.V.

J. Appl. Chem. 1957, 7, 435-9.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethyl ester in water at 30°C was reported to be 2.2 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0040.

The solubility of water in propanoic acid ethyl ester at 30°C was reported to be 1.4 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.074.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system propanoic acid ethyl ester-water-methanol.

SOURCE AND PURITY OF MATERIALS:

(1) Naarden, reagent grade; b.p. 99.1°C, d^{30} 0.8790, n_D^{30} 1.3812.

(2) Distilled; free from CO_2.

ESTIMATED ERROR:

Temp. ±0.02°C.

REFERENCES:

COMPONENTS:

(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Venkataratnam, A.; Rao, J.R.; Rao, C.V.

Chem. Eng. Sci. 1957, *7*, 102-10.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethyl ester in water at 30°C was reported to be 2.7 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.049.

The solubility of water in propanoic acid ethyl ester at 30°C was reported to be 1.8 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.094.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system propanoic acid ethyl ester-water-2-propanone (*ethylpropionate-water-acetone*). No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Naarden, analytical grade; used as received; b.p. 99.1°C, d^{30} 0.8790, n^{30} 1.3812.

(2) Distilled; free of CO_2.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rao, R.J.; Rao, C.V.

J. Appl. Chem. <u>1959</u>, *9*, 69-73.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethyl ester in water at 30°C was reported to be 2.2 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0040.

The solubility of water in propanoic acid ethyl ester at 30°C was reported to be 1.0 g(2)/100g sln and 98.6 g(1)/100g sln[a]. The corresponding mole fraction, x_2, values calculated by the compiler are 0.054 and 0.074[a].

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration method described by Rao and Rao (ref 1) was used. The data were reported together with the ternary system propanoic acid ethyl ester-water-1-propanol.

SOURCE AND PURITY OF MATERIALS:

(1) Naarden, analytical grade; b.p. 99.1°C, d^{30} 0.8790, n_D^{30} 1.3812.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Rao, R.J.; Rao, C.V. *J. Appl. Chem.* <u>1957</u>, *7*, 435.

COMPONENTS:

(1) Propanoic acid ethyl ester *(ethyl propionate)*; $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bomshtein, A.L.; Trofimov, A.N.; Serafimov, L.A.

Zh. Prikl. Khim. 1978, *51*, 1280-2.

VARIABLES:

$T/K = 293 - 353$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of propanoic acid ethyl ester and water

$t/^{\circ}C$	x_1		g(1)/100g sln (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	0.0011	0.9255	0.62	98.60
30	0.0029	0.9107	1.62	98.30
40	0.0038	0.8916	2.12	97.90
50	0.0041	0.8731	2.28	97.50
60	0.0045	0.8509	2.50	97.00
70	0.0052	0.8295	2.88	96.50
80	0.0066	0.8090	3.63	96.00

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used at constant temperature. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; without impurities by glc, b.p. 99.1°C, n_D^{20} 1.383.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E.

J. Chem. Eng. Data 1982, *27*, 451-4.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethyl ester in water at 25°C was reported to be 0.148 mol(1)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 15.1 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of a water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible-with-water solution and then analyzed by a gas chromatographic technique.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purity >99% by glc.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. ±1.0%.

REFERENCES:

COMPONENTS:

(1) Propanoic acid ethyl ester (*ethyl propionate*); $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid ethyl ester in water at 298.1 K was reported to be 0.0172 mol(1)/100g(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 1.726 g(1)/100g sln and 0.00309.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) BDH: purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.

COMPONENTS:

(1) Propanoic acid ethyl ester *(ethyl propionate)*; $C_5H_{10}O_2$; [105-37-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

$T/K = 273 - 364$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of propanoic acid ethyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	3.26	99.11	0.00591	0.9516
9.7	2.59	98.96	0.00467	0.9438
19.5	2.23	98.76	0.00401	0.9335
29.7	1.93	98.50	0.00346	0.9205
39.5	1.75	98.30	0.00313	0.9107
50.0	1.66	98.14	0.00297	0.9030
60.1	1.61	98.08	0.00288	0.9001
70.2	1.58	98.02	0.00282	0.8972
80.3	1.59	97.80	0.00284	0.8869
90.5	-	97.61	-	0.8781
std. dev.	0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 97%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Propanoic acid, 2-methly-, methyl ester (*methyl isobutyrate*); $C_5H_{10}O_2$; [547-63-7]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 353

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of 2-methylpropanoic acid methyl ester and water

t/°C	g(1)/100g sln (2)-rich phase	g(1)/100g sln (1)-rich phase	x_1 (compiler) (2)-rich phase	x_1 (compiler) (1)-rich phase
0	2.68	98.97	0.00483	0.9442
9.1	2.23	98.79	0.00401	0.9350
18.9	1.96	98.70	0.00351	0.9305
29.5	1.69	98.52	0.00302	0.9215
39.9	1.52	98.38	0.00271	0.9146
49.8	1.46	98.21	0.00260	0.9063
60.4	1.38	97.75	0.00246	0.8845
70.5	1.40	97.93	0.00250	0.8930
80.3	1.32	97.85	0.00235	0.8892
std. dev.	0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid 2-methoxyethyl ester
(*2-methoxyethyl acetate*);
$C_5H_{10}O_3$; [110-49-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Alvarez, J.R.; Neila, J.J.

An. Quim. 1978, *74*, 326-32.

VARIABLES:

T/K = 298

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-methoxyethyl ester in water at 25°C was reported to be 45.5 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.1129.

The solubility of water in acetic acid 2-methoxyethyl ester at 25°C was reported to be 46.4 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.850.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration method was used. The data were reported together with the ternary system 2-methoxyethyl acetate-water-phenol. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; used as received; $d_4^{18.1}$ 1.0051, n_D^{20} 1.4048.

(2) Twice distilled over $KMnO_4$.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Carbonic acid diethyl ester (*diethyl carbonate*); $C_5H_{10}O_3$; [105-58-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the carbonic acid diethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Carbonic acid diethyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Doolittle (ref 1)	293	mutual	unspecified
Stephenson and Stuart (ref 2)	273-363	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF CARBONIC ACID DIETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of carbonic acid diethyl ester (1) in water (2) are summarized in Table 2. At 293 K, the only temperature where comparison is possible, the data (ref 1,2) are in excellent agreement and the average "Best" value is Recommended. At other temperatures only the data of Stephenson and Stuart (ref 2) are available and, pending further studies, these must be regarded as Tentative.

TABLE 2: Recommended (*R*) and Tentative Solubilities of Carbonic acid diethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
273	2.49 (ref 2)	2.5	3.9
283	2.14* (ref 2)	2.1	3.3
293	1.88 (ref 1), 1.90* (ref 2)	1.89 ± 0.01 $(R)^b$	2.93
298	1.77* (ref 2)	1.8	2.6

[a] Rounded values of ref 2 unless otherwise indicated.

[b] Average value.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Carbonic acid diethyl ester (*diethyl carbonate*); $C_5H_{10}O_3$; [105-58-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
303	1.67 (ref 2)	1.7	2.5
313	1.58 (ref 2)	1.6	2.4
323	1.53 (ref 2)	1.5	2.3
333	1.53* (ref 2)	1.5	2.3
343	1.6* (ref 2)	1.6	2.4
353	1.6* (ref 2)	1.6	2.4
363	1.6* (ref 2)	1.6	2.4

[a] Rounded values of ref 2 unless otherwise indicated.

In Table 2, σ_n has no statistical significance; mole fraction solubility (x_1) has same status and (relative) percentage uncertainty as mass% solubility.

2. SOLUBILITY OF WATER (2) IN CARBONIC ACID DIETHYL ESTER (1)

As for the solubility of carbonic acid diethyl ester (1) in water (2) the only comparable data available for the solubility of (2) in (1) are at 293 K. However, unlike the H_2O-rich phase the datum of 2.60 g(2)/100 g sln of Doolittle (ref 1) is in poor agreement with the interpolated value of 0.86 g(2)/100 g sln of Stephenson and Stuart (ref 2). In the absence of confirmatory studies it is not possible to decide between these data although it may be noted that the data of Doolittle often differ significantly from reliable values in other systems.

The interested user is referred to the Data Sheet for the experimental solubilities of Stephenson and Stuart for water in carbonic acid diethyl ester.

REFERENCES

1. Doolittle, A. K. *Ind. Eng. Chem.* 1935, *27*, 1169-79.

2. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

COMPONENTS:

(1) Carbonic acid diethyl ester (*diethyl carbonate*); $C_5H_{10}O_3$; [105-58-8]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Doolittle, A.K.

Ind. End. Chem. 1935, *27*, 1169-79.

VARIABLES:

T/K = 293

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of carbonic acid diethyl ester in water at 20°C was reported to be 1.88 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00291.

The solubility of water in carbonic acid diethyl ester at 20°C was reported to be 2.60 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.1490.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; purity 91%, b.p. range 87-127°C, d_4^{20} 0.957.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Carbonic acid diethyl ester (*diethyl carbonate*); $C_5H_{10}O_3$; [105-58-8]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 363

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of carbonic acid diethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	2.49	99.35	0.00388	0.9589
9.9	2.15	99.28	0.00334	0.9546
20.1	1.90	99.11	0.00294	0.9444
30.0	1.67	98.94	0.00258	0.9343
40.0	1.58	98.88	0.00244	0.9309
50.0	1.53	98.68	0.00236	0.9193
60.2	1.54	98.38	0.00238	0.9025
70.1	1.63	98.27	0.00252	0.8965
80.1	1.69	97.63	0.00261	0.8627
90.3	1.63	97.22	0.00252	0.8421
std. dev.	0.02	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) 2-Butenedioic acid dimethyl ester (*dimethyl maleate*); $C_6H_8O_4$; [624-48-6]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 364

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of 2-butenedioic acid dimethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	7.7	97.90	0.0103	0.8535
9.6	7.3	97.46	0.0097	0.8275
19.8	7.6	96.82	0.0102	0.7919
29.7	7.8	96.24	0.0105	0.7619
39.5	8.1	95.50	0.0109	0.7262
50.0	8.7	94.50	0.0118	0.6823
59.9	8.9	93.57	0.0121	0.6453
69.8	9.6	92.40	0.0131	0.6031
80.1	10.4	90.92	0.0143	0.5559
90.5	10.9	89.62	0.0151	0.5190
std. dev.	0.2	0.03		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) 1-Methyl-2-propen-1-ol acetate *(1-methylallyl acetate)*; $C_6H_{10}O_2$; [6737-11-7]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Othmer, D.F.; Bergen, W.S.; Shlechter, N.; Bruins, P.F.

Ind. Eng. Chem. 1945, *37*, 890-4.

VARIABLES:

T/K = 299 - 348

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of 1-Methyl-2-propen-1-ol acetate and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
26	1.32	99.0	0.0021	0.940
50	0.8	98.9	0.0013	0.934
75	2.0	98.1	0.0032	0.891

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration method reported by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system 1-Methyl-2-propen-1-ol acetate-water-1,2-butanediol *(1-methylallyl acetate-water-butylene glycol)*.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized from methyl vinyl carbinol; washed with water, dried with $CaCl_2$, distilled; b.p. range 112-113°C.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Butanoic acid, 3-oxo-, ethyl ester (*ethyl acetoacetate*); $C_6H_{10}O_3$; [141-97-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Pai, M.U.; Sane, A.G.

Indian J. Technol. 1966, *4*, 373-5.

VARIABLES:

T/K = 273 and 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of 3-oxobutanoic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	12.15	93.55	0.01879	0.6675
30	10.04	92.02	0.01521	0.6148

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The turbidity method described by Othmer, White and Trueger (ref 1) was used. Mutual solubilities were determined in a 25 mL glass stoppered flask placed in a thermostat. The data were reported together with the ternary system 3-oxobutanoic acid ethyl ester-water-acetic acid ethyl ester (*ethyl acetoacetate-water-ethyl acetate*).

SOURCE AND PURITY OF MATERIALS:

(1) Merc CP grade; distilled at 10 ±1 mm Hg and the middle cut at 67 ±0.5°C was used; purity 99.9%, b.p. 180.9°C, d_{20}^{20} 1.025.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.1°C.

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger,E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Ethanedioic acid diethyl ester (*diethyl oxalate*); $C_6H_{10}O_4$; [95-92-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

$T/K = 273 - 364$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of ethanedioic acid diethyl ester and water

$t/°C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	5.47	99.40	0.00708	0.9533
9.5	4.45	99.23	0.00571	0.9408
19.7	3.82	98.92	0.00487	0.9186
30.9	3.71	98.80	0.00473	0.9103
39.8	3.17	98.65	0.00402	0.9001
49.7	2.74	98.30	0.00346	0.8770
60.0	-	97.92	-	0.8530
70.2	-	97.48	-	0.8266
80.4	-	96.68	-	0.7821
90.7	-	96.12	-	0.7533
std. dev.	0.09	0.03		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,1-Ethanediol diacetate (*ethylidene diacetate*); $C_6H_{10}O_4$; [542-10-9] (2) Water; H_2O; [7732-18-5]	Smith, J.C. *J. Phys. Chem.* 1942, *46*, 229-32.
VARIABLES:	**PREPARED BY:**
$T/K = 298$	Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of 1,1-ethanediol diacetate in water at 25°C was reported to be 5 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.006.

The solubility of water in 1,1-ethanediol diacetate at 25°C was reported to be 5 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.3.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration method was used. The data and method were reported together with the ternary system 1,1-ethanediol diacetate-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2-Ethanediol diacetate (*ethylene glycol diacetate*); $C_6H_{10}O_4$; [111-55-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the 1,2-ethanediol diacetate (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 1,2-Ethanediol diacetate (1) - Water (2) System

Reference	T/K	Solubility	Method
Doolittle (ref 1)	293	mutual	unspecified
Othmer *et al.* (ref 2)	298	mutual	unspecified
Kraus *et al.* (ref 3)	298	mutual	analytical

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 1,2-ETHANEDIOL DIACETATE (1) IN WATER (2)

All the available data for the solubility of 1,2-ethanediol diacetate (1) in water (2) are summarized in Table 2. As can be seen, the data are in only fair agreement with the value of Doolittle looking to be high. However, pending further studies, none of these data can be rejected at this stage.

TABLE 2: Tentative Solubilities of 1,2-Ethanediol diacetate (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^2x_1
293	21.3 (ref 1)	21^b	3.2
298	17.8^c (ref 2), 16 (ref 3)	17 ± 1	2.5

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] But see text.

[c] 297.7 K.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1,2-Ethanediol diacetate (*ethylene glycol diacetate*); $C_6H_{10}O_4$; [111-55-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 1,2-ETHANEDIOL DIACETATE (1)

All the available data for the solubility of water (2) in 1,2-ethanediol diacetate (1) are summarized in Table 3. The data of Othmer *et al.* (ref 2) and Kraus *et al.* (ref 3) at *ca.* 298 K are in fair agreement but the value of Doolittle (ref 1) is very much higher. However, in the absence of confirmatory studies no Critical Evaluation is possible.

TABLE 3: Tentative Solubilities of Water (2) in 1,2-Ethanediol diacetate (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	x_2
293	21.2 (ref 1)	21^b	0.68
298	10.0^c (ref 2), 7.65 (ref 3)	9 ± 1	0.45

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] But see text.

[c] 297.7 K.

REFERENCES

1. Doolittle, A. K. *Ind. Eng. Chem.* 1935, *27*, 1169-79.
2. Othmer, D. F.; White, R. E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240-8.
3. Kraus, K. A.; Rardon, R. J.; Baldwin, W. H. *J. Am. Chem. Soc.* 1964, *86*, 2571-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Ethanediol diacetate *(ethylene glycol diacetate)*; $C_6H_{10}O_4$; [111-55-7] (2) Water; H_2O; [7732-18-5]	Doolittle, A.K. *Ind. End. Chem.* 1935, *27*, 1169-79.
VARIABLES:	**PREPARED BY:**
T/K = 293	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 1,2-ethanediol diacetate in water at 20°C was reported to be 21.3 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0323.

The solubility of water in 1,2-ethanediol diacetate at 20°C was reported to be 21.2 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.686.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commercial product; purity 99%, b.p. range 184-191°C, d_4^{20} 1.107. (2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:

(1) 1,2-Ethanediol diacetate
(ethylene glycol diacetate);
$C_6H_{10}O_4$; [111-55-7]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Othmer, D.F.; White, R.E.;
Trueger, E.

Ind. Eng. Chem. 1941, *33*, 1240-8.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of 1,2-ethanediol diacetate in water at 24.5°C was reported to be 17.8 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0260.

The solubility of water in 1,2-ethanediol diacetate at 24.5°C was reported to be 10.0 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.474.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Nothing was specified in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.5°C (mean of reported range).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Ethanediol diacetate (*ethylene glycol diacetate*); $C_6H_{10}O_4$; [111-55-7] (2) Water; H_2O; [7732-18-5]	Kraus, K.A.; Raridon, R.J.; Baldwin, W.H. *J. Am. Chem. Soc.* 1964, *86*, 2571-6.
VARIABLES:	**PREPARED BY:**
T/K = 298	Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of 1,2-ethanediol diacetate in water at 25°C was reported to be 16 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.023.

The solubility of water in 1,2-ethanediol diacetate at 25°C was reported to be 7.65 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.402.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical methods were used. The mutual solubilities of (1) and (2) were determined by shaking mixtures in stoppered tubes in a constant temperature bath. The (1)-rich phases were analyzed for water by the use of Karl Fischer titrations. The (2)-rich phases were analyzed for acetate by a semimicro adaptation of the standard saponification technique whereby back titration of excess alkali is performed on a boiling solution to minimize carbonate error, and in a flask under a reflux condenser to minimize loss of acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Obtained by distillation under reduced pressure of commercially available material; fraction of unacetylated hydroxyl groups was less than 0.03.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±5 g(1)/100g sln and
±1 g(2)/100g sln (precision).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid butyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid butyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Bridgman (ref 1)	283-303	(2) in (1)	synthetic
Park and Hopkins (ref 2)	298	(1) in (2)	unspecified
Park and Hofmann (ref 3)	298	mutual	unspecified
Doolittle (ref 4)	293	mutual	unspecified
Othmer *et al.* (ref 5)	297	mutual	unspecified
Othmer *et al.* (ref 6)	323	mutual	synthetic
Donahue and Bartell (ref 7)	298	mutual	interferometric, Karl Fischer
Rao and Rao (ref 8)	303	mutual	titration
Bushmakin and Lutugina (ref 9)	364	mutual	analytical
Schuberth and Leibnitz (ref 10)	318	mutual	titration, analytical
Schuberth (ref 11)	318-342	mutual	titration, Karl Fischer
Rao and Rao (ref 12)	303	mutual	titration
Schuberth (ref 13)	293,318	mutual	titration, analytical
Rao *et al.* (ref 14)	308	mutual	titration
Narasimhan (ref 15)	303	mutual	titration, refractometric
Hirata and Hirose (ref 16)	303-364	mutual	titration
Ramanarao *et al.* (ref 17)	303	mutual	turbidometric
Blank and Popova (ref 18)	303	(2) in (1)	titration
Krupatkin and Glagoleva (ref 19)	298	mutual	titration
Pop *et al.* (ref 20)	293	mutual	titration
Bergovykh *et al.* (ref 21)	364	mutual	unspecified
Iguchi and Fuse (ref 22)	298	mutual	titration
Krupatkin and Shcherbakova (ref 23)	298	mutual	titration

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

Reference	*T*/K	Solubility	Method
Utkin *et al.* (ref 24)	298,313	mutual	titration
Andreeva *et al.* (ref 25)	363	mutual	titration
Skrzecz (ref 26)	291-362	mutual	synthetic, Karl Fischer
Tewari *et al.* (ref 27)	298	(1) in (2)	GLC
Cho *et al.* (ref 28)	364	mutual	titration
Ouyang *et al.* (ref 29)	323	mutual	GLC
Richon and Viallard (ref 30)	298	mutual	calorimetric, refractometric
Stephenson and Stuart (ref 31)	273-364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID BUTYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid butyl ester (1) in water (2) are summarized in Table 2 with the following exceptions.

The data of Park and Hofmann (ref 3), Iguchi and Fuse (ref 22), and Richon and Viallard (ref 30) at 298 K, and of Bergovykh *et al.* (ref 21), Hirata and Hirose (ref 16), and Andreeva *et al.* (ref 25) at *ca.* 364 K are all much higher than other values and are rejected. Similarly, the data of Doolittle (ref 4), Bushmakin and Lutugina (ref 9), Narasimhan *et al.* (ref 15) and Ouyang *et al.* (ref 29) are much lower than other studies and are also rejected. The data of Park and Hopkins (ref 2) and Tewari *et al.* (ref 27) reported in v/v and w/v units are also excluded from consideration and the various data of Rao and co-workers (ref 8,12) at 303 K and of Schuberth (ref 10,11,13) at 318 K are not regarded as independent determinations for the purpose of this Evaluation.

At lower temperatures the plethora of remaining data are in reasonable agreement although the σ_n values are too large for most of the averaged "Best" values to be Recommended. Outside the range 293-323 K most of the data are due to Skrzecz (ref 26) and to Stephenson and Stuart (ref 31). These two studies diverge somewhat at higher temperatures. Selected data are plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubilities of Acetic acid butyl ester (1) in Water (2)

T/K	Solubilities Reported values g(1)/100g sln	"Best" values ($\pm\sigma_n$)[a] g(1)/100g sln	 10^3x_1
273	0.96 (ref 31)	0.96	1.50
283	0.75* (ref 31)	0.75	1.17
293	0.7 (ref 13), 0.712 (ref 20), 0.64* (ref 26), 0.62* (ref 31)	0.67 ± 0.04	1.04
298	0.68[b] (ref 5), 0.638 (ref 7), 0.73 (ref 19), 0.76 (ref 23), 0.8 (ref 24), 0.61* (ref 26), 0.57* (ref 31)	0.68 ± 0.08	1.06
303	0.9 (ref 8,12), 0.70 (ref 16), 0.94 (ref 17), 0.58* (ref 26), 0.53* (ref 31)	0.73 ± 0.17	1.13
313	0.60 (ref 10,11,13), 0.6 (ref 24), 0.55* (ref 26), 0.50* (ref 31)	0.55 ± 0.04	0.85
323	0.69 (ref 6), 0.57[c] (ref 11), 0.54* (ref 26), 0.50* (ref 31)	0.58 ± 0.07	0.90
333	0.54[c] (ref 11), 0.55* (ref 26), 0.50* (ref 31)	0.53 ± 0.02 (*R*)	0.83
343	0.53[c] (ref 11), 0.58* (ref 26), 0.49* (ref 31)	0.53 ± 0.04	0.83
353	0.65* (ref 26), 0.48* (ref 31)	0.57 ± 0.09	0.89
363	0.73* (ref 26), 0.83[d] (ref 28), 0.47* (ref 31)	0.7 ± 0.2	1.1

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] 297 K.

[c] Calculated from the original author's fitting equation.

[d] 364.2 K.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

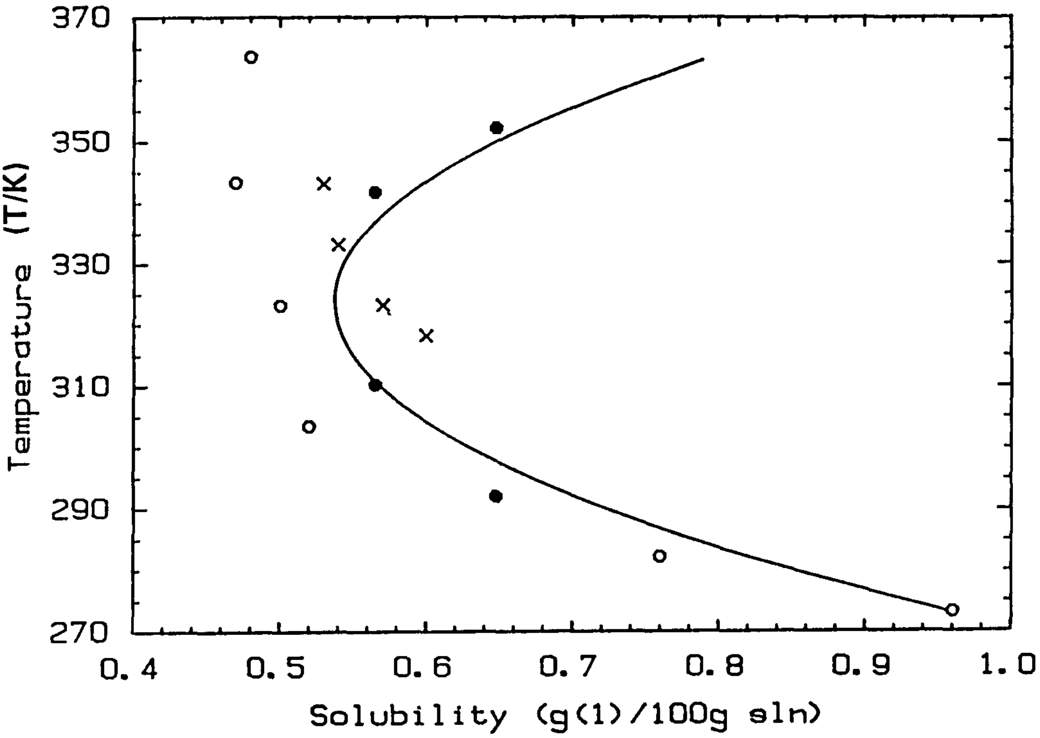

FIGURE 1. Selected data for the solubility of acetic acid butyl ester (1) in water (2): ref 10, 11, 13 (X); ref 26 (●); ref 31 (O). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID BUTYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid butyl ester (1) are summarized in Table 3 with the following exceptions.

The data of Park and Hofmann (ref 3), Doolittle (ref 4), Othmer *et al.* (ref 6), Hirata and Hirose (ref 16), Ramanarao *et al.* (ref 17), Krupatkin and Glagoleva (ref 19), at various temperatures (Table 1) are higher than other studies and are rejected. Similarly, the data of Pop *et al.* (ref 20) and Richon and Viallard (ref 30) are lower than all other studies and are also rejected.

As for the water-rich phase, the numerous independent studies at lower temperatures are in reasonable agreement, although none of the averaged "Best" values have been Recommended because of the high spread of the expeimental solubilities. At higher temperatures (T > 323 K) the data,

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

mainly due to Schuberth (ref 11), Skrzecz (ref 26), and Stephenson and Stuart (ref 31) are in poor agreement. Further studies are clearly warranted. Selected data are plotted in Figure 2.

TABLE 3: Tentative Solubilities of Water (2) in Acetic acid butyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values ($\pm\sigma_n$)[a]	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
273	0.78 (ref 31)	0.8	5
283	1.21^* (ref 1), 0.85^* (ref 31)	1.0 ± 0.2	6
293	1.36^* (ref 1), 1.2 (ref 13), 1.04^* (ref 26), 0.99^* (ref 31)	1.15 ± 0.15	7.0
298	1.46^* (ref 1), 1.2[b] (ref 5), 1.23 (ref 7), 1.07 (ref 22), 1.46 (ref 23), 1.3 (ref 24), 1.08^* (ref 26), 1.12^* (ref 31)	1.24 ± 0.15	7.5
303	1.56^* (ref 1), 1.1 (ref 8,12), 1.45 (ref 15), 1.13 (ref 16), 1.04 (ref 18), 1.13^* (ref 26), 1.24^* (ref 31)	1.24 ± 0.18	7.5
313	1.5 (ref 24), 1.28^* (ref 26), 1.35 (ref 31)	1.38 ± 0.09	8.3
318	1.69[c] (ref 10,11,13), 1.38^* (ref 26), 1.37^* (ref 31)	1.48 ± 0.15	8.8
323	1.82[d] (ref 11), 1.49^* (ref 26), 1.91 (ref 29), 1.37^* (ref 31)	1.65 ± 0.22	9.8
333	2.07[d] (ref 11), 1.76^* (ref 26), 1.38^* (ref 31)	1.7 ± 0.3	10
343	2.36[d] (ref 11), 2.08^* (ref 26), 1.37^* (ref 31)	1.9 ± 0.4	11
353	2.47^* (ref 26), 1.44^* (ref 31)	2.0 ± 0.5	12
363	2.60[e] (ref 9), 4.19[e](ref 21), 2.91 (ref 26), 3.55[e] (ref 28), 1.55^* (ref 31)	3.0 ± 0.9	17

---

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] 297 K.

[c] 317.6 K.

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COMPONENTS:	EVALUATOR:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

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[d] Obtained using the original author's fitting equation.

[e] 364.0 ± 0.2 K.

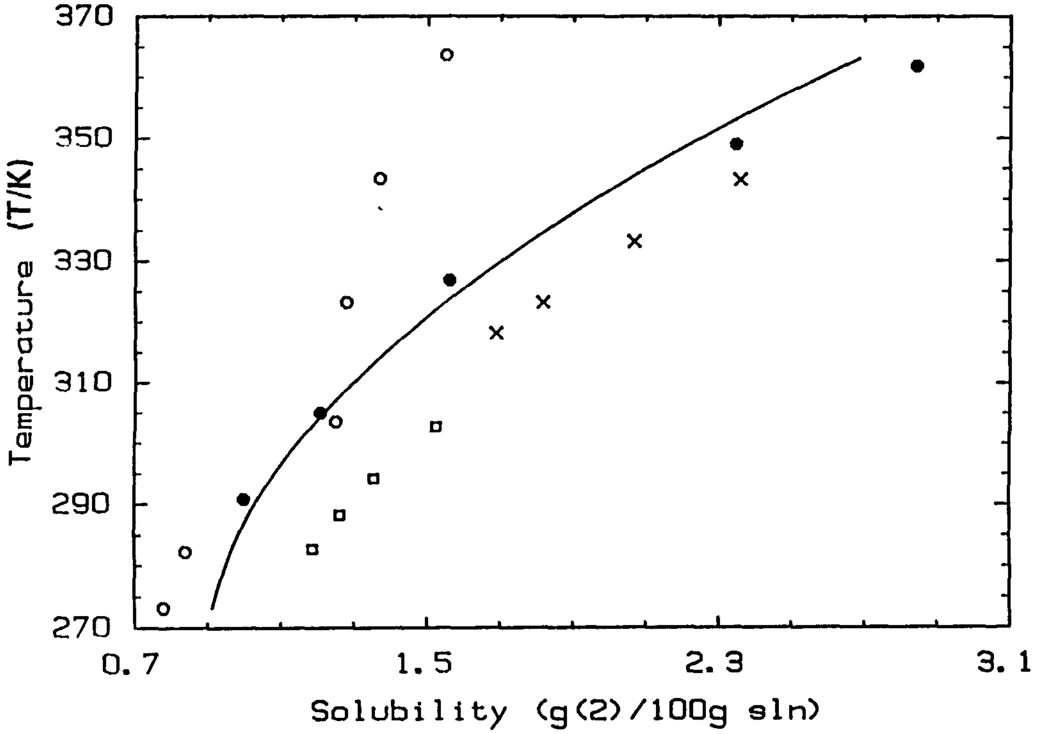

FIGURE 2. Selected data for the solubility of water (2) in acetic acid butyl ester (1): ref 1 (□); ref 10, 11, 13 (X); ref 26 (●); ref 31 (O). Solid line is a least square polynomial fitted to the "Best" values from Table 3.

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COMPONENTS:	EVALUATOR:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

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COMPONENTS:	EVALUATOR:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

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ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bridgman, J.A.

Ind. End. Chem. <u>1928</u>, *20*, 184-7.

VARIABLES:

T/K = 283 - 303

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in acetic acid butyl ester

t/°C	g(2)/100g(1)	g(2)/100g sln (compiler)	x_2 (compiler)
9.5	1.202	1.188	0.0719
15.0	1.279	1.263	0.0762
21.0	1.375	1.356	0.0814
29.5	1.549	1.525	0.0908

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method similar to that described by Groschuff (ref 1) was used. A glass tube of about 100 mL capacity with a stopcock was filled with weighed (1) and (2). By shaking the tube after it had been warmed somewhat, the water was dissolved completely in the ester, after which the tube was placed in a 2-liter beaker filled with water and equipped with an agitator. By alternate slow cooling and warming, it was possible to determine, within about 0.5°C, the temperature at which water was precipitated from the solution, as shown by the clouding of the liquid which would clear again when the temperature was slightly increased.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; b.p. range 124-126°C; boiled for some time in open flask before used.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.25°C (author).
Soly. about ±0.3 g(2)/100g sln (compiler).

REFERENCES:

1. Groschuff, E. *Z. Elektrochem.* <u>1911</u>, *17*, 348.

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Park, J.G.; Hopkins, M.B.

Ind. Eng. Chem. <u>1930</u>, *22*, 826-30.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 25°C was reported to be 0.7 mL(1)/100mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial samples; used as received.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester
(*butyl acetate*); $C_6H_{12}O_2$;
[123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Park, J.G.; Hofmann, H.E.

Ind. Eng. Chem. 1932, *24* 132-4.

VARIABLES:

T/K = 298

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 25°C was reported to be 2.3 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0036.

The solubility of water in acetic acid butyl ester at 25°C was reported to be 2.4 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.137.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Nothing was specified in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±1.7 g(1)/100g sln
and ±1.4 g(2)/100g sln
(compiler).

REFERENCES:

COMPONENTS: (1) Acetic acid butyl ester *(butyl acetate)*; $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Doolittle, A.K. *Ind. End. Chem.* <u>1935</u>, *27*, 1169-79.
VARIABLES: $T/K = 293$	PREPARED BY: A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 20°C was reported to be 0.43 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 6.7×10^{-4}.

The solubility of water in acetic acid butyl ester at 25°C was reported to be 1.86 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.109.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The method was not specified.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commercial product; purity 90%, b.p. range 119-127°C, d_4^{20} 0.876. (2) Not specified.
	ESTIMATED ERROR: Soly. about ±0.2 g(1)/100g sln and ±0.9 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Carbide and Carbon Chemicals Corporation, *Solvent Chart.* Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240-8, 1513.
VARIABLES:	PREPARED BY:
$T/K = 297$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 24°C was reported to be 0.68 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00106.

The solubility of water in acetic acid butyl ester at 24°C was reported to be 1.2 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.073.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing was specified in the paper.	(1) Not specified. (2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.06 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Othmer, D.F.; Bergen, W.S.; Shlechter, N.; Bruins, P.F. *Ind. Eng. Chem.* 1945, *37*, 890-4.
VARIABLES:	PREPARED BY:
$T/K = 323$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 50°C was reported to be 0.69 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00108.

The solubility of water in acetic acid butyl ester at 50°C was reported to be 3.19 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.1752.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not described. Presumably the indirect or synthetic method reported by Othmer, White and Trueger (ref 1) was used. The solution was kept at the desired temperature using a constant temperature water bath. The data and method were reported together with the ternary system acetic acid butyl ester-water-2,3-butanediol (*butyl acetate- water-2,3-butylene glycol*).

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; carefully fractionated from commercial material; b.p. range 1°C.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.15 g(1)/100g sln and ±1.7 g(2)/100g sln (compiler).

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Acetic acid butyl ester
(butyl acetate); $C_6H_{12}O_2$;
[123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Donahue, D.J.; Bartell, F.E.

J. Phys. Chem. 1952, *56*, 480-4.

VARIABLES:

T/K = 298

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 25°C was reported to be $x_1 = 0.000995$. The corresponding mass per cent value calculated by the compiler is 0.638 g(1)/100g sln.

The solubility of water in acetic acid butyl ester at 25°C was reported to be $x_2 = 0.0745$. The corresponding mass per cent value calculated by the compiler is 1.233 g(2)/100g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Samples of (1) with (2) were placed in glass stoppered flasks and were shaken intermittently for at least three days in a water bath held at 25°C.The (1)-rich phases were analyzed for (2) content by the Karl Fischer method and the (2)-rich phases were analyzed using interferometery.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; best reagent grade; purified by fractional distillation and treatment with silica gel; purity not specified.

(2) Purified.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±0.03 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rao, J.R.; Rao, C.V.

J. Appl. Chem. 1957, *7*, 435-9.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 30°C was reported to be 0.9 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0014.

The solubility of water in acetic acid butyl ester at 30°C was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.067.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system acetic acid butyl ester-water-methanol.

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House Ltd., reagent grade; b.p. 126.0°C, d^{30} 0.8710, n_D^{30} 1.3916.

(2) Distilled; free from CO_2.

ESTIMATED ERROR:

Temp. ±0.02°C (authors).
Soly. about ±0.3 g(1)/100g sln and ±0.05 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bushmakin, I.N.; Lutugina, N.V.

Vestn. Leningrad. Univ., Fiz., Khim. 1958, *(10)*, 75-83.

VARIABLES:

T/K = 364

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 91.04°C[a] was reported to be x_1 = 0.001. The corresponding mass per cent value calculated by the compiler is 0.6 g(1)/100g sln.

The solubility of water in acetic acid butyl ester at 91.04°C[a] was reported to be x_2 = 0.147. The corresponding mass per cent value calculated by the compiler is 2.60 g(2)/100g sln.

[a] Boiling temperature of the two-phase mixture at 760 mm Hg.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The two-phase mixture was boiled 2h. under reflux. Next, the heating was decreased and the temperature allowed to drop a few degrees so that the phases could be separated and analyzed. Butyl acetate was determined by saponification with an excess of 0.1N NaOH and titration of the unreacted mixture with HCl. The data were reported together with the ternary system acetic acid butyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Synthesized; several times distilled; b.p. 125.2°C, n_D^{20} 1.3942.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C, pressure ±0.1 mm Hg (authors).

Soly. about ±0.2 g(1)/100g sln and ±0.4 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Schuberth, H.; Leibnitz, E. *J. Prakt. Chem.* 1958, *6*, 31-45.
VARIABLES:	PREPARED BY:
T/K = 318	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 44.4°C was reported to be 0.60 g(1)/100g sln with a corresponding mole fraction, x_1, value of 0.0009.

The solubility of water in acetic acid butyl ester at 44.4°C was reported to be 1.7 g(2)/100g sln with a corresponding mole fraction, x_2, value of 0.100.
The measurments were made at 760 mm Hg.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the analytical and titration methods were used. In the analytical method, contained samples of 15 mL were stirred in a thermostat to establish equilibrium, separated for few hours, and then the refractive index and density of both homogeneous phases were measured. For the titration procedure, the method and apparatus similar to that described by Roethlin, Cruetzen and Schultze (ref 1) were used. The experiments were repeated several times and the mean values were reported. Only the ternary measurements were described.

SOURCE AND PURITY OF MATERIALS:

(1) Buna-Werke Merseburg, technical grade; dried over $CuSO_4$, twice distilled; without impurities by IR spectroscopy method, 0.03% water by the K. Fischer method, b.p. 126.1°C, d^{20} 0.882, n_D^{20} 1.3941.

(2) Twice distilled; $n_D^{44.4}$ 1.3300, $d_4^{44.4}$ 0.9904.

ESTIMATED ERROR:

Temp. ±0.05°C.
Soly. ±0.0001 mole fraction.

REFERENCES:

1. Roethlin, S.; Cruetzen, J.L.; Schultze, G.R. *Chem. Ing. Techn.* 1957, *29*, 211.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Schuberth, H. *J. Prakt. Chem.* 1958, *6*, 266-88.
VARIABLES:	PREPARED BY:
$T/K = 318$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 317.6 K was reported to be $x_1 = 0.0009$. The corresponding mass per cent value calculated by the compiler is 0.6 g(1)/100g sln.

The solubility of water in acetic acid butyl ester at 317.6 K was reported to be $x_2 = 0.0999$. The corresponding mass per cent value calculated by the compiler is 1.692 g(2)/100g sln.

Saturation lines in the range 317.6-341.7 K were described by equations:

$x_2 = 5.21\times10^{-6}\ (T/K)^2 - 2.077\times10^{-3}\ (T/K) + 0.2340$ (1)-rich phase

$x_2 = -8.6\times10^{-8}\ (T/K)^2 + 6.06\times10^{-5}\ (T/K) + 0.98851$ (2)-rich phase

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used, as described by Schuberth and Leibnitz (ref 1). Water was analyzed by the Karl Fischer titration method and butyl acetate by saponification and titration up to neutralization.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, technical grade; dried, twice distilled; b.p. 126.1°C, d^{20} 0.8815, n_D^{20} 1.3941, IR in agreement with literature.

(2) Twice distilled.

ESTIMATED ERROR:

Soly. about ±0.05 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).

REFERENCES:

1. Schuberth, H.; Leibnitz, E. *J. Prakt. Chem.* 1958, *6*, 31.

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rao, R.J.; Rao, C.V.

J. Appl. Chem. 1959, *9*, 69-73.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 30°C was reported to be 0.9 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0014.

The solubility of water in acetic acid butyl ester at 30°C was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.067.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration method described by Rao and Rao (ref 1) was used. The data were reported together with the ternary system acetic acid butyl ester-water-1-propanol.

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House Ltd., analytical grade; b.p. 126.0°C, d^{30} 0.8710, n_D^{30} 1.3916.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.3 g(1)/100g sln and ±0.05 g(2)/100g sln (compiler).

REFERENCES:

1. Rao, R.J.; Rao, C.V. *J. Appl. Chem.* 1957, *7*, 435.

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schuberth, H.

Abh. Deut. Akad. Wiss. Berlin, Kl. Chem. Geol. Biol. 1960, *3*, 1-82.

VARIABLES:

$T/K = 293$ and 318

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid butyl ester and water

$t/^\circ C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20.0	0.7	98.8	0.0011	0.927
44.4	0.59	98.3	0.00092	0.900

Author's smoothed equations for mutual solubilities presented graphically at 308-341 K:

$x_1 = 0.086\text{x}10^{-6}\ (T/K)^2 - 0.606\text{x}10^{-4}\ (T/K) + 1.149\text{x}10^{-2}$ (2)-rich phase

$x_1 = -5.21\text{x}10^{-6}\ (T/K)^2 + 20.77\text{x}10^{-4}\ (T/K) + 76.60\text{x}10^{-2}$ (1)-rich phase

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration and analytical methods were used. The data and method were reported with the ternary system acetic acid butyl ester-water-acetic acid propyl ester (*butyl acetate-water-propyl acetate*).

SOURCE AND PURITY OF MATERIALS:

(1) Buna-Werke Merseburg, technical product; washed with H_2O, dried over $CuSO_4$, twice distilled; b.p. 126.2°C, d^{20} 0.8818, n_D^{20} 1.3941.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.01°C.
Soly. ±0.05 g(1)/100g sln.

REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester
(butyl acetate); $C_6H_{12}O_2$;
[123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rao, M.V.R.; Rao, K.S.; Rao, C.V.

J. Sci. Ind. Res. 1961, *20B*,
379-81.

VARIABLES:

T/K = 308

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 35°C was reported to be 0.9 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0014.

The solubility of water in acetic acid butyl ester at 35°C was reported to be 2.0 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.116.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system acetic acid butyl ester- water-formic acid. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, technical grade; distilled; b.p. 126.5°C.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.3 g(1)/100g sln and
±0.9 g(2)/100g sln
(compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester *(butyl acetate)*; $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Narasimhan, K.S.; Reddy, C.C.; Chari, K.S. *J. Chem. Eng. Data* <u>1962</u>, *7*, 340-3.
VARIABLES:	PREPARED BY:
T/K = 303	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 30°C was reported to be 0.29 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 4.5×10^{-4}.

The solubility of water in acetic acid butyl ester at 30°C was reported to be 1.45 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0866.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration and the analytical methods were used as reported for the ternary system butyl acetate-water-phenol. In the titration procedure, a known weight of mixture was taken in 100mL stoppered conical flask and kept in a thermostat for 1/2 h. which was found to be sufficient for equilibrium. Then, the selected component was added dropwise until a permanent turbidity appeared in the solution. In the analytical method, the mixture was stirred for 1 h. in a thermostated equilibrium apparatus. After separation the refractive indexes of both layers were measured and the corresponding compositions were obtained graphically from a previously drawn plot relating the refractive index and composition.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; commercial grade; twice-distilled; purity 98.25-98.56%, b.p. range 124-126°C, d_{20}^{30} 0.8714, n_D^{25} 1.3890.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. ±0.03 g(1)/100g sln.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester *(butyl acetate)*; $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Hirata, M.; Hirose, Y. *Kagaku Kogaku* <u>1963</u>, *27(6)*, 407-14.
VARIABLES:	PREPARED BY:
T/K = 303 - 364	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid butyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
30.0	0.70[b]	98.87[c]	0.00109	0.9314
90.7[a]	-	92.91[e]	-	0.6702
91.0[a]	1.61[d]	-	0.00253	-
91.3[a]	-	93.2[e]	-	0.6801

[a] Boiling temperature at atmospheric pressure (the value of the pressure was not specified).

The relative densities of the water-rich phase and the ester-rich phase were reported to be d_4^{30} 0.9954 and d_4^{30} 0.8715 respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method as proposed by Othmer (ref 1) was used at 30°C. The mixture was thermostated for 3-4 h. and shaken each 15 min. The temperature titration method was used at the boiling point. The second component was added in portions to the mixture placed in a four-necked flask and the temperature of the boiling liquid was measured as proposed by Ogawa (ref 2). The boiling temperatures were about 0.8°C higher than the literature values because of superheating. The method and data were reported together with the ternary system acetic acid butyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial grade; used as received; d_4^{25} 0.8750, n_D^{25} 1.3920.

(2) Not specified; d_4^{25} 0.9971, n_D^{25} 1.3325.

ESTIMATED ERROR:

Soly. about ±0.1[b], ±0.05[c], ±0.8[d] and ±4.[e] g(1)/100g sln (compiler).

REFERENCES:

1. Othmer, D.F. *et al.* *Ind. Eng. Chem.* <u>1941</u>, *33*, 1240.

2. Ogawa, S. *Kagaku Kikai Gijyutsu* <u>1954</u>, *(6)*, 22.

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Ramanarao, M.V.; Husain, A.; Chari, K.S.

Indian J. Technol. 1964, *2*, 252-4.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 30°C was reported to be 0.9368 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0014645.

The solubility of water in acetic acid butyl ester at 30°C was reported to be 1.8110 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.10629.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The turbidity end point method described by Narasimhan, Reddy and Chari (ref 1) was used. Only the method for the ternary system was described. A known weight of mixture was placed into a 100 mL stoppered conical flask and kept in a thermostat for 1/2 h. which was found to be sufficient for equilibrium. Then, the selected component was added dropwise until a permanent turbidity appeared in the solution.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; twice distilled; b.p. 126.0°C.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±0.3g(1)/100g sln.
and ±0.7g(2)/100g sln.
(compiler).

REFERENCES:

1. Narasimhan, K.S.; Reddy, C.C.; Chari, K.S. *J. Chem. Eng. Data* 1962, *7*, 340.

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Blank, M.G.; Popova, T.V.

Ukr. Khim. Zh. 1970, *36*, 563-6.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of water in acetic acid butyl ester at 30°C was reported to be x_2 = 0.0637. The corresponding mass per cent value calculated by the compiler is 1.044 g(2)/100g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The titrations were made from burettes protected from moisture. The volume proportions of (1) and (2) were measured. The same amounts of components were weighed separately and the composition of the solution was calculated. Experiments were repeated several times. The data were reported together with the ternary system acetic acid butyl ester-water-ethanol. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; washed with NaCl and Na_2CO_3 solutions, dried with $MgSO_4$, fractionated; b.p. 126.1°C, d_4^{20} 0.8815, n_D^{20} 1.3941.

(2) Distilled three times (second distillation with $KMnO_4$ and KOH).

ESTIMATED ERROR:

Soly. <±0.1 g(2)/100g sln.

REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Krupatkin, I.L.; Glagoleva, M.F.

Zh. Obshch. Khim. 1970, *40*, 17-21.

VARIABLES:

$T/K = 298$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 25°C was reported to be 0.73 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00114.

The solubility of water in acetic acid butyl ester at 25°C was reported to be 1.92 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.112.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system acetic acid butyl ester-water-2-furancarbonal (*butyl acetate- water-furfural*). No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, analytical reagent; b.p. 125°C, d_4^{15} 0.8800.

(2) Twice distilled.

ESTIMATED ERROR:

Soly. about ±0.1 g(1)/100g sln and ±0.9 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Pop. A.; Weiss, G.; Cormos, L. *Stud. Univ. Babes-Bolyai, Ser. Chem.* 1970, *15(2)*, 77-82.
VARIABLES:	**PREPARED BY:**
T/K = 293	Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 20°C was reported to be 0.712 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00111.

The solubility of water in acetic acid butyl ester at 20°C was reported to be 0.750 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0465.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data were reported together with the ternary system acetic acid butyl ester-water-2-hydroxybenzoic acid (*butyl acetate-water-salicylic acid*). No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; 99% purity.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.07 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Beregovykh, V.V.; Timofeev, V.S.; Luk'yanova, R.N.; Yakushchev, V. M.; Serafimov, L.A.

Uch. Zap., Mosk. Inst. Tonkoi Khim. Tekhnol. 1971, *1(3)*, 31-8.

VARIABLES:

$T/K = 364$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 91.04°C[a] was reported to be $x_1 = 0.017$. The corresponding mass per cent value calculated by the compiler is 10.0 g(1)/100g sln.

The solubility of water in acetic acid butyl ester at 91.04°C[a] was reported to be $x_2 = 0.220$. The corresponding mass per cent value calculated by the compiler is 4.19 g(2)/100g sln.

[a] Boiling temperature of the two-phase mixture at 760 mm Hg.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±9.2 g(1)/100g sln and ±1.2 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Iguchi, A.; Fuse, K. *Kagaku Kogaku* 1971, *35(9)*, 1035-7.
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 25°C was reported to be 0.96 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00150.

The solubility of water in acetic acid butyl ester at 25°C was reported to be 1.07 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0652.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The samples were titrated with the second component to obtain turbidity. The method and data were reported together with the ternary system acetic acid butyl ester-water-acetic acid. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial grade of high purity, used as received.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. about ±0.3 g(1)/100g sln and ±0.05 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Krupatkin, I.L.; Shcherbakova, T.A. *Zh. Prikl. Khim.* 1971, *44*, 307-11.
VARIABLES:	PREPARED BY:
$T/K = 298$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 25°C was reported to be 0.76 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00119.

The solubility of water in acetic acid butyl ester at 25°C was reported to be 1.46 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0872.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The amount of water in pure ester was taken into account. The data were reported together with the ternary system acetic acid butyl ester-water-phosphoric acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, analytical grade; b.p. range 125-126°C, d_4^{15} 0.880-0.890.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.1°C (authors).
Soly. about ±0.15 g(1)/100g sln and ±0.4 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Utkin, G.K.; Zamyatina, V.K.; Andronnikov, N.V.; Golikov, L.V. *Gidroliz. Lesokhim. Prom.* 1971, *24(8)*, 9-10.
VARIABLES:	**PREPARED BY:**
T/K = 298 and 313	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid butyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
25	0.8^a	98.7^c	0.0012	0.922
40	0.6^b	98.5^c	0.0009	0.911

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. A one-phase mixture was titrated and mixed in a thermostated apparatus with a reflux condenser for 1 h. until an opalescence appeared. Only the measurements for the ternary systems were described. The data were reported together with the ternary system acetic acid butyl ester-water-propanoic acid (*butyl acetate-water-propionic acid*).

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, pure for analysis; distilled, fraction boiling at 125-126°C was used; purity 99.3-99.5%, dry residue 0.001%, without ashes, d^{20} 0.875.

(2) Distilled; without CO_2.

ESTIMATED ERROR:

Soly. about $\pm0.2^a$, $\pm0.05^b$ and $\pm0.3^c$ g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Andreeva, N.G.; Komarova, L.F.; Garber, Yu.N.

Zh. Prikl. Khim. 1978, *51*, 2031-6.

VARIABLES:

$T/K = 363$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at its boiling temperature at atmospheric pressure (90.2°C)[a] was reported to be $x_1 = 0.017$. The corresponding mass per cent value calculated by the compiler is 10.0 g(1)/100g sln.

The solubility of water in acetic acid butyl ester at its boiling temperature at atmospheric pressure (90.2°C)[a] was reported to be $x_2 = 0.022$. The corresponding mass per cent value calculated by the compiler is 0.35 g(2)/100g sln.

[a] Numerical value of the boiling temperature at atmospheric pressure was not reported in the paper. The value 90.2°C was adopted from Horsley (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method of Mozzhukhin, Tyurikov and Mitropolskaya (ref 2) was used. The data were reported together with the ternary system acetic acid butyl ester-water-acetic acid 3-methyl-1-butanol (*butyl acetate-water-isopentyl acetate*). No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±9 g(1)/100g sln and ±2.7 g(2)/100g sln (compiler).

REFERENCES:

1. Horsley, L.E. *Azeotrpic Data III*, Advances in Chemistry Series 116, American Chemical Society, Washington, 1973.
2. Mozzhukhin, A.S.; Tyurikov, I.D.; Mitropolskaya, V.A. in *Fiz. Khim. Osn. Rektifikatsii*, Moskva, 1970.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Skrzecz, A. *Pol. J. Chem.* 1980, *54*, 1101-4. Skrzecz, A. *Thesis*, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.
VARIABLES:	PREPARED BY:
T/K = 291 - 362	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid butyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
290.8	-	0.9388[a]	-	98.999
292.1	0.00101	-	0.648	-
305.0	-	0.9269	-	98.792
310.3	0.00088	-	0.565	-
326.9	-	0.9072	-	98.438
337.1	-	0.8922	-	98.161
341.8	0.00088	-	0.565	-
349.0	-	0.8658	-	97.652
352.2	0.00101	-	0.648	-
361.9	-	0.8412	-	97.156

[a] By the Karl Fischer method.

Author's smoothing equations:

$$x_1 = 1.3088\text{x}10^{-3} - 1.90\text{x}10^{-5}\ (T/K - 273.15) + 1.90\text{x}10^{-7}\ (T/K - 273.15)^2$$

st. dev. = 3.01×10^{-5} (2)-rich phase

$$x_2 = 0.059761 - 1.010\text{x}10^{-4}\ (T/K - 273.15) + 1.378\text{x}10^{-5}\ (T/K - 273.15)^2$$

st. dev. = 2.70×10^{-3} (1)-rich phase

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The synthetic method of Alexejew and the analytical method were used. An ampoule with the solution of fixed concentration was placed into a glass tube connected with a thermostat filled completely with distilled water. The temperature of the bath was changed continuously during the measurements and the appearance and disappearance of turbidity within the ampoule was observed visually. For the analytical method, The amount of water in the saturated organic-phase was determined using a Karl Fischer titration procedure. The amount of water in the pure ester was taken into account.	(1) POCH Gliwice, pure grade; distilled; purity 99.99% by glc, 0.19 wt% water by the Karl Fischer method. (2) Distilled.
	ESTIMATED ERROR: Temp. ±(0.2-0.6)°C. Soly. see above.
	REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tewari, Y.B.; Miller, M.M.; Wasik, S.P.; Martire, D.E.

J. Chem. Eng. Data 1982, *27*, 451-4.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 25°C was reported to be 0.0577 mol(1)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 6.70 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of a water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible-with-water solution and then analyzed by a gas chromatographic technique.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purity >99% by glc.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C.
Soly. ±1.0%.

REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Cho, T.-H.; Ochi, K.; Kojima, K.

Fluid Phase Equilib. 1983, *11*, 137-52.

VARIABLES:

T/K = 364

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid butyl ester in water at 363.89 K[a] was reported to be x_1 = 0.0013. The corresponding mass per cent value calculated by the compiler is 0.83 g(1)/100g sln.

The solubility of water in acetic acid butyl ester at 363.89 K[a] was reported to be x_2 = 0.1918. The corresponding mass per cent value calculated by the compiler is 3.550 g(2)/100g sln.

[a] Boiling temperature at 101.32 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The liquid-liquid equilibrium at the boiling point was determined directly in a modified ebulliometer with a boiling flask of about 600 mL charge. The bubble-point of the homogenous solution was measured and the second component was added until a cloudiness appeared.

SOURCE AND PURITY OF MATERIALS:

(1) Wako Pure Chem. Ind. Ltd., special grade; used as received; 99.99 wt% by glc, b.p. 126.11°C.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.01°C.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid butyl ester *(butyl acetate)*; $C_6H_{12}O_2$; [123-86-4] (2) Water; H_2O; [7732-18-5]	Ouyang, F.; Wang, G.; Gao, W. *Hua Kung Hsueh Pao* 1985, *(1)*, 110-18.
VARIABLES:	PREPARED BY:
$T/K = 323$	J. Fu

EXPERIMENTAL VALUES:

The proportion of acetic acid butyl ester in the water-rich phase at equilibrium at 50°C was reported to be 0.15 g(1)/100 g sln. The corresponding mole fraction solubility, x_1, is 0.0002.

The proportion of water in the acetic acid butyl ester-rich phase at equilibrium at 50°C was reported to be 1.91 g(2)/100g sln. The corresponding mole fraction solubility, x_2, is 0.1115.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An analytical method was used. Sample mixtures in an equilibrium cell immersed in a constant temperature water bath were stirred with a magnetic agitator to be emulsified. Then, the mixture was settled for 4 h. and samples withdrawn from the upper and lower layers were analyzed by gas chromatograph.	(1) Analytical pure reagent. (2) Twice distilled; b.p. 100.00°C.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid butyl ester and water

T/K	mol(1)/100g(2)	x_1 (2)-rich ph.	x_1 (1)-rich ph.	g(1)/100g sln (compiler) (2)-rich ph.	g(1)/100g sln (compiler) (1)-rich ph.
298.1[a]	-	9.95×10^{-4}	0.928	0.638[d]	98.81[e]
298.1[b]	0.00570	10.26×10^{-4} [c]	-	0.658[d]	-

[a] Calorimetric method.

[b] Refractometric method.

[c] Compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The calorimetric and differential refractometric methods were used. The calorimetric method was described by Richon (ref 1) and by Richon and Villard (ref 2). For the refractometric measurements, a Phoenix model 1-2000T differential refractometer from Texas Instruments was used, and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) Fluka (puriss); purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.05[d] and ±0.15[e] g(1)/100g sln (compiler).

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.
2. Richon, D.; Villard, A. *Can. J. Chem.* 1976, *54*, 2584.

COMPONENTS:

(1) Acetic acid butyl ester (*butyl acetate*); $C_6H_{12}O_2$; [123-86-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 364

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid butyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	0.96	99.22	0.00150	0.9518
9.1	0.76	99.16	0.00119	0.9482
19.7	0.64	99.02	0.00100	0.9400
30.3	0.52	98.75	0.00081	0.9245
39.6	0.50	98.65	0.00078	0.9189
50.0	0.50	98.72	0.00078	0.9228
60.2	0.50	98.62	0.00078	0.9172
70.2	0.47	98.63	0.00073	0.9178
80.1	0.48	98.56	0.00075	0.9139
90.5	0.48	98.45	0.00075	0.9078
std. dev.	0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid 1,1-dimethyl ethyl ester (*tert-butyl acetate*); $C_6H_{12}O_2$; [540-88-5]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 361

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 1,1-dimethyl ethyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.170	99.17	0.001832	0.9488
9.2	1.000	99.03	0.001564	0.9406
19.2	0.803	98.87	0.001253	0.9313
29.6	0.703	98.70	0.001096	0.9217
40.0	0.620	98.68	0.000966	0.9206
50.0	0.573	98.65	0.000893	0.9189
60.5	0.526	98.53	0.000819	0.9122
70.5	0.538	98.29	0.000838	0.8991
80.5	0.499	98.31	0.000777	0.9002
88.0	-	98.34	-	0.9018
std. dev.	0.004	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid 1-methylpropyl ester (*sec-butyl acetate*); $C_6H_{12}O_2$; [105-46-4]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 1-methylpropyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid 1-methylpropyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Park and Hopkins (ref 1)	298	(1) in (2)	unspecified
Doolittle (ref 2)	293	mutual	unspecified
Stephenson and Stuart (ref 3)	273-364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID 1-METHYLPROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid 1-methylpropyl ester (1) in water (2) are summarized in Table 2 with the exception of the approximate value of Park and Hopkins (ref 1) which is reported in v/v units and is therefore excluded from consideration. At 293 K, the only temperature where comparison is possible, the datum of Doolittle (ref 2) is only in fair agreement with the interpolated value of Stephenson and Stuart (ref 3). Consequently, in the absence of confirmatory studies, all the available data must be regarded as Tentative. For uniformity, the rounded data of Stephenson and Stuart (ref 3) have been chosen as the "Best" values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 1-methylpropyl ester (*sec-butyl acetate*); $C_6H_{12}O_2$; [105-46-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Solubilities of Acetic acid 1-methylpropyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values [a]	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
273	1.33 (ref 3)	1.3	2.1
283	0.88* (ref 3)	0.9	1.4
293	0.62 (ref 2), 0.86* (ref 3)	0.9	1.4
298	0.82* (ref 3)	0.8	1.1
303	0.77* (ref 3)	0.8	1.1
313	0.66* (ref 3)	0.7	1.0
323	0.63 (ref 3)	0.6	1.0
333	0.61* (ref 3)	0.6	0.9
343	0.61* (ref 3)	0.6	0.9
353	0.61* (ref 3)	0.6	0.9
363	0.60* (ref 3)	0.6	0.9

[a] Rounded values of ref 3, see text.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID 1-METHYLPROPYL ESTER (1)

As for the solubility of (1) in (2), the only data available for comparison of the solubilities of water (2) in acetic acid 1-methylpropyl ester (1) are those of Doolittle (ref 2) and Stephenson and Stuart (ref 3) at 293 K. However, unlike the H_2O-rich phase the datum of 1.65 g(2)/100 g sln reported by Doolittle is considerably higher than the value of 1.10 g(2)/100 g sln interpolated from the data of Stephenson and Stuart. In the absence of confirmatory studies it is not possible to choose between these data although it may be noted that the solubilities of Doolittle (ref 2) are often higher than reliable values for other systems. The interested user is referred to the Data Sheet for Stephenson and Stuart (ref 3) for what appear to be the most reliable experimental values available for the solubility of water in acetic acid 1-methylpropyl ester.

REFERENCES

1. Park, J. G.; Hopkins, M. B. *Ind. Eng. Chem.* 1930, *22*, 826-30.
2. Doolittle, A. K. *Ind. Eng. Chem.* 1935, *27*, 1169-79.
3. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 1-methylpropyl ester (*sec-butyl acetate*); $C_6H_{12}O_2$; [105-46-4] (2) Water; H_2O; [7732-18-5]	Park, J.G.; Hopkins, M.B. *Ind. Eng. Chem.* 1930, *22*, 826-30.
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 1-methylpropyl ester in water at 25°C was reported to be 1.0 mL(1)/100mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commercial samples; used as received; 85-88% of ester, b.p. range 107-114°C. (2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 1-methylpropyl ester *(sec-butyl acetate)*; $C_6H_{12}O_2$; [105-46-4] (2) Water; H_2O; [7732-18-5]	Doolittle, A.K. *Ind. End. Chem.* 1935, *27*, 1169-79.
VARIABLES:	**PREPARED BY:**
T/K = 293	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 1-methylpropyl ester in water at 20°C was reported to be 0.62 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 9.7×10^{-4}.

The solubility of water in acetic acid 1-methylpropyl ester at 20°C was reported to be 1.65 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0976.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; purity 82%, b.p. range 105-127°C, d_4^{20} 0.858.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 1-methylpropyl ester (*sec-butyl acetate*); $C_6H_{12}O_2$; [105-46-4] (2) Water; H_2O; [7732-18-5]	Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 364	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 1-methylpropyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.330	99.17	0.002086	0.9488
9.6	0.879	99.05	0.001373	0.9417
19.5	0.869	98.94	0.001357	0.9353
29.7	0.753	98.70	0.001175	0.9217
39.9	0.663	98.64	0.001034	0.9183
50.0	0.629	98.54	0.000981	0.9128
60.1	0.613	98.40	0.000955	0.9051
70.5	0.605	98.38	0.000943	0.9040
80.2	0.622	98.16	0.000969	0.8921
90.5	0.604	98.31	0.000941	0.9002
std. dev.	0.005	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 2-methylpropyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid 2-methylpropyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Hemptinne (ref 2)	298	(1) in (2)	analytical
Fuehner (ref 3)	293	(1) in (2)	titration
Doolittle (ref 4)	293	mutual	unspecified
Frolov *et al.* (ref 5)	293	mutual	titration
Linek (ref 6)	288-420	mutual	synthetic
Heyberger *et al.* (ref 7)	298,323	mutual	titration
Bomshtein *et al.* (ref 8)	293-353	mutual	analytical
Skrzecz (ref 9)	291-360	mutual	synthetic, Karl Fischer
Richon and Viallard (ref 10)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 11)	273-363	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID 2-METHYLPROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid 2-methylpropyl ester (1) in water (2) are summarized in Table 2, with the following exceptions.

The datum of Heyberger *et al.* (ref 7) at 298K is lower than other studies and is rejected. The data of Bomshtein *et al.* (ref 8) over a wide temperature range are higher than other studies (ref 6,9,11) especially at lower temperatures ($T < 343$K) and show a quite different temperature dependence so are rejected. The data of Stephenson and Stuart (ref 11) at higher temperatures are rather scattered and appear lower than the other

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

studies (ref 6,9) but have been retained pending further independent investigations. The approximate value of Traube (ref 1) has, however, been excluded from consideration in view of the ready availability of more recent and precise data. Selected data are plotted in Figure 1.

TABLE 2: Tentative Solubilities of Acetic acid 2-methylpropyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
273	1.026 (ref 11)	1.03	1.61
283	0.827 (ref 11)	0.83	1.29
293	0.67 (ref 3), 0.67 (ref 4), 0.80 (ref 5), 0.765* (ref 6), 0.706* (ref 9), 0.67* (ref 11)	0.71 ± 0.05	1.11
298	0.63 (ref 2). 0.740* (ref 6), 0.668* (ref 9), 0.693 (ref 10), 0.63* (ref 11)	0.67 ± 0.04	1.04
303	0.710* (ref 6), 0.635* (ref 9) 0.60* (ref 11)	0.65 ± 0.05	1.01
313	0.695* (ref 6), 0.587* (ref 9), 0.53* (ref 11)	0.60 ± 0.07	0.94
323	0.670 (ref 7), 0.695* (ref 6), 0.567* (ref 9), 0.51* (ref 11)	0.61 ± 0.08	0.95
333	0.702* (ref 6), 0.58* (ref 9), 0.51* (ref 11)	0.60 ± 0.08	0.94
343	0.730* (ref 6), 0.628* (ref 9), 0.53* (ref 11)	0.63 ± 0.08	0.98
353	0.780* (ref 6), 0.718* (ref 9), 0.55* (ref 11)	0.68 ± 0.10	1.06
363	0.830* (ref 6), 0.851* (ref 9)	0.84 ± 0.01[b]	1.31
373	0.890* (ref 6)	0.89	1.39
393	1.030* (ref 6)	1.03	1.61
413	1.160* (ref 6)	1.16	1.82

[a] Obtained by averaging where appropriate.

[b] Tentative, see text.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

In Table 2, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

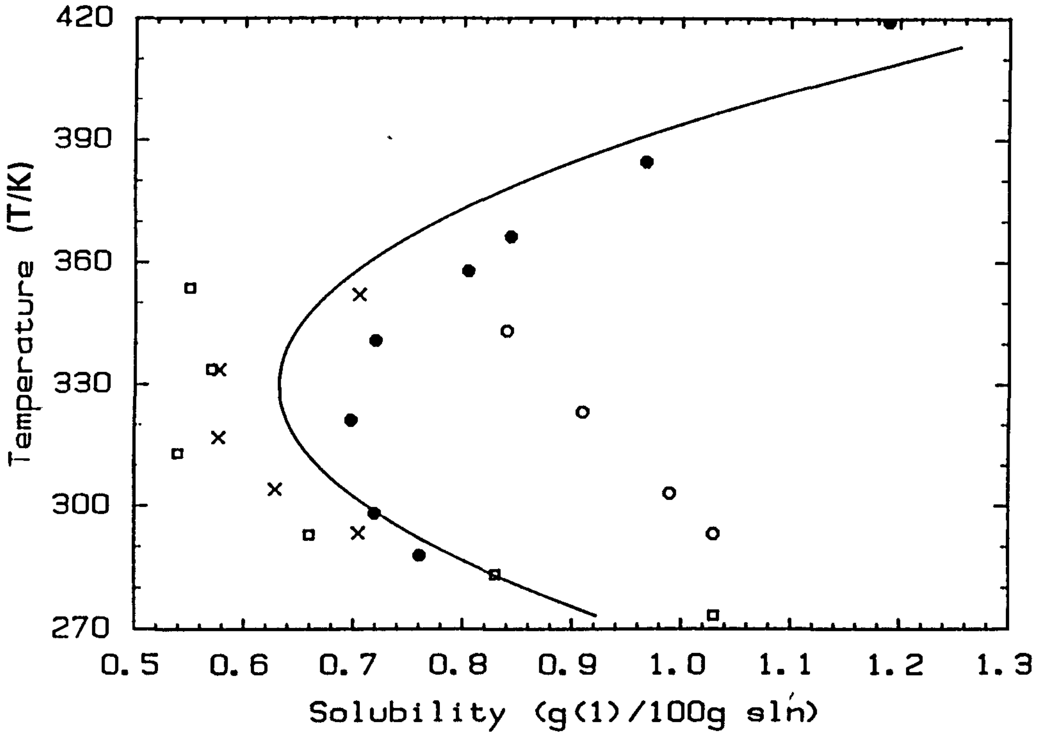

FIGURE 1. Selected data for the solubility of acetic acid 2-methylpropyl ester (1) in water (2): ref 6 (●); ref 8, rejected data, (O); ref 9 (X); ref 11 (□). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID 2-METHYLPROPYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid 2-methylpropyl ester (1) are summarized in Table 3 with the following exceptions. The data of Doolittle (ref 4), Frolov *et al.* (ref 5) and Heyberger *et al.* (ref 6) at various temperatures are substantially higher than other studies and are rejected. The data of Bomshtein *et al.* (ref 8), as for the water-rich phase, are higher than other studies (ref 6,9,11) and are also rejected. The data of Stephenson and Stuart (ref 11) are somewhat lower than other studies (ref 6,9) at higher temperatures ($T >$ 323K) but, pending further independent investigations, have been retained.

Selected data are plotted in Figure 2.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 3: Recommended (*R*) and Tentative Solubilities of Water (2) in Acetic acid 2-methylpropyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
273	0.72 (ref 11)	0.72	4.5
283	0.82 (ref 11)	0.82	5.1
293	1.03^* (ref 9), 0.95^* (ref 11)	0.99 ± 0.04 (*R*)	6.1
298	1.14^* (ref 9), 1.05^* (ref 11)	1.10 ± 0.05 (*R*)	6.7
303	1.25^* (ref 9), 1.12^* (ref 11)	1.18 ± 0.07	7.2
313	1.33^* (ref 6), 1.44^* (ref 9), 1.21^* (ref 11)	1.33 ± 0.09	8.0
323	1.47^* (ref 6), 1.64^* (ref 9), 1.26^* (ref 11)	1.5 ± 0.2	9.0
333	1.70^* (ref 6), 1.87^* (ref 9), 1.32^* (ref 11)	1.6 ± 0.2	9.5
343	2.05^* (ref 6), 2.16^* (ref 9), 1.37^* (ref 11)	1.9 ± 0.3	11
353	2.42^* (ref 6), 2.55^* (ref 9), 1.42^* (ref 11)	2.1 ± 0.5	12
363	2.90^* (ref 6), 1.47^* (ref 11)	2.2 ± 0.7	13
373	3.42^* (ref 6)	3.4	19
393	4.47^* (ref 6)	4.5	23
413	5.62^* (ref 2)	5.6	28

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

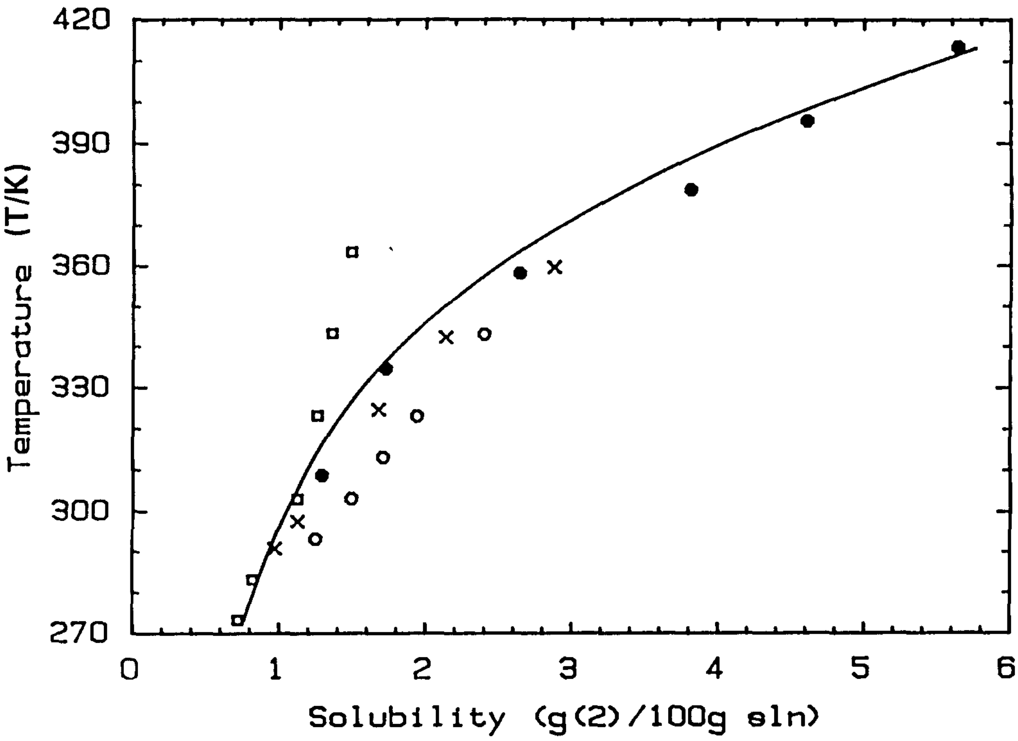

FIGURE 2. Selected data for the solubility of water (2) in acetic acid 2-methylpropyl ester (1): ref 6 (●); ref 8, rejected data, (O); ref 9 (X); ref 11 (□). Solid line is a least square polynomial fitted to the "Best" values from Table 3.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-2316.

2. Hemptinne, A. *Z. Phys. Chem.* 1894, *13*, 561-9.

3. Fuehner, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-5.

4. Doolittle, A. K. *Ind. Eng. Chem.* 1935, *27*, 1169-79.

5. Frolov, A. F.; Loginova, M. A.; Fadeeva, G. S.; Ustavshchikov, B. F. *Zh. Fiz. Khim.* 1966, *40*, 145-7; see also Loginova, M. A.; Frolov, A. F.; Ustavshchikov, B. F.; Fadeeva, G. S. *Khim. Prom.* 1967, *43*, 11-15.

6. Linek, J. *Collect. Czech. Chem. Commun.* 1976, *41*, 1714-6.

7. Heyberger, A.; Horacek, J.; Bulicka, J.; Prochazka, J. *Collect. Czech. Chem. Commun.* 1977, *42*, 3355-62.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

8. Bomshtein, A. L.; Trofimov, A. N.; Gotlib, V. A.; Serafimov, L. A. *Zh. Prikl. Khim.* 1978, *51*, 440-2.

9. Skrzecz, A. *Pol. J. Chem.* 1981, *55*, 1177-80; see also Skrzecz, A. *Thesis, I. Ch. F. PAN*, Warszawa, 1979.

10. Richon, D.; Viallard, A. *Fluid Phase Equil.* 1985, *21*, 279-93.

11. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-316.
VARIABLES:	**PREPARED BY:**
T/K = 295	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-methylpropyl ester in water at 22°C was reported to be 1 part of isobutyl acetate in 190-210 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 0.50 g(1)/100g sln and 7.8×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Not specified. (2) Not specified.
	ESTIMATED ERROR:
	Soly. ±0.03 g(1)/100g sln.
	REFERENCES:

COMPONENTS:

(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hemptinne, A.

Z. Phys. Chem. 1894, *13*, 561-9.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-methylpropyl ester in water at 25°C was reported to be 6.332 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture of water with excess ester was heated for some time in a water bath and the ester phase was filtered. A sample of known volume was then transferred to a smaller flask, heated with the known amount of baryta until complete saponification was obtained and then titrated. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Fuehner, H.

Ber. Dtsch. Chem. Ges. 1924, 57, 510-5.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-methylpropyl ester in water at 20°C was reported to be 0.75 vol%, 0.67 g(1)/100g sln and 0.058 mol(1)/L sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00104.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The ester was added from pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.03 g(1)/100g (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	Doolittle, A.K. *Ind. End. Chem.* 1935, *27*, 1169-79.
VARIABLES:	PREPARED BY:
$T/K = 293$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-methylpropyl ester in water at 20°C was reported to be 0.67 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00105.

The solubility of water in acetic acid 2-methylpropyl ester at 20°C was reported to be 1.64 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.0971.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commercial product; purity 96%, b.p. range 114-118°C, d_4^{20} 0.870. (2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.03 g(1)/100g sln and ±0.6 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:

(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Frolov, A.F.; Loginova, M.A. Fadeeva, G.S.; Ustavshchikov, B.F.

Zh. Fiz. Khim. 1966, *40*, 145-7. Loginova, M.A.; Frolov, A.F.; Ustavshchikov, B.F.; Fadeeva, G.S.

Khim. Prom. 1967, *43*, 11-5.

VARIABLES:

T/K = 293

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-methylpropyl ester in water at 20°C was reported to be 0.80 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.00125.

The solubility of water in acetic acid 2-methylpropyl ester at 20°C was reported to be 1.74 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.102.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. A sample of one component was titrated by a second component at constant temperature until a turbidity was observed for 20-30 min. The data were reported together with the ternary system acetic acid 2-methylpropyl ester-water-2-methylpropenamide (*isobutyl acetate-water-methacrylamide*).

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; b.p. 117°C, d_4^{20} 0.8695, $n_D^{18.8}$ 1.3910.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.1 g(1)/100g sln and ±0.7 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Linek, J.

Collect. Czech. Chem. Commun. 1976, *41*, 1714-6.

VARIABLES:

$T/K = 288 - 420$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 2-methylpropyl ester and water

$t/^\circ C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
14.6	0.761	-	0.001188	-
24.9	0.720	-	0.001123	-
35.6	-	98.71	-	0.9223
47.9	0.698	-	0.001089	-
61.5	-	98.27	-	0.8981
67.6	0.720	-	0.001123	-
74.9	0.760	-	0.001186	-
75.2	0.761	-	0.001188	-
84.8	0.805	-	0.001257	-
85.0	-	97.36	-	0.8512
93.2	0.844	-	0.001318	-

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The sealed tube method was used with the modification described by Matous, Novak, Sobr and Pick (ref 1). An ampoule with a solution of a given composition together with a ferrite magnet was heated in a thermostated glass tube which was connected into the circuit of a thermostat filled with triethylene glycol. The temperature of the bath was changed continuously and the appearance or disappearance of the second phase in the ampoule was observed visually. Ester hydrolysis was not observed.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, technical product; refluxed with acetic anhydride, washed with saturated solution of K_2CO_3 and water, dried and distilled; free of acetic acid and alcohols, about 1.5% butyl acetate by glc; b.p. 117.5°C, d_4^{20} 0.8715, n_D^{20} 1.3902.

(2) Distilled; specific conductivity 4×10^{-6} ohm^{-1}cm^{-1}.

ESTIMATED ERROR:

Temp. ±0.1°C (author).
Soly. about ±0.1 g(1)/100g sln [(2)-rich phase] and <±0.2 g(1)/100g sln [(1)-rich phase] (compiler).

REFERENCES:

1. Matous, J.; Novak, J.P.; Sobr, J.; Pick, J. *Collect. Czech. Chem. Commun.* 1972, *37*, 2653.

COMPONENTS:

(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Linek, J.

Collect. Czech. Chem. Commun. 1976, *41*, 1714-6.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid 2-methylpropyl ester and water

$t/^{\circ}C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
99.7	-	96.59	-	0.8146
105.7	-	96.19	-	0.7966
111.5	0.968	-	0.001514	-
115.7	1.002	-	0.001567	-
122.4	-	95.39	-	0.7624
140.3	-	94.36	-	0.7218
147.1	1.206	-	0.001890	-

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	Heyberger, A.; Horacek, J.; Bulicka, J.; Prochazka, J. *Collect. Czech. Chem. Commun.* <u>1977</u>, *42*, 3355-62.
VARIABLES:	**PREPARED BY:**
T/K = 298 and 323	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 2-methylpropyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
25	0.400[a]	98.640[a]	0.000622	0.9184
50	0.670[b]	96.400[c]	0.001045	0.8059

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The samples were titrated until a turbidity or droplets of the second phase appeared. The data and method were reported together with the ternary system acetic acid 2-methylpropyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, technical grade; shaken with Na_2CO_3(aq), distilled from H_2O after addition of chloroform.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.2[a], ±0.1[b] and ±1.9[c] g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	Bomshtein, A.L.; Trofimov, A.N.; Gotlib, V.A.; Serafimov, L.A. *Zh. Prikl. Khim.* 1978, *51*, 440-2.
VARIABLES:	**PREPARED BY:**
T/K = 293 - 353	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 2-methylpropyl ester and water

t/°C	x_1		g(1)/100g sln (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	0.00161	0.92458	1.03	98.751
25	0.00158	0.91784	1.01	98.631
30	0.00155	0.91118	0.99	98.511
40	0.00149	0.89919	0.95	98.291
50	0.00142	0.88692	0.91	98.061
60	0.00136	0.87493	0.87	97.831
70	0.00131	0.86321	0.84	97.601
80	0.00125	0.85174	0.80	97.371

Authors' smoothing equations:

g(1)/100g sln = 1.109 - 0.0039 t/°C (2)-rich phase

g(2)/100g sln = 0.812 + 0.0229 t/°C (1)-rich phase

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical methods were used. The component (1) was analyzed by saponification and the component (2) was analyzed by the Karl Fischer method. The experiments were made at normal pressure.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; without impurities by glc, b.p. 117.7°C, n_D^{20} 1.390.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±(0.1 - 0.4) g(1)/100g sln in both phases (compiler).

REFERENCES:

COMPONENTS:

(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skrzecz, A.

Pol. J. Chem. 1981, *55*, 1177-80.

Skrzecz, A.

Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

VARIABLES:

T/K = 291 - 360

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 2-methylpropyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
290.8[a]	-	0.9404	-	99.027
293.3	0.00110	-	0.705	-
297.6	-	0.9317	-	98.876
304.1	0.00098	-	0.629	-
316.9	0.00090	-	0.577	-
324.8	-	0.9008	-	98.321
333.6	0.00090	-	0.577	-
342.4	-	0.8765	-	97.861
342.6	0.00098	-	0.629	-
352.1	0.00110	-	0.705	-

[a] By the Karl Fischer method.

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew and the analytical method were used. An ampoule with the solution of fixed concentration was placed in a glass tube connected with a thermostat filled completely with distilled water. During the measurements the temperature of the bath was changed continuously and the appearance and disappearance of turbidity within the ampoule was observed visually. For the analytical method, The amount of water in the saturated organic phase was determined using a Karl Fischer titration procedure. The amount of water in the pure ester was taken into account.

SOURCE AND PURITY OF MATERIALS:

(1) POCH, pure grade; distilled; purity 99.98% by glc, 0.11 wt% water by the Karl Fischer method.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±(0.2-0.6)°C.
Soly. see above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	Skrzecz, A. *Pol. J. Chem.* 1981, *55*, 1177-80. Skrzecz, A. *Thesis*, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, 1979.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid 2-methylpropyl ester and water

T/K	x_1		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
353.2	-	0.8559	-	97.455
359.7	-	0.8397	-	97.124

Author's smoothing equations:

$$x_1 = 1.5088\text{x}10^{-3} - 2.50\text{x}10^{-5}\ (T/K - 273.15) + 2.51\text{x}10^{-7}\ (T/K - 273.15)^2$$

st. dev. = 9.55×10^{-6} (2)-rich phase

$$x_2 = 0.050721 + 4.192\text{x}10^{-4}\ (T/K - 273.15) + 9.52\text{x}10^{-6}\ (T/K - 273.15)^2$$

st. dev. = 2.30×10^{-3} (1)-rich phase

COMPONENTS:

(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-methylpropyl ester in water at 298.1 K was reported to be 0.00601 mol(1)/100g(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 0.693 g(1)/100g sln and 0.001082.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) Fluka (puriss); purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.04 g(1)/100g sln (compiler).

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 2-methylpropyl ester (*isobutyl acetate*); $C_6H_{12}O_2$; [110-19-0] (2) Water; H_2O; [7732-18-5]	Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* <u>1986</u>, *31*, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 363	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 2-methylpropyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.03	99.28	0.00161	0.9553
10.0	0.83	99.18	0.00130	0.9494
19.7	0.66	99.05	0.00103	0.9417
29.9	0.61	98.88	0.00095	0.9319
39.7	0.54	98.79	0.00084	0.9268
50.0	0.49	98.74	0.00076	0.9240
60.5	0.57	98.71	0.00089	0.9223
70.1	0.53	98.64	0.00082	0.9183
80.2	0.55	98.35	0.00086	0.9024
90.2	-	98.51	-	0.9111
std. dev.	0.02	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the butanoic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Butanoic acid ethyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Hemptinne (ref 2)	298	(1) in (2)	analytical
Bancroft (ref 3)	293	mutual	titration
Fuehner (ref 4)	295	(1) in (2)	titration
Doolittle (ref 5)	293	mutual	unspecified
Rao and Rao (ref 6)	303	mutual	titration
Venkataratnam *et al.* (ref 7)	303	mutual	titration
Rao and Rao (ref 8)	303	mutual	titration
Richon and Viallard (ref 9)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 10)	273-364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF BUTANOIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of butanoic acid ethyl ester (1) in water (2) are summarized in Table 2 with the following exclusions.

The data of Hemptinne (ref 2) and Bancroft (ref 3), expressed in w/v and v/v units have been excluded from consideration. The data of Traube (ref 1) and Doolittle (ref 5) at *ca.* 293 K have been rejected as they are considerably lower than other reported values (ref 4,9,10). The data of Rao *et al.* (ref 6-8), whilst not rejected, have for the purpose of uniformity not been included in calculating the "Best" values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

The remaining data (Table 2) are in general in good agreement although the lack of independent studies over a wide temperature range precludes Recommendation at most temperatures.

TABLE 2: Recommended (*R*) and Tentative Solubilities of Butanoic acid ethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
273	1.06 (ref 10)	1.1	1.7
283	0.81* (ref 10)	0.8	1.3
293	0.616^b (ref 4), 0.68 (ref 10)	0.65 ± 0.03 (*R*)	1.01
298	0.666 (ref 9), 0.63* (ref 10)	0.65 ± 0.02 (*R*)	1.01
303	0.8^c (ref 6-8), 0.58* (ref 10)	0.58	0.9
313	0.51* (ref 10)	0.5	0.8
323	0.47* (ref 10)	0.5	0.8
333	0.46* (ref 10)	0.5	0.7
343	0.46* (ref 10)	0.5	0.7
353	0.46* (ref 10)	0.5	0.7
363	0.44* (ref 10)	0.4	0.7

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] 295 K.

[c] Not included in calculation of "Best" value, see text.

2. SOLUBILITY OF WATER (2) IN BUTANOIC ACID ETHYL ESTER (1)

All the available data for the solubility of water (2) in butanoic acid ethyl ester (1) are summarized in Table 3. In general, agreement is satisfactory although the lack of independent studies over a wide temperature range precludes Recommendation of any of the "Best" values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 3: Tentative Solubilities of Water (2) in Butanoic acid ethyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
273	0.56 (ref 10)	0.6	4
283	0.70* (ref 10)	0.7	4
293	0.75 (ref 5), 0.86 (ref 10)	0.80 ± 0.06	4.9
298	0.92* (ref 10)	0.9	6
303	1.1 (ref 6), 0.6 (ref 7,8), 0.98* (ref 10)	0.9 ± 0.2	6
313	1.09* (ref 10)	1.1	7
323	1.16* (ref 10)	1.2	7
333	1.21* (ref 10)	1.2	7
343	1.23* (ref 10)	1.2	7
353	1.29* (ref 10)	1.3	8
363	1.30* (ref 10)	1.3	8

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-2316.
2. Hemptinne, A. *Z. Phys. Chem.* 1894, *13*, 561-9.
3. Bancroft, W. D. *Phys. Rev.* 1895, *3*, 114-36.
4. Fuehner, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-5.
5. Doolittle, A. K. *Ind. Eng. Chem.* 1935, *27*, 1169-79.
6. Rao, J. R.; Rao, C. V. *J. Appl. Chem.* 1957, *7*, 435-9.
7. Venkataratnam, A.; Rao, J. R.; Rao, C. V. *Chem. Eng. Sci.* 1957, *7*, 102-10.
8. Rao, J. R.; Rao, C. V.; *J. Appl. Chem.* 1959, *9*, 69-73.
9. Richon, D.; Viallard, A. *Fluid Phase Equil.* 1985, *21*, 279-93.
10. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

COMPONENTS:

(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Traube, J.

Ber. Dtsch. Chem. Ges. 1884, *17*, 2294-316.

VARIABLES:

$T/K = 295$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 22°C was reported to be 1 part of ethyl butyrate in 190-210 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 0.50 g(1)/100g sln and 7.8×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±0.03 g(1)/100g sln.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butanoic acid ethyl ester *(ethyl butyrate)*; $C_6H_{12}O_2$; [105-54-4] (2) Water; H_2O; [7732-18-5]	Hemptinne, A. *Z. Phys. Chem.* 1894, *13*, 561-9.
VARIABLES:	PREPARED BY:
$T/K = 298$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 25°C was reported to be 6.862 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The mixture of water with excess ester was heated for some time in a water bath and the ester phase was filtered. A sample of known volume was then transferred to a smaller flask, heated with the known amount of baryta until complete saponification was obtained and then titrated. No further details were reported in the paper.	(1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4] (2) Water; H_2O; [7732-18-5]	Bancroft, W.D. *Phys. Rev.* 1895, *3*, 114-36.
VARIABLES:	**PREPARED BY:**
$T/K = 293$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 20°C was reported to be 0.08 mL(1)/10mL(2).

The solubility of water in butanoic acid ethyl ester at 20°C was reported to be 0.04-0.05 mL(2)/10mL(1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used.
10 mL of solvent in a test tube was titrated with the second component until the solution became cloudy.

SOURCE AND PURITY OF MATERIALS:

(1) Laboratory source; dried over $CaCl_2$, distilled.

(2) Not specified.

ESTIMATED ERROR:

Soly. ±0.01 mL.

REFERENCES:

COMPONENTS:

(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Fuehner, H.

Ber. Dtsch. Chem. Ges. 1924, 57, 510-5.

VARIABLES:

$T/K = 295$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 22°C was reported to be 0.725 vol%, 0.616 g(1)/100g sln and 0.0531 mol(1)/L sln. The corresponding mole fraction, x_1, value calculated by the compiler is 9.60×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Butanoic acid ethyl ester
(ethyl butyrate); $C_6H_{12}O_2$;
[105-54-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Doolittle, A.K.

Ind. End. Chem. 1935, *27*, 1169-79.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 20°C was reported to be 0.49 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 7.6×10^{-4}.

The solubility of water in butanoic acid ethyl ester at 20°C was reported to be 0.75 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.046.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; purity 99%, b.p. range 107-131°C, d_4^{20} 0.880.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4] (2) Water; H_2O; [7732-18-5]	Rao, J.R.; Rao, C.V. *J. Appl. Chem.* 1957, 7, 435-9.
VARIABLES:	**PREPARED BY:**
$T/K = 303$	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 30°C was reported to be 0.8 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0012.

The solubility of water in butanoic acid ethyl ester at 30°C was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.067.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The data and method were reported together with the ternary system butanoic acid ethyl ester-water-methanol.

SOURCE AND PURITY OF MATERIALS:

(1) Naarden, reagent grade; b.p. 121.5°C, d^{30} 0.8685, n_D^{30} 1.3880.

(2) Distilled; free from CO_2.

ESTIMATED ERROR:

Temp. ±0.02°C.

REFERENCES:

COMPONENTS:

(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Venkataratnam, A.; Rao, J.R.; Rao, C.V.

Chem. Eng. Sci. 1957, *7*, 102-10.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 30°C was reported to be 0.8 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0012.

The solubility of water in butanoic acid ethyl ester at 30°C was reported to be 0.6 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.04.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system butanoic acid ethyl ester-water-2-propanone (*ethyl butyrate-water-acetone*).

SOURCE AND PURITY OF MATERIALS:

(1) Naarden, analytical grade; used as received; b.p. 121.5°C, d^{30} 0.8685, n^{30} 1.3880.

(2) Distilled; free of CO_2.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Butanoic acid ethyl ester *(ethyl butyrate)*; $C_6H_{12}O_2$; [105-54-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rao, R.J.; Rao, C.V.

J. Appl. Chem. 1959, *9*, 69-73.

VARIABLES:

T/K = 303

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 30°C was reported to be 0.8 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0012.

The solubility of water in butanoic acid ethyl ester at 30°C was reported to be 0.6 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.04.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the titration method described by Rao and Rao (ref 1) was used. The data were reported together with the ternary system butanoic acid ethyl ester-water-1-propanol.

SOURCE AND PURITY OF MATERIALS:

(1) Naarden, analytical grade; b.p. 121.5°C, d^{30} 0.8685, n_D^{30} 1.3880.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Rao, R.J.; Rao, C.V. *J. Appl. Chem.* 1957, *7*, 435.

COMPONENTS:

(1) Butanoic acid ethyl ester (*ethyl butyrate*); $C_6H_{12}O_2$; [105-54-4]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Richon, D.; Viallard, A.

Fluid Phase Equilib. 1985, *21*, 279-93.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 298.1 K was reported to be 0.00577 mol(1)/100g(2). The corresponding mass per cent and mole fraction, x_1, values calculated by the compiler are 0.666 g(1)/100g sln and 0.001038.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

(1) BDH: purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, 1974.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butanoic acid ethyl ester *(ethyl butyrate)*; $C_6H_{12}O_2$; [105-54-4] (2) Water; H_2O; [7732-18-5]	Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 364	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of butanoic acid ethyl ester and water

$t/°C$	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.06	99.44	0.00166	0.9650
9.5	0.81	99.32	0.00126	0.9577
20.0	0.69	99.21	0.00108	0.9512
31.0	0.58	98.98	0.00090	0.9377
39.9	0.52	98.93	0.00081	0.9348
50.0	0.46	98.78	0.00072	0.9262
60.4	0.46	98.83	0.00072	0.9291
70.2	0.46	98.72	0.00072	0.9228
80.3	0.46	98.82	0.00072	0.9285
90.5	0.44	98.74	0.00068	0.9240
std. dev.	0.01	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Formic acid 3-methyl-1-butyl ester (*isopentyl formate*); $C_6H_{12}O_2$; [110-45-2]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the formic acid 3-methyl-1-butyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Formic acid 3-methyl-1-butyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Trofimov (ref 2)	293-363	mutual	GLC
Stephenson and Stuart (ref 3)	273-364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF FORMIC ACID 3-METHYL-1-BUTYL ESTER (1) IN WATER (2)

All the available data for the solubility of formic acid 3-methyl-1-butyl ester (1) in water (2) are summarized in Table 2 and plotted in Figure 1. The data are in poor agreement with the two major studies (ref 2,3) showing a quite different temperature dependence. In the absence of confirmatory studies it is not possible at this stage to prefer either data set although it may be noted that ester solubilities in water do *not* usually show a monotonic increase with temperature as observed by Trofimov (ref 2). This system clearly warrants further study.

TABLE 2: Solubilities of Formic acid 3-methyl-1-butyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values ($\pm\sigma_n$)[a]	
	g(1)/100g sln	g(1)/100g sln	$10^4 x_1$
273	0.198 (ref 3)	0.2	3
283	0.15* (ref 3)	0.2	3
293	0.31[b] (ref 1), 0.244 (ref 2), 0.13* (ref 3)	0.19 ± 0.06	2.9

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid 3-methyl-1-butyl ester (*isopentyl formate*); $C_6H_{12}O_2$; [110-45-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities		
	Reported values	"Best" values ($\pm\sigma_n$)[a]	
	g(1)/100g sln	g(1)/100g sln	10^4x_1
298	0.25* (ref 2), 0.12* (ref 3)	0.2 ± 0.1	3
303	0.26* (ref 2), 0.12* (ref 3)	0.2 ± 0.1	3
313	0.28* (ref 2), 0.11* (ref 3)	0.2 ± 0.1	3
323	0.29* (ref 2), 0.11* (ref 3)	0.2 ± 0.1	3
333	0.34* (ref 2), 0.11* (ref 3)	- [c]	-
343	0.46* (ref 2), 0.11* (ref 3)	- [c]	-
353	0.66* (ref 2), 0.12* (ref 3)	- [c]	-
363	0.95* (ref 2), 0.13* (ref 3)	- [c]	-

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] 295 K, not included in calculation of average.

[c] Disagreement too marked for meaningful calculation of "Best" values.

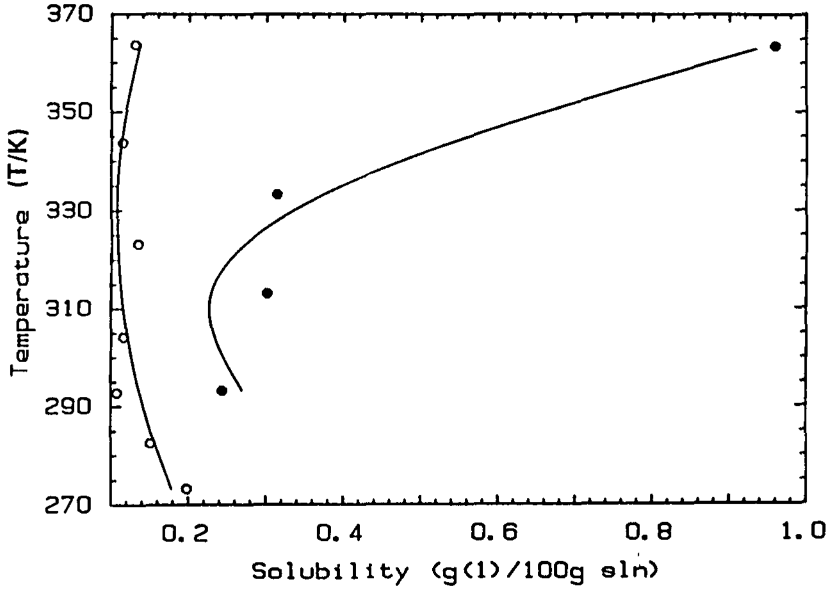

FIGURE 1. Selected data for the solubility of formic acid 3-methyl-1-butyl ester (1) in water (2): ref 2 (●); ref 3 (O). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid 3-methyl-1-butyl ester (*isopentyl formate*); $C_6H_{12}O_2$; [110-45-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN FORMIC ACID 3-METHYL-1-BUTYL ESTER (1)

Only Trofimov (ref 2) and Stephenson and Stuart (ref 3) have reported solubilities of water (2) in formic acid 3-methyl-1-butyl ester (1). Their data are summarized in Table 3 and plotted in Figure 2. As for the H_2O-rich phase, the data of refs 2 and 3 are not in very good agreement although they both show an increase in solubility with increasing temperature. The average "Best" values should be regarded as very Tentative pending further studies.

TABLE 3: Tentative Solubilities of Water (2) in Formic acid 3-methyl-1-butyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
273	0.80* (ref 3)	0.8	5
283	0.92* (ref 3)	0.9	6
293	0.535 (ref 2), 1.05* (ref 3)	0.8 ± 0.3	5
298	0.58* (ref 2), 1.13* (ref 3)	0.9 ± 0.3	6
303	0.63* (ref 2), 1.19* (ref 3)	0.9 ± 0.3	6
313	0.725 (ref 2), 1.35* (ref 3)	1.0 ± 0.3	6
323	0.83* (ref 2), 1.53* (ref 3)	1.2 ± 0.4	7
333	0.934 (ref 2), 1.70* (ref 3)	1.3 ± 0.4	8
343	1.05* (ref 2), 1.91* (ref 3)	1.5 ± 0.4	9
353	1.18* (ref 2), 2.11* (ref 3)	1.6 ± 0.5	9
363	1.32* (ref 2), 2.35* (ref 3)	1.8 ± 0.5	11

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Formic acid 3-methyl-1-butyl ester (*isopentyl formate*); $C_6H_{12}O_2$; [110-45-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

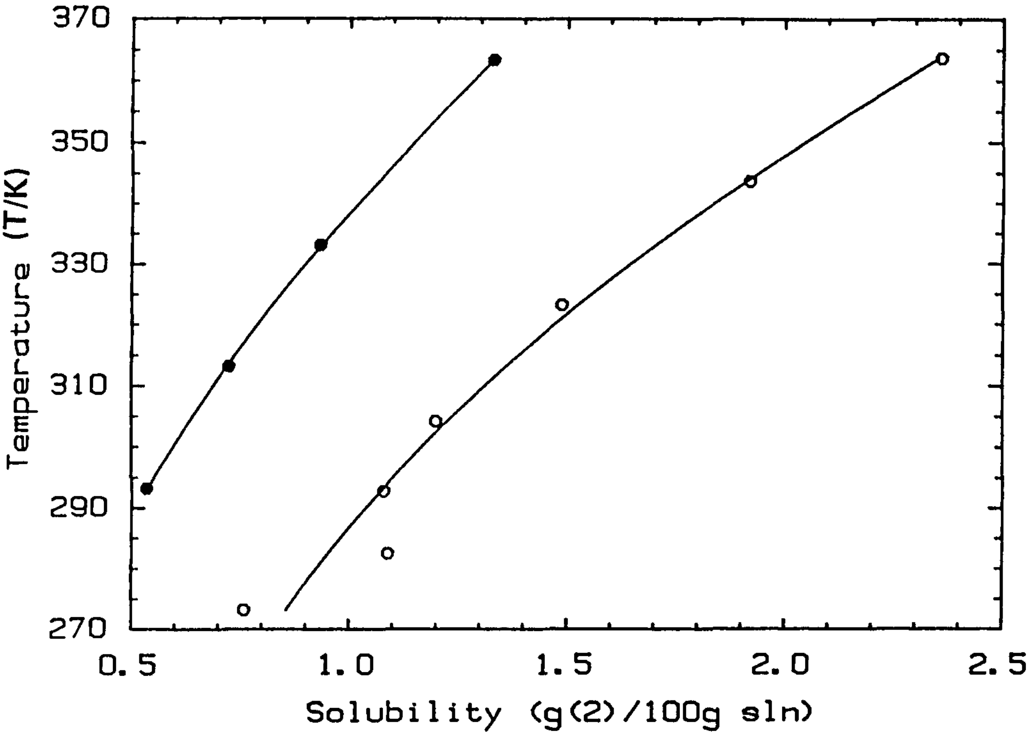

FIGURE 2. Selected data for the solubility of water (2) in formic acid 3-methyl-1-butyl ester (1): ref 2 (●); ref 3 (O). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

REFERENCES

1. Traube, J. *Ber. Dtsch. Chem. Ges.* 1884, *17*, 2294-2316.

2. Trofimov, A. N. *Gidroliz. Lesokhim. Prom.* 1969, *22*(8), 9.

3. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Formic acid 3-methyl-1-butyl ester (*isopentyl formate*); $C_6H_{12}O_2$; [110-45-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Traube, J.

Ber. Dtsch. Chem. Ges. 1884, *17*, 2294-316.

VARIABLES:

T/K = 295

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of formic acid 3-methyl-1-butyl ester in water at 22°C was reported to be 1 part of isopentyl formate in 325 parts of water. The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 0.31 g(1)/100g sln and 4.8×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Formic acid 3-methyl-1-butyl ester (*isopentyl formate*); $C_6H_{12}O_2$; [110-45-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Trofimov, A.N.

Gidroliz. Lesokhim. Prom. 1969, *22(8)*, 9.

VARIABLES:

$T/K = 293 - 363$

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of formic acid 3-methyl-1-butyl ester and water

$t/°C$	x_1		g(1)/100g sln (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	0.00038	0.9665	0.244	99.465
40	0.00047	0.9550	0.302	99.275
60	0.00049	0.9427	0.315	99.066
90.2[a]	0.0015	0.9200	0.96	98.669

[a] Boiling temperature at atmospheric pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The two-phase mixture was placed in a thermostated apparatus with a magnetic stirrer and reflux condenser and mixed for 1 h. (at the boiling temperature for 1/2 h. only), separated for 20 min, and analyzed by glc. The ester hydrolysis was less than 2%.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; properties were described in the publication of Trofimov, Chashchin and Botsharnikov (ref 1).

(2) Not specified.

ESTIMATED ERROR:

Soly. ±1.5% (max. relative error of analysis).

REFERENCES:

1. Trofimov, A.N.; Chashchin, A.; Botsharnikov, E.V. *Gidroliz. Lesokhim. Prom.* 1968, *(5)*.

COMPONENTS:

(1) Formic acid 3-methyl-1-butyl ester (*isopentyl formate*); $C_6H_{12}O_2$; [110-45-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 364

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of formic acid 3-methyl-1-butyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	0.198	99.24	0.000307	0.9529
9.3	0.151	98.91	0.000234	0.9336
19.6	0.108	98.92	0.000168	0.9342
31.0	0.116	98.80	0.000180	0.9274
39.6	0.111	98.66	0.000172	0.9195
50.0	0.135	98.51	0.000209	0.9111
60.4	-	98.25	-	0.8970
70.5	0.115	98.08	0.000178	0.8879
80.3	0.082	97.93	0.000127	0.8800
90.5	0.131	97.64	0.000203	0.8651
std. dev.	0.005	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 96%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Formic acid pentyl ester (*pentyl formate*); $C_6H_{12}O_2$; [638-49-3]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 364

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of formic acid pentyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	0.36	99.01	0.00056	0.9394
9.1	0.31	99.03	0.00048	0.9406
19.9	0.27	98.93	0.00042	0.9348
30.9	0.26	98.89	0.00040	0.9325
39.6	0.26	98.75	0.00040	0.9245
50.0	0.27	98.66	0.00042	0.9195
60.1	0.24	98.63	0.00037	0.9178
70.2	0.27	98.51	0.00042	0.9111
80.0	0.29	98.51	0.00045	0.9111
90.5	0.26	97.59	0.00040	0.8626
std. dev.	0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 95%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Pentanoic acid methyl ester (*methyl valerate*); $C_6H_{12}O_2$; [624-24-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the pentanoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Pentanoic acid methyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Bomshtein *et al.* (ref 1)	293-353	mutual	titration
Stephenson and Stuart (ref 2)	273-363	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF PENTANOIC ACID METHYL ESTER (1) IN WATER (2)

All the available data are summarized in Table 2 and plotted in Figure 1. As can be seen the values are in poor agreement, showing an opposite dependence on temperature. Although ester solubilities in water commonly exhibit a minimum when plotted against temperature (as found for the present system by Stephenson and Stuart (ref 2)), in the absence of any independent studies it is not possible to prefer any one data set. Consequently, no "Best" values have been derived and this system clearly requires further study. The interested user is referred to the relevant Data Sheets for further information.

TABLE 2: Reported Solubilities of Pentanoic acid methyl ester (1) in Water (2)

T/K	Reported Solubilities g(1)/100g sln
273	0.80 (ref 2)
283	0.63* (ref 2)
293	0.06 (ref 1), 0.52* (ref 2)
298	0.13* (ref 1), 0.49* (ref 2)
303	0.19 (ref 1), 0.47* (ref 2)
313	0.32 (ref 1), 0.45* (ref 2)

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Pentanoic acid methyl ester (*methyl valerate*); $C_6H_{12}O_2$; [624-24-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Reported Solubilities g(1)/100g sln
323	0.45 (ref 1), 0.45* (ref 2)
333	0.58 (ref 1), 0.44* (ref 2)
343	0.77 (ref 1), 0.46* (ref 2)
353	0.96 (ref 1), 0.46* (ref 2)
363	0.45* (ref 2)

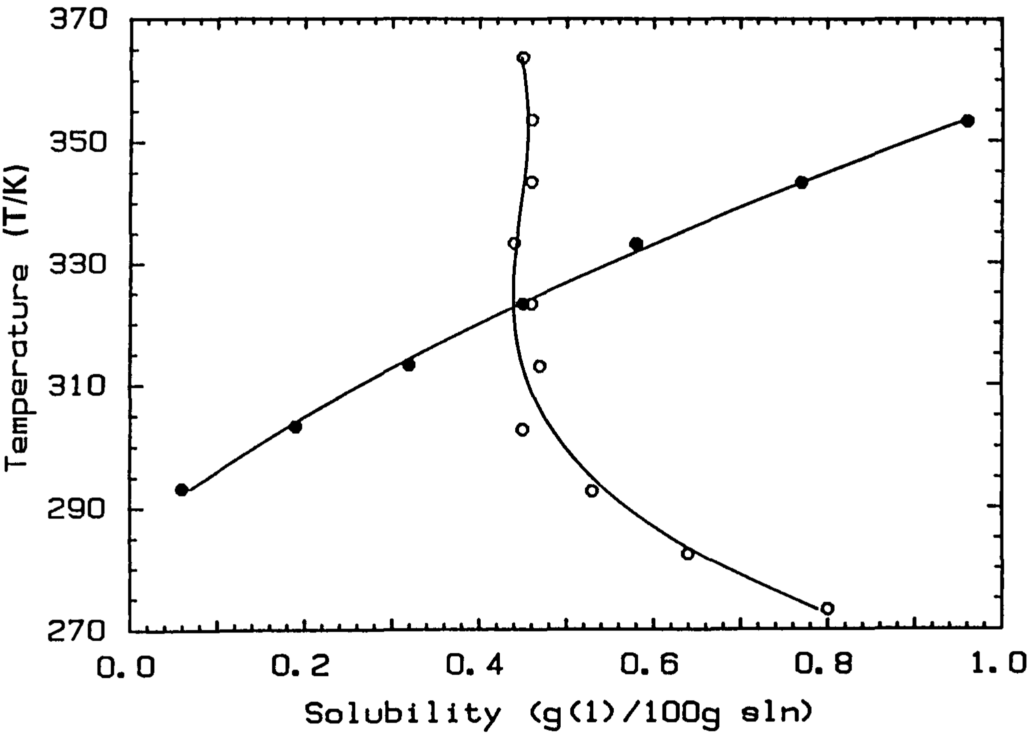

FIGURE 1. Data for the solubility of pentanoic acid methyl ester (1) in water (2): ref 1 (●); ref 2 (O). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Pentanoic acid methyl ester (*methyl valerate*); $C_6H_{12}O_2$; [624-24-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN PENTANOIC ACID METHYL ESTER (1)

All the available data (ref 1,2) for the solubility of water (2) in pentanoic acid methyl ester (1) are summarized in Table 3 and plotted in Figure 2. As for the H_2O-rich phase, the data of Bomshtein *et al.* (ref 1) differ markedly from those of Stephenson and Stuart (ref 2), albeit both studies at least give a similar dependence on temperature in this phase although the data are rather scattered. In the absence of confirmatory studies it is not possible at this stage to prefer one of these sets and no "Best" values have been calculated. Nevertheless, it may be noted that the solubilities of water in the organic-rich phase reported by Bomshtein *et al.* in other systems are often higher than reliable values. This system clearly requires re-investigation. The interested user is referred to the relevant Data Sheets for further information.

TABLE 3: Reported Solubilities of Water (2) in Pentanoic acid methyl ester (1)

T/K	Reported Solubilities g(2)/100 g sln
273	0.56 (ref 2)
283	0.64^* (ref 2)
293	2.30 (ref 1), 0.76^* (ref 2)
298	2.45^* (ref 1), 0.90^* (ref 2)
303	2.60 (ref 1), 1.02^* (ref 2)
313	2.80 (ref 1), 1.05 (ref 2)
323	3.10 (ref 1), 1.06 (ref 2)
333	3.40 (ref 1), 1.09 (ref 2)
343	4.10 (ref 1), 1.14 (ref 2)
353	5.50 (ref 1), 1.30 (ref 2)
363	1.55 (ref 2)

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Pentanoic acid methyl ester (*methyl valerate*); $C_6H_{12}O_2$; [624-24-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

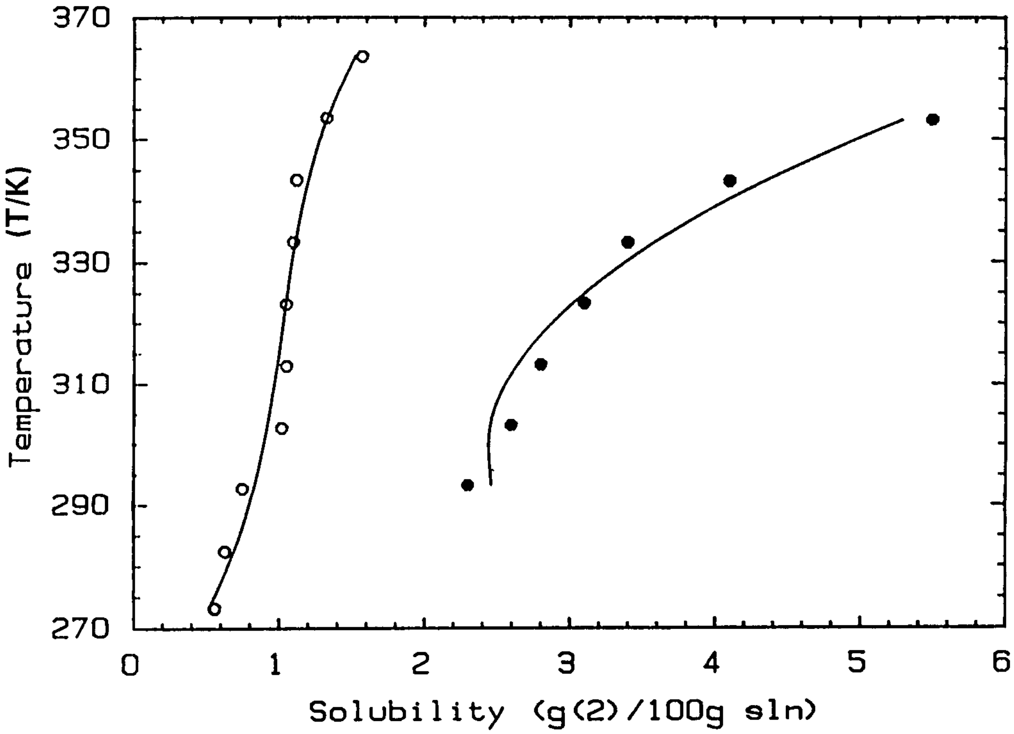

FIGURE 2. Data for the solubility of water (2) in pentanoic acid methyl ester (1): ref 1 (●); ref 2 (O). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

REFERENCES

1. Bomshtein A. L.; Trofimov, A. N.; Serafimov, L. A. *Zh. Prikl. Khim.* 1978, *51*, 1280-2.

2. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Pentanoic acid methyl ester (*methyl valerate*); $C_6H_{12}O_2$; [624-24-8]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bomshtein, A.L.; Trofimov, A.N.; Serafimov, L.A.

Zh. Prikl. Khim. 1978, *51*, 1280-2.

VARIABLES:

T/K = 293 - 353

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of pentanoic acid methyl ester and water

t/°C	x_1		g(1)/100g sln (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	0.0001	0.8683	0.06	97.70
30	0.0003	0.8532	0.19	97.40
40	0.0005	0.8434	0.32	97.20
50	0.0007	0.8291	0.45	96.90
60	0.0009	0.8151	0.58	96.60
70	0.0012	0.7840	0.77	95.90
80	0.0015	0.7272	0.96	94.50

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used at constant temperature. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; without impurities by glc, b.p. 127.2°C, n_D^{20} 1.398.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Pentanoic acid methyl ester (*methyl valerate*); $C_6H_{12}O_2$; [624-24-8]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 363

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of pentanoic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	0.80	99.44	0.00125	0.9650
9.2	0.64	99.37	0.00100	0.9607
19.5	0.53	99.25	0.00083	0.9535
29.5	0.45	98.98	0.00070	0.9377
39.8	0.47	98.95	0.00073	0.9360
50.0	0.46	98.95	0.00072	0.9360
60.1	0.44	98.90	0.00068	0.9331
70.2	0.46	98.88	0.00072	0.9319
80.3	0.46	98.67	0.00072	0.9200
90.5	0.45	98.43	0.00070	0.9067
std. dev.	0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid, 2,2-dimethyl-, methyl ester *(methyl trimethylacetate)*; $C_6H_{12}O_2$; [598-98-1] (2) Water; H_2O; [7732-18-5]	Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* <u>1986</u>, *31*, 56-70.
VARIABLES:	**PREPARED BY:**
T/K = 273 - 364	Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of 2,2-dimethylpropanoic acid methyl ester and water

t/°C	g(1)/100g sln (2)-rich phase	g(1)/100g sln (1)-rich phase	x_1 (compiler) (2)-rich phase	x_1 (compiler) (1)-rich phase
0	0.81	99.51	0.00126	0.9692
9.7	0.66	99.43	0.00103	0.9643
19.7	0.56	99.34	0.00087	0.9589
29.7	0.51	99.20	0.00079	0.9506
40.0	0.45	99.07	0.00070	0.9429
50.1	0.43	98.97	0.00067	0.9371
60.5	0.42	98.99	0.00065	0.9382
70.4	0.39	98.90	0.00061	0.9331
80.5	0.41	98.82	0.00064	0.9285
90.5	0.33	98.85	0.00051	0.9302
std. dev.	0.02	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Propanoic acid, 2-methyl-, ethyl ester (*ethyl isobutyrate*); $C_6H_{12}O_2$; [97-62-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 364

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of 2-methylpropanoic acid ethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.01	99.41	0.00158	0.9631
10.0	0.77	99.33	0.00120	0.9583
19.8	0.68	99.18	0.00106	0.9494
29.7	0.58	98.90	0.00090	0.9331
40.1	0.51	98.87	0.00079	0.9314
50.1	0.45	98.84	0.00070	0.9296
60.2	0.44	98.87	0.00068	0.9314
70.4	0.45	98.84	0.00070	0.9296
80.5	0.44	98.54	0.00068	0.9128
90.5	0.38	98.49	0.00059	0.9100
std. dev.	0.01	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A., Australia
January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the propanoic acid propyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Propanoic acid propyl ester (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Hemptinne (ref 1)	298	(1) in (2)	analytical
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Mozzhukhin *et al*. (ref 3)	293	mutual	titration
Bomshtein *et al*. (ref 4)	293-353	mutual	titration
Stephenson and Stuart (ref 5)	273-364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF PROPANOIC ACID PROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of propanoic acid propyl ester (1) in water (2) are summarized in Table 2 except for the value of Mozzhukhin *et al*. (ref 3) which is significantly lower than all other reports and is therefore rejected. Selected data (ref 4,5) are also plotted in Figure 1. Although the independent studies which cover the widest temperature range (ref 4,5) are in good agreement with each other and the values of Rayman (ref 2) at $T < 303$, they diverge markedly at higher temperatures. In the absence of confirmatory studies it is not possible to prefer either data set at this stage and no "Best" values have been derived at higher temperatures. Further studies of this system are clearly desirable.

(continued next page)

COMPONENTS:

(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences,
Murdoch University, Perth, W.A.,
Australia
January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubilities of Propanoic acid propyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values ($\pm\sigma_n$)[a]	
	g(1)/100g sln	g(1)/100g sln	10^3x_1
273	1.05 (ref 2), 1.01 (ref 5)	1.03 ± 0.02 (*R*)	1.61
283	0.84 (ref 2), 0.79* (ref 5)	0.82 ± 0.03 (*R*)	1.28
293	0.68 (ref 2), 0.51 (ref 4), 0.64* (ref 5)	0.61 ± 0.07	0.95
298	0.56 (ref 1), 0.68* (ref 2), 0.61* (ref 4), 0.59* (ref 5)	0.61 ± 0.04	0.95
303	0.60 (ref 2), 0.71 (ref 4), 0.54* (ref 5)	0.62 ± 0.07	0.97
313	1.02 (ref 4), 0.48* (ref 5)	0.8 ± 0.3	1.2
323	1.21 (ref 4), 0.44* (ref 5)	0.8 ± 0.4	1.2
333	1.78 (ref 4), 0.42* (ref 5)	-[b]	-[b]
343	2.59 (ref 4), 0.41* (ref 5)	-[b]	-[b]
353	3.50 (ref 4), 0.40* (ref 5)	-[b]	-[b]
363	0.39* (ref 5)	-[b]	-[b]

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] See text.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

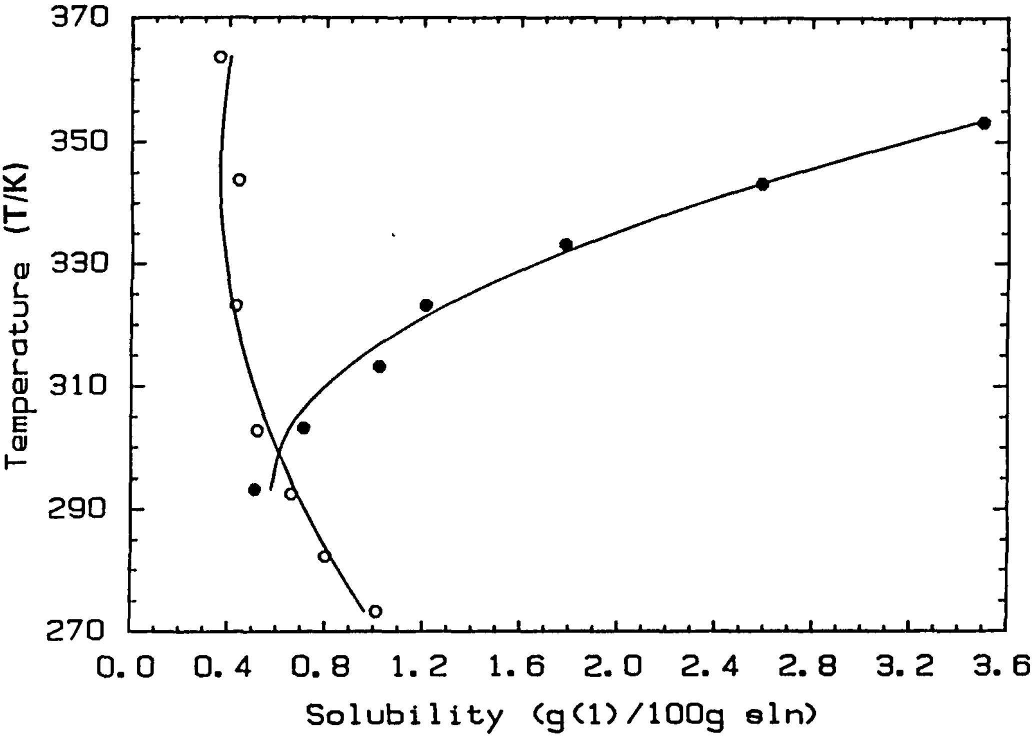

FIGURE 1. Selected data for the solubility of propanoic acid propyl ester (1) in water (2): ref 4 (●); ref 5 (O). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

2. SOLUBILITY OF WATER (2) IN PROPANOIC ACID PROPYL ESTER (1)

All the available solubility data for water (2) in propanoic acid propyl ester (1) are summarized in Table 3 except for the value of Mozzhukhin *et al*. (ref 3) which is an order of magnitude higher than other studies (ref 4,5) and is therefore rejected. The data are also plotted in Figure 2.

As for the H_2O rich phase, the data of Bomshtein *et al*. (ref 4) and Stephenson and Stuart (ref 5) are in good agreement near 298 K but differ markedly at higher temperatures. Again, in the absence of other independent studies it is not possible to prefer either data set and so no "Best" values have been derived at T > 333 K. Further studies of this system are clearly desirable.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 3: Recommended (*R*) and Tentative Solubilities of Water (2) in Propanoic acid propyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln	10^2x_2
273	0.63 (ref 5)	0.6	4
283	0.71* (ref 5)	0.7	4
293	0.90 (ref 4), 0.81* (ref 5)	0.86 ± 0.05 (*R*)	5.3
298	1.00* (ref 4), 0.88* (ref 5)	0.94 ± 0.06	5.8
303	1.10 (ref 4), 0.93* (ref 5)	1.02 ± 0.09	6.2
313	1.40 (ref 4), 1.03* (ref 5)	1.2 ± 0.2	7
323	1.50 (ref 4), 1.12* (ref 5)	1.3 ± 0.2	8
333	1.90 (ref 4), 1.19* (ref 5)	1.5 ± 0.4	9
343	2.80 (ref 4), 1.25* (ref 5)	– [b]	– [b]
353	3.90 (ref 4), 1.28* (ref 5)	– [b]	– [b]
363	1.31* (ref 5)	– [b]	– [b]

[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

[b] No "Best" values derived, see text.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

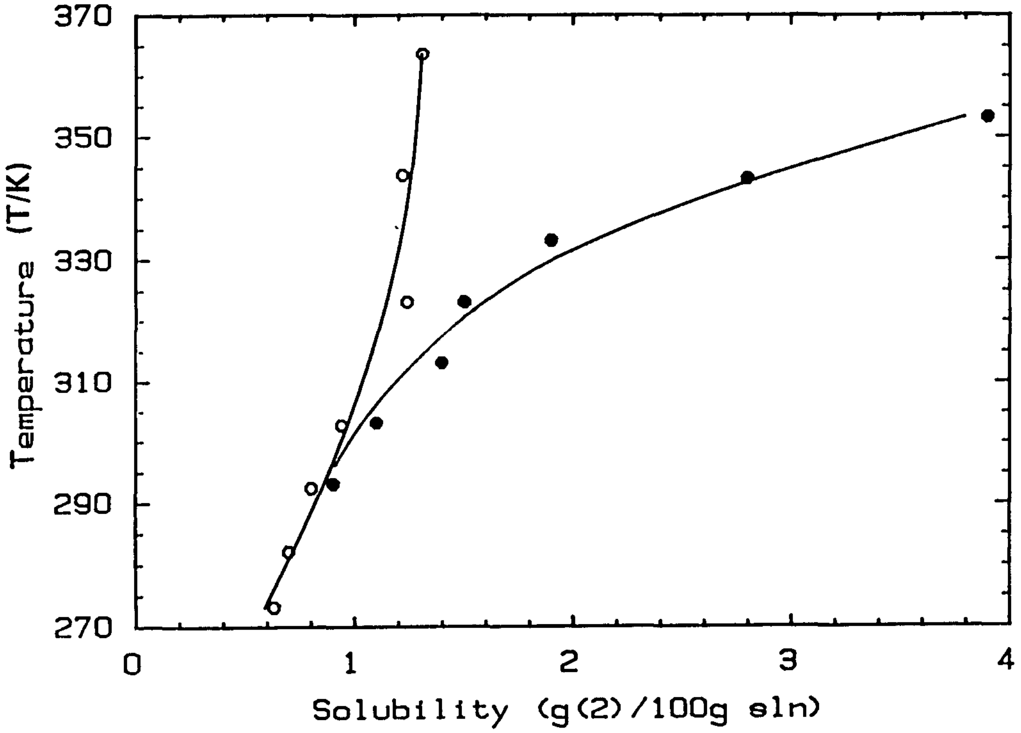

FIGURE 2. Selected data for the solubility of water (2) in propanoic acid propyl ester (1): ref 4 (●); ref 5 (O). Solid lines are smooth curves through the data points, drawn only for illustrative purposes.

REFERENCES

1. Hemptinne, A. *Z. Phys. Chem.* 1894, *13*, 561-9.
2. Rayman, J. *Thesis*, Budapest 1906.
3. Mozzhukhin, A. S.; Serafimov, L. A.; Mitropol'skaya, V. A.; Sankina, L. M. *Zh. Fiz. Khim.* 1967, *41*, 1687-90.
4. Bomshtein, A. L.; Trofimov, A. N.; Serafimov, L. A. *Zh. Prikl. Khim.* 1978, *51*, 1280-2.
5. Stephenson, R.; Stuart, J. *J. Chem. Eng. Data* 1986, *31*, 56-70.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

COMPONENTS:

(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hemptinne, A.

Z. Phys. Chem. <u>1894</u>, *13*, 561-9.

VARIABLES:

T/K = 298

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid propyl ester in water at 25°C was reported to be 5.623 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The mixture of water with excess ester was heated for some time in a water bath and the ester phase was filtered. A sample of known volume was then transferred to a smaller flask, heated with the known amount of baryta until complete saponification was obtained and then titrated. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rayman, J.

Thesis, Budapest, 1906.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of propanoic acid propyl ester in water

t/°C	g(1)/100g(2)	g(1)/100g solution (compiler)	x_1 (compiler)
0.	1.09	1.05	0.00164
10.	0.85	0.84	0.00131
20.	0.69	0.68	0.00106
30.	0.60	0.60	0.00094

These data have also been published in (ref 2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum or Merck; washed with salt water; dried over $CaCl_2$ or $CuSO_4$; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Winkler, L. *Z. Phys. Chem.* 1906, *55*, 360.
2. Hill, A.E. *International Critical Tables* (Washburn, E.W., Ed.) McGraw Hill, New York, 1928, Vol. 3, 387-98.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5] (2) Water; H_2O; [7732-18-5]	Mozzhukhin, A.S.; Serafimov, L.A.; Mitropol'skaya, V.A.; Sankina, L.M. *Zh. Fiz. Khim.* 1967, *41*, 1687-90.
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of propanoic acid propyl ester in water at 20°C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 1.6×10^{-4}.

The solubility of water in propanoic acid propyl ester at 20°C was reported to be 6.5 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.31.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described by Mozzhukhin, Serafimov, Mitropol'skaya and Rudakovskaya (ref 1) was used. The data were reported together with the ternary system propanoic acid propyl ester-water-1-propanol.

SOURCE AND PURITY OF MATERIALS:

(1) By Mozzhukhin, Mitropl'skaya, Serafimov, Torubarov and Rudakovskaya (ref 2): synthesized; distilled; impurities <0.5wt% by glc, 0.01wt% H_2O, b.p.121°C, d_4^{20} 0.8826, n_D^{20} 1.3933.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C by (ref 1).

REFERENCES:

1. Mozzhukhin, A.S.; Serafimov, L.A.; Mitropol'skaya, V.A.; Rudakovskaya, T.S. *Khim. Tekhnol. Topl. Masel* 1966, *4*, 11.
2. Mozzhukhin, A.S.; Mitropl'skaya, V.A.; Serafimov, L.A.; Torubarov, A.I.; Rudakovskaya, T.S. *Zh. Fiz. Khim.* 1967, *41*, 227.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5] (2) Water; H_2O; [7732-18-5]	Bomshtein, A.L.; Trofimov, A.N.; Serafimov, L.A. *Zh. Prikl. Khim.* 1978, *51*, 1280-2.
VARIABLES:	PREPARED BY:
T/K = 293 - 353	A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of propanoic acid propyl ester and water

t/°C	x_1 (2)-rich phase	x_1 (1)-rich phase	g(1)/100g sln (compiler) (2)-rich phase	g(1)/100g sln (compiler) (1)-rich phase
20	0.0008	0.9448	0.51	99.10
30	0.0011	0.9331	0.71	98.90
40	0.0016	0.9162	1.02	98.60
50	0.0019	0.9106	1.21	98.50
60	0.0028	0.8890	1.78	98.10
70	0.0041	0.8434	2.59	97.20
80	0.0056	0.7927	3.50	96.10

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used at constant temperature. No further details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; distilled; without impurities by glc, b.p. 122.9°C, n_D^{20} 1.392.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Propanoic acid propyl ester (*propyl propionate*); $C_6H_{12}O_2$; [106-36-5]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Stephenson, R.; Stuart, J.

J. Chem. Eng. Data 1986, *31*, 56-70.

VARIABLES:

T/K = 273 - 364

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

Mutual solubility of propanoic acid propyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	1.01	99.37	0.00158	0.9607
9.1	0.80	99.30	0.00125	0.9565
19.3	0.66	99.20	0.00103	0.9506
29.6	0.52	99.06	0.00081	0.9423
39.5	0.50	98.88	0.00078	0.9319
50.0	0.43	98.76	0.00067	0.9251
60.3	0.43	98.78	0.00067	0.9262
70.6	0.44	98.78	0.00068	0.9262
80.3	0.44	98.79	0.00068	0.9268
90.5	0.36	98.69	0.00056	0.9211
std. dev.	0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial sample; purity 98%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:

(1) Acetic acid 2-ethoxyethyl ester (*2-ethoxyethyl acetate*); $C_6H_{12}O_3$; [111-15-9]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Doolittle, A.K.

Ind. End. Chem. 1935, *27*, 1169-79.

VARIABLES:

T/K = 293

PREPARED BY:

A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 2-ethoxyethyl ester in water at 20°C was reported to be 24.7 g(1)/100g sln. The corresponding mole fraction, x_1, value calculated by the compiler is 0.0428.

The solubility of water in acetic acid 2-ethoxyethyl ester at 20°C was reported to be 9.4 g(2)/100g sln. The corresponding mole fraction, x_2, value calculated by the compiler is 0.43.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not specified.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified, commercial product; purity 96%, b.p. range 145-166°C, d_4^{20} 0.974.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

SYSTEM INDEX

Pages preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables.

REGISTRY NUMBER INDEX

Pages preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables.

AUTHOR INDEX

Pages preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables.

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