

IUPAC-NIST Solubility Data Series. 78. Acetonitrile Binary Systems

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The mutual solubilities and liquid–liquid equilibria of acetonitrile binary systems with different compounds exhaustively and critically are reviewed. The compounds include water, inorganic compounds, and a variety of organic compounds (hydrocarbons, halogenated hydrocarbons, alcohols, carboxylic acids and esters, nitrogen, and sulfur compounds). A total of 353 systems reported in the primary literature through 2000 are compiled. For 25 systems sufficient data are available to allow critical evaluation. All data are expressed as mass and mole fractions as well as the originally reported units. Similar reviews of gas, liquid, and solid solubilities for other systems are published in the of Solubility Data Series. This is the 78th volume of this series. © 2002 American Institute of Physics. [DOI: 10.1063/1.1494086]

Key words: acetonitrile; inorganic compounds; liquid–liquid equilibrium; organic solvents; solubility; water.

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1. Preface

1.1. Scope of the Volume

This volume presents a review of experimentally determined solubility data for well defined binary systems in

which one component is acetonitrile and the second component is a liquid at or near standard conditions. Acetonitrile is partially miscible in binary systems formed by various organic substances such as hydrocarbons, halogenated hydrocarbons, alcohols, acids, ethers, esters, etc., with a miscibility gap below an upper critical solubility point (UCSP).

Acetonitrile is among the best extractive solvents for the separation of paraffinic and olefinic hydrocarbons with similar boiling points. This is related to the large dipole moment of acetonitrile (3.95 D) and its molecule structure which favors association as a pure substance as well as in mixtures.

Second components for which data were found in the chemical literature include water, hydrocarbons of several structural types, halogenated hydrocarbons, mono and polyhydroxy alcohols, mono and polybasic carboxylic acids, ethers, carboxylic esters, amines, sulfur compounds and inorganic substances. An exhaustive search of the chemical literature published prior to 2000 found solubility data for 353 systems. From these, 191 compilation sheets were prepared.

Most compilations present the solubility data for one system as reported in one publication. For some original publications which report very limited data for several systems, data are grouped into a single compilation. Where two or more reliable compilations were found for a system, a critical evaluation was prepared. This was possible for only 25 systems, reflecting the sparseness of study of many acetonitrile systems. In this review the systems are ordered on the basis of the chemical formula according to the Hill system (described in the Introduction), with the exception those compilations more than one system is treated.

To the extent allowed by the available data, this volume considers mutual solubility of binary systems. That is, data for both the solubility of acetonitrile in the second component and the solubility of the second component in acetonitrile are compiled and evaluated when available.

Other solubility data which are compiled when available include the upper critical solution temperature (UCST) of binary mixtures and the influence of pressure on mutual solubility or UCST of binary systems. Numerical data reported in the primary sources were used for preparation of compilations. When data were presented only in graphical form, the compilers attempted to obtain numerical data from the original investigators. In some cases where numerical data could not be obtained in this way, the compilers extracted the numerical data from published diagrams.

This volume is the result of an exhaustive search of the chemical literature using both Chemical Abstracts and Russian Abstract Journal for Chemistry (Referativnyi Zhurnal "Khimiya"). The goal of the search was to include all published data for systems designated in the title. Russian archival sources including Deposited Documents of VINITI, scientific works (Nauchnye Trudy or Uchenye Zapiski) of Universities, Research Institutes and Educational Institutions, and materials from conferences, meetings, and symposia are also included. Each critical evaluation includes the date at the literature search closed for the system evaluated

(usually 2000). In spite of all efforts, some sources of experimental data, may have been missed. The editors will gratefully receive information about omissions.

In some original sources solubility data is reported as incidental or ancillary information to other studies. If, for this or other reasons, details concerning experimental methods, source and purity of materials, or estimated errors are brief or absent, correspondingly short entries appear in the compilations, sometimes with the note, "No further details were reported." Estimated errors were sometimes provided by the compiler with appropriate notation.

For convenience of comparison of experimental data, compilers and the evaluators of this volume, in so far as is possible, expressed all initial results in mass percent and mole fraction terms as well as in units reported in the original source. Conversions, where they were made, are clearly attributed to the compiler. Some unit conversions required numerical data for the density of pure components and/or the mixtures. Approximate values of mixture densities were obtained using calculations recommended in standard handbooks, for example Reid *et al.*¹ Definitions of mass percent and mole fraction as well as their relation to other units of solubility are given in the Introduction.

Solubility data, for a particularly system in which UCST is reported, can be described by an equation based on the scaling law with corrections terms. This equation has been also discussed by Shaw *et al.*² and has the form given by Wegner:³

$$x_1 = x_{c1} + b_1 \cdot \Theta + b_2 \cdot \Theta^{1-\alpha} + b_3 \cdot \Theta^{1-\alpha+\omega} \pm a_1 \cdot \Theta^{\beta} \pm a_2 \cdot \Theta^{\beta+\omega} \pm a_3 \cdot \Theta^{\beta+2\omega}, \quad (1)$$

where

$$\Theta = (T_c - T)/T_c. \quad (2)$$

The parameters a_1 , b_1 are adjustable. According to the above literature, the equation factors are assumed to be: $\beta = 0.329$; $\alpha = 0.11$; and $\omega = 0.5$. The equation is valid usually when $(T_c - T)/T_c > 10^{-3}$, which in the discussed systems is equivalent to the temperature range of about 0.3–0.4 K below the UCST. For the systems discussed further in the evaluation tables the equation was used generally in the simplified version without b_3 and a_3 elements.

The general properties of binary systems exhibiting liquid–liquid equilibrium and the modern theories of critical solution behavior have recently been treated in detail.²

1.2. Experimental Methods

Most solubility measurements of binary systems containing nitromethane have been made between room temperature and the UCST of the system under study. Temperatures studied range from 163 K (acetonitrile + trichlorofluoromethane) to 495 K (acetonitrile + 1,2,3-tris(octadecyloxy)propane) while the range of pressure examined extends from 0.1 to 157 MPa (acetonitrile + water). Three basic approaches to solubility measurement for binary systems are known: synthetic, titration, and ana-

lytical. Of these the synthetic (visual-polythermal, or cloud-point) method is most commonly used. Almost 75% (143) of the compilations in this volume are for data obtained using the synthetic method. In this method the temperature is determined at which turbidity associated with a second phase appears and/or disappears for a mixture of known composition, often in a sealed ampoule. This method was introduced by Alekseev (also transliterated in some older German language publications as "Alexeev" or "Alexejew") in 1876.⁴ The method has been refined and improved by Rothmund,⁵ and by Timmermans⁶ and is capable of measuring solution temperature with an error (± 0.3 mK). System pressure at the solution temperature is seldom reported since it is assumed that the effect of pressure is minor.

Two other methods are used for isothermal measurements of solubility. In the titration method one component is added to the second in small portions with vigorous mixing until persistent turbidity is observed. In the analytical method the samples of equilibrium liquid phases are analyzed by various methods: chemical or physical. Sources of error in these three methods include gravitational effects and impurities in materials whose solubilities are being determined. This has been discussed in detail.² For binary mixtures of acetonitrile and organic substances, water is a common impurity since it is difficult to remove completely from most organic liquids and is reabsorbed on exposure to air. The presence of small quantities of water can either lower the temperature of solubility (e.g., in systems of acetonitrile and alcohols) or raise these temperatures (e.g., in mixtures of acetonitrile and hydrocarbons). These effects have previously been noted in systems with nitromethane.^{7,8}

1.3. Procedure Used in Critical Evaluations

A Critical Evaluation was prepared for each system for which two or more independent reports of solubility data are available. In evaluating the available data the evaluators have considered both the data quality of individual original sources to the extent that can be established from the content (and omissions) of those reports and by comparing the results obtained independently in more than one laboratory. Several aspects of the solubility data have been considered: purity of substances and date of experiment; accuracy of the method and reproducibility of the experiment; experience of the researcher(s), and previous publications.

In critical evaluations data may be classified as *Recommended*, *Tentative*, or *Rejected*. Data are recommended if the results of two or more independent groups are in good agreement and the evaluator has no doubt of the adequacy of the experimental and computational procedures used. Data are classified as tentative if only one set of measurements is available or if the evaluator considers some aspect of the experimental or computational procedures to be mildly questionable. Data determined by an inadequate or ill-defined method are rejected. Where it is possible, Recommended or Tentative values of mutual solubility, critical solution composition, and critical solution temperature are specified at 0.1

MPa. For some systems the value (dT_c/dP) over the experimental range of pressure is given. Where sufficient data exist, the arithmetic mean of experimentally determined recommended or tentative values has been calculated.

Graphical representations of all reported data are often useful for comparing data and identifying outliers and are included in some Evaluations. These diagrams, representing the solubility data (expressed in mole fraction) can reveal whether or not a trend exists among the data in addition to highlighting any discrepancies of experimental solubility measurements.

In critical evaluations for which the UCST of the system was available, data have been described by an equation based on the scaling law. This equation allows interpolation and (less confidently) some extrapolation for the system treated. Additional equations for estimating the solubility of acetonitrile in homologous series of alcohols and alkanes are presented below; further details and backgrounds have been also presented in the preface to the IUPAC SDS, Vols. 56² and 71.⁸

For the series, alcohol–acetonitrile, and hydrocarbon–acetonitrile systems, there was a sufficient number of independently measured solubility determinations to find the general rules of behavior in the series.

The experimental solubility data of the binary acetonitrile and *n*-alcohol systems have been reported in the literature at temperatures over 293 K. The following equations have been found to describe the relationships in the acetonitrile–*n*-alcohol series (from decanol to eicosanol; *n*—number of carbon atoms):

$$T_c/K = 128.45 + 72.513 \cdot \ln(n) \quad 10 \leq n \leq 20, \quad (3)$$

$$x_{c1} = 0.2744 + 0.2099 \cdot \ln(n) \quad 10 \leq n \leq 18. \quad (4)$$

The mean standard errors of estimate in the series were 0.56 K and 0.0103 mole fraction, for Eqs. (3) and (4), respectively.

The following equations have been found to describe the relationships in the acetonitrile–*n*-alkane series:

$$T_c/K = 298.25 + 9.4961 \cdot n - 0.1295 \cdot (n)^2 \quad 4 \leq n \leq 18, \quad (5)$$

$$x_{c1} = 0.103 + 0.2712 \cdot \ln(n) \quad 4 \leq n \leq 16. \quad (6)$$

The mean standard errors of estimate in the series were 0.20 K and 0.0146 mole fraction, for Eqs. (5) and (6), respectively.

The editors wish to acknowledge with thanks the help of Dr. A. Skrzecz (Poland) and Dr. S. I. Sinegubova (Russia) who provided copies of several of the articles reviewed in this volume.

1.4. References for the Preface

- ¹R. C. Reid, J. M. Prauznitz, and B. E. Poling, *The Properties of Gases and Liquids*, 4th ed. (McGraw–Hill, New York, 1987).
²D. Shaw, A. Skrzecz, J. W. Lorimer, and A. Maczynski, *Alcohols with Hydrocarbons*, Vol. 56 of the Solubility Data Series (Oxford University Press, Oxford, 1994).

³F. Wegner, *Phys. Rev. B* **5**, 4529 (1981).

⁴V. F. Alekseev, *Zh. Fiz.-Khim. O-va* **8**, 249 (1876).

⁵V. Rothmund, *Z. Phys. Chem.* **26**, 433 (1898).

⁶J. Timmermans, *Z. Phys. Chem.* **58**, 129 (1907).

⁷V. P. Sazonov, *Zh. Obshch. Khim.* **42**, 1884 (1972).

⁸V. P. Sazonov, K. N. Marsh, and G. T. Hefter, *Niromethane with Water or Organic Solvents: Binary Systems*, Vol. 71 of the Solubility Data Series (Oxford University Press, Oxford); *J. Phys. Chem. Ref. Data* **29**, 1165 (2000).

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2. Introduction to the Solubility Data Series: Solubility of Liquids in Liquids

2.1. The Nature of the Project

The solubility data project (SDP) has as its aim a comprehensive review of published data for solubilities of gases, liquids, and solids in liquids or solids. Data of suitable precision are compiled for each publication on data sheets in a uniform format. The data for each system are evaluated and, where data from different sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values, and compiled data sheets are published on consecutive pages.

This series is concerned primarily with liquid–liquid systems, but a limited number of related solid–liquid, fluid–fluid, and multicomponent (organic–water–salt) systems are included where it is considered logical and appropriate. Solubilities at elevated and low temperatures and at elevated pressures have also been included, as it is considered inappropriate to establish artificial limits on the data presented if they are considered relevant or useful.

For some systems, the two components may be miscible in all proportions at certain temperatures and pressures. Data on reported miscibility gaps and upper and lower critical solution temperatures are included where appropriate and when available.

2.2. Compilations and Evaluations

The formats for the compilations and critical evaluations have been standardized for all volumes. A description of these formats follows.

2.2.1. Compilations

The format used for the compilations is, for the most part, self-explanatory. A compilation sheet is divided into boxes, with detailed contents described below.

Components: Each component is listed according to IUPAC name, formula, and Chemical Abstracts (CA) Registry Number. The CA name is also included if this differs from the IUPAC name, as are trivial names if appropriate. IUPAC and common names are cross-referenced to CA names in the System Index. The formula is given either in terms of the IUPAC or Hill¹ system and the choice of formula is governed

by what is usual for most current users: i.e., IUPAC for inorganic compounds, and Hill system for organic compounds. Components are ordered on a given compilation sheet according to:

- (a) saturating components;
- (b) nonsaturating components in alphanumerical order; and
- (c) solvents in alphanumerical order.

The saturating components are arranged in order according to the IUPAC 18-column periodic table with two additional rows: Columns 1 and 2: H, alkali elements, ammonium, alkaline earth elements

Columns 3–12: transition elements

Columns 13–17: boron, carbon, nitrogen groups; chalcogenides, halogens

Column 18: noble gases

Row 1: Ce–Lu

Row 2: Th to the end of the known elements, in order of atomic number.

Organic compounds within each Hill formula are ordered in the following succession:

- (a) by degree of unsaturation;
- (b) by order of increasing chain length in the parent hydrocarbon;
- (c) by order of increasing chain length of hydrocarbon branches;
- (d) numerically by position of unsaturation;
- (e) numerically by position by substitution; and
- (f) alphabetically by IUPAC name.

Example:

C ₅ H ₈	cyclopentane
	2-methyl-1,3-butadiene
	1,4-pentadiene
	1-pentyne
C ₅ H ₁₀	cyclopentane
	3-methyl-1-butene
	2-methyl-2-butene
	1-pentene
C ₅ H ₁₂	2,2-dimethylpropane
	2-methylbutane
	pentane
C ₅ H ₁₂ O	2,2-dimethyl-1-propanol
	2-methyl-1-butanol
	2-methyl-2-butanol
	3-methyl-1-butanol
	3-methyl-2-butanol
	1-pentanol
	2-pentanol
3-pentanol	
C ₆ H ₁₂ O	cyclohexanol
	4-methyl-1-penten-3-ol
	1-hexen-3-ol
	4-hexen-3-ol

Deuterated (²H) compounds immediately follow the corresponding H compounds.

Original Measurements: References are abbreviated in the forms given by Chemical Abstracts Service Source Index (CASSI). Names originally in other than Roman alphabets are given as transliterated by Chemical Abstracts. In the case of multiple entries (for example, translations) an asterisk indicates the publication used for compilation of the data.

Variables: Ranges of temperature, pressure, etc. are indicated here.

Prepared by: The names of all compilers are given here.

Experimental Values: Components are described as (1), (2), etc., as defined in the "Components" box. Data are reported in the units used in the original publication, with the exception that modern names for units and quantities are used; e.g., mass percent for weight percent; mol dm⁻³ for molar; etc. In most cases, both mass and molar values are given. Usually, only one type of value (e.g., mass percent) is found in the original paper, and the compiler has added the other type of value (e.g., mole percent) from computer calculations based on 1989 atomic weights.² Temperatures are expressed as *t*/°C, *t*/°F or *T*/K as in the original; if necessary, conversions to *T*/K are made, sometimes in the compilations, and always in the critical evaluation. However, the author's units are expressed according to IUPAC recommendations³ as far as possible.

Errors in calculations, fitting equations, etc., are noted, and where possible corrected. Material inserted by the compiler is identified by the word "compiler" or by the compiler's name in parentheses or in a footnote. In addition, compiler-calculated values of mole or mass fractions are included if the original data do not use these units. If densities are reported in the original paper, conversions from this are done in the evaluation, with the values and sources of the densities concentrations to mole fractions are included, but otherwise being quoted and referenced.

Details of smoothing equations (with limits) are included if they are present in the original publication and if the temperature or pressure ranges are wide enough to justify this procedure and if the compiler finds that the equations are consistent with the data.

The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure. In some cases graphs have been included, either to illustrate presented data more clearly, or if this is the only information in the original. Full grids are not usually inserted as it is not intended that users should read data from the graphs.

Method: The apparatus and procedure are mentioned briefly. Abbreviations used in Chemical Abstracts are often used here to save space, reference being made to sources of further detail if these are cited in the original paper.

Source and Purity of Materials: For each component, referred to as (1), (2), etc., the following information (in this order and in abbreviated form) is provided if available in the original paper: source and specified method of preparation; properties; degree of purity.

Estimated Error: If estimated errors were omitted by the original authors, and if relevant information is available, the compilers have attempted to estimate errors (identified by “compiler” or the compiler’s name in parentheses or in a footnote) from the internal consistency of data and type of apparatus used. Methods used by the compilers for estimating and reporting errors are based on Ku and Eisenhart.⁴

Comments and/or Additional Data: Many compilations include this section which provides short comments relevant to the general nature of the work or additional experimental and thermodynamic data which are judged by the compiler to be of value to the reader.

References: The format for these follows the format for the Original Measurements box, except that final page numbers are omitted. References (usually cited in the original paper) are given where relevant to interpretation of the compiled data, or where cross-reference can be made to other compilations.

2.2.2. Evaluations

The evaluator’s task is to assess the reliability and quality of the data, to estimate errors where necessary, and to recommend “best” values. The evaluation takes the form of a summary in which all the data supplied by the compiler have been critically reviewed. There are only three boxes on a typical evaluation sheet, and these are described below.

Components: The format is the same as on the Compilation sheets.

Evaluator: The name and affiliation of the evaluator(s) and date up to which the literature was checked.

Critical Evaluation: (a) Critical text. The evaluator checks that the compiled data are correct, assesses their reliability and quality, estimates errors where necessary, and recommends numerical values based on all the published data (including theses, reports, and patents) for each given system. Thus, the evaluator reviews the merits or shortcomings of the various data. Only published data are considered. Documented rejection of some published data may occur at this stage, and the corresponding compilations may be removed.

The solubility of comparatively few systems is known with sufficient accuracy to enable a set of recommended values to be presented. Although many systems have been studied by at least two workers, the range of temperatures is often sufficiently different to make meaningful comparison impossible.

Occasionally, it is not clear why two groups of workers obtained very different but internally consistent sets of results at the same temperature, although both sets of results were obtained by reliable methods. In such cases, a definitive assessment may not be possible. In some cases, two or more sets of data have been classified as tentative even though the sets are mutually inconsistent.

(b) Fitting equations. If the use of a smoothing equation is justifiable the evaluator may provide an equation representing the solubility as a function of the variables reported on

all the compilation sheets, stating the limits within which it should be used.

(c) Graphical summary. In addition to (b) above, graphical summaries are often given.

(d) Recommended values. Data are recommended if the results of at least two independent groups are available and they are in good agreement, and if the evaluator has no doubt as to the adequacy and reliability of the applied experimental and computational procedures. Data are reported as tentative if only one set of measurements is available, or if the evaluator considers some aspect of the computational or experimental method as mildly undesirable but estimates that it should cause only minor errors. Data are considered as doubtful if the evaluator considers some aspect of the computational or experimental method as undesirable but still considers the data to have some value where the order of magnitude of the solubility is needed. Data determined by an inadequate method or under ill-defined conditions are rejected. However, references to these data are included in the evaluation together with a comment by the evaluator as to the reason for their rejection.

(e) References. All pertinent references are given here, including all those publications appearing in the accompanying compilation sheets and those which, by virtue of their poor precision, have been rejected and not compiled.

(f) Units. While the original data may be reported in the units used by the investigators, the final recommended values are reported in SI units³ when the data can be converted accurately.

2.3. Quantities and Units Used in Compilation and Evaluation of Solubility Data

2.3.1. Mixtures, Solutions, and Solubilities

A *mixture*^{5,6} describes a gaseous, liquid or solid phase containing more than one substance, where the substances are all treated in the same way.

A *solution*^{5,6} describes a liquid or solid phase containing more than one substance, when for convenience one of the substances, which is called the *solvent*, and may itself be a mixture, is treated differently than the other substances, which are called *solutes*. If the sum of the mole fractions of the solutes is small compared to unity, the solution is called a *dilute solution*.

The *solubility* of a solute 1 (solid, liquid or gas) is the analytical composition of a saturated solution, expressed in terms of the proportion of the designated solute in a designated solvent.⁷

“Saturated” implies equilibrium with respect to the processes of dissolution and demixing; the equilibrium may be stable or metastable. The solubility of a substance in metastable equilibrium is usually greater than that of the same substance in stable equilibrium. (Strictly speaking, it is the activity of the substance in metastable equilibrium that is greater.) Care must be taken to distinguish true metastability from supersaturation, where equilibrium does not exist.

Either point of view, mixture or solution, may be taken in describing solubility. The two points of view find their expression in the reference states used for definition of activities, activity coefficients and osmotic coefficients. Note that the composition of a saturated mixture (or solution) can be described in terms of any suitable set of thermodynamic components.

2.3.2. Physicochemical Quantities and Units

Solubilities of solids have been the subject of research for a long time, and have been expressed in a great many ways, as described below. In each case, specification of the temperature and either partial or total pressure of the saturating gaseous component is necessary. The nomenclature and units follow, where possible.³ A few quantities follow the ISO standards⁸ or the German standard;⁹ see a review by Cvitas¹⁰ for details.

A note on nomenclature

The nomenclature of the IUPAC Green Book³ calls the solute component B and the solvent component A. In compilations and evaluations, the first-named component (component 1) is the solute, and the second (component 2 for a two-component system) is the solvent. The reader should bear these distinctions in nomenclature in mind when comparing equations given here with those in the Green Book.

1. *Mole fraction* of substance 1, x_1 or $x(1)$ (condensed phases), y_1 (gases):

$$x_1 = n_1 / \sum_{s=1}^c n_s, \quad (1)$$

where n_s is the amount of substance of s , and c is the number of distinct substances present (often the number of thermodynamic components in the system). *Mole percent* of substance 1 is $100x_1$.

2. *Ionic mole fractions* of salt i , x_{i+} , x_{i-} : For a mixture of binary salts i , each of which ionizes completely into ν_{s+} cations and ν_{s-} anions, with $\nu_s = \nu_{s+} + \nu_{s-}$ and a mixture of p nonelectrolytes j , of which some may be solvent components, a generalization of the definition in Ref. 11 gives:

$$x_{i+} = \frac{\nu_{i+}x_{i+}}{1 + \sum_{i=1}^s (\nu_i - 1)x_i}, \quad x_{i-} = \frac{\nu_{i-}x_{i-}}{\nu_{i+}}, \quad i = 1, \dots, s, \quad (2)$$

$$x_j' = \frac{x_j}{1 + \sum_{i=1}^s (\nu_i - 1)x_i}, \quad j = (s+1), \dots, p. \quad (3)$$

The sum of these mole fractions is unity, so that, with $c = s + p$,

$$\sum_{i=1}^s (x_{i+} + x_{i-}) + \sum_{i=s+1}^c x_i' = 1. \quad (4)$$

General conversions to other units in multicomponent systems are complicated. For a three-component system containing nonelectrolyte 1, electrolyte 2 and solvent 3.

$$x_1 = \frac{\nu_{2+}x_1'}{\nu_{2+} - (\nu_2 - 1)x_{2+}}, \quad x_2 = \frac{x_{2+}}{\nu_{2+} - (\nu_2 - 1)x_{2+}}. \quad (5)$$

These relations are used in solubility equations for salts, and for tabulation of salt effects on solubilities of gases (see below).

3. *Mass fraction* of substance 1, w_1 or $w(1)$:

$$w_1 = g_1 / \sum_{s=1}^c g_s, \quad (6)$$

where g_s is the mass of substance s . *Mass percent* of substance 1 is $100 w_1$. The equivalent terms *weight fraction*, *weight percent*, and *g(1)/100g solution* are no longer used.

4. *Molality* of solute 1 in a solvent 2, m_1 :

$$m_1 = n_1 / n_2 M_2. \quad (7)$$

SI base units: mol kg^{-1} . Here, M_2 is the molar mass of the solvent.

5. *Aquamolality*, *Solvomolality* of substance 1 in a mixed solvent with components 2, 3 (12), $m_1^{(3)}$:

$$m_1^{(3)} = m_1 \bar{M} / M_3 \quad (8)$$

SI base units: mol kg^{-1} . Here, the average molar mass of the solvent is

$$\bar{M} = x_2' M_2 + (1 - x_2') M_3 \quad (9)$$

and x_2' is the solvent mole fraction of component 2. This term is used most frequently in discussing comparative solubilities in water (component 2) and heavy water (component 3) and in their mixtures.

6. *Amount concentration* of solute 1 in a solution of volume V , c_1 :

$$c_1 = [\text{formula of solute}] = n_1 / V \quad (10)$$

SI base units: mol m^{-3} . The symbol c_1 is preferred to [formula of solute], but both are used. The old terms *molarity*, *molar*, and *moles per unit volume* are no longer used.

7. *Mass concentration* of solute 1 in a solution of volume V , ρ_1 : SI base units: kg m^{-3}

$$\rho_1 = g_1 / V. \quad (11)$$

8. *Mole ratio*, $r_{A,B}$ (dimensionless)¹⁰

$$r_{A,B} = n_1 / n_2. \quad (12)$$

Mass ratio, symbol $\zeta_{A,B}$, may be defined analogously.¹⁰

Mole and mass fractions are appropriate to either the mixture or the solution point of view. The other quantities are appropriate to the solution point of view only. Conversions between pairs of these quantities can be carried out using the equations given in Table 1 at the end of this Introduction. Other useful quantities will be defined in the prefaces to individual volumes or on specific data sheets.

9. *Density*, ρ :

$$\rho = g / V \quad (13)$$

TABLE 1. Interconversions between quantities used as measures of solubilities c -component systems containing $c-1$ solutes i and single solvent c (ρ —density of solution; M_i —molar masses of i . For relations for two-component systems, set summations to 0.)

	x_i	w_i	m_i	c_i
$x_i =$	x_i	$\frac{1}{1 + \frac{M_i}{M_c} \left(\frac{1}{w_i} - 1 + \sum_{j \neq i}^{c-1} \left(\frac{M_c}{M_j} - 1 \right) \frac{w_j}{w_i} \right)}$	$\frac{1}{1 + \frac{1}{m_i M_c} + \sum_{j \neq i}^{c-1} \frac{m_j}{m_i}}$	$\frac{1}{1 + \frac{1}{M_c} \left(\frac{\rho}{c_i} - M_i \right) + \sum_{j \neq i}^{c-1} \frac{c_j}{c_i} \left(1 - \frac{M_j}{M_c} \right)}$
$w_i =$	$\frac{1}{1 + \frac{M_c}{M_i} \left(\frac{1}{x_i} - 1 + \sum_{j \neq i}^{c-1} \left(\frac{M_j}{M_c} - 1 \right) \frac{x_j}{x_i} \right)}$	w_i	$\frac{1}{1 + \frac{1}{m_i M_i} \left(1 + \sum_{j \neq i}^{c-1} m_j M_j \right)}$	$\frac{c_i M_i}{\rho}$
$m_i =$	$\frac{1}{M_c \left(\frac{1}{x_i} - 1 - \sum_{j \neq i}^{c-1} \frac{x_j}{x_i} \right)}$	$\frac{1}{M_i \left(\frac{1}{w_i} - 1 - \sum_{j \neq i}^{c-1} \frac{w_j}{w_i} \right)}$	m_i	$\frac{1}{\frac{1}{c_i} \left(\rho - \sum_{j \neq i}^{c-1} c_j M_j \right) - M_i}$
$c_i =$	$\frac{\rho}{M_i + M_c \left(\frac{1}{x_i} - 1 + \sum_{j \neq i}^{c-1} \left(\frac{M_j}{M_c} - 1 \right) \frac{x_j}{x_i} \right)}$	$\frac{\rho w_i}{M_i}$	$\frac{\rho}{\frac{1}{m_i} \left(1 + \sum_{j \neq i}^{c-1} m_j M_j \right) + M_j}$	c_i

SI base units: kg m^{-3} . Here g is the total mass of the system.

10. *Relative density*, $d = \rho/\rho^\circ$: the ratio of the density of a mixture at temperature t , pressure p to the density of a reference substance at temperature t' , pressure p' . For liquid solutions, the reference substance is often water at 4°C , 1 bar. (In some cases 1 atm is used instead of 1 bar.) The term *specific gravity* is no longer used.

Thermodynamics of Solubility Thermodynamic analysis of solubility phenomena provides a rational basis for the construction of functions to represent solubility data, and thus aids in evaluation, and sometimes enables thermodynamic quantities to be extracted. Both these are often difficult to achieve because of a lack of experimental or theoretical activity coefficients. Where thermodynamic quantities can be found, they are not evaluated critically, since this task would involve examination of a large body of data that is not directly relevant to solubility. Where possible, procedures for evaluation are based on established thermodynamic methods. Specific procedures used in a particular volume will be described in the Preface to that volume.

2.4. References for the Introduction

¹E. A. Hill, *J. Am. Chem. Soc.* **22**, 478 (1900).

²IUPAC Commission on Atomic Weights and Isotopic Abundances, *Pure Appl. Chem.* **63**, 975 (1989).

³I. Mills *et al.*, eds., *Quantities, Units and Symbols in Physical Chemistry*

(The Green Book) (Blackwell Scientific Publications, Oxford, UK, 1993).

⁴H. H. Ku, p. 73; C. Eisenhart, p. 69; in H. H. Ku, ed., *Precision Measurement and Calibration*, NBS Special Publication 300 (Washington, 1969), Vol. 1.

⁵J. Regaudy and S. P. Klesney, *Nomenclature of Organic Chemistry* (IUPAC), (The Blue Book) (Pergamon, Oxford, 1979).

⁶V. Gold *et al.*, eds. *Compendium of Chemical Technology* (The Gold Book) (Blackwell Scientific Publications, Oxford, UK, 1987).

⁷H. Freiser and G. H. Nancollas, eds., *Compendium of Analytical Nomenclature* (The Orange Book) (Blackwell Scientific Publications, Oxford, UK, 1987), Sect. 9.1.8.

⁸ISO Standards Handbook, *Quantities and Units* (International Standards Organization, Geneva, 1993).

⁹German Standard, DIN 1310, *Zusammensetzung von Mischphasen* (Beuth Verlag, Berlin, 1984).

¹⁰T. Cvitaš, *Chem. International* **17**, 123 (1995).

¹¹R. A. Robinson and R. H. Stokes, *Electrolyte Solutions*, 2nd ed. (Butterworths, London, 1959).

¹²J. W. Lorimer, R. Cohen-Adad, and J. W. Lorimer, *Alkali Metal and Ammonium Chlorides in Water and Heavy Water (Binary Systems)*, IUPAC Solubility Data Series, Vol. 47 (Pergamon Press, Oxford, UK, 1991), p. 495.

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3. Acetonitrile+Water, Deuterium Compounds

3.1. Acetonitrile + Water

Components:	Evaluator:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Water; H ₂ O; [7732-18-5]	Valerii P. Sazonov, Technical University, Samara, Russia, August, 2001.

Critical Evaluation

Quantitative solubility data for the acetonitrile (1) + water (2) have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system acetonitrile+water

Reference	T/K	Solubility	Method
Evert ¹	269–272	Mutual	Synthetic
Schneider ²	249–272	Mutual	Synthetic
Armitage <i>et al.</i> ³	269–272	Mutual	Synthetic
Moollel and Schneider ⁴	259–273	Mutual	Synthetic
Benter and Schneider ⁵	264–272	Mutual	Titration
Pavlova <i>et al.</i> ⁶	271	UCST	Synthetic
Vuks <i>et al.</i> ⁷	270–273	Mutual	Synthetic
Szydowski and Szykula ⁸	260–272	Mutual	Synthetic

In addition to these data Francis⁹ reported the upper critical solution temperature and Schneider² reported extensive measurements of the mutual solubility of components (1) and (2) determined between 0.1 and 157 MPa. All original data are compiled in the data sheets immediately following this Critical Evaluation.

The water-rich phase data of Evert¹ and Moollel and Schneider⁴ and acetonitrile-rich phase data of Armitage *et al.*³ disagree markedly from all other studies and are rejected. All other reported data are included in the tables below.

Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*) and (#) respectively. "Best" values are arithmetic means. The variance values (σ_n) attached to these values solubilities are best regarded only as a convenient representation of the spread of values rather than as error limits. The letter (R) designates "recommended" data. Data are "recommended" if two or more apparently reliable studies are in reasonable ($\pm 5\%$ relative) agreement. All other data are regarded as tentative only. (See Tables 2 and 3.)

TABLE 2. Tentative and recommended (R) values for the solubility of acetonitrile (1) in water (2)

T/K	Solubility, 100 w ₁	
	Reported values	"Best" values ($\pm \sigma_n$)
		100 w ₁ x ₁
263.0	31.8# (Ref. 5), 31.6* (Ref. 8)	31.7±0.1 (R) 0.169
265.0	32.0# (Ref. 4), 33.0* (Ref. 5), 33.8* (Ref. 8)	32.9±0.7 (R) 0.177
267.0	34.8 (Ref. 2), 34.0* (Ref. 4), 35.9* (Ref. 5), 36.0* (Ref. 8)	35.2±0.8 (R) 0.193
269.0	38.7* (Ref. 2), 34.8* (Ref. 3), 37.3* (Ref. 4), 39.5* (Ref. 5), 39.9* (Ref. 8)	38.2±1.8 (R) 0.213
270.0	38.5* (Ref. 1), 41.9* (Ref. 2), 38.7* (Ref. 3), 39.6* (Ref. 4), 42.1* (Ref. 5), 42.1* (Ref. 8)	40.5±1.6 (R) 0.230
271.0	43.6* (Ref. 1), 48.2* (Ref. 2), 42.8* (Ref. 3), 41.9* (Ref. 4), 46.2* (Ref. 5), 47.8* (Ref. 7), 45.3* (Ref. 8)	45.1±2.3 0.265
271.5	46.1 (Ref. 1), 51.3* (Ref. 2), 47.6* (Ref. 3), 49.8* (Ref. 5), 50.5* (Ref. 7), 48.7* (Ref. 8)	48.1±1.8 (R) 0.289

TABLE 3. Tentative and Recommended (R) values for the solubility of water (2) in acetonitrile (1)

T/K	Solubility, 100 w ₂	
	Reported values	"Best" values ($\pm \sigma_n$)
		100 w ₂ x ₂
259.0	14.8* (Ref. 4)	14.8 0.283
261.0	16.0* (Ref. 4), 16.6* (Ref. 8)	16.3±0.3 (R) 0.307
263.0	17.3* (Ref. 4), 18.3* (Ref. 8)	17.8±0.5 (R) 0.330
265.0	18.8* (Ref. 4), 20.7* (Ref. 5), 20.2* (Ref. 8)	19.9±0.8 (R) 0.361
267.0	20.9* (Ref. 4), 23.3* (Ref. 5), 22.5* (Ref. 8)	22.2±1.0 (R) 0.394
269.0	25.1* (Ref. 1), 26.9* (Ref. 2), 24.3* (Ref. 4), 26.8* (Ref. 5), 25.7* (Ref. 8)	25.8±1.0 (R) 0.442
270.0	29.8* (Ref. 1), 26.8* (Ref. 4), 29.6* (Ref. 5), 28.0* (Ref. 8)	28.6±1.2 (R) 0.477
271.0	33.6* (Ref. 1), 30.0* (Ref. 4), 33.8* (Ref. 5), 31.3* (Ref. 8)	32.2±1.6 (R) 0.520
271.5	35.5* (Ref. 1), 31.6* (Ref. 4), 37.2* (Ref. 5), 34.7* (Ref. 8)	34.8±2.0 0.549

The interpolated values reported in the tables above were approximated using an equation based on the scaling law (described in the preface) for which following parameters were derived:

$$a_1=0.6490, a_2=0.6548, b_1=-3.9498, b_2=3.8298$$

(mean standard error of estimate was 0.0065).

For this approximation the recommended values of UCST and x_{c1} have been used. The calculated compositions are within the stated accuracy of the tables at each point. The calculated relationship is presented in Fig. 1 together with the values from Refs. 1–5, 8.

The UCST was reported to be 271.0 K,⁶ 271.80 K,⁵ 271.812 K,⁸ 272.1 K,² 272.10 K,³ 272.3 K,⁹ 272.7 K,⁷ and 272.9 K.⁴ Thus, the recommended value is: UCST=(272.1±0.6) K.

The corresponding critical solution composition was reported to be $x_{c1}=0.350$,⁴ $x_{c1}=0.353$,² $x_{c1}=0.360$,³ $x_{c1}=0.365$,⁸ $x_{c1}=0.380$,³ and $x_{c1}=0.40$.⁷ The data Vuks *et al.*⁷ is rejected. The remaining data give an average $x_{c1}=0.36\pm 0.01$ (100 w₁=56), which is recommended.

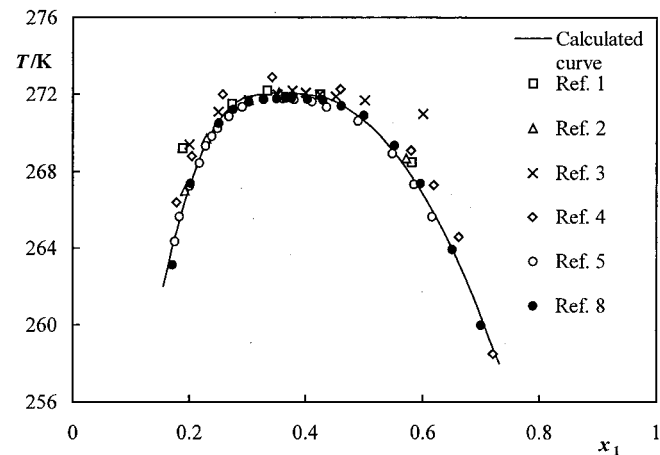


FIG. 1. Mutual solubility of acetonitrile and water.

Components:(1) Acetonitrile; C₂H₃N; [75-05-8]
(2) Water; H₂O; [7732-18-5]**Original Measurements:**M. Evert, Bull. Soc. Chim. Belg. **46**, 90-2 (1937).**Variables:**

T/K = 269-272

Prepared By:

Valerii P. Sazonov

Experimental Data

Mutual solubility of acetonitrile (1) and water (2)

t/°C	T/K (complier)	x ₁		x ₁	100 w ₁ (complier)	100 w ₁ (complier)
		Water-rich phase	Acetonitrile-rich phase			
-47	268.5	—	—	0.580	—	75.0
-4.0	269.2	0.188	—	—	34.5	—
-1.7	271.5	0.273	—	—	46.1	—
-1.2	272.0	—	—	0.424	—	62.6
-1.0	272.2	0.333	—	—	53.2	—

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used.

Source and Purity of Materials:(1) Koch-Light; puriss; dried over phosphorus pent oxide and twice distilled.
(2) Not specified.**Estimated Error:**

Not reported.

References:

- ¹M. Evert, Bull. Soc. Chim. Belg. **46**, 90 (1937).
- ²G. Schneider, Z Phys. Chem. (Munich) **41**, 327 (1964).
- ³D. A. Armitage, M. J. Blandamer, M. J. Foster, N. J. Hadden, K. W. Morcom, M. C. R. Symons, and M. J. Wooten, Trans. Faraday Soc. **64**, 1193 (1968).
- ⁴M. Moolle and H. Schneider, Z Phys. Chem. (Munich) **74**, 237 (1971).
- ⁵G. Benter and H. Schneider, Ber. Bunsen-Ges. Phys. Chem. **77**, 997 (1973).
- ⁶O. P. Pavlova, A. A. Gailé, V. A. Proskuryakov, and I. F. Li, Zh. Fiz. Khim. **49**, 2874 (1975).
- ⁷M. F. Vaks, E. P. Kulikova, and L. V. Shurpova, Molecular Physic and Biophysic Aqua-systems (in Russian), Leningrad (4), 65 (1979).
- ⁸J. Szydlowski and M. Szykula, Fluid Phase Equilib. **154**, 79 (1999).
- ⁹A. W. Francis, Critical Solution Temperature, Washington, Adv. Chem. Ser. **31** (1961).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	G. Schneider, Z Phys. Chem. (Munich) 41 , 327-38 (1964).
(2) Water; H ₂ O; [7732-18-5]	
Variables:	Prepared By:
T/K = 228-272; P/MPa 0.1-157	Valerii P. Sazonov

Experimental Data

TABLE 1. Mutual solubility of acetonitrile (1) and water (2) at 0.1 Mpa

t/°C	T/K (compiler)	Water-rich phase		Acetonitrile-rich phase	
		100 w ₁	x ₁ (compiler)	100 w ₁	x ₁ (compiler)
-10.7 ^a	262.5	—	—	90.0	0.801
-7.4 ^a	265.8	15.7	0.077	—	—
-6.2	267.0	34.8	0.192	—	—
-4.5	268.7	—	—	74.9	0.571
-3.5	269.7	40.0	0.229	—	—
-1.2	272.0	—	—	55.3	0.356
-1.1	272.1	55.0	0.353	55.0	0.353 (UCST)

^aSolid-liquid equilibrium.

Monotectic equilibrium occurs at -10.0 °C (263.2 K, compiler).

A eutectic was reported at -45.6 °C (227.6 K, compiler).

TABLE 2. Solubility temperatures of mixtures of (1) and (2) depending on pressure

100 w ₁	x ₁ (compiler)	P/MPa	t/°C	T/K (compiler)	100 w ₁	x ₁ (compiler)	P/MPa	t/°C	T/K (compiler)
34.8	0.192	39.6	-14.5	258.7	57.8	0.379	62.6	-9.7	263.5
		73.2	-18.6	254.6			64.6	-9.7	263.5
		84.3	-19.8	253.4			79.8	-11.7	261.5
		94.9	-20.7	252.5			90.9	-13.0	260.2
40.0	0.229	29.7	-9.1	264.1			94.9	-13.4	259.8
		59.6	-13.6	259.6			140.4	-17.5	255.7
		88.9	-17.3	255.9	74.9	0.571	19.8	-7.7	265.5
		119.2	-20.0	252.2			39.4	-9.8	263.4
57.8	0.379	19.8	-3.9	269.3			59.6	-12.8	260.4
		24.8	-4.7	268.5			78.8	-14.9	258.3
		34.3	-5.9	267.3			99.0	-16.8	256.4
		49.5	-7.9	265.3			119.2	-18.5	254.7
							138.4	-20.2	252.0

Four-phase (two liquid and two solid) equilibrium is realized at -24.2 °C (249.0 K, compiler) and 125.2 MPa.

Region of immiscibility disappears at -19.0 °C (254.2 K, compiler) and 156.6 MPa.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used as reported elsewhere.¹

Source and Purity of Materials:

(1) Fluka AG; pure grade; twice distilled; purity better than 99.8 mole %; melting point = -43.9 °C.
(2) Twice distilled.

Estimated Error:

Not reported.

References:

¹G. Schneider, Z Phys. Chem. (Munich) **37**, 333 (1963).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	D. A. Armitage, M. J. Blandamer, M. J. Foster, N. J. Hiden, K. W. Morcom, M. C. R. Symons, and M. J. Wooten, Trans. Faraday Soc. 64 , 1193-1200 (1968).
(2) Water; H ₂ O; [7732-18-5]	
Variables:	Prepared By:
T/K = 269-272	Valerii P. Sazonov

Experimental Data

The mutual solubility of acetonitrile (1) and water (2) in mole fractions was reported over the temperature range in graphical form. The data presented here were extracted from the published graphs by the compiler.

t/°C	T/K (compiler)	Mutual solubility of acetonitrile (1) and water (2)	
		Water-rich phase	Acetonitrile-rich phase
-3.8	269.4	0.200	36.3
-2.2	271.0	—	—
-2.1	271.1	0.250	43.2
-1.5	271.7	0.302	49.6
-1.3	271.9	—	—
-1.2	272.0	0.351	55.2
-1.1	272.1	—	—
-1.0	272.2	0.377	58.00

The upper critical solution temperature is -1.05 ± 0.15 °C at x₁ = 0.38 ± 0.02.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A mixture of (1) and (2) contained in a spectrophotometer cell, was placed in a Unicam SP770 thermostated cell holder. The temperature was measured using a thermocouple inside the cell. The transition of the liquid mixture was monitored at 16 000 cm⁻¹ as a function of temperature, the temperature falling by approximately 1° in 3 min. Dry nitrogen was passed through the cell compartment to stop condensation on the cell windows. The temperature was noted at which the transmittance fell sharply below 100%, the experiment being repeated for a series of liquid mixtures of various compositions.

Source and Purity of Materials:

(1) Koch-Light; puriss; dried over phosphorus pentoxide and twice distilled.
(2) Millipore Milli-Q; quality.

Estimated Error:

Temperature: ± 0.1 K.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	G. Benter and H. Schneider; Ber. Bunsen-Ges. Phys. Chem. 77, 997-9 (1973).
(2) Water; H ₂ O; [7732-18-5]	
Variables:	Prepared By:
T/K = 264-272	Valerii P. Sazonov

Experimental Data

The mutual solubility of acetonitrile (1) and water (2) in mole fractions was reported over the temperature range in graphical form. The data presented here were extracted from the published graphs by the compiler.

t/°C	T/K (compiler)	Mutual solubility of acetonitrile (1) and water (2)		100 w ₁ (compiler)	100 w ₂ (compiler)
		x ₁	x ₂		
-8.80	264.35	0.174	—	32.4	—
-7.50	265.65	0.182	—	33.6	78.4
-5.90	267.25	0.200	—	36.3	—
5.80	267.35	—	0.584	—	76.2
-4.70	268.45	0.216	—	38.6	—
-4.20	268.95	—	0.547	—	73.3
-3.80	269.35	0.227	—	40.1	—
-3.30	269.85	0.238	—	41.6	—
-2.90	270.25	0.248	—	42.9	—
-2.50	270.65	—	0.488	—	68.5
-2.30	270.85	0.267	—	45.3	—
-1.80	271.35	0.290	—	48.2	63.7
-1.50	271.65	—	0.410	—	61.3
-1.40	271.75	0.327	—	52.5	58.2
-1.35	271.80	0.360	—	56.2	56.2 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The turbidimetric titration method was used. A weighed amount of solution was placed in the mixing chamber described in work¹ and the temperature was varied until the opalescence showed that a phase separation occurred.

Source and Purity of Materials:

(1) Merck; synthetic grade; dried using molecular sieves and twice distilled in a fractionating column under a nitrogen atmosphere; concentration of impurities to be less than 0.003 mole % by GLC.
(2) De-ionized; twice distilled in a quartz apparatus.

Estimated Error:

Temperature: ±0.05 K.

References:

¹M. Moollel and H. Schneider; Zh. Phys. Chem. (Munich) 74, 237 (1971).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	M. Moollel and H. Schneider, Z. Phys. Chem. (Munich) 74, 237-47 (1971).
(2) Water; H ₂ O; [7732-18-5]	
Variables:	Prepared By:
T/K = 259-273	Valerii P. Sazonov

Experimental Data

Mutual solubility of acetonitrile (1) and water (2)

t/°C	T/K (compiler)	Mutual solubility of acetonitrile (1) and water (2)		100 w ₁ (compiler)	100 w ₂ (compiler)
		x ₁	x ₂		
-14.7	258.5	—	0.7216	—	85.52
-8.6	264.6	—	0.6625	—	81.72
-6.8*	266.4	0.1777	—	32.99	—
-5.9	267.3	—	0.6186	—	78.70
-4.4	268.8	0.2044	—	36.92	—
-4.1	269.1	—	0.5797	—	75.86
-1.2	272.0	0.2571	—	44.08	—
-0.9	272.3	—	0.4591	—	65.91
-0.3	272.9	0.3420	—	54.21	—

UCST was reported at 272.9 K at x_{1,c} = 0.350 (100 w₁ = 55.1, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solutions were prepared by weighing the components. Phase separation was followed optically by determining the temperature at which opalescence in a single phase or the disappearance of the phase boundary in a mixed phase occurred. This temperature was measured by means of a thermistor, which dipped into the experimental solution; about 4 mL in volume, kept stirred in a three-walled container and directly observed through a glass window. Through the inner mantle of the container, thermostated water was circulated; the outer mantle was evacuated to avoid condensation of atmospheric moisture on the observation window, as the temperature was lowered. The temperature variation was at the rate of about 0.2 °C·min⁻¹.

Source and Purity of Materials:

(1) Fluka; puriss.; purity > 99.5 mole %; not purified.
(2) Twice distilled.

Estimated Error:

Temperature: ±0.1 K.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	M. F. Vaks, E. P. Kulikova, and L. V. Shurupova, Molecular Physics and Biophysical aqua-systems (in Russian), Leningrad (4), 65-71 (1979).
(2) Water; H ₂ O; [7732-18-5]	
Variables:	Prepared By:
T/K = 270-273	Valerii P. Sazonov

Experimental Data

The mutual solubility of acetonitrile (1) and water (2) in mole fractions was reported over the temperature range in graphical form. The data presented here were extracted from the published graphs by the compiler.

t/°C	T/K (compiler)	Mutual solubility of acetonitrile (1) and water (2)		100 w ₁ (compiler)	x ₁	100 w ₁ (compiler)
		Water-rich phase	Acetonitrile-rich phase			
-2.9	270.3	0.26	—	44	—	—
-0.7	272.5	0.36	—	56	—	—
-0.6	272.6	—	0.43	—	0.43	63
-0.5	272.7	0.40	0.40	60	0.40	60 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. No experimental details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified.
(2) Source not specified; purity not specified.

Estimated Error:

Not reported.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	O. P. Pavlova, A. A. Galle, V. A. Proskuryakov, and I. F. Li, Zh. Fiz. Khim. 49 , 2874-6 (1975).
(2) Water; H ₂ O; [7732-18-5]	
Variables:	Prepared By:
T/K = 271	Valerii P. Sazonov

Experimental Data

The UCST was reported to be -2.2 °C (271.0 K, compiler).

Auxiliary Information

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not reported.

Method/Apparatus/Procedure:

The synthetic method was used. No experimental details given.

3.2. + Water-d₂

Components:		Evaluator:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valerii P. Sazonov, Technical University, Samara, Russia, August, 2001.		
(2) Water-d ₂ ; D ₂ O; [7789-20-0]			

Critical Evaluation

Solubilities in the system comprising acetonitrile and water-d₂ have been reported in three publications. Poppe¹ determined the upper critical solution temperature by the synthetic method. Vukš *et al.*² measured the mutual solubilities of (1) and (2) between 275 and 279 K using the synthetic method and these data were presented in graphical form only. Szydlowski and Szykula³ studied the mutual solubility of (1) and (2) between 253 and 279 K by the synthetic method.

The upper critical solution temperature has been reported as 278.3 K,¹ 278.534 K,³ and 278.8 K.² The data¹⁻³ are in reasonable agreement and thus their average value: UCST = (278.5 ± 0.2) K is recommended. The corresponding critical solution composition has been reported in as $x_{c1} = 0.362^3$ and $x_{c1} = 0.40^2$.

All experimental values reported in Vukš *et al.*² and Szydlowski and Szykula³ (treated with the same weighing factor) have been approximated by an equation based on the scaling law (described in the introduction to this volume) with the following parameters:

$$a_1 = 0.7317, \quad a_2 = 0.0619, \quad b_1 = -0.4528, \quad b_2 = 1.2268$$

(mean standard error of estimate was 0.0098).

For approximation values of x_{c1} and UCST determined by Szydlowski and Szykula³ have been used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with experimental points,^{2,3} are also presented in Fig. 2.

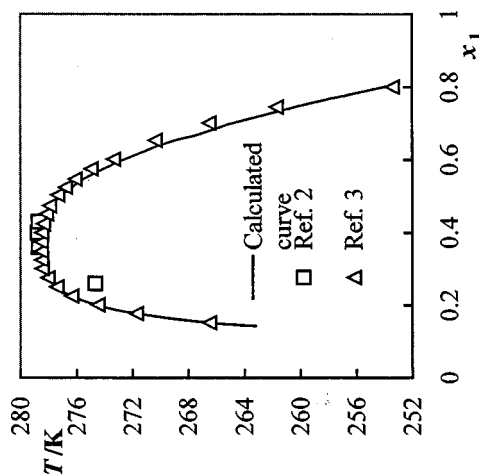


FIG. 2. Mutual solubility of acetonitrile and water-d₂.

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	J. Szydlowski and M. Szykula, Fluid Phase Equilib. 154 , 79–87 (1999).		
(2) Water; H ₂ O; [7732-18-5]			
Variables:		Prepared By:	
T/K = 260–272		Valerii P. Sazonov	

		Experimental Data		Mutual solubility of acetonitrile (1) and water (2)	
T/K	t/°C (compiler)	Water-rich phase		Acetonitrile-rich phase	
		x_1	100 w ₁ (compiler)	x_1	100 w ₁ (compiler)
259.969	-13.181	—	—	0.700	84.2
263.143	-10.007	0.170	31.8	—	—
263.925	-9.225	—	—	0.650	80.9
267.387	-5.763	0.201	36.4	—	—
267.387	-5.763	—	—	0.595	77.0
269.365	-3.785	—	—	0.550	73.6
270.519	-2.631	0.250	43.2	—	—
270.924	-2.226	—	—	0.498	69.3
271.231	-1.919	0.274	46.2	—	—
271.433	-1.717	—	—	0.460	66.0
271.611	-1.539	0.301	49.5	—	—
271.732	-1.418	—	—	0.428	63.0
271.766	-1.384	0.326	52.4	—	—
271.778	-1.372	—	—	0.402	60.5
271.802	-1.348	0.349	55.0	—	—
271.812	-1.338	—	—	0.375	57.7
271.812	-1.338	0.365	56.7	0.365	56.7 (UCST)

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used with a simplified version of the apparatus described in Ref. 1. Temperature was changed at the rate <0.01 K/min; there was no visible influence of the rate on the transition temperature up to the rate 0.1 K/min. Due to the very weak turbidity a long capillary cell was employed. A 5 mW Polytec HeNe laser was used as a probe for detecting the phase separation.

Source and Purity of Materials:

(1) Byk-Malinekrodt; AR; carefully purified by the column distillation; purity of the collected fractions: at least 99.95 mass %.
(2) Millipore Milli-Q; quality.

Estimated Error:

Temperature: ± 5 mK.

References:

J. Szydlowski, L. P. Rebelo, and W. A. Van Hook, Rev. Sci. Instrum. **63**, 1717 (1992).

Tentative values of mutual solubility of acetonitrile and water- d_2

T/K	Water- d_2 -rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
263.2	0.143	25.5	0.717	83.9
265.2	0.148	26.3	0.697	82.5
267.2	0.155	27.3	0.670	80.6
269.2	0.163	28.5	0.650	79.2
271.2	0.174	30.2	0.622	77.1
273.2	0.188	32.2	0.591	74.8
275.2	0.208	35.0	0.553	71.7
276.2	0.223	37.0	0.528	69.6
277.2	0.244	39.8	0.497	66.9
277.7	0.259	41.7	0.476	65.1
278.0	0.272	43.4	0.459	63.5
278.2	0.285	45.0	0.444	62.1
278.3	0.293	45.9	0.435	61.2
278.4	0.304	47.2	0.422	59.9

References:

- ¹G. Poppe, Bull. Soc. Chim. Belg. **44**, 640 (1935).
²M. F. Yaks, E. P. Kulikova, and L. V. Shurpova, Molecular Physic and Biophysic aqua-systems (in Russian), Leningrad (4), 65 (1979).
³J. Szydłowski and M. Szykula, Fluid Phase Equilib. **154**, 79 (1999).

Components:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) Water- d_2 ; D₂O; [7789-20-0]

Original Measurements:

G. Poppe, Bull. Soc. Chim. Belg. **44**, 640–57 (1935).

Variables:

T/K = 278

Prepared By:

Valerii P. Sazonov

Experimental Data

The UCST was reported to be 5.1 °C (278.3 K, compiler).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Observations were carried out in sealed tubes in the presence of the vapor phase. A thermostating cylinder was also used to control the temperature.

Source and Purity of Materials:

- (1) Obtained from the Bureau Etalons Physico-Chimiques.
 (2) Obtained from the Bureau Etalons Physico-Chimiques.

Estimated Error:

Not reported.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	J. Szydłowski and M. Szykula, Fluid Phase Equilib. 154 , 79–87 (1999).
(2) Water-d ₂ ; D ₂ O; [7789-20-0]	
Variables:	Prepared By:
T/K = 253–279	Valerii P. Sazonov

		Experimental Data			
		Mutual solubility of acetonitrile (1) and water-d ₂ (2)			
		Water-d ₂ -rich phase		Acetonitrile-rich phase	
T/K	t/°C (compiler)	x ₁	100 w ₁ (compiler)	x ₁	100 w ₁ (compiler)
253.417	-19.733	—	—	0.800	89.1
261.701	-11.449	—	—	0.745	85.7
266.526	-6.624	0.152	26.9	0.702	82.8
270.346	-2.804	—	—	0.653	79.4
271.757	-1.393	0.177	30.6	—	—
273.361	0.211	—	—	0.601	75.5
274.498	1.348	0.201	34.0	—	—
274.988	1.838	—	—	0.575	73.5
276.103	2.953	—	—	0.547	71.2
276.359	3.209	0.226	37.4	—	—
276.811	3.661	—	—	0.524	69.3
277.359	4.209	—	—	0.503	67.5
277.427	4.277	0.250	40.6	—	—
277.936	4.786	—	—	0.473	64.8
278.056	4.906	0.276	43.9	—	—
278.155	5.005	—	—	0.450	62.6
278.391	5.241	—	—	0.424	60.1
278.463	5.313	0.302	47.0	—	—
278.490	5.340	—	—	0.400	57.7
278.504	5.354	0.326	49.8	—	—
278.534	5.384	0.350	52.5	—	—
278.535	5.385	—	—	0.375	55.2

UCST was reported at 278.534±0.005 K at x_{1,c}=0.362±0.002 (100 w₁=53.8, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used with a simplified version of the apparatus described in the work.¹ Temperature was changed at the rate <0.01 K/min—there was no visible influence of the rate on the transition temperature up to the rate 0.1 K/min. Due to the very weak turbidity a long capillary cell was employed. A 5 mW Polytec HeNe laser was used as a probe for detecting the phase separation.

Source and Purity of Materials:

- (1) Byk-Malincrodt; AR; carefully purified by the column distillation; purity of the collected fractions at least 99.95 mass %.
- (2) From Institute of Atomic Energy, Isotope Distribution Center; 99.92 % D₂; twice distilled.

Estimated Error:

Temperature: ±5 mK.

References:

- ¹J. Szydłowski, L. P. Rebelo, and W. A. Van Hook, Rev. Sci. Instrum. **63**, 1717 (1992).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	M. F. Vuks, E. P. Kulikova, and L. V. Shurupova, Molecular Physic and Biophysic aqua-systems (in Russian), Leningrad (4), 65–71 (1979).
(2) Water-d ₂ ; D ₂ O; [7789-20-0]	
Variables:	Prepared By:
T/K = 275–279	Valerii P. Sazonov

		Experimental Data			
		Mutual solubility of acetonitrile (1) and water-d ₂ (2)			
		Water-d ₂ -rich phase		Acetonitrile-rich phase	
T/K	t/°C (compiler)	x ₁	100 w ₁ (compiler)	x ₁	100 w ₁ (compiler)
274.7	42	0.26	—	—	—
278.7	54	0.36	54	0.43	61
278.8	58	0.40	58	0.40	58 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. No experimental details were reported.

Source and Purity of Materials:

- (1) Source not specified; purity not specified.
- (2) Source not specified; purity not specified.

Estimated Error:

Not reported.

3.3. Acetonitrile- d_3 + Water

Components:	
(1) Acetonitrile- d_3 ; C_2D_3N ; [2206-26-0]	Original Measurements:
(2) Water; H_2O ; [7732-18-5]	J. Szydłowski and M. Szykula, Fluid Phase Equilib. 154 , 79–87 (1999).
Variables:	
$T/K = 256-273$	Prepared By:
	Valerii P. Sazonov

Experimental Data				
Mutual solubility of acetonitrile- d_3 (1) and water (2)				
T/K	$t/^\circ C$ (compiler)	x_1		100 w_1 (compiler)
		Water-rich phase	Acetonitrile- d_3 -rich phase	
256.289	-16.861	—	0.742	87.5
260.497	-12.653	—	0.701	85.1
264.933	-8.217	0.174	—	—
265.497	-7.653	—	0.642	81.4
268.088	-5.062	—	0.600	78.6
268.490	-4.660	0.203	—	—
270.325	-2.825	—	0.550	74.9
271.675	-1.475	—	0.500	71.0
271.722	-1.428	0.253	—	—
272.598	-0.552	—	0.451	66.8
272.740	-0.410	0.300	—	—
272.961	-0.189	0.362	—	—

UCST was reported at 272.961 \pm 0.005 K at $x_{1,c} = 0.365 \pm 0.002$ (100 $w_1 = 58.4$, compiler).

Auxiliary Information

Method/Apparatus/Procedure: The synthetic method was used with a simplified version of the apparatus described in the work.¹ Temperature was changed at the rate < 0.01 K/min; there was no visible influence of the rate on the transition temperature up to the rate 0.1 K/min. Due to the very weak turbidity a long capillary cell was employed. A 5 mW Polytec HeNe laser was used as a probe for detecting the phase separation.

Source and Purity of Materials:

- (1) Sigma; 99.5% D; carefully dried over 5 Å molecular sieves; not purified.
- (2) Millipore Milli-Q; quality.

Estimated Error:

Temperature: ± 5 mK.

References:

- J. Szydłowski, L. P. Rebelo, and W. A. Van Hook, Rev. Sci. Instrum. **63**, 1717 (1992).

3.4. + Water- d_2

Components:	
(1) Acetonitrile- d_3 ; C_2D_3N ; [2206-26-0]	Original Measurements:
(2) Water- d_2 ; D_2O ; [7789-20-0]	J. Szydłowski and M. Szykula, Fluid Phase Equilib. 154 , 79–87 (1999).
Variables:	
$T/K = 255-279$	Prepared By:
	Valerii P. Sazonov

Experimental Data				
Mutual solubility of acetonitrile- d_3 (1) and water- d_2 (2)				
T/K	$t/^\circ C$ (compiler)	x_1		100 w_1 (compiler)
		Water- d_2 -rich phase	Acetonitrile- d_3 -rich phase	
254.635	-18.515	—	0.804	90.0
263.376	-9.774	—	0.739	86.2
266.669	-6.481	0.150	—	—
267.619	-5.531	—	0.697	83.5
271.559	-1.591	—	0.649	80.3
274.769	1.619	—	0.595	76.4
275.186	2.036	0.201	—	—
276.765	3.615	—	0.549	72.8
278.177	5.027	—	0.496	68.4
278.248	5.098	0.252	—	—
278.878	5.728	—	0.453	64.6
279.099	5.949	0.300	—	—
279.245	6.095	0.349	—	—

UCST was reported at 279.244 \pm 0.006 K at $x_{1,c} = 0.360 \pm 0.003$ (100 $w_1 = 55.3$, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used with a simplified version of the apparatus described in the work.¹ Temperature was changed at the rate < 0.01 K/min; there was no visible influence of the rate on the transition temperature up to the rate 0.1 K/min. Due to the very weak turbidity a long capillary cell was employed. A 5 mW Polytec HeNe laser was used as a probe for detecting the phase separation.

Source and Purity of Materials:

- (1) Sigma; 99.5% D; carefully dried over 5 Å molecular sieves; not purified.
- (2) From Institute of Atomic Energy, Isotope Distribution Center; 99.92% D; twice distilled.

Estimated Error:

Temperature: ± 5 mK.

References:

- J. Szydłowski, L. P. Rebelo, and W. A. Van Hook, Rev. Sci. Instrum. **63**, 1717 (1992).

4. Acetonitrile+Inorganic Compounds

4.1. + Carbon Disulfide

Components:	Evaluator:
(1) Acetonitrile; C_2H_3N ; [75-05-8]	Valerii P. Sazonov, Technical University, Samara, Russia, August, 2001.
(2) Carbon disulfide; CS_2 ; [75-15-0]	

Critical Evaluation

Solubilities in the system comprising acetonitrile and carbon disulfide have been reported in four publications.

Poppe¹ determined the upper critical solution temperature and the effect of pressure (0.58–9.8 MPa) by the synthetic method. Dorby² determined the upper critical solution temperature. Mutual solubility of (1) and (2) was studied also by Govindarajan *et al.*³ between 320 and 323 K by the visual observation method. Sivaraman *et al.*⁴ between 319 and 324 K, and between 0.1 and 4.05 MPa measured the mutual solubilities of (1) and (2) using the synthetic method and these data were reported in graphical form, numerical data were extracted from the published graphs for this evaluation.

The upper critical solution temperature has been reported as 323.36 K,^{3,4} 324.05 K¹ and 324.2 K.² The data^{1–3} are in reasonable agreement and thus their average value: UCST = 323.7 ± 0.4 K is recommended. The corresponding critical solution composition has been reported in as $x_{c1} = 0.408^3$ and $x_{c1} = 0.409^4$. These data give an average $x_{c1} = (0.408 \pm 0.001)$, which is recommended.

The value of dT_c/dP was reported to be 0.0197 K·MPa⁻¹ by Poppe¹ and be 0.247 K·MPa⁻¹ by Sivaraman *et al.*⁴ All experimental values reported in Govindarajan *et al.*³ and Sivaraman *et al.*⁴ have been approximated by an equation based on the scaling law (described in the introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.7194, \quad a_2 = 1.5113, \quad b_1 = 10.9953, \quad b_2 = -6.4110$$

(mean standard error of estimate was 0.0115).

For approximation x_{c1} and UCST from data^{3,4} have been used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with experimental points reported in the data,^{3,4} are also presented in Fig. 3.

Interpolated mutual solubility of acetonitrile and carbon disulfide

T/K	Carbon disulfide-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
318.2	0.189	11.2	0.656	50.7
319.2	0.204	12.1	—	—
320.2	0.222	13.3	0.601	44.8
321.2	0.245	14.9	0.569	41.6
322.2	0.278	17.2	0.532	38.0
322.7	0.302	18.9	0.507	35.7
322.8	0.308	19.4	0.501	35.1
322.9	0.315	19.9	0.495	34.6
323.0	0.323	20.5	0.487	33.9
323.1	0.332	21.1	0.479	33.1
323.2	0.345	22.1	0.468	32.2
323.3	0.363	23.5	0.451	30.7

References:

- G. Poppe, Bull. Soc. Chim. Belg. **44**, 640 (1935).
- A. Dorby, Makromol. Chem. **18/19**, 317 (1956).
- K. Govindarajan, S. V. Subramanyam, and E. S. R. Gopal, J. Chem. Phys. **56**, 4235 (1972).
- A. Sivaraman, M. K. Tiwari, S. Iyothi, and E. S. R. Gopal, Ber. Bunsen-Ges. Phys. Chem. **84**, 196 (1980).

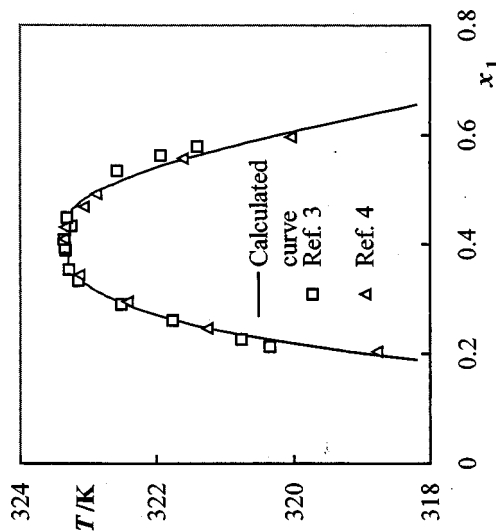


FIG. 3. Mutual solubility of acetonitrile and carbon disulfide.

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Carbon disulfide; CS ₂ ; [75-15-0]	Original Measurements: A. Dorby, Makromol. Chem. 18/19 , 317–21 (1956).
Variables: T/K = 324	Prepared By: Valerii P. Sazonov

Experimental Data

The UCST was reported to be 51.0 °C (324.2 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure: No details were reported.	Source and Purity of Materials: (1) Not specified. (2) Not specified.
	Estimated Error: Not reported.

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Carbon disulfide; CS ₂ ; [75-15-0]	Original Measurements: G. Poppe, Bull. Soc. Chim. Belg. 44 , 640–57 (1935).
Variables: T/K = 324 and P/kPa = 582–9803	Prepared By: Valerii P. Sazonov

Experimental Data

The UCST was reported to be 50.90 °C (324.05 K, compiler).
The value of dT_c/dP was reported to be 0.0197 K·kPa⁻¹ in the pressure range 582–9803 kPa.

Auxiliary Information

Method/Apparatus/Procedure: The synthetic method was used. Observations were carried out in sealed tubes in the presence of the vapor phase. A Caillietet tube with a Kuenen electromagnetic stirrer was used in the experiments at higher pressure. A thermostating cylinder was also used to control the temperature.	Source and Purity of Materials: (1) Obtained from the Bureau Etalons Physico-Chimiques. (2) Obtained from the Bureau Etalons Physico-Chimiques.
	Estimated Error: Pressure: ± 100 kPa.

Components:

(1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) Carbon disulfide; CS₂; [75-15-0]

Original Measurements:

A. Sivaraman, M. K. Tiwari, S. Jyothi, and E. S. R. Gopal, Ber. Bunsen-Ges. Phys. Chem. **84**, 196–2200 (1980).

Variables:

T/K = 319–324; P/MPa = 0.10–4.05

Prepared By:

Valerii P. Sazonov

Experimental Data

The mutual solubility of acetonitrile (1) and carbon disulfide (2) in mole fractions was reported over the temperature range in graphical form. Numerical data was extracted from the published graphs by the compiler.

P/MPa	t/°C	T/K (compiler)	Carbon disulfide-rich phase		100 w ₁ (compiler)		x ₁	Acetonitrile-rich phase	
			x ₁	T/K (compiler)	x ₁	T/K (compiler)		x ₁	100 w ₁ (compiler)
0.10	45.63	318.78	0.204	—	12.1	—	—	—	—
	46.89	320.04	—	—	—	—	0.596	—	44.3
	48.12	321.27	0.246	—	15.0	—	—	—	40.4
	48.47	321.62	—	—	—	—	0.557	—	—
	49.28	322.43	0.294	—	18.3	—	—	—	34.3
	49.92	322.89	—	—	—	—	0.492	—	32.2
	49.99	323.07	—	—	—	—	0.468	—	—
	49.99	323.14	—	—	22.0	—	—	—	29.0
	50.20	323.35	—	—	—	—	0.431	—	—
	50.21	323.36	—	—	27.2	—	0.409	—	27.2 (UCST)
2.03	46.09	319.24	0.194	—	11.5	—	—	—	—
	47.36	320.51	—	—	—	—	0.600	—	44.7
	48.60	321.75	0.250	—	15.2	—	—	—	—
	49.77	322.92	0.291	—	18.1	—	—	—	—
	50.25	323.40	—	—	—	—	0.527	—	37.5
	50.48	323.63	0.341	—	21.8	—	—	—	—
	50.60	323.75	—	—	—	—	0.468	—	—
	50.64	323.79	—	—	—	—	0.458	—	31.3
	50.70	323.85	—	—	—	—	0.429	—	28.8
	50.71	323.86	—	—	27.2	—	0.409	—	27.2 (UCST)
4.05	46.54	319.69	0.194	—	11.5	—	—	—	—
	47.83	320.98	—	—	—	—	0.596	—	44.3
	49.08	322.23	0.250	—	15.2	—	—	—	—
	49.39	322.54	—	—	—	—	0.557	—	40.4
	50.26	323.41	0.291	—	18.1	—	—	—	—
	50.70	323.85	—	—	—	—	0.503	—	35.3
	50.98	324.13	0.341	—	21.8	—	—	—	—
	51.09	324.24	—	—	—	—	0.468	—	32.2
	51.20	324.35	—	—	25.5	—	—	—	—
	51.21	324.36	—	—	27.2	—	0.409	—	27.2 (UCST)

The value of dT_c/dP was reported to be 0.247 K·MPa⁻¹ in the above pressure range.

Components:

(1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) Carbon disulfide; CS₂; [75-15-0]

Original Measurements:

K. Govindarajan, S. V. Subramanyam, and E. S. R. Gopal, J. Chem. Phys. **56**, 4235–36 (1972).

Variables:

T/K = 320–323

Prepared By:

Valerii P. Sazonov

Experimental Data

The mutual solubility of acetonitrile (1) and carbon disulfide (2) in mole fractions was reported over the temperature range in graphical form. Numerical data was extracted from the published graphs by the compiler.

t/°C	T/K (compiler)	Carbon disulfide-rich phase		100 w ₁ (compiler)		x ₁	Acetonitrile-rich phase	
		x ₁	T/K (compiler)	x ₁	T/K (compiler)		x ₁	100 w ₁ (compiler)
47.20	320.35	0.213	—	12.7	—	—	—	—
47.61	320.76	0.226	—	13.6	—	—	—	—
48.26	321.41	—	—	—	—	0.579	—	42.6
48.62	321.77	0.261	—	16.0	—	—	—	—
48.79	321.94	—	—	—	—	0.563	—	41.0
49.37	322.52	0.290	—	18.0	—	—	—	—
49.43	322.58	—	—	—	—	0.535	—	38.3
50.00	323.15	0.333	—	21.2	—	—	—	—
50.14	323.29	0.353	—	22.7	—	—	—	—
50.17	323.32	—	—	—	—	0.449	—	30.5
50.19	323.34	0.389	—	25.6	—	—	—	—
50.20	323.35	0.393	—	25.9	—	0.434	—	29.2
50.21	323.36	0.408	—	27.1	—	0.408	—	27.1 (UCST)

The value of dT_c/dP was reported to be 0.247 K·MPa⁻¹ in the above pressure range.

Auxiliary Information**Source and Purity of Materials:**

(1) E. Merck Co., Germany; not purified; water content certified to be less than 0.1 mole %.
 (2) E. Merck Co., Germany; not purified.

Estimated Error:

Temperature: ±0.05 K.

References:

¹B. Viswanathan, R. D. Gambhir, and E. S. R. Gopal, J. Chem. Phys. **53**, 4405 (1970).

Method/Apparatus/Procedure:

The synthetic method was used. The visual observation of the phase-transition temperatures has been used as in Viswanathan *et al.*¹ The samples were all raised to the one phase region, and after allowing them to stand at this temperature for about 1 h, gradual cooling in steps of 10 mdeg was started. Deep brown coloration near x_c was observed, when viewed through transmitted light, and the opalescence was very strong because of the large difference in the refractive indices of the liquids. They were reproduced in a slow heating cycle also.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The visual observation of the phase-transition temperatures has been used as in Viswanathan *et al.*¹ The samples were all raised to the one phase region, and after allowing them to stand at this temperature for about 1 h, gradual cooling in steps of 10 mdeg was started. Deep brown coloration near x_c was observed, when viewed through transmitted light, and the opalescence was very strong because of the large difference in the refractive indices of the liquids. They were reproduced in a slow heating cycle also.

Source and Purity of Materials:

(1) Source not specified; analytical reagent grade; distilled.
 (2) Source not specified; analytical reagent grade.

Estimated Error:

Temperature: ±0.05 K.

References:

¹B. Viswanathan, R. D. Gambhir, and E. S. R. Gopal, J. Chem. Phys. **53**, 4405 (1970).

4.2. + Cesium Chloride

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		A. P. Krasnoperova, L. S. Kovalenko, and E. N. Gracheva, Zh. Strukt. Khim. 19 , 82–85 (1978).	
(2) Cesium chloride; CsCl; [7647-17-8]			
Variables:		Prepared By:	
T/K=288–318		Valerii P. Sazonov	
Experimental Data			
Solubility of cesium chloride (2) in acetonitrile (1)			
t/°C	T/K (complier)	100 w ₂ (complier)	x ₂ (complier)
15.0	288.2	8.55	0.0223
25.0	298.2	9.60	0.0252
35.0	308.2	10.2	0.0269
45.0	318.2	10.5	0.0278
Auxiliary Information			
Method/Apparatus/Procedure:			
The method of radioactive indicators was used. The apparatus, filling procedure and method of the measurements were described elsewhere. ¹			
Source and Purity of Materials:			
(1) Source not specified; pure grade reagent; dried and purified; water content by the method Fischer less than 0.005 mass %.			
(2) Source not specified; analytical purity.			
Estimated Error:			
Solubility: relative error did not exceed 1%–2%.			
References:			
¹ A. P. Krasnoperova, Dissertation, Khar'kov University, 1973.			

4.3. + Cesium Iodide

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		T. M. Varlamova and S. I. Sinegubova, Neorg. Mater. 28 , 1288–91 (1992).	
(2) Cesium iodide; CsI; [7789-17-5]			
Variables:		Prepared By:	
T/K=283 and 313		Valerii P. Sazonov	
Experimental Data			
Solubility of cesium iodide (2) in acetonitrile (1)			
t/°C	T/K (complier)	100 w ₂	x ₂ (complier)
10.0	283.2	0.98	0.0016
40.0	313.2	0.97	0.0015
Auxiliary Information			
Method/Apparatus/Procedure:			
The analytical method was used. No experimental details were reported.			
Source and Purity of Materials:			
(1) Source not specified; pure grade reagent; dried over P ₂ O ₅ and distilled over Na ₂ CO ₃ ; boiling point=81.6 °C. n(25 °C,D)=1.3416.			
(2) Source not specified; analytical purity; dried in vacuum at 200 °C.			
Estimated Error:			
Not reported.			

4.4. + Potassium Iodide

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	P. Walden, Z. Phys. Chem. 55 , 683–720 (1906).	
(2) Potassium iodide; KI; [7681-11-0]	(2) Potassium iodide; KI; [7681-11-0]		
Variables:		Prepared By:	
T/K = 273 and 298		Valerii P. Sazonov	
Experimental Data			
Solubility of potassium iodide (2) in acetonitrile (2)			
<i>t</i> /°C	<i>T</i> /K (complier)	100 w ₂	<i>x</i> ₂ (complier)
0.0	273.2	2.259	0.0057
25.0	298.2	2.003	0.0050

Method/Apparatus/Procedure:		Source and Purity of Materials:	
The analytical method was used. Method A: 10–20 mL of (1) and an appropriate amount of fine dry (2) were placed in a glass retort in a thermostat and stirred for many hours. Aliquots of the saturated solution were taken by pipette for titration. Method B: 15–25 mL of (1) and finely divided (2) were equilibrated at 40 °C with intensive stirring for 1 h. The flask was then placed in a thermostat (25 or 0 °C) and stirred for 2 h. After this, stirring was halted and the flask kept at the given temperature for 17–18 h. The saturated solutions were then sampled and titrated.		(1) Not specified. (2) Not specified.	
Auxiliary Information		Estimated Error:	
		Not specified.	

Components:		Evaluator:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valerii P. Sazonov, Technical University, Samara, Russia, July, 2001.	
(2) Potassium iodide; KI; [7681-11-0]	(2) Potassium iodide; KI; [7681-11-0]		

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and potassium iodide (2) have been reported in three publications over a very limited range of temperatures. No data appear to have been reported for the solubility of (1) in (2). Walden¹ determined solubility of potassium iodide in acetonitrile at 273 and 298 K by an analytical method. Varlamova *et al.*² carried out measurements of the solubility of (2) in (1) at 298 K by an analytical method. Il'in *et al.*³ studied the solubility of (2) in (1) between 283 and 333 K by the analytical method.

At the one temperature (298 K) where comparison is possible, the three studies are in good agreement. These values $x_2 = 0.005$,² $x_2 = 0.0050$,¹ and $x_2 = 0.0052$.³ These data give an average $x_2 = 0.0051 \pm 0.0001$ (100 w₂ = 2.03), which is recommended. Accordingly, all the available data (see the relevant data sheets) must be regarded as very tentative.

References:

- ¹P. Walden, Z. Phys. Chem. **55**, 683 (1906).
- ²T. M. Varlamova, K. K. Il'in, A. G. Demakhin, and N. I. Nikurashina, Zh. Fiz. Khim. **58**, 2730 (1984).
- ³K. K. Il'in, T. M. Varlamova, and S. V. Lelyukhin, Phase Equilibria and Thermal Analysis (in Russian), Perm', 124 (1988).

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		K. K. Il'in, T. M. Varlamova, and S. V. Lelyukhin, Phase Equilibria and Thermal Analysis (in Russian), Perm', 124-9 (1988).	
(2) Potassium iodide; KI; [7681-11-0]			
Variables:		Prepared By:	
T/K = 283-333		Valerii P. Sazonov	
Experimental Data			
Solubility of potassium iodide (2) in acetonitrile (1)			
<i>t</i> /°C	<i>T</i> /K (compiler)	100 <i>w</i> ₂	<i>x</i> ₂ (compiler)
10.0	283.2	2.25	0.0057
20.0	293.2	2.07	0.0052
25.0	298.2	1.98	0.0050
30.0	303.2	1.96	0.0049
40.0	313.2	1.84	0.0046
50.0	323.2	1.71	0.0043
60.0	333.2	1.60	0.0040

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. (1) and (2) were placed in a vessel without contact to atmospheric moisture. With continuous stirring equilibrium was established in 6-7 h. Salt content in saturated solutions determined by gravimetrically.

Source and Purity of Materials:

- (1) Source not specified; pure grade reagent; dried and purified.
- (2) Source not specified; very pure reagent; dried in vacuum.

Estimated Error:

Temperature: ±0.1 K.
Solubility: relative error ±0.1%.

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		T. M. Varlamova, K. K. Il'in, A. G. Demakhin, and N. I. Nikurashina, Zh. Fiz. Khim. 58 , 2730-5 (1984).	
(2) Potassium iodide; KI; [7681-11-0]			
Variables:		Prepared By:	
T/K = 298		Valerii P. Sazonov	
Experimental Data			
Solubility of potassium iodide (2) in acetonitrile (1)			
<i>t</i> /°C	<i>T</i> /K (compiler)	100 <i>w</i> ₂	<i>x</i> ₂ (compiler)
25.0	298.2	2.0	0.005
Auxiliary Information			
Method/Apparatus/Procedure:			
The analytical method was used. No experimental details were reported.			
Source and Purity of Materials:			
(1) Source not specified; pure grade reagent; dried over P ₂ O ₅ and distilled over Na ₂ CO ₃ ; boiling point=81.6 °C, <i>n</i> (25 °C,D)=1.3416.			
(2) Source not specified; very pure reagent; dried in vacuum.			
Estimated Error:			
Not reported.			

4.6. + Lithium Perchlorate

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. P. T. Tomkins and P. J. Turner, <i>J. Chem. Eng. Data</i> 20, 50–2 (1975).
(2) Lithium perchlorate; LiClO ₄ ; [7791-03-9]	
Variables:	Prepared By:
T/K = 297–323	Valerii P. Sazonov

Experimental Data			
Solubility of lithium perchlorate (2) in acetonitrile (1)			
t/°C	T/K (compiler)	mol·kg ⁻¹	x ₂
24.20	297.35	1.5419	14.093
29.16	302.31	1.8632	16.545
32.8	306.0	2.1402	18.547
36.33	309.48	2.4615	20.755
40.12	313.27	2.9548	23.919
41.21	314.36	7.5868	44.67
41.94	315.09	3.2253	25.550
45.43	318.58	8.4018	47.14
45.66	318.81	7.7932	45.33
45.67	318.82	3.9402	29.538
48.28	321.43	4.4614	32.189
48.85	322.00	7.1865	43.33
49.41	322.56	6.1452	39.535
49.50	322.65	5.2365	35.781
50.17	323.32	6.2239	39.84

Auxiliary Information

Method/Apparatus/Procedure:

The cooling method was used. The system was examined with an apparatus which consists essentially of a Pyrex test tube with a 24/40 ground joint as container, and a Teflon-coated magnetic stirring bar. Several indentations were made in walls to improve mixing by breaking up the cylindrical flow pattern, which tended to promote nonuniform cooling. A mercury-in-glass thermometer graduated in 0.1° intervals was inserted and the whole unit was placed in a 250 mL Erlenmeyer flask which acted as both support and air jacket; cooling with laboratory air was sufficient over the temperature range studied. Supercooling of 2–5 °C was normal in this system and was corrected in the usual manner by back extrapolation.

Source and Purity of Materials:

(1) Source not specified; purified.
(2) Source not specified; purified.

Estimated Error:

Not reported.

4.5. + Lithium Bromide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	T. M. Varlamova, T. S. Mankevich, and Zh. V. Bukhun, <i>Chemistry, Technology and Industrial Ecology of Inorganic Compounds (in Russian)</i> , Perm, 36–42, (1999).
(2) Lithium bromide; LiBr; [7550-35-8]	
Variables:	Prepared By:
T/K = 283–422	Valerii P. Sazonov

Experimental Data			
Solubility of lithium bromide (2) in acetonitrile (1)			
t/°C	T/K (compiler)	100 w ₂	x ₂ (compiler)
10.0	283.2	6.94	0.0341
20.0	293.2	8.50	0.0421
25.0	298.2	9.40	0.0468
30.0	303.2	10.47	0.0524
40.0	313.2	12.20	0.0616
50.0	323.2	14.04	0.0717
60.0	333.2	16.31	0.0844
70.8	344.0	19.94	0.1053
79.3	352.5	24.72	0.1344
91.0	364.2	34.97	0.2027
96.0	369.2	40.08	0.2402
100.4	373.6	45.16	0.2802
101.6	374.8	46.83	0.2940
102.0	375.2	47.30	0.2979
102.4	375.6	47.67	0.3100
103.0	376.2	48.47	0.3078
103.4	376.6	49.00	0.3123
116.0	389.2	48.47	0.3078
123.6	396.8	47.67	0.3100
135.0	408.2	47.30	0.2979
149.2	422.4	46.83	0.2940

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic and analytical methods were used. No experimental details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; dried and purified.
(2) Source not specified; analytical purity; dried in vacuum.

Estimated Error:

Temperature: ±0.1 K.
Solubility: relative error ±0.1%.

4.7.+ Sodium Bromide

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	
(2) Sodium bromide; NaBr; [7647-15-6]	
Variables:	
T/K=283–333	Prepared By: Valerii P. Sazonov
Original Measurements:	
T. M. Varlamova, M. I. Smushkin, and S. P. Mushatkova, Chemical Sciences-99 (in Russian), Saratov, 30–4 (1999).	
Experimental Data	
Solubility of sodium bromide (2) in acetonitrile (1)	
<i>t</i> /°C	<i>T</i> /K (compiler)
	100 <i>w</i> ₂
10.0	283.2
20.0	293.2
25.0	298.2
30.0	303.2
40.0	313.2
50.0	323.2
60.0	333.2
	<i>x</i> ₂ (compiler)
	3.0E-06
	3.9E-06
	4.0E-06
	4.0E-06
	4.4E-06
	4.4E-06
	4.8E-06

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. (1) and (2) were placed in a vessel without contact to atmospheric moisture. With continuous stirring equilibrium was established in 6–7 h. Salt content in saturated solutions determined by gravimetrically.

Source and Purity of Materials:

- (1) Source not specified; pure grade reagent; dried and purified.
 (2) Source not specified; analytical purity; dried in vacuum.

Estimated Error:

Temperature: ±0.1 K.
 Solubility: relative error ±0.1%.

4.8.+ Sodium Iodide

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	
(2) Sodium iodide; NaI; [7681-82-5]	
Evaluator:	
Valerii P. Sazonov, Technical University, Samara, Russia, July, 2001.	

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and sodium iodide (2) have been reported in two publications over a very limited range of temperatures. No data appear to have been reported for the solubility of (1) in (2). Kushchenko *et al.*¹ determined solubility of potassium iodide in acetonitrile at 298 and 323 K by an analytical method. Nikurashina *et al.*² carried out measurements of the solubility of (2) in (1) at 298 K by an analytical method.

At the one temperature (298 K) where comparison is possible, the reported solubilities, $x_2=0.063^1$ and $x_2=0.070^2$ are in agreement. Accordingly, all the available data (see the relevant data sheets) must be regarded as tentative.

References:

- ¹V. V. Kushchenko, L. B. Litvinov, and K. P. Mishchenko, Zh. Obshch. Khim., **41**, 955 (1971).
²N. I. Nikurashina, T. M. Varlamova, A. G. Demakhin, and K. K. Il'in, Zh. Fiz. Khim., **53**, 2654 (1979).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	N. I. Nikurashina, T. M. Varlamova, A. G. Demakhin, and K. K. Il'in, <i>Zh. Fiz. Khim.</i> 53 , 2654-8 (1979).
(2) Sodium iodide; NaI; [7681-82-5]	
Variables:	Prepared By:
T/K = 298	Valerii P. Sazonov

Experimental Data	
Solubility of sodium iodide (2) in acetonitrile (1)	
t/°C	x_2 (complier)
25.0	100 w ₂
298.2	21.5
50.0	0.070

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. No experimental details given.

Source and Purity of Materials:

- (1) Source not specified; pure grade reagent; dried over P₂O₅ and distilled over Na₂CO₃; boiling point=81.6 °C; n(25 °C,D)=1.3416.
 (2) Source not specified; analytical purity; dried in vacuum at 200 °C.

Estimated Error:
Not reported.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	V. V. Kushchenko, L. B. Litvinov, and K. P. Mishchenko, <i>Zh. Obshch. Khim.</i> 41 , 955-8 (1971).
(2) Sodium iodide; NaI; [7681-82-5]	
Variables:	Prepared By:
T/K = 298 and 323	Valerii P. Sazonov

Experimental Data	
Solubility of sodium iodide (2) in acetonitrile (1)	
t/°C	x_2 (complier)
25.0	100 w ₂
298.2	19.8
323.2	17.1
50.0	0.063
	0.054

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. (1) and an appropriate amount of fine dry (2) were placed in an ampoule, which was sealed, and then maintained at constant temperature for 50 h. After that time the ampoule was opened and the equilibrium concentration determined gravimetrically.

Source and Purity of Materials:

- (1) Source not specified; purity not specified; distilled.
 (2) Source not specified; very pure reagent; not purified.

Estimated Error:
Not reported.

4.10. Silver, Potassium, Sodium Nitrates

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		M. Moolle and H. Schneider; Z Phys. Chem. (Munich) 74 , 237-47 (1971).	
(2) Silver nitrate; AgNO ₃ ; [7761-88-8]			
(3) Potassium nitrate; KNO ₃ ; [7557-79-1]			
(4) Sodium nitrate; NaNO ₃ ; [7631-99-4]			
Variables:		Prepared By:	
T/K = 298		Valerii P. Sazonov	
Experimental Data			
Solubility of nitrates (2), (3) or (4) in acetonitrile (1) at 25.0 °C (298.2 K compiler)			
Nitrate	Mole(2)/1000 g(1)	100 w ₂ (compiler)	x ₂ (compiler)
Acetonitrile+Silver nitrate	17.7	75.0	0.421
Acetonitrile+Potassium nitrate	0.0023	0.023	0.0001
Acetonitrile+Sodium nitrate	0.003	0.025	0.0001
Auxiliary Information			
Method/Apparatus/Procedure:		Source and Purity of Materials:	
No experimental details given.		(1) Fluka; puriss.; purity > 99.5 mole%; not purified. (2), (3), (4) Merck; pure grade reagent.	
		Estimated Error:	
		Temperature: ±0.1 K.	

4.9. + Rubidium Iodide

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		K. K. Il'in, A. G. Demakhin, N. I. Nikurashina, and T. M. Varlamova, Zh. Fiz. Khim. 55 , 2499-2502 (1981).	
(2) Rubidium iodide; RbI; [7790-29-6]			
Variables:		Prepared By:	
T/K = 253-333		Valerii P. Sazonov	
Experimental Data			
Solubility of rubidium iodide (2) in acetonitrile (1)			
t/°C	T/K (compiler)	100 w ₂	x ₂ (compiler)
-20.0	253.2	2.58	0.0051
-10.0	263.2	2.47	0.0049
0.0	273.2	2.34	0.0046
10.0	283.2	2.28	0.0045
20.0	293.2	2.15	0.0042
25.0	298.2	2.08	0.0041
30.0	303.2	2.06	0.0040
40.0	313.2	1.97	0.0039
50.0	323.2	1.90	0.0037
60.0	333.2	1.87	0.0036
Auxiliary Information			
Method/Apparatus/Procedure:		Source and Purity of Materials:	
The analytical method was used. (1) and (2) were placed in a vessel without contact to atmospheric moisture. With continuous stirring equilibrium was established in 6-7 h. Salt content in saturated solutions determined by gravimetrically.		(1) Source not specified; pure grade reagent; dried and purified. (2) Source not specified; analytical purity; dried in vacuum.	
		Estimated Error:	
		Temperature: ±0.1 K. Solubility: relative error ±0.1%.	

4.11. + Silicon Tetrachloride

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		S. S. Alikberov, L. P. Shklover, A. S. Syromyamikova, and T. M. Sheherbakova, Zh. Fiz. Khim. 44 , 935-6 (1960).	
(2) Silicon tetrachloride; SiCl ₄ ; [10026-04-7]			
Variables:		Prepared By:	
T/K = 301-325		Valerii P. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and silicon tetrachloride (2)			
<i>t</i> /°C	T/K (compiler)	100 <i>w</i> ₁	<i>x</i> ₁ (compiler)
		Acetonitrile-rich phase	
		Silicon tetrachloride-rich phase	
27.8	301.0	2.28	0.088
28.1	301.3	—	—
31.1	304.3	—	—
33.0	306.2	—	—
34.4	307.6	—	—
36.1	309.3	5.54	0.195
37.9	311.1	—	—
38.0	311.2	7.03	0.238
40.1	313.3	—	—
42.4	315.6	8.56	0.279
43.6	316.8	—	—
43.9	317.1	10.12	0.318
48.2	321.4	11.68	0.354
48.8	322.0	—	—
50.7	323.9	15.02	0.422
51.3	324.5	18.48	0.484
51.5	324.7	—	—
51.8	325.0	22.19	0.541

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Determinations were made in sealed tubes, which were heated and allowed to cool slowly in water bath. Total volume of a mixture was 20 mL. Thermometers were calibrated to 0.1 K.

Source and Purity of Materials:

(1) Source not specified; purity not specified; distilled in the laboratory quartz column; boiling point=80.5 °C.
(2) Source not specified; purity not specified; distilled in the laboratory quartz column; boiling point=57.4 °C.

Estimated Error:

Not reported.

4.12. + Sulfur Dioxide

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		J. J. Byerley, G. L. Rempel, and V. Thang Le, J. Chem. Eng. Data 25 , 55-6 (1980).	
(2) Sulfur dioxide; SO ₂ ; [7446-09-5]			
Variables:		Prepared By:	
T/K = 298 and 323; <i>P</i> /kPa = 101.3		Valerii P. Sazonov	
Experimental Data			
Solubility of sulfur dioxide (2) in acetonitrile (1) at 101.3 kPa total pressure			
<i>t</i> /°C	T/K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	<i>x</i> ₂ (compiler)
25.0	298.2	84.6	45.8
50.0	323.2	25.64	20.41
Auxiliary Information			
Method/Apparatus/Procedure:			
The analytical method was used. The solubility of sulfur dioxide was studied in a 50 mL buret equipped with a water jacket. Sulfur dioxide was bubbled at a slow flow rate approximately 60 mL/min with the gas flow being from bottom to top of the buret. The gas exited through a spiral condenser in order to avoid excessive loss of acetonitrile. The sulfur dioxide concentration after saturation was measured by titrating excess iodine with standard thiosulfate solution using starch as the indicator.			
Source and Purity of Materials:			
(1) J. T. Baker; reagent grade; not purified. (2) Union Carbide Canada, Ltd.; reagent grade; not purified.			
Estimated Error:			
Temperature: ±0.1 K.			

5. Acetonitrile+Hydrocarbons

5.1. + Propane

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	M. S. Gruszkiewicz, J. B. Ott, and J. T. Sipowska, <i>Thermochim. Acta</i> 245 , 155-61 (1994).
(2) Propane; C ₃ H ₈ ; [74-98-6]	
Variables:	Prepared By:
T/K = 298-336 K; P/MPa = 5.0-10.0	Valerii P. Sazonov

Experimental Data

The mutual solubilities of acetonitrile (1) and propane (2) in mole fractions over the specified temperature range were reported in the original publication in form of the equation:

$$T = T_c + k[\alpha x / (1 + x(\alpha - 1))] - [\alpha x_c / (1 + x_c(\alpha - 1))]^{1/\beta}$$

The data presented here were calculated from the published equation by the compiler (see Tables 1 and 2).

TABLE 1. Mutual solubility of acetonitrile (1) and propane (2) at high pressure

P/MPa	T/K	t/°C	x ₁		100 w ₁		Acetonitrile-rich phase	
			Hydrocarbon-rich phase	Acetonitrile-rich phase	Hydrocarbon-rich phase	Acetonitrile-rich phase		
5.0	300.2	27.0	—	—	—	—	—	78.8
	302.1	28.9	0.05	—	4.7	—	—	—
	313.4	40.2	—	—	—	4.7	—	73.6
	314.1	40.9	0.10	—	9.4	—	—	—
	322.7	49.5	—	—	—	—	—	68.5
	322.9	49.7	0.15	—	14.1	—	—	—
	328.8	55.6	0.20	—	18.9	—	—	—
	328.9	55.7	—	—	—	—	—	63.4
	332.5	59.3	0.25	—	23.7	—	—	—
	332.7	59.5	—	—	—	—	—	58.3
	334.6	61.4	0.30	—	28.5	—	—	—
	334.7	61.5	—	—	—	—	—	53.2
	335.4	62.2	0.35	—	33.4	—	—	—
	335.5	62.3	—	—	—	—	—	48.2
	335.6	62.4	0.40	—	38.3	—	—	43.2
10.0	294.2	21.0	—	—	—	—	—	78.8
	309.3	36.1	—	—	—	—	—	73.6
	309.4	36.2	0.05	—	4.7	—	—	—
	318.5	45.3	0.10	—	9.4	—	—	—
	319.5	46.3	—	—	—	—	—	68.5
	324.8	51.6	0.15	—	14.1	—	—	—
	326.0	52.8	—	—	—	—	—	63.4
	328.8	55.6	0.20	—	18.9	—	—	—
	329.8	57.6	—	—	—	—	—	58.3
	331.1	57.9	0.25	—	23.7	—	—	—
	331.7	58.5	—	—	—	—	—	53.2
	332.2	59.0	0.30	—	28.5	—	—	—
	332.4	59.2	—	—	—	—	—	48.2
	332.5	59.3	0.35	—	33.4	—	—	—
	332.6	59.4	0.40	—	38.3	—	—	43.2

TABLE 2. Dependence of the UCST and x_{1c} on pressure and equation coefficients

P/MPa	5.0	6.0	7.5	10.0
UCST, T/K	335.66	334.82	333.81	332.60
t/°C (compiler)	62.51	61.67	60.66	59.45
x _{1c}	0.4276	—	—	0.4126
K	-793	—	—	-975
α	0.959	—	—	0.900
β	0.315	—	—	0.287

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The phase apparatus consists of a 50 mm long sapphire capillary with a 3.8 mm inside diameter and a 6.35 outside diameter, inserted in the exit line of the calorimeter. Samples of (1) and (2) are mixed in a flow calorimeter at a temperature above the UCST so that complete mixing occurs. The mixture (of known composition) exits the calorimeter through a stainless steel capillary line that is heated to keep the temperature above the UCST, and enters the thermostated bath surrounding the sapphire capillary. The mixture passes through coils of stainless steel capillary tubing inside the thermostat to equilibrate the mixture with the bath temperature, flows through the sapphire capillary, and exits the apparatus through the back pressure regulator. A Sodev Model CFC thermostat circulates fluid through the bath. The temperature of this thermostat, which can be programmed to linearly increase or decrease with time, is lowered slowly until the fluid in the sapphire capillary becomes cloudy. The bath temperature where this occurs is read with a Hart Model 1506 resistance thermometer calibrated against a Rosemount thermometer (ITS-90), and is taken as the equilibrium temperature at the mole fraction of the mixture.

Source and Purity of Materials:

- (1) Fisher Scientific HPLC; purity of 99.9 mass %; used without further purification.
- (2) Phillips; purity of 99.5 mass %; used without further purification.

Estimated Error:

Temperature: ±0.02 K.
Pressure: ±0.1 MPa.

5.2. + Butane

Components:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) Butane; C₄H₁₀; [106-97-8]

Evaluator:

Valerii P. Sazonov, Technical University, Samara, Russia, August, 2001.

Critical Evaluation

Solubilities in the system comprising acetonitrile and butane have been reported in three publications.

Pavlov *et al.*¹ determined the mutual solubilities of acetonitrile and butane between 276 and 335 K for unknown pressure by the synthetic method and these data were presented in graphical form only. Gruszkiewicz *et al.*² measured the mutual solubilities of (1) and (2) between 298 and 334 K and pressure 5–10 MPa using the synthetic method and reported their results only in the form of an equation. Warowny³ studied the phase equilibrium of the liquid–liquid–gas system and the mutual solubility of (1) and (2) between 319 and 336 K and over the pressure range 0.45–0.68 MPa by the synthetic method.

The upper critical solution temperature has been reported as 333.59 K² (at 5 MPa), 335.2 K¹ (for unknown pressure) and 336.22 K³ (at 0.68 MPa). The data^{1–3} are in reasonable agreement and thus their average value: UCST = 335.7 ± 0.5 K is recommended. The corresponding critical solution composition has been reported in as $x_{c1} = 0.4753^2$ (at 5 MPa), $x_{c1} = 0.478^1$ (for unknown pressure), and $x_{c1} = 0.571^3$ (at 0.68 MPa).

All experimental values reported^{1,3} have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.7339, \quad a_2 = 0.1976, \quad b_1 = -0.1453, \quad b_2 = 0.0325$$

(mean standard error of estimate was 0.0262).

For approximation x_{c1} and UCST determined by Pavlov *et al.*¹ have been used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with experimental points reported by Pavlov *et al.*¹ and Warowny³ are also presented in Fig. 4.

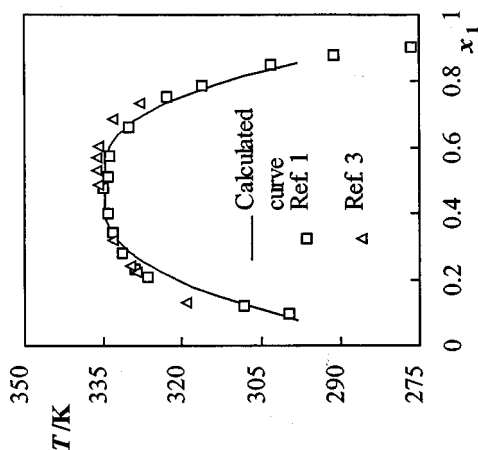


FIG. 4. Mutual solubility of acetonitrile and butane.

Calculated mutual solubility of acetonitrile and butane

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w ₁	x_1	100 w ₁
298.2	0.079	5.7	0.854	80.5
303.2	0.101	7.4	0.835	78.1
308.2	0.125	9.2	0.815	75.7
313.2	0.151	11.2	0.792	72.9
318.2	0.181	13.5	0.765	69.7
323.2	0.217	16.4	0.732	65.9
328.2	0.262	20.0	0.690	61.1
329.2	0.274	21.0	0.679	59.9
330.2	0.287	22.1	0.667	58.6
331.2	0.301	23.3	0.653	57.1
332.2	0.318	24.8	0.637	55.3
333.2	0.339	26.6	0.616	53.1
334.2	0.368	29.1	0.588	50.2
334.7	0.391	31.2	0.565	47.8

References:

- ¹S. Yu. Pavlov, V. A. Goshkov, T. G. Zakina, A. N. Bushin, and V. V. Skorikova, *Khim. Prom.-st (Moscow)* **11**, 810 (1970).
²M. S. Gruszkiewicz, J. B. Ort, and J. T. Sipowska, *Thermochim. Acta* **245**, 155 (1994).
³W. Warowny, *J. Chem. Eng. Data* **41**, 689 (1996).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	M. S. Gruszkiewicz, J. B. Ott, and J. T. Sipowska, <i>Thermochim. Acta</i> 245 , 155–61 (1994).
(2) Butane; C ₄ H ₁₀ ; [106-97-8]	
Variables:	Prepared By:
T/K = 298–334 K; P/MPa = 5.0–10.0	Valerii P. Sazonov

Experimental Data

The mutual solubilities of acetonitrile (1) and butane (2) in mole fractions over the specified temperature range were reported in the original publication in form of the equation:

$$T = T_c + k \left[\frac{\alpha x}{1 + x(\alpha - 1)} \right] - \left[\frac{\alpha x_c}{1 + x_c(\alpha - 1)} \right]^{1/\beta}$$

The data presented here were calculated from the published equation by the compiler (see Tables 1 and 2).

TABLE 1. Mutual solubility of acetonitrile (1) and butane (2) at high pressure

P/MPa	T/K	t/°C	x ₁		100 w ₁	
			Hydrocarbon-rich phase	Acetonitrile-rich phase	Hydrocarbon-rich phase	Acetonitrile-rich phase
5.0	298.6	25.4	0.10	—	7.3	—
	307.1	33.9	—	0.85	—	80.0
	313.7	40.5	0.15	—	11.1	—
	318.0	34.8	—	0.80	—	73.9
	323.3	50.1	0.20	—	15.0	—
	325.2	52.0	—	0.75	—	67.9
	328.9	55.7	0.25	—	19.1	—
	329.7	56.5	—	0.70	—	62.2
	331.8	58.6	0.30	—	23.2	—
	332.1	58.9	—	0.65	—	56.7
	333.1	59.9	0.35	—	27.6	—
	333.2	60.0	—	0.60	—	51.4
	333.5	60.3	0.40	—	32.0	—
	333.6	60.4	0.45	—	36.6	—
	302.5	29.3	—	0.85	—	80.0
10.0	307.2	34.0	0.10	—	7.3	—
	315.6	42.4	—	0.80	—	73.9
	318.8	45.6	0.15	—	11.1	—
	324.1	50.9	—	0.75	—	67.9
	326.1	52.9	0.20	—	15.0	—
	329.2	56.0	—	0.70	—	62.2
	330.3	58.1	0.25	—	19.1	—
	331.9	58.7	—	0.65	—	56.7
	332.5	59.3	0.30	—	23.2	—
	333.1	59.9	—	0.60	—	51.4
	333.3	60.1	0.35	—	27.6	—
	333.5	60.3	0.40	—	32.0	—
	333.6	60.4	0.45	—	36.6	—

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	S. Yu. Pavlov, V. A. Gornshkov, T. G. Zaikina, A. N. Bushin, and V. V. Skorikova, <i>Khim. Prom-st (Moscow)</i> 11 , 810–4 (1970).
(2) Butane; C ₄ H ₁₀ ; [106-97-8]	
Variables:	Prepared By:
T/K = 276–335 K	Valerii P. Sazonov

Experimental Data

The mutual solubilities of acetonitrile (1) and butane (2) in mass percent over the specified temperature range were reported in graphical form in the original publication. The data presented here were extracted from the published graphs by the compiler.

Mutual solubility of acetonitrile (1) and butane (2)

t/°C	T/K	100 w ₁		x ₁	
		Hydrocarbon rich phase	Acetonitrile-rich phase	Hydrocarbon rich phase	Acetonitrile-rich phase
3.2	276.4	—	87.0	—	0.905
17.9	291.1	—	83.4	—	0.877
26.5	299.7	7.2	—	0.099	—
30.0	303.2	—	80.0	—	0.850
35.0	308.2	9.0	—	0.123	—
43.1	316.3	—	72.3	—	0.787
49.6	322.8	—	68.2	—	0.752
53.2	326.4	15.8	—	0.210	—
55.9	329.1	17.5	—	0.231	—
57.0	330.2	—	58.0	—	0.662
58.2	331.4	21.5	—	0.279	—
60.0	333.2	26.8	—	0.341	—
60.5	333.7	—	48.7	—	0.573
60.8	334.0	32.3	—	0.403	—
61.0	334.2	—	42.8	—	0.514
62.0	335.2	39.3	—	0.478	0.478 (UCST)

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. No experimental details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified.
(2) Source not specified; purity not specified.

Estimated Error:

Not reported.

TABLE 2. Dependence of the UCST and x_{1c} on pressure and equation coefficients

P/MPa	5.0	7.5	10.0
UCST, T/K	333.59	333.58	333.63
$t/^\circ\text{C}$ (compiler)	62.51	60.66	59.45
x_{1c}	0.4753	—	0.4661
k	-1289	—	-1363
α	1.100	—	1.007
β	0.261	—	0.254

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The phase apparatus consists of a 50 mm long sapphire capillary with a 3.8 mm inside diameter and a 6.35 outside diameter, inserted in the exit line of the calorimeter. Samples of (1) and (2) are mixed in a flow calorimeter at a temperature above the UCST so that complete mixing occurs. The mixture (of known composition) exits the calorimeter through a stainless steel capillary line that is heated to keep the temperature above the UCST, and enters the thermostated bath surrounding the sapphire capillary. The mixture passes through coils of stainless steel capillary tubing inside the thermostat to equilibrate the mixture with the bath temperature, flows through the sapphire capillary, and exits the apparatus through the back pressure regulator. A Sodev Model CT-C thermostat circulates fluid through the bath. The temperature of this thermostat, which can be programmed to linearly increase or decrease with time, is lowered slowly until the fluid in the sapphire capillary becomes cloudy. The bath temperature where this occurs is read with a Hart Model 1506 resistance thermometer calibrated against a Rosemount thermometer (ITS-90), and is taken as the equilibrium temperature at the mole fraction of the mixture.

Source and Purity of Materials:

(1) Fisher Scientific HPLC; purity of 99.9 mass %; used without further purification.
 (2) Phillips; purity of 99.5 mass %; used without further purification.

Estimated Error:

Temperature: ± 0.02 K.
 Pressure: ± 0.1 MPa.

Components:

(1) Acetonitrile; $\text{C}_2\text{H}_3\text{N}$; [75-05-8]
 (2) Butane; C_4H_{10} ; [106-97-8]

Original Measurements:

W. Warowny, J. Chem. Eng. Data **41**, 689–97 (1996).

Variables:

$T/\text{K} = 319\text{--}336$ K; $P/\text{MPa} = 0.45\text{--}0.68$

Prepared By:

Valerii P. Sazonov

Experimental Data

Mutual solubility of acetonitrile (1) and butane (2) at moderate pressure

T/K	$t/^\circ\text{C}$ (compiler)	P/kPa	x_1		100 w ₁ (compiler)	100 w ₁ (compiler)
			Hydrocarbon-rich phase	Acetonitrile-rich phase		
319.30	46.15	449.1	0.1312	9.64	—	—
328.11	54.96	563.1	—	—	0.7354	66.25
328.60	54.45	570.0	0.2229	16.85	—	—
329.82	55.67	586.3	0.2422	18.42	—	—
333.15	60.00	636.2	0.3167	24.66	0.6868	60.77
335.85	62.70	677.8	0.4858	40.02	—	—
336.02	62.87	680.6	—	—	0.6051	51.98
336.15	63.00	682.5	0.5338	44.71	—	—
336.22	63.07	683.5	0.571	48.5	0.571	48.5 (UCST)

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The apparatus, filling procedure, and method of the measurements were described elsewhere.¹

Source and Purity of Materials:

(1) Source not specified; purity not specified; degassed and dried over molecular sieves.
 (2) Fluka A. G.; purity of 99.9 mole %; used without further purification.

Estimated Error:

Temperature: ± 0.02 K.
 Pressure: ± 0.006 MPa.

References:

¹W. Warowny, J. Chem. Eng. Data **39**, 275 (1994).

5.3. + 2-Methylbutane

Components:		Evaluators:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, September, 2001.
(2) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4]		

Critical Evaluation

Quantitative solubility data for the system of acetonitrile (1) + 2-methylbutane (2) have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system acetonitrile + 2-methylbutane

Reference	T/K	Solubility	Method
Burova <i>et al.</i> ¹	295–330	Mutual	Synthetic
Pavlov <i>et al.</i> ²	275–338	Mutual	Synthetic
Pavlov <i>et al.</i> ³	282–328	(2) in (1)	Synthetic
Rakotondramanana <i>et al.</i> ⁴	293	Mutual	Titration

All original data are compiled in the data sheets immediately following this Critical Evaluation. The upper critical solution temperature has been reported as 338.2 K.² The corresponding critical solution composition has been calculated by evaluators as $x_{c1} = 0.50$ from the data.²

All experimental values reported^{1–4} have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.9283, \quad a_2 = -0.2839, \quad b_1 = 0.7857, \quad b_2 = -0.7455$$

(mean standard error of estimate was 0.0191).

For approximation x_{c1} and UCST determined by Pavlov *et al.*² have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in Table 2. This relationship together with experimental points reported^{1–4} are also presented in Fig. 5.

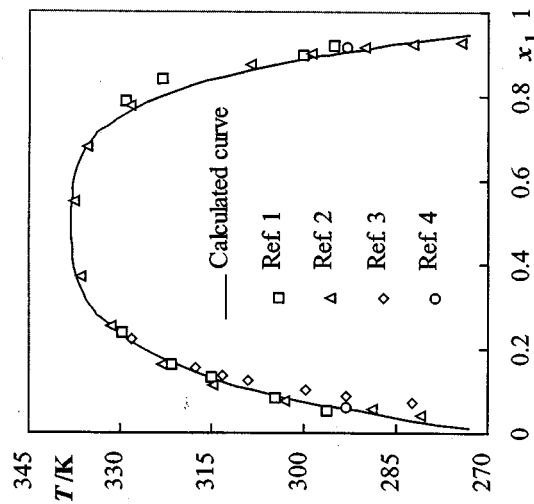


FIG. 5. Mutual solubility of acetonitrile and 2-methylbutane.

TABLE 2. Calculated mutual solubility of acetonitrile (1) and 2-methylbutane (2)

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w ₁	x_1	100 w ₁
273.2	0.012	0.7	0.946	90.9
283.2	0.032	1.8	0.927	87.8
293.2	0.056	3.3	0.905	84.4
298.2	0.070	4.1	0.893	82.6
303.2	0.085	5.0	0.879	80.5
308.2	0.103	6.1	0.864	78.3
313.2	0.123	7.4	0.846	75.8
318.2	0.147	8.9	0.825	72.8
323.3	0.177	10.9	0.799	69.3
328.2	0.215	13.5	0.767	65.2
333.2	0.271	17.5	0.718	59.2
334.2	0.286	18.6	0.703	57.4
335.2	0.305	20.0	0.686	55.4
336.2	0.329	21.8	0.665	53.0
337.2	0.364	24.6	0.633	49.5
337.7	0.391	26.8	0.606	46.7

References:

- ¹G. V. Burova, V. B. Kogon, and M. S. Nemtsov, Zh. Prikl. Khim. (Leningrad) **36**, 988 (1963).
- ²S. Yu. Pavlov, L. A. Serafimov, S. P. Pavlova, and L. S. Kofman, Zh. Fiz. Khim. **40**, 2719 (1966).
- ³S. Yu. Pavlov, S. P. Pavlova, L. A. Serafimov, and L. S. Kofman, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **10**, 915 (1967).
- ⁴S. Rakotondramanana, M.-E. Borredon, and J. Moliner, J. Chem. Eng. Data **32**, 308 (1987).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	S. Yu. Pavlov, L. A. Serafimov, S. P. Pavlova, and L. S. Kofman, Zh. Fiz. Khim. 40 , 2719–2724 (1966).
(2) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4]	
Variables:	Prepared By:
T/K = 275–338	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The mutual solubilities of acetonitrile (1) and 2-methylbutane (2) in mass percent over the specified temperature range were reported in graphical form in the original publication. Numerical data were extracted from the published graphs by the compilers.

t/°C	Mutual solubility of acetonitrile (1) and 2-methylbutane (2)	
	100 w ₁	x ₁
	Hydrocarbon-rich phase	Acetonitrile-rich phase
	T/K	x ₁
1.3	274.5	—
7.8	281.0	0.043
9.1	282.3	—
15.6	288.8	0.057
17.0	290.2	—
25.6	298.8	—
29.8	303.0	0.077
35.5	308.7	—
41.7	314.9	0.114
50.0	323.2	0.163
55.4	328.6	—
58.3	331.5	0.254
62.3	335.5	—
63.5	336.7	0.370
64.5	337.7	—
	100 w ₁	x ₁
	Hydrocarbon-rich phase	Acetonitrile-rich phase
	T/K	x ₁
	—	88.1
	2.5	—
	—	87.7
	3.3	—
	—	86.2
	—	83.8
	4.5	—
	—	80.0
	6.8	—
	10.0	—
	—	66.2
	16.2	—
	—	54.5
	25.1	—
	—	41.0

UCST was reported as 65.0 °C (338.2 K, compilers).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. No experimental details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; distilled; purity ≥ 99.80 mass %; boiling point = 81.6 °C, $n(20^\circ\text{C}, D) = 1.3442$, $d(20^\circ\text{C}, 4^\circ\text{C}) = 0.7828$.
 (2) Source not specified; purity not specified; distilled through a column of 70 theoretical plates; purity ≥ 99.75 mass %; $n(20^\circ\text{C}, D) = 1.3538$, $d(20^\circ\text{C}, 4^\circ\text{C}) = 0.6197$.

Estimated Error:

Not reported.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	G. V. Burova, V. B. Kogan, and M. S. Nemtsov, Zh. Prikl. Khim. (Leningrad) 36 , 988–94 (1963).
(2) 2-Methylbutane; C ₅ H ₁₂ ; [78-78-4]	
Variables:	Prepared By:
T/K = 295–330	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The mutual solubilities of acetonitrile (1) and 2-methylbutane (2) in mass percent over the specified temperature range were reported in graphical form in the original publication. Numerical data were extracted from the published graphs by the compilers.

t/°C	Mutual solubility of acetonitrile (1) and 2-methylbutane (2)	
	100 w ₁	x ₁
	Hydrocarbon-rich phase	Acetonitrile-rich phase
	T/K	x ₁
22.0	295.2	—
23.0	296.2	0.052
27.0	300.2	—
31.5	304.7	0.085
42.0	315.2	0.133
48.5	321.7	0.163
50.0	323.2	—
56.0	329.2	—
56.5	329.7	0.237
	100 w ₁	x ₁
	Hydrocarbon-rich phase	Acetonitrile-rich phase
	—	86.5
	3.0	—
	—	83.5
	5.0	—
	8.0	—
	10.0	—
	—	75.0
	—	68.0
	15.0	—

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. A sample of (1) was placed in a 10 mL ampoule, cooled, and a given amount of hydrocarbon was added. Sealed ampoules were placed into a glass-walled thermostat. The temperature of the thermostat was increased gradually with periodic stirring and a preliminary determination of the clear-point temperature in every ampoule was made. A more precise value of the cloud-point temperature was determined by allowing the thermostat to cool. The determination was repeated several times.

Source and Purity of Materials:

(1) Source not specified; purity not specified; distilled as in Ogorodnikov *et al.*¹; boiling point = 81.8 °C, $n(20^\circ\text{C}, D) = 1.3440$, $d(20^\circ\text{C}, 4^\circ\text{C}) = 0.7818$.
 (2) Source not specified; purity not specified; distilled through a column of 90 theoretical plates as in Ogorodnikov *et al.*²; boiling point = 27.88 °C, $n(20^\circ\text{C}, D) = 1.35383$.

Estimated Error:

Not reported.

References:

- ¹S. K. Ogorodnikov, V. B. Kogan, M. S. Nemtsov, and G. V. Burova, Zh. Prikl. Khim. (Leningrad) **34**, 1096 (1961).
²S. K. Ogorodnikov, V. B. Kogan, and M. S. Nemtsov, Zh. Prikl. Khim. (Leningrad) **33**, 1599 (1960).

Components:	Original Measurements:
(1) Acetonitrile; C_2H_3N ; [75-05-8]	S. Rakotoniramaana, M.-E. Borredon, and J. Mollner, J. Chem. Eng. Data 32 , 308-11 (1987).
(2) 2-Methylbutane; C_5H_{12} ; [78-78-4]	
Variables:	Prepared By:
$T/K = 293$	Valerii P. Sazonov

Experimental Data				
Mutual solubility of acetonitrile (1) and 2-methylbutane (2)				
	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
$t/^\circ C$	T/K (compiler)	Hydrocarbon-rich phase	Acetonitrile-rich phase	
20.0	293.2	3.5	0.060	85.9
				0.915

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The titration method was used. No experimental details were reported.	(1) Source not specified; commercial product; minimum purity of 99 mass %; dried with a 4 A molecular sieve.
	(2) Source not specified; commercial product; minimum purity of 99 mass %.
	Estimated Error:
	Temperature: ± 0.5 K.

Components:	Original Measurements:
(1) Acetonitrile; CH_3CN ; [75-05-8]	S. Yu. Pavlov, S. P. Pavlova, L. A. Serafimov, and L. S. Kofman, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. 10 , 915-20 (1967).
(2) 2-Methylbutane; C_5H_{12} ; [78-78-4]	
Variables:	Prepared By:
$T/K = 282-328$	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data			
Solubility of 2-methylbutane (2) in acetonitrile (1)			
	T/K (compilers)	100 w_2	x_2 (compilers)
$t/^\circ C$			
9.0*	282.2	12.1	0.073
20.0	293.2	14.4	0.087
26.5*	299.7	16.6	0.102
36.0*	309.2	20.1	0.125
40.0	313.2	21.8	0.137
44.5*	317.7	24.4	0.155
55.0*	328.2	33.8	0.225

*The compilers extracted these data from published graphs.

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The synthetic method was used. No details were reported.	(1) Source not specified; pure grade reagent; fractionally distilled.
	(2) Source not specified; purity 99.7 mass %.
	Estimated Error:
	Not specified.

5.4. + Pentane

Components:	Evaluators
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valeriy P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, September, 2001.
(2) Pentane; C ₅ H ₁₂ ; [109-66-0]	

Critical Evaluation

Solubilities in the system comprising acetonitrile and pentane have been reported in three publications.

Sinegubova¹ studied the mutual solubilities of acetonitrile (1) and pentane (2) between 298 and 341 K by the synthetic method. Rakotondramanana *et al.*² measured the mutual solubilities of (1) and (2) by the titration method between 298 and 303 K. McLure *et al.*³ determined the upper critical solution temperature of (1) and (2) by the synthetic method.

The upper critical solution temperature has been reported as 341.2 K³ and 341.4 K.¹ These data are in reasonable agreement and thus their average value: UCST=341.3±0.1 K is recommended. The corresponding critical solution composition has been not reported but was calculated by the evaluators from reported data¹ to be $x_{c1}=0.53$.

Reported^{1,2} experimental values have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.9063, \quad a_2 = -0.1988, \quad b_1 = 3.1067, \quad b_2 = -2.7492$$

(mean standard error of estimate was 0.0036).

For approximation x_{c1} and UCST determined by Sinegubova¹ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship together with experimental data^{1,2} are also presented in Fig. 6.

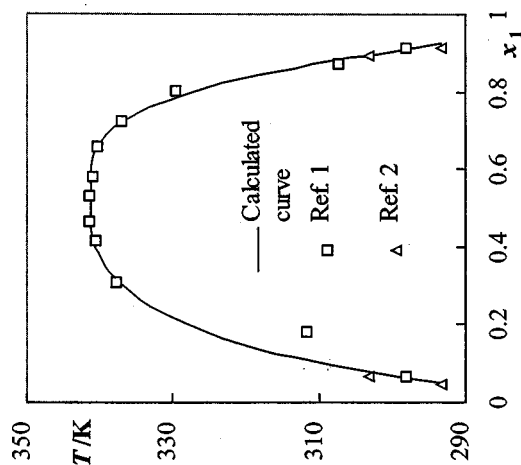


FIG. 6. Mutual solubility of acetonitrile and pentane.

Interpolated mutual solubility of acetonitrile (1) and pentane (2)

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w ₁	x_1	100 w ₁
293.2	0.050	2.9	0.924	87.4
298.2	0.063	3.7	0.910	85.2
303.2	0.078	4.6	0.895	82.9
308.2	0.094	5.6	0.879	80.5
313.2	0.114	6.8	0.862	78.0
318.2	0.137	8.3	0.843	75.3
323.3	0.166	10.2	0.821	72.3
328.2	0.201	12.5	0.795	68.8
333.2	0.248	15.8	0.762	64.6
338.2	0.325	21.5	0.707	57.9
339.2	0.350	23.5	0.689	55.8
340.2	0.384	26.2	0.662	52.7
340.7	0.408	28.2	0.642	50.5
341.2	0.450	31.8	0.606	46.7

References:

- ¹S. I. Sinegubova, Dissertation, Saratov University, 1978.
- ²S. Rakotondramanana, M.-E. Borredon, and J. Molliet, *J. Chem. Eng. Data* **32**, 308 (1987).
- ³J. A. McLure, A. T. Rodriguez, P. A. Ingham, and J. F. Steele, *Fluid Phase Equilib.* **8**, 271 (1982).

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Pentane; C ₅ H ₁₂ ; [109-66-0]	Original Measurements: S. Raktondranana, M.-E. Borredon, and J. Mollner, J. Chem. Eng. Data 32 , 308–11 (1987).
Variables: T/K = 293–303	Prepared By: Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data				
Mutual solubility of acetonitrile (1) and pentane (2)				
t/°C	T/K (computers)	100 w ₁		x ₁ (computers)
		Hydrocarbon-rich phase	Acetonitrile-rich phase	
20.0	293.2	2.7	0.047	0.915
30.0	303.2	3.9	0.067	0.892

*Value corrected by computers from the published graphs; reported in original as 88.8.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. No experimental details were reported.

Source and Purity of Materials:

- (1) Source not specified; commercial product; minimum purity of 99 mass %; dried with a 4 Å molecular sieve.
(2) Source not specified; commercial product; minimum purity of 99 mass %.

Estimated Error:

Temperature: ±0.5 K.

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Pentane; C ₅ H ₁₂ ; [109-66-0]	Original Measurements: S. I. Sinegubova, Dissertation, Saratov University, 1978.
Variables: T/K = 298–341	Prepared By: Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data				
Mutual solubility of acetonitrile (1) and pentane (2)				
t/°C	T/K	100 w ₁		x ₁ (computers)
		Hydrocarbon-rich phase	Acetonitrile-rich phase	
25.0	298.2	3.95	0.067	0.913
34.2	307.4	—	—	0.871
38.5	311.7	11.1	0.180	—
56.5	329.7	—	—	0.802
63.9	337.1	—	—	0.726
64.5	337.7	20.3	0.309	—
67.2	340.4	—	—	0.658
67.3	340.5	28.7	0.414	—
67.9	341.1	—	—	0.579
68.2	341.4	32.9	0.463	—
68.2	341.4	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Sealed ampoules were placed in a glass-walled thermostat. The temperature of the thermostat was increased gradually with periodic stirring and a preliminary determination of the clear-point temperature in every ampoule was made. A more precise value of the cloud-point temperature was determined by allowing the thermostat to cool. The determination was repeated several times.

Source and Purity of Materials:

- (1) Source not specified; pure grade product; distilled over anhydrous soda, boiling point = 81.6 °C; n(20 °C,D) = 1.3441, ρ(25 °C) = 777 g·L⁻¹.
(2) Source not specified; for chromatography; not purified; boiling point = 36.0 °C, n(20 °C,D) = 1.3578, ρ(20 °C) = 626 g·L⁻¹.

Estimated Error:

Temperature: ±0.2 K.

5.6. + Benzene

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Benzene; C ₆ H ₆ ; [71-43-2]	Original Measurements: O. S. Chistozonova, G. M. Dugacheva, and A. G. Anikin, Zh. Fiz. Khim. 41 , 82-5 (1967).
Variables: T/K = 224–279	Prepared By: Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

No region of liquid–liquid immiscibility was observed. A full solid–liquid phase diagram in mole percent over the specified temperature range was presented in graphical form in the original publication. The compilers extracted these data from published graphs.

Melting temperatures of acetonitrile (1) and benzene (2) system			
x ₁	100 w ₁ (compilers)	t/°C	T/K (compilers)
0.000	0.0	5.5	278.7
0.015	0.8	4.3	277.5
0.049	2.6	1.9	275.1
0.156	8.95	–3.3	269.9
0.396	25.6	–15.0	258.2
0.500	34.4	–19.6	253.6
0.548	38.9	–22.1	251.1
0.603	44.4	–24.1	249.1
0.725	58.1	–29.6	243.6
0.869	77.7	–43.9	229.3
0.915	85.0	–49.5	223.7
0.967	93.9	–46.6	226.6
0.982	96.6	–45.9	227.3
1.000	100.0	–44.9	228.3

A eutectic was reported at –49.5 °C (223.7 K, compilers) at x₁ = 0.915 (100 w₁ = 85.0, compilers).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Solutions of various compositions were transferred to glass vessels, and placed in a cooling mixture. The change of temperature was measured by the thermocouple. No experimental details given.

Source and Purity of Materials:

(1) Source not specified; purity 99.73 mole %, melting point = –44.9 °C.
(2) Source not specified; purity 99.90 mole %, melting point = 5.5 °C.

Estimated Error:

Temperature: ±0.05 K.

5.5. + Alkanes: C₅–C₁₈

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Alkanes; C ₅ H ₁₂ –C ₁₈ H ₃₈	Original Measurements: I. A. McLure, A. T. Rodriguez, P. A. Ingham, and J. F. Steele, Fluid Phase Equilib. 8 , 271–84 (1982).
Variables: T/K = 341–426	Prepared By: Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

Upper critical solution temperatures (USCT) and critical solution compositions (x_{1,c}) of the systems acetonitrile (1) + alkane (2)

Alkane	Source and grade	Purity (mol %)	T/K	t/°C (compilers)	x _{1,c}
Pentane; C ₅ H ₁₂ ; [109-66-0]	Fisons; A. R.	>99	341.2	68.0	—
Hexane; C ₆ H ₁₄ ; [110-54-3]	Fisons; S. L. R.	>99	350.2	77.0	—
Heptane; C ₇ H ₁₆ ; [142-82-5]	Fisons; S. L. R.	>99.5	358.0	84.8	0.63
Octane; C ₈ H ₁₈ ; [111-65-9]	Fisons; S. L. R.	>99.5	365.1	91.9	0.67
Nonane; C ₉ H ₂₀ ; [111-84-2]	Phillips Petroleum; Research	99.31	374.2	101.0	0.70
Decane; C ₁₀ H ₂₂ ; [124-18-5]	Phillips Petroleum; Pure	>99	381.7	108.5	0.75
Undecane; C ₁₁ H ₂₄ ; [1120-21-4]	Phillips Petroleum; Research	99.97	386.2	113.0	0.77
Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	Fisons; S. L. R.	>99	398.2	125.0	—
Tetradecane; C ₁₄ H ₃₀ ; [629-59-4]	Phillips Petroleum; Pure	>99	403.7	130.5	—
Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	Koch-Light; Puriss.	>99	420.2	147.0	—
Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	B. Newton Maine Ltd.	99	426.2	153.0	—

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The UCST was determined in Pyrex tubes of samples containing approximately equal volumes of the two components, the exact amounts being determined by weight. Each sample was thoroughly degassed by several freeze–pump–thaw cycles before being sealed off under vacuum. The heating and cooling rates close to the phase transition were ±0.1 K·min^{–1}. The mixtures were stirred by means of a couple of stainless-steel ball bearings activated magnetically. The measurement of temperature was carried out at ambient temperature and above using a mercury-in-glass thermometer.

Source and Purity of Materials:

(1) Fisons; S. L. R.; purity >99 mol. %; dried, and redistilled before use.
(2) Dried and redistilled.

Estimated Error:

Temperature: ±0.5 K.

5.7. + Cyclohexane

Components:	Evaluator:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valeri P. Sazonov, Technical University, Samara, Russia,
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	October, 2001.

Critical Evaluation

Quantitative solubility data for the system acetonitrile (1) and cyclohexane (2) have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system acetonitrile+cyclohexane.

Reference	T/K	Solubility	Method
Poppe ¹	350	UCST	Synthetic
Nagata and Kaoh ²	313 and 323	Mutual	Titration
Lakhanpal <i>et al.</i> ³	298–321	Mutual	Analytical
Nagata and Ohta ⁴	298 and 318	Mutual	Titration
Vani <i>et al.</i> ⁵	277–350	Mutual	Synthetic
Rakotondramanana <i>et al.</i> ⁶	293–313	Mutual	Titration
Ott <i>et al.</i> ⁷	319–348	Mutual	Synthetic
Francis ⁸	349	UCST	Synthetic

In addition to these data Ott *et al.*⁷ reported extensive measurements of the mutual solubility of components (1) and (2) determined between 0.4 and 15 MPa. The work of Poppe¹ defines the influence of pressure on upper critical solution temperature between 0.5 and 12.4 MPa. All original data are compiled in the data sheets immediately following this Critical Evaluation.

The upper critical solution temperature of this system has been reported as 347.84 K,⁷ 349.2 K,⁸ 349.70 K,¹ and 349.789 K.⁵ These data are in reasonable agreement and thus their average value: UCST=349.1±0.8 K is recommended. The corresponding critical solution composition was reported to be $x_{c1}=0.5269$.

All experimental values reported^{2–7} have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1=1.0175, a_2=-0.5082, b_1=2.0121, b_2=-1.8689$$

(mean standard error of estimate was 0.0052).

For approximation x_{c1} and UCST from Vani *et al.*⁵ have been used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in Table 2. This relationship together with experimental points reported^{2–7} are also presented in Fig. 7.

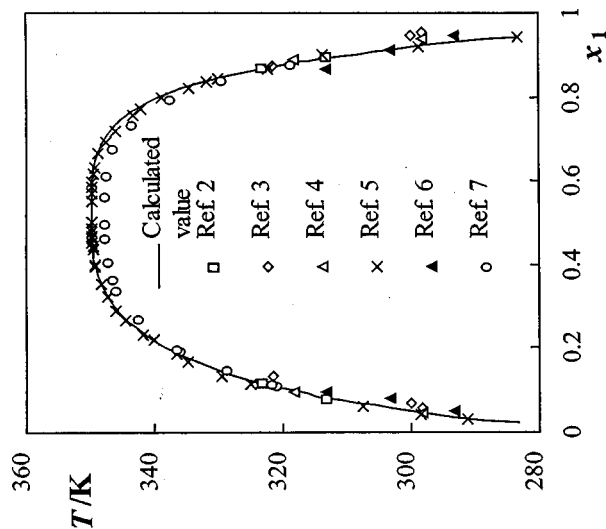


FIG. 7. Mutual solubility of acetonitrile and cyclohexane.

TABLE 2. Calculated mutual solubility of acetonitrile (1) and cyclohexane (2).

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w ₁	x_1	100 w ₁
283.2	0.022	1.1	0.944	89.2
293.2	0.036	1.8	0.930	86.6
303.2	0.056	2.8	0.913	83.7
313.2	0.081	4.1	0.893	80.3
318.2	0.097	5.0	0.881	78.3
323.2	0.115	6.0	0.867	76.1
328.2	0.138	7.2	0.851	73.6
333.2	0.166	8.8	0.831	70.6
338.2	0.202	11.0	0.805	66.8
343.2	0.254	14.2	0.767	61.6
344.2	0.268	15.2	0.756	60.2
345.2	0.283	16.1	0.744	58.6
346.2	0.302	17.4	0.730	56.9
347.2	0.324	18.9	0.712	54.7
348.2	0.354	21.1	0.687	51.7
348.7	0.374	22.6	0.670	49.8
349.2	0.402	24.7	0.646	47.1
349.4	0.418	25.9	0.632	45.6

References:

- ¹G. Poppe, Bull. Soc. Chim. Belg. **44**, 640 (1935).
- ²L. Nagata and K. Kaoh, Thermochim. Acta **39**, 45 (1980).
- ³M. L. Lakhanpal, N. J. Mandul, and S. C. Ahuja, Indian J. Chem. **20A**, 1008 (1981).
- ⁴L. Nagata and T. Ohta, J. Chem. Eng. Data **28**, 256 (1983).
- ⁵V. Vani, S. Guha, E. S. R. Gopal, and S. M. Madhusudana Rao, Phys. Lett. **99A**, 441 (1983); V. Vani, S. Guha, and E. S. R. Gopal, J. Chem. Phys. **86**, 3999 (1986).
- ⁶S. Rakotondramanana, M.-E. Borredon, and J. Moliner, J. Chem. Eng. Data **32**, 306 (1987).
- ⁷J. B. Ott, J. E. Purdy, B. J. Neely, and R. A. Harris, J. Chem. Thermodyn. **20**, 1079 (1988).
- ⁸A. W. Francis, Ind. Eng. Chem. **36**, 1096 (1944).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	I. Nagata and K. Katoh, <i>Thermochim. Acta</i> 39 , 45–62 (1980).
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	
Variables:	Prepared By:
T/K = 313 and 323	Valerii P. Sazonov

Experimental Data			
Mutual solubility of acetonitrile (1) and cyclohexane (2)			
<i>t</i> /°C	T/K (compiler)	<i>x</i> ₁	<i>x</i> ₁
		Hydrocarbon-rich phase	100 <i>w</i> ₁ (compiler)
			Acetonitrile-rich phase
40.00	313.15	0.0787	4.00
50.00	323.15	0.1184	6.15
			80.79
			76.90

Auxiliary Information

Method/Apparatus/Procedure:
The titration method was used. Component (1) was added from a burette to a known amount of (2) until the mixture became turbid. The upper face of an equilibrium vessel which was polished flat and fitted with a lid and Teflon O-ring held tightly by six bolts. The lid contained two feed tubes to introduce the second component, two sampling tubes, a thermometer, and a pressure measuring tube connected to a mercury manometer. Nitrogen gas was used to pressurize the lower sampling tube, so that the mixture could not enter into it during the mixing process. During titration, the samples were maintained at a desired temperature by means of a water thermostat.

Source and Purity of Materials:
(1) Source not specified; reagent grade; not purified; *n*(25 °C,D) = 1.341 70.
(2) Source not specified; spectrograde; not purified; *n*(25 °C,D) = 1.423 52.

Estimated Error:
Temperature: ±0.01 K.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	G. Poppe, <i>Bull. Soc. Chim. Belg.</i> 44 , 640–57 (1935).
(2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	
Variables:	Prepared By:
T/K = 350 and P/kPa = 582–12412	Valerii P. Sazonov

Experimental Data
The UCST was reported to be 76.55 °C (349.70 K, compiler). A value of dT_c/dP of 0.0235 K·kPa⁻¹ was reported in the above pressure range.

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. Observations were carried out in sealed tubes in the presence of the vapor phase. A Cailliet tube with a Kuenen electromagnetic stirrer was used in the experiments at higher pressure. A thermostating cylinder was also used to control the temperature.

Source and Purity of Materials:
(1) Obtained from the Bureau Etalons Physico-Chimiques.
(2) Obtained from the Bureau Etalons Physico-Chimiques.

Estimated Error:
Pressure: ± 100 kPa.

Components:		Original Measurements:	
(1) Acetonitrile; C_2H_3N ; [75-05-8]		I. Nagata and T. Ohta, <i>J. Chem. Eng. Data</i> 28 , 256-9 (1983).	
(2) Cyclohexane; C_6H_{12} ; [110-82-7]			
Variables:		Prepared By:	
$T/K = 298$ and 318		Valerii P. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and cyclohexane (2)			
$t/^\circ C$	T/K (compiler)	x_1 Hydrocarbon-rich phase	x_1 100 w_1 (compiler) Acetonitrile-rich phase
25.00	298.15	0.0440	2.20
45.00	318.15	0.0935	4.79
			88.41
			79.50

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Component (1) was added from a burette to a known amount of (2) until the mixture became turbid. The upper face of an equilibrium vessel which was polished flat and fitted with a lid and Teflon O-ring held tightly by six bolts. The lid contained two feed tubes to introduce the second component, two sampling tubes, a thermometer, and a pressure measuring tube connected to a mercury manometer. Nitrogen gas was used to pressurize the lower sampling tube, so that the mixture could not enter into it during the mixing process. During titration, the samples were maintained at a desired temperature by means of a water thermostat.

Source and Purity of Materials:

(1) Wako Chemical Co.; guaranteed reagent grade; not purified.
(2) Wako Chemical Co.; guaranteed reagent grade; purified by fractional distillation from a 1 m column packed with McMahon packing.

Estimated Error:

Temperature: ± 0.01 K.

Components:		Original Measurements:	
(1) Acetonitrile; C_2H_3N ; [75-05-8]		M. L. Lakhanpal, N. J. Mandal, and S. C. Ahuja, <i>Indian J. Chem.</i> 20A , 1008-13 (1981).	
(2) Cyclohexane; C_6H_{12} ; [110-82-7]			
Variables:		Prepared By:	
$T/K = 298-321$		Valerii P. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and cyclohexane (2)			
$t/^\circ C$	T/K (compiler)	x_1 Hydrocarbon-rich phase	x_1 100 w_1 (compiler) Acetonitrile-rich phase
25.0	298.2	0.0569	2.86
26.9	300.1	0.06924	3.50
48.2	321.4	0.1348	7.06
			90.87
			90.00
			76.99

Auxiliary Information

Method/Apparatus/Procedure:

The mutual solubilities of the components were determined with the help of Zeiss interferometer. No experimental details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade; twice distilled at first over P_2O_5 , then over anhydrous potassium carbonate, boiling point = $80^\circ C$.
(2) AR; containing traces of benzene as an impurity; purified as in Lakhanpal *et al.*¹

Estimated Error:

Not reported.

References:

¹M. L. Lakhanpal, K. K. Kapoor, Lal Gurcharan, and H. G. Mandal, *Indian J. Chem.* **11**, 471 (1973).

T/K	$100 w_1$	x_1	ϕ_1^a	$100 w_1$	x_1	ϕ_1^a	$100 w_1$	x_1	ϕ_1^a
76.390	349.540	27.79	0.4410	0.2772	—	43.89	0.6159	—	0.4379
76.402	349.552	—	—	—	—	—	—	—	—
76.430	349.580	28.01	0.4437	0.2794	—	—	—	—	—
76.502	349.652	28.77	0.4530	0.2870	—	—	—	—	—
76.503	349.653	—	—	—	—	—	—	—	—
76.522	349.672	—	—	—	—	41.90	0.5965	—	0.4181
76.546	349.696	—	—	—	—	41.50	0.5926	—	0.4141
76.564	349.714	—	—	—	—	41.15	0.5891	—	0.4106
76.570	349.720	—	—	—	—	40.62	0.5838	—	0.4054
76.574	349.724	29.83	0.4657	0.2916	—	40.64	0.5840	—	0.4056
76.580	349.730	30.03	0.4680	0.2995	—	—	—	—	—
76.580	349.730	30.34	0.4717	0.3026	—	—	—	—	—
76.582	349.732	30.18	0.4698	0.3010	—	—	—	—	—
76.584	349.734	30.02	0.4679	0.2994	—	—	—	—	—
76.586	349.736	30.20	0.4701	0.3013	—	—	—	—	—
76.590	349.740	30.38	0.4722	0.3030	—	40.24	0.5799	—	0.4015
76.591	349.741	30.46	0.4731	0.3038	—	—	—	—	—
76.591	349.741	30.42	0.4727	0.3035	—	—	—	—	—
76.604	349.754	30.96	0.4790	0.3088	—	—	—	—	—
76.606	349.756	30.84	0.4776	0.3076	—	—	—	—	—
76.609	349.759	—	—	—	—	39.52	0.5726	—	0.3943
76.613	349.763	31.29	0.4828	0.3121	—	39.35	0.5708	—	0.3926
76.620	349.770	31.78	0.4885	0.3170	—	—	—	—	—
76.624	349.774	32.14	0.4927	0.3207	—	38.38	0.5608	—	0.3829
76.628	349.778	32.35	0.4950	0.3227	—	38.18	0.5586	—	0.3809
76.632	349.782	—	—	—	—	37.73	0.5540	—	0.3764
76.633	349.783	32.92	0.5013	0.3284	—	—	—	—	—
76.634	349.784	—	—	—	—	37.45	0.5511	—	0.3737
76.635	349.785	33.30	0.5058	0.3323	—	—	—	—	—
76.636	349.786	33.46	0.5076	0.3338	—	—	—	—	—
76.637	349.787	33.81	0.5115	0.3373	—	36.67	0.5428	—	0.3659
76.638	349.788	34.23	0.5162	0.3415	—	36.20	0.5377	—	0.3612
76.639	349.789	34.62	0.5205	0.3453	—	35.67	0.5320	—	0.3558
76.639	349.789	35.17	0.5265	0.3544	—	35.54	0.5304	—	0.3454

^aVolume fraction.

UCST was reported as 349.789 K (76.639 °C, compiler) at $100 w_1 = 35.20$, $x_1 = 0.5269$, and $\phi_1 = 0.3512$.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Samples of (1) and (2) were placed in Pyrex glass bulbs which were nearly 2 cm high and were cylindrical with a diameter nearly 2 cm. The cleaned bulbs were filled with the liquids in a glove box using Finn pipettes. The weight of the liquid filled was then measured using a monopan balance which can measure 5×10^{-5} g. The composition of the liquids in the cell was then calculated using these weights. The experiment was carried out in a paraffin oil bath of capacity 35 L. Its temperature is controlled using a proportional integral derivative type controller, though the short term stability is nearly 0.0005 K. A thermostat operated at microwave levels of power dissipation was used as a temperature sensor for the controller. For measuring the temperature, a platinum resistance thermometer was used with a resistance bridge made by the Automatic Systems Laboratories (model F-17). The temperature of the bath was raised until the liquids were in the one phase region. The temperature was then slowly reduced in steps of a few mK and the separation temperature of each composition was determined by visually observing the phase separation temperature which is indicated by the meniscus formation. Near the critical concentration, critical slowing down sets and long relaxation times, of a few hours, were allowed for the liquids to attain equilibrium.

Source and Purity of Materials:

(1) S. D. Fine Chemicals Pvt. Ltd.; analytical reagent grade; purity 99.8 mass %; dried and distilled over a molecular sieve; no impurities detected by GLC.
(2) S. D. Fine Chemicals Pvt. Ltd.; analytical reagent grade; purity 99.8 mass %; distilled over a lithium aluminum hydride; no impurities detected by GLC.

Estimated Error:

Temperature: ± 0.001 K.

Original Measurements:

V. Vani, S. Guha, E. S. R. Gopal, and S. M. Madhusudana Rao, Phys. Lett. **99A**, 441-4 (1983).
*V. Vani, S. Guha, and E. S. R. Gopal, J. Chem. Phys. **86**, 3999-4007 (1986).

Prepared By:

Valerii P. Sazonov

Experimental Data

Mutual solubility of acetonitrile (1) and cyclohexane (2)

$T/^\circ\text{C}$ (compiler)	Hydrocarbon-rich phase		Acetonitrile-rich phase		ϕ_1
	$100 w_1$	x_1	$100 w_1$	x_1	
3.350	276.500	—	90.08	0.9490	0.9004
5.300	278.450	1.00	0.0100	—	—
10.100	283.250	—	—	0.9437	0.8907
18.100	291.250	1.53	0.0308	—	—
25.340	298.490	2.00	0.0402	—	—
25.600	298.750	—	—	0.9205	0.8491
33.790	306.940	3.01	0.0599	—	—
34.350	307.500	2.97	0.0590	—	—
40.600	313.750	—	—	0.9019	0.8171
49.100	322.250	—	—	0.8662	0.7588
51.814	324.964	5.81	0.1123	—	—
56.242	329.392	7.00	0.1336	—	—
56.736	329.886	—	—	0.8454	0.7266
58.485	331.635	—	—	0.8381	0.7156
61.132	334.282	—	—	0.8229	0.6931
61.356	334.506	—	—	0.8204	0.6894
61.650	334.800	9.01	0.1687	—	—
63.302	336.452	9.94	0.1846	—	—
65.628	338.778	—	—	0.7979	0.6574
66.834	339.984	12.02	0.2188	—	—
68.131	341.281	—	—	0.7782	0.6303
68.550	341.700	12.91	0.2331	—	—
68.968	342.118	—	—	0.7711	0.6208
69.238	342.388	—	—	0.7682	0.6169
69.512	342.662	—	—	0.7611	0.6076
70.072	343.222	—	—	0.7576	0.6044
70.097	343.247	—	—	0.7587	0.6030
71.250	344.400	15.00	0.2657	—	—
71.275	344.425	—	—	0.7439	0.5853
72.770	345.920	16.47	0.2879	—	—
72.818	345.968	—	—	0.7205	0.5561
73.428	346.578	—	—	0.7093	0.5425
73.746	346.896	—	—	0.7061	0.5387
74.071	347.221	—	—	0.7009	0.5325
74.203	347.353	19.00	0.3248	—	—
74.455	347.605	—	—	0.6908	0.5206
75.028	348.178	21.00	0.3528	—	—
75.164	348.314	—	—	0.6746	0.5019
75.486	348.636	—	—	0.6638	0.4897
75.890	349.040	—	—	0.6463	0.4703
76.006	349.156	—	—	—	—
76.019	349.169	24.22	0.3958	—	—
76.020	349.170	24.25	0.3962	—	—
76.032	349.182	24.53	0.3999	—	—
76.128	349.278	25.46	0.4119	0.6409	0.4645
76.188	349.338	—	—	—	—
76.252	349.402	—	—	0.6308	0.4537
76.368	349.518	27.46	0.4370	0.6260	0.4486

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	Original Measurements: J. B. Ott, J. E. Purdy, B. J. Neely, and R. A. Harris, J. Chem. Thermodyn. 20 , 1079-87 (1988).
Variables: T/K = 319-348 K; P/MPa = 0.1-15	Prepared By: Valerii P. Sazonov

t/°C	T/K	Experimental Data			
		Mutual solubility of acetonitrile (1) and cyclohexane (2) at ambient pressure		100 w ₁ (complier)	
		Hydrocarbon-rich phase	Acetonitrile-rich phase	Hydrocarbon-rich phase	Acetonitrile-rich phase
45.53	318.68	—	—	—	—
47.81	320.96	0.1105	5.71	—	—
48.68	321.83	0.1139	5.90	—	—
55.48	328.63	0.1477	7.79	—	—
56.44	329.59	—	—	—	71.72
62.76	335.91	0.1951	10.57	—	—
63.47	336.62	0.1996	10.84	—	—
64.44	337.59	—	—	—	65.14
69.39	342.54	0.2692	15.23	—	—
70.46	343.61	—	—	—	57.20
72.79	345.94	0.3375	19.90	—	—
73.24	346.39	—	—	—	50.34
73.31	346.46	0.3633	21.77	—	—
74.15	347.30	0.4077	25.14	—	—
74.46	347.61	—	—	—	43.57
74.62	347.77	0.4633	29.63	—	—
74.68	347.83	0.4978	32.59	—	—
74.69	347.84	—	—	—	38.56

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	Original Measurements: S. Rakotondramanana, M.-E. Borredon, and J. Molliner, J. Chem. Eng. Data 32 , 306-8 (1987).
Variables: T/K = 293-313	Prepared By: Valerii P. Sazonov

t/°C	T/K	Experimental Data			
		Mutual solubility of acetonitrile (1) and cyclohexane (2)		100 w ₁ (complier)	
		Hydrocarbon-rich phase	Acetonitrile-rich phase	Hydrocarbon-rich phase	Acetonitrile-rich phase
20.0	293.2	2.4	0.048	89.6	0.946
30.0	303.2	4.1	0.081	83.8	0.914
40.0	313.2	4.9	0.096	76.2	0.868

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. No experimental details were reported.

Source and Purity of Materials:

(1) Source not specified; commercial product; dried with a 4 A molecular sieve.
(2) Source not specified; commercial product; minimum purity of 99 mass %.

Estimated Error:

Temperature: ±0.5 K.

5.8. + Cycloalkanes: C₆-C₁₀

TABLE 2. Mutual solubility of acetonitrile (1) and cyclohexane (2) at high pressure

P/MPa	T/K (compiler)	x_1	x_1	100 w ₁ (compiler)	100 w ₁ (compiler)
0.4	323.15	0.1198	0.8649	6.23	77.86
15.0	323.15	0.1355	0.8782	7.10	75.74
15.0	348.15	0.3042	0.7077	17.58	54.15

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The liquids to be mixed were injected into the sample vessel through the capillary tube. This tube was then sealed so that a sample was completely enclosed in an all-glass container except for a Teflon-coated magnetic stirring rod placed in the vessel during construction. The volume of the sample vessel was approximately 25 mL and the total sample size was approximately 15 mL. The sample vessel was placed inside a temperature-control jacket, which in turn was surrounded by a vacuum jacket. A Rosemount platinum thermometer passed down the tube at the top of the apparatus and into the thermometer well of the sample vessel. To measure the temperature, fluid was pumped through the circulating jacket and through a temperature controller programmed to heat or cool at a slow rate. The sample was stirred rapidly with a magnetic stirrer using the Teflon-coated stirring bar in the sample vessel. A glass spiral was fused to the thermometer well inside the mixing vessel to break up the swirling action of the stirrer and give better mixing. The equilibrium temperature was obtained visually as the value where the mixture became clear upon heating or cloudy upon cooling. Care was taken not to confuse critical opalescence with phase separation.

Source and Purity of Materials:

(1) B and J Chrompure; purity of 99.9 mass %; used without further purification; dried over Davison 3 A molecular sieve.
(2) MCB Spectro-grade; purity of 99.9 mass %; used without further purification; dried over sodium ribbon.

Estimated Error:

Temperature: ± 0.02 K.

Components:

(1) Acetonitrile; C₂H₃N; [75-05-8]
(2) Cycloalkanes; C₆H₁₂, C₇H₁₄ and C₁₀H₁₈

Original Measurements:

A. W. Francis, Ind. Eng. Chem. **36**, 1096-104 (1944).

Variables:

T/K = 349-379

Prepared By:

Valerii P. Sazonov

Experimental Data

Critical solution temperatures of mixtures of acetonitrile (1) and cycloalkane (2)

Cycloalkane	Boiling point cycloalkane/ ^o C	t/ ^o C	T/K (compiler)
Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	80.8	76.0	349.2
Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2]	100.8	78.0	351.2
Decahydronaphthalene; C ₁₀ H ₁₈ ; [91-17-8]	194.6	106.0	379.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The reagents, about 1 mL of (1) and 1-1.5 mL of (2), were placed in tubes and stirred with a thermometer while the tubes were warmed gradually in a bath of water or glycerol. The temperature of disappearance or reappearance of the cloud due to two liquid phases was read three or four times in each direction. If the final position of the interface was not near the middle of the liquid, the volumes of the reagents were adjusted to make it so.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent.
(2) Not specified.

Estimated Error:

Not reported.

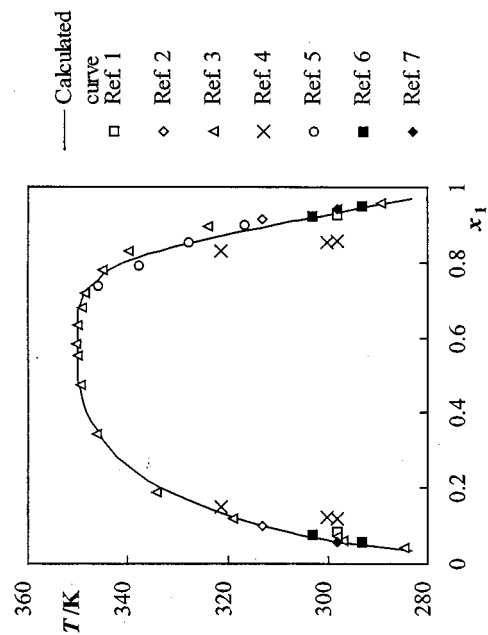


FIG. 8. Mutual solubility of acetonitrile and hexane.

TABLE 2. Calculated mutual solubility of acetonitrile and hexane

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w ₁	x_1	100 w ₁
283.2	0.035	1.7	0.970	93.9
293.2	0.050	2.4	0.945	89.1
303.2	0.071	3.5	0.919	84.4
308.2	0.085	4.2	0.906	82.1
313.2	0.100	5.0	0.893	79.9
318.2	0.119	6.0	0.880	77.7
323.2	0.141	7.3	0.865	75.3
328.2	0.168	8.8	0.849	72.8
333.2	0.201	10.7	0.832	70.2
338.2	0.243	13.3	0.811	67.1
343.2	0.301	17.0	0.782	63.1
348.2	0.403	24.3	0.727	55.9
349.2	0.442	27.4	0.702	52.9
349.7	0.473	29.9	0.680	50.3
350.0	0.503	32.5	0.657	47.7

References:

- ¹J. F. Rusling, R. J. Bertsch, R. A. Barford, and H. L. Rothbart, *J. Chem. Eng. Data* **14**, 169 (1969).
- ²H. Sugi and T. Katayama, *J. Chem. Eng. Jpn.* **11**, 167 (1978).
- ³S. I. Sinegubova, Dissertation, Saratov University, 1978.
- ⁴M. L. Lakhampal, N. J. Mandil, and S. C. Ahuja, *Indian J. Chem.* **20A**, 1008 (1981).
- ⁵L. M. Vinogradova and A. E. Shcherbina, *Zh. Fiz. Khim.* **57**, 1268 (1983).
- ⁶S. Rakotondramanana, M.-E. Borredon, and J. Moliner, *J. Chem. Eng. Data* **32**, 308 (1987).
- ⁷I. Nagata, *Thermochim. Acta* **114**, 227 (1987).
- ⁸L. A. McLure, A. T. Rodriguez, P. A. Ingham, and J. F. Steele, *Fluid Phase Equilib.* **8**, 271 (1982).

5.9. + Hexane

Components:		Evaluators:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, October, 2001.	
(2) Hexane; C ₆ H ₁₄ ; [110-54-3]			
Critical Evaluation:			
Quantitative solubility data for the system acetonitrile (1) and hexane (2) have been reported in the publications listed in Table 1.			
TABLE 1. Summary of solubility data for the system acetonitrile+hexane			
Reference	T/K	Solubility	Method
Rusling <i>et al.</i> ¹	298	Mutual	Titration
Sugi and Katayama ²	313	Mutual	Synthetic
Sinegubova ³	279 to 350	Mutual	Synthetic
Lakhampal <i>et al.</i> ⁴	298 to 321	Mutual	Analytical
Vinogradova and Shcherbina ⁵	317 to 348	(2) in (1)	Synthetic
Rakotondramanana <i>et al.</i> ⁶	293 and 303	Mutual	Titration
Nagata ⁷	298	Mutual	Analytical

In addition to these data, McLure *et al.*⁸ determined the upper critical solution temperatures of binary systems composed of acetonitrile+alkanes (C₂-C₁₀). All original data are compiled in the data sheets immediately following this Critical Evaluation. The hydrocarbon-rich phase data and especially acetonitrile-rich phase data of Lakhampal *et al.*⁴ disagree markedly from all other studies and are rejected.

The upper critical solution temperature of this system has been reported as 350.2 K,^{3,8} these data are in excellent agreement and this value is recommended. The corresponding critical solution composition has been reported as $x_{c1} = 0.583$.³

All experimental values reported¹⁻⁷ (except Lakhampal *et al.*⁴) have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.9035, \quad a_2 = -0.2252, \quad b_1 = 5.4260, \quad b_2 = -4.8743$$

(mean standard error of estimate was 0.0198).

For approximation values of x_{c1} and UCST determined by Sinegubova³ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in Table 2. This relationship together with experimental data¹⁻⁷ are also presented in Fig. 8.

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		H. Sugi and T. Katayama, J. Chem. Eng. Jpn. 11 , 167-72 (1978).	
(2) Hexane; C ₆ H ₁₄ ; [110-54-3]			
Variables:		Prepared By:	
T/K = 313		Valerii P. Sazonov and Nikolai V. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and hexane (2)			
<i>t</i> /°C	<i>T</i> /K (compilers)	<i>x</i> ₁	<i>x</i> ₁
40.00	313.15	0.0985	0.9143
		Hydrocarbon-rich phase	Acetonitrile-rich phase
		100 <i>w</i> ₁ (compilers)	100 <i>w</i> ₁ (compilers)
			83.56

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		J. F. Rusling, R. J. Bertsch, R. A. Barford, and H. L. Rothbart, J. Chem. Eng. Data 14 , 169-73 (1969).	
(2) Hexane; C ₆ H ₁₄ ; [110-54-3]			
Variables:		Prepared By:	
T/K = 298		Valerii P. Sazonov and Nikolai V. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and hexane (2)			
<i>t</i> /°C	<i>T</i> /K (compilers)	<i>x</i> ₁ (compilers)	<i>x</i> ₁ (compilers)
25.0	298.2	0.084	0.925
		Hydrocarbon-rich phase	Acetonitrile-rich phase
		100 <i>w</i> ₁	100 <i>w</i> ₁
			85.5

Method/Apparatus/Procedure:		Auxiliary Information	
Mutual solubility was determined by a cloud-point method described elsewhere. ¹ No experimental details were reported.			
Source and Purity of Materials:			
(1) Merck Uvasol; spectrograde chemical; minimum purity 99.7 mole %; not purified; $\rho(25\text{ }^\circ\text{C}) = 776.71\text{ g}\cdot\text{L}^{-1}$.			
(2) Merck Uvasol; spectrograde chemical; minimum purity 99 mole %; not purified; $\rho(25\text{ }^\circ\text{C}) = 654.72\text{ g}\cdot\text{L}^{-1}$.			
Estimated Error:			
Temperature: $\pm 0.01\text{ K}$.			
References:			
¹ H. Sugi, T. Niita, and T. Katayama, J. Chem. Eng. Jpn. 9 , 12 (1976).			

Method/Apparatus/Procedure:		Auxiliary Information	
The titration method was used. No experimental details were reported.			
Source and Purity of Materials:			
(1) Source not specified; analytical grade; twice distilled; $\rho(25\text{ }^\circ\text{C}) = 777\text{ g}\cdot\text{L}^{-1}$.			
(2) Source not specified; analytical grade; twice distilled; $\rho(25\text{ }^\circ\text{C}) = 664\text{ g}\cdot\text{L}^{-1}$.			
Estimated Error:			
Temperature: $\pm 0.1\text{ K}$.			

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	M. L. Lakhapal, N. J. Mandal, and S. C. Ahuja, Indian J. Chem.
(2) Hexane; C ₆ H ₁₄ ; [110-54-3]	20A, 1008-13 (1981).
Variables:	Prepared By:
T/K = 298-321	Valerii P. Sazonov and Nikolai V. Sazonov

t/°C	T/K (compilers)	Mutual solubility of acetonitrile (1) and hexane (2)		100 w ₁ (compilers)	x ₁	100 w ₁ (compilers)	x ₁
		Hydrocarbon-rich phase	Acetonitrile-rich phase				
25.0	298.2	0.1185	6.02	0.8588	74.34		
26.9	300.1	0.1250	6.37	0.8550	73.74		
48.2	321.4	0.1500	7.75	0.8312	70.11		

Method/Apparatus/Procedure:
The mutual solubilities of the components were determined with the help of Zeiss interferometer. No experimental details were reported.

Auxiliary Information

Source and Purity of Materials:
(1) Source not specified; pure grade; twice distilled at first over P₂O₅, then over anhydrous potassium carbonate, collected the fraction at 80 °C.
(2) Source not specified; spectroscopy grade; not purified.

Estimated Error:
Not reported.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	S. I. Sinegubova, Dissertation, Saratov University, 1978.
(2) Hexane; C ₆ H ₁₄ ; [110-54-3]	
Variables:	Prepared By:
T/K = 279-350	Valerii P. Sazonov and Nikolai V. Sazonov

t/°C	T/K (compiler)	Mutual solubility of acetonitrile (1) and hexane (2)		100 w ₁	x ₁ (compiler)	100 w ₁	x ₁ (compilers)
		Hydrocarbon-rich phase	Acetonitrile-rich phase				
6.0	279.2	—	—	92.5	—	0.963	—
11.5	284.7	2.0	0.041	—	—	—	—
16.1	289.3	—	—	91.1	—	0.956	—
19.9	293.1	—	—	90.0*	—	0.950	—
23.9	297.1	3.0	0.061	—	—	—	—
25.0	298.2	3.7	0.075	88.3	—	0.941	—
45.8	319.0	6.0	0.118	—	—	—	—
50.7	323.9	—	—	80.2	—	0.895	—
61.1	334.3	10.0	0.189	—	—	—	—
66.7	339.9	—	—	70.0	—	0.831	—
72.0	345.2	—	—	63.0	—	0.781	—
73.0	346.2	20.0	0.344	—	—	—	—
75.3	348.5	—	—	55.1	—	0.720	—
76.1	349.3	—	—	50.1	—	0.678	—
76.3	349.5	30.0	0.474	—	—	—	—
76.9	350.1	36.9	0.551	45.0	—	0.632	—
77.0	350.2	40.0	0.583	40.0	—	0.583 (UCST)	—

*Value corrected by compiler from the published graphs; reported in original as 80.0.

Method/Apparatus/Procedure:
The synthetic method was used. Sealed ampoules were placed in a glass-walled thermostat. The temperature of the thermostat was increased gradually with periodic stirring and a preliminary determination of the clear-point temperature in every ampoule was made. A more precise value of the cloud-point temperature was determined by allowing the thermostat to cool. The determination was repeated several times.

Auxiliary Information

Source and Purity of Materials:
(1) Source not specified; pure grade product; distilled over anhydrous soda, boiling point = 81.6 °C, n(20 °C,D) = 1.3441, ρ(25 °C) = 777 g·L⁻¹.
(2) Source not specified; for chromatography; not purified; boiling point = 68.8 °C, n(20 °C,D) = 1.3752, ρ(20 °C) = 660 g·L⁻¹.

Estimated Error:
Temperature: ±0.2 K.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	S. Rakotondramana, M.-E. Borredon, and J. Molinier, J. Chem. Eng. Data 32 , 308-11 (1987).
(2) Hexane; C ₆ H ₁₄ ; [110-54-3]	
Variables:	Prepared By:
T/K = 293 and 303	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data					
Mutual solubility of acetonitrile (1) and hexane (2)					
<i>t</i> /°C	T/K (computers)	100 w ₁ Hydrocarbon-rich phase	^x ₁ (computers)	100 w ₁ Acetonitrile-rich phase	^x ₁ (computers)
20.0	293.2	2.9	0.059	90.1	0.950
30.0	303.2	3.8	0.077	85.1	0.923

Method/Apparatus/Procedure:
The titration method was used. No experimental details were reported.

Source and Purity of Materials:
(1) Source not specified; commercial product; minimum purity of 99 mass %; dried with a 4 A molecular sieve.
(2) Source not specified; commercial product; minimum purity of 99 mass %.

Estimated Error:
Temperature: ±0.5 K.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	L. M. Vinogradova and A. E. Shcherbina, Zh. Fiz. Khim. 57 , 1268-9 (1983).
(2) Hexane; C ₆ H ₁₄ ; [110-54-3]	
Variables:	Prepared By:
T/K = 317-346	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data			
Solubility of hexane (2) in acetonitrile (1)			
<i>t</i> /°C	<i>x</i> ₂	100 w ₂	
316.5	0.100	18.9	
327.9	0.145	26.3	
337.8	0.209	35.7	
346.0	0.263	42.8	

Method/Apparatus/Procedure:
The synthetic method was used. No experimental details were reported.

Source and Purity of Materials:
(1) Source not specified; purity not specified; dried and purified.
(2) Source not specified; purity not specified; dried and purified.

Estimated Error:
Not reported.

5.10. + 1-Heptene

Components:	Evaluator:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valerii P. Sazonov, Technical University, Samara, Russia, July, 2001.
(2) 1-Heptene; C ₇ H ₁₄ ; [592-76-7]	

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and 1-heptene (2) have been reported in three publications over a very limited range of temperatures. Francis¹ reported the upper critical solution temperature, Kikic and Alessi² studied the mutual solubility of (1) and (2) at 291 K by an analytical method. Pavlova *et al.*³ measured the upper critical solution temperature by a synthetic method. The upper critical solution temperature has been reported as 311.2 K¹ and 314.4 K,³ these data are in reasonable agreement and thus their average value: UCST = 312.8 ± 1.6 K. The corresponding critical solution composition has not been reported. Accordingly, all the available data (see the relevant data sheets) must be regarded as tentative.

References:

- ¹A. W. Francis, Critical Solution Temperature, Washington, Adv. Chem. Ser. **31** (1961).
²L. Kikic and P. Alessi, Ann. Chim. (Rome) **64**, 363 (1974).
³O. P. Pavlova, A. A. Gaile, V. A. Proskuryakov, and I. F. Li, Zh. Fiz. Khim. **49**, 2874 (1975).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	I. Nagata, Thermochim. Acta 114 , 227-38 (1987).
(2) Hexane; C ₆ H ₁₄ ; [110-54-3]	
Variables:	Prepared By:
T/K = 298	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

Mutual solubility of acetonitrile (1) and hexane (2)	
x_1	x_1
T/K (compilers)	100 w ₁ (compilers)
	100 w ₁ (compilers)
	Acetonitrile-rich phase
	Acetonitrile-rich phase
t/°C	
25.00	2.87
	0.9433
	88.79

Auxiliary Information**Method/Apparatus/Procedure:**

The analytical method was used. Each two-phase mixture in a 70 mL equilibrium cell was stirred intensely for 2 h and then was allowed to settle for 2 h at 25.00 °C in a thermostated water bath. Two liquid samples in equilibrium were withdrawn with Hamilton syringes and were analyzed by means of a gas chromatograph and an electronic integrator.

Source and Purity of Materials:

- (1) Source not specified; guaranteed reagent; not purified.
 (2) Source not specified; not purified; GLC did not detect any appreciable impurities.

Estimated Error:

Temperature: ±0.01 K.
 Composition: ±0.002 mole fractions.

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) 1-Heptene; C ₇ H ₁₄ ; [592-76-7]	Original Measurements: O. P. Pavlova, A. A. Gaile, V. A. Proskuryakov, and I. F. Li, Zh. Fiz. Khim. 49 , 2874-6 (1975).
Variables: T/K = 314	Prepared By: Valerii P. Sazonov

Experimental Data
The UCST was reported to be 41.2 °C (314.4 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. No experimental details given.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not reported.

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) 1-Heptene; C ₇ H ₁₄ ; [592-76-7]	Original Measurements: I. Kikic and P. Alessi, Ann. Chim. (Rome) 64 , 363-7 (1974).
Variables: T/K = 291	Prepared By: Valerii P. Sazonov

Experimental Data
Mutual solubility of acetonitrile (1) and 1-heptene (2)

t/°C	T/K (compiler)	x ₁	100 w ₁ (compiler)	x ₁	100 w ₁ (compiler)
18.0	291.2	0.181	8.46	0.873	74.2
			Hydrocarbon-rich phase		Acetonitrile-rich phase

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A sample of each phase was withdrawn with a syringe and immediately analyzed by GLC. No experimental details given.

Source and Purity of Materials:
(1) 3M Minnesota; used without any preliminary treatment, since the analysis by GLC did not indicate any detectable impurity.
(2) Fluka; 99.9 mole % minimum purity; not purified.

Estimated Error:
Temperature: ±0.1 K.

5.11. + Methylcyclohexane

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		I. Nagata and S. Nakamura, J. Chem. Thermodyn. 17 , 1103–10 (1985).	
(2) Methylcyclohexane; C ₇ H ₁₄ ; [108-87-2]			
Variables:		Prepared By:	
T/K = 298		Valerii P. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and methylcyclohexane (2)			
	x_1	$100 w_1$ (computer)	$100 w_1$ (computer)
			Acetonitrile-rich phase
T/K	x_1	x_1	x_1
298.15	0.0546	2.36	0.9446
			Acetonitrile-rich phase
			87.70

Auxiliary Information**Method/Apparatus/Procedure:**

The analytical method was used. Liquid-liquid equilibrium measurement was performed by use of a thermostated equilibrium cell containing about 70 mL of mixture in the absence of a vapor phase. A two-phase mixture in the cell was vigorously mixed by use of a magnetic stirrer for 2 h and allowed to settle for 2 h at 298.15 K so as to ensure phase separation. After equilibrium was established, samples of two layers were withdrawn with precision Hamilton syringes and their compositions were determined by use of gas chromatograph with an electronic integrator.

Source and Purity of Materials:

- (1) Source not specified; spectrograde reagent; not purified.
- (2) Source not specified; spectrograde reagent; not purified.

Estimated Error:

Composition: ± 0.002 mole fractions.

5.12. + Heptane

Components:		Evaluators:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, October, 2001.	
(2) Heptane; C ₇ H ₁₆ ; [142-85-2]			

Critical Evaluation

Quantitative solubility data for the system acetonitrile (1) and heptane (2) have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system acetonitrile+heptane

Reference	T/K	Solubility	Method
Cornish <i>et al.</i> ¹	357	UCST	Synthetic
Kharitonova ²	298	Mutual	Titration
Palmer and Smith ³	318	Mutual	Analytical
Kikic and Alessi ⁴	291	Mutual	Analytical
Tripathi and Asselineau ⁵	343	Mutual	Analytical
Lakhanpal <i>et al.</i> ⁶	298–321	Mutual	Analytical
Vinogradova and Shcherbina ⁷	330–355	(2) in (1)	Synthetic
Negata ⁸	298	Mutual	Analytical

In addition to these data Francis⁹ reported the upper critical solution temperature and McLure *et al.*¹⁰ determined of the upper critical temperature solution and critical solution composition for binary solutions of acetonitrile and alkanes (C₅–C₁₀). All original data are compiled in the data sheets immediately following this Critical Evaluation.

The upper critical solution temperature of this system has been reported as 356.85 K,⁷ 357.2 K,¹ 357.8 K,⁹ and 358.0 K,¹⁰ these data are in reasonable agreement and thus their mean value: UCST = 357.5 \pm 0.5 K is recommended. The corresponding critical solution composition has been reported as $x_{c1} = 0.63$.¹⁰

All experimental values reported^{2–8} have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.9488, \quad a_2 = -0.3334, \quad b_1 = 5.2227, \quad b_2 = -4.8685$$

(mean standard error of estimate was 0.0138).

For this approximation x_{c1} and UCST values from McLure *et al.*¹⁰ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in Table 2. This relationship together with experimental points^{2–8} are also presented in Fig. 9.

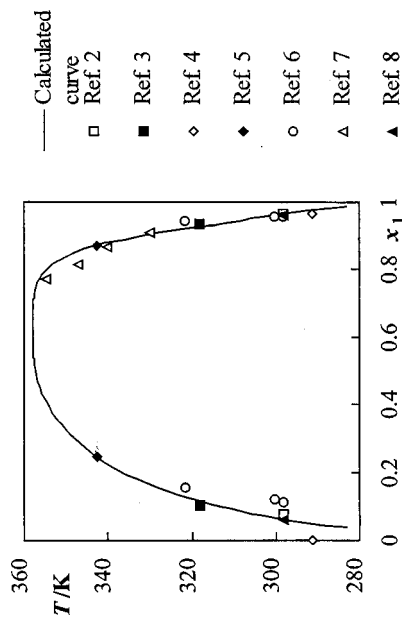


FIG. 9. Mutual solubility of acetonitrile and heptane.

TABLE 2. Calculated mutual solubility of acetonitrile (1) and heptane (2)

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
283.2	0.037	1.6	0.989	97.4
293.2	0.052	2.2	0.972	93.4
303.2	0.072	3.1	0.955	89.7
313.2	0.098	4.3	0.937	85.9
318.2	0.115	5.1	0.928	84.1
323.2	0.134	6.0	0.919	82.3
328.2	0.156	7.0	0.908	80.2
333.2	0.182	8.4	0.897	78.1
338.2	0.213	10.0	0.884	75.7
343.2	0.251	12.1	0.869	73.1
348.2	0.301	15.0	0.849	69.7
353.2	0.375	19.7	0.815	64.4
354.2	0.395	21.1	0.805	62.8
355.2	0.420	22.9	0.792	60.9
356.2	0.450	25.1	0.775	58.5
357.2	0.495	28.7	0.746	54.6
357.7	0.534	32.0	0.717	50.9

Components:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) Heptane; C₇H₁₆; [142-85-2]

Original Measurements:

R. E. Cornish, R. C. Archibald, E. A. Murphy, and H. M. Evans, Ind. Eng. Chem **26**, 397-406 (1934).

Variables:

T/K = 357

Prepared By:

Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The UCST was reported to be 84.0 °C (357.2 K, compilers).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Determinations were made in test tubes, which were heated and allowed to cool slowly in air. Thermometers were roughly calibrated.

Source and Purity of Materials:

(1) Prepared from sodium cyanide and dimethyl sulfate; the crude product was distilled and successively washed with solid sodium hydroxide and P₂O₅; carefully fractionated in a 6.09 m column; $d(20\text{ }^\circ\text{C}, 4\text{ }^\circ\text{C}) = 0.782\text{ }15$.

(2) Source not specified; commercial high-grade reagent.

Estimated Error:

Not reported

References:

- ¹R. E. Cornish, R. C. Archibald, E. A. Murphy, and H. M. Evans, Ind. Eng. Chem **26**, 397 (1934).
²G. I. Kharitonova, Dissertation, Saratov University, 1971.
³D. A. Palmer and B. D. Smith, J. Chem. Eng. Data **17**, 71 (1972).
⁴I. Kikić and P. Alessi, Ann. Chim. (Rome) **64**, 363 (1974).
⁵R. Tripathi and L. Asselineau, J. Chem. Eng. Data **20**, 33 (1975).
⁶M. L. Lakhappal, N. J. Mandial, and S. C. Ahuja, Indian J. Chem. **20A**, 1008 (1981).
⁷L. M. Vinogradova and A. E. Shcherbina, Zh. Fiz. Khim. **57**, 1268 (1983).
⁸I. Nagata, Thermochim. Acta **114**, 227 (1987).
⁹A. W. Francis, Critical Solution Temperature, Washington, Adv. Chem. Ser. **31** (1961).
¹⁰J. A. McLure, A. T. Rodriguez, P. A. Ingham, and J. F. Steele, Fluid Phase Equilib. **8**, 271 (1982).

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(2) Heptane; C ₇ H ₁₆ ; [142-85-2]	D. A. Palmer and B. D. Smith, J. Chem. Eng. Data 17 , 71-6 (1972).	
Variables:		Prepared By:	
T/K = 318		Valerii P. Sazonov and Nikolai V. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and heptane (2)			
<i>t</i> /°C	T/K (compilers)	<i>x</i> ₁	<i>x</i> ₁
45.0	318.2	Hydrocarbon-rich phase	Acetonitrile-rich phase
		0.1016	4.43
			0.9372
			85.94

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(2) Heptane; C ₇ H ₁₆ ; [142-82-5]	G. I. Kharitonova, Dissertation, Saratov University, 1971.	
Variables:		Prepared By:	
T/K = 298		Valerii P. Sazonov and Nikolai V. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and heptane (2)			
<i>t</i> /°C	T/K (compilers)	<i>x</i> ₁	<i>x</i> ₁
25.0	298.2	Hydrocarbon-rich phase	Acetonitrile-rich phase
		3.4	91.6
		0.079	0.964

Method/Apparatus/Procedure:
The analytical method was used. No experimental details were reported.

Source and Purity of Materials:
(1) Fisher Scientific Co.; purity 99.9 mass % by GLC; not purified.
(2) Phillips Petroleum Co.; purity 99.89 mass % by GLC; not purified.

Estimated Error:
Temperature: ±0.1 K.

Method/Apparatus/Procedure:
The titration method was used. No experimental details given.

Source and Purity of Materials:
(1) Source not specified; purity not specified; distilled; boiling point = 82.0 °C, *n*(25 °C,D) = 1.3425.
(2) Source not specified; purity not specified; distilled.

Estimated Error:
Temperature: ±0.1 K.

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		R. Tripathi and L. Asselmeau, <i>J. Chem. Eng. Data</i> 20 , 33–40 (1975).	
(2) Heptane; C ₇ H ₁₆ ; [142-85-2]			
Variables:		Prepared By:	
T/K = 343		Valerii P. Sazonov and Nikolai V. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and heptane (2)			
<i>t</i> /°C	T/K (compilers)	<i>x</i> ₁	100 <i>w</i> ₁ (compilers)
			Hydrocarbon-rich phase
69.5	342.7	0.245	11.7
			Acetonitrile-rich phase
		<i>x</i> ₁	100 <i>w</i> ₁ (compilers)
			Acetonitrile-rich phase
		0.871	73.4

Auxiliary Information**Method/Apparatus/Procedure:**

The analytical method was used. No experimental details were reported.

Source and Purity of Materials:

- (1) Prolabo Rhone-Poulenc, France; purified by fractional distillation in a Oldershaw column; boiling point = 81.6 °C, *n*(20 °C,D)=1.343 50, ρ (20 °C)=782.8 g·L⁻¹.
 (2) Phillips Petroleum Co.; purity more 99.0 mole %; not purified; boiling point=98.4 °C, *n*(20 °C,D)=1.387 60, ρ (20 °C)=683.7 g·L⁻¹.

Estimated Error:

Temperature: ±0.1 K.

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		I. Kikic and P. Alessi, <i>Ann. Chim. (Rome)</i> 64 , 363–7 (1974).	
(2) Heptane; C ₇ H ₁₆ ; [142-85-2]			
Variables:		Prepared By:	
T/K = 291		Valerii P. Sazonov and Nikolai V. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and heptane (2)			
<i>t</i> /°C	T/K (compilers)	<i>x</i> ₁	100 <i>w</i> ₁ (compilers)
			Hydrocarbon-rich phase
18.0	291.2	0.0004	0.016
			Acetonitrile-rich phase
		0.9655	91.98

Auxiliary Information**Method/Apparatus/Procedure:**

The analytical method was used. A sample of each phase was withdrawn with a syringe and immediately analyzed by GLC. No experimental details given.

Source and Purity of Materials:

- (1) 3M Minnesota; used without any preliminary treatment, since the analysis by GLC did not indicate any detectable impurity.
 (2) Fluka; 99.9 mole percent minimum purity; not purified.

Estimated Error:

Temperature: ±0.1 K.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	M. L. Lakhanpal, N. J. Mandal, and S. C. Ahuja, Indian J. Chem. 20A , 1008-13 (1981).
(2) Heptane; C ₇ H ₁₆ ; [142-85-2]	
Variables:	Prepared By:
T/K = 298-321	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data				
Mutual solubility of acetonitrile (1) and heptane (2)				
t/°C	T/K (compilers)	x ₁	100 w ₁	100 w ₁
			Hydrocarbon-rich phase	(compilers)
25.0	298.2	0.1110	4.87	90.07
26.9	300.1	0.1187	5.23	89.69
48.2	321.4	0.1562	7.05	87.04

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The mutual solubilities of the components were determined with the help of Zeiss interferometer. No experimental details were reported.	(1) Source not specified; pure grade; twice distilled, first over P ₂ O ₅ , then over anhydrous potassium carbonate, collected the fraction at 80 °C. (2) Web Laborchemie Apolda, Germany; pure grade; dried over anhydrous CaCl ₂ and distilled over sodium; collected the fraction distilling at 98.4 °C.
Estimated Error:	Estimated Error:
Not reported.	Not reported.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	L. M. Vinogradova and A. E. Shcherbina, Zh. Fiz. Khim. 57 , 1268-9 (1983).
(2) Heptane; C ₇ H ₁₆ ; [142-82-5]	
Variables:	Prepared By:
T/K = 330-355	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data		
The solubilities of heptane (2) in acetonitrile (1) were reported in graphical form in mole fractions terms over the indicated temperature range. These data were extracted by the compilers from the published graphs.		
T/K	t/°C	x ₂
330.0	56.8	0.089
340.1	66.9	0.132
347.2	74.0	0.186
354.6	81.4	0.229

The UCST was reported to be 356.85 K (83.70 °C, compilers).	
Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The synthetic method was used. No experimental details were reported.	(1) Source not specified; purity not specified; dried and purified. (2) Source not specified; purity not specified; dried and purified.
Estimated Error:	Estimated Error:
Not reported.	Not reported.

5.13. + Alkenes: C₈-C₁₀

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. P. Karaseva, M. A. Lognova, T. A. Egorova, and N. A. Simanov, Sb. Khim. Tekhnol. Yaroslavl, 99-103 (1974).
(2) Alkenes; C ₈ H ₁₆ -C ₁₀ H ₂₀	
Variables:	Prepared By:
T/K = 298	Valerii P. Sazonov

Experimental Data

The solubilities of alkenes (2) in acetonitrile (1) in mass percent at 25.0 °C (298.2 K) were presented in graphical form and in a table.

Alkene	Solubility of alkenes (2) in acetonitrile (1) at 25.0 °C (298.2 K)	
	Boiling point (°C)	$n(20\text{ °C}, D)$
1-Octene; C ₈ H ₁₆ ; [111-66-0]	122	1.4087
1-Nonene; C ₉ H ₁₈ ; [124-11-8]	53/4 kPa	1.4157
1-Decene; C ₁₀ H ₂₀ ; [872-05-9]	170.5	1.4214

*These data were extracted by the compiler from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. No experimental details were reported.

Source and Purity of Materials:

- (1) Source not specified; analytical purity; not purified.
- (2) Prepared by dehydration of pure 1-alcohols; distilled.

Estimated Error:

Temperature: ±0.1 K.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	I. Nagata, Thermochim. Acta 114 , 227-38 (1987).
(2) Heptane; C ₇ H ₁₆ ; [142-82-5]	
Variables:	Prepared By:
T/K = 298	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

Mutual solubility of acetonitrile (1) and hexane (2)

<i>t</i> /°C	T/K (compilers)	x_1	x_2	Phase	
25.00	298.15 K	0.0621	2.64	0.9622	91.25

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Each two-phase mixture in a 70 mL equilibrium cell was stirred intensely for 2 h and then was allowed to settle for 2 h at 25.00 °C in a thermostated water bath. Two liquid samples in equilibrium were withdrawn with Hamilton syringes and were analyzed by means of a gas chromatograph and an electronic integrator.

Source and Purity of Materials:

- (1) Source not specified; guaranteed reagent; not purified.
- (2) Source not specified; not purified; GLC did not detect any appreciable impurities.

Estimated Error:

Temperature: ±0.01 K.

Composition: ±0.002 mole fractions.

5.14. +2,2,4-Trimethylpentane

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. E. Cornish, R. C. Archibald, E. A. Murphy, and H. M. Evans, Ind. Eng. Chem. 26 , 397-406 (1934).
(2) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	
Variables:	Prepared By:
T/K=354	Valerii P. Sazonov

Experimental Data

The UCST was reported to be 81.0 °C (354.2 K, compiler).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Determinations were made in test tubes, which were heated and allowed to cool slowly in air. Thermometers were roughly calibrated.

Source and Purity of Materials:

(1) Prepared from sodium cyanide and dimethyl sulfate; the crude product was distilled and successively washed with solid sodium hydroxide and P₂O₅; carefully fractionated in a 6.09 m column; $d(20\text{ °C}, 4\text{ °C})=0.78215$.

(2) Source not specified; fractionated in a 6.09 m column; boiling point=99.3±0.05 °C, melting point=-107.5±0.5 °C; $n(20\text{ °C}, D)=1.39162$; $d(20\text{ °C}, 20\text{ °C})=0.69314$.

Estimated Error:

Not reported.

5.15. + Octane

Components:	Evaluators:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, October, 2001.
(2) Octane; C ₈ H ₁₈ ; [111-65-9]	

Critical Evaluation

Quantitative solubility data for the system acetonitrile (1) and octane (2) have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system acetonitrile+octane

Reference	T/K	Solubility	Method
Francis ¹	365	UCST	Non stated
Schmid <i>et al.</i> ²	366	UCST	Synthetic
Kharitonova ³	298	Mutual	Titration
Vinogradova and Shcherbina ⁴	343 to 365	(2) in (1)	Synthetic
Nagata ⁵	298	Mutual	Analytical

In addition to these data McLure *et al.*⁶ determined the upper critical temperature solution and critical solution composition binary systems containing acetonitrile+alkanes (C₅-C₁₈). All original data are compiled in the data sheets immediately following this Critical Evaluation.

The upper critical solution temperature has been reported as 364.7 K,¹ 364.85 K,⁴ 365.1 K,⁶ and 365.7 K.² These data are in reasonable agreement and thus their mean value: UCST=365.1±0.3 K is recommended. The corresponding critical solution composition has been reported as $x_{c1}=0.67$.

All experimental values reported³⁻⁶ have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = -0.9488, \quad a_2 = -0.3334, \quad b_1 = 5.2227, \quad b_2 = -4.8685$$

(mean standard error of estimate was 0.0138).

For approximation x_{c1} and UCST from McLure *et al.*⁶ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for selected temperatures are presented in Table 2. This relationship together with experimental points³⁻⁶ are also presented in Fig. 10.

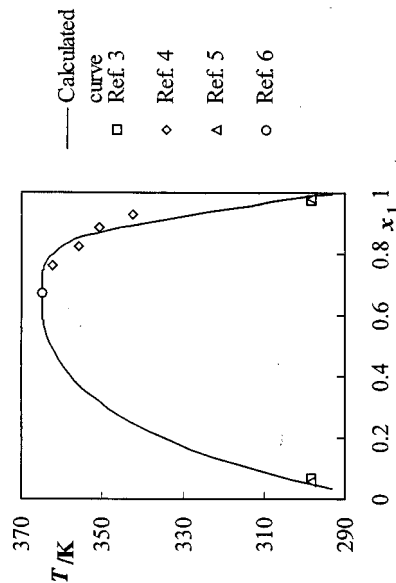


FIG. 10. Mutual solubility of acetonitrile and octane.

TABLE 2. Calculated mutual solubility of acetonitrile and octane

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
293.2	0.035	1.3	0.999	99.9
303.2	0.064	2.4	0.979	94.4
313.2	0.098	3.8	0.959	89.4
323.2	0.139	5.5	0.938	84.5
333.2	0.190	7.8	0.916	79.7
343.2	0.254	10.9	0.892	74.8
353.2	0.342	15.7	0.861	69.0
358.2	0.406	19.7	0.837	64.9
363.2	0.510	27.2	0.791	57.6
364.2	0.550	30.5	0.768	54.3
364.7	0.580	33.2	0.748	51.6
364.8	0.589	34.0	0.741	50.7
364.9	0.600	35.0	0.733	49.7
365.0	0.615	36.5	0.721	48.2

References:

- ¹A. W. Francis, Critical Solution Temperature, Washington, Adv. Chem. Ser. **31** (1961).
- ²H. H. O. Schmidt, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).
- ³G. I. Kharitonova, Dissertation, Saratov University, 1971.
- ⁴L. M. Vinogradova and A. E. Shcherbina, Zh. Fiz. Khim. **57**, 1268 (1983).
- ⁵I. Nagata, Thermochim. Acta **114**, 227 (1987).
- ⁶I. A. McLure, A. T. Rodriguez, P. A. Ingham, and J. F. Steele, Fluid Phase Equilib. **8**, 271 (1982).

Components:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
- (2) Octane; C₈H₁₈; [111-65-9]

Original Measurements:

G. I. Kharitonova, Dissertation, Saratov University, 1971.

Variables:

T/K = 298

Prepared By:

Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

Mutual solubility of acetonitrile (1) and octane (2)

t/°C	100 w_1		x_1 (compilers)		x_1 (compilers)
	Hydrocarbon-rich phase	Acetonitrile-rich phase	Hydrocarbon-rich phase	Acetonitrile-rich phase	
25.0	2.6	0.069	93.3	0.975	0.975

Auxiliary Information**Method/Apparatus/Procedure:**

The titration method was used. No experimental details given.

Source and Purity of Materials:

- (1) Source not specified; purity not specified; distilled; boiling point=82.0 °C, $n(25\text{ °C,D}) = 1.3425$
- (2) Source not specified; purity not specified; distilled.

Estimated Error:

Temperature: ±0.1 K.

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Octane; C ₈ H ₁₈ ; [111-65-9]	Original Measurements: I. Nagata, <i>Thermochim. Acta</i> 114 , 227–38 (1987).
Variables: T/K = 298	Prepared By: Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data			
Mutual solubility of acetonitrile (1) and octane (2)			
<i>t</i> /°C	T/K (compilers)	<i>x</i> ₁	<i>x</i> ₁
25.00	298.15 K	0.0568	0.9801
		100 <i>w</i> ₁ (compilers)	100 <i>w</i> ₁ (compilers)
		Hydrocarbon-rich phase	Acetonitrile-rich phase

Auxiliary Information	
Method/Apparatus/Procedure: The analytical method was used. Each two-phase mixture was stirred intensely in a 70 mL equilibrium cell for 2 h and then was allowed to settle for 2 h at 25.00 °C in a thermostated water bath. Two liquid samples in equilibrium were withdrawn with Hamilton syringes and were analyzed by means of a gas chromatograph and an electronic integrator.	Source and Purity of Materials: (1) Source not specified; guaranteed reagent; not purified. (2) Source not specified; not purified; GLC did not detect any appreciable impurities.
Estimated Error: Temperature: ±0.01 K. Composition: ±0.002 mole fractions.	

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Octane; C ₈ H ₁₈ ; [111-65-9]	Original Measurements: L. M. Vinogradova and A. E. Shcherbina, <i>Zh. Fiz. Khim.</i> 57 , 1268–9 (1983).
Variables: T/K = 343–365	Prepared By: Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data		
Solubility of octane (2) in acetonitrile (1)		
T/K	<i>t</i> /°C	<i>x</i> ₂
342.5	69.3	0.072
350.9	77.7	0.112
355.9	82.7	0.174
362.3	89.1	0.240
		100 <i>w</i> ₂
		17.8
		26.0
		37.0
		46.8

The UCST was reported to be 364.85 K (91.70 °C; compilers).

Auxiliary Information	
Method/Apparatus/Procedure: The synthetic method was used. No experimental details were reported.	Source and Purity of Materials: (1) Source not specified; purity not specified; dried and purified. (2) Source not specified; purity not specified; dried and purified.
Estimated Error: Not reported.	

5.16. + Alkanes: C₈C₁₈

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₂ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372-81 (1965).
(2) Alkanes; C ₈ H ₁₈ ; C ₁₀ H ₂₂ ; C ₁₂ H ₂₆ ; C ₁₄ H ₃₀ ; C ₁₆ H ₃₄ ; and C ₁₈ H ₃₈	
Variables:	Prepared By:
T/K = 366-428	Valerii P. Sazonov

Experimental Data		T/K (compilers)
Upper critical solution temperatures of the systems acetonitrile (1) + alkane (2)		
Alkane	t/°C	
Octane; C ₈ H ₁₈ ; [111-65-9]	92.5	365.7
Decane; C ₁₀ H ₂₂ ; [124-18-5]	107.5	380.7
Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	121.5	394.7
Tetradecane; C ₁₄ H ₃₀ ; [629-59-4]	133.5	406.7
Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	144.0	417.2
Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	155.0	428.2

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. A Reichert microscope, type RCH, with a heating stage was used. A 26×38 mm slide was adapted to hold capillaries on the stage. Two glass strips were glued, using water glass, to the slide, leaving a 0.5 mm channel. The slide was then placed in the adjustable device of the heating stage. (1) and (2) were put into capillary tubing (0.2-0.3 mm diameters) by dipping consecutively into both liquids. The height of the liquid was 7-10 mm. Room temperature solids were melted on a glass slide over a micro-burner. The capillary was sealed at both ends to a length of 30-35 mm, then inserted into the channel on the slide and heated on the stage. The UCST was determined by following the appearance and disappearance of the meniscus.

Source and Purity of Materials:

(1) Baker Chemical Co.; reagent, No. 9011; n(20 °C/D) = 1.3445; d(20 °C/4 °C) = 0.780.

(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

5.17. + Aromatic Hydrocarbons: C₉-C₂₀

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₂ N; [75-05-8]	A. W. Francis, <i>Ind. Eng. Chem.</i> 36 , 1096-104 (1944).
(2) Aromatic hydrocarbons; C ₉ H ₁₂ -C ₂₀ H ₂₈	
Variables:	Prepared By:
T/K = 195-357	Valerii P. Sazonov

Experimental Data		Boiling point Hydrocarbon/°C	t/°C	T/K (compilers)
Upper critical solution temperatures of the systems acetonitrile (1) and aromatic hydrocarbon (2)				
Aromatic hydrocarbon				
(1-Methylethyl)benzene; C ₉ H ₁₂ ; [98-82-8]		152	< -78	< 195
1-Methyl-3-(1-methylethyl)benzene; C ₁₀ H ₁₄ ; [535-77-3]		176	-60	213
1,3-Diethylbenzene; C ₁₀ H ₁₄ ; [141-93-5]		181	-60	213
(1-Methylpropyl)benzene; C ₁₀ H ₁₄ ; [135-98-8]		173	-50	223
(1-Methylethyl)naphthalene; C ₁₃ H ₁₄ ; [29253-36-9]		264	-30	243
1-Ethyl-4-(1-methylethyl)benzene; C ₁₁ H ₁₆ ; [4218-48-8]		195	-30	243
1-Methyl-3,5-diethylbenzene; C ₁₁ H ₁₆ ; [2050-24-0]		203	-23	250
Bis(1-methylethyl)benzene; C ₁₂ H ₁₈ ; [25321-09-9]		205	-15	258
1,3,5-Triethylbenzene; C ₁₂ H ₁₈ ; [102-25-0]		216	-7	266
(1-Methylbutyl)benzene; C ₁₁ H ₁₆ ; [2719-52-0]		192	-5	268
1-Methyl-2,4-bis(1-methylethyl)benzene; C ₁₃ H ₂₀ ; [1460-98-6]		217	2	275
(1-Methylbutyl)naphthalene; C ₁₃ H ₁₈ ; [26763-59-7]		300	4	277
Bis(1-methylethyl)naphthalene; C ₁₆ H ₂₀ ; [38640-62-9]		310	12	285
1,2,3,4-Tetrahydro-2-(1-methylethyl)naphthalene; C ₁₃ H ₁₈ ; [33451-66-0]		261	14	287
1,2-Dipentylbenzene; C ₁₆ H ₂₆ ; [635-89-2]		265	67	340
Dipentyl-naphthalene; C ₂₀ H ₂₈ ; [71784-99-1]		360	84	357

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The reagents, about 1 mL of (1) and 1-1.5 mL of (2), were introduced and stirred with a thermometer while the tubes were warmed gradually in a bath of water. The temperature of disappearance or reappearance of the cloud due to two liquid phases was read three or four times in each direction. If the final position of the interface was not near the middle of the liquid, the volumes of the reagents were adjusted to make it so.

Source and Purity of Materials:

(1) Source not specified, pure grade reagent.
(2) Prepared by alkylation of benzene, toluene, ethyl benzene, naphthalene or tetralin with ethene, propene, 2-butene, isobutene or pentene, using aluminum chloride as catalyst.

Estimated Error:

Temperature: ±1 K.

5.18. + trans-Decahydronaphthalene

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		M. Antosik, A. Stafiej, and R. Stryjek, Fluid Phase Equil. 58 , 325–33 (1990).	
(2) trans-Decahydronaphthalene (trans-bicyclo [4.4.0] decane, trans-decalin); C ₁₀ H ₁₈ ; [493-02-7]			
Variables:		Prepared By:	
T/K = 319–384		Valerii P. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and trans-decahydronaphthalene (2)			
T/K	t/°C (compiler)	x ₁	100 w ₁ (compiler)
		Hydrocarbon-rich phase	Acetonitrile-rich phase
318.98	45.83	—	99.07
337.78	64.63	—	98.53
362.14	88.99	—	97.44
372.83	99.68	0.3482	—
375.66	102.51	0.3818	—
375.90	102.75	—	96.08
376.11	102.96	—	95.74
377.17	104.02	0.4039	—
379.26	106.11	0.4400	—
379.50	106.35	0.4442	—
383.20	110.05	0.5253	—
383.52	110.37	0.6052	—
383.60	110.45	—	90.44
383.62	110.47	—	89.47
383.69	110.54	0.6750	87.49 (UCST)

5.19. + Decane

Components:		Evaluators:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, November, 2001.	
(2) Decane; C ₁₀ H ₂₂ ; [124-18-5]			

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and decane (2) have been reported in four publications. Francis¹ reported the upper critical solution temperature. Schmid *et al.*² determined the upper critical solution temperature by the synthetic method. McLure *et al.*³ measured of the upper critical temperature solution and critical solution composition of components (1) and (2) during a study of solubilities of acetonitrile with alkanes (C₅–C₁₈). Antosik *et al.*⁴ studied the mutual solubility of (2) and (1) between 295 and 380 K by a synthetic method.

The upper critical solution temperature has been reported as 380.46 K,¹ 380.7 K,^{1,2} and 381.7 K,³ these data are in reasonable agreement and thus their average value; UCST = 380.9 ± 0.5 K and are recommended. The corresponding critical solution composition has been reported as x_{c1} = 0.7143⁴ and x_{c1} = 0.75.³

All experimental values reported^{1–4} have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.8399, a_2 = -0.1090, b_1 = 3.9660, b_2 = -4.1114$$

(mean standard error of estimate was 0.0173).

For approximation x_{c1} and UCST from Antosik *et al.*⁴ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with experimental results,⁴ are also presented in Fig. 11.

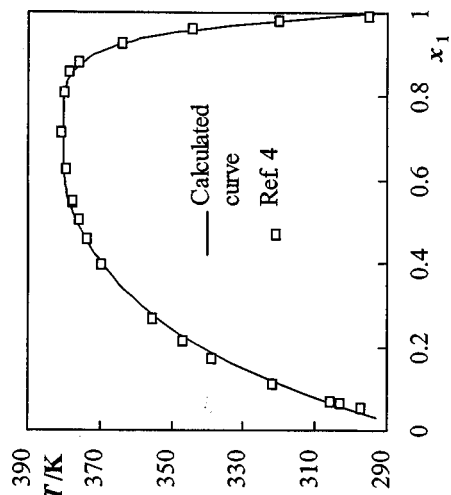


FIG. 11. Mutual solubility of acetonitrile and decane.

Auxiliary Information

Method/Apparatus/Procedure:

The method used was as described elsewhere.¹ Samples of varying composition and 4 g total weight were sealed in glass ampoules and then immersed in a thermostated bath equipped with a platinum resistance thermometer. The ampoule contents were continuously mixed by a rolling glass bead inside the ampoule, which was swung mechanically. The miscibility temperature was determined by repeatedly observing the disappearance/appearance of turbidity when heating or cooling.

Source and Purity of Materials:

(1) Source not specified; purified by fractional distillation at atmospheric pressure; purity 99.9 mass % by GLC.
(2) Source not specified; purified by fractional distillation at sub atmospheric pressure; purity greater than 99.8 mass % by GLC.

Estimated Error:

Temperature: ±0.01 K.
Composition: better than 0.0001 mole fraction.

References:

¹M. Luszczczyk and R. Stryjek, Bull. Pol. Acad. Sci. Chim. **32**, 371 (1984).

Calculated mutual solubility of acetonitrile (1) and decane (2)

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
293.2	0.030	0.9	0.999	99.9
303.2	0.057	1.7	0.993	97.6
313.2	0.087	2.7	0.985	95.0
323.2	0.121	3.8	0.977	92.5
333.2	0.161	5.2	0.968	89.7
343.2	0.208	7.0	0.958	86.8
353.2	0.264	9.4	0.945	83.2
363.2	0.337	12.8	0.927	78.6
368.2	0.384	15.2	0.914	75.4
373.2	0.444	18.7	0.893	70.7
378.2	0.541	25.4	0.849	61.9
379.2	0.575	28.1	0.829	58.3
379.7	0.598	30.0	0.814	55.8
380.2	0.635	33.4	0.787	51.6
380.3	0.647	34.6	0.777	50.1
380.4	0.666	36.5	0.760	47.7

References:

- ¹A. W. Francis, Critical Solution Temperature, Washington, Adv. Chem. Ser. **31** (1961).
²H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).
³J. A. McLure, A. T. Rodriguez, P. A. Ingham, and J. F. Steele, Fluid Phase Equilib. **8**, 271 (1982).
⁴M. Antosik, A. Stafiej, and R. Stryjek, Fluid Phase Equilib. **58**, 325 (1990).

Components:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) Decane; C₁₀H₂₂; [124-18-5]

Original Measurements:

- M. Antosik, A. Stafiej, and R. Stryjek, Fluid Phase Equilib. **58**, 325-33 (1990).

Variables:

T/K = 295-380

Prepared By:

Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

Mutual solubility of acetonitrile (1) and decane (2)

T/K	t/°C (compliers)	Hydrocarbon-rich phase		Acetonitrile-rich phase	
		x_1	100 w_1 (compliers)	x_1	100 w_1 (compliers)
294.90	21.75	—	—	0.9930	99.80
297.17	24.02	0.0534	16.36	—	—
302.74	29.59	0.0639	19.13	—	—
305.76	32.61	0.0687	20.36	—	—
319.91	47.76	—	—	0.9826	99.49
321.50	48.35	0.1092	29.82	—	—
338.53	65.38	0.1724	41.93	—	—
343.81	70.66	—	—	0.9625	98.89
346.80	73.65	0.2126	48.34	—	—
355.24	82.09	0.2681	55.94	—	—
363.69	90.54	—	—	0.9288	97.84
369.41	96.26	0.3988	69.69	—	—
373.37	100.22	0.4584	74.58	—	—
375.75	102.60	0.5037	77.87	—	—
375.88	102.73	—	—	0.8820	96.28
377.35	104.20	0.5442	80.54	—	—
377.48	104.33	0.5511	80.97	—	—
378.43	105.28	—	—	0.8598	95.51
379.27	106.12	0.6274	85.37	—	—
379.86	106.71	—	—	0.8082	93.59
380.46	107.31	0.7143	89.65 (UCST)	0.7143	89.65

Auxiliary Information**Method/Apparatus/Procedure:**

The method used was as described elsewhere.¹ Samples of varying composition and 4 g total weight were sealed in glass ampoules and then immersed in a thermostated bath equipped with a platinum resistance thermometer. The ampoule contents were continuously mixed by a rolling glass bead inside the ampoule, which was swung mechanically. The miscibility temperature was determined by repeatedly observing the disappearance/appearance of turbidity when heating or cooling.

Source and Purity of Materials:

- (1) Source not specified; purified by fractional distillation at atmospheric pressure; purity 99.9 mass % by GLC.
 (2) Source not specified; purified by fractional distillation at sub atmospheric pressure; purity greater than 99.9 mass % by GLC.

Estimated Error:

Temperature: ±0.01 K.
 Composition: better than 0.0001 mole fraction.

References:

- ¹M. Luszczyk and R. Stryjek, Bull. Pol. Acad. Sci. Chim. **32**, 371 (1984).

5.20. + Hexadecane

Components:	Evaluators:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valeriy P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, November, 2001.
(2) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and hexadecane (2) have been reported in four publications. Schmid *et al.*¹ determined the upper critical solution temperature by the synthetic method. Rogalski and Stryjek² studied the mutual solubility of (1) and (2) between 298 and 418 K by a synthetic method. Stryjek *et al.*³ reported the mutual solubility of (1) and (2) between 298 and 413 K at standard temperatures. McLure *et al.*⁴ measured the upper critical temperature solution of components (1) and (2) as part of a study of the binary solubilities of acetonitrile-alkanes (C₅-C₁₈).

The upper critical solution temperature has been reported as 403.7 K,⁴ 417.2 K,¹ and 417.65 K.² The UCST of McLure *et al.*⁴ is rejected. The remaining values give an average recommended value of: UCST=417.5±0.4 K. The corresponding critical solution composition has been reported as $x_{c1}=0.8358$.²

All experimental values reported¹⁻⁴ have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1=0.4482, \quad a_2=0.5602, \quad b_1=3.0206, \quad b_2=-3.6064$$

(mean standard error of estimate was 0.0254).

For approximation x_{c1} and UCST from Rogalski and Stryjek² have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship together with experimental points¹⁻⁴ are also presented in Fig. 12.

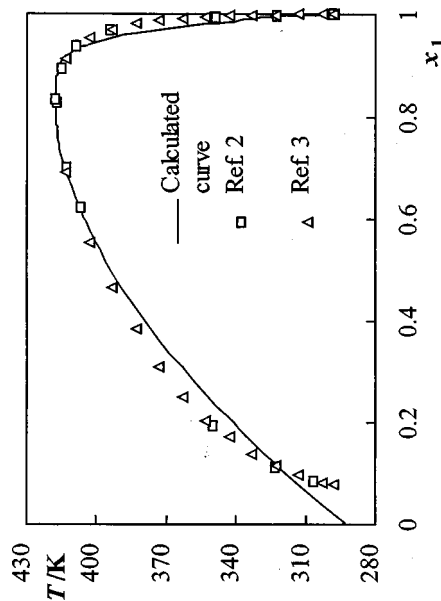


FIG. 12. Mutual solubility of acetonitrile and hexadecane.

T/K	Hydrocarbon-rich phase		Acetonitrile-rich phase	
	x_1	100 w ₁	x_1	100 w ₁
	313.2	0.079	1.7	0.999
333.2	0.163	3.9	0.991	95.8
343.2	0.209	5.2	0.985	93.1
353.2	0.257	6.7	0.980	91.0
363.2	0.309	8.5	0.974	88.6
373.2	0.364	10.6	0.968	86.2
383.2	0.426	13.3	0.962	84.0
393.2	0.495	16.9	0.954	81.1
403.2	0.577	22.0	0.942	77.1
408.2	0.627	25.8	0.933	74.2
413.2	0.691	31.6	0.918	69.9
414.2	0.707	33.3	0.913	68.5
415.2	0.726	35.4	0.907	66.9
416.2	0.748	38.0	0.898	64.6
416.7	0.763	40.0	0.891	62.8
417.2	0.782	42.6	0.880	60.3

References:

- ¹H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).
- ²M. Rogalski and R. Stryjek, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **28**, 139 (1980).
- ³R. Stryjek, M. Luszczek, and M. Fedorko-Amosik, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **29**, 203 (1981).
- ⁴A. McLure, A. T. Rodriguez, P. A. Ingham, and J. F. Steele, *Fluid Phase Equilib.* **8**, 271 (1982).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. Stryjek, M. Luszczek, and M. Fedorko-Antosik, Bull. Acad. Pol. Sci., Ser. Sci. Chim. 29 , 203–11 (1981).
(2) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	
Variables:	Prepared By:
T/K = 298–413	Valerii P. Sazonov and Nikolai V. Sazonov

T/K	t/°C (compilers)	Mutual solubility of acetonitrile (1) and hexadecane (2)		100 w ₁ (compilers)	100 w ₁ (compilers)
		x ₁	x ₁		
298.15	25.00	0.0775	1.50	0.9995	99.72
303.15	30.00	0.0823	1.60	0.9993	99.62
313.15	40.00	0.0965	1.90	0.9985	99.18
323.15	50.00	0.1149	2.30	0.9978	98.80
333.15	60.00	0.1371	2.80	0.9967	98.21
343.15	70.00	0.1708	3.60	0.9954	97.51
353.15	80.00	0.2025	4.40	0.9937	96.62
363.15	90.00	0.2500	5.70	0.9911	95.28
373.15	100.00	0.3090	7.50	0.9876	93.52
383.15	110.00	0.3852	10.20	0.9815	90.58
393.15	120.00	0.4668	13.70	0.9697	85.30
403.15	130.00	0.5543	18.40	0.9540	78.99
413.15	140.00	0.6905	28.80	0.9135	65.69

Auxiliary Information

Method/Apparatus/Procedure:
No details were reported.

Source and Purity of Materials:
(1) Source not specified; purified by fractional distillation; 99.9 mass % purity.
(2) Source not specified; purified by crystallization; 99.9 mass % purity.

Estimated Error:
Not reported.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	M. Rogalski and R. Stryjek, Bull. Acad. Pol. Sci., Ser. Sci. Chim. 28 , 139–47 (1980).
(2) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	
Variables:	Prepared By:
T/K = 298–418	Valerii P. Sazonov and Nikolai V. Sazonov

T/K	t/°C (compilers)	Mutual solubility of acetonitrile (1) and hexadecane (2)		100 w ₁ (compilers)	100 w ₁ (compilers)
		x ₁	x ₁		
297.95	24.80	—	—	0.9994	99.67
306.15	33.00	0.0852	1.66	—	—
322.45	49.30	—	—	0.9977	98.74
322.95	49.80	0.1140	2.28	—	—
348.15	75.00	—	—	0.9947	97.14
350.15	77.00	0.1928	4.15	—	—
394.35	121.20	—	—	0.9681	84.62
406.65	133.50	0.6216	22.95	—	—
408.65	135.50	—	—	0.9379	73.25
412.95	139.80	0.7010	29.82	—	—
414.75	141.60	—	—	0.8930	60.21
417.15	144.00	0.8271	46.44	—	—
417.65	144.50	0.8358	47.99	0.8358	47.99 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic (Alekseev) and, below 353 K, the titration methods were used. A glass device with a magnetic stirrer was filled with 5–10 mL of (1) then placed in a thermostat, stirred, and small amounts of (2) added until turbidity appeared. The sample was then heated to above the complete homogeneity temperature, and then cooled until turbidity reappeared. Repeated determinations were made. Above 353 K, the method of Alekseev was used. Samples 4–5 g were sealed in glass, placed in thermostat, and the solubility temperature determined as above.

Source and Purity of Materials:
(1) Source not specified; purified by fractional distillation; 99.9 mass % purity.
(2) Source not specified; purified by crystallization; 99.9 mass % purity.

Estimated Error:
Temperature: ±0.1 K.
Composition: ±0.001 mole fraction.

6. Acetonitrile+Halogenated Hydrocarbons

6.1. + Trichloromethane

Components:	Original Measurements:
(1) Acetonitrile; CH ₃ CN; [75-05-8] (2) Trichloromethane (chloroform); CHCl ₃ ; [67-66-3]	J. B. Ott, B. F. Woodfield, C. Guanquan, J. Boerio-Goates, and J. R. Goates, <i>J. Chem. Thermodyn.</i> 19 , 177–84 (1987).
Variables:	Prepared By:
T/K=182–228	Valerii P. Sazonov

Experimental Data

No region of liquid–liquid immiscibility was observed. A full solid–liquid phase diagram in mole fractions over the specified temperature range was reported in the original publication.

Melting temperatures of acetonitrile (1)+trichloromethane (2) system

x_1	100 w_1 (compiler)	T/K	$t/^\circ\text{C}$ (compiler)
0.0000	0.000	209.73	–63.42
0.0245	0.856	208.87	–64.28
0.0776	2.81	206.76	–66.39
0.1441	5.472	203.32	–69.83
0.1976	7.807	200.01	–73.14
0.2478	10.18	196.27	–76.88
0.2972	12.70	191.94	–81.21
0.3476	15.48	187.06	–86.09
0.3935	18.24	181.73	–91.42
0.3951	18.34	182.20	–90.95
0.4198	19.92	187.41	–85.74
0.4502	21.97	192.23	–80.92
0.4923	25.01	197.44	–75.71
0.5345	28.31	201.78	–71.37
0.5731	31.58	205.16	–67.99
0.6339	37.32	209.62	–63.53
0.6898	43.33	212.85	–60.30
0.727	47.8	214.7	–58.5
0.7479	50.50	216.11	–57.04
0.8080	59.13	219.50	–53.65
0.8588	67.65	222.07	–51.08
0.9191	79.62	225.18	–47.97
0.9808	94.61	228.33	–44.82
1.0000	100.00	229.28	–43.87

A eutectic was reported at 181.73 K (–91.42 °C, compiler) at $x_1=0.3935$ (100 $w_1=18.24$, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The freezing–temperature apparatus has been described previously¹ but the temperature–measurement system is new. Temperatures were measured with a Leeds and Northrup platinum resistance thermometer and with a Solartron Model 7081 digital multimeter which has a sensitivity on the 100 Ω scale of 10 μΩ. The multimeter used a 1 mA current for measurements of resistance less than 100 Ω. The resistance meter was interfaced to a Hewlett-Packard Model 9845C computer through an IEEE bus. The computer read and stored a resistance measurement every 4 s from which cooling and warming curves of time against temperature could be constructed. The computer could be signaled to record visual melting temperatures during the recording process. The results were continually plotted on a video monitor, recorded on disk, and eventually plotted to provide a permanent record of the time–against–temperature cooling and warming curves.

Source and Purity of Materials:

- MBC Omnisolv; purified by fractional distillation in a vacuum-jacketed 2 m column packed with glass helices and operated at a reflux ratio of approximately 100; purity 0.9998 mole fractions; melting point= –43.87 °C.
- Fisher; reagent grade; purified by fractional distillation in a vacuum-jacketed 2 m column packed with glass helices and operated at a reflux ratio of approximately 100; care was taken to exclude light and to use it soon after the purification since it slowly decomposes; purity 0.9997 mole fractions; melting point= –63.42 °C.

Estimated Error:

Temperature: ±0.05 K.

References:

- J. R. Goates, J. B. Ott, and A. H. Budge, *J. Phys. Chem.* **65**, 2162 (1961).

6.2. + Trichlorofluoromethane

Components:	Original Measurements:
(1) Acetonitrile; CH ₃ CN; [75-05-8] (2) Trichlorofluoromethane; CCl ₃ F; [75-69-4]	J. B. Ott, B. F. Woodfield, C. Guanquan, J. Boerio-Goates, and J. R. Goates, <i>J. Chem. Thermodyn.</i> 19 , 177–84 (1987).
Variables:	Prepared By:
T/K=163–228	Valerii P. Sazonov

Experimental Data

No region of liquid–liquid immiscibility was observed. A full solid–liquid phase diagram in mole fractions over the specified temperature range was reported in the original publication.

Melting temperatures of acetonitrile (1)+trichlorofluoromethane (2) system

x_1	100 w_1 (compiler)	T/K	$t/^\circ\text{C}$ (compiler)
0.000	0.00	162.72	–110.43
0.002	0.06	162.60	–110.55
0.0082	0.25	183.0	–90.2
0.0200	0.61	198.0	–75.2
0.0416	1.28	208.0	–65.2
0.0698	2.19	213.0	–60.2
0.080	2.5	214.5	–58.7
0.0905	2.89	215.4	–57.8
0.0958	3.07	215.6	–57.6
0.1192	3.887	216.7	–56.5
0.1617	5.450	217.75	–55.40
0.1981	6.875	218.15	–55.00
0.3002	11.36	218.75	–54.40
0.3949	16.32	218.92	–54.23
0.5037	23.27	219.12	–54.03
0.5487	26.65	219.27	–53.88
0.5781	29.05	219.41	–53.74
0.6056	31.45	219.62	–53.53
0.6463	35.32	219.80	–53.35
0.6931	40.29	220.39	–52.76
0.7969	53.97	222.14	–51.01
0.8969	72.22	224.97	–48.18
0.9466	84.12	226.83	–46.32
0.9793	93.39	228.41	–44.74
1.0000	100.00	229.28	–43.87

A eutectic was reported at 162.60 K (–110.55 °C, compiler) at $x_1=0.002$ (100 $w_1=0.06$, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The freezing–temperature apparatus has been described previously¹ but the temperature–measurement system is new. Temperatures were measured with a Leeds and Northrup platinum resistance thermometer and with a Solartron Model 7081 digital multimeter which has a sensitivity on the 100 Ω scale of 10 μΩ. The multimeter used a 1 mA current for measurements of resistance less than 100 Ω. The resistance meter was interfaced to a Hewlett-Packard Model 9845C computer through an IEEE bus. The computer read and stored a resistance measurement every 4 s from which cooling and warming curves of time against temperature could be constructed. The computer could be signaled to record visual melting temperatures during the recording process. The results were continually plotted on a video monitor, recorded on disk, and eventually plotted to provide a permanent record of the time–against–temperature cooling and warming curves.

Source and Purity of Materials:

- MBC Omnisolv; purified by fractional distillation in a vacuum-jacketed 2 m column packed with glass helices and operated at a reflux ratio of approximately 100; purity 0.9998 mole fractions; melting point= –43.87 °C.
- Aldrich; reagent grade; purified by fractional distillation in a vacuum-jacketed 2 m column packed with glass helices and operated at a reflux ratio of approximately 100; purity 0.9989 mole fractions; melting point= –110.43 °C.

Estimated Error:

Temperature: ±0.05 K.

References:

- J. R. Goates, J. B. Ott, and A. H. Budge, *J. Phys. Chem.* **65**, 2162 (1961).

6.3. + Tetrachloromethane

Components:(1) Acetonitrile; CH₃CN; [75-05-8](2) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]**Variables:**

T/K=222–247

Original Measurements:J. B. Ott, B. F. Woodfield, C. Guanquan, J. Boerio-Goates, and J. R. Goates, *J. Chem. Thermodyn.* **19**, 177–84 (1987).**Prepared By:**

Valerii P. Suzonov

Experimental Data

No region of liquid–liquid immiscibility was observed. A full solid–liquid phase diagram in mole fractions over the specified temperature range was reported in the original publication.

Melting temperatures of acetonitrile (1) + tetrachloromethane (2) system

x_1	100 w_1 (complier)	T/K	$t/^\circ\text{C}$ (complier)
0.0000	0.000	250.39	–22.76
0.0307	0.838	246.60	–26.55
0.0659	1.848	243.69	–29.46
0.1144	3.333	241.20	–31.95
0.1489	4.461	240.00	–33.15
0.1961	6.112	238.74	–34.41
0.2372	7.663	237.94	–35.21
0.2779	9.314	237.24	–35.91
0.3256	11.41	236.58	–36.57
0.3775	13.93	235.86	–37.29
0.4399	17.33	234.90	–38.25
0.4990	21.00	233.79	–39.36
0.5477	24.42	232.76	–40.39
0.5971	28.34	231.18	–41.97
0.6201	30.34	230.10	–43.05
0.6445	32.61	228.59	–44.56
0.6642	34.55	227.28	–45.87
0.6738	35.54	226.55	–46.60
0.689	37.2	225.37	–47.78
0.7055	39.00	225.02	–48.13
0.7203	40.73	224.53	–48.62
0.7455	43.88	223.14	–50.01
0.765	46.5	221.55	–51.60
0.7724	47.53	221.75	–51.40
0.7925	50.48	222.03	–51.12
0.8257	55.84	222.82	–50.33
0.8819	66.59	224.39	–48.76
0.9287	77.66	226.02	–47.13
0.9808	93.17	228.30	–44.85
1.0000	100.00	229.28	–43.87

A eutectic was reported at 221.55 K (–51.60 °C, compiler) at $x_1=0.765$ (100 $w_1=46.5$, compiler).**Auxiliary Information****Method/Apparatus/Procedure:**

The synthetic method was used. The freezing-temperature apparatus has been described previously¹ but the temperature-measurement system is new. Temperatures were measured with a Leeds and Northrup platinum resistance thermometer and with a Solartron Model 7081 digital multimeter which has a sensitivity on the 100- Ω scale of 10 $\mu\Omega$. The multimeter used a 1 mA current for measurements of resistance less than 100 Ω . The resistance meter was interfaced to a Hewlett-Packard Model 9845C computer through an IEEE bus. The computer read and stored a resistance measurement every 4 s from which cooling and warming curves of time against temperature could be constructed. The computer could be signaled to record visual melting temperatures during the recording process. The results were continually plotted on a video monitor, recorded on disk, and eventually plotted to provide a permanent record of the time-against-temperature cooling and warming curves.

Source and Purity of Materials:

(1) MBC Omnisolv; purified by fractional distillation in a vacuum-jacketed 2 m column packed with glass helices and operated at a reflux ratio of approximately 100; purity 0.9998 mole fractions; melting point= –43.87 °C.
 (2) Fisher; reagent grade; purified by fractional distillation in a vacuum-jacketed 2 m column packed with glass helices and operated at a reflux ratio of approximately 100; purity 0.9999 mole fractions; melting point= –22.76 °C.

Estimated Error:Temperature: ± 0.05 K.**References:**

¹J. R. Goates, J. B. Ott, and A. H. Budge, *J. Phys. Chem.* **65**, 2162 (1961).

6.4. + 1,1,1-Trichloro-2,2,2-trifluoroethane

Components:	Original Measurements:
(1) Acetonitrile; CH ₃ CN; [75-05-8]	J. B. Ott, B. F. Woodfield, C. Guanquan, J. Boerio-Goates, and J. R. Goates, <i>J. Chem. Thermodyn.</i> 19 , 177–84 (1987).
(2) 1,1,1-Trichloro-2,2,2-trifluoroethane; C ₂ Cl ₃ F ₃ ; [354-58-5]	
Variables:	Prepared By:
T/K = 226–284	Valerii P. Sazonov

Experimental Data

No region of liquid–liquid immiscibility was observed. A full solid–liquid phase diagram in mole fractions over the specified temperature range was reported in the original publication.

Melting temperatures of acetonitrile (1) + 1,1,1-trichloro-2,2,2-trifluoroethane (2) system

x_1	100 w_1 (compiler)	T/K	$t/^\circ\text{C}$ (compiler)
0.0000	0.000	287.52	14.37
0.0257	0.575	284.41	11.26
0.0523	1.19	281.86	8.71
0.0922	2.18	279.15	6.00
0.1341	3.281	277.04	3.89
0.1891	4.860	275.04	1.89
0.2861	8.071	272.66	−0.49
0.3839	12.01	271.22	−1.93
0.4918	17.49	269.99	−3.16
0.5974	24.53	268.54	−4.61
0.6961	33.41	265.90	−7.25
0.7917	45.43	259.99	−13.16
0.8721	59.90	246.20	−26.95
0.9136	69.85	231.20	−41.95
0.922	72.1	226.14	−47.01
0.9399	77.41	226.70	−46.45
0.9591	83.71	227.36	−45.79
0.9803	91.60	228.32	−44.83
1.0000	100.00	229.28	−43.87

A eutectic was reported at 226.14 K (−47.01 °C, compiler) at $x_1 = 0.922$ (100 $w_1 = 72.1$, compiler).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The freezing-temperature apparatus has been described previously¹ but the temperature-measurement system is new. Temperatures were measured with a Leeds and Northrup platinum resistance thermometer and with a Solartron Model 7081 digital multimeter which has a sensitivity on the 100 Ω scale of 10 μΩ. The multimeter used a 1 mA current for measurements of resistance less than 100 Ω. The resistance meter was interfaced to a Hewlett-Packard Model 9845C computer through an IEEE bus. The computer read and stored a resistance measurement every 4 s from which cooling and warming curves of time against temperature could be constructed. The computer could be signaled to record visual melting temperatures during the recording process. The results were continually plotted on a video monitor, recorded on disk, and eventually plotted to provide a permanent record of the time-against-temperature cooling and warming curves.

Source and Purity of Materials:

(1) MBC Omnisolv; purified by fractional distillation in a vacuum-jacketed 2 m column packed with glass helices and operated at a reflux ratio of approximately 100; purity 0.9998 mole fractions; melting point = −43.87 °C.
(2) Aldrich; reagent grade; purified by fractional distillation in a vacuum-jacketed 2 m column packed with glass helices and operated at a reflux ratio of approximately 100; purity 0.9998 mole fractions; melting point = 14.37 °C.

Estimated Error:

Temperature: ±0.05 K.

References:

¹J. R. Goates, J. B. Ott, and A. H. Budge, *J. Phys. Chem.* **65**, 2162 (1961).

6.5. + Tetrachloroethane

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. E. Cornish, R. C. Archibald, E. A. Murphy, and H. M. Evans, <i>Ind. Eng. Chem.</i> 26 , 397–406 (1934).
(2) Tetrachloroethane; C ₂ Cl ₄ ; [127-18-4]	
Variables:	Prepared By:
T/K = 286	Valerii P. Sazonov

Experimental Data

UCST was reported to be 13 °C (286 K, compiler).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Determinations were made in test tubes, which were heated and allowed to cool slowly in air. Thermometers were roughly calibrated.

Source and Purity of Materials:

(1) Prepared from sodium cyanide and dimethyl sulfate; the crude product was distilled off and successively washed with solid sodium hydroxide and P₂O₅; carefully fractionated in the 6.09 m column; $d(20^\circ\text{C}, 4^\circ\text{C}) = 0.78215$.
(2) Source not specified; commercial high-grade reagent.

Estimated Error:

Not reported.

6.7. + Hexadecafluorooxoctane

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(2) Hexadecafluorooxoctane; C ₈ F ₁₆ O; [1978-24-1]	I. Kikic and P. Alessi, Ann. Chim. (Rome) 64 , 363-7 (1974).	
Variables:		Prepared By:	
T/K = 291		Valerii P. Sazonov	

Experimental Data			
Mutual solubility of acetonitrile (1) and hexadecafluorooxoctane (2)			
<i>t</i> /°C	T/K (compiler)	100 w ₁ (compiler)	x ₁
18.0	291.2	0.0096	0.9993
		Fluorocarbon-rich phase	Acetonitrile-rich phase
			99.30

Method/Apparatus/Procedure:
The analytical method was used. A sample of each phase was withdrawn with a syringe and immediately analyzed by GLC. No experimental details given.

Source and Purity of Materials:
(1) 3M Minnesota; used without any preliminary treatment, since the analysis by GLC did not indicate any detectable impurity.
(2) 3M Minnesota; used without any preliminary treatment, since the analysis by GLC did not indicate any detectable impurity.

Estimated Error:
Temperature: ±0.1 K.

6.6. + 1-Hydropentadecafluoroheptane

Components:		Original Measurements:	
(1) Acetonitrile; CH ₃ CN; [75-05-8]	(2) 1-Hydropentadecafluoroheptane; C ₇ HF ₁₅ ; [375-83-7]	J. O. Konecky and C. H. Deal, J. Phys. Chem. 67 , 504-6 (1963).	
Variables:		Prepared By:	
T/K = 256-317		Valerii P. Sazonov and Nikolai V. Sazonov	

Experimental Data					
The mutual solubility of acetonitrile and 1-hydropentadecafluoroheptane in volume fractions were reported over the temperature range in graphical form. Data presented here were extracted by the compilers from the reported graphs.					
<i>t</i> /°C	T/K	100 $\bar{\phi}_1$	x ₁	100 w ₁	x ₁
-17.1	256.1	16.4	0.639	—	—
1.4	274.6	18.5	0.672	—	—
6.4	279.6	—	—	94.9	0.994
28.5	301.7	—	—	88.9	0.986
28.6	301.8	28.6	0.783	78.3	—
39.2	312.4	38.5	0.850	—	—
42.5	315.7	—	—	73.5	0.962
42.8	316.0	46.8	0.890	—	—
43.7	316.9	57.1	0.923	—	—
43.8	317.0	—	—	—	— (UCST)

Timmermans¹ values of density of acetonitrile, $\rho(25^\circ\text{C}) = 776.8 \text{ g} \cdot \text{L}^{-1}$, was used in the above conversions.

Method/Apparatus/Procedure:
The synthetic (cloud point) method using sealed Pyrex tubes was employed. All values reported are an average of at least three determinations agreeing within 0.2 °C or better. No details were reported.

Source and Purity of Materials:
(1) Source not specified; spectroscopic grade; not purified.
(2) Prepared by the decarboxylation of perfluoro-*n*-octanoic acid; dried over phosphorus pent oxide and distilled on a ten plate microhelipod column at a reflux ratio of 5/1; boiling point = 95 °C/100.1 kPa, $\rho(25^\circ\text{C}) = 1718 \text{ g} \cdot \text{L}^{-1}$.

Estimated Error:
Not reported.

References:
¹J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

6.8. + 1-Bromoalkanes: C₈-C₁₈

Components: (1) Acetonitrile; C ₂ H ₅ N; [75-05-8] (2) 1-Bromoalkanes: C ₈ H ₁₇ Br; C ₁₀ H ₂₁ Br; C ₁₂ H ₂₅ Br; C ₁₄ H ₂₉ Br; C ₁₆ H ₃₃ Br; and C ₁₈ H ₃₇ Br	Original Measurements: H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372-81 (1965).
Variables: T/K = 291-393	Prepared By: Valerii P. Sazonov
Experimental Data	
Upper critical solution temperatures of the systems acetonitrile (1) + 1-bromoalkane (2)	
1-Bromoalkane	T/K (compiler)
1-Bromooctane; C ₈ H ₁₇ Br; [111-83-1]	290.7
1-Bromodecane; C ₁₀ H ₂₁ Br; [112-29-8]	318.7
1-Bromododecane; C ₁₂ H ₂₅ Br; [143-15-7]	342.2
1-Bromotetradecane; C ₁₄ H ₂₉ Br; [112-71-0]	360.7
1-Bromohexadecane; C ₁₆ H ₃₃ Br; [112-82-3]	377.7
1-Bromooctadecane; C ₁₈ H ₃₇ Br; [112-89-0]	393.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, with a heating stage was used. A 26 × 38 mm slide was adapted to hold capillaries on the stage. Two glass strips were glued, using water glass, to the slide, leaving a 0.5 mm channel. The slide was then placed in the adjustable device of the heating stage. (1) and (2) were put into capillary tubing (0.2-0.3 mm diameters) by dipping consecutively into both liquids. The height of the liquid was 7-10 mm. Room temperature solids were melted on a glass slide over a microburner. The capillary was sealed at both ends to a length of 30-35 mm, then inserted in to the channel on the slide and heated on the stage. The UCST was determined by following the appearance and disappearance of the meniscus.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent, No. 9011; *n*(20 °C/D) = 1.3445; *d*(20 °C, 4 °C) = 0.780.
(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

6.9. + Tetraalkylammonium Iodides: C₈ and C₁₂

Components: (1) Acetonitrile; C ₂ H ₅ N; [75-05-8] (2) Tetraalkylammonium iodides: C ₈ H ₃₀ IN and C ₁₂ H ₂₈ IN	Original Measurements: P. Walden, <i>Z. Phys. Chem.</i> 55 , 683-720 (1906).			
Variables: T/K = 273 and 298	Prepared By: Valerii P. Sazonov			
Experimental Data				
Solubility of tetraalkylammonium iodides (2) in acetonitrile (1)				
Salt	<i>t</i> /°C	T/K (compiler)	100 <i>w</i> ₂	<i>x</i> ₂ (compiler)
Tetraethylammonium iodide; C ₄ H ₉ IN; [68-05-3]	0.0 25.0	273.2 298.2	2.74 3.834	0.0045 0.0063
Tetrapropylammonium iodide; C ₁₂ H ₂₈ IN; [631-40-3]	0.0 25.0	273.2 298.2	15.24 21.77	0.0230 0.0352

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used.
Method A: 10-20 mL of (1) and an appropriate amount of fine dry salt (2) were placed in a glass retort in a thermostat and stirred for many hours. Aliquots of the saturated solution were taken by pipette for titration.

Method B: 15-25 mL of (1) and finely divided salt (2) were equilibrated at 40 °C with intensive stirring for 1 h. The flask was then placed in a thermostat (25 or 0 °C) and stirred for 2 h. After this, stirring was halted and the flask kept at the given temperature for 17-18 h. The saturated solutions were then sampled and titrated.

Source and Purity of Materials:

- (1) Not specified.
(2) Not specified.

Estimated Error:

Not reported.

7. Acetonitrile+Alcohols (mono- and poly-)

7.1. +1,2,3-Propanetriol

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	V. P. Sazonov and L. V. Gudkina, Zh. Prikl. Khim. (Leningrad)	
(2) 1,2,3-Propanetriol (glycerol); C ₃ H ₈ O ₃ ; [56-81-5]	(2) 1,2,3-Propanetriol (glycerol); C ₃ H ₈ O ₃ ; [56-81-5]	46, 1076-9 (1973).	
Variables:		Prepared By:	
T/K = 299-320		Valerii P. Sazonov	

Experimental Data

Mutual solubility of acetonitrile (1) and 1,2,3-propanetriol (2)

<i>t</i> /°C	<i>T</i> /K (complier)	100 <i>w</i> ₁	<i>x</i> ₁ (complier)	100 <i>w</i> ₁	<i>x</i> ₁ (complier)
25.4	298.6	8.35	0.170	—	—
31.3	304.5	—	—	95.0	0.977
37.4	310.6	10.0	0.200	—	—
39.3	312.5	—	—	94.0	0.972
46.7	319.9	—	—	92.4	0.965

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Determinations were made in sealed tubes, which were heated and allowed to cool slowly in water bath. Thermometers were calibrated to 0.01 K.

Source and Purity of Materials:

(1) Soyuzreaktiv, USSR; CP reagent, dried over P₂O₅ and twice distilled in a laboratory packed column; *n*(20 °C,D)=1.3440, *d*(20 °C,4 °C)=0.7828.
 (2) Soyuzreaktiv, USSR; pure grade reagent; purified by two vacuum distillations; water content by the method Fischer less than 0.04 mass %.

Estimated Error:

Temperature: ±0.02 K.

7.2. + 1,4-Benzenediol

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	G. N. Chekhova, Dissertation, Novosibirsk Institute of Inorganic Chemistry, 1975.	
(2) 1,4-Benzenediol (hydroquinone); C ₆ H ₆ O ₂ ; [123-31-9]	(2) 1,4-Benzenediol (hydroquinone); C ₆ H ₆ O ₂ ; [123-31-9]		
Variables:		Prepared By:	
T/K = 229-444		Valerii P. Sazonov and Nikolai V. Sazonov	

Experimental Data

No region of liquid-liquid immiscibility was observed. A full solid-liquid phase diagram in mole percent over the specified temperature range was reported in the original publication.

Melting temperatures of acetonitrile (1) and 1,4-benzenediol (2) system

<i>x</i> ₁	100 <i>w</i> ₁ (compliers)	<i>t</i> /°C	<i>T</i> /K (compliers)
0.000	0.0	170.3	443.5
0.011	0.4	169.9	443.1
0.049	1.9	169.2	442.4
0.109	4.4	166.5	439.7
0.157	6.5	163.3	436.5
0.192	8.1	161.2	434.4
0.240	10.5	156.5	429.7
0.246	10.8	156.0	429.2
0.341	16.2	149.1	422.3
0.396	19.6	142.0	415.2
0.454	23.7	134.0	407.2
0.523	29.0	124.1	397.3
0.625	39.3	103.7	376.9
0.679	44.1	97.5	370.7
0.720	48.9	91.1	364.3
0.734	50.7	89.8	363.0
0.833	65.0	70.1	343.3
0.895	76.1	50.0	323.2
0.952	88.1	20.0	293.2
0.975	93.6	-44.5	228.7
0.996	98.9	-43.3	229.9
1.000	100.0	-42.2	231.0

A eutectic was reported at -44.5 °C (228.7 K, compliers) at *x*₁ = 0.975 (100 *w*₁ = 93.6, compliers).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Solutions of various compositions were located in glass vessels and placed in a cooling mixture. The change of temperature was measured by the thermocouple. No experimental details given.

Source and Purity of Materials:

(1) Source not specified; for chromatography; not purified; melting point = -42.2 °C.
 (2) Source not specified; purified by the recrystallization; melting point = 170.3 °C.

Estimated Error:

Temperature: ±0.2 K.

7.3. + 1-Decanol

Components:	Evaluators:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, October, 2001.
(2) 1-Decanol; C ₁₀ H ₂₂ O; [112-30-1]	

Critical Evaluation

Quantitative solubility data for the system acetonitrile (1) and 1-decanol (2) have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system acetonitrile+ 1-decanol

Reference	T/K	Solubility	Method
Hoerr <i>et al.</i> ¹	269–295	Mutual	Synthetic
Francis ²	296	UCST	Synthetic
Majgler-Baranowska <i>et al.</i> ³	290–297	Mutual	Synthetic
Szydlowski and Szykula ⁴	295–297	Mutual	Synthetic

In addition to these data Schmid *et al.*⁵ determined of the upper critical temperature solution of components (1) and (2) in the course of a study of binary solubilities of acetonitrile and (C₁₀–C₂₀) alcohols. All original data are compiled in the data sheets immediately following this Critical Evaluation.

The upper critical solution temperature has been reported as 295.6 K,¹ 295.9 K,² 296.2 K,⁵ 296.61 K,⁴ and 297.1 K,⁵ these data are in reasonable agreement and thus their average value: UCST=296.3±0.5 K and is recommended. The corresponding critical solution composition has been reported as $x_{c1}=0.756^3$ and as $x_{c1}=0.767^4$ and averaged value, $x_{c1}=0.762\pm 0.005$ is recommended.

Monotectic equilibrium has been reported to occur at 278.3 K.¹ All experimental values reported^{1,3,4} have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1=0.4740, \quad a_2=1.8944, \quad b_1=-3.8277, \quad b_2=0.6260$$

(mean standard error of estimate was 0.0269).

For approximation x_{c1} and UCST from Szydlowski and Szykula⁴ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in Table 2. This relationship together with experimental points^{1,3,4} are also presented in Fig. 13.

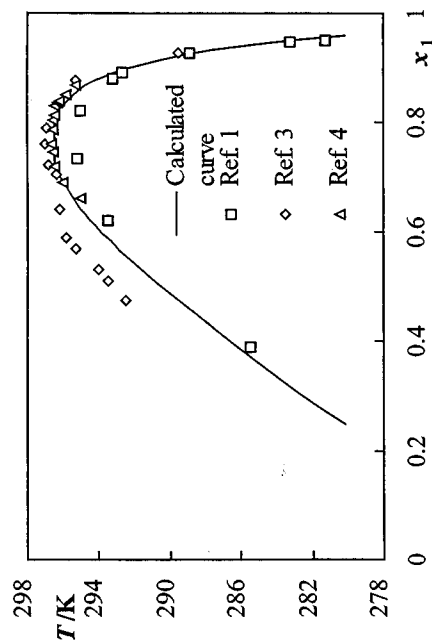


FIG. 13. Mutual solubility of acetonitrile and 1-decanol.

TABLE 2. Calculated mutual solubility of acetonitrile (1) and 1-decanol (2)

T/K	Alcohol-rich phase		Acetonitrile-rich phase	
	x_1	100 w ₁	x_1	100 w ₁
280.2	0.248	7.9	0.958	85.5
283.2	0.317	10.7	0.950	83.1
286.2	0.389	14.2	0.940	80.2
289.2	0.465	18.4	0.925	76.2
292.2	0.548	23.9	0.901	70.2
294.2	0.612	29.0	0.877	64.9
296.2	0.650	32.5	0.858	61.0
296.3	0.701	37.8	0.826	55.2
296.3	0.708	38.6	0.820	54.2
296.4	0.717	39.7	0.814	53.2

References:

- ¹C. W. Hoerr, H. J. Harwood, and A. W. Ralston, *J. Org. Chem.* **9**, 267 (1944).
- ²A. W. Francis, *J. Phys. Chem.* **60**, 20 (1956).
- ³H. Majgler-Baranowska, W. Pyzuk, W. Jente, and J. Ziolo, *J. Chem. Eng. Data* **26**, 51 (1981).
- ⁴J. Szydlowski and M. Szykula, *Fluid Phase Equilib.* **154**, 79 (1999).
- ⁵H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *Microchem. J.* **9**, 134 (1965).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	H. Májlinger-Baranowska, W. Pyzak, W. Jeute, and J. Ziolo, <i>J. Chem. Eng. Data</i> 26 , 51–3 (1981).
(2) 1-Decanol; C ₁₀ H ₂₂ O; [112-30-1]	
Variables:	Prepared By:
T/K = 290–297	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The mutual solubility of acetonitrile (1) and 1-decanol (2) in volume fractions was reported over the temperature range in graphical form. Data were extracted from the published graphs by the compilers.

T/K	t/°C	Mutual solubility of acetonitrile (1) and 1-decanol (2)			
		100 ϕ_1	100 w ₁	x ₁	100 ϕ_1
289.5	16.3	—	—	—	76.9
292.5	19.3	20.0	19.0	0.475	—
293.5	20.3	22.2	21.2	0.509	—
294.0	20.8	23.7	22.6	0.530	—
295.3	22.1	26.5	25.4	0.568	65.0
295.8	22.6	28.1	27.0	0.588	—
296.2	23.0	32.7	31.4	0.640	—
296.4	23.2	39.6	38.2	0.704	—
296.8	23.6	41.5	40.1	0.721	—
296.9	23.7	—	—	—	49.3
297.0	23.8	—	—	—	44.9
297.1	23.9	45.9	44.5	0.756	44.5

Timmermans' values of the density of acetonitrile, $\rho(20\text{ }^\circ\text{C}) = 782.2\text{ g}\cdot\text{L}^{-1}$, and Marsden and Mann² value for 1-decanol, $\rho(20\text{ }^\circ\text{C}) = 829.2\text{ g}\cdot\text{L}^{-1}$, were used for conversions.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Miscibility temperature was determined by observing turbidity changes during heating and cooling of vigorously shaken solutions. No experimental details given.

Source and Purity of Materials:

(1) Fluka; purity 99.5 mass %; dried and distilled over CaH₂.
(2) Source not specified; purity 98 mass %; dried, vacuum fractionated and redistilled over CaH₂.

Estimated Error:

Temperature: $\pm 0.05\text{ K}$.

References:

1. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).
2. Marsden and S. Mann, *Solvents Guide* (Cleveland-Hume Press Ltd., London, 1963).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr, H. J. Harwood, and A. W. Ralston, <i>J. Org. Chem.</i> 9 , 267–80 (1944).
(2) 1-Decanol; C ₁₀ H ₂₂ O; [112-30-1]	
Variables:	Prepared By:
T/K = 269–295	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of acetonitrile (1) and 1-decanol (2) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical and tabular form.

t/°C	T/K (compilers)	g ₂ /100 g ₁	Mutual solubility of acetonitrile (1) and 1-decanol (2)	
			100 w ₁	x ₁ (compilers)
—4.4 ^c	268.8	—	—	0.993
0.0	273.2	5.8	—	0.985
0.9 ^c	274.1	—	—	0.983
3.9 ^c	277.1	—	—	0.966
5.2 ^c	278.4	—	7.7 ^a	—
5.7 ^c	278.9	—	3.6 ^b	—
8.0 ^c	281.2	—	—	0.951
10.0	283.2	21.6	—	0.947
12.3 ^c	285.5	—	14.2 ^b	—
15.7 ^c	288.9	—	—	0.926
19.5 ^c	292.7	—	—	0.893
20.0	293.2	52.0	—	0.881
20.3 ^c	293.5	—	29.7 ^b	—
21.8 ^c	295.0	—	—	0.822
22.0 ^c	295.2	—	41.8 ^b	—

^aSolid–liquid equilibrium.

^bLiquid–liquid equilibrium.

^cData extracted from the published graphs by the compilers.

Monotectic equilibrium occurs at 5.1 °C (278.3 K, compilers).

The upper critical solution temperature was extracted by the compilers to be 22.2 °C (295.6 K).

Auxiliary Information

Method/Apparatus/Procedure:

The solubility measurements were made with the equipment and in the manner described elsewhere.^{1,2}

Source and Purity of Materials:

- (1) Source not specified; purity not specified.
- (2) Prepared by catalytic hydrogenation of ethyl decanoate; purified by vacuum distillation; freezing point = 6.88 °C.

Estimated Error:

Not specified.

References:

1. C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).
2. A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, *J. Org. Chem.* **9**, 102 (1944).

7.4. 1-Alcohols: C₁₀ and C₁₂

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		J. Szydłowski and M. Szykula, Fluid Phase Equilib. 154 , 79–87 (1999).	
(2) 1-Decanol; C ₁₀ H ₂₂ O; [112-30-1]			
Variables:		Prepared By:	
T/K = 295–297		Valerii P. Sazonov and Nikolai V. Sazonov	
Experimental Data			
Mutual solubility of acetonitrile (1) and 1-decanol (2)			
T/K	t/°C (compilers)	x ₁	100 w ₁ (compilers)
		Acetonitrile-rich phase	
295.07	21.92	0.660	33.5
295.34	22.19	—	—
295.88	22.73	—	—
295.99	22.84	0.690	36.6
296.17	23.02	—	—
296.29	23.14	—	—
296.45	23.30	—	—
296.48	23.33	—	—
296.51	23.36	—	—
296.57	23.42	0.720	40.0
296.59	23.44	0.746	43.2
296.60	23.45	—	—
296.62	23.47	0.760	45.1
		Alcohol-rich phase	
295.07	21.92	—	—
295.34	22.19	0.868	63.0
295.88	22.73	0.850	59.5
296.17	23.02	—	—
296.29	23.14	0.840	57.7
296.45	23.30	0.835	55.9
296.48	23.33	0.830	53.0
296.51	23.36	0.813	51.7
296.57	23.42	—	—
296.59	23.44	—	—
296.60	23.45	0.805	49.1
296.62	23.47	0.788	47.9

The UCST was reported to be 296.61 ± 0.016 K (23.46 °C, compilers) at x_c = 0.767 ± 0.002 (100 w = 46.0, compilers).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A simplified version of the apparatus described elsewhere was used.¹ Temperature was changed at the rate < 0.01 K/min and there was no visible influence of the rate on the transition temperature up to the rate 0.1 K/min. Due to the very weak turbidity a long capillary cell was employed. A 5 mW Polytec HeNe laser was used as a probe for detecting the phase separation.

Source and Purity of Materials:

(1) Byk-Malinkrodt; AR; purified by a column distillation; purity of the collected fractions at least 99.9 mole % by GLC.
 (2) Aldrich; dried over molecular sieves and distilled.

Estimated Error:

Temperature: ± 5 mK.

References:

¹J. Szydłowski, L. P. Rebelo, and W. A. Van Hook, Rev. Sci. Instrum. **63**, 1717 (1992).

Components:

(1) Acetonitrile; C₂H₅N; [75-05-8]
 (2) 1-Alcohols; C₁₀H₂₂O and C₁₂H₂₆O

Original Measurements:

A. W. Francis, J. Phys. Chem. **60**, 20–7 (1956).

Variables:

T/K = 296–308

Prepared By:

Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

Upper critical solution temperatures of the systems acetonitrile (1) + 1-alcohol (2)

Alcohol	Melting point/°C	ρ, (20 °C) g·L ⁻¹	n(20 °C,D)	t/°C	T/K (compilers)
1-Decanol; C ₁₀ H ₂₂ O; [112-30-1]	6.8	831.8	1.4372	22.7	295.9
1-Dodecanol; C ₁₂ H ₂₆ O; [112-53-8]	22.7	832.24	1.4410/24 °C	35.2	308.4

Auxiliary Information

Method/Apparatus/Procedure:

Observations were made after vigorous shaking in glass-stoppered graduated tubes of 15 mL capacity, immersed in water baths in large Dewar flasks. The water was agitated with a rapid stream of air bubbles. The temperature was adjusted by adding cooler or warmer water occasionally.

Source and Purity of Materials:

(1) Source not specified; purity not specified.
 (2) Source not specified; purified by crystallization.

Estimated Error:

Not reported.

7.6. + 2-Alcohols: C₁₁-C₁₉

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) 2-Alcohols; C ₁₁ H ₂₄ O-C ₁₉ H ₄₀ O	Original Measurements: H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 9 , 134-44 (1965).
Variables: T/K = 296-339	Prepared By: Valerii P. Sazonov

Experimental Data		T/K (complier)
Upper critical solution temperatures of the systems acetonitrile (1)+2-alcohol (2)		
2-Alcohol	t/°C	
2-Undecanol; C ₁₁ H ₂₄ O; [1653-30-1]	22.5	295.7
2-Dodecanol; C ₁₂ H ₂₆ O; [10203-28-8]	29.0	302.2
2-Tridecanol; C ₁₃ H ₂₈ O; [1653-31-2]	35.0	308.2
2-Tetradecanol; C ₁₄ H ₃₀ O; [4706-81-4]	39.5	312.7
2-Pentadecanol; C ₁₅ H ₃₂ O; [1653-34-5]	45.0	318.2
2-Hexadecanol; C ₁₆ H ₃₄ O; [34019-44-8]	50.0	323.2
2-Heptadecanol; C ₁₇ H ₃₆ O; [16813-18-6]	55.5	328.7
2-Nonadecanol; C ₁₉ H ₄₀ O; [26533-36-8]	66.0	339.2

Auxiliary Information	
Method/Apparatus/Procedure: The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere. ¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.	Source and Purity of Materials: (1) Baker Chemical Co.; reagent, No. 9011; n(20 °C,D) = 1.3445, d(20 °C,4 °C) = 0.780. (2) Some alcohols obtained from Aldrich Chemical Co.; all other alcohols prepared by reduction of the corresponding methyl ketones with lithium aluminum hydride; purified by gas-liquid partition chromatography.
Estimated Error: Temperature: ±0.5 K.	References: ¹ H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372 (1965).

7.5. + 1-Alcohols: C₁₀-C₂₀

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) 1-Alcohols; C ₁₀ H ₁₈ O-C ₂₀ H ₄₂ O	Original Measurements: H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 9 , 134-44 (1965).
Variables: T/K = 296-347	Prepared By: Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data		T/K (compliers)
Upper critical solution temperatures of the binary systems acetonitrile (1)+1-alcohol (2)		
1-Alcohol	t/°C	
1-Decanol; C ₁₀ H ₂₂ O; [112-30-1]	23.0	296.2
1-Undecanol; C ₁₁ H ₂₄ O; [112-42-5]	29.0	302.2
1-Dodecanol; C ₁₂ H ₂₆ O; [112-53-8]	34.5	307.7
1-Tridecanol; C ₁₃ H ₂₈ O; [112-70-9]	40.0	313.2
1-Tetradecanol; C ₁₄ H ₃₀ O; [112-72-1]	44.5	317.7
1-Pentadecanol; C ₁₅ H ₃₂ O; [629-76-5]	50.0	323.2
1-Hexadecanol; C ₁₆ H ₃₄ O; [36653-82-4]	54.5	327.7
1-Heptadecanol; C ₁₇ H ₃₆ O; [1454-85-9]	59.5	332.7
1-Octadecanol; C ₁₈ H ₃₈ O; [112-92-5]	64.0	337.2
1-Nonadecanol; C ₁₉ H ₄₀ O; [1454-84-8]	69.0	342.2
1-Eicosanol; C ₂₀ H ₄₂ O; [629-96-9]	74.0	347.2

Auxiliary Information	
Method/Apparatus/Procedure: The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere. ¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.	Source and Purity of Materials: (1) Baker Chemical Co.; reagent, No. 9011; n(20 °C,D) = 1.3445, d(20 °C,4 °C) = 0.780. (2) Some alcohols obtained from the Homel Institute and from Lachat Chemicals; all other alcohols prepared by reduction of the corresponding methyl esters with lithium aluminum hydride; purified by gas-liquid partition chromatography.
Estimated Error: Temperature: ±0.5 K.	References: ¹ H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372 (1965).

7.7. + 1-Dodecanol

Components:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) 1-Dodecanol; C₁₂H₂₆O; [112-53-8]

Evaluators:

Valeriy P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, November, 2001.

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and 1-dodecanol (2) have been reported in four publications. Hoerr *et al.*¹ studied the phase equilibrium of the liquid-liquid-solid system and the mutual solubility of (1) and (2) between 273 and 309 K by the synthetic method. Francis² determined the upper critical solution temperature of (1) and (2) by the synthetic method. Schmidt *et al.*³ measured the upper critical temperature solution of components (1) and (2) in the course of a study of solubilities of binary systems of acetonitrile and (C₁₀-C₂₀) alcohols. Sazonov and Gudkina⁴ defined the mutual solubilities of acetonitrile and 1-dodecanol between 299 and 308 K by the synthetic method.

The upper critical solution temperature has been reported as 307.7 K,³ 308.4 K,² 308.45 K,⁴ and 308.9 K,¹ these data are in reasonable agreement and thus their average value: UCST = 308.4 ± 0.5 K and is recommended. The corresponding critical solution composition has been reported as $x_{c1} = 0.788$.⁴

Monotectic equilibrium has been reported to occur at 293.2 K.¹

All experimental values reported^{1,4} have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.6791, \quad a_2 = 0.7569, \quad b_1 = -0.4051, \quad b_2 = -1.8542$$

(mean standard error of estimate was 0.0105).

For approximation x_{c1} and UCST⁴ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with experimental points,^{1,4} are also presented in Fig. 14.

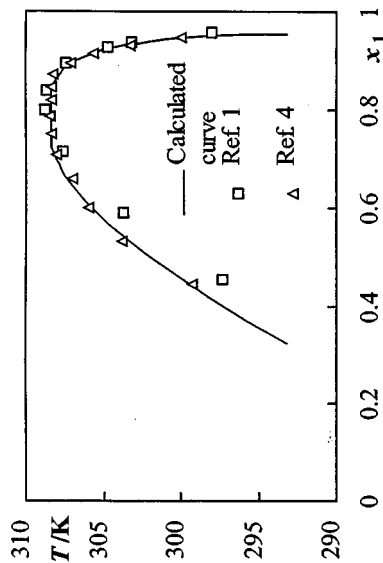


FIG. 14. Mutual solubility of acetonitrile and 1-dodecanol.

Calculated mutual solubility of acetonitrile (1) and 1-dodecanol (2)

T/K	Alcohol-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
293.2	0.325	9.6	0.955	82.4
298.2	0.418	13.7	0.952	81.4
303.2	0.528	19.8	0.935	76.0
304.2	0.554	21.5	0.929	74.2
305.2	0.582	23.5	0.921	72.0
306.2	0.614	25.9	0.909	68.8
307.2	0.654	29.4	0.891	64.3
307.7	0.679	31.8	0.877	61.1
308.2	0.717	35.8	0.852	55.9
308.3	0.729	37.2	0.842	54.0

References:

- ¹C. W. Hoerr, H. J. Harwood, and A. W. Ralston, *J. Org. Chem.* **9**, 267 (1944).
²A. W. Francis, *J. Phys. Chem.* **60**, 20 (1956).
³H. O. Schmidt, H. K. Mangold, and W. O. Lundberg, *Microchem. J.* **9**, 134 (1965).
⁴V. P. Sazonov and L. V. Gudkina, *Zh. Prikl. Khim. (Leningrad)* **46**, 1076 (1973).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	V. P. Sazonov and L. V. Gudkina, Zh. Prikl. Khim. (Leningrad)
(2) 1-Dodecanol; C ₁₂ H ₂₆ O; [112-53-8]	46, 1076-9 (1973).
Variables:	Prepared By:
T/K = 299-308	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data					
Mutual solubility of acetonitrile (1) and 1-dodecanol (2)					
t/°C	T/K (compilers)	100 w ₁		x ₁ (compilers)	
		Alcohol-rich phase	Acetonitrile-rich phase	Alcohol-rich phase	Acetonitrile-rich phase
26.10	299.25	15.0	—	0.445	—
26.85	300.00	—	—	—	80.0
30.15	303.30	—	—	—	75.0
30.70	303.85	20.0	—	0.532	—
32.50	305.65	—	—	—	70.0
32.85	306.00	25.0	—	0.602	—
33.90	307.05	30.0	—	0.661	—
34.00	307.15	—	—	—	65.0
34.90	308.05	35.0	—	0.710	—
35.10	308.25	—	—	—	60.0
35.20	308.35	40.0	—	0.752	—
35.25	308.40	—	—	—	55.0
35.30	308.45	45.0	—	0.788	—
					45.0
					0.788 (UCST)

Auxiliary Information	
Method/Apparatus/Procedure:	The synthetic method was used. Determinations were made in sealed tubes, which were heated and allowed to cool slowly in water bath. Thermometers were calibrated to 0.01 K.
Source and Purity of Materials:	(1) Soyuzreaktiv, USSR; CP reagent; dried over P ₂ O ₅ and twice distilled in a laboratory packed column; n(20 °C,D)=1.3440, d(20 °C,4 °C)=0.7828. (2) Soyuzreaktiv, USSR; pure grade reagent; purified by two vacuum distillations; n(20 °C,D)=1.4410, d(20 °C,4 °C)=0.8349.
Estimated Error:	Temperature: ±0.02 K.

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr, H. J. Harwood, and A. W. Ralston, J. Org. Chem. 9,
(2) 1-Dodecanol; C ₁₂ H ₂₆ O; [112-53-8]	267-80 (1944).
Variables:	Prepared By:
T/K = 273-309	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data					
Mutual solubility of acetonitrile (1) and 1-dodecanol (2)					
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₁		x ₁ (compilers)
			Alcohol-rich phase	Acetonitrile-rich phase	
0.0	273.2	1.0	—	99.0 ^a	0.998
0.2 ^c	273.4	—	—	98.9 ^a	0.998
6.2 ^c	279.4	—	—	97.8 ^a	0.995
10.0	283.2	3.9	—	96.2 ^a	0.991
12.8 ^c	286.0	—	—	94.5 ^a	0.987
15.5 ^c	288.7	—	—	92.7 ^a	0.983
19.0 ^c	292.2	—	—	88.6 ^a	0.972
20.0	293.2	16.7	—	85.7 ^a	0.965
20.2 ^c	293.4	—	—	—	—
21.5 ^c	294.7	—	—	0.348	—
24.1 ^c	297.3	—	—	0.193	—
24.8 ^c	298.0	—	—	0.454	—
30.0	303.2	29.9	—	83.4 ^b	0.958
30.5 ^c	303.7	—	—	76.9 ^b	0.938
31.5 ^c	304.7	—	—	—	—
34.2 ^c	307.4	—	—	73.9 ^b	0.928
34.4 ^c	307.6	—	—	65.0 ^b	0.894
35.5 ^c	308.7	—	—	0.715	—
35.6 ^c	308.8	—	—	53.8 ^b	0.841
				0.801	—
				47.0 ^b	—

^aSolid-liquid equilibrium.
^bLiquid-liquid equilibrium.
^cData extracted from the published graphs by the compilers.
 Monotectic equilibrium occurs at 20.0 °C (293.2 K, compilers). The upper critical solution temperature was extracted from the reported graphs by the compilers and found to be 35.7 °C (308.9 K).

Auxiliary Information	
Method/Apparatus/Procedure:	The solubility measurements were made with the equipment and in the manner described elsewhere. ^{1,2}
Source and Purity of Materials:	(1) Source not specified; purity not specified. (2) Source not specified; commercial product; purified by vacuum distillation in a Stedman packed column; freezing point=23.95 °C.
Estimated Error:	Not specified.
References:	¹ C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9, 68 (1944). ² A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, Org. Chem. 9, 102 (1944).

7.8. + 1-Tetradecanol

Components:	Evaluators:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, November, 2001.
(2) 1-Tetradecanol; C ₁₄ H ₃₀ O; [112-72-1]	

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and 1-tetradecanol (2) have been reported in two publications. Hoerr *et al.*¹ studied the phase equilibrium of the liquid-liquid-solid system and the mutual solubility of (1) and (2) between 283 and 322 K by the synthetic method. Schmid *et al.*² measured the upper critical temperature solution of components (1) and (2) in the course of study of binary solubilities of acetonitrile and (C₁₀-C₂₀) alcohols. In addition to these data Francis³ reported the upper critical solution temperature of this system.

The upper critical solution temperature has been reported as 317.7 K,² 321.2 K,³ and 321.6 K.¹ The UCST by Schmid *et al.*² is rejected. The average of the remaining values, UCST = 321.4 ± 0.2 K, is treated as tentative. The corresponding critical solution composition has been calculated by the evaluator as $x_{c1} = 0.84$ from the data.¹

Monotectic equilibrium has been reported to occur at 306.7 K.¹

All experimental values reported¹ have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = -0.4516, \quad a_2 = 1.1462, \quad b_1 = 0.2848, \quad b_2 = -2.0623$$

(mean standard error of estimate was 0.0020).

For approximation x_{c1} and UCST from Hoerr *et al.*¹ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with experimental results,¹ are also presented in Fig. 15.

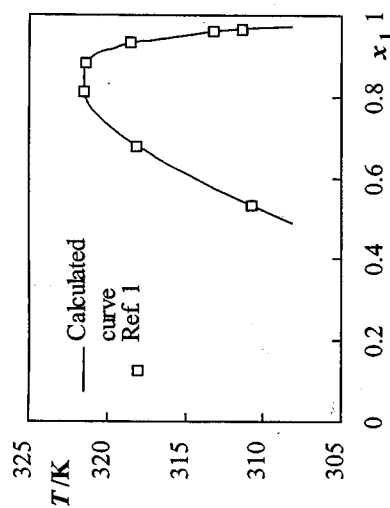


FIG. 15. Mutual solubility of acetonitrile and 1-tetradecanol.

Calculated mutual solubility of acetonitrile (1) and 1-tetradecanol (2)

T/K	Alcohol-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
308.2	0.489	15.5	0.971	86.5
313.2	0.575	20.6	0.959	81.7
318.2	0.680	28.9	0.935	73.4
319.2	0.706	31.5	0.926	70.6
320.2	0.737	34.9	0.913	66.8
320.7	0.756	37.2	0.904	64.3
321.2	0.781	40.6	0.889	60.5
321.4	0.795	42.6	0.888	58.4
321.5	0.805	44.1	0.872	56.6

References:

- ¹C. W. Hoerr, H. J. Harwood, and A. W. Ralston, *J. Org. Chem.* **9**, 267 (1944).
- ²H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *Microchem. J.* **9**, 134 (1965).
- ³A. W. Francis, *Critical Solution Temperature*, Washington, Adv. Chem. Ser. **31** (1961).

7.9. + 1-Hexadecanol

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr, H. J. Harwood, and A. W. Ralston, <i>J. Org. Chem.</i> 9 , 267-80 (1944).
(2) 1-Tetradecanol; C ₁₄ H ₃₀ O; [112-72-1]	
Variables:	Prepared By:
T/K = 283-322	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data
The solubilities of acetonitrile (1) and 1-tetradecanol (2) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical and tabular form.

Mutual solubility of acetonitrile (1) and 1-tetradecanol (2)						
<i>t</i> /°C	T/K (compilers)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₁	<i>x</i> ₁ (compilers)	100 <i>w</i> ₁	<i>x</i> ₁ (compilers)
			Alcohol-rich phase	Acetonitrile-rich phase		
10.0	283.2	<0.1	—	—	>99.9 ^a	0.999
20.0	293.2	1.3	—	—	98.7 ^a	0.998
21.5 ^c	294.7	—	—	—	98.2 ^a	0.997
28.2 ^c	301.4	—	—	—	94.7 ^a	0.989
30.0	303.2	7.7	—	—	92.9 ^a	0.986
31.9 ^c	305.1	—	—	—	90.0 ^a	0.979
33.6 ^c	306.8	—	11.8 ^a	0.411	—	—
35.2 ^c	308.4	—	5.9 ^a	0.247	—	—
37.5 ^c	310.7	—	17.8 ^b	0.531	—	—
38.2 ^c	311.4	—	—	—	83.8 ^b	0.964
40.0	313.2	22.1	—	—	81.9 ^b	0.959
44.9 ^c	318.1	—	28.5 ^b	0.676	—	—
45.3 ^c	318.5	—	—	—	72.5 ^b	0.932
48.2 ^c	321.4	—	—	—	58.9 ^b	0.882
48.3 ^c	321.5	—	45.0 ^b	0.810	—	—

^aSolid-liquid equilibrium.

^bLiquid-liquid equilibrium.

^cThese data were extracted by the compilers from the published graphs.

Monotectic equilibrium occurs at 33.5 °C (306.7 K, compilers).

The upper critical solution temperature was extracted from the reported graphs by the compilers and found to be 48.4 °C (321.6 K).

Auxiliary Information

Method/Apparatus/Procedure:

The solubility measurements were made with the equipment and in the manner described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; purity not specified.
(2) Prepared by catalytic hydrogenation of methyl myristate; purified by vacuum distillation; freezing point = 38.26 °C.

Estimated Error:

Not specified.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).
²A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, *J. Org. Chem.* **9**, 102 (1944).

Components:

(1) Acetonitrile; C₂H₃N; [75-05-8]
(2) 1-Hexadecanol; C₁₆H₃₄O; [36653-82-4]

Evaluators:

Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, November, 2001.

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and 1-hexadecanol (2) have been reported in two publications. Hoerr *et al.*¹ studied the phase equilibrium of the liquid-liquid-solid system and the mutual solubility of (1) and (2) between 293 and 331 K by the synthetic method. Schmid *et al.*² measured the upper critical temperature solution of components (1) and (2) in the course of a study of binary solubilities of acetonitrile and (C₁₀-C₂₀) alcohols. In addition to these data Francis³ reported the upper critical solution temperature of this system.

The upper critical solution temperature has been reported as 327.7 K,² 330.7 K,¹ and 331.2 K.³ The UCST by Schmid *et al.*² is rejected. The average of the remaining values, UCST = 331.0 ± 0.3 K, is treated as tentative. The corresponding critical solution composition has been calculated by the evaluators as *x*_{c1} = 0.86 from the data of Hoerr *et al.*¹

Monotectic equilibrium has been reported to occur at 317.7 K.¹

All experimental values reported¹ have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = -0.4132, a_2 = 1.0803, b_1 = -0.3432, b_2 = -1.5032$$

(mean standard error of estimate was 0.0057).

For approximation *x*_{c1} and UCST from Hoerr *et al.*¹ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with experimental results,¹ are also presented in Fig. 16.

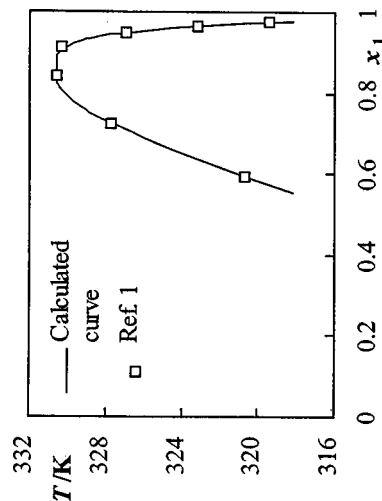


FIG. 16. Mutual solubility of acetonitrile and 1-hexadecanol.

Calculated mutual solubility of acetonitrile (1) and 1-tetradecanol (2)

T/K	Alcohol-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
318.2	0.553	17.3	0.978	88.3
323.2	0.635	22.8	0.966	82.8
328.2	0.736	32.1	0.940	72.6
329.2	0.764	35.4	0.928	68.6
329.7	0.780	37.5	0.920	66.0
330.2	0.801	40.5	0.909	62.8
330.4	0.812	42.2	0.901	60.6
330.5	0.819	43.4	0.896	59.3

References:

- ¹C. W. Hoerr, H. J. Harwood, and A. W. Ralston, *J. Org. Chem.* **9**, 267 (1944).
²H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *Microchem. J.* **9**, 134 (1965).
³A. W. Francis, *Critical Solution Temperature*, Washington, Adv. Chem. Ser. **31** (1961).

Original Measurements:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) 1-Hexadecanol; C₁₆H₃₄O; [36653-82-4]

Variables:

T/K = 293–331

Prepared By:

Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of acetonitrile (1) and 1-hexadecanol (2) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical and tabular form.

Mutual solubility of acetonitrile (1) and 1-hexadecanol (2)

t/°C	T/K (compilers)	$g_2/100g_1$	100 w_1		x_1 (compilers)	100 w_1	x_1 (compilers)
			Alcohol-rich phase	Acetonitrile-rich phase			
20.0	293.2	≈0.1	—	—	—	99.9 ^a	0.999
30.0	303.2	1.1	—	—	—	98.9 ^a	0.998
38.4 ^c	311.6	—	—	—	—	96.4 ^b	0.994
40.0	313.2	5.6	—	—	—	94.7 ^a	0.991
42.9 ^c	316.1	—	—	—	—	91.5 ^b	0.985
45.0 ^c	318.2	—	12.5 ^b	—	0.458	—	—
46.2 ^c	319.4	—	—	—	—	86.8 ^b	0.975
46.5 ^c	319.7	—	6.4 ^a	—	0.288	—	—
47.5 ^c	320.7	—	19.8 ^b	—	0.593	—	—
50.0	323.2	20.9	—	—	—	82.7 ^b	0.966
53.8 ^c	327.0	—	—	—	—	76.1 ^b	0.950
54.5	327.7	—	30.6 ^b	—	0.723	—	—
57.1 ^c	330.3	—	—	—	—	63.6 ^b	0.912
57.4 ^c	330.6	—	47.5 ^b	—	0.842	—	—

^aSolid–liquid equilibrium.

^bLiquid–liquid equilibrium.

^cThese data were extracted by the compilers from the published graphs.

Monotectic equilibrium occurs at 44.5 °C (317.7 K, compilers).

The upper critical solution temperature was extracted from the reported graphs by the compilers and found to be 57.5 °C (330.7 K).

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility measurements were made with the equipment and in the manner described elsewhere.^{1,2}

Source and Purity of Materials:

- (1) Source not specified; purity not specified.
 (2) Source not specified; commercial product; purified by recrystallization; freezing point = 49.62 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).
²A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, *J. Org. Chem.* **9**, 102 (1944).

7.10. + Unsaturated 1-Alcohols: C₁₈

Components:		
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(2) Unsaturated 1-alcohols; C ₁₈ H ₃₄ O and C ₁₈ H ₃₆ O	
Variables:		
T/K= 304 and 319		
Original Measurements:		
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 9 , 134-44 (1965).		
Prepared By:		
Valerii P. Sazonov		
Experimental Data		
Upper critical solution temperatures of the systems acetonitrile (1)+unsaturated 1-alcohol (2)		
Unsaturated 1-alcohol	<i>t</i> /°C	<i>T</i> /K (compiler)
1-Octadecadienol; C ₁₈ H ₃₄ O; [506-43-4]	30.5	303.7
1-Octadecenol; C ₁₈ H ₃₆ O; [143-28-2]	46.0	319.2

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere.¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent, No. 9011; *n*(20 °C, D) = 1.3445; *d*(20 °C, 4 °C) = 0.780.
- (2) Obtained by reduction of the respective α -chloroketones with lithium aluminum hydride; purified by gas-liquid partition and thin-layer adsorption chromatography.

Estimated Error:

Temperature: ± 0.5 K.

References:

- ¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).

7.11. + 1-Octadecanol

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(2) 1-Octadecanol; C ₁₈ H ₃₈ O; [112-92-5]
Evaluators:	
Valerii P. Sazonov and Nikolai V. Sazonov, Technical University, Samara, Russia, November, 2001.	

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and 1-octadecanol (2) have been reported in two publications. Hoerr *et al.*¹ studied the phase equilibrium of the liquid-liquid-solid system and the mutual solubility of (1) and (2) between 303 and 337 K by the synthetic method. Schmid *et al.*² measured the upper critical temperature solution of components (1) and (2) in the course of a study of binary solubilities of acetonitrile and (C₁₀-C₂₀) alcohols. In addition to these data, Francis³ reported the upper critical solution temperature of this system.

The upper critical solution temperature has been reported as 336.2 K,³ 336.8 K,¹ and 337.2 K,² these data are in reasonable agreement and thus their average value: UCST = 336.7 \pm 0.4 K and is recommended. The corresponding critical solution composition has been calculated by evaluators as $x_{c1} = 0.88$ from the data of Hoerr *et al.*¹

Monotectic equilibrium has been reported to occur at 325.7 K.¹

All experimental values reported¹ have been approximated by an equation based on the scaling law (described in the introduction to this volume) for which the following parameters have been derived:

$$a_1 = -0.3143, a_2 = 1.5386, b_1 = -0.4256, b_2 = -1.6183$$

(mean standard error of estimate was 0.0080).

For approximation x_{c1} and UCST from Hoerr *et al.*¹ have been used. In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with experimental results,¹ are also presented in Fig. 17.

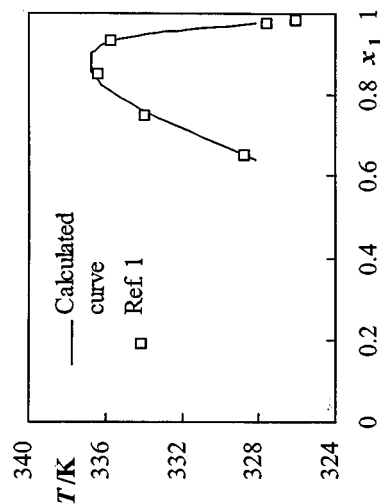


FIG. 17. Mutual solubility of acetonitrile and 1-octadecanol.

Calculated mutual solubility of acetonitrile (1) and 1-octadecanol (2)

T/K	Alcohol-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
328.2	0.640	21.2	0.975	85.5
333.2	0.741	30.3	0.953	75.5
334.2	0.765	33.1	0.946	72.7
335.2	0.792	36.6	0.936	68.9
335.7	0.808	39.0	0.930	66.8
336.2	0.826	41.9	0.921	63.9
336.4	0.835	43.4	0.916	62.3
336.6	0.847	45.7	0.908	60.0

References:

- ¹C. W. Hoerr, H. J. Harwood, and A. W. Ralston, *J. Org. Chem.* **9**, 267 (1944).
²H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *Microchem. J.* **9**, 134 (1965).
³A. W. Francis, *Critical Solution Temperature*, Washington, Adv. Chem. Ser. **31** (1961).

Components:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) 1-Octadecanol; C₁₈H₃₈O; [112-92-5]

Original Measurements:

- C. W. Hoerr, H. J. Harwood, and A. W. Ralston, *J. Org. Chem.* **9**, 267–80 (1944).

Variables:

T/K = 303–336

Prepared By:

Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of acetonitrile (1) and 1-octadecanol (2) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical form and in a table.

Mutual solubility of acetonitrile (1) and 1-octadecanol (2)

t/°C	T/K (compilers)	$g_2/100 g_1$	x_1 (compilers)		100 w_1	x_1 (compilers)	100 w_1	x_1 (compilers)
			Alcohol-rich phase	Acetonitrile-rich phase				
30.0	303.2	0.3	—	—	—	—	99.7 ^a	0.999
36.4 ^c	309.6	—	—	—	—	—	99.1 ^a	0.999
40.0	313.2	1.6	—	—	—	—	98.4 ^a	0.998
42.0 ^c	315.2	—	—	—	—	—	98.2 ^a	0.997
48.2 ^c	321.4	—	—	—	—	—	95.3 ^a	0.993
50.0	323.2	7.6	—	—	—	—	92.9 ^a	0.989
51.8 ^c	325.0	—	—	—	—	—	90.0 ^b	0.983
52.9 ^c	326.1	—	15.0 ^a	0.538	—	—	—	—
54.0 ^c	327.2	—	9.3 ^a	0.403	—	—	—	—
54.4 ^c	327.6	—	—	—	—	—	86.2 ^b	0.976
55.5 ^c	328.7	—	4.8 ^a	0.249	—	—	—	—
55.6 ^c	328.8	—	22.3 ^b	0.654	—	—	—	—
60.8 ^c	334.0	—	31.2 ^b	0.749	—	—	—	—
62.5 ^c	335.7	—	—	—	—	—	68.2 ^b	0.934
63.2 ^c	336.4	—	46.4 ^b	0.851	—	—	—	—

^aSolid–liquid equilibrium.

^bLiquid–liquid equilibrium.

^cThese data were extracted by the compiler from the published graphs.

Monotectic equilibrium occurs at 52.5 °C (325.7 K, compiler).

The upper critical solution temperature was extracted from the reported graphs by the compiler and found to be 63.6 °C (336.8 K).

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility measurements were made with the equipment and in the manner described elsewhere.^{1,2}

Source and Purity of Materials:

- (1) Source not specified; purity not specified.
 (2) Prepared by catalytic hydrogenation of ethyl stearate; purified by vacuum distillation; freezing point = 57.98 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).
²A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, *J. Org. Chem.* **9**, 102 (1944).

8. Acetonitrile+Aldehydes, Ketones

8.1. + Aldehydes: C₁₈

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements:
(2) Aldehydes; C ₁₈ H ₃₆ O and C ₁₈ H ₃₆ O	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 11 , 376-83 (1966).
Variables:	
T/K = 284 and 313	Prepared By:
	Valerii P. Sazonov
Experimental Data	
Upper critical solution temperatures of the systems acetonitrile (1) + aldehyde (2)	
Aldehyde	T/K (complier)
cis-9-Octadecanal; C ₁₈ H ₃₄ O; [2423-10-1]	11.0
Octadecanal; C ₁₈ H ₃₆ O; [638-66-4]	40.0
	284.2
	313.2

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The synthetic method was used. As described elsewhere, ¹ a microscope equipped with a heating stage was used. The sealed glass capillary, containing (1) and (2), was held on the heating stage by an aluminum slide. The stage was cooled by acetone/CO ₂ , and heated electrically by a regulating transformer. For capillaries with inner diameter (0.2-0.3) mm, the amount required for one CST determination is about 0.2-2 μ L.	(1) Baker Chemical Co.; reagent No. 9011. (2) Not specified.
Estimated Error:	Not reported.
References:	¹ H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372 (1965).

7.12. + Unsaturated 2-Alcohols: C₁₉

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements:
(2) Unsaturated 2-alcohols; C ₁₉ H ₃₆ O and C ₁₉ H ₃₈ O	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 9 , 134-44 (1965).
Variables:	
T/K = 306 and 323	Prepared By:
	Valerii P. Sazonov
Experimental Data	
Upper critical solution temperatures of the systems acetonitrile (1) + unsaturated 2-alcohol (2)	
Unsaturated 2-alcohol	T/K (complier)
2-Nonadecadienol; C ₁₉ H ₃₆ O	306.2
2-Nonadecenol; C ₁₉ H ₃₈ O	322.7

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere. ¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.	(1) Baker Chemical Co.; reagent, No. 9011; $n(20^\circ\text{C}, \text{D}) = 1.3445$; $d(20^\circ\text{C}, 4^\circ\text{C}) = 0.780$. (2) Prepared by reduction of the respective α -chloro-ketones with lithium aluminum hydride; purified by gas-liquid partition chromatography.
Estimated Error:	Temperature: ± 0.5 K.
References:	¹ H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372 (1965).

8.3. + 12-Tricosanone

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. 8, 344-57 (1943).
(2) 12-Tricosanone; C ₂₃ H ₄₆ O; [540-09-0]	
Variables:	Prepared By:
T/K=283-355	Valerii P. Sazonov

Experimental Data

The solubilities of 12-tricosanone (2) in acetonitrile (1) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical form and in a table.

Solubility of 12-tricosanone (2) in acetonitrile (1)

t/°C	T/K (compiler)	g ₂ /100g ₁	100 w ₂ (compiler)	x ₂ (compiler)
10.0	283.2	<0.1	<0.1 ^a	0.0001
23.3 ^c	296.5	—	0.3 ^a	0.0004
30.0	303.2	0.4	0.4 ^a	0.0005
35.0 ^c	308.2	—	0.5 ^a	0.0006
45.9 ^c	319.1	—	0.7 ^a	0.0009
50.0	323.2	1.2	1.2 ^a	0.0015
53.0 ^c	326.2	—	1.9 ^a	0.002
56.1 ^c	329.3	—	3.1 ^a	0.004
60.4 ^c	333.6	—	6.2 ^a	0.008
62.7 ^c	335.9	—	82.3 ^a	0.361
63.4 ^c	336.6	—	87.8 ^a	0.466
64.5 ^c	337.7	—	91.8 ^a	0.576
65.5 ^c	338.7	—	9.3 ^b	0.012
65.9 ^c	339.1	—	95.0 ^a	0.697
66.4 ^c	339.6	—	79.5 ^b	0.320
70.0	343.2	12.4	11.0 ^b	0.015
72.7 ^c	345.9	—	78.0 ^b	0.301
74.8 ^c	348.0	—	13.2 ^b	0.018
75.1 ^c	348.3	—	77.1 ^b	0.290
80.5 ^c	353.7	—	16.2 ^b	0.023
81.1 ^c	354.3	—	74.3 ^b	0.260
82.0	355.2	22.8	18.6 ^b	0.027

^aSolid-liquid equilibrium.

^bLiquid-liquid equilibrium.

^cThe compiler extracted these data from the published graphs.

Monotectic equilibrium is realized at 62.3 °C (335.5 K, compiler).

The upper critical solution temperature was reported to be above 82 °C.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketesters by hydrolyzing with 5% alcoholic potassium hydroxide; purified by several recrystallizations from ethanol; freezing point=69.3 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. 64, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. 64, 2824 (1942).

8.2. + 10-Nonadecanone

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. 8, 344-57 (1943).
(2) 10-Nonadecanone; C ₁₉ H ₃₈ O; [504-57-4]	
Variables:	Prepared By:
T/K=283-333	Valerii P. Sazonov

Experimental Data

The solubilities of 10-nonadecanone (2) in acetonitrile (1) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical form and in a table.

Solubility of 10-nonadecanone (2) in acetonitrile (1)

t/°C	T/K (compiler)	g ₂ /100 g ₁	100 w ₂ (compiler)	x ₂ (compiler)
10.0	283.2	0.8	0.8 ^a	0.001
21.8 ^c	295.0	—	0.9 ^a	0.001
30.0	303.2	1.6	1.6 ^a	0.002
30.2 ^c	303.4	—	1.8 ^a	0.003
40.0 ^c	313.2	—	4.1 ^a	0.006
44.2 ^c	317.4	—	6.5 ^a	0.010
47.5 ^c	320.7	—	11.5 ^a	0.019
49.0 ^c	322.2	—	16.8 ^a	0.029
49.1 ^c	322.3	—	19.1 ^a	0.033
49.5 ^c	322.7	—	72.2 ^a	0.274
50.0	323.2	27.0	21.3 ^b	0.038
50.4 ^c	323.6	—	70.8 ^b	0.261
50.9 ^c	324.1	—	80.4 ^b	0.374
51.1 ^c	324.3	—	21.3 ^b	0.038
52.3 ^c	325.5	—	89.5 ^b	0.553
53.6 ^c	326.8	—	24.5 ^b	0.045
55.0 ^c	328.2	—	95.6 ^b	0.759
55.3 ^c	328.5	—	65.5 ^b	0.216
58.9 ^c	332.1	—	35.1 ^b	0.073
59.1 ^c	332.3	—	56.9 ^b	0.161
59.5 ^c	332.7	—	37.7 ^b	0.081
60.0 ^c	333.2	—	52.0 ^b	0.136

^aSolid-liquid equilibrium.

^bLiquid-liquid equilibrium.

^cThe compiler extracted these data from the published graphs.

Monotectic equilibrium is realized at 49.3 °C (322.5 K, compiler).

The upper critical solution temperature was extracted from the reported graphs by the compiler and found to be 60.4 °C (333.6 K).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketesters by hydrolyzing the latter with 5% alcoholic potassium hydroxide; purified by several recrystallization from ethanol; freezing point=57.8 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹H. J. Harwood, A. W. Ralston, and W. M. Selby, J. Am. Chem. Soc. 63, 1916 (1941).
²A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. 64, 1516 (1942).

8.5. + 16-Hentriacontanone

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. 8 , 344-57 (1943).
(2) 16-Hentriacontanone; C ₃₁ H ₆₂ O; [502-73-8]	
Variables:	Prepared By:
T/K = 323-355	Valerii P. Sazonov

Experimental Data

The solubilities of 16-hentriacontanone (2) in acetonitrile (1) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical form and in a table.

Solubility of 16-hentriacontanone (2) in acetonitrile (1)				
<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
50.0	323.2	≈0.1	≈0.1 ^a	0.0001
61.4 ^c	334.6	—	0.2 ^a	0.0002
67.8 ^c	341.0	—	0.9 ^a	0.0008
70.0	343.2	1.0	1.0 ^a	0.0009
76.4 ^c	349.6	—	2.3 ^a	0.002
78.5 ^c	351.7	—	90.0 ^a	0.450
79.1 ^c	352.3	—	91.6 ^a	0.498
80.5 ^c	353.7	—	95.5 ^a	0.659
81.4 ^c	354.6	—	96.6 ^a	0.721
82.0	355.2	3.3	3.2 ^b	0.003

^aSolid-liquid equilibrium.

^bLiquid-liquid equilibrium.

^cThese data were extracted by the compiler from the published graphs.

Monotectic equilibrium is realized at 78.2 °C (351.4 K, compiler).

The upper critical solution temperature was reported to be above 82 °C.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketesters by hydrolyzing with 5% alcoholic potassium hydroxide; purified by several crystallizations from ethanol; freezing point=83.7 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

8.4. + 14-Heptacosanone

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. 8 , 344-57 (1943).
(2) 14-Heptacosanone; C ₂₇ H ₅₄ O; [542-50-7]	
Variables:	Prepared By:
T/K = 303-355	Valerii P. Sazonov

Experimental Data

The solubilities of 14-heptacosanone (2) in acetonitrile (1) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical form and in a table.

Solubility of 14-heptacosanone (2) in acetonitrile (1)				
<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
30.0	303.2	≈0.1	≈0.1 ^a	0.0001
50.0	323.2	0.2	0.2 ^a	0.0002
55.6 ^c	328.8	—	0.3 ^a	0.0003
62.1 ^c	335.3	—	1.0 ^a	0.001
68.2 ^c	341.4	—	2.7 ^a	0.003
70.0	343.2	4.1	3.9 ^a	0.004
70.9 ^c	344.1	—	4.5 ^a	0.005
72.0 ^c	345.2	—	85.9 ^b	0.388
72.2 ^c	345.4	—	88.2 ^a	0.437
72.5 ^c	345.7	—	91.8 ^a	0.538
74.5 ^c	347.7	—	96.4 ^a	0.736
77.3 ^c	350.5	—	6.4 ^b	0.007
77.3 ^c	350.5	—	84.8 ^b	0.367
82.0	355.2	8.1	7.5 ^b	0.008
82.0 ^c	355.2	—	83.6 ^b	0.347

^aSolid-liquid equilibrium.

^bLiquid-liquid equilibrium.

^cData extracted from the published graphs by the compiler.

Monotectic equilibrium is realized at 71.8 °C (345.0 K, compiler).

The upper critical solution temperature was reported to be above 82 °C.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketesters by hydrolyzing with 5% alcoholic potassium hydroxide; purified by several crystallizations from ethanol; freezing point=77.2 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

8.6. + 18-Pentatriacontanone

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements:
(2) 18-Pentatriacontanone; C ₃₈ H ₇₆ O; [504-53-0]	F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. 8 , 344–57 (1943).
Variables:	Prepared By:
T/K = 323–355	Valerii P. Sazonov

Experimental Data

The solubilities of 18-pentatriacontanone (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

t/°C	T/K (compiler)	Solubility of 18-pentatriacontanone (2) in acetonitrile (1)	
		g ₂ /100g ₁	100 w ₂ (compiler) x ₂
50.0	323.2	<0.1	<0.1
70.0	343.2	0.2	0.0002
76.1 [*]	349.3	—	0.0003
82.0	355.2	1.1	0.001

^{*}Data extracted from the published graphs by the compiler.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

- (1) Source not specified; best grade reagent; dried and twice distilled.
- (2) Obtained from the ketesters by hydrolyzing with 5% alcoholic potassium hydroxide; purified by several crystallizations from ethanol; freezing point = 88.7 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
- ²C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

9. Acetonitrile+Ethers
9.1. + 2,2'-Oxybispropane

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements:
(2) 2,2'-Oxybispropane (dipropyl ether); C ₆ H ₁₄ O; [108-20-3]	R. E. Cornish, R. C. Archibald, E. A. Murphy, and H. M. Evans, Ind. Eng. Chem. 26 , 397–406 (1934).
Variables:	Prepared By:
T/K = 233	Valerii P. Sazonov

Experimental Data

The UCST was reported as < -40 °C (<233 K, compiler).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Determinations were made in test tubes, which were heated and allowed to cool slowly in air. Thermometers were roughly calibrated.

Source and Purity of Materials:

- (1) Prepared from sodium cyanide and dimethyl sulfate; the crude product was distilled off and successively washed with solid sodium hydroxide and P₂O₅; carefully fractionated in a 6.09 m column; d(20 °C, 4 °C) = 0.782 15.
- (2) Source not specified; purified by fractionating in a 6.09 m column.

Estimated Error:

Not reported.

9.3. + Dialkyl Ethers: C₁₂-C₂₀

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. 9, 134-44 (1965).
(2) Dialkyl ethers; C ₁₂ H ₂₆ O, C ₁₄ H ₃₀ O, C ₁₆ H ₃₄ O, C ₁₈ H ₃₈ O, and C ₂₀ H ₄₂ O	
Variables:	Prepared By:
T/K = 311-399	Valeri P. Sazonov

Experimental Data			
Upper critical solution temperatures of the binary systems acetonitrile (1) + dialkyl ether (2)			
	Dialkyl ether	t/°C	T/K (compiler)
1-Methoxyundecane (methyl-undecyl ether); C ₁₂ H ₂₆ O; [7289-53-4]		38.0	311.2
1-Ethoxydecane (ethyl-decyl ether); C ₁₂ H ₂₆ O; [16976-29-6]		48.0	321.2
1-Butoxyoctane (butyl-octyl ether); C ₁₂ H ₂₆ O; [53839-23-9]		59.5	332.7
1-Hexoxyhexane (diethyl ether); C ₁₂ H ₂₆ O; [112-58-3]		60.0	333.2
1-Methoxytridecane (methyl-tridecyl ether); C ₁₄ H ₃₀ O; [7289-55-9]		62.0	335.2
1-Ethoxydodecane (ethyl-dodecyl ether); C ₁₄ H ₃₀ O; [7289-37-4]		70.0	343.2
1-Butoxydecane (butyl-decyl ether); C ₁₄ H ₃₀ O; [111082-32-7]		78.5	351.7
1-Hepoxyheptane (diheptyl ether); C ₁₄ H ₃₀ O; [629-64-1]		80.5	353.7
1-Methoxypentadecane (methyl-pentadecyl ether); C ₁₆ H ₃₄ O		81.5	354.7
1-Ethoxytetradecane (ethyl-tetradecyl ether); C ₁₆ H ₃₄ O; [4813-58-5]		88.0	361.2
1-Butoxydodecane (butyl-dodecyl ether); C ₁₆ H ₃₄ O; [7289-38-5]		96.5	369.7
1-Methoxyheptadecane (methyl-heptadecyl ether); C ₁₈ H ₃₈ O		97.5	370.7
1-Octoxyoctane (dioctyl ether); C ₁₆ H ₃₄ O; [629-82-3]		98.0	371.2
1-Ethoxyhexadecane (ethyl-hexadecyl ether); C ₁₈ H ₃₈ O; [13933-61-4]		103.5	376.7
1-Butoxytetradecane (butyl-tetradecyl ether); C ₁₈ H ₃₈ O; [111082-34-9]		110.5	383.7
1-Methoxynonadecane (methyl-nonadecyl ether); C ₂₀ H ₄₂ O		112.5	385.7
1-Hexoxydodecane (hexyl-dodecyl ether); C ₁₈ H ₃₈ O		113.0	386.2
1-Octoxydecane (octyl-decyl ether); C ₁₈ H ₃₈ O; [17088-93-6]		113.0	386.2
1-Ethoxyoctadecane (ethyl-octadecyl ether); C ₂₀ H ₄₂ O; [62435-06-7]		117.5	390.7
1-Butoxyhexadecane (butyl-hexadecyl ether); C ₂₀ H ₄₂ O; [18302-77-7]		124.0	397.2
1-Decoxydecane (didecyl ether); C ₂₀ H ₄₂ O; [2456-28-2]		126.0	399.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere.¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent, No. 9011; n(20 °C,D) = 1.3445, d(20 °C,4 °C) = 0.780.
- (2) Symmetrical dialkyl ethers from Lachat Chemicals Co.; other ethers prepared by reaction of the potassium salts of the respective alcohols with dimethyl sulfate, diethyl sulfate, butyl bromide, hexyl bromide, or octyl bromide; purified.

Estimated Error:

Temperature: ±0.5 K.

References:

- H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. 42, 372 (1965).

9.2. + 1,1'-Oxybis-pentane

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	V. P. Sazonov and L. V. Gudkina, Zh. Prikl. Khim. (Leningrad)
(2) 1,1'-Oxybis-pentane (dipentyl ether); C ₁₀ H ₂₂ O; [693-65-2]	47, 2515-8 (1974).
Variables:	Prepared By:
T/K = 298-306	Valeri P. Sazonov

Experimental Data				
Mutual solubility of acetonitrile (1) and 1,1'-oxybis-pentane (2)				
t/°C	100 w ₁	100 w ₂	x ₁ (compiler)	x ₁ (compiler)
			Ether-rich phase	Acetonitrile-rich phase
24.50	—	—	—	0.900
28.60	297.65	—	—	0.877
29.00	301.75	—	—	—
30.80	302.15	24.6	0.557	—
31.55	303.95	—	—	0.853
32.40	304.70	29.3	0.615	—
32.65	305.55	—	—	0.823
32.90	305.80	34.7	0.672	—
32.95	306.05	39.9	0.719	0.794
	306.10	44.6	0.756	0.756 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. No experimental details were reported.

Source and Purity of Materials:

- (1) Soyuzreaktiv, USSR; CP reagent; dried over P₂O₅ and twice distilled in a laboratory packed column; n(20 °C,D) = 1.3440, d(20 °C,4 °C) = 0.7828.
- (2) Soyuzreaktiv, USSR; pure grade reagent; dried over CaCl₂ and purified by two vacuum distillations over sodium; d(20 °C,4 °C) = 0.7838.

Estimated Error:

Not reported.

9.4. + 1-Alkyl Glycosyl Ethers: C₁₃-C₂₄

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, <i>Microchem. J.</i> 11 , 306-14 (1966).	
(2) 1-Alkyl glyceryl ethers; C ₁₃ H ₂₆ O ₃ -C ₂₄ H ₄₈ O ₃			
Variables:		Prepared By:	
T/K = 295-349		Valerii P. Sazonov	
Experimental Data			
Upper critical solution temperatures of the binary systems acetonitrile (1) + alkyl glyceryl ether (2)			
Ether	<i>t</i> /°C	<i>T</i> /K (compiler)	
1-(<i>cis,cis,cis</i> -9,12,15-Octadecatrienoxy)-2,3-propanediol; C ₂₁ H ₃₈ O ₃	21.5	294.7	
1-Deoxy-2,3-propanediol; C ₁₃ H ₂₆ O ₃ ; [92219-12-0]	25.5	298.7	
1-Undecyloxy-2,3-propanediol; C ₁₄ H ₂₈ O ₃ ; [126923-57-7]	32.5	305.7	
1-(<i>cis,cis</i> -9,12-Octadecadienoxy)-2,3-propanediol; C ₂₁ H ₄₀ O ₃ ; [70518-62-6]	33.5	306.7	
1-Dodecyloxy-2,3-propanediol; C ₁₄ H ₃₀ O ₃ ; [1561-07-5]	38.0	311.2	
1-(<i>cis</i> -9-Hexadecenoxy)-2,3-propanediol; C ₁₆ H ₃₂ O ₃	40.0	313.2	
1-Tridecyloxy-2,3-propanediol; C ₁₆ H ₃₄ O ₃ ; [126923-58-8]	43.5	316.7	
1-Tetradecyloxy-2,3-propanediol; C ₁₇ H ₃₆ O ₃ ; [92219-13-1]	48.0	321.2	
1-(<i>cis</i> -9-Octadecenoxy)-2,3-propanediol; C ₂₁ H ₄₂ O ₃ ; [2929-07-9]	49.0	322.2	
1-(<i>trans</i> -9-Octadecenoxy)-2,3-propanediol; C ₂₁ H ₄₂ O ₃ ; [593-31-7]	51.5	324.7	
1-Pentadecyloxy-2,3-propanediol; C ₁₈ H ₃₆ O ₃ ; [124770-96-3]	53.0	326.2	
1-Hexadecyloxy-2,3-propanediol; C ₁₉ H ₃₈ O ₃ ; [506-03-6]	57.0	330.2	
1-Heptadecyloxy-2,3-propanediol; C ₂₀ H ₄₀ O ₃ ; [113817-63-3]	61.0	334.2	
1-Octadecyloxy-2,3-propanediol; C ₂₁ H ₄₂ O ₃ ; [544-62-7]	65.0	338.2	
1-Nonadecyloxy-2,3-propanediol; C ₂₂ H ₄₄ O ₃ ; [10431-03-5]	68.5	341.7	
1-Eicosyloxy-2,3-propanediol; C ₂₃ H ₄₆ O ₃ ; [158850-88-5]	72.0	345.2	
1-Heneicosyloxy-2,3-propanediol; C ₂₄ H ₅₀ O ₃ ; [158789-24-3]	76.0	349.2	

Auxiliary Information

Method/Apparatus/Procedure:

A microscope equipped with a heating stage as in Schmid *et al.*¹ was employed for determining UCST values. No experimental details are given.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent No. 9011.
- (2) Synthesized as in Baumann and Mangold.²

Estimated Error:

Not specified.

References:

- ¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).
- ²W. J. Baumann and H. K. Mangold, *J. Org. Chem.* **29**, 3055 (1964).

9.5. + 1,2-Dialkyl Glyceryl Ethers: C₃₃-C₄₁

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, <i>Microchem. J.</i> 11 , 306-14 (1966).	
(2) 1,2-Dialkyl glyceryl ethers; C ₃₃ H ₆₈ O ₃ -C ₄₁ H ₈₄ O ₃			
Variables:		Prepared By:	
T/K = 392-430		Valerii P. Sazonov	
Experimental Data			
Upper critical solution temperatures of the binary systems acetonitrile (1) + 1,2-dialkyl glyceryl ether (2)			
Ether	<i>t</i> /°C	<i>T</i> /K (compiler)	
2-(Dodecyloxy)-3-(octadecyloxy)-1-propanol; C ₃₃ H ₆₈ O ₃ ; [6076-36-4]	118.5	391.7	
2,3-Bis(9-octadecenoxy)-(Z,Z)-1-propanol; C ₃₉ H ₇₆ O ₃ ; [6076-41-1]	121.5	394.7	
3-(Octadecyloxy)-2-(tetradecyloxy)-1-propanol; C ₃₃ H ₇₂ O ₃ ; [6076-37-5]	129.5	402.7	
2,3-Bis(hexadecyloxy)-1-propanol; C ₃₅ H ₇₂ O ₃ ; [6076-35-3]	130.0	403.2	
3-(Octadecyloxy)-2-(<i>cis</i> -9-octadecenoxy)-1-propanol; C ₃₉ H ₇₈ O ₃	135.5	408.7	
3-(Octadecyloxy)-2-(<i>trans</i> -9-octadecenoxy)-1-propanol; C ₃₉ H ₇₈ O ₃	135.5	408.7	
3-(Hexadecyloxy)-2-(octadecyloxy)-1-propanol; C ₃₇ H ₇₆ O ₃	138.5	411.7	
2-(Hexadecyloxy)-3-(octadecyloxy)-1-propanol; C ₃₇ H ₇₆ O ₃ ; [6110-57-2]	140.5	413.7	
2,3-Bis(octadecyloxy)-1-propanol; C ₃₉ H ₈₀ O ₃ ; [6110-58-3]	140.5	413.7	
2-(Eicosyloxy)-3-(octadecyloxy)-1-propanol; C ₄₁ H ₈₄ O ₃ ; [6068-26-4]	148.5	421.7	

Auxiliary Information

Method/Apparatus/Procedure:

A microscope equipped with a heating stage as in Schmid *et al.*¹ was employed for determining UCST values. No experimental details are given.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent No. 9011.
- (2) Synthesized as in work of Baumann and Mangold.²

Estimated Error:

Not specified.

References:

- ¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).
- ²W. J. Baumann and H. K. Mangold, *J. Org. Chem.* **29**, 3055 (1964).

9.6. + 1,2,3-Trialkyl Glyceryl Ethers: C₄₇-C₅₇

Components:		
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements:	
(2) 1,2,3-Trialkyl glyceryl ethers; C ₄₇ H ₉₆ O ₃ -C ₅₇ H ₁₁₆ O ₃	H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, <i>Microchem. J.</i> 11 , 306-14 (1966).	
Variables:		
T/K = 464-495	Prepared By:	
	Valerii P. Sazonov	
Experimental Data		
Upper critical solution temperatures of the binary systems acetonitrile (1)+1,2,3-trialkyl glyceryl ether (2)		
Ether	t/°C	T/K (complier)
1-(Dodecyl)-2,3-bis(hexadecyl)propane; C ₄₇ H ₉₆ O ₃ ; [6076-43-3]	191.0	464.2
(Z,Z)-1,2,3-Tris(9-octadecyl)propane; C ₅₇ H ₁₁₆ O ₃ ; [10431-15-9]	196.5	469.7
1-(Dodecyl)-2-(hexadecyl)-3-(octadecyl)propane; C ₄₉ H ₁₀₀ O ₃ ; [6068-27-5]	198.0	471.2
1,2,3-Tris(hexadecyl)propane; C ₅₁ H ₁₀₄ O ₃ ; [5896-48-0]	204.5	477.7
1,2,3-Tris(hexadecyl)propane; C ₅₁ H ₁₀₄ O ₃ ; [6110-59-4]	204.5	477.7
(Z,Z)-1,2-Bis(9-octadecyl)-3-(octadecyl)propane; C ₅₇ H ₁₁₂ O ₃ ; [10431-14-8]	206.0	479.2
(Z)-1-(9-Octadecyl)-2,3-bis(octadecyl)propane; C ₅₇ H ₁₁₄ O ₃ ; [13166-06-8]	213.5	486.7
1,2,3-Tris(octadecyl)propane; C ₅₇ H ₁₁₆ O ₃ ; [6076-42-2]	222.0	495.2

Auxiliary Information

Method/Apparatus/Procedure:

A microscope equipped with a heating stage as in Schmid *et al.*¹ was employed for determining UCST values. No experimental details are given.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent No. 9011.
 (2) Synthesized as in work of Baumann and Mangold.²

Estimated Error:

Not specified.

References:

- ¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).
²W. J. Baumann and H. K. Mangold, *J. Org. Chem.* **29**, 3055 (1964).

10. Acetonitrile+Acids
10.1. + 6-(Hydroxyimino)-6-Nitrohexanoic Acid

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements:
(2) 6-(Hydroxyimino)-6-nitrohexanoic acid; C ₆ H ₁₀ N ₂ O ₅ ; [1069-46-1]	Z. S. Smolyan, G. N. Matveeva, Y. K. Fukin, K. N. Korotavskii, A. P. Ignat'eva, A. N. Komilina, L. S. Zvereva, and A. S. Fomin, <i>Khim. Prom-st (Moscow)</i> 48 , 508-9 (1972).
Variables:	
T/K = 298	Prepared By:
	Valerii P. Sazonov

Experimental Data

The solubility of 6-(hydroxyimino)-6-nitrohexanoic acid in acetonitrile at 25 °C (298 K, compiler) was reported to be 100 w₂ = 35.6. The corresponding mole fraction x₂ calculated by the compiler is 0.0092.

Auxiliary Information

Method/Apparatus/Procedure:

No details were reported.

Source and Purity of Materials:

- (1) Source not specified; purity not specified.
 (2) Source not specified; purity not specified.

Estimated Error:

Temperature: ± 1 K.

10.3. +Nonanoic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329–37 (1944).
(2) Nonanoic acid; C ₉ H ₁₈ O ₂ ; [112-05-0]	
Variables:	Prepared By:
T/K = 273–283	Valerii P. Sazonov

Experimental Data

The solubilities of nonanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of nonanoic acid (2) in acetonitrile (1)				
<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
0.0	273.2	51	33.8	0.117
0.8*	274.0	—	38.8	0.141
2.5*	275.7	—	56.3	0.251
3.1*	276.3	—	72.0	0.400
5.8*	279.0	—	88.0	0.656
10.0	283.2	3470	97.2	0.900

*The compiler extracted these data from the published graphs.

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The synthetic method, as described elsewhere, ¹ was used. No details were reported.	(1) Source not specified; purity not specified; dried and twice distilled.
	(2) Source not specified; purified according to Pool and Ralston; ² freezing point = 12.25 °C.
Estimated Error:	Not reported.

References:
¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.2. + Octanoic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329–37 (1944).
(2) Octanoic acid; C ₈ H ₁₆ O ₂ ; [124-07-2]	
Variables:	Prepared By:
T/K = 273 and 285	Valerii P. Sazonov

Experimental Data

The solubilities of octanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of octanoic acid (2) in acetonitrile (1)				
<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
0.0	273.2	44.5	30.8	0.112
2.5*	275.7	—	38.2	0.150
3.4*	276.6	—	43.5	0.180
5.0*	278.2	—	57.4	0.277
6.1*	279.3	—	72.5	0.429
9.2*	282.4	—	88.6	0.689
10.0	283.2	1020	91.1	0.745
12.0*	285.2	—	95.0	0.844

*These data were extracted by the compiler from the published graphs.

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The synthetic method, as described elsewhere, ¹ was used. No details were reported.	(1) Source not specified; purity not specified; dried and twice distilled.
	(2) Source not specified; purified according to Pool and Ralston; ² freezing point = 16.3 °C.
Estimated Error:	Not reported.

References:
¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.5. + Undecanoic Acid

Components:		Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329–37 (1944).
(2) Undecanoic acid; C ₁₁ H ₂₂ O ₂ ; [112-37-8]		
Variables:		Prepared By:
T/K = 273–296		Valerii P. Sazonov

Experimental Data

The solubilities of undecanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of undecanoic acid (2) in acetonitrile (1)				
t/°C	T/K (compiler)	g ₂ /100 g ₁	100 w ₂ (compiler)	x ₂ (compiler)
0.0	273.2	8.7	8.0	0.019
6.1*	279.3	—	11.4	0.0276
10.0	283.2	17.3	14.7	0.0366
14.8*	288.0	—	20.8	0.0547
18.3*	291.5	—	34.7	0.105
19.7*	292.9	—	53.0	0.199
20.0	293.2	185	64.9	0.290
20.3*	293.5	—	65.6	0.296
22.8*	296.0	—	87.5	0.607

*The compilers extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Purified according to Pool and Ralston;² freezing point = 28.13 °C.

Estimated Error:

Not specified.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.4. + Decanoic Acid

Components:		Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329–37 (1944).
(2) Decanoic acid; C ₁₀ H ₂₀ O ₂ ; [534-48-5]		
Variables:		Prepared By:
T/K = 273–303		Valerii P. Sazonov

Experimental Data

The solubilities of decanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of decanoic acid (2) in acetonitrile (1)				
t/°C	T/K (compiler)	g ₂ /100 g ₁	100 w ₂ (compiler)	x ₂ (compiler)
0.0	273.2	11.8	10.6	0.0275
3.0*	276.2	—	12.1	0.0318
8.2*	281.4	—	15.4	0.0416
10.0	283.2	21.0	17.4	0.0478
13.7*	286.9	—	21.4	0.0609
19.7*	292.9	—	36.5	0.121
20.0	293.2	66.0	39.8	0.136
20.9*	294.1	—	44.5	0.160
22.3*	295.5	—	63.0	0.289
24.2*	297.4	—	81.8	0.517
27.5*	300.7	—	92.5	0.746
30.0	303.2	7600	98.7	0.948

*These data were extracted by the compiler from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Purified according to Pool and Ralston;² freezing point = 31.24 °C.

Estimated Error:

Not specified.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.6. + Dodecanoic Acid

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329–37 (1944).	
(2) Dodecanoic acid; C ₁₂ H ₂₄ O ₂ ; [143-07-7]			
Variables:		Prepared By:	
T/K = 273–314		Valerii P. Sazonov	

Experimental Data

The solubilities of dodecanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

<i>t</i> /°C	T/K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
0.0	273.2	2.1	2.1	0.0044
8.6*	281.8	—	2.5	0.0052
10.0	283.2	2.8	2.7	0.0057
14.3*	287.5	—	4.0	0.0085
20.0	293.2	7.6	7.1	0.015
21.6*	294.8	—	8.1	0.018
28.0*	301.2	—	15.0	0.0349
30.0	303.2	24.4	19.6	0.0476
30.3*	303.5	—	20.3	0.0496
33.8*	307.0	—	34.4	0.0970
34.5*	307.7	—	41.5	0.127
35.8*	309.0	—	55.8	0.206
36.3*	309.5	—	66.3	0.287
37.2*	310.4	—	80.9	0.465
39.1*	312.3	—	90.4	0.659
40.0	313.2	1540	93.9	0.759
40.5*	313.7	—	95.0	0.796

*These data were extracted by the compiler from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;² freezing point = 43.92 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.7. + Tridecanoic Acid

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329–37 (1944).	
(2) Tridecanoic acid; C ₁₃ H ₂₆ O ₂ ; [638-53-9]			
Variables:		Prepared By:	
T/K = 273–313		Valerii P. Sazonov	

Experimental Data

The solubilities of tridecanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

<i>t</i> /°C	T/K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
0.0	273.2	1.4	1.4	0.0027
6.4*	279.6	—	1.7	0.0033
10.0	283.2	2.0	2.0	0.0039
20.0	293.2	5.8	5.5	0.011
24.1*	297.3	—	8.2	0.017
30.0	303.2	21.4	17.6	0.0393
31.2*	304.4	—	22.1	0.0515
32.1*	305.3	—	28.3	0.0703
33.1*	306.3	—	40.5	0.115
34.2*	307.4	—	61.3	0.233
35.4*	308.6	—	84.1	0.503
40.0	313.2	8600	98.9	0.945

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;² freezing point = 41.76 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.8. + Tetradecanoic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329-37 (1944).
(2) Tetradecanoic acid; C ₁₄ H ₂₈ O ₂ ; [544-63-8]	
Variables:	Prepared By:
T/K = 273-323	Valerii P. Sazonov

Experimental Data

The solubilities of tetradecanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
0.0	273.2	0.7	0.7	0.001
10.0	283.2	0.9	0.9	0.0016
12.0*	285.2	—	1.1	0.0020
20.0	293.2	1.8	1.8	0.0033
30.0	303.2	4.1	3.9	0.0072
32.0*	305.2	—	4.6	0.0086
40.0	313.2	13.0	11.5	0.0228
41.6*	314.8	—	14.1	0.0287
44.5*	317.7	—	23.5	0.0523
45.0*	318.2	—	29.6	0.0703
45.7*	318.9	—	42.7	0.118
46.5*	319.7	—	70.6	0.302
48.0*	321.2	—	80.7	0.429
49.2*	322.4	—	88.3	0.576
50.0	323.2	1210	92.4	0.686

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

- (1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;² freezing point = 54.15 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.9. + Fatty Acids: C₁₄-C₂₄

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. 42 , 372-81 (1965).
(2) Fatty acids; C ₁₄ H ₂₈ O ₂ -C ₂₄ H ₄₈ O ₂	
Variables:	Prepared By:
T/K = 327-382	Valerii P. Sazonov

Experimental Data

Upper critical solution temperatures of the binary systems acetonitrile (1) + fatty acid (2)

Acid	<i>t</i> /°C	<i>T</i> /K (compiler)
Tetradecanoic acid; C ₁₄ H ₂₈ O ₂ ; [544-63-8]	53.5	326.7
Hexadecanoic acid; C ₁₆ H ₃₂ O ₂ ; [57-10-3]	68.5	341.7
Octadecanoic acid; C ₁₈ H ₃₆ O ₂ ; [57-11-4]	81.5	354.7
Eicosanoic acid; C ₂₀ H ₄₀ O ₂ ; [506-30-9]	91.5	364.7
Docosanoic acid; C ₂₂ H ₄₄ O ₂ ; [112-85-6]	101.0	374.2
Tetracosanoic acid; C ₂₄ H ₄₈ O ₂ ; [557-59-5]	109.0	382.2

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. A Reichert microscope, type RCH, with a heating stage was used. A 26×38 mm slide was adapted to hold capillaries on the stage. Two glass strips were glued, using water glass, to the slide, leaving a 0.5 mm channel. The slide was then placed in the adjustable device of the heating stage. Samples of (1) and (2) were put into capillary tubing (0.2-0.3 mm diameters) by dipping consecutively into both liquids. The height of the liquid was 7-10 mm. Room temperature solids were melted on a glass slide over a micro burner. The capillary was sealed at both ends to a length of 30-35 mm, then inserted in to the channel on the slide and heated on the stage. The UCST was determined by following the appearance and disappearance of a meniscus.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent, No. 9011; *n*(20 °C, D) = 1.3445, *d*(20 °C, 4 °C) = 0.780.
(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

10.11. + Hexadecanoic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329–37 (1944).
(2) Hexadecanoic acid; C ₁₆ H ₃₂ O ₂ ; [57-10-3]	
Variables:	Prepared By:
T/K = 273–333	Valerii P. Sazonov

Experimental Data

The solubilities of hexadecanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of hexadecanoic acid (2) in acetonitrile (1)				
<i>t</i> /°C	T/K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
0.0	273.2	<0.1	<0.1	0.0001
10.0	283.2	0.2	0.2	0.0003
20.0	293.2	0.4	0.4	0.0006
23.8*	297.0	—	0.9	0.0015
30.0	303.2	1.0	1.0	0.0016
38.6*	311.8	—	2.7	0.0044
40.0	313.2	2.8	3.0	0.0049
44.0*	316.5	—	8.3	0.014
44.0*	317.2	—	9.0	0.016
45.0*	318.0	—	14.8	0.0271
47.2*	320.4	—	28.6	0.0603
50.0	323.2	—	59.4	0.190
		—	81.8	0.418
		1200	92.3	0.657

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;² freezing point = 62.82 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.10. + Pentadecanoic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9 , 329–37 (1944).
(2) Pentadecanoic acid; C ₁₅ H ₃₀ O ₂ ; [1002-84-2]	
Variables:	Prepared By:
T/K = 273–323	Valerii P. Sazonov

Experimental Data

The solubilities of pentadecanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of pentadecanoic acid (2) in acetonitrile (1)				
<i>t</i> /°C	T/K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
0.0	273.2	0.4	0.4	0.0007
10.0	283.2	0.5	0.5	0.0009
20.0	293.2	1.1	1.1	0.0019
23.8*	297.0	—	1.3	0.0022
30.0	303.2	2.9	2.8	0.0049
38.6*	311.8	—	7.3	0.013
40.0	313.2	10.5	9.5	0.018
43.3*	316.5	—	17.7	0.0351
44.0*	317.2	—	25.5	0.0548
44.8*	318.0	—	49.0	0.140
45.0*	318.2	—	71.4	0.297
47.2*	320.4	—	88.2	0.559
50.0	323.2	2460	96.1	0.807

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;² freezing point = 52.54 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

10.12. + Heptadecanoic Acid

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements: C. W. Hoerr and A. W. Ralston, J. Org. Chem. 9, 329-37 (1944).
(2) Heptadecanoic acid; C ₁₇ H ₃₄ O ₂ ; [506-12-7]	
Variables:	
T/K = 283-333	Prepared By: Valeri P. Sazonov

Experimental Data

The solubilities of heptadecanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
10.0	283.2	<0.1	<0.1	0.0001
20.0	293.2	0.2	0.2	0.0003
30.0	303.2	0.6	0.6	0.0009
32.6*	305.8	—	0.8	0.0012
40.0	313.2	1.9	1.9	0.0029
44.1*	317.3	—	3.3	0.0052
50.0	323.2	8.3	7.7	0.013
51.1*	324.3	—	9.5	0.016
53.5*	326.7	—	16.4	0.0289
54.5*	327.7	—	30.5	0.0624
56.0*	329.2	—	57.4	0.170
56.6*	329.8	—	78.0	0.350
58.7*	331.9	—	91.0	0.606
60.0	333.2	3600	97.3	0.845

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;² freezing point = 60.94 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9, 68 (1944).
²W. O. Pool and A. W. Ralston, Ind. Eng. Chem. 34, 1104 (1942).

10.13. + cis,cis-9,12-Octadecadienoic Acid

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements: C. W. Hoerr and H. J. Harwood, J. Phys. Chem. 56, 1068-73 (1952).
(2) cis,cis-9,12-Octadecadienoic acid (linoleic acid); C ₁₈ H ₃₂ O ₂ ; [60-33-3]	
Variables:	
T/K = 243-303	Prepared By: Valeri P. Sazonov

Experimental Data

Solubility of cis,cis-9,12-octadecadienoic acid (2) in acetonitrile (1)

<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
-30.0	243.2	0.2	0.2	0.0003
-20.0	253.2	0.4	0.4	0.0006
-10.0	263.2	4.9	4.7	0.0071
0.0	273.2	7.5	7.0	0.011
20.0	293.2	11.2	10.1	0.0161
30.0	303.2	17.7	15.0	0.0253

UCST reported as 39.5 °C (312.7 K, compiler).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Solubilities were determined by weighing 2-5 g portions of (2) into 2 cm×15 cm Pyrex test tubes which were fitted with a Nichrome stirrer and a thermocouple well, the test tube being inserted into a larger tube which served as an air bath. Upon successive additions of weighed amounts of (1), the solubilities were determined by measuring the temperatures at which crystals precipitated and dissolved upon alternate cooling and heating the systems in an acetone-dry ice bath or water bath as required.

Source and Purity of Materials:

(1) Source not specified; best grade reagent; distilled.
(2) Chemical Division, Armour and Co.; purified by stepwise fractional crystallization and vacuum distilled a short Vigreux column; melting point = -5.2 °C, *n*(20 °C, D) = 1.4703.

Estimated Error:

Temperature: ±0.1 K.

10.14. + cis-9-Octadecenoic Acid

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		C. W. Hoerr and H. J. Harwood, <i>J. Phys. Chem.</i> 56 , 1068–73 (1952).	
(2) cis-9-Octadecenoic acid (oleic acid); C ₁₈ H ₃₄ O ₂ ; [112-80-1]			
Variables:		Prepared By:	
T/K = 233–303		Valerii P. Sazonov	
Experimental Data			
Solubility of cis-9-octadecenoic acid (2) in acetonitrile (1)			
t/°C	T/K (complier)	g ₂ /100 g ₁	x ₂ (complier)
–40.0	233.2	0.1	0.0001
–30.0	243.2	0.3	0.0004
–20.0	253.2	0.7	0.0010
–10.0	263.2	1.1	0.0016
0.0	273.2	1.8	0.0026
20.0	293.2	7.7	0.011
30.0	303.2	9.1	0.013
UCST reported as 61.0 °C (334.2 K, complier).			
Auxiliary Information			
Method/Apparatus/Procedure:			
The synthetic method was used. Solubilities were determined by weighing 2–5 g portions of (2) into 2 cm × 15 cm Pyrex test tubes which were fitted with a Nichrome stirrer and a thermocouple well, the test tube being inserted into a larger tube which served as an air-bath. Upon successive additions of weighed amounts of (1), the solubilities were determined by measuring the temperatures at which crystals precipitated and dissolved upon alternately cooling and heating the systems in an acetone-dry ice bath or water bath as required.			
Source and Purity of Materials:			
(1) Source not specified; best grade reagent; distilled.			
(2) Prepared from high quality oil by saponification; purified by recrystallization and by vacuum distillation in packed column; melting point = 16.30 °C, n _D (20 °C, D) = 1.4599.			
Estimated Error:			
Temperature: ±0.1 K.			

10.15. + 12-Hydroxy-cis-9-Octadecenoic Acid

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Mikrochem. J.</i> 11 , 376–83 (1966).	
(2) 12-Hydroxy-cis-9-octadecenoic acid; C ₁₈ H ₃₄ O ₃ ; [141-22-0]			
Variables:		Prepared By:	
T/K = 298		Valerii P. Sazonov	
Experimental Data			
Upper critical solution temperature of the binary system acetonitrile+hydroxy acid			
Hydroxy acid	t/°C	T/K (complier)	
12-Hydroxy-cis-9-octadecenoic acid	25.0	298.2	
Auxiliary Information			
Method/Apparatus/Procedure:			
The synthetic method was used. As described elsewhere, ¹ a microscope equipped with a heating stage was used. The sealed glass capillary, containing (1) and (2), was held on the heating stage by an aluminum slide. The stage was cooled by acetone/CO ₂ , and heated electrically by a regulating transformer. For capillaries with inner diameter 0.2–0.3 mm, the amount required for one CST determination is about 0.2–2 μL.			
Source and Purity of Materials:			
(1) Baker Chemical Co.; reagent No. 9011.			
(2) Not specified.			
Estimated Error:			
Not reported.			
References:			
¹ H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372 (1965).			

11. Acetonitrile+Two-Basic Acids and Salts

11.1. + Butanedioic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	H. Snaigowski, <i>Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem.</i> 3 , 45–53 (1974).
(2) Butanedioic acid; C ₄ H ₆ O ₄ ; [110-15-6]	
Variables:	Prepared By:
T/K = 273–308	Valerii P. Sazonov

Experimental Data			
Solubility of butanedioic acid (2) in acetonitrile (1)			
t/°C	T/K (compiler)	mol/L	x ₂ (compiler)
0.0	273.2	0.018	0.26
15.0	288.2	0.022	0.33
25.0	298.2	0.035	0.53
35.0	308.2	0.062	0.96

*For these calculations the compiler assumed that the densities of the solutions were those of acetonitrile¹ at the specified temperatures.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used: 25 mL of (1) and an amount of (2) exceeding the solubility were placed in 50 mL volumetric flasks. The flasks were closed by ground glass stoppers and stored at the required temperature in a thermostat for 45 h, with intensive stirring every several hours. After this, 5 mL samples of the saturated solution were taken by pipette, diluted to 25 mL with water, and titrated against 0.1 N sodium hydroxide solutions by using phenolphthalein indicator.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over anhydrous K₂CO₃ and repeatedly distilled over P₂O₅.
 (2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

¹J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

10.16. + Octadecanoic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr and A. W. Ralston, <i>J. Org. Chem.</i> 9 , 329–37 (1944).
(2) Octadecanoic acid; C ₁₈ H ₃₆ O ₂ ; [57-11-4]	
Variables:	Prepared By:
T/K = 293–341	Valerii P. Sazonov

Experimental Data

The solubilities of octadecanoic acid (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of octadecanoic acid (2) in acetonitrile (1)				
t/°C	T/K (compiler)	g ₂ /100 g ₁	100 w ₂ (compiler)	x ₂ (compiler)
20.0	293.2	<0.1	<0.1	0.0001
30.0	303.2	0.3	0.3	0.0004
36.6*	309.8	—	0.6	0.0009
40.0	313.2	0.8	0.8	0.0012
46.7*	319.9	—	1.3	0.0019
50.0	323.2	2.0	2.0	0.0029
55.5*	328.7	—	4.1	0.0061
59.2*	332.4	—	8.0	0.012
60.0	333.2	10.3	9.3	0.015
62.6*	335.8	—	20.5	0.0359
63.0*	336.2	—	31.0	0.0609
63.2*	336.4	—	55.4	0.152
63.9*	337.1	—	72.4	0.275
65.3*	338.5	—	87.0	0.491
67.4*	340.6	—	96.0	0.776

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described elsewhere,¹ was used. No details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
 (2) Source not specified; purified according to Pool and Ralston;² freezing point = 69.32 °C.

Estimated Error:

Not specified.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).
²W. O. Pool and A. W. Ralston, *Ind. Eng. Chem.* **34**, 1104 (1942).

11.2. + Hexanedioic Acid

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Hexanedioic acid; C ₆ H ₁₀ O ₄ ; [124-04-9]	Original Measurements: Z. S. Smolyan, G. N. Matveeva, V. K. Fukin, K. N. Korotaevskii, A. P. Ignat'eva, A. N. Komilina, L. S. Zvereva, and A. S. Fomin, <i>Khim. Prom-st (Moscow)</i> 48 , 508-9 (1972).
Variables: T/K = 298	Prepared By: Valerii P. Sazonov

Experimental Data
The solubility of hexanedioic acid in acetonitrile at 25 °C (298 K, compiler) was reported to be $100 w_2 = 0.45$. The corresponding mole fraction x_2 calculated by the compiler is 0.0013.

Auxiliary Information	
Method/Apparatus/Procedure: No details were reported.	Source and Purity of Materials: (1) Source not specified; purity not specified. (2) Source not specified; purity not specified.
Estimated Error: Temperature: ± 1 K.	

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Hexanedioic acid; C ₆ H ₁₀ O ₄ ; [124-04-9]	Evaluator: Valerii P. Sazonov, Technical University, Samara, Russia, July, 2001.
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Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and hexanedioic acid (2) have been reported in two publications over a very limited range of temperatures. No data appear to have been reported for the solubility of (1) in (2). Smolyan *et al.*¹ determined solubility of hexanedioic acid in acetonitrile at 298 and 323 K. Smagowski² carried out measurements of the solubility of (2) in (1) between 273 and 308 K by the titration method.

At the one temperature (298 K) where comparison is possible, the two studies are in poor agreement. Accordingly, all the available data (see the relevant data sheets) must be regarded as doubtful.

References:

- ¹Z. S. Smolyan, G. N. Matveeva, V. K. Fukin, K. N. Korotaevskii, A. P. Ignat'eva, A. N. Komilina, L. S. Zvereva, and A. S. Fomin, *Khim. Prom-st (Moscow)* **48**, 508 (1972).
²H. Smagowski, *Zesz. Nauk. Wyzdz. Mat., Fiz. Chem., Univ. Gdanski, Chem.* **3**, 45 (1974).

11.3. + Heptanedioic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. 3, 45-53 (1974).
(2) Heptanedioic acid; C ₇ H ₁₂ O ₄ ; [111-16-0]	
Variables:	Prepared By:
T/K = 273-308	Valerii P. Sazonov

Experimental Data			
Solubility of heptanedioic acid (2) in acetonitrile (1)			
t/°C	T/K (compiler)	mol/L	100 w ₂ ^a (compiler) x ₂ (compiler)
0.0	273.2	0.015	0.30 0.0008
15.0	288.2	0.032	0.65 0.0017
25.0	298.2	0.055	1.1 0.0028
35.0	308.2	0.12	2.4 0.0063

^aFor these calculations the compiler assumed that the densities of the solutions were those of acetonitrile¹ at the specified temperatures.

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The titration method was used: 25 mL of (1) and an amount of (2) exceeding the solubility were placed in 50 mL volumetric flasks. The flasks were closed by ground glass stoppers and stored at the required temperature in a thermostat for 45 h, with intensive stirring every several hours. After this, 5 mL samples of the saturated solution were taken by pipette, diluted to 25 mL with water, and titrated against 0.1 N sodium hydroxide solutions by using phenolphthalein indicator.	(1) Source not specified; purity not specified; dried over anhydrous K ₂ CO ₃ and repeatedly distilled over P ₂ O ₅ . (2) Source not specified; purity not specified; purified by crystallization from ethyl acetate.
Estimated Error:	References:
Not reported.	¹ J. Timmermans, <i>Physico-Chemical Constants of Pure Organic Compounds</i> (Elsevier, New York, 1950).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. 3, 45-53 (1974).
(2) Hexanedioic acid; C ₆ H ₁₀ O ₄ ; [124-04-9]	
Variables:	Prepared By:
T/K = 273-308	Valerii P. Sazonov

Experimental Data			
Solubility of hexanedioic acid (2) in acetonitrile (1)			
t/°C	T/K (compiler)	mol/L	100 w ₂ ^a (compiler) x ₂ (compiler)
0.0	273.2	0.068	1.2 0.0034
15.0	288.2	0.089	1.6 0.0046
25.0	298.2	0.13	2.4 0.0069
35.0	308.2	0.18	3.3 0.0095

^aFor these calculations the compiler assumed that the densities of the solutions were those of acetonitrile¹ at the specified temperatures.

Auxiliary Information	
Method/Apparatus/Procedure:	Source and Purity of Materials:
The titration method was used: 25 mL of (1) and an amount of (2) exceeding the solubility were placed in 50 mL volumetric flasks. The flasks were closed by ground glass stoppers and stored at the required temperature in a thermostat for 45 h, with intensive stirring every several hours. After this, 5 mL samples of the saturated solution were taken by pipette, diluted to 25 mL with water, and titrated against 0.1 N sodium hydroxide solutions by using phenolphthalein indicator.	(1) Source not specified; purity not specified; dried over anhydrous K ₂ CO ₃ and repeatedly distilled over P ₂ O ₅ . (2) Source not specified; purity not specified; purified by crystallization from ethyl acetate.
Estimated Error:	References:
Not reported.	¹ J. Timmermans, <i>Physico-Chemical Constants of Pure Organic Compounds</i> (Elsevier, New York, 1950).

11.4. + Octanedioic Acid

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. 3, 45-53 (1974).	
(2) Octanedioic acid; C ₈ H ₁₆ O ₄ ; [505-48-6]			
Variables:		Prepared By:	
T/K = 273-308		Valerii P. Sazonov	

Experimental Data			
Solubility of octanedioic acid (2) in acetonitrile (1)			
t/°C	T/K (compiler)	mol/L	100 w ₂ ^a (compiler)
0.0	273.2	0.012	0.26
15.0	288.2	0.020	0.44
25.0	298.2	0.037	0.82
35.0	308.2	0.083	1.9

^aFor these calculations the compiler assumed that the densities of the solutions were those of acetonitrile¹ at the specified temperatures.

Auxiliary Information

Method/Apparatus/Procedure:
The titration method was used: 25 mL of (1) and an amount of (2) exceeding the solubility were placed in 50 mL volumetric flasks. The flasks were closed by ground glass stoppers and stored at the required temperature in a thermostat for 45 h, with intensive stirring every several hours. After this, 5 mL samples of the saturated solution were taken by pipette, diluted to 25 mL with water, and titrated against 0.07 0.1 N sodium hydroxide solutions by using phenolphthalein indicator.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over anhydrous K₂CO₃ and repeatedly distilled over P₂O₅.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

¹J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

11.5. + Nonanedioic Acid

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. 3, 45-53 (1974).	
(2) Nonanedioic acid; C ₉ H ₁₆ O ₄ ; [123-99-9]			
Variables:		Prepared By:	
T/K = 273-308		Valerii P. Sazonov	

Experimental Data			
Solubility of nonanedioic acid (2) in acetonitrile (1)			
t/°C	T/K (compiler)	mol/L	100 w ₂ ^a (compiler)
0.0	273.2	0.008	0.19
15.0	288.2	0.010	0.24
25.0	298.2	0.019	0.46
35.0	308.2	0.069	1.7

^aFor these calculations the compiler assumed that the densities of the solutions were those of acetonitrile¹ at the specified temperatures.

Auxiliary Information

Method/Apparatus/Procedure:
The titration method was used: 25 mL of (1) and an amount of (2) exceeding the solubility were placed in 50 mL volumetric flasks. The flasks were closed by ground glass stoppers and stored at the required temperature in a thermostat for 45 h, with intensive stirring every several hours. After this, 5 mL samples of the saturated solution were taken by pipette, diluted to 25 mL with water, and titrated against 0.1 N sodium hydroxide solutions by using phenolphthalein indicator.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over anhydrous K₂CO₃ and repeatedly distilled over P₂O₅.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

¹J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

11.7. + Dicarboxylic Acids, Monosodium Salts

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. 3, 45-53 (1974).
(2) Dicarboxylic acids monosodium salts; C ₂ HNaO ₄ -C ₁₁ H ₁₇ NaO ₄	
Variables:	Prepared By:
T/K = 298	Valerii P. Sazonov

Experimental Data

Solubility of monosodium salts of dicarboxylic acids (2) in acetonitrile (1) at 25.0 °C (298.2 K compiler)

Monosodium salt of dicarboxylic acid	mol/L	100 w ₂ ^a (compiler)	x ₂ (compiler)
Ethanedioate; C ₂ HNaO ₄ ; [1186-49-8]	0.009	0.13	0.0005
Propanedioate; C ₃ H ₃ NaO ₄ ; [2922-55-6]	0.008	0.13	0.0004
Butanedioate; C ₄ H ₂ NaO ₄ ; [2922-54-5]	0.006	0.10	0.0003
Pentanedioate; C ₅ H ₇ NaO ₄ ; [3343-88-2]	0.012	0.23	0.0006
Hexanedioate; C ₆ H ₉ NaO ₄ ; [18966-34-4]	0.007	0.15	0.0004
Heptanedioate; C ₇ H ₁₁ NaO ₄ ; [6142-21-8]	0.007	0.16	0.0004
Octanedioate; C ₈ H ₁₃ NaO ₄ ; [27796-70-9]	0.006	0.15	0.0003
Nonanedioate; C ₉ H ₁₅ NaO ₄ ; [17356-30-8]	0.005	0.13	0.0003
Decanedioate; C ₁₀ H ₁₇ NaO ₄ ; [19455-73-3]	0.004	0.11	0.0002

^aFor these calculations the compiler assumed that the densities of the solutions were those of acetonitrile¹ at the specified temperatures.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used: 25 mL of (1) and an amount of (2) exceeding the solubility were placed in 50 mL volumetric flasks. The flasks were closed by ground glass stoppers and stored at the required temperature in a thermostat for 45 h, with intensive stirring every several hours. After this, 2 mL samples of the saturated solution were taken by pipette, diluted to 25 mL with water—less acetic acid, and titrated by 0.05 N HClO₄ by using crystal violet indicator.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over anhydrous K₂CO₃ and repeatedly distilled over P₂O₅.
 (2) Obtained by mixing of methanol solutions of sodium hydroxide and the acid in stoichiometric amounts; purified by crystallization from a mixture of water and methanol; purity not less 99 mass %.

Estimated Error:

Not reported.

References:

¹J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

11.6. + Decanedioic Acid

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. 3, 45-53 (1974).
(2) Decanedioic acid; C ₁₀ H ₁₈ O ₄ ; [111-20-6]	
Variables:	Prepared By:
T/K = 273-308	Valerii P. Sazonov

Experimental Data

Solubility of decanedioic acid (2) in acetonitrile (1)

t/°C	T/K (compiler)	mol/L	100 w ₂ ^a (compiler)	x ₂ (compiler)
0.0	273.2	0.005	0.13	0.00026
15.0	288.2	0.009	0.23	0.00047
25.0	298.2	0.013	0.34	0.00069
35.0	308.2	0.027	0.71	0.00145

^aFor these calculations the compiler assumed that the densities of the solutions were those of acetonitrile¹ at the specified temperatures.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used: 25 mL of (1) and an amount of (2) exceeding the solubility were placed in 50 mL volumetric flasks. The flasks were closed by ground glass stoppers and stored at the required temperature in a thermostat for 45 h, with intensive stirring every several hours. After this, 5 mL samples of the saturated solution were taken by pipette, diluted to 25 mL with water, and titrated against 0.1 N sodium hydroxide solutions by using phenolphthalein indicator.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over anhydrous K₂CO₃ and repeatedly distilled over P₂O₅.
 (2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

¹J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

12.2. + Methyl Dodecanoate

Components:	Original Measurements:
(5) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, J. Org. Chem. 17, 327-37 (1952).
(6) Methyl dodecanoate; C ₁₃ H ₂₆ O ₂ ; [111-82-0]	
Variables:	Prepared By:
T/K=243-276	Valerii P. Sazonov

Experimental Data

The solubilities of methyl dodecanoate (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of methyl dodecanoate (2) in acetonitrile (1)				
<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
-30.0	243.2	0.4	0.4	0.0008
-28.6*	244.6	—	0.5	0.001
-23.5*	249.7	—	0.9	0.002
-20.0	253.2	2.1	2.1	0.004
-15.0*	258.2	—	3.3	0.007
-10.0	263.2	6.5	6.1	0.012
-8.9*	264.3	—	6.7	0.014
-4.4*	268.8	—	18.5	0.042
-3.1*	270.1	—	31.6	0.081
-1.4*	271.8	—	53.6	0.181
0.0	273.2	310	75.6	0.372
1.1*	274.3	—	82.3	0.471
2.8*	276.0	—	92.0	0.688

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

(1) Source not specified; best grade; freshly distilled.
(2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Stedman-packed column; freezing point=5.08 °C.

Estimated Error:

Not reported.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9, 68 (1944).

12. Acetonitrile+Esters
12.1. + Methyl Octanoate

Components:	Original Measurements:
(3) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, J. Org. Chem. 17, 327-37 (1952).
(4) Methyl octanoate; C ₉ H ₁₈ O ₂ ; [111-11-5]	
Variables:	Prepared By:
T/K=223-236	Valerii P. Sazonov

Experimental Data

The solubilities of methyl octanoate (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of methyl octanoate (2) in acetonitrile (1)				
<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler)	<i>x</i> ₂ (compiler)
-50.0	223.2	12.7	11.3	0.032
-46.8*	226.4	—	20.0	0.061
-43.6*	229.6	—	36.0	0.127
-41.5*	231.7	—	50.0	0.206
-40.0	233.2	177	63.9	0.315
-39.0*	234.2	—	67.1	0.346
-36.8*	236.4	—	84.0	0.577

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

(1) Source not specified; best grade; freshly distilled.
(2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Stedman-packed column; freezing point= -33.8 °C.

Estimated Error:

Not reported.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9, 68 (1944).

12.4. + Methyl Tetradecanoate

Components:	Original Measurements:
(9) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, J. Org. Chem. 17, 327-37 (1952).
(10) Methyl tetradecanoate; C ₁₅ H ₃₀ O ₂ ; [124-10-7]	
Variables:	Prepared By:
T/K = 263-288	Valerii P. Sizozov

Experimental Data

The solubilities of methyl tetradecanoate (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of methyl tetradecanoate (2) in acetonitrile (1)				
t/°C	T/K (compiler)	g ₂ /100 g ₁	100 w ₂ (compiler)	x ₂ (compiler)
-10.0	263.2	<0.1	<0.1	0.0002
0.0	273.2	0.9	0.9	0.002
2.5*	275.7	—	1.6	0.003
7.5*	280.7	—	5.0	0.009
9.9*	283.1	—	10.0	0.019
10.0	283.2	12.2	10.9	0.020
11.3*	284.5	—	17.1	0.034
11.5*	284.7	—	27.1	0.059
11.9*	285.1	—	43.5	0.115
12.5*	285.7	—	58.7	0.194
13.1*	286.3	—	77.5	0.368
15.0*	288.2	—	91.2	0.637

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating. The solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

(1) Source not specified; best grade; freshly distilled.
 (2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Stedman-packed column; freezing point= 18.39 °C.

Estimated Error:

Not reported.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9, 68 (1944).

12.3. + Methyl Tridecanoate

Components:	Original Measurements:
(7) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, J. Org. Chem. 17, 327-37 (1952).
(8) Methyl tridecanoate; C ₁₄ H ₂₈ O ₂ ; [1731-88-0]	
Variables:	Prepared By:
T/K = 243-276	Valerii P. Sizozov

Experimental Data

The solubilities of methyl tridecanoate (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of methyl tridecanoate (2) in acetonitrile (1)				
t/°C	T/K (compiler)	g ₂ /100 g ₁	100 w ₂ (compiler)	x ₂ (compiler)
-30.0	243.2	<0.1	<0.1	0.0002
-22.8*	250.4	—	0.8	0.001
-21.0*	252.2	—	1.3	0.002
-20.4*	252.8	—	1.5	0.003
-20.0	253.2	1.6	1.6	0.003
-12.8*	260.4	—	3.6	0.007
-10.0	263.2	5.8	5.5	0.010
-6.1*	267.1	—	8.4	0.016
-1.4*	271.8	—	25.1	0.057
0.0	273.2	86.0	46.2	0.134
0.3*	273.5	—	48.9	0.147
1.8*	275.0	—	64.8	0.249
3.1*	276.3	—	84.6	0.497

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating. The solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

(1) Source not specified; best grade; freshly distilled.
 (2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Stedman-packed column; freezing point= 6.52 °C.

Estimated Error:

Not reported.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9, 68 (1944).

12.5. + Esters C₁₆

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Esters; C ₁₆ H ₃₂ O ₂	Original Measurements: H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 9 , 134–44 (1965).
Variables: T/K = 290–307	Prepared By: Valerii P. Sazonov
Experimental Data	
Upper critical solution temperatures of the binary systems acetonitrile (1) + ester (2)	
Ester	t/°C
Methyl pentadecanoate; C ₁₅ H ₃₀ O ₂ ; [7132-64-1]	17.0
Ethyl tetradecanoate; C ₁₄ H ₂₈ O ₂ ; [124-06-1]	22.5
Tridecyl propanoate; C ₁₆ H ₃₂ O ₂ ; [6271-77-0]	23.0
Propyl tridecanoate; C ₁₆ H ₃₂ O ₂ ; [88591-28-0]	27.5
Dodecyl butanoate; C ₁₆ H ₃₂ O ₂ ; [3724-61-6]	28.0
Butyl dodecanoate; C ₁₆ H ₃₂ O ₂ ; [106-18-3]	30.5
Decyl hexanoate; C ₁₆ H ₃₂ O ₂ ; [152363-43-6]	31.5
Octyl octanoate; C ₁₆ H ₃₂ O ₂ ; [2306-88-9]	33.0
Hexyl decanoate; C ₁₆ H ₃₂ O ₂ ; [10448-26-7]	33.5
T/K (computer)	
	290.2
	295.7
	296.2
	300.7
	301.2
	303.7
	304.7
	306.2
	306.7

Auxiliary Information

Method/Apparatus/Procedure: The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described in Schmid <i>et al.</i> ¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.	Source and Purity of Materials: (1) Baker Chemical Co.; reagent No. 9011; n(20 °C,D) = 1.3445; d(20 °C,4 °C) = 0.780. (2) Methyl, ethyl and butyl esters purchased from Applied Science Laboratories; propyl and hexyl esters, propanoate and butyrate prepared by direct esterification; other esters synthesized by transesterification; purified.
Estimated Error: Temperature: ±0.5 K.	References: ¹ H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372 (1965).

12.6. + Methyl Hexadecanoate

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Methyl hexadecanoate; C ₁₇ H ₃₄ O ₂ ; [112-39-0]	Evaluator: Valerii P. Sazonov, Technical University, Samara, Russia, August, 2001.
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Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and methyl hexadecanoate (2) have been reported in three publications. Sedgwick *et al.*¹ studied the phase equilibrium of the liquid–liquid–solid system and the mutual solubility of (1) and (2) between 273 and 304 K by the synthetic method. Rusling *et al.*² determined the mutual solubility of acetonitrile and methyl hexadecanoate at 298 K by the titration method. Schmid *et al.*³ measured the upper critical solution temperature for binary solutions of acetonitrile and methyl esters of fatty acids.

The upper critical solution temperature has been reported as 303.2 K³ and 304.2 K.¹ These data are in reasonable agreement and thus their average value: UCST = 303.7 ± 0.5 K is recommended. The corresponding critical solution composition has been calculated by evaluator as $x_{c1} = 0.88$ from the data of Sedgwick *et al.*¹

Monotectic equilibrium has been reported to occur at 296.5 K.¹

All experimental values reported in the work¹ have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.2938, \quad a_2 = 0.8177, \quad b_1 = -12.0761, \quad b_2 = 7.2283$$

(mean standard error of estimate was 0.0063).

For this approximation x_{c1} and UCST values from Sedgwick *et al.*¹ have been used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship together with experimental data^{1,2} are also presented in Fig. 18.

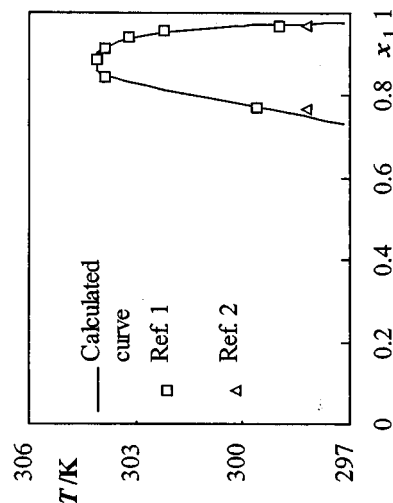


FIG. 18. Mutual solubility of acetonitrile and methyl hexadecanoate.

Calculated mutual solubility of acetonitrile (1) and methyl hexadecanoate (2)

T/K	Ester-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
297.2	0.733	29.4	0.975	85.5
299.2	0.765	33.1	0.971	83.6
300.2	0.781	35.1	0.967	81.6
301.2	0.797	37.3	0.961	78.9
302.2	0.814	39.9	0.952	75.1
303.2	0.833	43.1	0.937	69.3
303.7	0.845	45.3	0.924	64.9
303.9	0.851	46.4	0.916	62.3
304.0	0.854	47.0	0.911	60.8

References:

- ¹R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, *J. Org. Chem.* **17**, 327 (1952).
²J. F. Rusling, R. J. Bertsch, R. A. Barford, and H. L. Rothbart, *J. Chem. Eng. Data* **14**, 169 (1969).
³H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).

Components:

- (1) Acetonitrile; C₂H₃N; [75-05-8]
 (2) Methyl hexadecanoate; C₁₇H₃₅O₂; [112-39-0]

Original Measurements:

- R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, *J. Org. Chem.* **17**, 327–37 (1952).

Variables:

T/K = 273–304

Prepared By:

Valerii P. Sazonov

Experimental Data

The solubilities of acetonitrile (1) and methyl hexadecanoate (2) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical form and in a table.

Mutual solubility of acetonitrile (1) and methyl hexadecanoate (2)

t/°C	T/K (compiler)	$g_2/100g_1$	x_1 (compiler)		100 w_1	x_1 (compiler)		100 w_1
			Ester-rich phase	Acetonitrile-rich phase		Ester-rich phase	Acetonitrile-rich phase	
0.0	273.2	<0.1	—	—	>99.9 ^a	—	>99.9 ^a	0.999
10.0	283.2	0.9	—	—	99.1 ^a	—	99.1 ^a	0.998
10.2 ^c	283.4	—	—	—	99.0 ^a	—	99.0 ^a	0.998
15.0 ^c	288.2	—	—	—	97.6 ^a	—	97.6 ^a	0.996
19.9 ^c	293.1	—	—	—	94.5 ^a	—	94.5 ^a	0.991
20.0	293.2	7.1	—	—	93.4 ^a	—	93.4 ^a	0.989
22.1 ^c	295.3	—	—	—	90.0 ^a	—	90.0 ^a	0.983
23.5 ^c	296.7	—	—	29.8 ^b	—	0.737	—	—
24.2 ^c	297.4	—	—	17.3 ^a	—	0.580	—	—
25.3 ^c	298.5	—	—	8.4 ^a	—	0.377	—	—
25.8 ^c	299.0	—	—	—	—	—	—	—
27.4 ^c	299.6	—	—	34.0 ^b	—	0.772	—	0.970
29.0 ^c	302.2	—	—	—	—	—	—	—
30.0	303.2	42.5	—	—	76.7 ^b	—	76.7 ^b	0.956
30.7 ^c	303.9	—	—	45.2 ^b	70.2 ^b	—	70.2 ^b	0.940
					62.0 ^b	0.845	62.0 ^b	0.915

^aSolid–liquid equilibrium.

^bLiquid–liquid equilibrium.

^cThese data were extracted by the compiler from the published graphs.

Monotectic equilibrium occurs at 23.3 °C (296.5 K, compiler).

The upper critical solution temperature was reported to be 31.0 °C (304.2 K, compiler).

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

- (1) Source not specified; best grade; freshly distilled.
 (2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Steadman-packed column; freezing point=28.90 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).

12.7. + Methyl Esters Fatty Acids C₁₇-C₂₃

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Methyl esters fatty acids; C ₁₇ H ₃₃ O ₂ -C ₂₃ H ₄₆ O ₂	Original Measurements: H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372-81 (1965).
Variables: T/K = 303-361	Prepared By: Valerii P. Sazonov

Experimental Data		
Upper critical solution temperatures of the binary systems acetonitrile (1) + methyl ester fatty acid (2)		
<i>t</i> /°C	<i>T</i> /K (complier)	Methyl ester
		Methyl hexadecanoate; C ₁₇ H ₃₃ O ₂ ; [112-39-0]
	303.2	
		Methyl octadecanoate; C ₁₉ H ₃₉ O ₂ ; [112-61-8]
	324.2	
		Methyl eicosanoate; C ₂₁ H ₄₃ O ₂ ; [1120-28-1]
	344.2	
		Methyl docosanoate; C ₂₃ H ₄₇ O ₂ ; [929-77-1]
	361.2	

Auxiliary Information	
Method/Apparatus/Procedure: The synthetic method was used. A Reichert microscope, type RCH, with a heating stage was used. A 26×38 mm slide was adapted to hold capillaries on the stage. Two glass strips were glued, using water glass, to the slide, leaving a 0.5 mm channel. The slide was then placed in the adjustable device of the heating stage. (1) and (2) were put into capillary tubing (0.2-0.3 mm diameters) by dipping consecutively into both liquids. The height of the liquid was 7-10 mm. Room temperature solids were melted on a glass slide over a microburner. The capillary was sealed at both ends to a length of 30-35 mm, then inserted in to the channel on the slide and heated on the stage. The UCST was determined by following the appearance and disappearance of the meniscus.	Source and Purity of Materials: (1) Baker Chemical Co.; reagent, No. 9011; <i>n</i> (20 °C,D) = 1.3445, <i>d</i> (20 °C,4 °C) = 0.780. (2) Not specified.
Estimated Error: Temperature: ±0.5 K.	

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Methyl hexadecanoate; C ₁₇ H ₃₃ O ₂ ; [112-39-0]	Original Measurements: J. F. Rusling, R. J. Bertsch, R. A. Barford, and H. L. Rothbart, <i>J. Chem. Eng. Data</i> 14 , 169-73 (1969).
Variables: T/K = 298	Prepared By: Valerii P. Sazonov

Experimental Data				
Mutual solubility of acetonitrile (1) and methyl hexadecanoate (2)				
<i>t</i> /°C	<i>T</i> /K (complier)	100 <i>w</i> ₁	100 <i>w</i> ₂	<i>x</i> ₁ (complier)
25.0	298.2	33.1	0.765	81.9
				0.968

Auxiliary Information	
Method/Apparatus/Procedure: The titration method was used. No experimental details were reported.	Source and Purity of Materials: (1) Source not specified; analytical grade; twice distilled; $\rho(25\text{ }^\circ\text{C}) = 777\text{ g}\cdot\text{L}^{-1}$. (2) Obtained from methyl esters oils; purity 99 mass % by GLC; $\rho(25\text{ }^\circ\text{C}) = 847\text{ g}\cdot\text{L}^{-1}$.
Estimated Error: Temperature: ±0.1 K.	

12.9. + Methyl cis-9-Octadecenoate

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		J. F. Rusling, R. J. Bertsch, R. A. Barford, and H. L. Rothbart, J. Chem. Eng. Data 14 , 169-73 (1969).	
(2) Methyl cis-9-octadecenoate; C ₁₉ H ₃₆ O ₂ ; [112-62-9]			
Variables:		Prepared By:	
T/K = 298		Valerii P. Sazonov	

Experimental Data				
Mutual solubility of acetonitrile (1) and methyl cis-9-octadecenoate (2)				
<i>t</i> /°C	T/K (compiler)	100 w ₁	<i>x</i> ₁ (compiler)	<i>x</i> ₁ (compiler)
25.0	298.2	44.2	0.851	71.4
			Ester-rich phase	Acetonitrile-rich phase

Auxiliary Information**Method/Apparatus/Procedure:**

The titration method was used. No experimental details were reported.

Source and Purity of Materials:

- (1) Source not specified; analytical grade; twice distilled; $\rho(25\text{ }^\circ\text{C}) = 777\text{ g}\cdot\text{L}^{-1}$.
 (2) Obtained from methyl esters oils; purity 99 mass % by GLC, $\rho(25\text{ }^\circ\text{C}) = 859\text{ g}\cdot\text{L}^{-1}$.

Estimated Error:

Temperature: $\pm 0.1\text{ K}$.

12.8. + Hexadecyl Esters C₁₈-C₃₄

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. 42 , 372-81 (1965).	
(2) Hexadecyl esters; C ₁₈ H ₃₆ O ₂ -C ₃₄ H ₆₈ O ₂			
Variables:		Prepared By:	
T/K = 321-426		Valerii P. Sazonov	

Experimental Data		
Upper critical solution temperatures of the systems acetonitrile (1) + hexadecyl ester (2)		
Hexadecyl ester	<i>t</i> /°C	T/K (compiler)
Hexadecyl ethanoate; C ₁₈ H ₃₆ O ₂ ; [629-70-9]	36.0	309.2
Hexadecyl butanoate; C ₂₀ H ₄₀ O ₂ ; [6221-99-4]	68.0	331.2
Hexadecyl hexanoate; C ₂₂ H ₄₄ O ₂ ; [14331-11-4]	89.0	362.2
Hexadecyl octanoate; C ₂₄ H ₄₈ O ₂ ; [29710-31-4]	104.0	377.2
Hexadecyl decanoate; C ₂₆ H ₅₂ O ₂ ; [29710-34-7]	118.0	391.2
Hexadecyl dodecanoate; C ₂₈ H ₅₆ O ₂ ; [20834-06-4]	130.0	403.2
Hexadecyl tetradecanoate; C ₃₀ H ₆₀ O ₂ ; [2599-01-1]	140.5	413.7
Hexadecyl hexadecanoate; C ₃₂ H ₆₄ O ₂ ; [540-10-3]	150.5	423.7
Hexadecyl octadecanoate; C ₃₄ H ₆₈ O ₂ ; [1190-63-2]	159.5	432.7

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. A Reichert microscope, type RCH, with a heating stage was used. A 26×38 mm slide was adapted to hold capillaries on the stage. Two glass strips were glued, using water glass, to the slide, leaving a 0.5 mm channel. The slide was then placed in the adjustable device of the heating stage. (1) and (2) were put into capillary tubing (0.2-0.3 mm diameters) by dipping consecutively into both liquids. The height of the liquid was 7-10 mm. Room temperature solids were melted on a glass slide over a microburner. The capillary was sealed at both ends to a length of 30-35 mm, then inserted into the channel on the slide and heated on the stage. The UCST was determined by following the appearance and disappearance of the meniscus.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent, No. 9011; $n(20\text{ }^\circ\text{C,D}) = 1.3445$, $d(20\text{ }^\circ\text{C,4 }^\circ\text{C}) = 0.780$.
 (2) Not specified.

Estimated Error:

Temperature: $\pm 0.5\text{ K}$.

12.10+ Methyl Octadecanoate

Components:

- (1) Acetonitrile; C_2H_3N ; [75-05-8]
 (2) Methyl octadecanoate; $C_{19}H_{38}O_2$; [112-61-8]

Evaluator:

Valeri P. Sazonov, Technical University, Samara, Russia, August, 2001.

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and methyl octadecanoate (2) have been reported in two publications. Sedgwick *et al.*¹ studied the phase equilibrium of the liquid-liquid-solid system and the mutual solubility of (1) and (2) between 283 and 326 K by the synthetic method. Schmid *et al.*² measured the upper critical solution temperature for binary solutions of acetonitrile and methyl esters of fatty acids.

The upper critical solution temperature has been reported as 324.2 K² and 326.3 K.¹ These data are in reasonable agreement and thus their average value: UCST = 325.3 ± 1 K is recommended. The corresponding critical solution composition has been calculated by the evaluator as $x_{c1} = 0.90$ from the data.¹ Monoteic equilibrium has been reported to occur at 305.5 K.¹

All experimental values reported¹ have been approximated by an equation based on the scaling law (described in the Introduction to this volume) for which the following parameters have been derived:

$$a_1 = 0.2912, \quad a_2 = 0.4908, \quad b_1 = -0.1608, \quad b_2 = -0.8262$$

(mean standard error of estimate was 0.0036).

For this approximation x_{c1} and UCST values from Sedgwick *et al.*¹ have been used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship together with experimental points^{1,2} are also presented in Fig. 19.

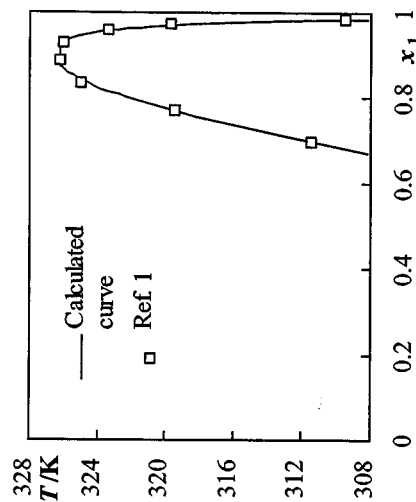


FIG. 19. Mutual solubility of acetonitrile and methyl octadecanoate.

Calculated mutual solubility of acetonitrile (1) and methyl octadecanoate (2)

T/K	Ester-rich phase		Acetonitrile-rich phase	
	x_1	100 w_1	x_1	100 w_1
308.2	0.671	21.9	0.985	90.0
313.2	0.711	25.3	0.982	88.2
318.2	0.756	29.9	0.974	83.7
323.2	0.812	37.3	0.959	76.3
324.2	0.827	39.7	0.953	73.6
325.2	0.845	42.8	0.943	69.5
325.7	0.857	45.2	0.936	66.8
325.9	0.864	46.6	0.932	65.3
326.0	0.868	47.5	0.929	64.3
326.1	0.872	48.4	0.925	62.9

References:

- ¹R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, *J. Org. Chem.* **17**, 327 (1952).
²H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).

12.11. + Ethyl Octadecanoate

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, <i>J. Org. Chem.</i> 17 , 327-37 (1952).
(2) Methyl octadecanoate; C ₁₉ H ₃₈ O ₂ ; [112-61-8]	
Variables:	Prepared By:
T/K = 283-326	Valerii P. Sazonov

Experimental Data

The solubilities of acetonitrile (1) and methyl octadecanoate (2) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical form and in a table.

t/°C	T/K (compiler)	Mutual solubility of acetonitrile (1) and methyl octadecanoate (2)		100 w ₁	x ₁ (compiler)	100 w ₁	x ₁ (compiler)
		g ₂ /100 g ₁	Ester-rich phase				
10.0	283.2	<0.1	—	>99.9 ^a	—	—	0.999
20.0	293.2	1.1	—	98.9 ^a	—	—	0.999
22.9 ^c	296.1	—	—	98.8 ^a	—	—	0.998
26.7 ^c	299.9	—	—	97.3 ^a	—	—	0.996
29.4 ^c	302.6	—	—	95.5 ^a	—	—	0.994
30.0	303.2	5.9	—	94.4 ^a	—	—	0.992
31.7 ^c	304.9	—	—	92.3 ^a	—	—	0.989
32.5 ^c	305.7	—	—	—	0.632	—	—
33.2 ^c	306.4	—	—	—	0.505	—	—
34.6 ^c	307.8	—	—	—	0.350	—	—
36.3 ^c	309.5	—	—	89.5 ^b	—	—	0.984
38.3 ^c	311.5	—	—	—	0.697	—	—
46.3 ^c	319.5	—	—	31.5 ^b	0.770	—	—
46.5 ^c	319.7	—	—	—	—	82.7 ^b	0.972
50.2 ^c	323.4	—	—	—	—	75.6 ^b	0.958
51.8 ^c	325.0	—	—	41.2 ^b	0.836	—	—
52.8 ^c	326.0	—	—	—	—	63.9 ^b	0.928
53.0 ^c	326.2	—	—	52.0 ^b	0.887	—	—

^aSolid-liquid equilibrium.

^bLiquid-liquid equilibrium.

^cThese data were extracted by the compiler from the published graphs.

Monotectic equilibrium occurs at 32.3 °C (305.5 K, compiler).

The upper critical solution temperature was reported to be 53.1 °C (326.3 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

(1) Source not specified; best grade; freshly distilled.
(2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Stedman-packed column; freezing point = 37.85 °C.

Estimated Error:

Not specified.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).

Components:

(1) Acetonitrile; C₂H₃N; [75-05-8]
(2) Ethyl octadecanoate; C₂₀H₄₀O₂; [111-61-5]

Evaluator:

Valerii P. Sazonov, Technical University, Samara, Russia, July, 2001.

Critical Evaluation

Solubilities in the system comprising acetonitrile (1) and ethyl octadecanoate (2) have been reported in two publications over a very limited range of temperatures. No data appear to have been reported for the solubility of (1) in (2). Sedgwick *et al.*¹ determined solubility of ethyl octadecanoate (2) in acetonitrile (1) between 283 and 303 K by the synthetic method. Schmid *et al.*² measured the upper critical solution temperature for binary solutions of acetonitrile and esters of fatty acids by the synthetic method. The corresponding critical solution composition has not been reported.

The upper critical solution temperature has been reported as 338.2 K² and 338.7 K.¹ These data are in reasonable agreement and thus their average value: UCST = 338.5 ± 0.3 K is recommended. Accordingly, all the available data (see the relevant data sheets) must be regarded as tentative.

References:

¹R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, *J. Org. Chem.* **17**, 327 (1952).

²H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *Microchem. J.* **9**, 134 (1965).

12.12. + Esters: C₂₀

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, <i>J. Org. Chem.</i> 17 , 327-37 (1952).
(2) Ethyl octadecanoate; C ₂₀ H ₄₀ O ₂ ; [111-61-5]	
Variables:	Prepared By:
T/K = 283-303	Valerii P. Sazonov

Experimental Data			
Solubility of ethyl octadecanoate (2) in acetonitrile (1)			
t/°C	T/K (compiler)	g ₂ /100g ₁	x ₂ (compiler)
10.0	283.2	0.2	0.0003
20.0	293.2	1.5	0.002
30.0	303.2	7.2	0.009

Miscible above 65.5 °C (338.7 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

(1) Source not specified; best grade; freshly distilled.
 (2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Steidman-packed column; freezing point = 31.36 °C.

Estimated Error:

Not reported.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 9 , 134-44 (1965).
(2) Esters; C ₂₀ H ₄₀ O ₂	
Variables:	Prepared By:
T/K = 328-348	V. P. Sazonov

Experimental Data			
Upper critical solution temperatures of the binary systems acetonitrile (1) + ester (2)			
Ester	t/°C	T/K (compiler)	
Nonadecyl methanoate; C ₂₀ H ₄₀ O ₂ ; [66455-49-0]	55.0	328.2	
Octadecyl ethanoate; C ₂₀ H ₄₀ O ₂ ; [822-23-1]	56.5	329.7	
Methyl nonadecanoate; C ₂₀ H ₄₀ O ₂ ; [1731-94-8]	61.0	334.2	
Heptadecyl propanoate; C ₂₀ H ₄₀ O ₂ ; [66455-48-9]	64.0	337.2	
Ethyl octadecanoate; C ₂₀ H ₄₀ O ₂ ; [111-61-5]	65.0	338.2	
Hexadecyl butanoate; C ₂₀ H ₄₀ O ₂ ; [6221-99-4]	68.0	341.2	
Propyl heptadecanoate; C ₂₀ H ₄₀ O ₂ ; [26718-84-3]	68.5	341.7	
Butyl hexadecanoate; C ₂₀ H ₄₀ O ₂ ; [111-06-8]	71.0	344.2	
Tetradecyl hexanoate; C ₂₀ H ₄₀ O ₂ ; [71801-23-5]	71.5	344.7	
Dodecyl octanoate; C ₂₀ H ₄₀ O ₂ ; [20292-09-5]	73.5	346.7	
Hexyl tetradecanoate; C ₂₀ H ₄₀ O ₂ ; [42231-99-2]	74.0	347.2	
Octyl dodecanoate; C ₂₀ H ₄₀ O ₂ ; [5303-24-2]	75.0	348.2	
Decyl decanoate; C ₂₀ H ₄₀ O ₂ ; [654-86-0]	75.0	348.2	

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere.¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Baker Chemical Co.; reagent, No. 9011; n(20 °C,D) = 1.3445, d(20 °C,4 °C) = 0.780.
 (2) Methyl, ethyl, and butyl esters purchased from Applied Science Laboratories; propyl and hexyl esters, formate, acetate, propanoate, and butyrate prepared by direct esterification; other esters synthesized by transesterification; purified.

Estimated Error:

Temperature: ±0.5 K.

References:

¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).

12.13. + Propyl Octadecanoate

Components:				
(3) Acetonitrile; C ₂ H ₃ N; [75-05-8]				
(4) Propyl octadecanoate; C ₂₁ H ₄₂ O ₂ ; [3634-92-2]				
Variables:				
T/K = 273–303				
Original Measurements:				
R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, J. Org. Chem. 17 , 327–37 (1952).				
Prepared By:				
Valerii P. Sazonov				
Experimental Data				
Solubility of propyl octadecanoate (2) in acetonitrile (1)				
t/°C	T/K (compiler)	g ₂ /100g ₁	100 w ₂ (compiler)	x ₂ (compiler)
0.0	273.2	0.1	0.1	0.0001
10.0	283.2	0.7	0.7	0.001
20.0	293.2	2.3*	2.2	0.003
30.0	303.2	3.4	3.3	0.004

*Recorded as 23.0 in original. Value corrected by the compiler.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

- (1) Source not specified; best grade; freshly distilled.
 (2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Stedman-packed column; freezing point = 28.87 °C.

Estimated Error:

Not reported.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).

12.14. + Butyl Octadecanoate

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	
(2) Butyl octadecanoate; C ₂₂ H ₄₄ O ₂ ; [123-95-5]	
Evaluator:	
Valerii P. Sazonov, Technical University, Samara, Russia, July, 2001.	
Critical Evaluation	
Solubilities in the system comprising acetonitrile (1) and butyl octadecanoate (2) have been reported in two publications over a very limited range of temperatures. No data appear to have been reported for the solubility of (1) in (2). Sedgwick <i>et al.</i> ¹ determined solubility of butyl octadecanoate (2) in acetonitrile (1) between 273 and 303 K by the synthetic method. Schmid <i>et al.</i> ² measured the upper critical solution temperature for binary solutions of acetonitrile and esters of fatty acids by the synthetic method. The corresponding critical solution composition has not been reported.	
The upper critical solution temperature has been reported as 360.2 K. ² Accordingly, all the available data (see the relevant data sheets) must be regarded as tentative.	
References:	
¹ R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, J. Org. Chem. 17 , 327 (1952).	
² H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. 9 , 134 (1965).	

12.15. + Esters: C₂₂

Components:	Original Measurements:
(5) Acetonitrile; C ₂ H ₃ N; [75-05-8]	R. S. Sedgwick, C. W. Hoerr, and H. J. Harwood, <i>J. Org. Chem.</i> 17 , 327-37 (1952).
(6) Butyl octadecanoate; C ₂₂ H ₄₄ O ₂ ; [123-95-5]	
Variables:	Prepared By:
T/K = 273-303	Valerii P. Sazonov

Experimental Data		
Solubility of butyl octadecanoate (2) in acetonitrile (1)		
t/°C	T/K (complier)	g ₂ /100g ₁
0.0	273.2	0.3
10.0	283.2	0.9
20.0	293.2	2.5
30.0	303.2	3.8
		x ₂ (complier)
		0.0004
		0.0011
		0.0031
		0.0047

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperature at which crystals appear upon cooling and dissolve upon heating solutions containing known concentrations of solutes. The procedure and equipment were described elsewhere.¹

Source and Purity of Materials:

(1) Source not specified; best grade; freshly distilled.
 (2) Prepared by direct esterification of highly purified fatty acid with the appropriate alcohol; fractionated under a vacuum in a Stedman-packed column; freezing point = 26.61 °C.

Estimated Error:

Not reported.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, *J. Org. Chem.* **9**, 68 (1944).

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Micromochem. J.</i> 9 , 134-44 (1965).
(2) Esters; C ₂₂ H ₄₄ O ₂	
Variables:	Prepared By:
T/K = 344-365	Valerii P. Sazonov

Experimental Data		
Upper critical solution temperatures of the binary systems acetonitrile (1) + ester (2)		
Ester	t/°C	T/K (complier)
Henicosyl methanoate; C ₂₂ H ₄₄ O ₂	71.0	344.2
Eicosyl ethanoate; C ₂₂ H ₄₄ O ₂ ; [822-24-2]	74.0	347.2
Methyl henicosanoate; C ₂₂ H ₄₄ O ₂ ; [6064-90-0]	79.0	352.2
Ethyl eicosanoate; C ₂₂ H ₄₄ O ₂ ; [18281-05-5]	82.0	355.2
Nonadecyl propanoate; C ₂₂ H ₄₄ O ₂ ; [66326-06-5]	82.0	355.2
Propyl nonadecanoate; C ₂₂ H ₄₄ O ₂ ; [27593-68-6]	85.0	358.2
Octadecyl butanoate; C ₂₂ H ₄₄ O ₂ ; [13373-83-6]	86.0	359.2
Butyl octadecanoate; C ₂₂ H ₄₄ O ₂ ; [123-95-5]	87.0	360.2
Hexadecyl hexanoate; C ₂₂ H ₄₄ O ₂ ; [14331-11-4]	89.0	362.2
Hexyl hexadecanoate; C ₂₂ H ₄₄ O ₂ ; [42232-25-7]	89.5	362.7
Tetradecyl octanoate; C ₂₂ H ₄₄ O ₂ ; [16456-36-3]	90.5	363.7
Octyl tetradecanoate; C ₂₂ H ₄₄ O ₂ ; [16260-26-7]	91.0	364.2
Dodecyl decanoate; C ₂₂ H ₄₄ O ₂ ; [42231-50-5]	91.0	364.2
Decyl dodecanoate; C ₂₂ H ₄₄ O ₂ ; [35528-28-6]	91.5	364.7

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere.¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Baker Chemical Co.; reagent, No. 9011; n(20 °C,D) = 1.3445, d(20 °C,4 °C) = 0.780.
 (2) Methyl, ethyl, and butyl esters purchased from Applied Science Laboratories; propyl and hexyl esters, formate, acetate, propanoate, and butyrate prepared by direct esterification; other esters synthesized by transesterification; purified.

Estimated Error:

Temperature: ±0.5 K.

References:

¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).

12.17. + Cholesteryl Esters: C₃₉ and C₄₁

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372-81 (1965).
(2) Cholesteryl esters; C ₃₉ H ₆₈ O ₂ and C ₄₁ H ₇₂ O ₂	
Variables:	Prepared By:
T/K = 474 and 485	Valerii P. Sazonov

Experimental Data
Upper critical solution temperatures of the binary systems acetonitrile (1) + cholesteryl ester (2)

Cholesteryl ester	t/°C	T/K (compiler)
Cholest-5-en-3-yl dodecanoate; C ₃₉ H ₆₈ O ₂ ; [1908-11-8]	201.0	474.2
Cholest-5-en-3-yl tetradecanoate; C ₄₁ H ₇₂ O ₂ ; [1989-52-2]	212.0	485.2

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. A Reichert microscope, type RCH, with a heating stage was used. A 26×38 mm slide was adapted to hold capillaries on the stage. Two glass strips were glued, using water glass, to the slide, leaving a 0.5 mm channel. The slide was then placed in the adjustable device of the heating stage. (1) and (2) were put into capillary tubing (0.2–0.3 mm diameters) by dipping consecutively into both liquids. The height of the liquid was 7–10 mm. Room

Source and Purity of Materials:

(1) Baker Chemical Co.; reagent, No. 9011; n(20 °C, D) = 1.3445, d(20 °C, 4 °C) = 0.780.
(2) Not specified.

Estimated Error:
Temperature: ±0.5 K.

temperature solids were melted on a glass slide over a microburner. The capillary was sealed at both ends to a length of 30–35 mm, then inserted into the channel on the slide and heated on the stage. The UCST was determined by following the appearance and disappearance of the meniscus.

12.16. + Esters: C₂₄–C₃₂

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 9 , 134–44 (1965).
(2) Esters; C ₂₄ H ₄₈ O ₂ , C ₂₆ H ₅₂ O ₂ , C ₂₈ H ₅₆ O ₂ , C ₃₀ H ₆₀ O ₂ , and C ₃₂ H ₆₄ O ₂	
Variables:	Prepared By:
T/K = 377–424	Valerii P. Sazonov

Experimental Data
Upper critical solution temperatures of the binary systems acetonitrile (1) + ester (2)

Ester	t/°C	T/K (compiler)
Hexadecyl octanoate; C ₂₄ H ₄₈ O ₂ ; [29710-31-4]	104.0	377.2
Octyl hexadecanoate; C ₂₆ H ₅₂ O ₂ ; [16958-85-3]	104.5	377.7
Decyl hexadecanoate; C ₂₈ H ₅₆ O ₂ ; [42232-27-9]	118.0	391.2
Hexadecyl decanoate; C ₂₆ H ₅₂ O ₂ ; [29710-34-7]	118.0	391.2
Dodecyl hexadecanoate; C ₂₈ H ₅₆ O ₂ ; [42232-29-1]	130.0	403.2
Hexadecyl dodecanoate; C ₂₈ H ₅₆ O ₂ ; [20834-06-4]	130.0	403.2
Tetradecyl hexadecanoate; C ₃₀ H ₆₀ O ₂ ; [4536-26-9]	140.5	413.7
Hexadecyl tetradecanoate; C ₃₀ H ₆₀ O ₂ ; [2599-01-1]	140.5	413.7
Hexadecyl hexadecanoate; C ₃₂ H ₆₄ O ₂ ; [540-10-3]	150.5	423.7

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere.¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Baker Chemical Co.; reagent, No. 9011; n(20 °C, D) = 1.3445, d(20 °C, 4 °C) = 0.780.

(2) Synthesized by transesterification of methyl esters and acetates using sodium methanolate as catalyst; purified by gas-liquid partition and thin-layer adsorption chromatography.

Estimated Error:
Temperature: ±0.5 K.

References:

¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).

13. Acetonitrile + Amines

13.1. + Decanamine

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(2) Decanamine; C ₁₀ H ₂₁ N; [2016-57-1]
Original Measurements:	
A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. 9, 102-112 (1944).	
Prepared By:	
Valerii P. Sazonov and Nikolai V. Sazonov	
Variables:	
T/K = 253-286	

Experimental Data

The solubilities of decanamine (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of decanamine (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
-20.0	253.2	2.8	2.7	0.007
-15.0*	258.2	—	3.8	0.010
-5.5*	267.7	—	7.5	0.021
0.0	273.2	12.7	11.3	0.032
1.4*	274.6	—	11.4	0.033
6.4*	279.6	—	23.4	0.074
8.0*	281.2	—	35.8	0.127
9.0*	282.2	—	48.8	0.199
10.0*	283.2	—	68.6	0.363
10.9*	284.1	—	80.7	0.522
13.2*	286.4	—	90.5	0.713

*The compilers extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility measurements were made with the equipment and in the manner previously described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; purity not specified; freshly distilled and cooled without access to the atmosphere, to prevent contamination with carbon dioxide.
(2) Prepared by hydrogenation of the highly purified nitrile as in the work,¹ purified by two vacuum distillations; freezing point = 16.11 °C.

Estimated Error:

Not specified.

References:

- C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9, 68 (1944).
- A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. 64, 1516 (1942).

13.2. + Dodecanamine

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	(2) Dodecanamine C ₁₂ H ₂₇ N; [124-22-1]
Original Measurements:	
A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. 9, 102-112 (1944).	
Prepared By:	
Nikolai V. Sazonov and Valerii P. Sazonov	
Variables:	
T/K = 273-299	

Experimental Data

The solubilities of dodecanamine (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of dodecanamine (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
0.0	273.2	0.2	0.2	0.0004
3.9*	277.1	—	1.3	0.003
10.5*	283.7	—	3.9	0.009
15.0*	288.2	—	8.0	0.019
17.6*	290.8	—	12.7	0.031
19.0*	292.2	—	17.6	0.045
20.0	293.2	27.7	21.7	0.058
21.2*	294.4	—	30.0	0.087
22.0*	295.2	—	45.9	0.158
23.4*	296.6	—	67.0	0.310
24.4*	297.6	—	80.5	0.478
25.9*	299.1	—	91.6	0.707

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility measurements were made with the equipment and in the manner previously described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; purity not specified; freshly distilled and cooled without access to the atmosphere to prevent contamination with carbon dioxide.
(2) Prepared by hydrogenation of the highly purified nitrile as in the work,¹ purified by two vacuum distillations; freezing point = 28.32 °C.

Estimated Error:

Not specified.

References:

- C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9, 68 (1944).
- A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. 64, 1516 (1942).

13.3. + Tetradecanamine

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements:
(2) Tetradecanamine; C ₁₄ H ₃₁ N; [2016-42-4]	A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. 9 , 102-112 (1944).
Variables:	Prepared By:
T/K = 290-308	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of tetradecanamine (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

<i>t</i> /°C	T/K (compilers)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compilers)	<i>x</i> ₂ (compilers)
16.7*	289.9	—	1.3	0.003
20.0	293.2	1.8	1.8	0.004
25.4*	298.6	—	5.4	0.011
30.0	303.2	14.9	13.0	0.028
32.0*	305.2	—	24.0	0.057
32.4*	305.6	—	44.9	0.136
33.0*	306.2	—	63.9	0.254
33.6*	306.8	—	77.4	0.397
35.0*	308.2	—	88.6	0.599

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility measurements were made with the equipment and in the manner previously described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; purity not specified; freshly distilled and cooled without access to the atmosphere to prevent contamination with carbon dioxide.
(2) Prepared by hydrogenation of the highly purified nitrile as in the work;¹ purified by two vacuum distillations; freezing point = 38.19 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
- ²A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).

13.4. + Hexadecanamine

Components:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Original Measurements:
(2) Hexadecanamine; C ₁₆ H ₃₃ N; [143-27-1]	A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. 9 , 102-112 (1944).
Variables:	Prepared By:
T/K = 293-317	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of hexadecanamine (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

<i>t</i> /°C	T/K (compilers)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compilers)	<i>x</i> ₂ (compilers)
20.0	293.2	0.2	0.2	0.0003
28.6*	301.8	—	1.2	0.002
30.0	303.2	1.3	1.3	0.002
35.4*	308.6	—	5.0	0.009
40.0	313.2	14.8	12.9	0.025
41.2*	314.4	—	28.8	0.064
41.3*	314.5	—	47.8	0.135
41.4*	314.6	—	65.4	0.243
42.0*	315.2	—	80.0	0.405
43.6*	316.8	—	90.9	0.629

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility measurements were made with the equipment and in the manner previously described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; purity not specified; freshly distilled and cooled without access to the atmosphere, to prevent contamination with carbon dioxide.
(2) Prepared by hydrogenation of the highly purified nitrile as in the work;¹ purified by two vacuum distillations; freezing point = 46.77 °C.

Estimated Error:

Not specified.

References:

- ¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
- ²A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).

13.5. + Octadecanamine

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. 9 , 102–112 (1944).	
(2) Octadecanamine; C ₁₈ H ₃₉ N; [124-30-1]			
Variables:		Prepared By:	
T/K = 303–349		Valerii P. Sazonov and Nikolai V. Sazonov	

Experimental Data

The solubilities of acetonitrile (1) and octadecanamine (2) in mass percent including the region of immiscibility over the indicated temperature range were reported in graphical form and in a table.

t/°C	T/K (compilers)	g ₂ /100g ₁	Mutual solubility of acetonitrile (1) and octadecanamine (2)		
			100 w ₁	x ₁ (compilers)	
		Amine-rich phase	Acetonitrile-rich phase		
30.0	303.2	0.3	—	99.7 ^a	0.999
36.0 ^c	309.2	—	—	98.7 ^a	0.998
40.0	313.2	1.9	—	98.1 ^a	0.997
41.4 ^c	314.6	—	—	97.3 ^a	0.995
45.2 ^c	318.4	—	—	95.0 ^a	0.992
47.0 ^c	320.2	—	—	94.1 ^a	0.990
49.0 ^c	322.2	—	—	—	—
49.8 ^c	323.0	—	0.443	—	—
50.0	323.2	10.5	0.582	90.5 ^b	0.984
50.6 ^c	323.8	—	0.257	—	—
52.7 ^c	325.9	—	—	90.0 ^b	0.983
63.0 ^c	336.2	—	0.700	—	—
66.7 ^c	339.9	—	—	83.2 ^b	0.970
73.0 ^c	346.2	—	0.800	—	—
73.1 ^c	346.3	—	—	74.4 ^b	0.950
76.1 ^c	349.3	—	0.897	57.1 ^b	0.897

^aSolid–liquid equilibrium.

^bLiquid–liquid equilibrium.

^cThese data were extracted by the compiler from the published graphs.

Monotectic equilibrium occurs at 48.2 °C (321.4 K, compilers).

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility measurements were made with the equipment and in the manner previously described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; purity not specified; freshly distilled and cooled without access to the atmosphere to prevent contamination with carbon dioxide.

(2) Prepared by hydrogenation of the highly purified nitrile as in the work;¹ purified by two vacuum distillations; freezing point = 53.06 °C.

Estimated Error:

Not specified.

References:

¹C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).

²A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).

14. Acetonitrile + Nitriles

14.1. + Decanenitrile

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9 , 68–80 (1944).	
(2) Decanenitrile; C ₁₀ H ₁₉ N; [1975-78-6]			
Variables:		Prepared By:	
T/K = 233–253		Valerii P. Sazonov and Nikolai I. Lisov	

Experimental Data

The solubilities of decanenitrile (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

t/°C	T/K (compilers)	g ₂ /100g ₁	Solubility of decanenitrile (2) in acetonitrile (1)	
			100 w ₂ (compilers)	x ₂ (compilers)
−40.0	233.2	15.6	13.5	0.040
−37.1 [*]	236.1	—	15.0	0.045
−32.1 [*]	241.1	—	20.9	0.066
−30.5 [*]	242.7	—	28.4	0.096
−28.2 [*]	245.0	—	43.6	0.172
−26.4 [*]	246.8	—	56.8	0.260
−23.5 [*]	249.7	—	75.0	0.446
−20.0	253.2	730	87.9	0.661

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm ×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron–constantan thermocouple. As the nitrile crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.

(2) Prepared by passing decanoic acid over aluminum oxide in the presence of ammonia at 673 °C; dried and purified by vacuum distillation in a Stedman-packed column; freezing point = −14.46 °C.

Estimated Error:

Temperature: ±0.4 K (below 248 K), ±0.2 K (above 248 K).

14.2. + Dodecanitrile

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9 , 68–80 (1944).
(2) Dodecanitrile; C ₁₂ H ₂₃ N; [2437-25-4]	
Variables:	Prepared By:
T/K = 233–273	Valerii P. Sazonov and Nikolai I. Lisov

Experimental Data

The solubilities of dodecanitrile (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of dodecanitrile (2) in acetonitrile (1)				
<i>t</i> /°C	<i>T</i> /K (compilers)	<i>g</i> ₂ /100 <i>g</i> 1	100 <i>w</i> ₂ (compilers)	<i>x</i> ₂ (compilers)
-40.0	233.2	0.9	0.9	0.002
-30.9*	242.3	—	2.0	0.005
-23.2*	250.0	—	4.5	0.011
-20.0	253.2	6.9	6.5	0.016
-17.1*	256.1	—	9.1	0.022
-15.0*	258.2	—	11.8	0.029
-13.2*	260.0	—	15.0	0.038
-11.8*	261.4	—	20.9	0.057
-10.0*	263.2	—	35.0	0.109
-8.4*	264.8	—	49.1	0.179
-7.3*	265.9	—	61.4	0.265
-4.1*	269.1	—	78.2	0.448
-1.4*	271.8	—	89.1	0.649
0.0	273.2	1200	92.3	0.731

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm ×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron–constantan thermocouple. As the nitriles crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing dodecanoic acid over aluminum oxide in the presence of ammonia at 673 °C; dried and purified by vacuum distillation in a Siedman-packed column; freezing point=4.02 °C.

Estimated Error:

Temperature: ±0.4 K (below 248 K), ±0.2 K (above 248 K).

14.3. + Tetradecanenitrile

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9 , 68–80 (1944).
(2) Tetradecanenitrile; C ₁₄ H ₂₇ N; [629-63-0]	
Variables:	Prepared By:
T/K = 233–286	Valerii P. Sazonov and Nikolai I. Lisov

Experimental Data

The solubilities of tetradecanenitrile (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of tetradecanenitrile (2) in acetonitrile (1)				
<i>t</i> /°C	<i>T</i> /K (compilers)	<i>g</i> ₂ /100 <i>g</i> 1	100 <i>w</i> ₂ (compilers)	<i>x</i> ₂ (compilers)
-40.0	233.2	≈0.1	0.1	0.0002
-20.0	253.2	1.1	1.1	0.002
-9.1*	264.1	—	2.7	0.005
-3.2*	270.0	—	5.7	0.012
0.0	273.2	9.6	8.8	0.019
2.5*	275.7	—	12.7	0.028
4.5*	277.7	—	25.0	0.061
6.4*	279.6	—	40.0	0.116
7.3*	280.5	—	47.3	0.150
8.9*	282.1	—	65.5	0.271
10.0	283.2	—	72.1	0.336
10.9*	284.1	258	78.4	0.416
12.7*	285.9	—	85.5	0.536

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm ×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron–constantan thermocouple. As the nitriles crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing tetradecanoic acid over aluminum oxide in the presence of ammonia at 673 °C; dried and purified by vacuum distillation in a Siedman-packed column; freezing point=19.25 °C.

Estimated Error:

Temperature: ±0.4 K (below 248 K), ±0.2 K (above 248 K).

14.4. + Hexadecanenitrile

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9 , 68–80 (1944).
(2) Hexadecanenitrile; C ₁₆ H ₃₁ N; [629-79-8]	
Variables:	Prepared By:
T/K = 253–303	Valerii P. Sazonov and Nikolai I. Lisov

Experimental Data

The solubilities of hexadecanenitrile (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of hexadecanenitrile (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100 g ₁	100 w ₂ (compilers)	x ₂ (compilers)
–20.0	253.2	≈0.1	0.1	0.0002
–2.5*	270.7	—	0.9	0.002
0.0	273.2	1.3	1.3	0.002
5.9*	279.1	—	2.0	0.004
10.0	283.2	4.8	4.6	0.008
12.7*	285.9	—	6.6	0.012
16.4*	289.6	—	12.9	0.025
17.7*	290.9	—	19.5	0.040
18.6*	291.8	—	28.2	0.064
20.0	293.2	94	48.5	0.140
22.7*	295.9	—	74.5	0.336
25.9*	299.1	—	88.5	0.571
30.0	303.2	4250	97.7	0.880

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm ×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron–constantan thermocouple. As the nitriles crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by passing hexadecanoic acid over aluminum oxide in the presence of ammonia at 400 °C; dried and purified by vacuum distillation in a Siedman-packed column; freezing point = 31.40 °C.

Estimated Error:

Temperature: ±0.4 K (below 248 K), ±0.2 K (above 248 K).

14.5. + Octadecanenitrile

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. 9 , 68–80 (1944).
(2) Octadecanenitrile; C ₁₈ H ₃₅ N; [638-65-3]	
Variables:	Prepared By:
T/K = 273–309	Valerii P. Sazonov and Nikolai I. Lisov

Experimental Data

The solubilities of octadecanenitrile (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of octadecanenitrile (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100 g ₁	100 w ₂ (compilers)	x ₂ (compilers)
0.0	273.2	≈0.1	0.1	0.0002
10.0	283.2	0.5	0.5	0.0008
15.0*	288.2	—	0.9	0.001
20.0	293.2	3.6	3.5	0.006
21.4*	294.6	—	4.1	0.007
25.5*	298.7	—	10.0	0.017
26.8*	300.0	—	12.7	0.022
28.2*	301.4	—	20.0	0.037
29.5*	302.7	—	41.8	0.100
30.0	303.2	115	53.5	0.151
30.5*	303.7	—	58.2	0.177
31.8*	305.0	—	72.7	0.292
35.7*	308.9	—	89.1	0.558

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm ×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron–constantan thermocouple. As the nitriles crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by passing octadecanoic acid over aluminum oxide in the presence of ammonia at 673 K; purified by several crystallizations; freezing point = 40.88 °C.

Estimated Error:

Temperature: ±0.2 K and ±0.4 K (below 248 K).

15.2. + Decanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. 8 , 473-88 (1943).
(2) Decanamide; C ₁₀ H ₂₁ NO; [2319-29-1]	
Variables:	Prepared By:
T/K = 283-355	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of decanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of decanamide (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100 g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	0.5	0.5	0.001
23.6*	296.8	—	1.1	0.003
30.0	303.2	1.4	1.4	0.004
34.9*	308.1	—	2.0	0.005
47.7*	320.9	—	4.5	0.011
50.0	323.2	6.0	5.7	0.014
59.1*	332.3	—	10.5	0.027
60.0	333.2	13.4	11.8	0.031
66.4*	339.6	—	20.9	0.060
70.0	343.2	44.5	30.8	0.096
73.2*	346.4	—	39.1	0.133
81.1*	354.3	—	61.4	0.276
82.0	355.2	178	64.0	0.299
10.0	283.2	0.5	0.5	0.001

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by passing of ammonia through decanoic acid at 190-210 °C for 10-14 h; purified by recrystallization; freezing point=98.5 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
- C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

15. Acetonitrile+Amides

15.1. + Octanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. 8 , 473-88 (1943).
(2) Octanamide; C ₈ H ₁₇ NO; [629-01-6]	
Variables:	Prepared By:
T/K = 283-355	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of octanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of octanamide (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100 g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	1.1	1.1	0.003
21.8*	295.0	—	2.8	0.008
30.0	303.2	5.4	5.1	0.015
40.5*	313.7	—	8.7	0.027
50.0	323.2	16.4	14.1	0.045
58.2*	331.4	—	20.9	0.070
60.0	333.2	31.6	24.0	0.083
69.1*	342.3	—	39.5	0.158
70.0	343.2	73.0	42.2	0.173
78.2*	351.4	—	58.7	0.289
82.0	355.2	200	66.7	0.365

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by passing of ammonia through octanoic acid at 190-210 °C for 10-14 h; purified by recrystallization; freezing point=105.9 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
- C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

15.4. + Tetradecanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, <i>J. Org. Chem.</i> 8 , 473-88 (1943).
(2) Tetradecanamide; C ₁₄ H ₂₉ NO; [638-58-4]	
Variables:	Prepared By:
T/K = 283-355	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of tetradecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of tetradecanamide (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	0.2	0.2	0.0004
30.0	303.2	0.6	0.6	0.001
35.0*	308.2	—	0.9	0.002
50.0	323.2	1.1	1.1	0.002
60.0	333.2	2.9	2.8	0.005
60.9*	334.1	—	3.0	0.006
70.0	343.2	7.8	7.2	0.014
73.4*	346.6	—	10.2	0.020
81.8*	355.0	—	30.0	0.072
82.0	355.2	43.3	30.2	0.072

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing of ammonia through tetradecanoic acid at 190-210 °C for 10-14 h; purified by recrystallization; freezing point = 105.1 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, *J. Am. Chem. Soc.* **64**, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, *J. Am. Chem. Soc.* **64**, 2824 (1942).

15.3. + Dodecanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, W. O. Pool, <i>J. Org. Chem.</i> 8 , 473-88 (1943).
(2) Dodecanamide; C ₁₂ H ₂₅ NO; [1120-16-7]	
Variables:	Prepared by:
T/K = 283 to 355	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of dodecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of dodecanamide (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	0.3	0.3	0.0006
30.0	303.2	0.9	0.9	0.002
32.5*	305.7	—	1.1	0.002
45.6*	318.8	—	3.5	0.007
50.0	323.2	5.1	4.9	0.010
51.5*	324.7	—	5.2	0.011
56.6*	329.8	—	8.0	0.018
60.0	333.2	12.1	10.8	0.024
66.0*	339.2	—	18.4	0.044
70.0	343.2	39.8	28.5	0.076
73.5*	346.7	—	37.3	0.109
77.7*	350.9	—	51.2	0.178
81.1*	354.3	—	61.4	0.247
82.0	355.2	175	63.6	0.265

*Data extracted from the published graphs by the compilers

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing of ammonia through dodecanoic acid at (190 to 210) °C for (10 to 14) hours; purified by recrystallization; f. p. = 102.4 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, *J. Am. Chem. Soc.* **64**, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, *J. Am. Chem. Soc.* **64**, 2824 (1942).

15.6. + Hexadecanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, <i>J. Org. Chem.</i> 8 , 473-88 (1953).
(2) Hexadecanamide; C ₁₆ H ₃₃ NO; [629-54-9]	
Variables:	Prepared By:
T/K = 283-355	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of hexadecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of hexadecanamide (2) in acetonitrile (1)				
<i>t</i> /°C	T/K (compilers)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compilers)	<i>x</i> ₂ (compilers)
10.0	283.2	0.2	0.2	0.0003
30.0	303.2	0.3	0.3	0.0005
37.7*	310.9	—	0.6	0.001
50.0	323.2	0.7	0.7	0.001
55.5*	328.7	—	1.0	0.002
60.0	333.2	1.6	1.6	0.003
70.0	343.2	5.9	5.6	0.009
70.8*	344.0	—	6.1	0.010
77.6*	350.8	—	15.2	0.028
82.0	355.2	34.8	25.8	0.053

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by passing of ammonia through hexadecanoic acid at 190-210 °C for 10-14 h; purified by recrystallization; freezing point = 107.0 °C.

Estimated Error:

Temperature: control ± 0.2 K.

References:

- A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, *J. Am. Chem. Soc.* **64**, 1516 (1942).
- C. W. Hoerr and A. W. Ralston, *J. Am. Chem. Soc.* **64**, 2824 (1942).

15.5. + N-Phenyldodecanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, <i>J. Org. Chem.</i> 8 , 473-88 (1943).
(2) N-Phenyldodecanamide; C ₁₆ H ₂₅ NO; [15473-32-2]	
Variables:	Prepared By:
T/K = 283-333	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of N-phenyldodecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of N-phenyldodecanamide (2) in acetonitrile (1)				
<i>t</i> /°C	T/K (compilers)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compilers)	<i>x</i> ₂ (compilers)
10.0	283.2	9.3	8.5	0.015
17.7*	290.9	—	10.0	0.018
30.0	303.2	18.0	15.3	0.029
33.2*	306.4	—	17.5	0.034
38.4*	311.6	—	26.4	0.056
40.0*	315.2	—	33.2	0.076
47.3*	320.5	—	66.5	0.248
50.0	325.2	297	74.8	0.330
54.8*	328.0	—	81.8	0.427
57.7*	330.9	—	85.7	0.499
60.0	333.2	825	89.2	0.578

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Obtained by heating of dodecanoic acid with redistilled aniline at 150-170 °C for 2-3 h; purified by recrystallization; freezing point = 69.5 °C.

Estimated Error:

Temperature: ± 0.2 K.

References:

- A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, *J. Am. Chem. Soc.* **64**, 1516 (1942).
- C. W. Hoerr and A. W. Ralston, *J. Am. Chem. Soc.* **64**, 2824 (1942).

15.8. + Octadecanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, <i>J. Org. Chem.</i> 8 , 473-88 (1943).
(2) Octadecanamide; C ₁₈ H ₃₇ NO; [124-26-5]	
Variables:	Prepared By:
T/K = 283-355	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of octadecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of octadecanamide (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	0.1	0.1	0.0001
30.0	303.2	0.2	0.2	0.0003
50.0	323.2	0.4	0.4	0.0006
55.4*	328.6	—	0.5	0.0007
60.0	333.2	0.9	0.9	0.001
70.0	343.2	2.6	2.5	0.004
70.2*	343.4	—	2.6	0.004
74.5*	347.7	—	4.7	0.007
80.2*	353.4	—	11.2	0.018
82.0	355.2	16.8	14.4	0.024

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by passing of ammonia through octadecanoic acid at 190-210 °C for 10-14 h; purified by recrystallization; freezing point = 109.7 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, *J. Am. Chem. Soc.* **64**, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, *J. Am. Chem. Soc.* **64**, 2824 (1942).

15.7. + N-Phenyldodecanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, <i>J. Org. Chem.</i> 8 , 473-88 (1943).
(2) N-Phenyldodecanamide; C ₁₈ H ₂₉ NO; [3430-95-3]	
Variables:	Prepared By:
T/K = 283-343	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of N-phenyldodecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of N-phenyldodecanamide (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	0.8	0.8	0.001
15.5*	288.7	—	1.1	0.002
30.0	303.2	3.0	2.9	0.004
30.5*	303.7	—	3.0	0.005
44.5*	317.7	—	9.6	0.016
50.0	323.2	24.1	19.4	0.035
50.5*	323.7	—	19.6	0.035
53.5*	326.7	—	32.2	0.066
57.7*	330.9	—	61.6	0.193
60.0	333.2	308	75.5	0.315
62.4*	335.6	—	79.5	0.366
70.0	343.2	1100	91.7	0.622

*The compiler extracted these data from the published graphs.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Obtained by heating of dodecanoic acid with redistilled aniline at 150-170 °C for 2-3 h; purified by recrystallization; freezing point = 77.2 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, *J. Am. Chem. Soc.* **64**, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, *J. Am. Chem. Soc.* **64**, 2824 (1942).

15.10. + N-Phenylhexadecanamide

Components:		Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. 8 , 473-88 (1943).
(2) N-Phenylhexadecanamide; C ₂₅ H ₃₇ NO; [6832-98-0]		
Variables:		Prepared By:
T/K=283-355		Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of N-phenylhexadecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of N-phenylhexadecanamide (2) in acetonitrile (1)					
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)	x ₂ (compilers)
10.0	283.2	0.3	0.3	0.0004	0.0004
30.0	303.2	0.7	0.7	0.0009	0.0009
40.0*	313.2	—	1.0	0.001	0.001
50.0	323.2	2.2	2.2	0.003	0.003
56.4*	329.6	—	4.3	0.006	0.006
60.0	333.2	5.5	5.2	0.007	0.007
62.9*	336.1	—	7.6	0.010	0.010
69.1*	342.3	—	19.3	0.029	0.029
70.0	343.2	32.5	24.5	0.039	0.039
72.3*	345.5	—	49.1	0.107	0.107
74.2*	347.4	—	68.2	0.210	0.210
76.2*	349.4	—	78.7	0.314	0.314
82.0	355.2	733	88.0	0.476	0.476

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Obtained by heating of hexadecanoic acid with redistilled aniline at 150-170 °C for 2-3 h; purified by recrystallization; freezing point=90.2 °C.

Estimated Error:

Temperature: ±0.2 K

References:

¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

15.9. + N,N-Diphenyldecanamide

Components:		Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. 8 , 473-88 (1943).
(2) N,N-Diphenyldecanamide; C ₂₂ H ₂₉ NO		
Variables:		Prepared By:
T/K=283-315		Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of N,N-diphenyldecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of N,N-diphenyldecanamide (2) in acetonitrile (1)					
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)	x ₂ (compilers)
10.0	283.2	39.3	28.2	0.048	0.048
15.9*	289.1	—	39.8	0.077	0.077
30.0	303.2	252	71.6	0.242	0.242
31.5*	304.7	—	74.3	0.268	0.268
39.5*	312.7	—	87.9	0.480	0.480
41.6*	314.8	—	91.1	0.565	0.565

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by heating the decanoyl chloride with diphenylamine for 2-4 h at 135-145 °C; purified by recrystallization; freezing point=47.5 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
²C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

15.11. + N,N-Diphenyldodecanamide

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. 8 , 473-88 (1943).	
(2) N, N-Diphenyldodecanamide; C ₂₃ H ₃₃ NO			
Variables:		Prepared By:	
T/K=283-323		Valerii P. Sazonov and Nikolai V. Sazonov	

Experimental Data

The solubilities of N,N-diphenyldodecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of N,N-diphenyldodecanamide (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	12.6	11.2	0.015
15.9*	289.1	—	14.3	0.019
25.9*	299.1	—	30.4	0.049
30.0	303.2	75.0	42.9	0.081
36.4*	309.6	—	59.1	0.144
47.3*	320.5	—	85.5	0.408
50.0	323.2	1075	91.5	0.557

*These data were extracted by the compilers from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by heating the dodecanoyl chloride with diphenylamine for 2-4 h 135-145 °C; purified by recrystallization; freezing point=57 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
- ²C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

15.12. + N-Phenyloctadecanamide

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]		A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. 8 , 473-88 (1943).	
(2) N-Phenyloctadecanamide; C ₂₄ H ₄₁ NO; [637-54-7]			
Variables:		Prepared By:	
T/K=283-355		Valerii P. Sazonov and Nikolai V. Sazonov	

Experimental Data

The solubilities of N-phenyloctadecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

Solubility of N-phenyloctadecanamide (2) in acetonitrile (1)				
t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	0.2	0.2	0.0002
30.0	303.2	0.5	0.5	0.0006
50.0	323.2	1.4	1.4	0.0016
52.9*	326.1	—	1.8	0.002
60.0	333.2	3.3	3.2	0.004
66.2*	339.4	—	6.8	0.008
70.0	343.2	13.8	12.1	0.016
70.4*	343.6	—	13.0	0.017
73.5*	346.7	—	23.0	0.033
75.0*	348.2	—	40.9	0.073
77.5*	350.7	—	67.5	0.192
78.6*	351.8	—	73.2	0.238
82.0	355.2	480	82.8	0.355

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
 (2) Prepared by addition of aniline to searoyl chloride at 50 °C; purified by recrystallization; freezing point=94.9 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
- ²C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

15.13. + N,N-Diphenylhexadecanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, <i>J. Org. Chem.</i> 8 , 473-88 (1943).
(2) N,N-Diphenylhexadecanamide; C ₂₈ H ₄₁ NO	
Variables:	Prepared By:
T/K=283-336	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of N,N-diphenylhexadecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	1.5	1.5	0.002
25.9*	299.1	—	4.2	0.004
30.0	303.2	5.8	5.5	0.006
37.5*	310.7	—	9.1	0.010
44.4*	317.6	—	17.7	0.021
50.0	323.2	75.0	42.9	0.070
52.2*	325.4	—	52.3	0.099
60.0*	333.2	635	85.6	0.374
63.2	336.4	—	91.8	0.530

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by heating the hexadecanoyl chloride with diphenylamine for 2-4 h at 135-145 °C; purified by recrystallization; freezing point=69.5 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, *J. Am. Chem. Soc.* **64**, 1516 (1942).
- ²C. W. Hoerr and A. W. Ralston, *J. Am. Chem. Soc.* **64**, 2824 (1942).

15.14. + N,N-Diphenyloctadecanamide

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]	A. W. Ralston, C. W. Hoerr, and W. O. Pool, <i>J. Org. Chem.</i> 8 , 473-88 (1943).
(2) N,N-Diphenyloctadecanamide; C ₃₀ H ₄₃ NO	
Variables:	Prepared By:
T/K=283-343	Valerii P. Sazonov and Nikolai V. Sazonov

Experimental Data

The solubilities of N,N-diphenyloctadecanamide (2) in acetonitrile (1) in mass percent over the indicated temperature range were reported in graphical form and in a table.

t/°C	T/K (compilers)	g ₂ /100g ₁	100 w ₂ (compilers)	x ₂ (compilers)
10.0	283.2	0.6	0.6	0.0006
15.5*	288.7	—	1.2	0.001
30.0	303.2	2.4	2.3	0.002
35.0*	308.2	—	4.7	0.005
46.5*	319.7	—	12.7	0.014
50.0	323.2	23.3	18.9	0.022
53.5*	326.7	—	32.2	0.043
57.3*	330.5	—	65.7	0.153
60.0	333.2	359	78.2	0.253
65.3*	338.5	—	89.8	0.453
70.0	343.2	3350	97.1	0.759

*The compiler extracted these data from the published graphs.

Auxiliary Information**Method/Apparatus/Procedure:**

The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described elsewhere.^{1,2}

Source and Purity of Materials:

(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by heating the octadecanoyl chloride with diphenylamine for 2-4 h at 135-145 °C; purified by crystallization; freezing point=72.3 °C.

Estimated Error:

Temperature: ±0.2 K.

References:

- ¹A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, *J. Am. Chem. Soc.* **64**, 1516 (1942).
- ²C. W. Hoerr and A. W. Ralston, *J. Am. Chem. Soc.* **64**, 2824 (1942).

16.2. + 1,3-Diglycerides C₃₁-C₃₉

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>J. Am. Oil Chem. Soc.</i> 42 , 372-81 (1965).	
(2) 1,3-Diglycerides; C ₃₁ H ₆₀ O ₅ -C ₃₉ H ₇₆ O ₅			
Variables:		Prepared By:	
T/K = 333-376		Valerii P. Sazonov	
Experimental Data			
Upper critical solution temperatures of the binary systems acetonitrile(1)+1,3-diglyceride(2)			
1,3-Diglyceride	<i>t</i> /°C	<i>T</i> /K (compiler)	
1,3-Ditridecanoyloxy-2-propanol; C ₃₁ H ₆₀ O ₅ ; [7770-09-4]	60.0	333.2	
1,3-Dihexadecanoyloxy-2-propanol; C ₃₅ H ₆₈ O ₅ ; [502-52-3]	82.0	255.2	
1,3-Dioctadecanoyloxy-2-propanol; C ₃₉ H ₇₆ O ₅ ; [504-40-5]	103.0	376.2	

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, with a heating stage was used. A 26×38 mm slide was adapted to hold capillaries on the stage. Two glass strips were glued, using water glass, to the slide leaving a 0.5 mm channel. The slide was then placed in the adjustable device of the heating stage. (1) and (2) were put into capillary tubing (0.2-0.3 mm diameter) by dipping consecutively into both liquids. The height of the liquid was 7-10 mm. Room temperature solids were melted on a glass slide over a microburner. The capillary was sealed at both ends to a length of 30-35 mm, then inserted into the channel on the slide and heated on the stage. The UCST was determined by following the appearance and disappearance of the meniscus.

Source and Purity of Materials:

(1) Baker Chemical Co.; reagent No. 9011; *n*(20 °C,D) = 1.3445, *d*(20 °C,4 °C) = 0.780.
(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

16. Acetonitrile+Glycerides

16.1. + Triglycerides C₃₃-C₆₉

Components:		Original Measurements:	
(1) Acetonitrile; C ₂ H ₃ N; [75-05-8]		H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, <i>Microchem. J.</i> 7 , 297-302 (1963).	
(2) Triglycerides; C ₃₃ H ₆₀ O ₆ -C ₆₉ H ₁₂₈ O ₆			
Variables:		Prepared By:	
T/K = 326-462		Valerii P. Sazonov	
Experimental Data			
Upper critical solution temperatures of the binary systems acetonitrile (1)+ triglyceride (2)			
Triglyceride	<i>t</i> /°C	<i>T</i> /K (compilers)	
1,2,3-Tridecanoyloxypropane (tricaprin); C ₃₃ H ₆₂ O ₆ ; [621-71-6]	53.0	326.2	
1,2,3-Tri(cis,cis,cis-9,12,15-octadecatrienoxyloxy)propane (trilinolenin); C ₃₇ H ₆₂ O ₆ ; [14465-08-0]	88.0	361.2	
1,2,3-Tri(dodecanoyloxy)propane (trilaurin); C ₃₉ H ₇₄ O ₆ ; [538-24-9]	91.5	364.7	
1,2,3-Tri(cis,cis,cis-9,12-octadecadienoxyloxy)propane (trilinolenin); C ₃₇ H ₆₂ O ₆ ; [537-40-6]	113.5	386.7	
1,2,3-Tri(cis-9-hexadecenoxyloxy)propane (tripalmitolein); C ₅₁ H ₉₂ O ₆ ; [20246-55-3]	114.5	387.7	
1,2,3-Tri(tritridecanoyloxy)propane (trimyrstin); C ₄₅ H ₈₆ O ₆ ; [555-45-3]	120.0	393.2	
1,2,3-Tri(cis-9-octadecenoxyloxy)propane (triolein); C ₅₇ H ₁₀₄ O ₆ ; [122-32-7]	140.0	413.2	
1-Hexadecanoyloxy-2,3-di(cis-9-octadecenoxyloxy)propane (1-palmito-2,3-diolein); C ₅₅ H ₁₀₂ O ₆ ; [27071-84-7]	142.0	415.2	
2-Hexadecanoyloxy-1,3-di(cis-9-octadecenoxyloxy)propane (2-palmito-1,3-diolein); C ₅₅ H ₁₀₂ O ₆ ; [1716-07-0]	142.0	415.2	
1,2,3-Tri(trans-9-octadecenoxyloxy)propane (trilaidin); C ₅₇ H ₁₀₄ O ₆ ; [537-39-3]	145.0	418.2	
1,2,3-Trihexadecanoyloxypropane (tripalmitin); C ₅₁ H ₉₆ O ₆ ; [555-44-2]	145.0	418.2	
1,3-Dihexadecanoyloxy-2-(cis-9-octadecenoxyloxy)propane (1,3-dipalmito-2-olein); C ₅₅ H ₁₀₀ O ₆ ; [28409-94-1]	145.5	418.7	
1-Octadecanoyloxy-2,3-di(cis-9-octadecenoxyloxy)propane (1-stearo-2,3-diolein); C ₅₇ H ₁₀₆ O ₆ ; [29590-02-1]	147.5	420.7	
2-Octadecanoyloxy-1,3-di(cis-9-octadecenoxyloxy)propane (2-stearo-1,3-diolein); C ₅₇ H ₁₀₆ O ₆ ; [2410-29-9]	147.5	420.7	
1-Hexadecanoyloxy-2-octadecenoxyloxy-3-(cis-9-octadecenoxyloxy)propane (1-palmito-2-stearo-3-olein); C ₅₅ H ₁₀₄ O ₆ ; [26836-31-7]	152.0	425.2	
1-Hexadecanoyloxy-3-octadecenoxyloxy-2-(cis-9-octadecenoxyloxy)propane (1-palmito-3-stearo-2-olein); C ₅₅ H ₁₀₄ O ₆	152.0	425.2	
1,3-Dioctadecanoyloxy-2-(cis-9-octadecenoxyloxy)propane (1,3-distearo-2-olein); C ₅₇ H ₁₀₈ O ₆ ; [28880-75-3]	158.0	431.2	
1,2,3-Tri-11-icosenoxyloxypropane (tri-11-icosenoin); C ₆₅ H ₁₁₀ O ₆ ; [115936-00-0]	160.5	433.7	
1,2,3-Trioctadecanoyloxypropane (tristearin); C ₅₇ H ₁₁₀ O ₆ ; [555-43-1]	170.0	443.0	
1,2,3-Tri(cis-13-docosenoxyloxy)propane (tristearin); C ₆₉ H ₁₂₈ O ₆ ; [2752-99-0]	182.0	455.2	
1,2,3-Triheicosanoyloxypropane (triarachidin); C ₆₉ H ₁₂₈ O ₆ ; [620-64-4]	189.0	462.2	

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described elsewhere.¹ The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Baker Chemical Co.; reagent, No. 9011; *n*(20 °C,D) = 1.3445, *d*(20 °C,4 °C) = 0.780.

(2) Monoacid triglycerides obtained from the Hormel Foundation, other triglycerides from Procter & Gamble Co.; purity verified by thin-layer adsorption chromatography.

Estimated Error:

Not specified.

References:

¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *Microchem. J.* **7**, 287 (1963).

16.3. + 1-Alkoxy-diglycerides C₄₅-C₆₁

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, <i>Microchem. J.</i> 11 , 306-14 (1966).
(2) 1-Alkoxy-diglycerides; C ₄₅ H ₈₈ O ₅ -C ₆₁ H ₁₂₀ O ₅	
Variables:	Prepared By:
T/K = 415-470	Valerii P. Sazonov

Experimental Data
Upper critical solution temperatures of the binary systems acetonitrile(1) + 1-alkoxy-diglyceride(2)

Ether	<i>t</i> /°C	<i>T</i> /K (compiler)
1-Alkoxy-diglyceride		
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester lauric acid; C ₄₃ H ₈₆ O ₅ ; [10322-28-8]	141.5	414.7
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester tetradecanoic acid; C ₄₉ H ₉₈ O ₅ ; [10322-29-9]	157.5	430.7
(Z)-[(9-Octadecenoxyloxy)methyl]-1,2-ethanediyl ester oleic acid; C ₅₇ H ₁₀₆ O ₅ ; [10322-38-0]	157.5	430.7
1-[(Decyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₄₉ H ₉₈ O ₅ ; [10431-17-1]	158.0	431.2
1-[(Undecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₉ H ₁₁₈ O ₅ ; [10322-31-3]	161.0	434.2
1-[(Dodecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₁ H ₁₀₂ O ₅ ; [10322-32-4]	164.0	437.2
1-[(Tridecyloxy)methyl]-1,2-ethanediyl ester oleic acid; C ₅₇ H ₁₀₆ O ₅ ; [10329-25-6]	167.0	440.2
1-[(Tetradecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₃ H ₁₀₆ O ₅ ; [10322-33-5]	167.5	440.7
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester palmitic acid; C ₅₃ H ₁₀₄ O ₅ ; [10322-30-2]	171.0	444.2
1-[(Tetradecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₅ H ₁₀₈ O ₅ ; [10322-34-6]	171.5	444.7
1-[(Pentadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₅ H ₁₀₆ O ₅ ; [10431-21-7]	174.5	447.7
(Z)-[(9-Octadecenoxyloxy)methyl]-ethylene ester stearic acid; C ₅₇ H ₁₀₆ O ₅ ; [10322-37-9]	175.0	448.2
1-[(Hexadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₅ H ₁₀₈ O ₅ ; [923-63-7]	178.0	451.2
1-[(Heptadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₉ H ₁₁₂ O ₅ ; [923-62-6]	181.5	454.7
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₇ H ₁₁₀ O ₅ ; [923-62-6]	184.5	457.7
1-[(Nonadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₈ H ₁₁₄ O ₅ ; [10322-39-1]	187.5	460.7
1-[(Eicosyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₅₉ H ₁₁₆ O ₅ ; [10322-40-4]	191.0	464.2
1-[(Heneicosyloxy)methyl]-1,2-ethanediyl ester stearic acid; C ₆₀ H ₁₁₈ O ₅ ; [10322-41-5]	194.0	467.2
1-[(Octadecyloxy)methyl]-ethylene ester eicosanoic acid; C ₆₁ H ₁₂₀ O ₅ ; [10322-36-8]	197.0	470.2

Auxiliary Information**Method/Apparatus/Procedure:**

A microscope equipped with a heating stage as in the work¹ was employed for determining UCST values. No experimental details are given.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent No. 9011.
- (2) Synthesized as described elsewhere.²

Estimated Error:

Not specified.

References:

- ¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).
- ²W. J. Baumann and H. K. Mangold, *J. Org. Chem.* **29**, 3055 (1964).

16.4. + 1,2-Dialkoxy-glycerides C₄₅-C₅₉

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, <i>Microchem. J.</i> 11 , 306-14 (1966).
(2) 1,2-Dialkoxy-glycerides; C ₄₅ H ₉₀ O ₄ -C ₅₉ H ₁₁₈ O ₄	
Variables:	Prepared By:
T/K = 435-483	Valerii P. Sazonov

Experimental Data
Upper critical solution temperatures of the binary systems acetonitrile(1) + 1,2-dialkoxy-glyceride(2)

Ether	<i>t</i> /°C	<i>T</i> /K (compiler)
2-(Dodecyloxy)-3-(octadecyloxy)propyl ester lauric acid; C ₄₃ H ₈₆ O ₄ ; [10322-44-8]	162.0	435.2
2,3-Bis(9-octadecenoxyloxy)-(ZZZ)-propyl ester oleic acid; C ₅₇ H ₁₀₆ O ₄ ; [10322-53-9]	176.0	449.2
2-(Hexadecyloxy)-3-(octadecyloxy)propyl ester lauric acid; C ₄₉ H ₉₈ O ₄ ; [10322-47-1]	177.0	450.2
2,3-Bis(hexadecyloxy)propyl ester hexadecanoic acid; C ₅₃ H ₁₀₆ O ₄ ; [10322-42-6]	182.5	455.7
2-(Dodecyloxy)-3-(octadecyloxy)propyl ester stearic acid; C ₅₁ H ₁₀₂ O ₄ ; [10322-45-9]	183.0	456.2
2-(9-octadecenoxyloxy)-(ZZ)-3-(octadecyloxy)propyl ester lauric acid; C ₅₁ H ₁₀₂ O ₄ ; [10322-49-3]	183.5	456.7
2-(9-octadecenoxyloxy)-(ZZ)-3-(octadecyloxy)propyl ester oleic acid; C ₅₇ H ₁₀₆ O ₄ ; [10322-52-8]	185.0	458.2
3-(Octadecyloxy)-2-(tetradecyloxy)propyl ester stearic acid; C ₅₃ H ₁₀₆ O ₄ ; [10322-46-0]	190.0	463.2
2,3-Bis(octadecyloxy)-propyl ester-(Z)-9-octadecenoic acid; C ₅₃ H ₁₁₂ O ₄ ; [10322-51-7]	193.0	466.2
2-(Hexadecyloxy)-3-(octadecyloxy)propyl ester stearic acid; C ₅₃ H ₁₁₀ O ₄ ; [10322-48-2]	197.0	467.2
3-(Hexadecyloxy)-2-(octadecyloxy)propyl ester stearic acid; C ₅₃ H ₁₁₀ O ₄ ; [10322-43-7]	197.0	467.2
3-Bis(octadecyloxy)propyl ester octadecanoic acid; C ₅₇ H ₁₁₄ O ₄ ; [10322-50-6]	203.0	476.2
2-(Eicosyloxy)-3-(octadecyloxy)propyl ester stearic acid; C ₅₉ H ₁₁₈ O ₄ ; [10322-54-0]	209.5	482.7

Auxiliary Information**Method/Apparatus/Procedure:**

A microscope equipped with a heating stage as in the work¹ was employed for determining UCST values. No experimental details are given.

Source and Purity of Materials:

- (1) Baker Chemical Co.; reagent No. 9011.
- (2) Synthesized as described elsewhere.²

Estimated Error:

Not specified.

References:

- ¹H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, *J. Am. Oil Chem. Soc.* **42**, 372 (1965).
- ²W. J. Baumann and H. K. Mangold, *J. Org. Chem.* **29**, 3055 (1964).

17. Acetonitrile+Sulfur Compounds

17.1. + Thiophenes: C₄ and C₈

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Thiophenes; C ₄ H ₄ S and C ₈ H ₁₂ S	Original Measurements: R. D. Obolentsev, M. N. Lebedeva, E. A. Kreis, N. K. Lyapina, and M. A. Parphenova, <i>Neftekhimiya</i> 11 , 893–901 (1971).
Variables: <i>T</i> / <i>K</i> =203 and 225	Prepared By: Valerii P. Sazonov

Experimental Data

Upper critical solution temperatures of the binary systems acetonitrile(1)+thiophene(2)

Thiophene	Boiling point (°C)	<i>n</i> (20 °C,D)	<i>d</i> (20 °C,4 °C)	<i>t</i> /°C	<i>T</i> / <i>K</i> (compiler)
Thiophene; C ₄ H ₄ S; [110-02-1]	84	1.5287	1.0700	−70	203
2-Butylthiophene; C ₈ H ₁₂ S; [1455-20-5]	186.6	1.5021	0.9562	−48	225

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Samples of (1) and (2) of weight about 0.2 g were placed in glass ampoules of length 3–4 cm and inner diameter of 4 mm. After cooling in a mixture of ice with salt ampoules were sealed. Three to four ampoules were attached to a thermometer and placed in a glass bath with glycerine (for heating) or with acetone and solid CO₂ (for cooling) with continuous stirring. The heating and cooling 2 K/min. The UCST was determined by following the appearance and disappearance of the meniscus.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and purified; boiling point=81.6 °C, *n*(20 °C,D)=1.3458.
(2) Synthesized in Institute of Chemistry (Upha, Russia).

Estimated Error:

Temperature: ±0.5 K (below 243 K).

17.2. + Thiophanes C₄–C₁₃

Components: (1) Acetonitrile; C ₂ H ₃ N; [75-05-8] (2) Thiophanes; C ₄ H ₈ S–C ₁₃ H ₂₆ S	Original Measurements: R. D. Obolentsev, M. N. Lebedeva, E. A. Kreis, N. K. Lyapina, and M. A. Parphenova, <i>Neftekhimiya</i> 11 , 893–901 (1971).
Variables: <i>T</i> / <i>K</i> =205–338	Prepared By: Valerii P. Sazonov

Experimental Data

Upper critical solution temperatures of the binary systems acetonitrile(1)+thiophane(2)

Thiophane	Boiling point (°C/kPa)	<i>n</i> (20 °C,D)	<i>d</i> (20 °C,4 °C)	<i>t</i> /°C	<i>T</i> / <i>K</i> (compiler)
Thiophane; C ₄ H ₈ S; [110-01-0]	121.2	1.5048	0.9980	−68	205
2-Butylthiophane; C ₈ H ₁₆ S; [1613-49-6]	201–203	1.4875	0.9217	−50	223
2-Propylthiophane; C ₇ H ₁₄ S; [1551-34-4]	184.1	1.4857	0.9290	−31	242
3-(2-Methylpropyl)thiophane; C ₈ H ₁₆ S; [1551-23-1]	190.5	1.4824	0.9168	−17.0	256.2
2-Hexylthiophane; C ₁₀ H ₂₀ S; [876-37-9]	239–240	1.4823	0.9005	22.0	295.2
2-Heptylthiophane; C ₁₁ H ₂₂ S; [24767-96-2]	122/1.07	1.4811	0.9114	37.0	310.2
2-Nonylthiophane; C ₁₃ H ₂₆ S; [36011-32-2]	292–293	1.4792	0.8940	65.0	338.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Samples of (1) and (2) of weight about 0.2 g were placed in glass ampoules of length 3–4 cm and inner diameter of 4 mm. After cooling in a mixture of ice with salt ampoules were sealed. Three to four ampoules were attached to a thermometer and placed in a glass bath with glycerine (for heating) or with acetone and solid CO₂ (for cooling) with continuous stirring, then heating and cooling 2 K/min. The UCST was determined by following the appearance and disappearance of the meniscus.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and purified; boiling point=81.6 °C, *n*(20 °C,D)=1.3458.
(2) Synthesized in Institute of Chemistry (Upha, Russia).

Estimated Error:

Temperature: ±0.1 K (243–373 K); ±0.5 K (below 243 K).

17.4. + 2-Undecylbenzothiazole

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	P. L. DuBrow, C. W. Hoerr, and H. J. Harwood, J. Am. Chem. Soc. 74 , 6241-5 (1952).
(2) 2-Undecylbenzothiazole; C ₁₈ H ₁₇ NS	
Variables:	Prepared By:
T/K = 273–323	Valerii P. Sazonov

Experimental Data				
Solubility of 2-undecylbenzothiazole (2) in acetonitrile (1)				
t/°C	T/K (compiler)	g ₂ /100 g ₁	100 w ₂ (compiler)	x ₂ (compiler)
0.0	273.2	0.1	0.1	0.0001
10.0	283.2	2.6	2.6	0.004
20.0	293.2	7.2	6.7	0.010
30.0	303.2	10.1	9.2	0.014
40.0	313.2	14.0	12.3	0.020
50.0	323.2	19.2	16.1	0.027

Miscible above 79 °C (352 K; compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperatures at which known concentrations precipitated upon cooling and dissolved upon heating.

Source and Purity of Materials:

(1) Source not specified; reagent grade; freshly distilled.
 (2) Prepared by the reaction of highly purified lauric acid with 2-aminobenzenethiol at elevated temperatures, using catalytic amounts of HCl; purified by vacuum distillation in a Vigreux column; freezing point=18.20 °C.

Estimated Error:

Temperature: ±0.1.

17.3. + Sulfides C₅–C₃₆

Components:	Original Measurements:
(1) Acetonitrile; C ₂ H ₅ N; [75-05-8]	R. D. Obolensov, M. N. Lebedeva, E. A. Kreis, N. K. Lyapina, and M. A. Parphenova, Neftekhimiya II , 893–901 (1971).
(2) Sulfides; C ₄ H ₈ S–C ₁₃ H ₂₆ S	
Variables:	Prepared By:
T/K = 207–450	Valerii P. Sazonov

Experimental Data				
Upper critical solution temperatures of the binary systems acetonitrile(1) + sulfide(2)				
Sulfide	Boiling point/°C/kPa	n(20 °C,D)	d(20 °C,4 °C)	T/K (compiler)
2,2'-Thiobispropane; C ₆ H ₁₄ S; [625-80-9]	120.05	1.4388	0.8195	207
1-(Ethylthio)propane; C ₅ H ₁₂ S; [4110-50-3]	118.5	1.4461	0.8370	208
(Ethylthio)benzene; C ₈ H ₁₀ S; [622-38-8]	81/1.60	1.5651	1.0284	212
(Propylthio)benzene; C ₉ H ₁₂ S; [874-79-3]	215–218	1.5530	0.9960	212
1,1'-Thiobispropane; C ₆ H ₁₄ S; [111-47-7]	142.8	1.4491	0.8377	225
1,1'-Thiobisbenzene; C ₈ H ₁₀ S; [139-66-2]	162.5/2.40	1.6325	1.1115	225
1,1'-Thiobisbutane; C ₈ H ₁₈ S; [544-40-1]	188.9	1.4529	0.8402	268.2
2,2'-Thiobisbutane; C ₈ H ₁₈ S; [626-26-6]	170.8	1.4468	0.8263	268.2
(Methylthio)benzene; C ₇ H ₈ S; [100-68-5]	194.2	1.5869	1.053	336.2
1,1'-Thiobisheptane; C ₁₄ H ₂₆ S; [629-65-2]	—	—	—	355.2
1,1'-Thiobisiodoacane; C ₃₆ H ₇₄ S; [1844-09-3]	melting point=61.5	—	—	450.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Samples of (1) and (2) of weight about 0.2 g were placed in glass ampoules of length 3–4 cm and inner diameter of 4 mm. After cooling in a mixture of ice with salt ampoules were sealed. Three to four ampoules were attached to a thermometer and placed in a glass bath with glycine (for heating) or with acetone and solid CO₂ (for cooling) with continuous stirring, then heating and cooling 2 K/min. The UCST was determined by following the appearance and disappearance of the meniscus.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and purified; boiling point=81.6 °C, n(20 °C,D)=1.3458.
 (2) Synthesized in Institute of Chemistry (Upha, Russia).

Estimated Error:

Temperature: ±0.1 K (243–373 K); ±0.3 (above 373 K); ±0.5 K (below 243 K).

17.5. + 2-Heptadecylbenzothiazole

Components:		Original Measurements:	
(1) Acetonitrile; C ₃ H ₅ N; [75-05-8]		P. L. DuBrow, C. W. Heerr, and H. J. Harwood, J. Am. Chem. Soc. 74 , 6241-5 (1952).	
(2) 2-Heptadecylbenzothiazole; C ₂₀ H ₃₁ NS			
Variables:		Prepared By:	
T/K= 313 and 323		Valerii P. Sazonov	
Experimental Data			
Solubility of 2-heptadecylbenzothiazole (2) in acetonitrile (1)			
<i>t</i> /°C	<i>T</i> /K (compiler)	<i>g</i> ₂ /100 <i>g</i> ₁	100 <i>w</i> ₂ (compiler) <i>x</i> ₂ (compiler)
40.0	313.2	<0.1	<0.1
50.0	323.2	1.0	1.0
Not miscible below 82 °C (355 K, compiler).			

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The solubilities were determined by observing visually the temperatures at which known concentrations precipitated upon cooling and dissolved upon heating.

Source and Purity of Materials:

(1) Source not specified; reagent grade; freshly distilled.
 (2) Prepared by the reaction of highly purified stearic acid with 2-aminobenzethiol at elevated temperatures, using catalytic amounts of HCl, purified by vacuum distillation in a Vigreux column; crystallized from 5% solution in ethanol; freezing point= 39.60 °C.

Estimated Error:

Temperature: ±0.1.

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	1-[(Tridecyloxy)methyl]-1,2-ethediyl ester stearic acid	1115
	Tridecyl propanoate	1092
	1,2,3-Tridodecanoyloxypropane	1114
	1,2,3-Trieicosanoyloxypropane	1114
	1,3,5-Triethylbenzene	1049
	1,2,3-Trihexadecanoyloxypropane	1114
	2,2,4-Trimethylpentane	1046
	1,2,3-Trioctadecanoyloxypropane	1114
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	1,2,3-Tris-(octadecyloxy)propane	1077
	1,2,3-Tritetradecanoyloxypropane	1114
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	Undecanoic acid	1079
	1-Undecanol	1063
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	1-[(Undecyloxy)methyl]-1,2-ethanediyl ester stearic acid	1115
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Acetonitrile- d_3 +	Water	1006
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[56-81-5]	C ₃ H ₈ O ₃	1,2,3-Propanetriol	1059
[57-10-3]	C ₁₆ H ₃₂ O ₂	Hexadecanoic acid	1081-1082
[57-11-4]	C ₁₈ H ₃₆ O ₂	Octadecanoic acid	1081, 1085
[60-33-3]	C ₁₈ H ₃₂ O ₂	cis,cis-9,12-Octadecadienioc acid	1083
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[68-05-3]	C ₈ H ₂₀ IN	Tetraethylammonium iodide	1058
[71-43-2]	C ₆ H ₆	Benzene	1027
[74-98-6]	C ₃ H ₈	Propane	1018
[75-05-8]	C ₂ H ₃ N	Acetonitrile	998-1005, 1007-1118
[75-15-0]	CS ₂	Carbon disulfide	E1007, 1008-1009
[75-69-4]	CCl ₃ F	Trichlorofluoromethane	1054
[78-78-4]	C ₅ H ₁₂	2-Methylbutane	E1022,1023-1024
[91-17-8]	C ₁₀ H ₁₈	Decahydronaphthalene	1033
[98-82-8]	C ₉ H ₁₂	(1-Methylethyl)benzene	1049
[100-68-5]	C ₇ H ₈ S	(Methylthio)benzene	1117
[102-25-0]	C ₁₂ H ₁₈	1,3,5-Triethylbenzene	1049
[106-14-9]	C ₁₆ H ₃₂ O ₂	Butyl dodecanoate	1092
[106-97-8]	C ₄ H ₁₀	Butane	E1019, 1020-1021
[108-20-3]	C ₆ H ₁₄ O	2,2'-Oxybispropane	1074
[108-87-2]	C ₇ H ₁₄	Methylcyclohexane	1033, 1040
[109-66-0]	C ₅ H ₁₂	Pentane	E1025, 1026-1027
[110-01-0]	C ₄ H ₈ S	Thiophane	1116
[110-02-1]	C ₄ H ₄ S	Thiophene	1116
[110-15-6]	C ₄ H ₆ O ₄	Butanedioic acid	1085
[110-54-3]	C ₆ H ₁₄	Hexane	1027, E1034, 1035-1038
[110-82-7]	C ₆ H ₁₂	Cyclohexane	E1028, 1029-1033
[111-06-8]	C ₂₀ H ₄₀ O ₂	Butyl hexadecanoate	1098
[111-11-5]	C ₉ H ₁₈ O ₂	Methyl octanoate	1090
[111-16-0]	C ₇ H ₁₂ O ₄	Heptanedioic acid	1087
[111-20-6]	C ₁₀ H ₁₈ O ₄	Decanedioic acid	1089
[111-47-7]	C ₆ H ₁₄ S	1,1'-Thiobispropane	1117
[111-61-5]	C ₂₀ H ₄₀ O ₂	Ethyl octadecanoate	E1097, 1098
[111-65-9]	C ₈ H ₁₈	Octane	1027, E1046-E1047, 1047-1049
[111-66-0]	C ₈ H ₁₆	1-Octene	1045
[111-82-0]	C ₁₃ H ₂₆ O ₂	Methyl dodecanoate	1090
[111-83-1]	C ₈ H ₁₇ Br	1-Bromooctane	1058
[111-84-2]	C ₉ H ₂₀	Nonane	1027

[112-05-0]	C ₉ H ₁₈ O ₂	Nonanoic acid	1078
[112-29-8]	C ₁₀ H ₂₁ Br	1-Bromodecane	1058
[112-30-1]	C ₁₀ H ₂₂ O	1-Decanol	E1060, 1061-1063
[112-37-8]	C ₁₁ H ₂₂ O ₂	Undecanoic acid	1079
[112-39-0]	C ₁₇ H ₃₄ O ₂	Methyl hexadecanoate	E1092-E1093, 1093-1094
[112-40-3]	C ₁₂ H ₂₆	Dodecane	1027, 1049
[112-42-5]	C ₁₁ H ₂₄ O	1-Undecanol	1063
[112-53-8]	C ₁₂ H ₂₆ O	1-Dodecanol	1062-1063, E1064, 1065
[112-58-3]	C ₁₂ H ₂₆ O	1-Hexoxyhexane	1075
[112-61-8]	C ₁₉ H ₃₈ O ₂	Methyl octadecanoate	1094, E1096, 1097
[112-62-9]	C ₁₉ H ₃₆ O ₂	Methyl-cis-9-octadecenoate	1095
[112-70-9]	C ₁₃ H ₂₈ O	1-Tridecanol	1063
[112-71-0]	C ₁₄ H ₂₉ Br	1-Bromotetradecane	1058
[112-72-1]	C ₁₄ H ₃₀ O	1-Tetradecanol	1063, E1066, 1067
[112-80-1]	C ₁₈ H ₃₄ O ₂	cis-9-Octadecenoic acid	1084
[112-82-3]	C ₁₆ H ₃₃ Br	1-Bromohexadecane	1058
[112-85-6]	C ₂₂ H ₄₄ O ₂	Docosanoic acid	1081
[112-89-0]	C ₁₈ H ₃₇ Br	1-Bromooctadecane	1058
[112-92-5]	C ₁₈ H ₃₈ O	1-Octadecanol	1063, E1069-E1070, 1070
[122-32-7]	C ₅₇ H ₁₀₄ O ₆	1,2,3-Tri(cis-9-octadecenoyloxy)propane	1114
[123-31-9]	C ₆ H ₆ O ₂	1,4-Benzenediol	1059
[123-95-5]	C ₂₂ H ₄₄ O ₂	Butyl octadecanoate	E1099, 1100
[123-99-9]	C ₉ H ₁₆ O ₄	Nonanedioic acid	1088
[124-04-9]	C ₆ H ₁₀ O ₄	Hexanedioic acid	E1086, 1086-1087
[124-06-1]	C ₁₆ H ₃₂ O ₂	Ethyl tetradecanoate	1092
[124-07-2]	C ₈ H ₁₆ O ₂	Octanoic acid	1078
[124-10-7]	C ₁₅ H ₃₀ O ₂	Methyl tetradecanoate	1091
[124-11-8]	C ₉ H ₁₈	1-Nonene	1045
[124-18-5]	C ₁₀ H ₂₂	Decane	1027, 1049, E1050-E1051, 1051
[124-22-1]	C ₁₂ H ₂₇ N	Dodecanamine	1102
[124-26-5]	C ₁₈ H ₃₇ NO	Dodecanamide or Octadecanamide	1110
[124-30-1]	C ₁₈ H ₃₉ N	Octadecanamine	1104
[127-18-4]	C ₂ Cl ₄	Tetrachloroethene	1056
[135-98-8]	C ₁₀ H ₁₄	(1-Methylpropyl)benzene	1049
[139-66-2]	C ₁₂ H ₁₀ S	1,1'-Thiobisbenzene	1117
[141-22-0]	C ₁₈ H ₃₄ O ₃	12-Hydroxy-cis-9-octadecenoic acid	1084
[141-93-5]	C ₁₀ H ₁₄	1,3-Diethylbenzene	1049
[142-82-5]	C ₇ H ₁₆	Heptane	1027, E1040-E1041, 1041-1045
[143-07-7]	C ₁₂ H ₂₄ O ₂	Dodecanoic acid	1080
[143-15-7]	C ₁₂ H ₂₅ Br	1-Bromododecane	1058
[143-27-1]	C ₁₆ H ₃₅ N	Hexadecanamine	1103
[143-28-2]	C ₁₈ H ₃₆ O	1-Octadecenol	1069
[334-48-5]	C ₁₀ H ₂₀ O ₂	Decanoic acid	1079
[354-58-5]	C ₂ Cl ₃ F ₃	1,1,1-Trichloro-2,2,2-trifluoroethane	1056
[375-83-7]	C ₇ HF ₁₅	1-Hydropentadecafluoroheptane	1057
[493-02-7]	C ₁₀ H ₁₈	trans-Decahydronaphthalene	1050
[502-52-3]	C ₃₅ H ₆₈ O ₅	1,3-Dihexadecanoyloxy-2-propanol	1114
[502-73-8]	C ₃₁ H ₆₂ O	16-Hentriacontanone	1073
[504-40-5]	C ₃₉ H ₇₆ O ₅	1,3-Dioctadecanoyloxy-2-propanol	1114
[504-53-0]	C ₃₅ H ₇₀ O	18-Pentatriacontanone	1074
[504-57-4]	C ₁₉ H ₃₈ O	10-Nonadecanone	1072
[505-48-6]	C ₈ H ₁₄ O ₄	Octanedioic acid	1088
[506-03-6]	C ₁₉ H ₄₀ O ₃	1-Hexadecoxy-2,3-propanediol	1076
[506-12-7]	C ₁₇ H ₃₄ O ₂	Heptadecanoic acid	1083
[506-30-9]	C ₂₀ H ₄₀ O ₂	Eicosanoic acid	1081
[506-43-4]	C ₁₈ H ₃₄ O	1-Octadecadienol	1069
[535-77-3]	C ₁₀ H ₁₄	1-Methyl-3-(1-methylethyl)benzene	1049
[537-39-3]	C ₅₇ H ₁₀₄ O ₆	1,2,3-Tri(trans-9-octadecenoyloxy)propane	1114
[537-40-6]	C ₅₇ H ₉₈ O ₆	1,2,3-Tri(cis,cis,cis-9,12-octadecadienoyloxy) propane	1114
[538-24-9]	C ₃₉ H ₇₄ O ₆	1,2,3-Tridodecanoyloxypropane	1114
[540-09-0]	C ₂₃ H ₄₆ O	12-Tricosanone	1072
[540-84-1]	C ₈ H ₁₈	2,2,4-Trimethylpentane	1046
[540-10-3]	C ₃₂ H ₆₄ O ₂	Hexadecyl hexadecanoate	1095, 1101
[542-50-7]	C ₂₇ H ₅₄ O	14-Heptacosanone	1073
[544-40-1]	C ₈ H ₁₈ S	1,1'-Thiobisbutane	1117
[544-62-7]	C ₂₁ H ₄₄ O ₃	1-Octadecoxy-2,3-propanediol	1076
[544-63-8]	C ₁₄ H ₂₈ O ₂	Tetradecanoic acid	1081
[544-76-3]	C ₁₆ H ₃₄	Hexadecane	1027, 1049, E1052, 1053

[555-43-1]	C ₅₇ H ₁₁₀ O ₆	1,2,3-Trioctadecanoyloxypropane	1114
[555-44-2]	C ₅₁ H ₉₈ O ₆	1,2,3-Trihexadecanoyloxypropane	1114
[555-45-3]	C ₄₅ H ₈₆ O ₆	1,2,3-Tritetradecanoyloxypropane	1114
[557-59-5]	C ₂₄ H ₄₈ O ₂	Tetracosanoic acid	1081
[592-76-7]	C ₇ H ₁₄	1-Heptene	E1038, 1039
[593-31-7]	C ₂₁ H ₄₂ O ₃	1-(trans-9-Octadecenoyloxy)-2,3-propanediol	1076
[593-45-3]	C ₁₈ H ₃₈	Octadecane	1027, 1049
[620-64-4]	C ₆₃ H ₁₂₂ O ₆	1,2,3-Trieicosanoyloxypropane	1114
[621-71-6]	C ₃₃ H ₆₂ O ₆	1,2,3-Tridecanoyloxypropane	1114
[622-38-8]	C ₈ H ₁₀ S	(Ethylthio)benzene	1117
[625-80-9]	C ₆ H ₁₄ S	2,2'-Thiobispropane	1117
[626-26-6]	C ₈ H ₁₈ S	2,2'-Thiobisbutane	1117
[629-01-6]	C ₈ H ₁₇ NO	Octanamide	1107
[629-65-2]	C ₁₄ H ₃₀ S	1,1'-Thiobisheptane	1117
[629-54-9]	C ₁₆ H ₃₃ NO	Hexadecanamide	1109
[629-59-4]	C ₁₄ H ₃₀	Tetradecane	1027, 1049
[629-63-0]	C ₁₄ H ₂₇ N	Tetradecanenitrile	1106
[629-64-1]	C ₁₄ H ₃₀ O	1-Heptoxyheptane	1075
[629-70-9]	C ₁₈ H ₃₆ O ₂	Hexadecyl ethanoate	1095
[629-76-5]	C ₁₅ H ₃₂ O	1-Pentadecanol	1063
[629-79-8]	C ₁₆ H ₃₁ N	Hexadecanenitrile	1106
[629-82-3]	C ₁₆ H ₃₄ O	1-Octoxyoctane	1075
[629-96-9]	C ₂₀ H ₄₂ O	1-Eicosanol	1063
[631-40-3]	C ₁₂ H ₂₈ IN	Tetrapropylammonium iodide	1058
[635-89-2]	C ₁₆ H ₂₆	1,2-Dipentylbenzene	1049
[637-54-7]	C ₂₄ H ₄₁ NO	N-Phenyltadecanamide	1112
[638-53-9]	C ₁₃ H ₂₆ O ₂	Tridecanoic acid	1080
[638-58-4]	C ₁₄ H ₂₉ NO	Tetradecanamide	1108
[638-65-3]	C ₁₈ H ₃₅ N	Octadecanenitrile	1106
[638-66-4]	C ₁₈ H ₃₆ O	Octadecanal	1071
[693-65-2]	C ₁₀ H ₂₂ O	1,1'-Oxybispentane	1075
[822-23-1]	C ₂₀ H ₄₀ O ₂	Octadecyl ethanoate	1098
[822-24-2]	C ₂₂ H ₄₄ O ₂	Eicosyl ethanoate	1100
[872-05-9]	C ₁₀ H ₂₀	1-Decene	1045
[874-79-3]	C ₉ H ₁₂ S	(Propylthio)benzene	1117
[876-37-9]	C ₁₀ H ₂₀ S	2-Hexylthiophane	1116
[923-62-6]	C ₅₇ H ₁₁₂ O ₅	1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester stearic acid	1115
[923-63-7]	C ₅₅ H ₁₀₈ O ₅	1-[(Hexadecyloxy)methyl]-1,2-ethanediyl ester stearic acid	1115
[929-77-1]	C ₂₃ H ₄₆ O ₂	Methyl docosanoate	1094
[1002-84-2]	C ₁₅ H ₃₀ O ₂	Pentadecanoic acid	1082
[1069-46-1]	C ₆ H ₁₀ N ₂ O ₅	6-(Hydroxyimino)-6-nitrohexanoic acid	1077
[1120-16-7]	C ₁₂ H ₂₅ NO	Dodecanamide	1108
[1120-21-4]	C ₁₁ H ₂₄	Undecane	1027
[1120-28-1]	C ₂₁ H ₄₂ O ₂	Methyl eicosanoate	1094
[1186-49-8]	C ₂ HNaO ₄	Ethanoic acid monosodium salt	1089
[1190-63-2]	C ₃₄ H ₆₈ O ₂	Hexadecyl octadecanoate	1095
[1454-84-8]	C ₁₉ H ₄₀ O	1-Nonadecanol	1063
[1454-85-9]	C ₁₇ H ₃₆ O	1-Heptadecanol	1063
[1455-20-5]	C ₈ H ₁₂ S	2-Butylthiophene	1116
[1460-98-6]	C ₁₃ H ₂₀	1-Methyl-2,4-bis(1-methylethyl)benzene	1049
[1551-23-1]	C ₈ H ₁₆ S	3-(2-Methylpropyl)thiophane	1116
[1551-34-4]	C ₇ H ₁₄ S	2-Propylthiophane	1116
[1561-07-5]	C ₁₅ H ₃₂ O ₃	1-Dodecoxy-2,3-propanediol	1076
[1613-49-6]	C ₈ H ₁₆ S	2-Butylthiophane	1116
[1653-30-1]	C ₁₁ H ₂₄ O	2-Undecanol	1063
[1653-31-2]	C ₁₃ H ₂₈ O	2-Tridecanol	1063
[1653-34-5]	C ₁₅ H ₃₂ O	2-Pentadecanol	1063
[1654-86-0]	C ₂₀ H ₄₀ O ₂	Decyl decanoate	1098
[1716-07-0]	C ₅₅ H ₁₀₂ O ₆	2-Hexadecanoyloxy-1,3-di(cis-9-octadecenoyloxy) propane	1114
[1731-88-0]	C ₁₄ H ₂₈ O ₂	Methyl tridecanoate	1091
[1731-94-8]	C ₂₀ H ₄₀ O ₂	Methyl nonadecanoate	1098
[1844-09-3]	C ₃₆ H ₇₄ S	1,1'-Thiobisoctadecane	1117
[1908-11-8]	C ₃₉ H ₆₈ O ₂	Cholest-5-en-3-ylidodecanoate	1101
[1975-78-6]	C ₁₀ H ₁₉ N	Decanenitrile	1104
[1978-24-1]	C ₈ F ₁₆ O	Hexadecafluorooxoctane	1057
[1989-52-2]	C ₄₁ H ₇₂ O ₂	Cholest-5-en-3-yltetradecanoate	1101
[2016-42-4]	C ₁₄ H ₃₁ N	Tetradecanamine	1103
[2016-57-1]	C ₁₀ H ₂₃ N	Decanamine	1102

[2050-24-0]	C ₁₁ H ₁₆	1-Methyl-3,5-diethylbenzene	1049
[2206-26-0]	C ₂ D ₃ N	Acetonitrile-d ₃	1006
[2306-88-9]	C ₁₆ H ₃₂ O ₂	Octyl octanoate	1092
[2319-29-1]	C ₁₀ H ₂₁ NO	Decanamide	1107
[2410-29-9]	C ₅₇ H ₁₀₆ O ₆	2-Octadecanoyloxy-1,3-di(cis-9-octadecenoyloxy) propane	1114
[2423-10-1]	C ₁₈ H ₃₄ O	cis-9-Octadecenal	1071
[2437-25-4]	C ₁₂ H ₂₃ N	Dodecanenitrile	1105
[2456-28-2]	C ₂₀ H ₄₂ O	1-Decoxydecane	1075
[2599-01-1]	C ₃₀ H ₆₀ O ₂	Hexadecyl tetradecanoate	1095, 1101
[2719-52-0]	C ₁₁ H ₁₆	(1-Methylbutyl)benzene	1049
[2752-99-0]	C ₆₉ H ₁₂₈ O ₆	1,2,3-Tri(cis-13-docosenoyloxy)propane	1114
[2922-55-6]	C ₃ H ₃ NaO ₄	Propanedioic acid monosodium salt	1089
[2922-54-5]	C ₄ H ₅ NaO ₄	Butanedioic acid monosodium salt	1089
[2929-07-9]	C ₂₁ H ₄₂ O ₃	1-(cis-9-Octadecenoxy)-2,3-propanediol	1076
[3343-88-2]	C ₅ H ₇ NaO ₄	Pentanedioic acid monosodium salt	1089
[3430-95-3]	C ₁₈ H ₂₉ NO	N-Phenyldodecanamide	1110
[3634-92-2]	C ₂₁ H ₄₂ O ₂	Propyl octadecanoate	1099
[3724-61-6]	C ₁₆ H ₃₂ O ₂	Dodecyl butanoate	1092
[4110-50-3]	C ₅ H ₁₂ S	1-(Ethylthio)propane	1117
[4218-48-8]	C ₁₁ H ₁₆	1-Ethyl-4-(1-methylethyl)benzene	1049
[4536-26-9]	C ₃₀ H ₆₀ O ₂	Tetradecyl hexadecanoate	1101
[4706-81-4]	C ₁₄ H ₃₀ O	2-Tetradecanol	1063
[4813-58-5]	C ₁₆ H ₃₄ O	1-Ethoxytetradecane	1075
[5303-24-2]	C ₂₀ H ₄₀ O ₂	Octyl dodecanoate	1098
[5896-48-0]	C ₅₁ H ₁₀₄ O ₃	1-(Dodecyloxy)-2,3-bis(octadecyloxy)propane	1077
[6064-90-0]	C ₂₂ H ₄₄ O ₂	Methyl heneicosanoate	1100
[6068-26-4]	C ₄₁ H ₈₄ O ₃	2-(Eicosyloxy)-3-(octadecyloxy)-1-propanol	1076
[6068-27-5]	C ₄₉ H ₁₀₀ O ₃	1-(Dodecyloxy)-2-(hexadecyloxy)-3-(octadecyloxy)propane	1077
[6076-35-3]	C ₃₅ H ₇₂ O ₃	2,3-Bis(hexadecyloxy)-1-propanol	1076
[6076-36-4]	C ₃₃ H ₆₈ O ₃	2-(Dodecyloxy)-3-(octadecyloxy)-1-propanol	1076
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[6076-38-6]	C ₃₉ H ₈₀ O ₃	2,3-Bis(octadecyloxy)-1-propanol	1076
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