IUPAC-NIST Solubility Data Series 71. Nitromethane with Water or Organic Solvents: Binary Systems

Volume Editors
Valerii P. Sazonov[a)]
Technical University, Samara, Russia

Kenneth N. Marsh
University of Canterbury, Christchurch, New Zealand

Glenn T. Hefter
Murdoch University, Perth, Australia
With the assistance of
Evaluators: Valerii P. Sazonov and Glenn T. Hefter
Compilers: Valerii P. Sazonov, Nikolai V. Sazonov, and Anatolii V. Morozov

Received February 10, 2000; accepted February 10, 2000

The mutual solubilities and liquid–liquid equilibrium of nitromethane binary systems with liquid solvents are reviewed. The solvents include water, inorganic compounds, and a variety of organic compounds as hydrocarbons, halogenated hydrocarbons, alcohols, acids, esters, and nitrogen compounds. A total 474 systems published through 1993 are compiled. For 39 systems sufficient data were 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 were published in the frame of Solubility Data Series.
[S0047-2689(00)00505-5]

Key words: solubility; liquid-liquid equilibrium; organic solvents; nitromethane; aqueous solution.

Contents

[a)]Electronic mail: sazonov@star.sstu.samara.ru

*The Critical Evaluation is prepared for this system.

List of Figures

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 nitromethane. Second components for which data were found in the chemical literature include water, organic substances of various classes (hydrocarbons of several structural types, halogenated hydrocarbons, mono and polyhydroxy alcohols, mono and polybasic acids, ethers, esters), rare gases, and inorganic substances. An exhaustive search of the chemical literature published prior to 1993 found solubility data for 474 systems. From these, 235 Compilations 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, those 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 39 systems, reflecting the sparseness of study of many nitromethane systems. The systems are ordered on the basis of the chemical formula according to the Hill system (described in the Introduction), with the exception of those compilations ordered on the basis of the chemical formula according where 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 nitromethane in the second component and the solubility of the second component in nitromethane 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 1993). 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 are 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 as well as in units reported in the original source. Conversions, where they were made, are clearly attributed to the compiler. Some unit conversions require numerical data for the density of pure components and/or the mixtures. Approximate values of mixture densities 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.

In a few systems where the second component is a gas, solubility data have been reported originally as the Ostwald coefficient (L). This dimensionless value is the volume of saturating gas absorbed by a volume of pure solvent at the temperature and pressure of the measurement. Thus, the Ostwald coefficient is equal to the ratio of the amount concentrations in the gas and in the liquid.

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 208 K (Nitromethane+1,2,3-Trimethylbenzene) to 471 K (Nitromethane+Cholest-5-yldocosanoate) while the range of pressure examined extends from 0.1 to 50 MPa (Nitromethane+1,2-Ethanediol). Three basic approaches to solubility measurement for binary systems are known: synthetic, titration, and analytical. Of these the synthetic (visual-polythermal, or cloud-point) method is most commonly used. Almost 80% (185) 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.[3] The method has been refined and improved by Rothmund,[4] and by Timmermans[5] 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 nitromethane 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 nitromethane and alcohols) or increase these temperatures (e.g., in mixtures of nitromethane and hydrocarbons).[6]

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 as 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 $(\mathrm{d}T_c/\mathrm{d}P)$ 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. The resulting mean is referred to as the ‘‘best’’ value. However, the user should note that these ‘‘best’’ values represent the best available data and vary in quality among evaluated systems.

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 many Critical Evaluations presented in this volume, when the UCST of the system was available, data have been described by the equation based on the scaling law. This equation allows for interpolation and some extrapolation of the data for the system. It is presented in the next chapter; some details and background have been also presented in the preface to the IUPAC SDS Vol. 56.[2]

For the series, alcohol–nitromethane, hydrocarbon–nitromethane, and acid–nitromethane systems, there were a sufficient number of systems, in each group, measured in independent laboratories to find the general rules of solubility behavior in the series. The obtained rules have been reported and discussed for temperature and composition at the critical point below in the chapter ‘‘Relation of Solubility Data for Binary Systems Containing Nitromethane.’’

The editors wish to acknowledge with thanks the help of Professor R. Riccardi (Italy) and Dr. I. K. Zhuravleva (Russia) who provided us with copies of several of the articles reviewed in this volume.

1.4. References for the Preface

[1] R. C. Reid, J. M. Prauznitz, and B. E. Poling, *The Properties of Gases and Liquids*, 4th ed. (McGraw-Hill, New York, 1987).
[2] D. Shaw, A. Skrzecz, J. W. Lorimer, and A. Maczynski, *Alcohols with Hydrocarbons*, IUPAC Solubility Data Series, Vol. 56 (Oxford University Press, Oxford, UK, 1994).
[3] V. F. Alekseev, Zh. Fiz.-Khim. O-va **8**, 249 (1876).
[4] V. Rothmund, Z. Phys. Chem. **26**, 433 (1898).
[5] J. Timmermans, Z. Phys. Chem. **58**, 129 (1907).
[6] V. P. Sazonov, Zh. Obshch. Khim. **42**, 1884 (1972).
[7] V. P. Sazonov, Samara, Russia, July, 1999

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 or 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

Chemical Abstracts 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 Chemical Abstracts names in the System Index. The formula is given either in terms of the IUPAC or Hill[1] 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) non-saturating components in alphanumerical order;
(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 to 12: transition elements

Columns 13 to 17: boron, carbon, nitrogen groups, chalcogenides, halogens

Column 18: noble gases

Row 1: Ce to 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
(f) alphabetically by IUPAC name.

Example:

C_5H_8	cyclopentane
	2-methyl-1,3-butadiene
	1,4-pentadiene
	1-pentyne
C_5H_{10}	cyclopentane
	3-methyl-1-butene
	2-methyl-2-butene
	1-pentene
	2-pentene
C_5H_{12}	2,2-dimethylpropane
	2-methylbutane
	pentane
$C_5H_{12}O$	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
$C_6H_{12}O$	cyclohexanol
	4-methyl-1-penten-3-ol
	1-hexen-3-ol
	4-hexen-3-ol

Deuterated (^2H) compounds follow immediately 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 in Refs. 1 and 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 recommendations[3] 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 is 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 Refs. 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 units[3] 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 references 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 standards[8] or the German standard;[9] see a review by Cvitaš[10] for details.

A note on nomenclature

The nomenclature of the IUPAC Green Book[3] 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):

$$x_1 = n_1 \Big/ \sum_{s=1}^{c} n_s , \tag{1}$$

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 s 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 non-electrolytes j, of which some may be solvent components, a generalization of the definition in Ref. 11 gives:

$$x_{i+} = \frac{\nu_{i+} x_{1+}}{1 + \Sigma_{i=1}^{s} (\nu_i - 1) x_s}, \quad x_{i-} = \frac{\nu_{i-} x_{1-}}{\nu_{1+}}, \quad i = 1,.....s, \tag{2}$$

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

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

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

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

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

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]

$$w_1 = g_1 \Big/ \sum_{s=1}^{c} g_s , \tag{6}$$

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 $g(1)/100$ *g solution* are no longer used.

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

$$m_1 = n_1 / n_2 M_2 . \tag{7}$$

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), $m_1^{(3)}$:

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

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

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

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:

$$c_1 = [\text{formula of solute}] = n_1/V. \tag{10}$$

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}.

$$\rho_1 = g_1/V. \tag{11}$$

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

$$r_{\mathrm{A,B}} = n_1/n_2 \tag{12}$$

Mass ratio, symbol $\zeta_{\mathrm{A,B}}$, 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:

$$\rho = g/V. \tag{13}$$

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

10. *Relative density*, $d = \rho/\rho^0$: 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

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

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

[3] I. Mills *et al.*, eds, *Quantities, Units and Symbols in Physical Chemistry* (The Green Book) (Blackwell Scientific, Oxford, UK, 1993).

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

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

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

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

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

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

[10] T. Cvitaš, Chem. International **17**, No. 4, 123 (1995).

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

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

This section was written by:

A. F. M. Barton	Perth, WA, Australia
G. T. Hefter	Perth, WA, Australia
F. W. Getzen	Raleigh, NC, USA
D. G. Shaw	Fairbanks, AK, USA

December, 1995

3. Relations of Solubility Data for Binary Systems Containing Nitromethane

Nitromethane is partially miscible in binary systems formed by various organic substances as hydrocarbons, halogenated hydrocarbons, alcohols, acids, ethers, esters, etc., and forms the miscibility gap with the Upper Critical Solubility Point (UCSP). The UPCP is represented by Upper Critical Solubility Temperature (UCST or written also as T_c) and Upper Critical Solubility Concentration (UCSC or written also as x_c). It is related to the large dipole moment of nitromethane (3.2 D) and its molecular structure which causes association of the pure substance as well as in mixtures. This volume of Solubility Data Series reviews experimental solubility, mutual solubility, and UCSP data reported in the literature.

3.1. Description of Data

The solubility data for the particular system in which UCSP appears, could be described by the equation based on the scaling law with the correction terms for which details have been presented in original papers.[1,2,9] This equation has also been discussed in detail by Lorimer, Skrzecz and Maczynski in the preface to the IUPAC Solubility Data Series Vol. 56.[5] The equation has the form:

$$x_1 = x_{\mathrm{c}1} + b_1 \cdot \Theta + b_2 \cdot \Theta^{1-\alpha} + b_3 \cdot \Theta^{1-\alpha+\omega} \pm a_1 \cdot \Theta^{\beta} \pm a_2 \cdot \Theta^{\beta+\omega} \pm a_3 \cdot \Theta^{\beta+2\omega}, \tag{1}$$

where

$$\Theta = (T_\mathrm{c} - T)/T_\mathrm{c}. \tag{2}$$

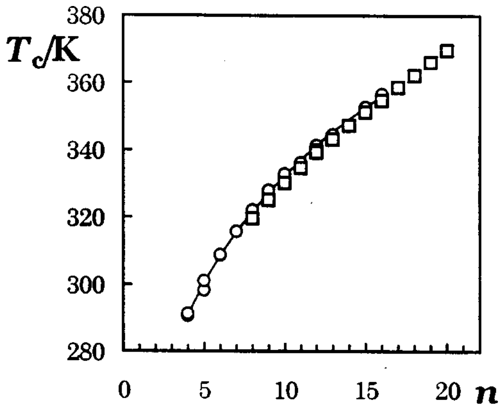

FIG. 1. T_c in the series nitromethane–n-alcohol as a function of carbon atoms of alcohol: (○) experimental T_c reported in literature, (□) experimental T_c reported in Ref. 6, and (—) calculated by Eq. (3).

The a_i, b_i are the adjustable parameters. According to the above literature, the equation factors are assumed to be: $\beta = 0.329$; $\alpha = 0.11$; $\omega = 0.5$. The equation is valid usually when $(T_c - T)/T_c > 10^{-3}$,[8] 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 experimental solubility data reported in the literature for binary systems containing nitromethane are scattered significantly one to another which presumably is the result of experimental errors, purity of components, contents of trace water, etc. Even small amounts of impurities could have a large influence on the UCST, while the influence on the UCSC is much smaller. Therefore the knowledge of the real UCST value is very important for proper evaluation of solubility data in any system. The relationship in the series of similar systems helps to solve this problem.

In binary systems containing nitromethane, in the series described below, the calculation of the UCST and UCSC relationships have been always made after rejection of the outliers. For nitromethane–n-alcohol and nitromethane–n-alkanoic acid, experimental values of the UCST and UCSC have been used to find the respective relationships in the series. The weighting factor has been taken as unity for each reported value.

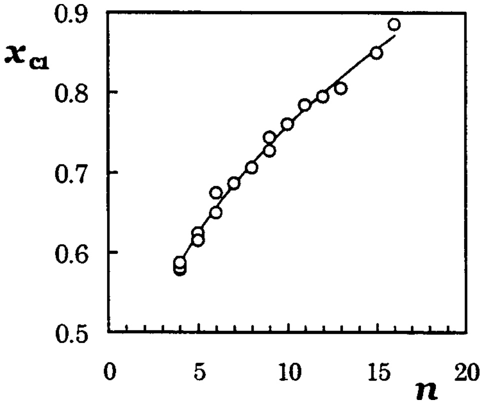

FIG. 2. x_{c1} in the series nitromethane–n-alcohol as a function of carbon atoms of alcohol: (○) experimental x_{c1} reported in literature, and (—) calculated by Eq. (4).

The references, data, and detailed information of each of the discussed systems have been presented as compilation and evaluation tables reported further.

3.2. Nitromethane–*n*-Alcohol Systems

The experimental solubility data of the binary nitromethane-n-alcohol systems have been reported in the literature at temperatures over 278 K. In many cases the highest observed temperatures were very close or equal to the UCST of the particular system. Using the above procedure, the following equations have been found to describe the relationships in the nitromethane–n-alcohol series (from butanol to hexadecanol; n—number of carbon atoms):

$$T_c/\mathrm{K} = 231.72 + 0.791 \cdot n + 40.34 \cdot \ln(n) \quad n \leqslant 16, \quad (3)$$

$$x_{c1} = 0.3733 + 0.0088 \cdot n + 0.1289 \cdot \ln(n) \quad n \leqslant 16. \quad (4)$$

The obtained relationships for the UCST and UCSC, together with experimental values are presented in Figs. 1 and 2 and in Table 1 (these values were used during evaluation of the systems). The mean standard errors of estimate in the series were 0.62 K and 0.0092 mole fraction, for Eqs. (3) and (4), respectively. The experimental values of the UCST reported by Schmid *et al.*[6] for 13 systems from octanol up to eicosanol, have been rejected in calculations of the UCST function, because they were systematically lower than other experimental results. The extrapolation to the systems containing higher alcohols gave satisfactory results.

TABLE 1. Calculated UCST and UCSC for the nitromethane-n-alcohol systems

n	T_c	x_{c1}	n	T_c	x_{c1}
4	290.8	0.587	13	345.5	0.818
5	300.6	0.625	14	349.3	0.837
6	308.7	0.657	15	352.8	0.854
7	315.8	0.685	16	356.2	0.871
8	321.9	0.711	17	359.5	—
9	327.5	0.735	18	362.6	—
10	332.5	0.758	19	365.5	—
11	337.2	0.779	20	368.4	—
12	341.5	0.799			

3.3. Nitromethane–*n*-Alkane Systems

The UCST data for nitromethane–n-alkane systems (C_5–C_9) measured by Riccardi *et al.*[3] were correlated with reasonable success by the authors by the similar equation:

$$T_c/\mathrm{K} = 346.05 + 4.57 \cdot n. \quad (5)$$

In the present studies, there have been taken into account all recommended/tentative values of UCST from evaluation tables of the binary nitromethane–n-alkane systems from

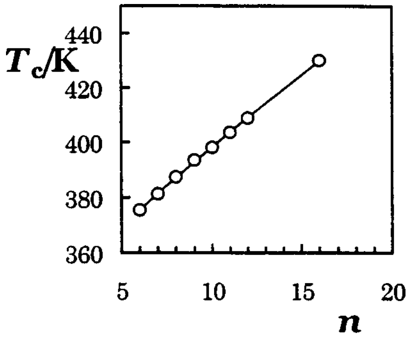

FIG. 3. T_c in the series nitromethane–n-alkane as a function of carbon atoms of alkane: (○) experimental T_c reported in literature, and (—) calculated by Eq. (6).

hexane up to hexadecane. These values have been compared and approximated by the models to find the relationship as a function of carbon atoms. The aim was to calculate UCST and UCSC values consistent in the series. The following equations have been found to describe the relationships in the series:

$$T_c/\mathrm{K}=331.17+4.472\cdot n+9.767\cdot\ln(n)\quad n\leqslant 16, \tag{6}$$

$$x_{c1}=-0.0086-0.0132\cdot n+0.3840\cdot\ln(n)\quad n\leqslant 16. \tag{7}$$

The obtained relationships for the UCST and UCSC, together with experimental values are presented in Figs. 3 and 4, and in Table 2. The mean standard errors of estimate in the series were 0.32 K and 0.0048 mole fraction, for Eqs. (6) and (7), respectively.

For the nitromethane–hexadecane system, the UCST measured by Schmid *et al.*[7] is lower over nearly 6 K than the value reported by Rogalski and Stryjek.[4] From the above relationship we found that this last value is in very good agreement with the value calculated in the series by Eq. (6). It makes a suggestion that data of Schmid and his co-workers are less accurate (also for other nitromethane systems) so they ought to be rejected or treated with lower weighting factor.

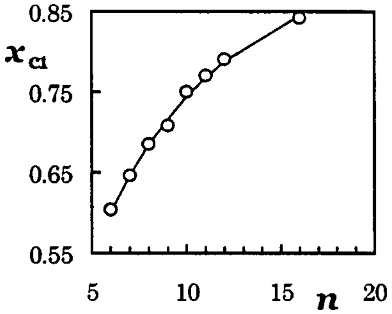

FIG. 4. x_{c1} in the series nitromethane–n-alkane as a function of carbon atoms of alkane: (○) experimental x_{c1} reported in literature, and (—) calculated by Eq. (7).

TABLE 2. Calculated UCST and UCSC for the nitromethane–n-alkane systems

n	T_c	x_{c1}	n	T_c	x_{c1}
6	375.5	0.600	10	398.4	0.744
7	381.5	0.646	11	403.8	0.767
8	387.3	0.684	12	409.1	0.787
9	392.9	0.716	16	429.8	0.845

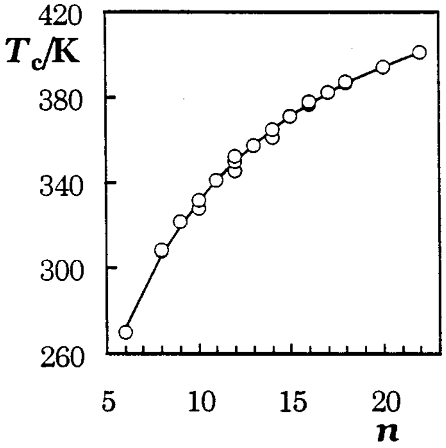

FIG. 5. T_c in the series nitromethane–n-alkanoic acid as a function of carbon atoms of acid: (○) experimental T_c reported in literature, and (—) calculated by Eq. (8).

3.4. Nitromethane–*n*-Alkanoic Acid Systems

All experimental values of UCST reported in compilation tables of the binary nitromethane–n-alkanoic acid systems (from hexanedioic acid to docosanoic acid) have been compared and approximated by the models to find the relationship as a function of carbon atoms. The aim of these calculations was to obtain UCST and UCSC values consistent in the series. The following equations have been found to describe the relationships in the series nitromethane–n-alkanoic acid systems:

$$T_c/\mathrm{K}=39.50-3.410\cdot n+141.274\cdot\ln(n)\quad n\leqslant 22, \tag{8}$$

$$x_{c1}=0.4531+0.1497\cdot\ln(n)\quad n\leqslant 18. \tag{9}$$

The obtained relationships for the UCST and UCSC, together with experimental values are presented in Figs. 5 and 6 and in Table 3. The mean standard errors of estimate in the series were 1.79 K and 0.0060 mole fraction, for Eqs. (8) and (9), respectively. The description of x_{c1} ought to be treated only as a rough estimation because the input data were of low quality.

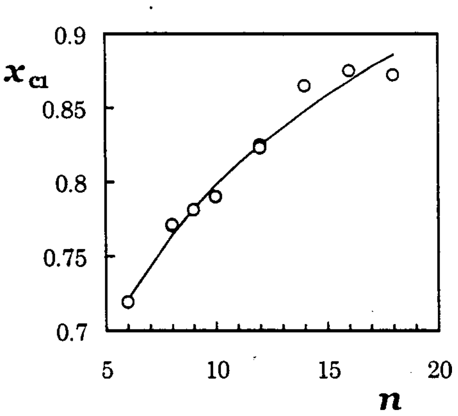

FIG. 6. x_{c1} in the series nitromethane–n-alkanoic acid as a function of carbon atoms of acid: (○) experimental x_{c1} reported in literature, and (—) calculated by Eq. (9).

TABLE 3. Calculated UCST and UCSC for the nitromethane–n-alkanoic acid systems

N	T_c	x_{c1}	n	T_c	x_{c1}
6	272.2	0.721	14	364.6	0.848
8	306/0	0.764	15	370.9	0.859
9	319.2	0.782	16	376.6	0.868
10	330.7	0.798	17	381.8	0.878
11	340.8	0.812	18	386.5	0.886
12	349.6	0.825	20	394.5	—
13	357.5	0.837	22	401.2	—

Conclusions

The obtained relationships of UCST and UCSC in the series of binary systems containing nitromethane, nitromethane systems, as functions of the second component carbon number, are consistent with one another, show outliers, allow for interpolation, and some extrapolations. These relationships were very useful during evaluation of the discussed systems.

Symbols

T–solubility temperature of a mixture, K;
T_c–temperature at UCSP, K, (UCST);
x_i–concentration of component in a mixture, mole fraction;
x_{ci}–concentration of component in a mixture at UCSP, mole fraction, (UCSC);
a_i, b_i–adjustable parameters of Eqs. (1) and (2).
n–number of carbon atoms in the molecule.

3.5. References

[1] M. Ley-Koo and M. S. Green, Phys. Rev. A **16**, 2483 (1977).
[2] M. Ley-Koo and M. S. Green, Phys. Rev. A **23**, 2650 (1981).
[3] R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816 (1968).
[4] M. Rogalski and R. Stryjek, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **28**, 139 (1980).
[5] D. Shaw, A. Skrzecz, J. W. Lorimer, and A. Maczynski, *Alcohols with Hydrocarbons*, IUPAC Solubility Data Series, Vol. 56. (Oxford University Press, Oxford, UK, 1994).
[6] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).
[7] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).
[8] R. R. Singh and W. A. van Hook, J. Chem. Phys. **87**, 6088 (1987).
[9] F. J. Wegner, Phys. Rev. B **5**, 4529 (1972).

Section 3 was written by:

Adam Skrzecz
Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.

Nikolai V. Sazonov
Technical University, Samara, Russia.

4. Nitromethane+Water

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Evaluator:
V. P. Sazonov, Technical University, Samara, Russia
September, 1999

Critical Evaluation

Quantitative solubility data for the nitromethane+water have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Wright *et al.*[2]	298	Mutual	Viscosimetric
Fowler and Hunt[3]	298 and 357	Mutual	Titration
Schumacher and Hunt[4]	298 and 357	Mutual	Refractometric
Corelli[5]	268–377	Mutual	Synthetic
Donahue and Bartell[6]	298	Mutual	Interferometric
Skrzec and Murphy[7]	300	Mutual	Titration
Friedman and Hauger[8]	298	Mutual	Not stated
Schuberth[9]	293–358	Mutual	Synthetic/titration
Mel'nikova[10]	280–378	Mutual	Synthetic
Schuberth and Kranke[11]	293–333	Mutual	Synthetic/titration
Erofeeva and Yunnikova[12]	278–377	Mutual	Synthetic
Zhuravlev and Maslovskaya[13]	293 and 313	Mutual	Titration
Hampe[14]	293	Mutual	Not stated
Sazonov[15]	294–339	Mutual	Synthetic
Rezanova *et al.*[16]	298–333	Mutual	Titration
Stephenson[17]	273–363	Mutual	Not stated

In addition to these data, Timmermans[1] determined the upper critical solution temperature and critical solution composition and the solubilities of nitromethane in water-d_2 ,D_2O, have been reported, by Rabinovich *et al.*[18] All original data are compiled in the data sheets immediately following this Critical Evaluation. From the available data (Table 1), those of Erofeeva and Yunnikova[12] were excluded as only a graphical presentation was given. The data of Donahue and Bartell,[6] Friedman and Hauger[8] (water-rich phase data only), Zhuravlev and Maslovskaya[13] (water-rich phase data only), disagree markedly from all other studies and are rejected. All other reported data are included in the tables below (Tables 2 and 3). Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). ''Best'' values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be 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 (±5% relative) agreement. All other data are regarded as tentative only.

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

	Solubility, w_1	''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_1	x_1
268	8.965 (Ref. 5)	9.0	0.028
273	9.3*(Ref. 5), 9.0 (Ref. 17)	9.2±0.2 (R)	0.029
278	9.6*(Ref. 5), 9.4*(Ref. 17)	9.5±0.1 (R)	0.030
283	10.0*(Ref. 5), 10.1*(Ref. 10), 9.8*(Ref. 17)	10.0±0.1 (R)	0.0320
288	10.7*(Ref. 5), 10.71 (Ref. 9), 11.1*(Ref. 10), 10.6 (Ref. 11)	10.3±0.2 (R)	0.0328
293	11.1 (Ref. 14), 10.4*(Ref. 17)	10.8±0.2 (R)	0.0345
298	10.0 (Ref. 2), 11.03 (Ref. 3), 11.03 (Ref. 4), 11.3*(Ref. 5), 10.6 (Ref. 8), 11.1*(Ref. 9), 11.6*(Ref. 10), 11.2*(Ref. 11), 11.2*(Ref. 15), 11.2 (Ref. 16), 11.1*(Ref. 17)	11.0±0.3 (R)	0.0352
303	11.8*(Ref. 5), 11.52 (Ref. 9), 12.1*(Ref. 10), 11.8 (Ref. 11), (Ref. 15), 11.8(Ref. 16), 11.6*(Ref. 17)	11.8±0.2 (R)	0.0380
308	12.3*(Ref. 5), 12.2*(Ref. 9), 12.8*(Ref. 10), 12.5*(Ref. 11), 12.4*(Ref. 15), 12.4*(Ref. 16), 12.2*(Ref. 17)	12.4±0.2 (R)	0.0401
313	13.1*(Ref. 5), 12.79 (Ref. 9), 13.5*(Ref. 10), 13.2 (Ref. 11), 13.3 (Ref. 15), 12.9 (Ref. 16), 12.7*(Ref. 17)	13.1±0.3 (R)	0.0426
318	13.9*(Ref. 5), 13.7*(Ref. 9), 14.2*(Ref. 10), 14.1*(Ref. 11), 13.9*(Ref. 15), 13.8*(Ref. 16), 13.8*(Ref. 17)	13.9±0.2 (R)	0.0455
323	14.8*(Ref. 5), 14.59 (Ref. 9), 15.2*(Ref. 10), 14.9*(Ref. 11), 14.3 (Ref. 16) 14.8 (Ref. 17)	14.8±0.3 (R)	0.0488
328	15.7*(Ref. 5), 15.7*(Ref. 9), 16.5*(Ref. 10), 16.0 (Ref. 11)	16.0±0.3 (R)	0.0532
333	16.8*(Ref. 5), 16.76 (Ref. 9), 17.7 (Ref. 10), 17.0*(Ref. 11), 15.4 (Ref. 16)	16.7±0.7 (R)	0.0559
338	18.1*(Ref. 5), 18.1*(Ref. 9), 18.8*(Ref. 10)	18.3±0.3 (R)	0.0620
343	19.5*(Ref. 5), 19.39 (Ref. 9), 19.9*(Ref. 10)	19.6±0.2 (R)	0.0671
348	21.4*(Ref. 5), 20.9*(Ref. 9), 21.2*(Ref. 10)	21.2±0.2 (R)	0.0736
353	23.5*(Ref. 5), 22.30 (Ref. 9), 23.5*(Ref. 10)	23.1±0.6 (R)	0.0815
358	25.7*(Ref. 5), 23.89 (Ref. 9), 25.8*(Ref. 10)	25.1±0.9 (R)	0.0900
363	29.1*(Ref. 5), 28.7*(Ref. 10)	28.9±0.2 (R)	0.107
368	33.2*(Ref. 5), 32.0*(Ref. 10)	32.6±0.6 (R)	0.125
373	40.3*(Ref. 5), 37.1*(Ref. 10)	39±2	0.16
375	45.2*(Ref. 5), 40.7*(Ref. 10)	43±2 (R)	0.18
376	49.3*(Ref. 5), 43.3*(Ref. 10)	46±3	0.20

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

	Solubility, 100 w_2	''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_2	x_2
273	1.1 (Ref. 17)	1.1	0.036
278	1.1*(Ref. 5), 1.3*(Ref. 17)	1.2±0.1	0.040
283	1.2*(Ref. 5), 1.5*(Ref. 17)	1.4±0.2	0.046
288	1.3*(Ref. 5), 1.7*(Ref. 17)	1.5±0.2	0.049
293	1.6*(Ref. 5), 2.00 (Ref. 9), 2.0 (Ref. 11), 2.0 (Ref. 13), 2.09 (Ref. 4), 1.91 (Ref. 17)	1.9±0.2	0.062
298	2.0 (Ref. 2), 2.28 (Ref. 3), 228 (Ref. 4), 1.9*(Ref. 5), (Ref. 6), 2.3* (Ref. 9), 2.3*(Ref. 11), 2.5*(Ref. 13), 2.3*(Ref. 15, 16), 2.2*(Ref. 17)	2.3±0.2	0.074
303	2.2*(Ref. 5), 2.49 (Ref. 9), 2.6 (Ref. 11), 3.0*(Ref. 13), 2.6*(Ref. 15), 2.9 (Ref. 16), 2.4*(Ref. 17)	2.6±0.3	0.083
308	2.6*(Ref. 5), 2.9*(Ref. 9), 2.8*(Ref. 10), 3.0*(Ref. 11), 3.5*(Ref. 13), 2.9*(Ref. 15), 3.1*(Ref. 16), 3.0*(Ref. 17)	3.0±0.2	0.095
313	3.3*(Ref. 5), 3.26 (Ref. 9), 3.4*(Ref. 10), 3.4 (Ref. 11), 4.0 (Ref. 13), 3.4*(Ref. 15), 3.3 (Ref. 16), 3.6*(Ref. 17)	3.5±0.2	0.11
318	4.0*(Ref. 5), 3.8*(Ref. 9), 3.9*(Ref. 10), 3.9*(Ref. 11), 3.9*(Ref. 15), 3.8*(Ref. 16), 4.4*(Ref. 17)	4.0±0.2 (R)	0.12
323	4.6*(Ref. 5), 4.36 (Ref. 9), 4.4*(Ref. 10), 4.4 (Ref. 11), 4.4*(Ref. 15), 4.2 (Ref. 16)	4.4±0.1 (R)	0.13
328	5.3*(Ref. 5), 5.1*(Ref. 9), 5.0*(Ref. 10), 5.1*(Ref. 11), 5.0*(Ref. 15), 4.6*(Ref. 16)	5.0±0.2 (R)	0.15
333	5.8*(Ref. 5), 5.84 (Ref. 9), 5.6*(Ref. 10), 5.8 (Ref. 11), 5.6*(Ref. 15), 5.0 (Ref. 16)	5.6±0.3	0.17
338	6.8*(Ref. 5), 6.8*(Ref. 9), 6.3*(Ref. 10), 6.2*(Ref. 15)	6.5±0.3 (R)	0.19
343	7.7*(Ref. 5), 7.76 (Ref. 9), 7.4*(Ref. 10), 8.0*(Ref. 17)	7.7±0.2 (R)	0.22
348	8.7*(Ref. 5), 8.9*(Ref. 9), 8.7*(Ref. 10), 9.1*(Ref. 17)	8.9±0.2 (R)	0.25
353	9.71 (Ref. 5), 10.21 (Ref. 9), 10.0*(Ref. 10), 10.3*(Ref. 17)	10.1±0.2 (R)	0.276
358	11.7*(Ref. 5), 11.68 (Ref. 9), 12.0*(Ref. 10)	11.8±0.1 (R)	0.312
363	14.4*(Ref. 5), 14.2*(Ref. 10)	14.3±0.1 (R)	0.361
368	17.6*(Ref. 5), 17.4*(Ref. 10)	17.5±0.1 (R)	0.418
373	24.8*(Ref. 5), 22.6*(Ref. 10)	24±1(R)	0.52
375	30.3*(Ref. 5), 25.7*(Ref. 10)	28±2	0.57
376	35.0*(Ref. 5), 28.0*(Ref. 10)	32±3	0.61

The tentative and recommended values reported in the Tables 2 and 3 above have been approximated by the equation based on scaling law (described in the introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted:

$$a_1=0.86790,\ a_2=-0.26960,\ b_1=-4.91434,\ b_2=4.90924$$

(mean standard error of estimate was 0.0062).

For approximation the recommended values of UCST and x_{c1} have been used. The calculated compositions are in each point inside declared inaccuracy. This relationship is presented in Fig. 7 together with the values reported in the above tables.

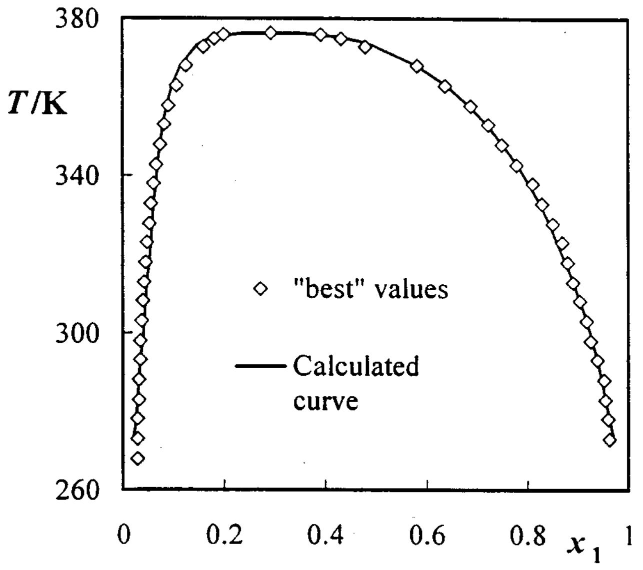

FIG. 7. Mutual solubility of nitromethane and water.

The upper critical solution temperature (UCST) has been reported as 376.2 K[1], 376.4 K,[18] 376.5 K,[12,19] 376.8 K.[5] The UCST reported by Mel'nikova[10] is considerably higher than these values and is therefore rejected. Thus, the recommended value is: UCST=(376.3 ±0.2) K. The corresponding critical solution composition has been reported as $x_1=0.35$ (Ref. 1), $x_1=0.303$ (Ref. 5), $x_1=0.290$ (Ref. 12), and $x_1=0.283$ (Ref. 10). The datum of Timmermans[1] is rejected. The remaining data give an average $x_{c1}=0.292\pm0.007$, $(100\ w_1=58.3)$, which is recommended.

References:

[1] J. Timmermans, Z. Phys. Chem. **58**, 129 (1907).

[2] C. P. Wright, D. M. Murray-Rust, and H. Hartley, J. Chem. Soc. **33**, 90 (1931).

[3] A. R. Fowler and H. Hunt, Ind. Eng. Chem. **33**, 90 (1941).

[4] J. E. Schumacher and H. Hunt, Ind. Eng. Chem. **34**, 701 (1942).

[5] R. M. Corelli, L'Aerotecnica (Italy) **30**, 32 (1950).

[6] A. E. Donahue and F. E. Bartell, J. Phys. Chem. **56**, 480 (1952).

[7] A. E. Skrzec and N. F. Murphy, Ind. Eng. Chem. **46**, 2245 (1952).

[8] H. L. Friedman and G. R. Hauger, J. Am. Chem. Soc. **76**, 2060 (1954).

[9] H. Schuberth, Z. Phys. Chem. (Leipzig) **225**, 305 (1964).

[10] I. K. Mel'nikova, Dissertation, Voronezh University, 1966.

[11] H. Schuberth and P. Kranke, Z. Phys. Chem. (Leipzig) **245**, 49 (1970).

[12] L. F. Erofeeva and N. V. Yunnikova, Sb. Nauch. Tr., Kusbas. Polytekh. Inst. **26**, 1 (1971).

[13] E. F. Zhuravlev and N. V. Maslovskaya, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 334 (1975); Deposited Doc., VINITI 1466 (1974).

[14] M. J. Hampe, Chem Ing. Tech. **57**, 669 (1985).

[15] V. P. Sazonov, Zn. Obshch. Khim. **59**, 2431 (1989).

[16] E. N. Rezanova, A. M. Tojkka, and N. P. Markuzin, Vestn. Leningr. Univ, Fiz., Khim. **18**, 53 (1991).

[17] R. M. Stephenson, J. Chem. Eng. Data **37**, 80 (1992).

[18] I. B. Rabinovich, V. D. Fedorov, N. R. Pashkin, M. A. Avdeshyak, and N. Ya. Pimenov, Dokl. Akad. Nauk. SSSR **105**, 108 (1955).

[19] A. W. Francis, Critical Solution Temperatures, Washington, Adv. Chem. Ser. **31** (1961).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Timmermans, Z. Phys. Chem. **58**, 129–213 (1907).

Variables:

T/K=376

Prepared By:

V. P. Sazonov

Experimental Data

The UCST was reported to be 103 °C at 100 w_1=65 (x_1=0.35,376.2 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Initial mixtures were prepared by weighing. Measurements were carried out in tubes with glass stoppers. These tubes were fixed with a rubber ring onto a thermometer and were placed into a water or glycerol bath.

Source and Purity of Materials:

(1) source not specified; pure grade reagent; fractionally distilled.
(2) distilled.

Estimated Error:

Composition: about 1%.
Temperature: ±0.1 K.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. R. Fowler and H. Hunt, Ind. Eng. Chem **33**, 90–5 (1941).

Variables:

T/K=298 and 357

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
25.0	298.2	11.03	0.0353	97.72	0.9268
83.7	356.9	34.0	0.132	81.5	0.565

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Commercial Solvents Corp.; fractionally distilled; b. p. range (100.9–101.5) °C at 99.73 kPa; d(25 °C)=1129.9 g·L^{-1}.
(2) Redistilled.

Estimated Error:

Temperature: control to ±0.5 K.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. P. Wright, D. M. Murray-Rust, and H. Hartley, J. Chem. Soc. 199–214 (1931).

Variables:

T/K=298

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
25.0	298.2	10.0	0.032	98.0	0.935

Auxiliary Information

Method/Apparatus/Procedure:

Viscosity measurements were used to determine mutual solubilities of (1) and (2). Layers of each liquid were allowed to reach mutual saturation at 25 °C and the time of flow for each layer was measured. The upper layer, a saturated solution of (1) in (2), was diluted with water so that solutions containing known amounts of the saturated solution were obtained. The times of flow for these solutions were measured and compared with those for water containing weighed quantities of nitromethane. Similar measurements were made with the lower layer after dilution with nitromethane.

Source and Purity of Materials:

(1) Poulenc Freres; dried over $CaCl_2$ and twice distilled in a 1m Hempel column; $d(25\ °C)=1131.2\ g\cdot L^{-1}$.
(2) Distilled.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. E. Schumacher and H. Hunt, Ind. Eng. Chem. **34**, 701–4 (1942).

Variables:

T/K=298 and 356

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
25.0	298.2	11.03	0.0353	97.72	0.9268
83.6	356.8	27.0	0.098	85.5	0.635

Auxiliary Information

Method/Apparatus/Procedure:

A refractometric method was used. No further details were reported.

Source and Purity of Materials:

(1) Commercial Solvents Corp.; technical grade; purified by fractional distillation; b.p. range (101.0–101.7) °C at 101.33 kPa; $d(25\ °C)=1129\ g\cdot L^{-1}$.
(2) Distilled.

Estimated Error:

Not specified.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. M. Corelli, L'Aerotecnica (Italy) **30**, 32–7 (1950).

Variables:

T/K=268–377

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
−5	268.2	8.965	0.0282	—	—
1	274.2	—	—	99.00	0.9969
16	289.2	—	—	98.66	0.9560
18	291.2	10.53	0.0336	—	—
34.5	307.7	—	—	97.49	0.9198
37	310.2	12.55	0.0406	—	—
48.5	321.7	14.48	0.0476	—	—
57	330.2	16.08	0.0535	—	—
62	335.2	—	—	93.75	0.8158
68.5	341.7	18.97	0.0646	—	—
75.5	348.7	21.54	0.0750	—	—
76.5	349.7	22.33	0.0782	—	—
80	353.2	—	—	90.29	0.7330
85.5	358.7	25.92	0.0936	—	—
88.5	361.7	—	—	86.73	0.6586
91	364.2	—	—	84.86	0.6233
94	367.2	32.02	0.1221	—	—
96	369.2	—	—	81.99	−0.5734
98	371.2	—	—	79.08	0.5274
99.5	372.7	39.19	0.1598	—	—
102	375.2	45.20	0.1958	—	—
102.5	375.7	—	—	67.57	0.3808
103.6	376.8	59.60	0.3030	59.60	0.3030 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1,2] was used. Initial mixtures of (1) and (2) were weighed into 10 mL test tubes. The sealed tubes were put into a heating bath filled with distilled water or aqueous glycerol or paraffin oil, at the required temperature. The bath and the submerged tube were heated until mixtures of (1) and (2) became homogeneous; heating was then stopped, and the complex cooled in air. While cooling, the tubes were observed. With the appearance of turbidity, the thermometer reading was recorded. The bath was then reheated and the tube shaken to determine the temperature when the turbidity disappeared. The average value between two determinations was accepted as mutual solubility temperature.

Source and Purity of Materials:

Synthesized by method Kolbe from monochloro-acetic acid and sodium nitrite; dried and purified; b.p.=(100–101) °C, d(25 °C)=1130 g·L^{-1}.
(2) Not specified.

Estimated Error:

Not reported.

References:

[1] W. Alexejew, Wied. Ann. **28**, 306 (1886).
[2] W. Rothmund, Z. Phys. Chem. **26**, 433 (1898).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. J. Donahue and F. E. Bartell, J. Phys. Chem. **56**, 480–4 (1952).

Variables:

T/K=298

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
25.0	298.2	8.0	0.025	97.4	0.918

Auxiliary Information

Method/Apparatus/Procedure:

Mixtures of (1) and (2) were placed in glass-stoppered flasks and shaken occasionally for 3 d in a water bath. The organic phase was analyzed for water content by the Karl Fischer method. The aqueous phase was analyzed interferometrically.

Source and Purity of Materials:

(1) Source not specified; best reagent grade; purified by fractional distillation.
(2) Distilled.

Estimated Error:

Temperature: ±0.1 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. E. Skrzec and N. F. Murphy, Ind. Eng. Chem. **46**, 2245–7 (1954).

Variables:
T/K=299

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
26.7	299.9	9.60	0.0304	98.11	0.9387

Auxiliary Information

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

Source and Purity of Materials:
(1) Commercial Solvents Corp.; technical grade; purity 99.5 mass %.
(2) Not specified.

Estimated Error:
Temperature: ±0.5 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. L. Friedman and G. R. Hauger, J. Am. Chem. Soc. **76**, 2060–3 (1954).

Variables:
T/K=298

Prepared By:
V. P. Sazonov

Experimental Data

The solubility of nitromethane (1) in water (2) at 298.2 K was reported to be 100 w_1=10.6. The corresponding mole fraction, x_1, calculated by the compiler is 0.034.

The solubility of water (2) in nitromethane (1) at 298.2 K was reported to be 100 w_2=1.5. The corresponding mole fraction, x_2, calculated by the compiler is 0.049.

Auxiliary Information

Method/Apparatus/Procedure:
No further details were reported.

Source and Purity of Materials:
(1) source not specified; purity not specified; distilled from phosphoric anhydride; b.p.=(100.4–100.6) °C.
(2) Redistilled.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Schuberth and P. Kranke, Z. Phys. Chem. (Leipzig) **245**, 49–67 (1970).

Variables:
T/K=293–333

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
20.0	293.2	0.034	10.6	0.936	98.0
30.0	303.2	0.038	11.8	0.916	97.4
40.0	313.2	0.043	13.2	0.893	96.6
50.0	323.2	0.049	14.9	0.865	95.6
60.0	333.2	0.057	17.0	0.827	94.2

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method and the titration method were used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled; b.p. =101.0 °C, $n(20\ °C,D)=1.38195$, $d(20\ °C)=1137.9\ g\cdot L^{-1}$.
(2) Distilled.

Estimated Error:
Not specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Schuberth, Z. Phys. Chem. (Leipzig) **225**, 305–12 (1964).

Variables:
T/K=293–358

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1 (compiler)	x_1	100 w_1 (compiler)	x_1
20.0	293.2	10.71	0.0342	98.00	0.9353
30.0	303.2	11.52	0.0370	97.51	0.9205
40.0	313.2	12.79	0.0415	96.74	0.8975
50.0	323.2	14.59	0.0480	95.64	0.8661
60.0	333.2	16.76	0.0561	94.16	0.8264
70.0	343.2	19.39	0.0663	92.24	0.7783
80.0	353.2	22.30	0.0781	89.79	0.7220
85.0	358.2	23.89	0.0848	88.32	0.6906

The solubility of nitromethane in water: $x_1=9.14\cdot 10^{-6}(T/\mathrm{K})^2-51.75\cdot 10^{-4}(T/\mathrm{K})+76.58\cdot 10^{-2}$.
The solubility of water in nitromethane: $x_2=41.61\cdot 10^{-6}(T/\mathrm{K})^2-233.37\cdot 10^{-4}(T/\mathrm{K})+333.01\cdot 10^{-2}$.

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method and the titration method were used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; purity not specified; distilled over a column of 40 theoretical plates; b.p.=101.2 °C, $n(20\ °C,D)=1.3819$, $d(20\ °C)=1139\ g\cdot L^{-1}$.
(2) Twice distilled.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2)Water; H_2O; [7732-18-5]

Variables:
T/K=280–378

Original Measurements:
I. K. Mel'nikova, Dissertation, Voronezh University, 1966.

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
7.0	280.2	9.8	0.031	—	—
31.7	304.9	12.3	0.0398	—	—
33.0	306.2	—	—	97.4	0.917
47.0	320.2	14.5	0.0477	—	—
54.5	327.7	—	—	95.1	0.851
60.0	333.2	17.7	0.0597	—	—
70.5	343.7	20.0	0.0687	—	—
73.5	346.7	—	—	91.8	0.768
82.0	355.2	24.6	0.0879	—	—
92.2	365.4	—	—	85.0	0.626
98.7	371.9	34.4	0.134	—	—
101.9	375.1	—	—	75.0	0.470
104.2	377.4	—	—	64.7	0.351
104.5	377.7	50.0	0.228	—	—
104.5	377.7	57.2	0.283	57.2	0.283 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Mixtures of (1) and (2) of a definite composition were sealed in glass tubes and placed in a thermostat. The turbidity temperature of each solution was determined under conditions of slow cooling and stirring.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; dried and purified.
(2) Distilled.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water: H_2O; [7732-18-5]

Variables:
T/K=279–376

Original Measurements:
L. F. Erofeeva and N. V. Yunnikova, Sb. Nauch. Tr., Kuzbas. Polytekh. Inst. **26**, 1–6 (1971).

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
6.2	279.4	10.1	0.0321	—	—
16.7	289.9	—	—	97.7	0.926
25.6	298.8	11.4	0.0366	—	—
45.0	318.2	14.0	0.0459	—	—
48.6	321.8	—	—	95.4	0.860
72.7	345.9	19.2	0.0656	—	—
76.9	350.1	—	—	91.1	0.751
80.0	353.2	22.7	0.0798	—	—
85.0	358.2	25.2	0.0905	—	—
90.1	363.3	27.9	0.103	—	—
97.7	370.9	—	—	79.0	0.526
100.0	373.2	41.5	0.173	—	—
101.4	374.6	—	—	71.7	0.428
102.3	375.5	50.9	0.234	—	—
102.9	376.1	—	—	64.2	0.346
103.2	376.4	55.4	0.268	—	—
103.3	376.5	—	—	59.5	0.303
103.3	376.5	58.0	0.290	58.0	0.290 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method [1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled.
(2) Twice distilled.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. F. Zhuravlev and N. V. Maslovskaya, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 334 (1975).
*Deposited Doc., VINITI 1466 (1974).

Variables:
T/K=293 and 313

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
20.0	293.2	9.0	0.028	98.0	0.935
40.0	313.2	10.0	0.032	96.0	0.876

Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; purity not specified; distilled.
(2) Twice distilled.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. J. Hampe, Chem.-Ing.-Tech. **57**, 669–81 (1985).

Variables:
T/K=293

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
20.0	293.2	11.1	0.036	97.91	0.933

Auxiliary Information

Method/Apparatus/Procedure:
No details were reported.

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

Estimated Error:
Not specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
V. P. Sazonov, Zh. Obshch. Khim. **59**, 2431–5 (1989).

Variables:
T/K=294–339

Prepared By:
N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
21.0	294.2	10.7	0.0342	97.9	0.932
23.3	296.5	11.0	0.0352	—	—
29.0	302.2	—	—	97.5	0.920
30.0	303.2	11.8	0.0380	—	—
32.4	305.6	12.0	0.0387	—	—
36.1	309.3	—	—	97.0	0.905
39.6	312.8	13.0	0.0422	—	—
40.0	313.2	13.3	0.0433	—	—
42.0	315.2	—	—	96.4	0.888
46.2	319.4	14.0	0.0459	—	—
46.4	319.7	—	—	96.0	0.876
54.0	327.2	—	—	95.1	0.851
65.7	338.9	—	—	93.7	0.815

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method of Alekseev was used. The apparatus which employs visual indication of turbidity was described by Sazonov and Chernysheva.[1] No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; fractionally distilled; 99.85 mass % purity; $n(20\ °C,D)=1.3819$, $d(20\ °C)=1138\ g\cdot L^{-1}$.
(2) Twice distilled.

Estimated Error:

Not reported.

References:

[1] V. P. Sazonov and M. F. Chernysheva, Zh. Obshch. Khim. **57**, 46 (1987).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. N. Rezanova, A. M. Tojkka, and N. P. Markuzin, Vestn. Leningr. Univ., Fiz., Khim. **18**, 53–6 (1991).

Variables:
T/K=298–333

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
25.00	298.15	11.2	0.0359	97.7	0.926
30.00	303.15	11.8	0.0380	97.1	0.909
40.00	313.15	12.9	0.0419	96.7	0.895
50.00	323.15	14.3	0.0469	95.8	0.870
60.00	333.15	15.4	0.0510	95.0	0.849

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. A 100 mL glass flask and a microburette with scale divisions of 0.01 mL were used. The solution was mixed by a magnetic stirrer. The titration was continued until the second phase appeared. The amount of added substance was obtained by weighing the mixture before and after the titration.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; dried over $CaCl_2$ and repeatedly distilled in a laboratory packed column of 20 theoretical plates;
b.p.=101.2 °C, $n(20\ °C,D)=1.3820$.
(2) Twice distilled.

Estimated Error:

Temperature: control to ± 0.02 K.
Solubility: ± 0.002 mole fraction.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. M. Stephenson, J. Chem. Eng. Data **37**, 80–95 (1992).

Variables:

T/K=273–363

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and water

		Water-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
0	273.2	9.0	0.028	98.9	0.964
9.5	282.8	9.7	0.031	98.56	0.9528
19.7	292.9	10.4	0.0331	98.09	0.9381
31.0	304.2	11.7	0.0376	97.50	0.9201
40.4	313.6	12.8	0.0415	96.35	0.8863
50.0	323.2	14.8	0.0488	93.87	0.8189
60.5	333.7	15.1	0.0499	92.08	0.7744
70.5	343.7	17.1	0.0574	91.82	0.7682
80.2	353.4	19.6	0.0671	89.58	0.7174
89.8	363.0	20.8	0.0720	—	—

Auxiliary Information

Method/Apparatus/Procedure:

No details were reported.

Source and Purity of Materials:

(1) Aldrich Chemical; not purified; purity more 99 mass%.
(2) Twice distilled.

Estimated Error:

Temperature: to ± 0.1 K.
Solubility: ± 0.2% (1) in (2), ± 0.05% (2) in (1).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2)Water-d_2; D_2O; [7789-20-0]

Original Measurements:

I. B. Rabinovich, V. D. Fedorov, N. R. Pashkin, M. A. Avdeshyak, and N. Ya. Pimenov, Dokl. Akad. Nauk SSSR **105**, 108–11 (1955).

Variables:

T/K=293–379

Prepared By:

V. P. Sazonov

Experimental Data

Effect of deuteration on solubility of nitromethane in water

t/°C	T/K	$100(L_H-L_D)/L_H$[a]
	(Compliler)	
20.0	293.2	5.5
26.0	299.2	5.5
40.0	313.2	4.1
66.0	339.2	4.3
80.0	353.2	5.4
100.0	373.2	10
103.0	376.2	43[b]

[a] L_H and L_D are the solubilities (in mole %) of nitromethane in H_2O and nitromethane in D_2O, respectively.
[b] This value refers to a temperature that corresponds to within ±0.5 °C to the UCST of the nitromethane+water system. USCT is 105.5 °C.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method (cloud-clear points) of Alekseev was used. This involves observing the temperature at which a measured mass of one liquid becomes visually soluble in a measured mass of the other liquid.

Source and Purity of Materials:

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

Estimated Error:

Temperature: ± 0.2 K.

5. Nitromethane+Inorganic Compounds

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Carbon disulfide; CS_2; [75-15-0]	V. P. Sazonov, Technical University, Samara, Russia A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and carbon disulfide have been reported in four references. Joukovsky[1] studied mutual solubilities of the components between 291 and 337 K probably by the synthetic method. Poppe[2] determined the upper critical solution temperature and effect of pressure (0.3–12.3 MPa) by synthetic method. Dorby[3] defined the upper critical solution temperature. Mutual solubility of (1) and (2) was studied also by Gopal *et al.*[4] between 270 and 336 K by the visual observation method.

It has been noticed that the older papers reported the higher UCST than those more recently. The paper of Joukovsky[1] presents the larger miscibility gap than the data reported in Gopal *et al.*[4] The corresponding critical solution composition has been reported as $x_{c1} = 0.505$ (Joukovsky[1]) and $x_{c1} = 0.4266$ (Poppe[2]). Therefore the data reported by Gopal *et al.*,[4] 70 experimental data points, consistent one to another, have been approximated by the equation based on scaling law (described in the introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted:

$$a_1 = 0.95793, \quad a_2 = -0.37187, \quad b_1 = 0.67505, \quad b_2 = -0.33301$$

(mean standard error of estimate was 0.0187).

As an approximation, the values of x_{c1} and UCST from Gopal *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 points reported in Joukovsky[1] and Gopal *et al.*[4] are also presented in Fig. 8.

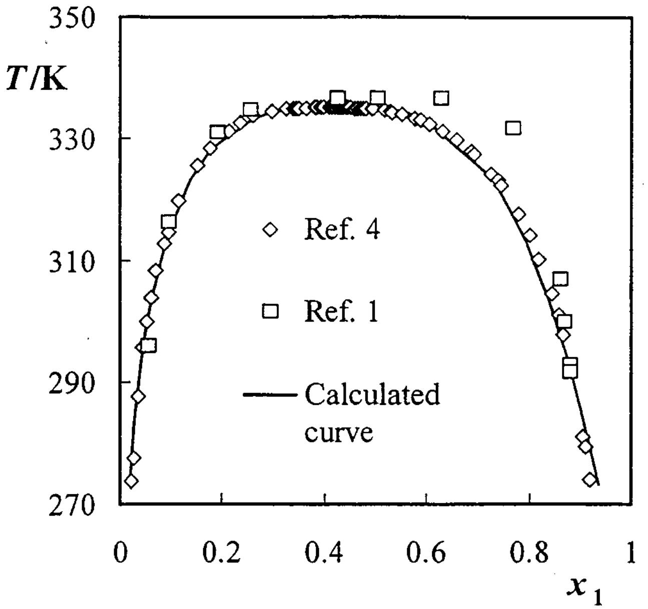

FIG. 8. Mutual solubility of nitromethane and carbon disulfide.

Mutual solubility of nitromethane and carbon disulfide

	Carbon disulfide-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
273.2	0.0193	2.72	0.9352	95.34
283.2	0.0284	3.99	0.9073	93.28
293.2	0.0416	5.80	0.8758	90.91
298.2	0.0503	6.99	0.8581	89.56
303.2	0.0608	8.41	0.8389	88.08
313.2	0.0895	12.24	0.7932	84.47
323.2	0.1372	18.41	0.7298	79.31
333.2	0.2567	32.88	0.5975	67.81
334.2	0.2914	36.85	0.5620	64.54
334.7	0.3209	40.14	0.5322	61.75

References:

[1] N. I. Joukovsky, Bull. Soc. Chim. Belg. **43**, 397 (1934).
[2] G. Poppe, Bull. Soc. Chim. Belg. **44**, 640 (1935).
[3] A. Dobry, Macromol. Chem. **18/19**, 317 (1956).
[4] E. S. R. Gopal, P. Chandra Sekhar, G. Ananthakrishna, R. Ramachandra, and S. V. Subraranyam, Proc. Roy. Soc. London A **350**, 91 (1976); S. C. Greer, B. K. Das, A. Kumar, and E. S. R. Gopal, J. Chem. Phys. **79**, 4545 (1983).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Carbon disulfide; CS_2; [75-15-0]

Original Measurements:
N. I. Joukovsky, Bull. Soc. Chim. Belg. **43**, 397–446 (1934).

Variables:
$T/K = 291-337$

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and carbon disulfide

		Carbon disulfide-rich phase		Nitromethane-rich phase	
$t/°C$	T/K (compiler)	100 w_1 (compiler)	x_1	100 w_1 (compiler)	x_1
18.5	291.7	—	—	85.5	0.880
19.5	282.7	—	—	85.5	0.880
22.5	295.7	4.5	0.055	—	—
26.5	299.7	—	—	84.0	0.867
33.6	306.8	—	—	83.0	0.859
43.0	316.2	7.8	0.095	—	—
57.7	330.9	15.9	0.190	—	—
58.5	331.7	—	—	72.5	0.767
61.5	334.7	21.6	0.255	—	—
63.4	336.6	—	—	57.6	0.628
63.5	336.7	37.3	0.425	—	—
63.5	336.7	45.0	0.505	45.0	0.505 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
No further details were reported.

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

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Carbon disulfide; CS_2; [75-15-0]

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

Variables:
$T/K = 338$; $P/\text{kPa} = 329-12412$

Prepared By:
V. P. Sazonov and A. V. Morozov

Experimental Data

The upper critical solution temperature (T_c) was reported to be 64.75 °C (337.90 K, compilers). The value of dT_c/dP was reported to be 0.0225 $K \cdot kPa^{-1}$ in the above pressure range.

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. The observations were carried out in sealed tubes in the presence of the vapor phase. A Cailletet 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) Nitromethane; CH_3NO_2; [75-52-5]
(2) Carbon disulfide; CS_2; [75-15-0]

Original Measurements:

A. Dorby, Makromol. Chem. **18/19**, 317–21 (1956).

Variables:

T/K=336

Prepared By:

V. P. Sazonov

Experimental Data

The upper critical solution temperature was reported to be 63.0 °C (336.2 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

No further details were reported.

Source and Purity of Materials:

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

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Carbon disulfide; CS_2; [75-15-0]

Original Measurements:

E. S. R. Gopal, P. Chandra Sekhar, G. Ananthakrishna, R. Ramachandra, and S. V. Subraranyam, Proc. R. Soc. London A **350**, 91–106 (1976).

*S. C. Greer, B. K. Das, A. Kumar, and E. S. R. Gopal, J. Chem. Phys. **79**, 4545–52 (1983).

Variables:

T/K=274–335

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and carbon disulfide

		Carbon disulfide-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1 (compiler)	x_1	100 w_1 (compiler)	x_1
0.5	273.7	1.76	0.0218	—	—
0.9	274.1	—	—	90.12	0.9192
4.3	277.5	2.25	0.0279	—	—
6.2	279.4	—	—	89.07	0.9104
7.8	281.0	—	—	88.43	0.9056
14.3	287.5	2.94	0.0364	—	—
19.5	292.7	—	—	85.47	0.8801
22.3	295.5	3.53	0.0440	—	—
24.5	297.7	—	—	83.84	0.8662
26.7	299.9	4.21	0.0520	—	—
27.7	300.9	—	—	82.66	0.8561
30.6	303.8	4.99	0.0615	—	—
31.3	304.5	—	—	81.09	0.8425
35.0	308.2	5.58	0.0689	—	—
36.9	310.1	—	—	78.41	0.8192
39.5	312.7	7.15	0.0876	—	—
40.8	314.0	—	—	76.28	0.8005
41.477	314.627	7.68	0.0940	—	—
44.473	317.623	—	—	73.83	0.7787
46.676	319.826	9.53	0.1161	—	—
49.173	322.323	—	—	70.23	0.7463
50.025	323.175	—	—	69.42	0.7390
51.033	324.183	—	—	67.90	0.7252
52.549	325.699	12.57	0.1520	—	—
54.224	327.374	—	—	64.18	0.6909
54.709	327.859	—	—	63.60	0.6855
55.379	328.529	14.76	0.1776	—	—
56.648	329.798	—	—	60.71	0.6584
58.103	331.253	—	—	57.53	0.6302
58.129	331.279	17.79	0.2125	—	—
59.244	332.394	—	—	55.14	0.6052
59.480	332.630	19.75	0.2349	—	—
59.920	333.070	—	—	53.46	0.5890
60.244	333.394	—	—	52.27	0.5773
60.568	333.718	21.99	0.2602	—	—
60.865	334.015	—	—	49.65	0.5516
61.200	334.350	—	—	47.83	0.5335
61.328	334.478	—	—	47.32	0.5284
61.387	334.537	25.20	0.2959	—	—

61.495	334.645	—	—	46.20	0.5172
61.761	334.911	—	—	44.09	0.4959
61.781	334.931	—	—	43.76	0.4925
61.783	334.933	27.91	0.3256	—	—
61.843	334.993	29.06	0.3382	—	—
61.863	335.013	—	—	42.64	0.4812
61.871	335.021	29.68	0.3449	—	—
61.888	335.038	—	—	42.18	0.4765
61.891	335.041	30.07	0.3491	—	—
61.913	335.063	—	—	41.56	0.4701
61.937	335.087	—	—	41.02	0.4645
61.942	335.092	31.53	0.3648	—	—
61.951	335.101	—	—	40.52	0.4594
61.968	335.118	32.97	0.3802	—	—
61.968	335.118	—	—	39.77	0.4516
61.971	335.121	—	—	39.62	0.4501
61.973	335.123	33.27	0.3835	—	—
61.976	335.126	34.05	0.3917	—	—
61.977	335.127	—	—	39.09	0.4446
61.979	335.129	34.62	0.3978	—	—
61.979	335.129	—	—	38.82	0.4418
61.981	335.131	35.70	0.4092	—	—
61.981	335.131	—	—	38.48	0.4383
61.982	335.132	36.25	0.4150	—	—
61.982	335.132	—	—	37.95	0.4328
61.983	335.133	36.83	0.4210	—	—
61.983	335.133	—	—	37.77	0.4309
61.983	335.133	37.23	0.4522	—	—
61.983	335.133	—	—	37.57	0.4288
61.983	335.133	37.32	0.4262	—	—
61.983	335.133	—	—	37.36	0.4266

The upper critical solution temperature was reported to be 335.13 K (61.98 °C) at $x_1 = 0.4266$ (100 $w_1 = 37.36$).

Auxiliary Information

Method/Apparatus/Procedure:

Mixtures of (1) and (2) were put in separate glass bulbs of 10 mL capacity, 1 cm height. The thermostat bath was triple-stage, controlled to 1 mK, basically consisting of a 10 L oil bath in a glass beaker. An inner thermostatic shield, with its own temperature sensor, heater, and viewing slits, was wrapped around the thermally insulated beaker. Room temperature was kept constant to 1–2 K. Sealed bulbs were mounted in the bath, which was then heated to the 1-phase region, followed by cooling in steps of 1 mK to the temperature at which separation into two phases occurred.

Source and Purity of Materials:

(1) Source not specified; analytical grade; no impurities detectable by gas chromatography.
(2) Source not specified; analytical grade; no impurities detectable by gas chromatography.

Estimated Error:

Temperature: ±0.001 K.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Tetraalkylammonium iodides

Original Measurements:

P. Walden, Z. Phys. Chem. **55**, 683–720 (1906).

Variables:

T/K = 273 and 298

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of tetraalkylammonium iodides in nitromethane

Salt	t/°C	T/K (compiler)	100 w_2	x_2 (compiler)
Tetramethylammonium iodide; $C_4H_{12}IN$; [75-58-1]	0.0	273.2	0.221	0.0007
	25.0	298.2	0.297	0.0009
Tetraethylammonium iodide; $C_8H_{20}IN$; [68-05-3]	0.0	273.2	3.002	0.0073
	25.0	298.2	4.887	0.0121
Tetrapropylammonium iodide; $C_{12}H_{28}IN$; [631-40-3]	0.0	273.2	12.52	0.0272
	25.0	298.2	19.21	0.0443

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 were placed into 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 were equilibrated at 40 °C with intensive stirring for 1 h. The flask was then placed into 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.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Alkali metal iodides; IK, ILi, INa and IRb

Original Measurements:
P. Walden, Z. Phys. Chem. **55**, 683–720 (1906).

Variables:
T/K=273 and 298

Prepared By:
V. P. Sazonov

Experimental Data

Solubility of alkali metal iodides in nitromethane

Salt	t/°C	T/K (compiler)	100 w_2	x_2 (compiler)
Potassium iodide; IK; [7681-11-0]	0.0	273.2	0.314	0.019
	25.0	298.2	0.289	0.017
Lithium iodide; ILi; [10377-51-2]	0.0	273.2	1.219	0.091
	25.0	298.2	2.519	0.188
Sodium iodide; INa; [7681-82-5]	0.0	273.2	0.339	0.023
	25.0	298.2	0.478	0.032
Rubidium iodide; IRb; [7790-29-6]	0.0	273.2	0.567	0.027
	25.0	298.2	0.518	0.024

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 were placed into 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 were equilibrated at 40 °C with intensive stirring for 1 h. The flask was then placed into 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 specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Gases; Kr, Ne, N_2 and Xe

Original Measurements:
H. L. Friedman, J. Am. Chem. Soc. **74**, 3294–7 (1954).

Variables:
T/K=298

Prepared By:
V. P. Sazonov

Experimental Data

Solubility of gases in nitromethane

			Ostwald solubility coefficient	
Gas	t/°C	T/K (compiler)	Experiment	Avg.
Krypton; Kr; [7439-90-9]	24.85	298.00	0.381; 0.378	0.380
Neon; Ne; [7440-01-9]	24.85	298.00	0.0241; 0.0249	0.0245
Nitrogen; N_2; [7727-37-9]	24.85	298.00	0.091	0.091
Xenon; Xe; [7440-63-3]	24.85	298.00	1.15; 1.11; 1.15	1.14

Auxiliary Information

Method/Apparatus/Procedure:

The method was essentially that employed by Eucken and Herzberg.[1] The solvent was degassed by alternately opening to the vacuum pump for 5–15 s and then stirring very rapidly to produce cavitation. This was repeated 5–10 times. In the solubility measurement itself gas, which had been previously saturated with solvent vapor, was admitted to the saturation vessel, holding about 80 mL of solution, and with 5–10 mL remaining space, volume–time measurements were taken and extrapolated back to the time the gas was admitted. Then the stirrer was turned on and driven very fast, producing a slightly (~1%) supersaturated solution. The approach to equilibrium was then followed from each direction while stirring as rapidly as possible without producing cavitation and bubbles.

Source and Purity of Materials:
(1) Source not specified; purity not specified; redistilled and dried by filtering at −20 °C.
(2) Krypton, neon, and xenon were reagent grade products of the Air Reduction Co.; purity 99.8 mass %; nitrogen was purified by passing over CaH_2 and CaO.

Estimated Error:
Solubility: relative error of 2–3 determinations less than 3%.

References:
[1] A. Eucken and G. Herzberg, Z. Phys. Chem. (Leipzig) **195**, 1 (1950).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Sulfur hexafluoride; SF_6; [2551-62-4]

Original Measurements:

H. L. Friedman, J. Am. Chem. Soc. **74**, 3294–7 (1954).

Variables:

T/K=273–298

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of sulfur hexafluoride in nitromethane

t/°C	T/K (compiler)	Ostwald solubility coefficient	
		Experiment	Avg.
0.10	273.25	0.374; 0.369	0.372
19.35	292.50	0.354; 0.364; 0.369	0.363
24.85	298.00	0.374; 0.380	0.377

Auxiliary Information

Method/Apparatus/Procedure:

The method was essentially that employed by Eucken and Herzberg.[1] The solvent was degassed by alternately opening to the vacuum pump for 5–15 s and then stirring very rapidly to produce cavitation. This was repeated 5–10 times. In the solubility measurement itself gas, which had been previously saturated with solvent vapor, was admitted to the saturation vessel, holding about 80 mL of solution, and with 5–10 mL remaining space, volume–time measurements were taken and extrapolated back to the time the gas was admitted. Then the stirrer was turned on and driven very fast, producing a slightly (~1%) supersaturated solution. The approach to equilibrium was then followed from each direction while stirring as rapidly as possible without producing cavitation and bubbles.

Source and Purity of Materials:

(1) Source not specified; purity not specified; redistilled and dried by filtering at −20 °C.
(2) Mathieson; purified from a more volatile impurity by fractional condensation at −190 °C.

Estimated Error:

Solubility: relative error of 2–3 determinations less than 3%.

References:

[1] A. Eucken and G. Herzberg, Z. Phys. Chem. (Leipzig) **195**, 1 (1950).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Uranium bis(nitrato-O)dioxohexahydrate; $UO_2(NO_3)_2 \cdot 6H_2O$; [13520-83-7]

Original Measurements:

R. K. Warner, Aust. J. Appl. Sci. **4**, 581–9 (1953).

Variables:

T/K=293

Prepared By:

V. P. Sazonov

Experimental Data

The solubility of uranyl nitrate in nitromethane at 20.0 °C (293.2 K, compiler) was reported to be 100 $w_2=14.0$. The corresponding mole fraction, x_2, calculated by the compiler is 0.025.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. A sample of (2) was placed with the appropriate amount of pure solvent in a small flask. The contents of the flask were warmed to 30–50 °C, agitated with excess crystals for 15 min, and then placed in a constant temperature bath at 20 °C with intermittent shaking for 6–8 h. Crystallization of the supersaturated solution occurred, and when equilibrium was reached the solution was quickly decanted, filtered from the fine crystals, and placed in a stoppered flask at 20 °C for analysis.

Source and Purity of Materials:

(1) Synthesized by standard method; thoroughly dried and fractionally distilled.
(2) Source not specified; A. R. grade; not purified.

Estimated Error:

Temperature: ±0.05 K.
Solubility: ±0.002 mass fraction.

6. Nitromethane+Hydrocarbons

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclopentene; C_5H_8; [142-29-0]

Original Measurements:

R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A (**2**), 26 (1982).

Variables:

T/K=302–307

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclopentene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
301.6	28.4	—	—	0.703	68.0
302.8	29.6	0.235	21.6	—	—
305.0	31.8	—	—	0.642	61.6
305.8	32.6	0.289	26.7	—	—
306.2	33.0	—	—	0.597	57.0
306.6	33.4	0.367	34.2	—	—
307.0	33.8	0.438	41.1	—	—
307.1	33.9	—	—	0.543	51.6
307.1	33.9	—	—	0.493	46.6
307.2	34.0	0.47	44.0	0.47	44.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.9 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclopentane; C_5H_{10}; [287-92-3]

Original Measurements:

R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 25 (1981).

Variables:

T/K=333–353

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclopentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
332.7	59.5	—	—	0.834	81.4
343.7	70.5	—	—	0.773	74.8
345.5	72.3	0.200	17.9	—	—
346.4	73.2	0.218	19.5	—	—
347.2	74.0	—	—	0.736	70.8
350.1	76.9	0.271	24.4	—	—
350.7	77.5	0.295	26.7	—	—
350.8	77.6	—	—	0.678	64.7
352.5	79.3	—	—	0.620	58.7
352.8	79.6	0.378	34.6	—	—
353.2	80.0	0.452	41.8	0.521	48.6
353.2	80.0	0.500	47.0	0.500	47.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.9 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5]	V. P. Sazonov, Technical University, Samara, Russia.
(2) 3-Methyl-1-butene; C_5H_{10}; [563-45-1]	A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, August 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 3-methyl-1-butene have been reported in two publications. Burova *et al.*[1] studied the mutual solubilities of the components between 292 and 326 K by the synthetic method. Riccardi *et al.*[2] carried out measurements of the mutual solubilities of (1) and (2) between 310 and 325 K, also using the synthetic method.

The experimental data reported in Burova *et al.*[1] and Riccardi *et al.*[2] differed significantly in the region close to the UCST. Solubility data of various other systems reported by Riccardi and co-workers were very close to the recommended/tentative values so only these data have been approximated by the equation based on scaling law (described in the introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted:

$$a_1=0.74092,\ a_2=0.19947,\ b_1=5.26510,\ b_2=-4.02929$$

(mean standard error of estimate was 0.0258).

The UCST=324.5 K and $x_{c1}=0.520$, reported in Riccardi *et al.*,[2] may be treated as tentative and these values have been used also for approximation. 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 all experimental points[1,2] are also presented in Fig. 9.

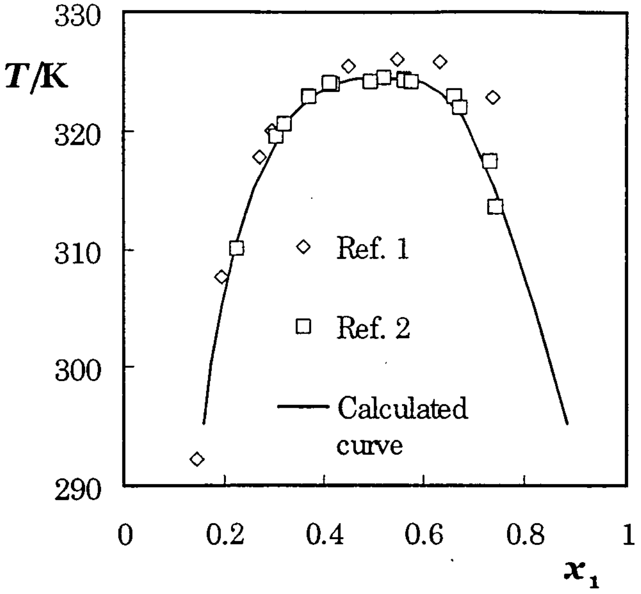

FIG. 9. Mutual solubility of nitromethane and 3-methyl-1-butene.

Mutual solubility of nitromethane and 3-methyl-1-butene

	Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
293.2	0.1532	17.21	0.8971	90.93
298.2	0.1672	18.74	0.8652	88.06
303.2	0.1854	20.73	0.8320	85.05
313.2	0.2425	26.89	0.7582	78.27
318.2	0.2914	32.08	0.7117	73.93
323.2	0.3889	42.24	0.6340	66.56
324.2	0.4418	47.63	0.5918	62.49

References:

[1] T. V. Burova, V. B. Kogan, and M. S. Nemtsev, Zh. Prikl. Khim. (Leningrad) **36**, 988 (1963).

[2] R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1818 (1968); P. L. Tonelli and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 1 (1985).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 3-Methyl-1-butene; C_5H_{10}; [563-45-1]

Original Measurements:

T. V. Burova, V. B. Kogan, and M. S. Nemtsev, Zh. Prikl. Khim. (Leningrad) **36**, 988–94 (1963).

Variables:

T/K = 292–326

Prepared By:

V. P. Sazonov

Experimental Data

The mutual solubility of nitromethane and 2-methylbutane in mass per cent over the specified temperature range were presented in graphical form in the original publication. The numeric data in the table below were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and 3-methyl-1-butene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
19.0	292.2	12.8	0.144	—	—
34.4	307.6	17.4	0.195	—	—
44.6	317.8	24.4	0.271	—	—
46.8	320.0	26.8	0.296	—	—
49.6	322.8	—	—	70.8	0.736
52.2	325.4	41.5	0.449	—	—
52.6	325.8	—	—	60.0	0.633
52.8	326.0	51.4	0.549	—	—

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A sample of (1) was poured into a 10 mL ampoule which was then cooled and a given amount of hydrocarbon added to it. The 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) Distilled through a column of 20 theoretical plates as in Ref. 1; b.p. = 101.5 °C at 101.33 kPa, n(20 °C, D) = 1.3820, d(20 °C) = 1138.0 g·L^{-1}.
(2) Distilled through a column of 90 theoretical plates as in Ref. 2; b.p. = 20.09 °C/101.33 kPa, n(20 °C, D) = 1.36715.

Estimated Error:

Not reported.

References:

[1] S. K. Ogorodnikov, V. B. Kogan, and M. S. Nemtsev, Zh. Prikl. Khim. (Leningrad) **34**, 841 (1961).
[2] S. K. Ogorodnikov, V. B. Kogan, and M. S. Nemtsev, Zh. Prikl. Khim. (Leningrad) **33**, 1599 (1960).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 3-Methyl-1-butene; C_5H_{10}; [563-45-1]

Original Measurements:

R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*P. L. Tonelli and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 1 (1985).

Variables:

T/K = 310–325

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 3-methyl-1-butene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
310.1	36.9	0.226	20.3	—	—
313.6	40.4	—	—	0.743	71.6
317.4	44.2	—	—	0.731	70.3
319.5	46.3	0.303	27.4	—	—
320.6	47.4	0.321	29.1	—	—
321.9	48.7	—	—	0.670	63.9
322.9	49.7	0.369	33.7	0.660	62.8
323.9	50.7	0.417	38.4	—	—
324.1	50.9	0.411	37.8	—	—
324.2	51.0	0.493	45.8	0.574	54.0
324.3	51.1	—	—	0.561	52.7
324.4	51.2	—	—	0.562	52.8
324.5	51.3	0.520	49.0	0.520	49.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methyl-2-butene; C_5H_{10}; [513-35-9]

Original Measurements:
L. Boublikova, Coll. Czech. Chem. Comm. **38**, 2033–42 (1973).

Variables:
T/K=293 and 303

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2-methyl-2-butene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	100 w_1 (compiler)	x_1	100 w_1 (compiler)	x_1
293.2	20.0	11.3	0.128	83.6	0.854
303.2	30.0	16.7	0.187	77.9	0.802

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Distilled over a column of 40 theoretical plates; $n(20\ °C, D)=1.3819$, $d(20\ °C)=1130.6\ g\cdot L^{-1}$.
(2) Prepared by dehydrating of 2-methyl-2-butanol; distilled over a column of 60 theoretical plates; $n(20\ °C, D)=1.3873$, $d(20\ °C)=662.1\ g\cdot L^{-1}$.

Estimated Error:

Not specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Pentene; C_5H_{10}; [109-67-1]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 25 (1982).

Variables:
T/K=309–320

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-pentene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
308.7	35.5	—	—	0.793	76.9
309.9	36.7	0.218	19.5	—	—
312.9	39.7	0.250	22.5	—	—
316.3	43.1	—	—	0.713	68.4
317.7	44.5	0.329	29.9	—	—
317.9	44.7	—	—	0.694	66.4
319.1	45.9	0.374	34.2	—	—
319.8	46.6	0.436	40.2	—	—
320.1	46.9	—	—	0.584	55.0
320.2	47.0	—	—	0.547	51.2
320.2	47.0	0.530	50.0	0.530	50.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.91 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5]	V. P. Sazonov, Technical University, Samara, Russia.
(2) 2-Methylbutane; C_5H_{12}; [78-78-4]	A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, August 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 2-methylbutane have been reported in three publications. Burova *et al.*[1] studied mutual solubilities of the components between 293 and 341 K, Rolla *et al.*[2] between 350 and 369 K, and Pavlov *et al.*[3] between 293 and 339 K, all using the synthetic method.

All experimental values reported in Burova *et al.*,[1] Rolla *et al.*,[2] and Pavlov *et al.*[3] (treated with the same weighing factor) have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted:

$$a_1=0.98413,\quad a_2=-0.43533,\quad b_1=1.13295,\quad b_2=-1.10745$$

(mean standard error of estimate was 0.0177).

For approximation x_{c1} and UCST from Rolla *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 the following table. This relationship together with experimental points reported in Burova *et al.*,[1] Rolla *et al.*,[2] and Pavlov *et al.*[3] are also presented in Fig. 10.

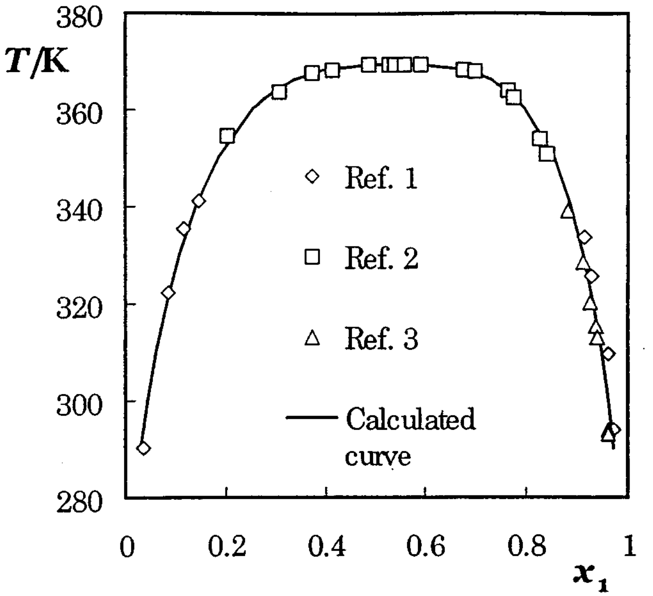

FIG. 10. Mutual solubility of nitromethane and 2-methylbutane.

Mutual solubility of nitromethane and 2-methylbutane

	Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	w_1
293.2	0.0341	4.01	0.9697	97.43
298.2	0.0412	4.84	0.9638	96.92
303.2	0.0490	5.74	0.9575	96.38
313.2	0.0669	7.81	0.9433	95.16
323.2	0.0888	10.33	0.9264	93.71
333.2	0.1162	13.45	0.9056	91.90
343.2	0.1519	17.48	0.8786	89.54
353.2	0.2023	23.06	0.8401	86.13
363.2	0.2887	32.42	0.7711	79.93
368.2	0.3933	43.38	0.6807	71.59
369.2	0.4647	50.64	0.6141	65.29

References:

[1] T. V. Burova, V. B. Kogan, and M. S. Nemtsev, Zh. Prikl. Khim. (Leningrad) **36**, 988 (1963).
[2] M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48 (1967).
[3] S. Y. Pavlov, S. P. Pavlova, L. A. Serafimov, and L. S. Kofman, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **10**, 915 (1967).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methylbutane; C_5H_{12}; [78-78-4]

Original Measurements:

T. V. Burova, V. B. Kogan, and M. S. Nemtsev, Zh. Prikl. Khim. (Leningrad) **36**, 988–94 (1963).

Variables:

T/K=290–341

Prepared By:

V. P. Sazonov

Experimental Data

The mutual solubility of nitromethane and 2-methylbutane in mass per cent over the specified temperature range were presented in graphical form in the original publication. The numeric data in the table below were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and 2-methylbutane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
17.2	290.4	3.0	0.035	—	—
20.8	294.0	—	—	96.8	0.973
36.6	309.8	—	—	95.4	0.961
49.0	322.2	7.2	0.084	—	—
52.5	325.7	—	—	91.6	0.928
60.6	333.8	—	—	90.0	0.914
62.2	335.4	10.0	0.116	—	—
68.0	341.2	12.6	0.146	—	—

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A sample of (1) was poured into a 10 mL ampoule which was then cooled and a given amount of hydrocarbon added to it. The 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) Distilled through a column of 20 theoretical plates as in Ref. 1; b.p.=101.5 °C at 101.33 kPa, $n(20\ °C,D)=1.3820$, $d(20\ °C)=1138.0\ g\cdot L^{-1}$.
(2) Distilled through a column of 90 theoretical plates; b.p. =27.88 °C at 101.33 kPa, $n(20\ °C,D)=1.3538$.

Estimated Error:

Not reported.

References:

[1] S. K. Ogorodnikov, V. B. Kogan, and M. S. Nemtsev, Zh. Prikl. Khim. (Leningrad) **34**, 841 (1961).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methylbutane; C_5H_{12}; [78-78-4]

Original Measurements:

M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:

T/K=351–369

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2-methylbutane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
77.7	350.9	—	—	0.840	81.6
80.9	354.1	—	—	0.827	80.2
81.3	354.5	0.202	17.6	—	—
89.4	362.6	—	—	0.776	74.6
90.5	363.7	0.307	27.3	—	—
90.8	364.0	—	—	0.765	73.4
94.4	367.6	0.372	33.4	—	—
94.8	368.0	—	—	0.698	66.2
95.1	368.3	0.414	37.4	—	—
95.2	368.4	—	—	0.678	64.0
96.1	369.3	0.489	44.7	0.593	55.2
96.2	369.4	0.528	48.6	0.558	51.6
96.2	369.4	0.540	49.8	0.540	49.8 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described in detail by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:

(1) Carlo Erba; RP material; dried by passing their vapors through a tube filled with P_2O_5; f.p.=−29.15 °C.
(2) Fluka AG; puriss grade material; purification as above.

Estimated Error:

Not specified.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methylbutane; C_5H_{12}; [78-78-4]

Original Measurements:
S. Y. Pavlov, S. P. Pavlova, L. A. Serafimov, and L. S. Kofman, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **10**, 915–20 (1967).

Variables:
T/K=293–339

Prepared By:
V. P. Sazonov

Experimental Data

The solubilities of 2-methylbutane in nitromethane in mass per cent are reported over the specified temperature range in graphical form and in a table.

Solubility of 2-methylbutane in nitromethane

t/°C	T/K (compiler)	100 w_2	x_2 (compiler)
20.0	293.2	4.5	0.038
20.9*	294.1	4.6	0.039
40.0	313.2	7.0	0.060
42.3*	315.5	7.2	0.062
47.1*	320.3	8.5	0.073
55.3*	328.5	10.3	0.088
66.0*	339.2	13.7	0.118

*These data were extracted graphically by the compiler.

Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; fractionally distilled.
(2) Source not specified; purity 99.7 mass %.

Estimated Error:
Not specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

Variables:
T/K=245–279

Prepared By:
V. P. Sazonov

Experimental Data

No region of liquid–liquid immiscibility was observed. A full solid–liquid phase diagram is presented.

Solubility of nitromethane and benzene

t/°C	T/K (compiler)	x_1	100 w_1 (compiler)
−28.50	244.65	1.000	100
−9.86	263.29	0.397	34.0
−6.86	266.29	0.248	20.5
−2.29	270.86	0.142	11.5
−1.41	271.74	0.123	9.88
0.30	273.45	0.0942	7.52
1.59	274.74	0.0654	5.18
5.45	278.60	0.000	0.00

A eutectic was reported at −37.2 °C.

Auxiliary Information

Method/Apparatus/Procedure:
Cooling curves were determined using a freezing point apparatus (Precision Scientific Co.), equipped with a Leeds & Northrup Mueller bridge, and a Pt resistance thermometer. Minimum sample size was 50 mL. A solution of (1) and (2) was prepared and its cooling curve recorded, then a known amount of (1) was added, and a second cooling curve taken.

Source and Purity of Materials:
(1) Fisher; reagent grade; distilled at 60 °C/60 kPa.
(2) Fisher ACS certified.

Estimated Error:
Not reported.

Components:

(1) Nitromethane-d_3; CD_3NO_2; [13031-32-8]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:

H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

Variables:

T/K=244–279

Prepared By:

V. P. Sazonov

Experimental Data

No region of liquid–liquid immiscibility was observed. A full solid–liquid phase diagram is presented.

Solubility of nitromethane-d_3 and benzene

t/°C	T/K (compiler)	x_1	100 w_1 (compiler)
−28.96	244.19	1.000	100
−26.03	247.12	0.780	74.4
−7.94	265.21	0.275	23.7
−0.68	272.47	0.116	9.71
2.07	275.22	0.0609	5.05
5.45	278.69	0.000	0.00

A eutectic was reported at −37.2 °C.

Auxiliary Information

Method/Apparatus/Procedure:

Cooling curves were determined using a freezing point apparatus (Precision Scientific Co.), equipped with a Leeds & Northrup Mueller bridge, and a Pt resistance thermometer. Minimum sample size was 50 mL. A solution of (1) and (2) was prepared and its cooling curve recorded, then a known amount of (1) was added, and a second cooling curve taken.

Source and Purity of Materials:

(1) Diaprep, Inc; 99 mole % minimum isotopic purity.
(2) Fisher ACS certified.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexene; C_6H_{10}; [110-83-8]

Original Measurements:

R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A(**1**), 27 (1982).

Variables:

T/K=301–323

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclohexene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
301.1	27.9	0.128	9.8	—	—
305.6	32.4	—	—	0.840	79.6
309.3	36.1	0.185	14.4	—	—
311.6	38.4	—	—	0.803	75.2
312.2	39.0	0.208	16.3	—	—
318.4	45.2	—	—	0.744	68.3
319.4	46.2	0.314	25.4	0.719	65.5
320.7	47.5	—	—	0.676	60.8
320.9	47.7	0.351	28.7	—	—
321.2	48.0	0.361	29.6	—	—
321.6	48.4	0.367	30.1	—	—
321.8	48.6	0.405	33.6	—	—
322.0	48.8	—	—	0.638	56.7
322.3	49.1	—	—	0.587	51.4
322.5	49.3	0.461	38.9	0.532	45.8
322.6	49.4	0.520	44.6	0.520	44.6 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2)Fluka AG; purity 99.5 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P Franzosini, Z. Naturforsch **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Quantitative solubility data for the nitromethane+cyclohexane have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Poppe[1]	367	UCST	Synthetic
Weck and Hunt[3]	299, 343	Mutual	Refractometric
Lakshmanan and Laddha[4]	303	Mutual	Titration
Hwa *et al.*[5]	288–303	Mutual	Analytical
Riccardi *et al.*[6]	352–366	Mutual	Synthetic
Sazonov *et al.*[7]	284–367	Mutual	Synthetic

All the original data are compiled in the data sheets immediately following this Critical Evaluation. The data of Weck and Hunt[3] in both phases disagree markedly with all other studies and are rejected.

All other reported data are included in the tables below. In Tables 2 and 3, values obtained by the evaluators by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk(*). ''Best'' values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be 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 (±5% relative) agreement. All other data are regarded as tentative only.

In general, the results of independent determinations are in excellent agreement, enabling their averaged values to be recommended over a wide range of temperatures (Tables 2 and 3).

TABLE 2. Tentative and recommended (R) values for the solubility nitromethane (1) in cyclohexane (2)

T/K	Solubility, 100 w_1 Reported values	''Best'' values ($\pm\sigma_n$) 100 w_1	 x_1
288	2.2 (Ref. 5), 2.3* (Ref. 7)	2.2±0.1 (R)	0.030
293	2.4*(Ref. 5), 2.6* (Ref. 7)	2.5±0.1 (R)	0.034
298	2.8* (Ref. 5), 3.0* (Ref. 7)	2.9±0.1 (R)	0.040
303	3.92 (Ref. 4), 3.4 (Ref. 5), 3.7* (Ref. 7)	3.7±0.2	0.050
313	4.6*(Ref. 7)	4.6	0.062
323	5.9*(Ref. 7)	5.9	0.080
333	8.1*(Ref. 7)	8.1	0.11
343	11.5*(Ref. 7)	11.5	0.152
353	17.5*(Ref. 7)	17.5	0.226
358	21.8*(Ref. 6), 21.3*(Ref. 7)	21.6±0.3 (R)	0.275
363	29.8*(Ref. 6), 29.6*(Ref. 7)	29.7±0.1 (R)	0.368
365	35.9*(Ref. 6), 38.0*(Ref. 7)	37±1 (R)	0.45

TABLE 3. Tentative and recommended (R) values for the solubility cyclohexane (2) in nitromethane (1)

T/K	Solubility, 100 w_2 Reported values	''Best'' values ($\pm\sigma_n$) 100 w_2	 x_2
288	4.3 (Ref. 5), 4.3*(Ref. 7)	4.3 (R)	0.032
293	4.8*(Ref. 5), 5.0*(Ref. 7)	4.9±0.1 (R)	0.036
298	5.1*(Ref. 3), 5.4 (Ref. 5), 5.6*(Ref. 7)	5.4±0.2 (R)	0.040
303	5.43 (Ref. 4), 6.6 (Ref. 5), 6.2*(Ref. 7)	6.1±0.5	0.045
313	7.9*(Ref. 7)	7.9	0.059
323	9.8* (Ref. 7)	9.8	0.073
333	12.4*(Ref. 7)	12.4	0.0931
343	16.8*(Ref. 7)	16.5	0.125
353	20.4*(Ref. 6), 22.2*(Ref. 7)	21±1 (R)	0.16
358	24.6*(Ref. 6), 26.6*(Ref. 7)	26±1 (R)	0.20
363	31.0*(Ref. 6), 33.2*(Ref. 7)	32±1 (R)	0.25
365	37.0*(Ref. 6), 39.2*(Ref. 7)	38±1 (R)	0.31

At system pressure the upper critical solution temperature has been reported as 352.2 K,[2] 365.8 K,[6] and 366.8 K.[1,7] The UCST of Francis[2] is therefore rejected. The average of the remaining values, UCST=(366.7±0.4) K is recommended.

The corresponding critical solution composition has been reported as $x_{c1}=0.555$ (Sazonov *et al.*[7]) and $x_{c1}=0.580$ (Riccardi *et al.*[6]) and their averaged value, $x_{c1}=0.568\pm0.012$ (100 $w_1=48.8$) is recommended. Poppe[1] has also determined the UCST at pressure from 3 to 123 atm (0.3–12.3) MPa. With a value of dT_c/dP of 0.0216 $K\cdot kPa^{-1}$.

The numerical values reported in the above tables have been approximated by the equation based on scaling law (described in the introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.942\,59$, $a_2=-0.320\,90$, $b_1=2.961\,49$, $b_2=-2.76752$ (mean standard error of estimate was 0.0135).

For approximation the recommended values of UCST and x_{c1} have been used. The calculated compositions are in each point inside declared inaccuracy. This relationship is presented in Fig. 11 together with data reported in the tables.

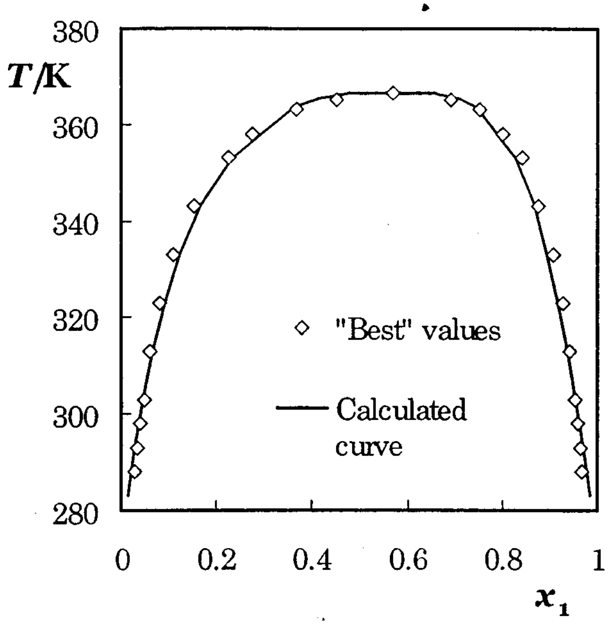

FIG. 11. Mutual solubility of nitromethane and cyclohexane.

References:

[1] G. Poppe, Bull. Soc. Chim. Belg. **44**, 640 (1935).

[2] A. W. Francis, Ind. Eng. Chem. **36**, 1096 (1944).

[3] H. I. Weck and H. Hunt, Ind. Eng. Chem. **46**, 2521 (1954).

[4] C. M. Lakshmanan and G. S. Laddha, J. Madras. Univ. **29**, 97 (1959).

[5] S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409 (1963).

[6] R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816 (1968), G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 26 (1981).

[7] V. P. Sazonov, I. N. Zhilyaeva, and L. V. Gudkina, Zh. Prikl. Khim. (Leningrad) **48**, 1953 (1975).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:

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

Variables:

$T/\mathrm{K}=367$, $P/\mathrm{kPa}=329-12412$

Prepared By:

V. P. Sazonov

Experimental Data

The upper critical solution temperature (T_c) was reported to be 93.6 °C (366.8 K, compiler).

A value of $\mathrm{d}T_c/\mathrm{d}P$ of 0.0216 $\mathrm{K\cdot kPa^{-1}}$ was reported in the above pressure range.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The observations were carried out in sealed tubes in the presence of the vapor phase. A Cailletet 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) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:
H. I. Weck and H. Hunt, Ind. Eng. Chem. **46**, 2521–3 (1954).

Variables:
T/K=298 and 343

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclohexane

		Cyclohexane-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
25.0	298.2	2.20	0.0301	94.90	0.9625
69.5	342.7	13.80	0.1808	91.50	0.9369

Auxiliary Information

Method/Apparatus/Procedure:
The refractometric method was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; technical grade; distilled; n(20 °C,D) $=1.3818$, d(20 °C)$=1135.2$ g·L^{-1}.
(2) Source not specified; purified by crystallization; n(20 °C,D)$=1.4262$, d(20 °C)$=777.4$ g·L^{-1}.

Estimated Error:
Temperature: ±0.05 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:
C. M. Lakshmanan and G. S. Laddha, J. Madras. Univ. **29**, 97–102 (1959).

Variables:
T/K=303

Prepared By:
V. P. Sazonov

Experimental Data

The solubility of nitromethane in the (2)-rich phase at 30 °C (303 K, complier) was reported as 100 $w_1=3.92$. The corresponding mole fraction solubility, x_1, calculated by the complier, is 0.0532.

The solubility of nitromethane in the (1)-rich phase at 30 °C (303 K, complier) was reported as 100 $w_1=94.57$. The corresponding mole fraction solubility, x_1, calculated by the complier is 0.9600.

Auxiliary Information

Method/Apparatus/Procedure:
The titration method by Othmer *et al.*[1] was used. No further experimental details were given.

Source and Purity of Materials:
(1) Fluka A. G.; Buchs S. G.; distilled through a rectification column; b.p.$=100.5-101.5$ °C, n(30 °C,D)$=1.3770$, d(30 °C)$=1123.7$ g·L^{-1}.
(2) B. D. H. Ltd.; laboratory reagent grade; rectified; b.p. $=(80.5-81.5$ °C), n(30 °C,D)$=1.4206$, d(30 °C) d(30 °C)$=772.5$ g·L-1.

Estimated Error:
Temperature: ±1 K.

References:
[1] D. F. Othmer, R. E. White, and E. Trueger, Ind. Eng. Chem. **33**, 1240 (1941).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

Variables:
T/K=288 and 303

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclohexane

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
15.0	288.2	2.2	0.030	95.7	0.968
25.0	298.2	2.8	0.038	94.6	0.960
30.0	303.2	3.4	0.046	93.4	0.951

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Analysis of the phases was made both by gas chromatography and by refractive index.

Source and Purity of Materials:

(1) Commercial Solvents Corp.; purity 99 mole %; not further purified.
(2) Phillips Petroleum Co.; purity 99 mole %; not further purified.

Estimated Error:

Not specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 26 (1981).

Variables:
T/K=352–366

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclohexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
352.3	79.1	—	—	0.851	80.6
354.9	81.7	0.242	18.8	—	—
359.6	86.4	0.300	23.7	—	—
362.8	89.6	—	—	0.770	70.8
363.2	90.9	0.369	29.8	—	—
365.1	91.9	0.437	36.0	—	—
365.5	92.3	—	—	0.696	62.4
365.5	92.3	—	—	0.647	57.1
365.6	92.4	0.492	41.3	—	—
365.7	92.5	0.542	46.2	—	—
365.8	92.6	0.580	50.0	0.580	50.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:
V. P. Sazonov, I. N. Zhilyaeva, and L. V. Gudkina, Zh. Prikl. Khim. (Leningrad) **48**, 1953–7 (1975).

Variables:
T/K = 284–367

Prepared By:
N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclohexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compilers)	100 w_1	x_1 (compilers)	100 w_1	x_1 (compilers)
11.00	284.15	1.75	0.0240	96.28	0.9727
50.75	323.90	—	—	90.01	0.9255
66.85	340.00	9.99	0.1327	—	—
76.55	349.70	—	—	90.01	0.8466
84.25	357.40	20.01	0.2564	—	—
87.90	361.05	—	—	69.98	0.7627
90.45	363.60	30.05	0.3720	—	—
91.85	365.00	—	—	60.04	0.6744
92.15	365.30	39.00	0.4685	—	—
93.25	366.40	—	—	50.01	0.5797
93.65	366.80	45.02	0.5303	—	—
93.65	366.80	47.5	0.555	47.5	0.555 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method of Alekseev[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled through a column of 15 theoretical plates; $n(20\ °C,D)=1.3819$, $d(20\ °C)=1138\ g\cdot L^{-1}$.
(2) Source not specified; pure grade reagent; distilled in a glass-packed fractionating column; $n(20\ °C,D)=1.4263$, $d(20\ °C)=778.5\ g\cdot L^{-1}$.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Methylcyclopentane; C_6H_{12}; [96-37-7]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 28 (1981).

Variables:
T/K = 342–363

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and methylcyclopentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
341.6	68.4	—	—	0.874	83.4
348.2	75.0	0.197	15.1	—	—
351.2	78.0	—	—	0.824	77.3
352.2	79.0	0.235	18.2	—	—
352.5	79.3	0.235	17.7	—	—
353.9	80.7	—	—	0.801	74.5
356.7	83.5	—	—	0.777	71.6
357.4	84.2	0.303	24.0	—	—
359.9	86.7	0.360	29.0	—	—
360.1	86.9	—	—	0.731	66.3
361.2	88.0	0.400	32.6	—	—
362.1	88.9	0.478	39.9	—	—
362.3	89.1	0.518	43.8	0.622	54.4
362.3	89.1	0.520	44.0	—	—
362.4	89.2	—	—	0.615	53.7
362.5	89.3	0.560	48.0	0.560	48.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:
(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.94 mole%; purification as above.

Estimated Error:
Temperature: reproduced better than 0.1 K.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,3-Dimethyl-1-butene; C_6H_{12}; [563-78-0]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:
T/K=319–334

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 2,3-dimethyl-1-butene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
319.1	45.9	—	—	0.838	79.0
326.9	53.7	—	—	0.786	72.7
329.3	56.1	0.325	25.9	—	—
331.7	58.5	—	—	0.709	63.9
332.0	58.8	0.412	33.7	—	—
333.1	59.9	0.430	35.4	—	—
333.3	60.1	0.447	37.0	0.633	55.6
333.6	60.4	0.507	42.7	—	—
333.9	60.7	0.568	48.8	0.595	51.6
333.9	60.7	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:
(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.99 mole %; purification as above.

Estimated Error:
Temperature: reproduced better than 0.1 K.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methyl-1-pentene; C_6H_{12}; [763-29-1]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:
T/K=323–336

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 2-methyl-1-pentene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
323.1	49.9	—	—	0.825	77.4
326.1	52.9	—	—	0.801	74.5
331.1	57.9	0.334	26.7	—	—
333.1	59.9	—	—	0.730	66.2
333.4	60.2	0.387	31.4	0.712	64.2
334.3	61.1	—	—	0.695	62.3
334.4	61.2	—	—	—	—
334.9	61.7	0.436	35.9	—	—
335.1	61.9	—	—	0.633	55.6
335.3	62.1	0.488	40.9	—	—
335.4	62.2	0.563	48.3	0.605	52.6
335.5	62.3	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:
(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.99 mole %; purification as above.

Estimated Error:
Temperature: reproduced better than 0.1 K.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2-Dimethylbutane; C_6H_{14}; [75-83-2]

Original Measurements:
M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:
T/K=333–370

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2-dimethylbutane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
59.5	332.7	—	—	0.915	88.4
77.7	350.9	0.188	14.1	—	—
85.3	358.5	—	—	0.829	77.4
86.9	360.1	0.271	20.8	—	—
93.5	366.7	0.383	30.5	—	—
94.7	367.9	—	—	0.733	66.0
95.1	368.3	0.441	35.8	—	—
95.9	369.1	—	—	0.697	62.0
96.4	369.6	0.517	43.1	—	—
96.5	369.7	0.492	40.7	—	—
96.6	369.8	—	—	0.619	53.5
96.7	369.9	0.585	50.0	0.585	50.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:
(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.=−29.15 °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:
Not specified.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8]

Original Measurements:
M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:
T/K=345–370

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,3-dimethylbutane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
71.4	344.6	—	—	0.892	85.4
78.7	351.9	—	—	0.863	81.7
85.4	358.6	0.255	19.5	—	—
87.4	360.0	0.282	21.8	—	—
88.6	361.8	0.296	22.9	—	—
91.3	364.5	0.345	27.2	—	—
91.8	365.0	—	—	0.773	70.7
93.2	366.4	—	—	0.759	69.0
93.9	367.1	0.403	32.3	—	—
95.4	368.6	0.469	38.5	—	—
95.5	368.7	0.461	37.7	—	—
96.1	369.3	0.523	43.7	0.643	56.1
96.2	369.4	0.585	50.0	0.585	50.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:
(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.=−29.15 °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:
Not specified.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methylpentane; C_6H_{14}; [107-83-5]

Original Measurements:
M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:
T/K=345–374

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2-methylpentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
71.9	345.1	—	—	0.904	87.0
82.9	356.1	0.203	15.3	—	—
88.0	361.2	—	—	0.846	79.6
90.7	363.9	0.288	22.3	—	—
97.2	370.4	0.392	31.3	0.770	70.3
97.5	370.7	0.392	31.3	—	—
97.9	371.1	—	—	0.745	67.4
98.4	371.6	0.417	33.6	—	—
99.4	373.6	0.458	37.4	—	—
100.3	373.5	0.575	48.9	—	—
100.4	373.6	—	—	0.657	57.6
100.4	373.6	—	—	0.592	50.7
100.5	373.7	—	—	0.586	50.1
100.4	373.6	0.585	50.0	0.585	50.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:
(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.= −29.15 °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:
Not specified.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 3-Methylpentane; C_6H_{14}; [96-14-0]

Original Measurements:
M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:
T/K=349–372

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 3-methylpentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
75.7	348.9	0.178	13.3	—	—
77.1	350.3	—	—	0.872	82.8
91.9	365.1	—	—	0.802	74.2
92.2	365.4	0.320	25.0	—	—
93.3	366.5	0.328	25.7	—	—
93.7	366.9	0.348	27.4	—	—
94.0	367.2	—	—	0.785	72.1
96.5	369.7	—	—	0.745	67.4
97.9	371.1	0.478	39.3	—	—
98.5	371.6	0.541	45.5	0.639	55.6
98.6	371.8	0.585	50.0	0.585	50.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:
(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.= −29.15 °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:
Not specified.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2 ; [75-52-5] (2) Hexane; C_6H_{14} ; [110-54-3]	V. P. Sazonov, Technical University, Samara, Russia. A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and hexane have been reported in three publications, all using the synthetic method.

Mulliken and Wakeman[1] determined the upper critical solution temperature, while Malesinska[2] and Rolla *et al.*[3] measured the mutual solubilities of the components between 366 and 376 K and between 357 and 376 K, respectively.

Values obtained by the graphical interpolation or extrapolation from the data sheets are presented in the following table. Data are ''recommended'' if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Recommended and tentative values for the mutual solubilities of nitromethane and hexane

	Hexane-rich phase			Nitromethane-rich phase		
T/K	100 w_1	x_1		100 w_2	x_2	
358	16.3	0.216	Tentative	—	—	—
363	19.2	0.251	Tentative	17.8	0.133	Tentative
368	25	0.32	Recommended	23.4	0.178	Recommended
373	34	0.42	Recommended	30	0.23	Recommended

The upper critical solution temperature has been reported as 375.4 K,[3] 375.55 K,[2] and 379 K.[1] The UCST of Mulliken and Wakeman[1] is rejected. The remaining values are in good agreement and their average, (375.5±0.1) K is recommended.

The corresponding critical solution composition has been reported as $x_{c1}=0.6225$ (Malesinska[2]) and $x_{c1}=0.585$ (Rolla *et al.*[3]). Their average value, $x_{c1}=(0.604\pm0.018)$, is recommended.

The recommended UCST and x_{c1} are consistent with the values calculated on the basis of critical evaluation of all experimental critical solution compositions in the nitromethane–*n*-alkane series and discussed at the beginning of this volume. The numerical values reported in the above tables have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.892\,57$, $a_2=0.196\,71$, $b_1=3.205\,60$, $b_2=-3.077\,72$ (mean standard error of estimate was 0.0049).

For approximation the recommended value of UCST and x_{c1} have been used. This relationship is presented in Fig. 12 together with experimental data reported in Malesinska[2] and Rolla *et al.*[3]

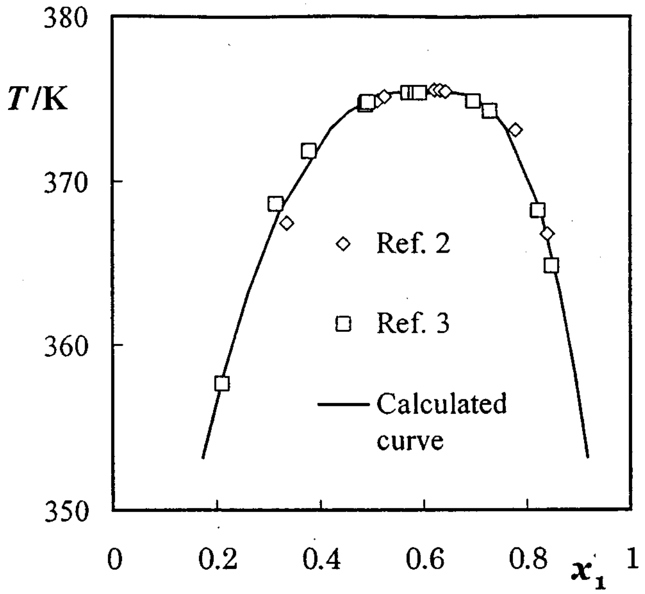

FIG. 12. Mutual solubility of nitromethane and hexane.

References:

[1]S. P. Mulliken and R. L. Wakeman, Rec. Trav. Chim. **54**, 366 (1935).
[2]B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53 (1960).
[3]M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48 (1967).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexane; C_6H_{14}; [110-54-3]

Original Measurements:

B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53–9 (1960).

Variables:

T/K=367–376

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and hexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
366.73	93.58	—	—	0.8387	78.65
367.43	94.28	0.3355	26.34	—	—
373.13	99.28	—	—	0.7779	71.27
374.88	101.73	0.5115	42.58	—	—
375.15	102.00	0.5261	44.02	—	—
375.42	102.27	—	—	0.6421	55.96
375.50	102.35	—	—	0.6330	54.99
375.55	102.40	0.6225	53.90	0.6225	53.90 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev[1]) method was used. Sealed samples, about 1.0–1.5 g, of various compositions were heated to a temperature higher than that required for complete homogeneity, then cooled at about 0.01 K·min^{-1} until turbidity and a meniscus appeared. Repeat determinations were made.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Isolated from a Fischer-Tropsch gasoline fraction freed from unsaturated hydrocarbons; fractionally distilled.

Estimated Error:

Not specified.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexane; C_6H_{14}; [110-54-3]

Original Measurements:

M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:

T/K=358–375

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and hexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
84.5	357.7	0.211	15.9	—	—
91.6	364.8	—	—	0.849	79.9
95.0	368.2	—	—	0.820	76.3
95.4	368.6	0.315	24.6	—	—
98.6	371.8	0.379	30.2	—	—
101.1	374.3	—	—	0.727	65.4
101.4	374.6	0.488	40.3	—	—
101.6	374.8	0.490	40.5	—	—
101.6	374.8	0.493	40.8	—	—
101.7	374.9	—	—	0.697	62.0
102.2	375.4	0.571	48.5	0.592	50.7
102.2	375.4	0.585	50.0	0.585	50.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described in Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:

(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.=−29.15 °C.
(2) Fluka AG; purist grade; purif5ication as above.

Estimated Error:

Not specified.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cycloheptane; C_7H_{14}; [291-64-5]

Original Measurements:

R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:

T/K=362–375

Prepared By:

V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and cycloheptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
362.0	88.8	—	—	0.850	77.9
369.4	96.2	—	—	0.792	70.3
369.5	96.3	0.333	23.7	—	—
370.5	97.3	—	—	0.779	68.7
371.9	98.7	0.363	26.2	—	—
372.5	99.3	—	—	0.743	64.3
373.4	100.2	0.415	30.6	—	—
374.0	100.8	0.477	36.2	—	—
374.1	100.9	0.511	39.4	—	—
374.5	101.3	0.590	47.2	—	—
374.6	101.4	—	—	0.670	55.8
374.6	101.4	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and methylcyclohexane have been reported in four publications. Francis[1] determined the upper critical solution temperature by the synthetic method. Kotarski[2] studied the mutual solubilities of the components at 293 K by the titration method. Riccardi *et al.*[3] measured the mutual solubilities between 345 and 371 K, also by the synthetic method. Finally, Lafyatis *et al.*[4] determined the mutual solubilities at 323, 348, and 363 K using an analytical method.

The UCST reported by Francis[1] is considerably lower than UCST reported by Riccardi *et al.*[3] (data from this laboratory are close to tentative/recommended values for many systems) and is rejected. The corresponding critical solution composition has been reported only in Riccardi *et al.*[3] Therefore, for approximate data from Riccardi *et al.*,[3] the UCST=370.3 K and $x_{c1}=0.600$ (100 $w_1=48.0$), have been used; these values are treated as tentative. The numerical values reported in Kotarski,[2] Riccardi *et al.*,[3] and Lafyatis *et al.*[4] have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted:

$$a_1=1.022\,82,\quad a_2=-0.441\,29,\quad b_1=3.285\,29,\quad b_2=-3.155\,35$$

(mean standard error of estimate was 0.0356).

As an approximation, the UCST=370.3 K and $x_{c1}=0.600$ (Riccardi *et al.*[3]) have been used. This relationship together with all experimental points[2–4] is presented in Fig. 13. The calculated results for the selected temperatures are presented in the following table. These mutual solubilities ought to be treated as tentative.

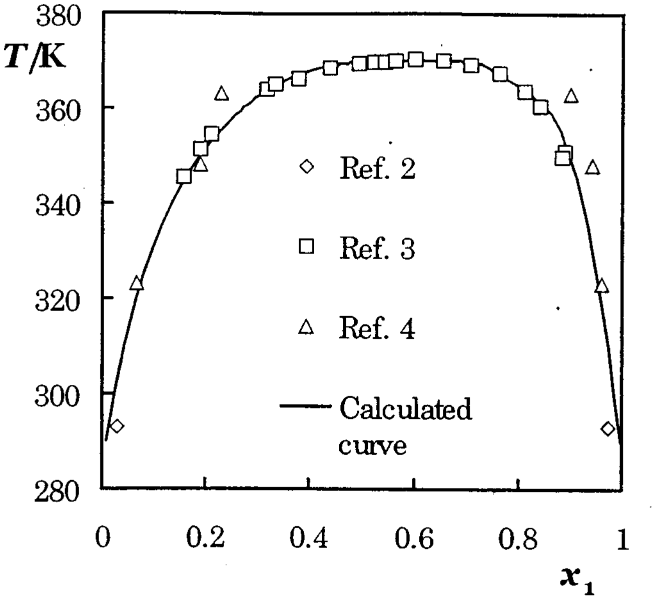

FIG. 13. Mutual solubility of nitromethane and methylcyclohexane.

Mutual solubility of nitromethane and methylcyclohexane

	Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
293.2	0.0131	0.82	0.9935	98.95
303.2	0.0294	1.85	0.9814	97.04
313.2	0.0497	3.15	0.9682	94.98
323.2	0.0752	4.81	0.9535	92.72
333.2	0.1077	6.98	0.9363	90.13
343.2	0.1504	9.91	0.9148	86.96
353.2	0.2099	14.18	0.8847	82.68
363.2	0.3077	21.65	0.8314	75.40
368.2	0.4066	29.87	0.7675	67.24
369.2	0.4447	33.24	0.7392	63.80
370.2	0.5308	41.29	0.6668	55.44

References:

[1]A. W. Francis, Ind. Eng. Chem. **36**, 1096 (1944).

[2]A. Kotarski, Przem. Chem. **42**, 413 (1963).

[3]R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816 (1968); G. Spinolo, Int. Data Ser., Sel. Data Mixtures. Ser. A (**1**), 29 (981).

[4]D. S. Lafyatis, L. S. Scott, D. M. Trampe, and C. A. Eckert, Ind. Eng. Chem. Res. **28**, 585 (1989).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Methylcyclohexane; C_7H_{14}; [108-87-2]	A. Kotarski, Przem. Chem. **42**, 431–6 (1963).

Variables:	**Prepared By:**
T/K=293	V. P. Sazonov

Experimental Data

The solubility of nitromethane in methylcyclohexane at 20.0 °C (293.2 K, compiler) was reported to be 100 $w_1=1.8$. The corresponding mole fraction, x_1, calculated by the compiler is 0.029.

The solubility of methylcyclohexane in nitromethane at 20.0 °C (293.2 K, compiler) was reported to be 100 $w_2=4.2$. The corresponding mole fraction, x_2, calculated by the compiler is 0.027.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Source not specified; purity not specified; distilled; $n(20\ °C,D)=1.3819$.

(2) Source not specified; purity not specified; distilled; $n(20\ °C,D)=1.4233$, $d(20\ °C)=769.5\ g\cdot L^{-1}$.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Methylcyclohexane; C_7H_{14} ; [108-87-2]

Original Measurements:

D. S. Lafyatis, L. S. Scott, D. M. Trampe, and C. A. Eckert, Ind. Eng. Chem. Res. **28**, 585–90 (1989).

Variables:

T/K=323–363

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and methylcyclohexane

t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
50.0	323.2	0.066	4.2	0.961	93.9
75.0	348.2	0.188	12.6	0.941	90.8
90.0	363.2	0.229	15.6	0.898	84.6

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The two partially miscible components were placed in the equilibration cell in approximately equal volumes, and the mixture was stirred for at least 15 min. The stirring was then stopped and the mixture allowed to separate into two phases for at least 15 min. Samples of each phase were taken and analyzed by gas chromatography.

Source and Purity of Materials:

(1) Source not specified; purity greater than 99.9 mole %; not purified.
(2) Source not specified; purity greater than 99.9 mole %; not purified.

Estimated Error:

Temperature: ±0.01 K.
Composition: ≤0.005 mole fraction.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

Original Measurements:

R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 29 (1981).

Variables:

T/K=345–370

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and methylcyclohexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
345.4	72.2	0.157	10.4	—	—
350.0	76.8	—	—	0.883	82.4
351.0	77.7	—	—	0.887	83.0
351.4	78.2	0.190	12.7	—	—
354.4	81.2	0.210	14.2	—	—
360.5	87.3	—	—	0.840	76.5
363.8	90.6	—	—	0.812	72.9
364.2	91.0	0.317	22.4	—	—
365.1	91.9	0.333	23.7	—	—
366.4	93.2	0.378	27.4	—	—
367.5	94.3	—	—	0.764	66.8
368.6	95.4	0.439	32.7	—	—
369.2	96.0	—	—	0.707	60.0
369.6	96.4	0.496	38.0	—	—
369.8	96.6	0.524	40.6	—	—
369.8	96.6	0.545	42.7	—	—
370.1	96.9	0.563	44.5	—	—
370.2	97.0	—	—	0.653	53.9
370.3	97.1	0.600	48.0	0.600	48.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99.99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,3-Dimethyl-1-pentene; C_7H_{14}; [3404-72-6]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:
T/K=330–343

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 2,3-dimethyl-1-pentene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
329.8	56.6	—	—	0.848	77.6
332.1	58.9	—	—	0.831	75.3
335.6	62.4	0.307	21.6	—	—
336.5	63.3	0.322	22.8	—	—
338.6	65.4	0.357	25.7	—	—
339.0	65.8	—	—	0.779	68.7
339.5	66.3	0.376	27.3	—	—
339.9	66.7	—	—	0.763	66.7
341.3	68.1	0.406	29.8	—	—
342.3	69.1	0.459	34.5	—	—
342.9	69.7	—	—	0.707	60.0
343.0	69.8	0.567	44.9	—	—
343.1	69.9	0.615	49.8	—	—
343.3	70.1	—	—	0.648	53.4
343.4	70.2	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:
(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:
Temperature: reproduced better than 0.1 K.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methyl-1-hexene; C_7H_{14}; [6094-02-6]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:
T/K=328–347

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 2-methyl-1-hexene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
328.1	54.9	—	—	0.885	82.7
334.1	60.9	—	—	0.855	78.6
340.6	67.4	—	—	0.832	75.5
340.8	67.6	0.372	26.9	—	—
343.1	69.9	—	—	0.793	70.4
343.3	70.1	0.406	29.8	—	—
344.7	71.5	0.456	34.3	—	—
345.9	72.7	—	—	0.723	61.9
346.4	73.2	0.544	42.6	0.607	49.0
346.4	73.2	0.572	45.4	—	—
346.5	73.3	0.521	40.3	0.666	55.3
346.6	73.6	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:
(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:
Temperature: reproduced better than 0.1 K.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 3-Methyl-1-hexene; C_7H_{14} ; [3404-61-3]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:
T/K=331–346

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 3-methyl-1-hexene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
330.6	57.4	—	—	0.870	80.6
339.1	65.9	—	—	0.820	73.9
340.1	66.9	0.348	24.9	—	—
342.1	68.9	—	—	0.773	67.9
342.3	69.1	0.379	27.5	—	—
343.5	70.3	0.445	33.3	—	—
344.3	71.1	—	—	0.728	62.5
345.1	71.9	0.515	39.8	—	—
345.6	72.4	0.573	45.5	0.662	54.9
345.6	72.4	—	—	0.622	50.6
345.6	72.4	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:
(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:
Temperature: reproduced better than 0.1 K.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 4-Methyl-1-hexene; C_7H_{14}; [3769-23-1]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:
T/K=321–341

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 4-methyl-1-hexene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
321.3	48.1	—	—	0.886	82.9
331.6	58.4	—	—	0.840	76.5
337.0	63.8	0.351	25.2	—	—
337.7	64.5	—	—	0.778	68.5
339.3	66.1	0.441	32.9	—	—
339.8	66.6	—	—	0.725	62.1
340.0	66.8	0.491	37.5	—	—
340.5	67.3	—	—	0.685	57.5
340.5	67.3	—	—	0.629	51.3
340.6	67.4	—	—	0.606	48.9
340.7	67.5	0.546	42.8	—	—
340.7	67.5	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:
(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:
Temperature: reproduced better than 0.1 K.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 5-Methyl-1-hexene; C_7H_{14}; [3524-73-0]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:
T/K=321–340

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 5-methyl-1-hexene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
321.3	48.1	—	—	0.875	81.3
331.6	58.4	—	—	0.834	75.7
333.0	59.8	0.311	21.9	—	—
335.3	62.1	0.360	25.9	0.781	68.9
335.7	62.5	0.367	26.5	—	—
336.0	62.8	0.399	29.2	—	—
337.8	64.6	—	—	0.739	63.9
338.7	65.5	0.493	37.7	—	—
339.2	66.0	—	—	0.714	60.8
339.4	66.2	—	—	0.610	49.3
339.6	66.4	0.553	43.5	—	—
339.7	66.5	0.577	45.9	0.634	51.9
		—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2-Dimethylpentane; C_7H_{16}; [590-35-2]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A **(2)**, 80 (1977).

Variables:
T/K=371–376

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2-dimethylpentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
370.5	97.3	0.385	27.6	—	—
370.9	97.7	—	—	0.830	74.8
370.9	97.7	—	—	0.828	74.6
372.8	99.6	—	—	0.785	69.0
372.9	99.9	0.441	32.5	—	—
374.6	101.4	0.510	38.8	—	—
375.1	101.9	—	—	0.791	60.9
375.1	101.9	—	—	0.681	56.5
375.3	102.1	0.586	46.3	—	—
375.5	102.3	0.608	48.6	—	—
376.6	102.4	0.635	51.1	0.635	51.5 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch, **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7]

Original Measurements:

M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch, **22A**, 48–53 (1967).

Variables:

$T/\mathrm{K}=356-377$

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,4-dimethylpentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
$t/°\mathrm{C}$	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
82.5	355.7	0.217	14.4	—	—
85.7	358.9	—	—	0.898	84.3
90.5	363.7	—	—	0.876	81.1
96.5	369.7	0.358	25.4	—	—
97.3	370.5	—	—	0.839	76.0
100.5	373.7	0.442	32.5	—	—
102.8	376.0	0.533	41.0	0.745	64.0
103.3	376.5	0.596	47.3	0.686	57.1
103.4	376.6	0.640	52.0	0.640	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:

(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p. = −29.15 °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:

Not specified.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methylhexane; C_7H_{16}; [591-76-4]

Original Measurements:

R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A **(2)**, 79 (1977).

Variables:

$T/\mathrm{K}=365-379$

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2-methylhexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	$t/°\mathrm{C}$ (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
365.2	92.0	—	—	0.882	82.0
368.7	95.5	—	—	0.857	78.5
369.8	96.6	—	—	0.843	76.6
373.2	100.0	0.376	26.9	—	—
374.0	100.8	—	—	0.823	73.9
374.8	101.6	0.398	28.7	—	—
375.6	102.4	0.435	31.9	—	—
376.5	103.3	—	—	0.787	69.2
377.3	104.1	—	—	0.758	65.6
377.5	104.3	0.462	34.3	—	—
377.8	104.6	0.503	38.1	—	—
377.9	104.7	—	—	0.742	63.7
378.6	105.4	—	—	0.690	57.6
378.7	105.5	—	—	0.662	54.4
378.7	105.5	0.626	50.5	—	—
378.8	105.6	0.560	43.7	—	—
379.0	105.8	0.578	45.5	—	—
379.4	106.2	0.609	48.7	—	—
379.3	106.1	0.635	51.5	0.635	51.5 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Heptane; C_7H_{16}; [142-82-5]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Quantitative solubility data for the nitromethane+heptane have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Kimura *et al.*[1]	303	Mutual	Titration
Malesinska[2]	289–382	Mutual	Synthetic
Komarova and Kogan[3]	293–343	Mutual	Analytical
Rolla *et al.*[4]	372–381	Mutual	Synthetic
Patel[5]	294	Mutual	Synthetic
Sazonov[6]	313–382	Mutual	Synthetic
Rezanova *et al.*[7]	298–333	Mutual	Titration

All original data are compiled in the data sheets immediately following this Critical Evaluation. The data of Patel,[5] in both phases, disagree markedly with all other studies and are rejected. All other data are included in Tables 2 and 3 below.

In these tables, values obtained by the Evaluators by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). ''Best'' values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to the ''best'' values do not have statistical significance and should be regarded only as a convenient representation of the spread of reported values and not as error limits. The letter (R) indicates ''Recommended'' data. Data are ''Recommended'' if two or more apparently reliable studies are in reasonable agreement (±5% relative).

It will be noted from Tables 2 and 3 that the solubility data reported by independent workers for this system are in only fair agreement. This is reflected in the σ_n values, which are typically 5%–10% relative. As the 'absolute' value of σ_n remains approximately constant, only the higher solubilities can therefore be recommended. Nitromethane and heptane have very similar values of their refractive index, so visual determination of the meniscus appearance or disappearance is difficult. This is probably one of the reasons for the discrepancies among different authors. From the Evaluator's point of view, further investigation of this system is required.

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

	Solubility, 100 w_i		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_1	x_1
293	2.13 (Ref. 3)	2.1	0.034
298	2.5* (Ref. 3), 2.54 (Ref. 7)	2.5 (R)	0.040
303	3.5 (Ref. 1), 2.9* (Ref. 3), 3.17 (Ref. 7)	3.2±0.2	0.052
308	3.3* (Ref. 3)	3.3	0.053
313	3.63 (Ref. 3), 4.00 (Ref. 7)	3.8±0.2	0.061
318	4.5* (Ref. 2), 4.2* (Ref. 3), 4.9* (Ref. 6)	4.5±0.3	0.072
323	5.2* (Ref. 2), 4.7* (Ref. 3), 5.5* (Ref. 6), 5.29 (Ref. 7)	5.2±0.3	0.083
328	6.0 (Ref. 2), 5.5* (Ref. 3), 6.4* (Ref. 6)	6.0±0.4	0.095
333	6.7* (Ref. 2), 6.4* (Ref. 3), 7.3* (Ref. 6), 6.47 (Ref. 7)	6.7±0.4	0.11
338	7.5* (Ref. 2), 7.4* (Ref. 3), 8.4* (Ref. 6)	7.8±0.5	0.12
343	8.6* (Ref. 2), 8.63 (Ref. 3), 10.0* (Ref. 6)	9.1±0.7	0.14
348	9.8* (Ref. 2), 11.2* (Ref. 6)	10.5±0.7	0.162
353	11.4* (Ref. 2), 13.0* (Ref. 6)	12.2±0.8	0.186
358	13.5 (Ref. 2), 14.9* (Ref. 6)	14.2±0.7 (R)	0.214
363	16.2* (Ref. 2), 17.4* (Ref. 4)	16.8±0.6 (R)	0.249
368	20.2* (Ref. 2), 20.7* (Ref. 6)	20.5±0.3 (R)	0.297
373	25.3* (Ref. 2), 25.7* (Ref. 6)	25.5±0.2 (R)	0.360
378	33.2* (Ref. 15), 33.5 (Ref. 4), 33.4* (Ref. 6)	33.4±0.1 (R)	0.452

TABLE 3. Tentative and recommended (R) values for the solubility of heptane (2) in nitromethane (1)

	Solubility, 100 w_1		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_2	x_2
293	2.0* (Ref. 2), 2.39 (Ref. 3)	2.2±0.2	0.013
298	2.1* (Ref. 2), 2.7* (Ref. 3), 2.1 (Ref. 7)	2.3±0.3	0.014
303	2.7* (Ref. 1), 2.2* (Ref. 2), 3.0* (Ref. 3), 2.6 (Ref. 7)	2.6±0.3	0.016
308	2.3* (Ref. 2), 3.3* (Ref. 3)	2.8±0.5	0.017
313	2.4* (Ref. 2), 3.64 (Ref. 3), 4.8* (Ref. 6), 2.9 (Ref. 7)	3.4±0.9	0.021
318	2.6* (Ref. 2), 3.7* (Ref. 3), 5.1* (Ref. 6)	3.9±1.0	0.024
323	3.5* (Ref. 2), 3.9* (Ref. 3), 5.4* (Ref. 6), 3.9 (Ref. 7)	4.2±0.7	0.026
328	3.9* (Ref. 2), 4.4* (Ref. 3), 5.9* (Ref. 6)	4.8±0.9	0.030
333	4.3* (Ref. 2), 5.2* (Ref. 3), 6.8* (Ref. 6), 4.5 (Ref. 7)	5.2±1.0	0.032
338	5.8* (Ref. 2), 6.1* (Ref. 3), 7.7* (Ref. 6)	6.6±0.8	0.041
343	6.7* (Ref. 2), 7.33 (Ref. 3), 8,8* (Ref. 6)	7.7±0.9	0.048
348	8.1* (Ref. 2), 9.9* (Ref. 6)	9.0±0.9	0.057
353	9.8* (Ref. 2), 11.6* (Ref. 6)	10.7±0.9	0.0680
358	11.9* (Ref. 2), 13.5* (Ref. 6)	12.7±0.8	0.0814
363	14.6* (Ref. 2), 16.0* (Ref. 6)	15.3±0.7 (R)	0.0991
368	17.8* (Ref. 2), 19.2* (Ref. 6)	18.5±0.7 (R)	0.122
373	22.2* (Ref. 2), 21.4* (Ref. 4), 23.7* (Ref. 6)	23±1	0.15
378	27.9* (Ref. 2), 28.6* (Ref. 4), 31.3* (Ref. 6)	29±1	0.20

The upper critical solution temperature has been reported as 381.0 K,[4] 381.45 K,[2] 381.5 K,[6] and 388 K.[8] The UCST reported by Francis,[8] is considerably higher than all other values and is rejected. The average of the remaining values, UCST=(381.3±0.2) K, is recommended. The corresponding critical solution composition has been reported as: $x_{c1}=0.640$,[4] $x_{c1}=0.647$,[6] and $x_{c1}=0.650$.[2] Their average value, $x_{c1}=0.646\pm0.004$, (100 $w_1=52.6$), has a spread equal to the estimated error given by Sazonov[6] and is therefore recommended. The recommended UCST and x_{c1} are consistent with the values calculated on the basis of critical evaluation of all experimental critical solution compositions in the nitromethane–*n*-alkane series and discussed at the beginning of this volume. The numerical values reported in the above tables have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted:

$$a_1=0.964\ 62,\quad a_2=-0.370\ 72,\quad b_1=3.884\ 02,\quad b_2=-3.794\ 83$$

(mean standard error of estimate was 0.0085).

For approximation the recommended values of UCST and x_{c1} have been used. The calculated compositions are in each point inside inaccuracy declared in the above tables. This relationship is presented in Fig. 14 together with the ''best values'' reported in Tables 2 and 3.

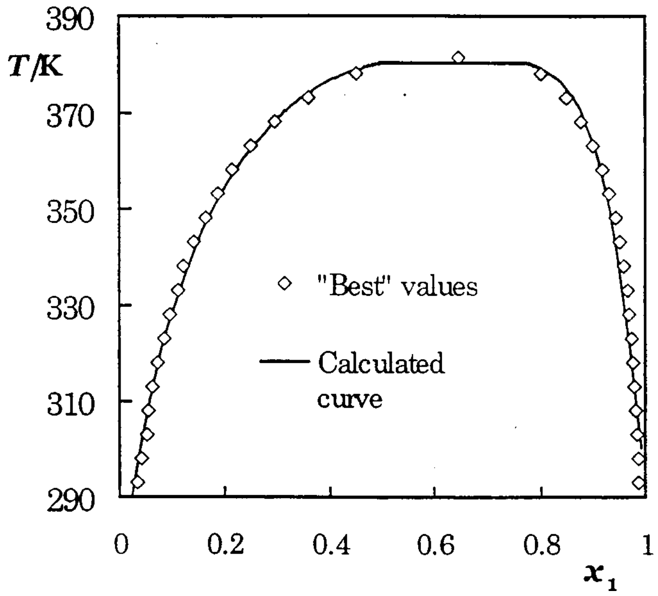

FIG. 14. Mutual solubility of nitromethane and heptane.

References:

[1] C. Kimura, K. Kashiwaya, and T. Acahara, Kogyo Kagaku Zasshi **59**, 1126 (1956).

[2] B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53 (1960).

[3] E. G. Komarova and V. B. Kogan, Zh. Prikl. Khim. (Leningrad) **37**, 1776 (1964).

[4] M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48 (1967).

[5] A. N. Patel, J. Chem. Eng. Data **26**, 124 (1981).

[6] V. P. Sazonov, Zh. Obshch. Khim. **59**, 2431 (1989).

[7] E. N. Rezanova, A. M. Tojkka, and N. P. Markuzin, Vestn. Leningr. Univ., Fiz., Khim. **18**, 53 (1991).

[8] A. W. Francis, Critical Solution Temperatures, Adv. Chem. Ser. **31** (1961).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Heptane; C_7H_{16}; [142-82-5]	C. Kimura, K. Kashiwaya, and T. Asahara, Kogyo Kagaku Zasshi **59**, 1126–8 (1956).
Variables:	**Prepared By:**
T/K = 303	V. P. Sazonov

Experimental Data

The solubility of nitromethane in the (2)-rich phase at equilibrium at 30 °C (303 K, compiler) was reported to be 100 $w_1 = 3.5$. The corresponding mole fraction, x_1, calculated by the compiler is 0.056.

The solubility of nitromethane in the (1)-rich phase at equilibrium at 30 °C (303 K, compiler) was reported to be 100 $w_1 = 97.3$. The corresponding mole fraction solubility, x_1, calculated by the compiler is 0.983.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. No further experimental details were given.

Source and Purity of Materials:

(1) Synthesized in the laboratory; purity not specified; b.p. = 101 °C, n(20 °C,D) = 1.3817, d(20 °C) = 1137.2 g·L^{-1}.

(2) Source not specified; commercial material; purity not specified; b.p. = 98 °C, n(20 °C,D) = 1.3878, d(20 °C)
d(20 °C) = 683.2 g·L^{-1}.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Heptane; C_7H_{16}; [142-82-5]

Original Measurements:

E. G. Komarova and V. B. Kogan, Zh. Prikl. Khim. (Leningrad) **37**, 1776–86 (1964).

Variables:

T/K = 293 and 343

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and heptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
20.0	293.2	0.0345	2.13	0.9853	97.61
40.0	313.2	0.0584	3.64	0.9775	96.36
70.0	343.2	0.1342	8.63	0.9540	92.67

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. A mixture of (1) and (2) was placed in a thermostated cell and stirred for 1 h. Compositions of phases were determined by chromatography.

Source and Purity of Materials:

(1) Source not specified; distilled in a 1.2 m packed fractionating column; b.p. = 101.2 °C, n(20 °C,D) = 1.3818, d(20 °C) d(20 °C) = 1138.0 g·L^{-1}.
(2) Source not specified; distilled in a 1.2 m packed fractionating column; b.p. = 98.4 °C, n(20 °C,D) = 1.3877.

Estimated Error:

Temperature: ±0.1 K.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Heptane; C_7H_{16}; [142-82-5]

Original Measurements:

B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chem. **8**, 53–9 (1960).

Variables:

T/K = 290–381

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and heptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
289.5	12.3	—	—	0.9877	98.00
318.2	45.0	—	—	0.9843	97.45
318.50	45.35	0.0729	4.57	—	—
328.0	54.8	0.0948	6.00	0.9759	96.10
335.5	62.3	0.1045	6.64	—	—
362.15	89.00	—	—	0.9096	85.97
372.47	99.32	0.3523	24.89	—	—
377.40	104.25	0.4339	31.83	—	—
378.83	105.68	—	—	0.8052	71.58
380.31	107.16	—	—	0.7750	67.72
380.56	107.41	0.5251	40.25	—	—
381.35	108.20	—	—	0.6991	58.60
381.43	108.28	0.6439	52.42	—	—
381.45	108.30	0.6500	53.10	0.6500	53.10 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev) method was used. Sealed samples, about 1.0–1.5 g, of various compositions were heated to a temperature higher than that required for complete homogeneity, then cooled at about 0.01 K·min^{-1} until turbidity and a meniscus appeared. Repeat determinations were made.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Isolated from a Fischer-Tropsch gasoline fraction freed from unsaturated hydrocarbons; fractionally distilled.

Estimated Error:

Not specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Heptane; C_7H_{16}; [142-82-5]

Original Measurements:
M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:
T/K=373–381

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and heptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
99.5	372.7	—	—	0.860	78.9
105.4	378.6	0.470	35.1	—	—
107.2	380.4	—	—	0.753	65.0
107.4	380.6	0.557	43.4	—	—
107.8	381.0	—	—	0.685	57.0
107.8	381.0	—	—	0.675	55.9
107.8	381.0	0.640	52.0	0.640	52.5 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was employed. No further details were reported.

Source and Purity of Materials:
(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.$=-29.15$ °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:
Not specified.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Heptane; C_7H_{16}; [142-82-5]

Original Measurements:
A. M. Patel, J. Chem. Eng. Data **26**, 124–7 (1981).

Variables:
T/K=294

Prepared By:
V. P. Sazonov

Experimental Data

The solubility of nitromethane in heptane at 20.5 °C (293.7 K, compiler) was reported to be 100 $w_1=6.2$. The corresponding mole fraction, x_1, calculated by the compiler is 0.098.

The solubility of heptane in nitromethane at 20.5 °C (293.7 K, compiler) was reported to be 100 $w_2=4.3$. The corresponding mole fraction, x_2, calculated by the compiler is 0.027.

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

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

Estimated Error:
Temperature: control to ±0.5 K.

References:
[1] D. F. Othmer, R. E. White, and E. Trueger, Ind. Eng. Chem. **33**, 1240 (1941).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Heptane; C_7H_{16}; [142-82-5]

Original Measurements:
E. N. Rezanova, A. M. Tojkka, and N. P. Markuzin, Vestn. Leningr. Univ., Fiz., Khim. **18**, 53–6 (1991).

Variables:
T/K=298–333

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane (1) and heptane (2)

T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
298.15	25.00	0.041	2.5	0.987	97.9
303.15	30.00	0.051	3.2	0.984	97.4
313.15	40.00	0.064	4.0	0.982	97.1
323.15	50.00	0.084	5.3	0.976	96.1
333.15	60.00	0.102	6.57	0.972	95.5

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. A 100 mL glass flask and a microburette with scale divisions of 0.01 mL were used. The solution was mixed by a magnetic stirrer. The titration was continued until the second phase appeared. The amount of added substance was obtained by weighing the mixture before and after the titration.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; dried over $CaCl_2$ and repeatedly distilled in a laboratory packed column of 20 theoretical plates; b.p.=101.20 °C, $n(20\ °C,D)=1.3820$.

(2) Source not specified; CP reagent; distilled; b.p.=98.42 °C, $n(20\ °C,D)=1.3877$.

Estimated Error:

Temperature: ±0.02 K
Solubility: ±0.002 mole fraction.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Heptane; C_7H_{16}; [142-82-5]

Original Measurements:
V. P. Sazonov, Zh. Obshch. Khim. **59**, 2431–5 (1989).

Variables:
T/K=313 and 382

Prepared By:
V. P. Sazonov and N. V. Sazonov

Experimental Data

Mutual solubility of nitromethane and heptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
313.3	40.1	—	—	95.0	0.969
318.2	45.0	5.0	0.080	—	—
342.8	69.6	10.0	0.154	—	—
347.2	74.0	—	—	90.0	0.937
357.2	84.0	14.0	0.211	—	—
362.1	88.9	—	—	85.0	0.903
365.5	92.3	20.0	0.291	—	—
370.3	97.1	—	—	80.0	0.868
370.5	97.3	24.0	0.341	—	—
373.6	100.4	—	—	75.0	0.831
376.7	103.5	30.0	0.413	—	—
377.2	104.0	—	—	70.0	0.793
378.4	105.2	35.0	0.469	—	—
379.8	106.6	40.0	0.522	—	—
380.2	107.0	—	—	62.0	0.728
380.8	107.6	45.0	0.573	—	—
381.0	107.8	50.0	0.621	—	—
381.2	108.0	52.5	0.645	57.5	0.689
381.5	108.3	—	—	55.0	0.667
381.5	108.3	52.8	0.647	52.8	0.647 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The apparatus with visual indication of turbidity was described by Sazonov *et al.*[1] No additional details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; fractionally distilled; 99.85 mass % purity; $n(20\ °C,D)=1.3819$, $d(20\ °C)=1138.0\ g\cdot L^{-1}$.

(2) Source not specified; reagent for chromatography; $n(20\ °C,D)=1.3877$, $d(20\ °C)=683.7\ g\cdot L^{-1}$.

Estimated Error:

Not reported.

References:

[1] V. P. Sazonov and M. F. Chernysheva, Zh. Obshch. Khim. **57**, 46 (1987).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,3-Dimethyl-1-hexene; C_8H_{16}; [16746-86-4]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–18 (1968).

Variables:
T/K=347–358

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 2,3-dimethyl-1-hexene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
346.9	73.7	—	—	0.871	78.6
348.3	75.1	0.298	18.8	—	—
352.6	79.4	0.381	25.1	—	—
353.8	80.6	—	—	0.822	71.5
354.2	81.0	0.401	26.7	—	—
355.4	82.4	0.433	29.3	—	—
355.5	82.3	—	—	0.800	68.5
357.4	84.2	0.517	36.8	—	—
357.5	84.3	0.631	48.2	0.748	61.8
357.8	84.6	—	—	0.706	56.6
357.9	84.7	0.566	41.5	0.649	50.1
358.0	84.8	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixture were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclooctane; C_8H_{16}; [292-64-8]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A** 1816-8 (1968).
*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A (**1**), 27 (1981).

Variables:
T/K=371–383

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclooctane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
370.6	97.4	—	—	0.855	76.2
375.0	101.8	0.306	19.3	—	—
377.2	104.0	—	—	0.814	70.4
379.7	106.5	—	—	0.773	64.9
381.1	107.9	—	—	0.744	61.3
381.4	108.2	0.472	32.7	—	—
381.8	108.6	0.486	34.0	—	—
382.4	109.2	0.544	39.4	—	—
382.4	109.2	0.577	42.6	—	—
382.5	109.3	—	—	0.654	50.7
382.7	109.5	0.620	47.0	0.620	47.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixture in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixture were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methyl-1-heptene; C_8H_{16}; [15870-10-7]

Original Measurements:
R. Riccardi, P. Franzosini, and M. Rolla, Z. Naturforsch. **23A**, 1816–8 (1968).

Variables:
T/K=344–356

Prepared By:
V. P. Sazonov

Experimental Data

The numerical data were not included in the original publication but were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 2-methyl-1-heptene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
343.7	70.5	0.277	17.2	—	—
344.8	71.6	—	—	0.878	79.7
348.0	74.8	0.351	22.7	—	—
352.3	79.1	—	—	0.830	72.6
354.7	81.5	0.479	33.3	—	—
355.5	82.3	—	—	0.760	63.3
355.8	82.6	0.539	38.9	—	—
356.2	83.0	0.580	42.9	—	—
356.4	83.2	0.627	47.8	0.697	55.6
356.4	83.2	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:
(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:
Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, August 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 2,2,4-trimethylpentane have been reported in two publications. Malesinska[1] carried out measurements of the mutual solubilities of the components between 363 and 379 K by synthetic method. Rolla *et al.*[2] studied mutual solubilities of (1) and (2) between 369 and 378 K by the synthetic method.

Values obtained by the graphical interpolation or extrapolation from the data sheets are presented in the following table. Data are ''recommended'' if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Recommended and tentative values for the mutual solubilities of nitromethane and 2,2,4-trimethylpentane

	Hydrocarbon-rich phase			Nitromethane-rich phase		
T/K	100 w_1	x_1		100 w_2	x_2	
363	18.8	0.302	Tentative	16.9	0.098	Tentative
368	22.8	0.356	Tentative	21.0	0.124	Tentative
373	29.3	0.437	Recommended	27.9	0.171	Recommended
375	33.6	0.486	Recommended	31.7	0.199	Recommended

The upper critical solution temperature has been reported as 377.8 K,[2] 378.20 K.[1] Thus, the recommended value is: (378.0±0.2) K.

The corresponding critical solution composition has been reported as $x_{c1}=0.665$ (Rolla *et al.*[2]) and $x_{c1}=0.670$ (Malesinska[1]). The data average $x_{c1}=0.668\pm0.003$, ($100\,w_1=51.8$) this value is recommended. The numerical values reported in the above table have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted:

$$a_1=0.718\,10,\quad a_2=0.785\,52,\quad b_1=5.745\,95,\quad b_2=-5.189\,87$$

(mean standard error of estimate was 0.0029).

For approximation the recommended values of UCST and x_{c1} have been used. This relationship is presented in Fig. 15 together with experimental data reported by Malesinska[1] and Rolla *et al.*[2]

Components:	**Original Measurements:**
(1) Nitromethane; CH_5NO_2; [75-52-5] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53–9 (1960).
Variables:	**Prepared By:**
T/K=363–378	V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2,4-trimethylpentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
363.30	90.15	0.3033	18.87	—	—
367.00	93.85	—	—	0.8814	79.89
370.30	97.15	0.3902	25.48	—	—
375.30	102.15	0.4962	34.48	—	—
377.37	104.22	0.5586	40.34	—	—
377.67	104.52	—	—	0.7661	63.64
378.13	104.98	0.6376	48.46	—	—
378.15	105.00	—	—	0.6707	52.12
378.20	105.05	0.6650	51.50	0.6650	51.50 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev) method was used. Sealed samples, about 1.0–1.5 g, of various compositions were heated to a temperature higher than that required for complete homogeneity, then cooled at about 0.01 K·min^{-1} until turbidity and a meniscus appeared. Repeat determinations were made.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Not specified.

Estimated Error:

Not specified.

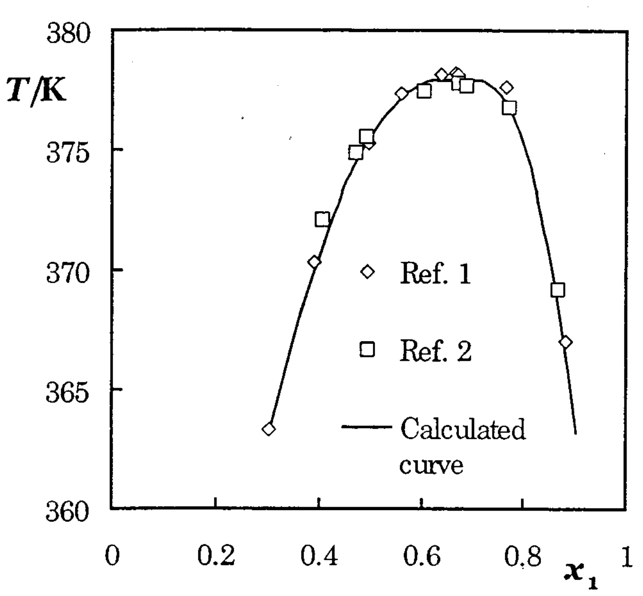

FIG. 15. Mutual solubility of nitromethane and 2,2,4-trimethylpentane.

References:

[1] B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53 (1960).
[2] M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48 (1967).

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) 2,2,4-Trimethylpentane; C_8H_{18} ; [540-84-1]

Original Measurements:

M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:

T/K=369–378

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2,4-trimethylpentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
96.0	369.2	—	—	0.868	77.8
98.9	372.1	0.406	26.8	—	—
101.7	374.9	0.469	32.1	—	—
102.4	375.6	0.491	34.0	—	—
103.6	376.9	—	—	0.769	64.0
104.3	377.5	0.602	44.7	—	—
104.5	377.7	—	—	0.686	53.9
104.6	377.8	0.670	52.0	0.670	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:

(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5 ; f.p.$=-29.15$ °C.
(2) Fulka AG; purist grade; purification as above.

Extimated Error:

Not specified.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) 2,3,4-Trimethylpentane; C_8H_{18} ; [565-75-3]

Original Measurements:

M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:

T/K=363–378

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,3,4-trimethylpentane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
89.4	362.6	—	—	0.897	82.3
92.0	365.2	—	—	0.882	80.0
92.2	365.4	0.303	18.9	—	—
93.5	366.7	0.317	19.9	—	—
98.8	372.0	—	—	0.845	74.4
98.9	372.1	0.397	26.0	—	—
99.1	372.3	0.396	25.9	—	—
100.7	373.9	—	—	0.826	71.7
103.3	376.5	0.532	37.8	—	—
103.4	376.6	0.531	37.7	—	—
103.9	377.1	—	—	0.744	60.8
104.2	377.4	0.621	46.7	—	—
104.3	377.5	0.670	52.0	0.670	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:

(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5 ; f.p.$=-29.15$ °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:

Not specified.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2-Dimethylhexane; C_8H_{18}; [590-73-8]

Original Measurements:

P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123-6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**2**), 84 (1977).

Variables:

T/K=366–381

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2-dimethylhexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
366.4	93.2	0.298	18.5	—	—
370.4	97.2	0.340	21.6	—	—
373.1	99.9	0.385	25.1	—	—
373.5	100.3	—	—	0.863	77.1
374.2	101.0	—	—	0.857	76.2
376.0	102.8	0.419	29.5	—	—
379.5	106.3	—	—	0.782	65.7
380.0	106.8	0.556	40.1	—	—
380.3	107.1	—	—	0.746	61.1
380.5	107.3	0.596	44.1	—	—
380.6	107.4	0.638	48.5	—	—
380.7	107.5	—	—	0.689	54.2
380.8	107.6	0.670	52.0	0.670	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,4-Dimethylhexane; C_8H_{18}; [589-43-5]

Original Measurements:

P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123-6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**2**), 85 (1977).

Variables:

T/K=360–381

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,4-dimethylhexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
359.7	86.5	0.238	14.3	—	—
368.7	95.5	0.309	19.3	—	—
373.8	100.6	0.373	24.1	—	—
375.5	102.3	—	—	0.853	75.6
375.9	102.7	0.422	28.1	—	—
379.6	106.4	0.509	35.6	0.795	67.5
381.1	107.9	0.607	45.2	0.734	59.6
381.2	108.0	0.633	48.0	—	—
381.3	108.1	—	—	0.714	57.2
381.4	108.2	0.670	52.0	0.670	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,5-Dimethylhexane; C_8H_{18}; [592-13-2]

Original Measurements:
P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).
*G. Spinolo, Int. Data Ser., Sel. Data Mixtures, Ser. A **(2)**, 111 (1981).

Variables:
T/K=364–382

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,5-dimethylhexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
363.6	90.4	0.270	16.5	—	—
368.9	95.7	0.317	19.9	—	—
371.1	97.9	—	—	0.882	80.0
373.0	99.8	0.375	24.3	—	—
375.6	102.4	0.411	27.2	—	—
378.1	104.9	—	—	0.841	73.9
378.1	104.9	—	—	0.840	73.7
378.9	105.7	0.489	33.8	—	—
380.6	107.4	—	—	0.789	66.7
381.2	108.0	0.548	39.3	—	—
381.3	108.1	—	—	0.735	59.7
381.5	108.3	0.605	45.0	—	—
381.7	108.5	—	—	0.698	55.3
382.0	108.8	0.650	49.8	—	—
381.9	108.7	0.670	52.0	0.670	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methylheptane; C_8H_{18}; [592-27-8]

Original Measurements:
P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A **(2)**, 81 (1977).

Variables:
T/K=371–385

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2-methylheptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
371.0	97.8	0.315	19.7	—	—
372.7	99.5	—	—	0.890	81.2
376.0	102.8	0.374	24.2	—	—
378.2	105.0	—	—	0.860	76.6
379.4	106.2	0.422	28.1	—	—
379.8	106.6	—	—	0.851	75.3
382.8	109.6	0.502	35.0	—	—
383.8	110.6	—	—	0.781	65.6
384.1	110.9	0.571	41.6	—	—
384.5	111.3	0.628	47.4	—	—
384.6	111.4	0.655	50.4	0.718	57.6
384.8	111.6	0.670	52.0	0.670	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 3-Methylheptane; C_8H_{18}; [589-81-1]

Original Measurements:

P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**2**), 82 (1977).

Variables:

T/K=372–384

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 3-methylheptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
371.6	98.4	0.323	20.3	—	—
372.1	98.9	—	—	0.885	80.4
375.5	102.3	0.372	24.0	—	—
378.5	105.3	0.422	28.1	—	—
380.0	106.8	0.459	31.2	—	—
381.2	108.0	—	—	0.814	70.0
382.0	108.8	0.514	36.1	—	—
382.3	109.1	—	—	0.787	66.4
382.7	109.5	—	—	0.778	65.2
383.2	110.0	0.582	42.7	—	—
383.6	110.4	0.613	45.8	—	—
383.6	110.4	0.669	51.9	—	—
383.6	110.4	0.670	52.0	0.670	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 4-Methylheptane; C_8H_{18}; [589-53-7]

Original Measurements:

P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**2**), 83 (1977).

Variables:

T/K=368–384

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 4-methylheptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
368.2	95.0	0.287	17.7	—	—
370.9	97.7	0.313	19.6	—	—
375.4	102.2	0.360	23.1	—	—
378.1	104.9	0.403	26.5	—	—
379.2	106.0	—	—	0.848	74.9
397.7	106.5	—	—	0.836	73.1
380.2	107.0	—	—	0.830	72.3
380.8	107.6	0.466	31.8	—	—
382.3	109.1	—	—	0.801	68.3
382.4	109.2	0.512	35.9	—	—
383.3	110.1	0.578	42.3	—	—
383.7	110.5	—	—	0.738	60.1
383.8	110.6	0.664	51.4	—	—
384.0	110.8	0.670	52.0	0.670	52.0 (UCST)

Auxiliary sInformation

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Octane; C_8H_{18}; [111-65-9]	V. P. Sazonov, Technical University, Samara, Russia. A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, August 1999.

Critical Evaluation

Quantitative solubility data for the system nitromethane+octane have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Malesinska[1]	308–388	Mutual	Synthetic
Schmid *et al.*[2]	384	UCST	Synthetic
Rolla *et al.*[3]	365–387	Mutual	Synthetic
Cherkasova *et al.*[4]	280–359	Mutual	Synthetic

Apart from the publication of Schmid *et al.*,[2] which did not contain sufficient information to justify its inclusion, all the original data are given in the data sheets following this Critical Evaluation.

In Tables 2 and 3, values obtained by the Evaluator by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). ''Best'' values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these ''best'' values do not have statistical significance and should be regarded only as a convenient representation of the spread of values and not as error limits. The letter (R) indicates ''recommended'' data. Data are ''recommended'' if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

In the hydrocarbon-rich phase the results of Malesinska,[2] Rolla *et al.*,[3] and Cherkasova *et al.*[4] are in reasonable agreement and the average values can be recommended at higher temperatures. At lower temperatures ($\leqslant$343 K), because of the lower solubilities, the relative uncertainty increases and fewer data are available so the average values can only be considered tentative. A similar situation prevails in the nitromethane-rich phase.

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

	Solubility, 100 w_1		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_1	x_1
283	1.0*(Ref. 4)	1.0	0.019
293	1.6*(Ref. 4)	1.6	0.030
303	2.5*(Ref. 4)	2.5	0.046
313	3.7*(Ref. 4)	3.7	0.067
323	4.3*(Ref. 1), 5.1*(Ref. 4)	4.7±0.4	0.085
333	5.7*(Ref. 1), 6.7*(Ref. 4)	6.2±0.5	0.11
338	6.6*(Ref. 1), 8.0*(Ref. 4)	7.3±0.7	0.13
343	7.4*(Ref. 1), 9.0*(Ref. 4)	8.2±0.8	0.14
348	9.2*(Ref. 1), 10.0 (Ref. 4)	9.6±0.4 (R)	0.17
353	10.7*(Ref. 1), 10.3*(Ref. 4)	10.5±0.2 (R)	0.180
358	12.4*(Ref. 1), 10.9*(Ref. 4)	11.7±0.7	0.199
363	14.6*(Ref. 1), 14.0*(Ref. 3)	14.3±0.3 (R)	0.238
368	17.0*(Ref. 1), 16.4*(Ref. 3)	16.7±0.3 (R)	0.273
373	20.3*(Ref. 1), 19.7*(Ref. 3)	20.0±0.3 (R)	0.319
378	24.8*(Ref. 1), 24.4*(Ref. 3)	24.6±0.2 (R)	0.379
383	32.0*(Ref. 1), 30.9*(Ref. 3)	31.5±0.6 (R)	0.463
385	36.7*(Ref. 1), 37.3*(Ref. 3)	37.0±0.3 (R)	0.524

TABLE 3. Tentative and recommended (R) values for the solubility of octane (2) in nitromethane (1)

	Solubility, 100 w_2		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_2	x_2
283	0.2 (Ref. 4)	0.2	0.0011
293	0.3*(Ref. 4)	0.3	0.0026
303	1.2*(Ref. 1), 1.8*(Ref. 4)	1.5±0.3	0.0081
313	1.8*(Ref. 1), 2.8*(Ref. 4)	2.3±0.5	0.012
323	2.7*(Ref. 1), 3.8*(Ref. 4)	3.3±0.6	0.018
333	4.2*(Ref. 1), 5.4*(Ref. 4)	4.8±0.6	0.026
338	4.5*(Ref. 1), 6.7*(Ref. 4)	6±1	0.033
343	6.1*(Ref. 1), 6.9*(Ref. 4)	6.5±0.4	0.036
348	7.2*(Ref. 1), 7.8*(Ref. 4)	7.6±0.4	0.042
353	8.8*(Ref. 1), 9.0*(Ref. 4)	8.9±0.1(R)	0.050
363	12.0*(Ref. 1)	12.0	0.0680
373	16.0*(Ref. 1), 16.1*(Ref. 3)	16.1±0.1 (R)	0.0930
378	19.0*(Ref. 1), 19.2*(Ref. 3)	19.1±0.1 (R)	0.112
383	25.0*(Ref. 1), 25.1*(Ref. 3)	25.1±0.1 (R)	0.152
385	29.2*(Ref. 2), 28.9*(Ref. 3)	29.1±0.1 (R)	0.180

The upper critical solution temperature has been reported as 383.7 K,[2] 387.2 K,[3] and 387.65 K.[1] The UCST of Schmid *et al.*[2] is much lower than the other values and is therefore rejected. The remaining values are in reasonable agreement and hence their average, UCST=(387.4±0.3) K, is recommended.

The corresponding critical solution composition has been reported as $x_{c1}=0.685$ (Malesinska[1]) and $x_{c1}=0.670$ (Rolla *et al.*[3]). The value of x_{c1} reported by Malesinska[1] is consistent with the value calculated on the basis of critical evaluation of all experimental critical solution compositions in the nitromethane–*n*-alkane series and discussed at the beginning of this volume. Therefore, $x_{c1}=0.685$ is recommended. The numerical values reported in the above tables have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted:

$a_1=0.932\,27$, $a_2=-0.314\,49$, $b_1=4.574\,95$, $b_2=-4.515\,74$ (mean standard error of estimate was 0.0088).

For approximation the recommended values of UCST and x_{c1} have been used. This relationship is presented in Fig. 16 together with data reported in Malesinska,[1] Rolla *et al.*,[3] and Cherkasova *et al.*[4] The calculated compositions are in each point inside inaccuracy declared in Tables 2 and 3.

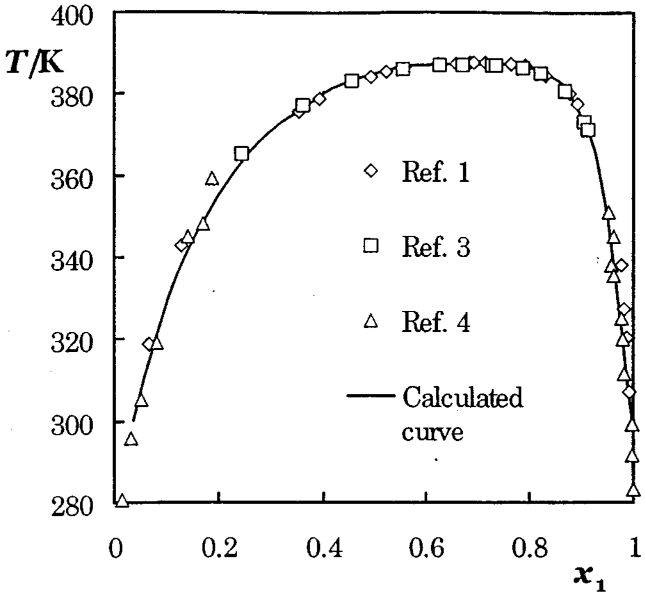

FIG. 16. Mutual solubility of nitromethane and octane.

References:

[1] B. Malesinska, Bull. Acad. Pol. Sci. Ser. Sci. Chim. **8**, 53 (1960).

[2] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

[3] M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48 (1967).

[4] N. M. Cherkasova, I. K. Zhuravleva, E. F. Zhuravlev, and V. B. Mukhametshina, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **17**, 1602 (1974); Deposited Doc., VINITI 1181 (1974).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Octane; C_8H_{18}; [111-65-9]	B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53–9 (1960).
Variables:	**Prepared By:**
T/K=307–388	V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and octane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
307.1	33.9	—	—	0.9927	98.64
318.7	45.5	0.0062	3.65	—	—
320.5	47.3	—	—	0.9974	97.67
327.5	54.3	—	—	0.9830	96.87
338.0	64.8	—	—	0.9765	95.69
342.9	69.7	0.1293	7.35	—	—
375.73	102.58	0.3530	22.57	—	—
377.50	104.35	—	—	0.8928	81.65
378.77	105.62	0.3926	25.67	—	—
380.26	107.11	—	—	0.8779	79.35
384.23	111.08	0.4924	34.14	—	—
384.51	111.36	—	—	0.8319	72.56
385.34	112.19	0.5228	36.93	—	—
386.95	113.80	—	—	0.7919	67.04
387.23	114.08	—	—	0.7648	63.47
387.25	114.10	0.6232	46.92	—	—
387.45	114.30	0.6591	50.82	—	—
387.55	114.40	—	—	0.7157	57.36
387.61	114.46	—	—	0.6920	54.56
387.65	114.50	0.6850	53.70	0.6850	53.70 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev) method was used. Sealed samples, about 1.0–1.5 g, of various compositions were heated to a temperature higher than that required for complete homogeneity, then cooled at about 0.01 K·min^{-1} until turbidity and a meniscus appeared. Repeat determinations were made.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.

(2) Isolated from a Fischer-Tropsch gasoline fraction freed from unsaturated hydrocarbons; fractionally distilled.

Estimated Error:

Not specified.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octane; C_8H_{18}; [111-65-9]

Original Measurements:

M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:

T/K=365–387

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and octane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
92.2	365.4	0.244	14.7	—	—
98.0	371.2	—	—	0.913	84.9
100.1	373.3	—	—	0.907	83.9
104.0	377.2	0.361	23.2	—	—
107.6	380.8	—	—	0.869	78.0
110.0	383.2	0.456	30.9	—	—
111.9	385.1	—	—	0.822	71.2
112.9	386.1	0.554	39.9	—	—
113.1	386.3	—	—	0.788	66.5
113.8	387.0	0.625	47.1	—	—
113.9	387.1	—	—	0.736	59.8
113.9	387.1	—	—	0.728	58.9
114.0	387.2	0.670	52.0	0.670	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:

(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.=−29.15 °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:

Not specified.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octane; C_8H_{18}; [111-65-9]

Original Measurements:

N. M. Cherkasova, I. K. Zhurvleva, E. F. Zhuravlev, and V. B. Mukhametshina, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **17**, 1602 (1974).
*Deposited Doc., VINITI 1181 (1974).

Variables:

T/K=281–359

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and octane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
7.5	280.7	0.8	0.015	—	—
10.0	283.2	—	—	99.8	0.999
18.5	291.7	—	—	99.7	0.998
22.5	295.7	1.8	0.033	—	—
26.0	299.2	—	—	99.5	0.997
32.0	305.2	2.8	0.051	—	—
38.5	311.7	—	—	96.8	0.983
46.0	319.2	4.5	0.081	—	—
46.9	320.1	—	—	96.4	0.980
52.0	325.2	—	—	96.0	0.978
62.5	335.7	—	—	93.5	0.964
65.0	345.2	8.0	0.140	93.3	0.963
72.0	338.2	—	—	92.5	0.958
75.0	348.2	10.0	0.172	—	—
78.0	351.2	—	—	91.5	0.953
86.0	359.2	11.0	0.188	—	—

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used.[1] No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; freshly distilled; b.p.=101 °C, n(20 °C,D)=1.3816.
(2) Source not specified; pure grade reagent; freshly distilled; b.p.=113 °C, n(20 °C,D)=1.3975.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6]

Original Measurements:
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

Variables:
T/K=208–242

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1,2,4-trimethylbenzene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
−65	208	0.25	14.5	—	—
−60	213	0.33	20.0	—	—
−44	229	0.44	28.5	—	—
−40	233	—	—	0.88	78.8
−33	240	0.66	49.6	—	—
−31	242	0.74	59.1	—	—
−31	242	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. Solutions of (1) and (2) were sealed in 5 mL glass vials. Cloud points were observed visually in an acetone bath slowly cooled by addition of dry ice. Temperatures were taken on an alcohol thermometer.

Source and Purity of Materials:
(1) Fisher; reagent grade; distilled at 60 °C at 24.4 kPa.
(2) Phillips; research grade; purity 99.89 mole %.

Estimated Error:
Temperature: ±3 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,3,5-Trimethylbenzene; C_9H_{12}; [108-67-8]

Original Measurements:
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

Variables:
T/K=230–257

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1,3,5-trimethylbenzene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
−43	230	0.30	17.9	—	—
033	240	0.38	23.7	—	—
029	244	0.39	24.5	—	—
−25	248	—	—	0.90	82.0
−21	252	0.51	34.6	—	—
−18	255	0.59	42.2	—	—
−16.5	256	—	—	0.79	65.6
−16	257	0.70	54.2	—	—
−16	257	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. Solutions of (1) and (2) were sealed in 5 mL glass vials. Cloud points were observed visually in an acetone bath slowly cooled by addition of dry ice. Temperatures were taken on an alcohol thermometer.

Source and Purity of Materials:
(1) Fisher, reagent grade; distilled at 60 °C at 24.4 kPa.
(2) Eastman; practical grade; dried over $CaSO_4$ and distilled once from CaH_2 and second time from over sodium at 79 °C/5.6 kPa.

Estimated Error:
Temperature: ±3 K.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2,4-Trimethylhexane; C_9H_{20}; [16747-26-5]

Original Measurements:

P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A(**2**), 89 (1977).

Variables:

T/K=372–383

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2,4-trimethylhexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
372.2	99.0	0.359	21.0	—	—
373.1	99.9	—	—	0.887	78.9
376.8	103.6	0.428	26.3	0.865	75.3
378.8	105.6	0.461	28.9	—	—
379.9	106.6	—	—	0.832	70.2
381.3	108.1	0.536	35.5	—	—
382.1	108.9	—	—	0.775	62.1
382.3	109.1	0.598	41.4	—	—
382.4	109.2	—	—	0.732	56.5
382.6	109.4	0.632	45.0	—	—
382.8	109.6	0.690	51.0	0.690	51.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9]

Original Measurements:

M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:

T/K=364–384

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2,5-trimethylhexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
90.4	363.6	—	—	0.930	86.3
91.6	364.8	0.278	15.5	—	—
99.5	372.7	0.356	20.8	—	—
105.9	379.1	0.454	28.4	—	—
106.2	379.4	—	—	0.862	74.8
109.0	382.2	0.530	34.9	—	—
109.9	383.1	0.576	39.3	—	—
110.3	383.5	—	—	0.790	64.2
110.5	383.7	0.616	43.3	—	—
110.8	384.0	0.695	52.0	0.695	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described by Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:

(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.=−29.15 °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:

Not specified.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,3,5-Trimethylhexane; C_9H_{20}; [1069-53-0]

Original Measurements:
P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**2**), 90 (1977).

Variables:
T/K=375–385

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,3,5-trimethylhexane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
374.9	101.7	0.372	22.0	—	—
375.0	101.8	—	—	0.883	78.2
379.3	106.1	—	—	0.849	72.8
379.6	106.4	0.443	27.5	—	—
381.9	108.7	—	—	0.825	69.2
382.3	109.1	0.511	33.2	—	—
383.8	110.6	0.566	38.3	—	—
383.9	110.7	0.608	42.5	—	—
384.3	111.1	0.610	42.7	0.760	60.1
384.4	111.2	0.671	49.3	—	—
384.5	111.3	—	—	0.709	53.7
384.8	111.6	0.690	51.0	0.690	51.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2-Dimethylheptane; C_9H_{20}; [1071-26-7]

Original Measurements:
P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).

Variables:
T/K=377–387

Prepared By:
V. P. Sazonov

Experimental Data

The mutual solubility of nitromethane and 2,2-dimethylheptane in mole fraction were reported over the specified temperature range in a graphical form in the original publication. The numerical data in the following table were provided by Professor R. Riccardi at the request of the compiler.

Mutual solubility of nitromethane and 2,2-dimethylheptane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
377.4	104.2	—	—	0.885	78.6
377.8	104.6	—	—	0.882	78.1
380.9	107.7	0.446	27.7	—	—
383.8	110.6	0.520	34.0	—	—
384.3	111.1	—	—	0.828	69.6
385.3	112.0	—	—	0.814	67.6
385.9	112.7	0.605	42.2	—	—
386.1	112.9	—	—	0.758	59.8
386.1	112.9	—	—	0.699	52.5
386.2	113.0	0.634	45.2	—	—
386.4	113.2	—	—	0.748	58.6
386.5	113.3	—	—	0.731	56.4
386.6	113.4	0.665	48.6	—	—
386.7	113.5	0.690	51.0	0.690	51.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methyloctane; C_9H_{20}; [3221-61-2]

Original Measurements:

P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**2**), 86 (1977).

Variables:

T/K=374–391

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2-methyloctane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
374.3	101.1	0.316	18.0	—	—
380.8	107.6	0.382	22.7	—	—
382.5	109.3	—	—	0.889	79.2
384.6	111.4	0.448	27.9	—	—
388.2	115.0	0.530	34.9	0.840	71.4
389.6	116.4	—	—	0.803	66.0
389.9	116.7	0.599	41.6	—	—
390.1	116.9	0.654	47.4	—	—
390.4	117.2	—	—	0.752	59.1
391.3	118.1	0.688	51.2	—	—
391.0	116.8	0.690	51.4	0.690	51.4 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 3-Methyloctane; C_9H_{20}; [2216-33-3]

Original Measurements:

P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968).
*P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A (**2**), 87 (1977).

Variables:

T/K=378–390

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 3-methyloctane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	T/C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
378.2	105.0	0.353	20.6	—	—
380.9	107.7	—	—	0.891	79.6
381.4	108.2	0.396	23.8	—	—
384.6	111.4	0.449	27.9	—	—
386.7	113.5	0.493	31.6	0.847	72.5
388.3	115.1	0.543	36.1	—	—
388.7	115.5	—	—	0.816	67.9
389.1	115.9	—	—	0.798	65.3
389.3	116.1	—	—	0.763	60.5
389.5	116.3	0.610	42.7	—	—
389.7	116.5	0.637	45.5	—	—
390.0	116.8	—	—	0.699	52.5
390.0	116.8	0.690	51.4	0.690	51.4 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 4-Methyloctane; C_9H_{20}; [2216-34-4]	P. Franzosini, R. Riccardi, and M. Rolla, Ric. Sci. **38**, 123–6 (1968). *P. Ferloni and R. Riccardi, Int. Data Ser., Sel. Data Mixtures, Ser. A. (**2**), 88 (1977).
Variables:	**Prepared By:**
T/K=366–390	V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 4-methyloctane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
366.4	93.2	0.245	13.4	—	—
378.2	105.0	0.361	21.2	—	—
381.2	108.0	0.399	24.0	—	—
384.5	111.3	0.455	28.4	—	—
386.4	113.2	—	—	0.853	73.4
386.7	113.5	0.498	32.1	—	—
388.2	115.0	0.550	36.8	—	—
288.8	115.6	—	—	0.812	67.3
389.1	115.9	—	—	0.791	64.3
389.2	116.0	0.595	41.1	—	—
389.6	116.4	0.651	47.0	0.694	51.9
389.8	116.6	—	—	0.741	57.7
389.8	116.6	0.690	51.4	0.690	51.4 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. Tubes were filled under vacuum with known masses of degassed and moisture-free components, sealed, and then placed in a thermostat bath filled with paraffin oil. The mixtures in the tubes were shaken by a Chemap vibromixer type E-1. Temperatures were measured with Degussa Pt resistance thermometers, which were checked against standards. Phase changes (cloud points) were observed as mixtures were cooled.

Source and Purity of Materials:

(1) Fluka AG; purity 99 mole %; fractionally distilled, degassed and finally distilled through a P_2O_5 filled tube.
(2) Fluka AG; purity 99 mole %; purification as above.

Estimated Error:

Temperature: reproduced better than 0.1 K.

References:

[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:	**Evaluator:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Nonane; C_9H_{20}; [111-84-2]	V. P. Sazonov, Technical University, Samara, Russia, August 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and nonane have been reported in two publications. Malesinska,[1] between 296 and 393 K, and Rolla *et al.*,[2] between 366 K and 393 K, measured the mutual solubilities of (1) and (2) using the synthetic method.

Values obtained by the graphical interpolation or extrapolation from the data sheets are presented in the following table. Data are ''recommended'' if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Recommended and tentative values for the mutual solubilities of nitromethane and nonane

	Hydrocarbon-rich phase			Nitromethane-rich phase		
T/K	100 w_1	x_1		100 w_2	x_2	
303	2.0	0.041	Tentative	1.7	0.008	Tentative
313	2.7	0.055	Tentative	2.1	0.010	Tentative
323	3.6	0.073	Tentative	2.8	0.014	Tentative
333	5.1	0.101	Tentative	3.8	0.018	Tentative
343	6.8	0.133	Tentative	5.2	0.025	Tentative
353	9.3	0.177	Tentative	7.0	0.035	Tentative
363	12.4	0.229	Tentative	9.6	0.048	Tentative
373	16.5	0.293	Recommended	12.6	0.064	Recommended
383	24.7	0.408	Recommended	18.2	0.096	Recommended
393	45	0.63	Tentative	35	0.204	Recommended

The upper critical solution temperature has been reported as 393.45 (Malesinska[1]) and 393.8 K (Rolla *et al.*[2]). Thus, the recommended value is (393.6±0.2) K. The corresponding critical solution composition has been reported as $x_{c1}=0.695$ (Rolla *et al.*[2]) and $x_{c1}=0.720$ (Malesinska[1]). Their average, $x_{c1}=0.708\pm0.012$, is recommended. These recommended values are consistent with the values calculated in the series nitromethane–*n*-alkane systems and described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane.'' The numerical values reported in the above table have been approximated by the equation based on scaling law and described also in the above introduction material to this volume. The following parameters have been adjusted: $a_1=0.871\ 00$, $a_2=-0.168\ 20$, $b_1=4.421\ 21$, $b_2=-4.476\ 26$ (mean standard error of estimate was 0.0106).

For approximation the recommended values of UCST and x_{c1} have been used. This relationship is presented in Fig. 17 together with experimental data reported in Malesinska[1] and Rolla *et al.*[2]

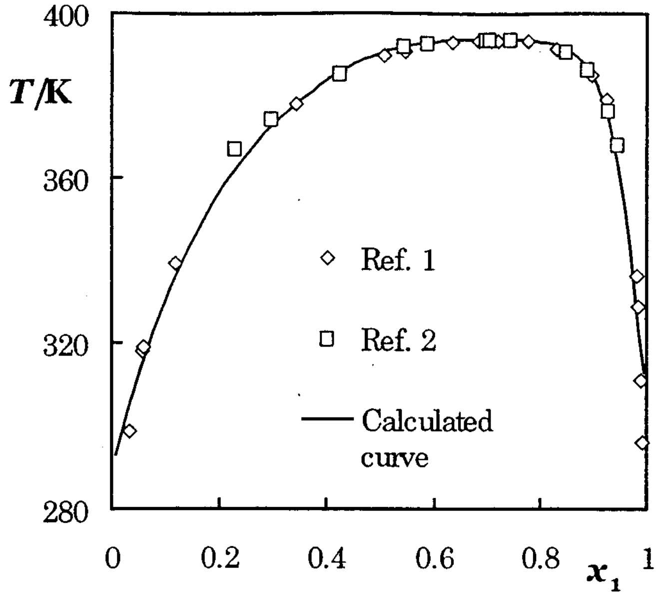

FIG. 17. Mutual solubility of nitromethane and nonane.

References:

[1]B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Ser. Sci. Chim. **8**, 53 (1960).

[2]M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48 (1967).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Nonane; C_9H_{20}; [111-84-2]

Original Measurements:

B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53–9 (1960).

Variables:

T/K=296–393

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and nonane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
296.0	22.8	—	—	0.9935	98.64
298.7	25.5	0.0347	1.68	—	—
311.0	37.8	—	—	0.9901	97.94
318.2	45.0	0.0567	2.78	—	—
219.0	45.8	0.0587	2.88	—	—
328.8	55.6	—	—	0.9840	96.70
336.0	62.8	—	—	0.9815	96.19
339.2	66.0	0.1194	6.06	—	—
377.80	104.65	0.3436	19.94	—	—
378.97	105.82	—	—	0.9252	85.48
385.07	111.92	—	—	0.8960	80.39
389.55	116.40	0.5086	33.00	—	—
390.48	117.33	0.5464	36.44	—	—
391.23	118.08	—	—	0.8306	70.00
392.93	119.78	0.6351	45.30	—	—
393.25	120.10	—	—	0.7764	62.30
393.30	120.15	0.6826	50.58	—	—
393.35	120.20	0.7057	53.30	—	—
393.45	120.30	0.7200	55.00	0.7200	55.00 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev) method was used. Sealed samples, about 1.0–1.5 g, of various compositions were heated to a temperature higher than that required for complete homogeneity, then cooled at about 0.01 K·min^{-1} until turbidity and a meniscus appeared. Repeat determinations were made.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Isolated from a Fischer-Tropsch gasoline fraction freed from unsaturated hydrocarbons; fractionally distilled.

Estimated Error:

Not specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Nonane; C_9H_{20}; [111-84-2]

Original Measurements:
M. Rolla, P. Franzosini, R. Riccardi, and L. Bottelli, Z. Naturforsch. **22A**, 48–53 (1967).

Variables:
T/K=367–394

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and nonane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
93.6	366.8	0.229	12.4	—	—
94.8	368.0	—	—	0.946	89.3
101.0	374.2	0.296	16.7	—	—
102.3	376.4	—	—	0.927	85.8
112.1	385.3	0.425	26.0	—	—
113.1	386.3	—	—	0.890	79.4
117.5	390.7	—	—	0.849	72.8
118.7	391.9	0.545	36.3	—	—
119.6	392.8	0.587	40.3	—	—
120.6	393.8	—	—	0.741	57.7
120.6	393.8	—	—	0.704	53.1
120.6	393.8	0.695	52.0	0.695	52.0 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, described in Franzosini,[1] was employed. No further details were reported.

Source and Purity of Materials:
(1) Carlo Erba; RP; distilled through a tube filled with P_2O_5; f.p.= −29.15 °C.
(2) Fluka AG; purist grade; purification as above.

Estimated Error:
Not specified.

References:
[1] P. Franzosini, Z. Naturforsch. **18A**, 224 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Naphthalene; $C_{10}H_8$; [91-20-3]

Original Measurements:
V. P. Sazonov and M. F. Chernysheva, Zh. Prikl. Khim. (Leningrad) **51**, 1019–22 (1978).

Variables:
T/K=289–348

Prepared By:
N. V. Sazonov and V. P. Sazonov

Experimental Data

Solubility of naphthalene (2) in nitromethane (1)

t/°C	T/K (compilers)	100 w_2	x_2 (compilers)
15.40	288.55	9.95	0.0500
23.70	293.85	15.00	0.0775
29.30	302.45	20.00	0.1064
33.90	307.05	25.00	0.1370
37.40	310.55	30.00	0.1695
42.90	316.05	40.00	0.2410
47.55	320.70	49.85	0.3213
52.05	325.20	59.95	0.4162
57.00	330.15	69.95	0.5258
62.80	335.95	79.90	0.6544
69.90	343.05	89.80	0.8074
75.15	348.30	95.35	0.9071

Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; fractionally distilled.
(2) Source not specified; analytical purity; purified by crystallization; m.p.= 80.2 °C.

Estimated Error:
Not reported.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene; $C_{10}H_{16}$; [7785-70-8]

Original Measurements:

M. Antosik and R. Stryjek, Fluid Phase Equil. **71**, 321–31 (1992).

Variables:

$T/K=298$

Prepared By:

V. P. Sazonov

Experimental Data

The solubility of nitromethane in α-pinene (2) at 298.15 K (25.00 °C, compiler) was reported to be $x_1=0.0691$. The corresponding mass percentage calculated by the compiler is 100 $w_1=3.22$.

The solubility ofα-pinene (2) in nitromethane at 298.15 K (25.00 °C, compiler) was reported to be $x_2=0.0239$. The corresponding mass percentage calculated by the compiler is 100 $w_2=5.18$.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. The apparatus and procedure were described in Antosik.[1]

Source and Purity of Materials:

(1) Purified as described in Ref. 1; purity 99.8 mass% by GLC; 0.025% by mass of water.
(2) Isolated from turpentine and purified by distillation at subambient pressure; purity above 99.9% by GLC; 0.01% by mass water.

Estimated Error:

Temperature: ±0.02 K.

References:

[1] M. Antosik, J. Chem. Thermodyn. **22**, 85 (1990).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 3,7,7-Trimethylbicyclo[4.1.0]hept-2-ene; $C_{10}H_{16}$; [13466-78-9]

Original Measurements:

M. Antosik and R. Stryjek, Fluid Phase Equil. **71**, 321–31 (1992).

Variables:

$T/K=298$

Prepared By:

V. P. Sazonov

Experimental Data

The solubility of nitromethane in Δ-pinene (2) at 298.15 K (25.00 °C, compiler) was reported to be $x_1=0.1010$. The corresponding mass percentage calculated by the compiler is 100 $w_1=4.79$.

The solubility of Δ-pinene (2) in nitromethane at 298.15 K (25.00 °C, compiler) was reported to be $x_2=0.0365$. The corresponding mass percentage calculated by the compiler is 100 $w_2=7.80$.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. The apparatus and procedure were described in Antosik.[1]

Source and Purity of Materials:

(1) Purified as described in Ref. 1; purity 99.8 mass% by GLC; 0.025% by mass of water.
(2) Isolated from turpentine and purified by distillation at subambient pressure; purity above 99.9% by GLC; 0.01% by mass water.

Estimated Error:

Temperature: ±0.02 K.

References:

[1] M. Antosik, J. Chem. Thermodyn. **22**, 85 (1990).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) trans-Decahydronaphthalene; $C_{10}H_{18}$; [493-02-7]	M. Antosik, A. Stafiej, and R. Stryjek, Fluid Phase Equil. **58**, 325–33 (1990).
Variables:	**Prepared By:**
T/K=370–393	V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and trans-decahydronaphthalene

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
369.85	96.70	—	—	0.9292	85.28
376.93	103.78	0.2923	15.42	—	—
379.32	106.17	—	—	0.9028	80.40
383.82	110.67	0.3635	20.14	—	—
385.28	112.13	—	—	0.8783	76.11
385.28	112.13	—	—	0.8780	76.06
388.77	115.62	—	—	0.8477	71.08
389.87	116.72	0.4632	27.59	—	—
390.72	117.57	—	—	0.8247	67.50
391.69	118.54	—	—	0.8061	64.73
391.95	118.80	—	—	0.8003	63.89
392.41	119.26	—	—	0.7887	62.24
392.67	119.52	0.5627	36.23	—	—
393.28	120.13	—	—	0.7302	54.44
393.32	120.17	0.6447	44.48	—	—
393.36	120.21	0.6775	48.12	0.6899	49.55
393.37	120.22	0.6875	49.27	0.6875	49.27 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The method used was as described in Luszczyk and Stryjek.[1] 4 g samples of varying composition 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 99.8 mass % by GLC.

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

Estimated Error:

Temperature: ±0.02 K,
Composition: better than 0.0001 mole fraction.

References:

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

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Decane; $C_{10}H_{22}$; [124-18-5]	V. P. Sazonov, Technical University, Samara, Russia. A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and decane have been reported in two publications. Malesinska[1] measured the mutual solubilities of the two components between 381 and 399 K by the synthetic method. Schmid *et al.*[2] determined the upper critical solution temperature also using the synthetic method.

At the UCST, the only temperature where direct comparison is possible, the two studies are in rather poor agreement: 395.7 K (Schmid *et al.*[2]) and 398.15 K (Malesinska[1]). Accordingly, in the absence of confirmatory studies, all data must be regarded as tentative. However, it may be noted that the UCST values of Schmid *et al.*[2] in well characterized systems are generally lower than other reports and thus the value from Malesinska[1] is probably more realistic. The corresponding critical solution composition[1] has been reported as 100 $w_1=56.3$, $x_{c1}=0.750$. Interested users are referred to the following data sheet for the numerical solubility values. The numerical values reported in Malesinska[1] have been approximated by the equation based on scaling law (described in the Introduction material to this volume ‘‘Relations of Solubility Data in Binary Systems Containing Nitromethane’’) and the following parameters have been adjusted: $a_1=0.582\,79$, $a_2=1.693\,58$, $b_1=9.839\,78$, $b_2=-7.948\,65$ (mean standard error of estimate was 0.0382).

For approximation also x_{c1} and UCST from Malesinska[1] have been used. Measured values of mutual solubility, T_c and x_{c1} for each reported system by Malesinska[1] are very close to the values calculated in the series. Therefore 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 reported in Malesinska,[1] are also presented in Fig. 18.

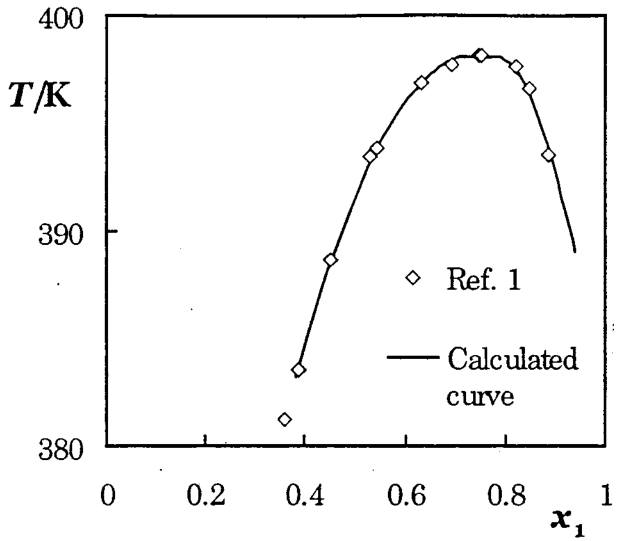

FIG. 18. Mutual solubility of nitromethane and decane.

Mutual solubility of nitromethane and decane

	Decane-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
383.2	0.3818	20.95	—	—
388.2	0.4452	35.61	0.9505	89.18
393.2	0.5300	32.61	0.8944	78.42
394.2	0.5519	34.57	0.8814	76.12
395.2	0.5768	36.90	0.8670	73.66
396.2	0.6064	39.80	0.8502	70.88
397.2	0.6453	43.84	0.8279	67.36
397.7	0.6735	46.95	0.8108	64.77

References:

[1] B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53 (1960).
[2] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Decane; $C_{10}H_{22}$ [124-18-5]

Original Measurements:
B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53–9 (1960).

Variables:
T/K=381–398

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and decane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
381.25	108.10	0.3609	19.50	—	—
383.55	110.40	0.3883	21.40	—	—
388.65	115.50	0.4510	26.06	—	—
393.48	120.33	0.5288	32.50	—	—
393.50	120.35	—	—	0.8874	77.17
393.86	120.70	0.5419	33.66	—	—
396.59	123.44	—	—	0.8485	70.61
396.89	123.74	0.6318	42.40	—	—
397.64	124.49	—	—	0.8186	65.94
397.69	124.54	0.6928	49.17	—	—
398.14	124.99	0.7444	55.55	—	—
398.15	125.00	0.7500	56.30	0.7500	56.30 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev) method was used. Sealed samples, about 1.0–1.5 g, of various compositions were heated to a temperature higher than that required for complete homogeneity, then cooled at about 0.01 K·min^{-1} until turbidity and a meniscus appeared. Repeat determinations were made.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Isolated from a Fischer-Tropsch gasoline fraction freed from unsaturated hydrocarbons; fractionally distilled.

Estimated Error:
Not specified.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Undecane; $C_{11}H_{24}$ [1120-21-4]

Original Measurements:

B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53–9 (1960).

Variables:

T/K=375–404

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and undecane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
374.65	101.50	0.2930	13.93	—	—
387.70	114.55	0.4022	20.81	—	—
391.65	118.50	0.4443	23.79	—	—
392.34	11.19	—	—	0.9321	84.28
398.72	125.57	—	—	0.9002	77.89
400.85	127.70	0.5966	36.61	—	—
403.05	129.90	0.7006	47.75	—	—
403.33	130.18	—	—	0.8008	61.09
403.35	130.20	—	—	0.7915	59.72
403.53	130.38	0.7582	55.05	—	—
403.55	130.40	0.7700	56.70	0.7700	56.70 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev) method was used. Sealed samples, about 1.0–1.5 g, of various compositions were heated to a temperature higher than that required for complete homogeneity, then cooled at about 0.01 K·min^{-1} until turbidity and a meniscus appeared. Repeat determinations were made.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Isolated from a Fischer-Tropsch gasoline fraction freed from unsaturated hydrocarbons; fractionally distilled.

Estimated Error:

Not specified.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Dodecane; $C_{12}H_{26}$; [112-40-3]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland.
G. T. Hefter, Murdoch University, Perth, Australia, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and dodecane have been reported in two publications. Malesinska[1] measured the mutual solubilities of the two components between 389 and 409 K by the synthetic method. Schmid *et al.*[2] determined the upper critical solution temperature, also using the synthetic method.

At the UCST, the only temperature where direct comparison is possible, the two studies are in rather poor agreement: 405.7 K (Schmid *et al.*[2]) and 408.80 K (Malesinska[1]). Accordingly, in the absence of confirmatory studies, all data must be regarded as tentative. However, it may be noted that the UCST values of Schmid *et al.*[2] in well characterized systems are generally lower than other reports and thus the value from Malesinska[1] is probably more realistic. The corresponding critical solution composition has been reported[1] as 100 $w_1=57.4$,
$x_{c1}=0.790$.

The numerical values reported in Malesinska[1] have been approximated by the equation based on scaling law (described in the Introduction material to this volume "Relations of Solubility Data in Binary Systems Containing Nitromethane") and the following parameters have been adjusted: $a_1=0.625\ 15$, $a_2=0.755\ 09$, $b_1=7.914\ 27$, $b_2=-7.270\ 33$ (mean standard error of estimate was 0.0173).

For approximation also x_{c1} and UCST from Malesinska[1] have been used. T_c, x_{c1} and mutual solubility data in nitromethane–*n*-alkane series reported by Malesinska[1] are very close to these values calculated in the series as well as to the particular recommended data in each of the investigated systems. Therefore 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 reported in Malesinska,[1] is also presented in Fig. 19.

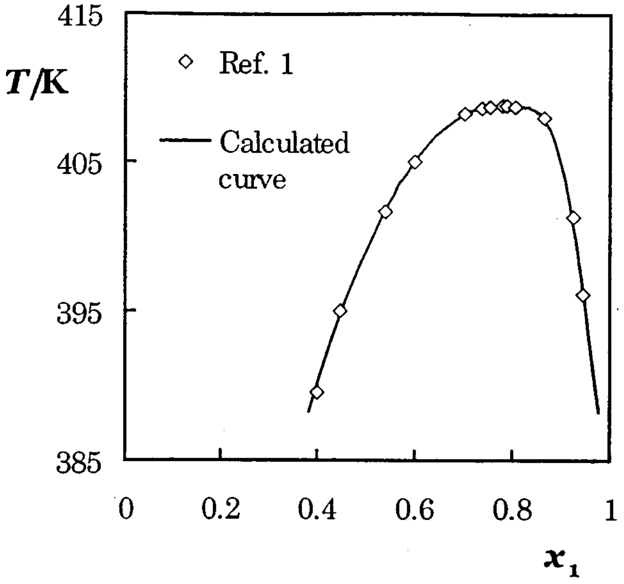

FIG. 19. Mutual solubility of nitromethane and dodecane.

Mutual solubility of nitromethane and dodecane

	Dodecane-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
388.2	0.3825	18.17	0.9772	93.89
393.2	0.4308	21.34	0.9585	89.22
398.2	0.4889	25.53	0.9380	84.43
403.2	0.5648	31.75	0.9127	78.93
404.2	0.5839	33.46	0.9062	77.58
405.2	0.6052	35.46	0.8987	76.06
406.2	0.6299	37.88	0.8895	74.25
407.2	0.6601	41.03	0.8772	71.90
408.2	0.7033	45.93	0.8562	68.09

References:

[1] B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53 (1960).

[2] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Dodecane; $C_{12}H_{26}$ [112-40-3]

Original Measurements:

B. Malesinska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 53–9 (1960).

Variables:

T/K=389–409

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and dodecane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
389.55	116.40	0.3977	19.13	—	—
395.02	121.87	0.4462	22.40	—	—
396.10	122.95	—	—	0.9449	86.01
401.26	128.11	—	—	0.9267	81.92
401.72	128.57	0.5413	29.72	—	—
405.05	131.90	0.6009	35.05	—	—
408.01	134.86	—	—	0.8671	70.04
408.20	135.05	0.7026	45.85	—	—
408.65	135.50	0.7373	50.14	—	—
408.73	135.58	—	—	0.8057	59.77
408.74	135.59	0.7546	52.43	—	—
408.80	135.65	0.7819	56.23	—	—
408.80	135.65	0.7900	57.40	0.7900	57.40 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev[1]) method was used. Sealed samples, about 1.0–1.5 g, of various compositions were heated to a temperature higher than that required for complete homogeneity, then cooled at about 0.01 K·min^{-1} until turbidity, and a meniscus appeared. Repeat determinations were made.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried and twice distilled.
(2) Isolated from a Fischer-Tropsch gasoline fraction freed from unsaturated hydrocarbons; fractionally distilled.

Estimated Error:

Not specified.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) cis-9-Octadecene; $C_{18}H_{36}$; [7206-25-9]

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **11**, 376–83 (1966).

Variables:

T/K=416

Prepared By:

V. P. Sazonov

Experimental Data

The upper critical solution temperature of nitromethane and cis-9-octadecene was reported to be 143 °C (416 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. As described in Schmid *et al.*,[1] a microscope equipped with a heating stage was used. A 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) Fisher Scientific Co.
(2) Not specified.

Estimated Error:

Not reported.

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexadecane; $C_{16}H_{34}$; [544-76-3]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland.
G. T. Hefter, Murdoch University, Perth, Australia, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and hexadecane have been reported in three publications. Schmid *et al.*[1] determined the upper critical solution temperature by the synthetic method. Rogalski and Stryjek[2] measured the mutual solubilities of the two components between 305 and 430 K using the synthetic method. Stryjek *et al.*[3] also reported the mutual solubilities of (1) and (2) at rounded temperatures between 298 and 413 K by an unknown method. In view of the close coincidence between the latter data[3] and those in the earlier publication[2] it is possible that both are based on a single set of measurements. Regardless, coming from the same group, they cannot be treated as independent results.

At the UCST, the only temperature where direct comparison between independent measurements is possible, the two available studies are in rather poor agreement: 424.2 K (Schmid *et al.*[1]) and 429.95 K (Rogalski and Stryjik[2]). However, it may be noted that the UCST values of Schmid *et al.*[1] in well characterized systems are generally lower than other reports and thus the value from Rogalski and Stryjek[2] is probably more realistic. The corresponding critical solution composition[2] has been reported as $x_{c1}=0.8422$, 100 $w_1=58.99$.

The UCST and x_{c1} values[2] are consistent with the values calculated in the series nitromethane–*n*-alkane and described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane.'' The numerical values on mutual solubility reported in Rogalski and Stryjek[2] and Stryjek *et al.*[3] have been approximated by the equation based on scaling law and described in the above Introduction material to this volume. The following parameters have been adjusted: $a_1=0.220\ 87$, $a_2=2.164\ 18$, $b_1=-2.863\ 54$, $a_3=-2.332\ 79$, $b_3=2.871\ 17$ (mean standard error of estimate was 0.0102).

For approximation $x_{c1}=0.8442$ and UCST=429.25 K (Rogalski and Stryjik[2]) have been used. Therefore in the opinion of the evaluators, mutual solubilities calculated by this equation may be treated as tentative (for nitromethane-rich phase at $T>393$ K). These calculated results, for the selected temperatures, are presented in the following table. This relationship, together with experimental points,[2,3] are also presented in Fig. 20.

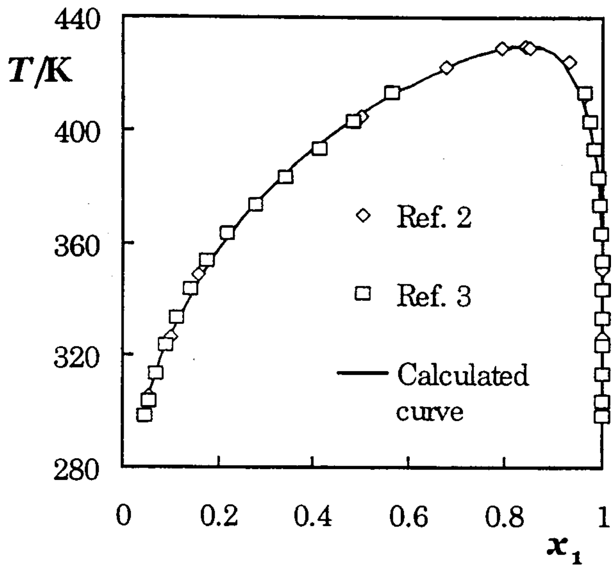

FIG. 20. Mutual solubility of nitromethane and hexadecane.

Mutual solubility of nitromethane and hexadecane

	Hexadecane-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
298.2	0.0423	1.18	—	—
303.2	0.0498	1.39	—	—
313.2	0.0678	1.92	—	—
323.2	0.0900	2.60	—	—
333.2	0.1166	3.44	—	—
343.2	0.1481	4.48	—	—
353.2	0.1850	5.77	—	—
363.2	0.2277	7.36	—	—
373.2	0.2771	9.37	—	—
383.2	0.3341	11.92	—	—
393.2	0.4002	15.25	0.9827	93.88
403.2	0.4777	19.78	0.9714	90.15
413.2	0.5706	26.38	0.9537	84.75
418.2	0.6257	31.06	0.9407	81.06
423.2	0.6901	37.51	0.9223	76.18
424.2	0.7046	39.14	0.9174	74.97
425.2	0.7201	40.95	0.9120	73.64
426.2	0.7366	42.98	0.9058	72.15
427.2	0.7545	45.31	0.8984	70.44
428.2	0.7748	48.11	0.8891	68.36
429.2	0.7996	51.82	0.8756	65.49

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

[2] M. Rogalski and R. Stryjek, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **28**, 139 (1980).

[3] R. Stryjek, M. Luszczyk, and M. Fedorko-Antosik, Bull. Acad. Pol. Sci., Ser. Sci. Chim., **29**, 203 (1981).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexadecane; $C_{16}H_{34}$[544-76-3]

Original Measurements:

M. Rogalski and R. Stryjek, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **28**, 139–47 (1980).

Variables:

T/K=305–430

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and hexadecane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
305.05	31.9	0.0555	1.56	—	—
326.15	53.0	—	—	0.9994	99.78
326.25	53.1	0.0994	2.89	—	—
348.65	75.5	0.1581	4.82	—	—
350.55	77.4	—	—	0.9991	99.67
405.05	131.9	0.5025	21.40	—	—
412.05	138.9	—	—	0.9626	87.40
422.65	149.5	0.6780	36.21	—	—
424.65	151.5	—	—	0.9301	78.20
429.25	156.1	0.7929	50.79	—	—
429.45	156.3	—	—	0.8517	60.75
429.95	156.8	0.8422	58.99	0.8422	58.99 UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev[1]) 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 the other component added until turbidity appeared. The sample was then heated to above the complete homogeneity temperature, then cooled until turbidity reappeared. Repeat determinations were made. Above 353 K, Alekseev's method was used. Samples, 4–5 g, were sealed in glass, placed in the 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:

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

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:

R. Stryjek, M. Luszczyk, and M. Fedorko-Antosik, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **29**, 203–11 (1981).

Variables:

T/K=298–413

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and hexadecane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
298.5	25.00	0.0466	1.30	0.9997	99.89
303.15	30.00	0.0535	1.50	0.9997	99.89
313.15	40.00	0.0704	2.00	0.9997	99.89
323.15	50.00	0.0901	2.60	0.9995	99.81
333.15	60.00	0.1124	3.30	0.9995	99.81
343.15	70.00	0.1399	4.20	0.9995	99.81
353.15	80.00	0.1747	5.40	0.9986	99.48
363.15	90.00	0.2183	7.00	0.9973	99.01
373.15	100.00	0.2779	9.40	0.9945	97.99
383.15	110.00	0.3422	12.30	0.9906	96.60
393.15	120.00	0.4140	16.00	0.9834	94.11
403.15	130.00	0.4843	20.20	0.9740	90.99
413.15	140.00	0.5671	26.10	0.9616	87.10

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:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Tricosane; $C_{23}H_{48}$; [638-67-5]

Original Measurements:

V. A. Rakhmanova and L. M. Kozlov, Khim. Tekhnol. Topl. Masel **8**, 9–13 (1970).

Variables:

T/K=317–357

Prepared By:

V. P. Sazonov

Experimental Data

The mutual solubility of nitromethane and tricosane in mass percent over the specified temperature range were presented in a graphical form in the original publication. The numerical data in the following table were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and tricosane

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
43.8	317.0	—	—	99.0	0.998
52.8	326.0	—	—	98.8	0.998
55.3	328.5	18.3	0.544	—	—
61.7	334.9	—	—	98.5	0.997
64.2	337.4	20.7	0.581	—	—
71.0	344.2	—	—	98.3	0.997
74.7	347.9	22.7	0.610	—	—
82.2	355.4	—	—	98.2	0.997
83.7	356.9	24.0	0.627	—	—

The upper critical solution temperature was reported to be greater than 90 °C (363 K, compiler). Monotectic equilibrium is realized at 47.5 °C (320.7 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Source not specified; purity not specified; purified.
(2) Source not specified; purity not specified; b.p.=383.8 °C, m.p.=47.7 °C.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Alkenes; C_5H_{10}–$C_{22}H_{44}$

Original Measurements:

S. P. Mulliken and R. L. Wakeman, Rec. Trav. Chim. **54**, 366–72 (1935).

Variables:

T/K=291–398

Prepared By:

V. P. Sazonov

Experimental Data

Solubility temperatures of mixtures with equal volumes of nitromethane and alkene

Alkene	B. p. alkene/°C	t/°C	T/K (compiler)
2-Pentene; C_5H_{10} ; [109-68-2]	36	18	291
2,3-Dimethyl-2-butene*; C_6H_{12} ; [563-79-1]	(71.5–72.0)	51	324
2-Hexene*; C_6H_{12} ; [592-43-8]	(68.0–68.2)	65	338
2,4-Dimethyl-2-pentene; C_7H_{14} ; [625-65-0]	(82.9–83.4)	65	338
3-Heptene; C_7H_{14} ; [592-78-9]	(95.8–96.3)	65	338
2-Heptene; C_7H_{14} ; [592-77-8]	(98.6–99.6)	67	340
4-Methyl-2-heptene; C_8H_{16} ; [3404-56-6]	(113.8–114.1)	81	354
1-Nonene; C_9H_{18} ; [124-11-8]	(145.3–145.8)	84	357
4-Nonene; C_9H_{18} ; [10405-85-3]	(147.5–148.1)	84	357
4,5,5-Trimethyl-2-hexene; C_9H_{18} ; [55702-61-9]	(128.7–129.5)	88	361
4,5-Dimethyl-2-heptene; C_9H_{18} ; [64780-96-7]	(129.5–130.1)	98	371
4-Methyl-2-octene; C_9H_{18}	(137.3–137.9)	101	374
4-Butyl-2-octene; $C_{12}H_{24}$	(197–198)	107	380
Hexadecene; $C_{16}H_{32}$; [26952-14-7]	(274–275)	120	393
Docosene; $C_{22}H_{44}$; [29730-67-4]	(150–155)/0.2 kPa	125	398

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Miscibility was determined in a glass-stoppered tube of 4 mm inside diameter. Equal volumes (0.1 mL) of (1) and (2) were measured into the tube which was then strapped to a thermometer, warmed to 5 or 10 °C above the solubility temperature, mixed well by shaking, and then allowed to cool slowly, still shaking, in a bath of white oil (above 30 °C) or water (below 30 °C).

Source and Purity of Materials:

(1) Not specified.
(2) 2-pentene synthesized in the Research Laboratory of Organic Chemistry Massachusetts Institute of Technology; some alkenes (*) were obtained from Dr. H. E. Buc, Standard Oil Development Co.; the others were the purest commercial samples available from BDH.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Cycloalkenes; C_6H_{12}, C_7H_{14}, and $C_{10}H_{18}$

Original Measurements:

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

Variables:

T/K=352–389

Prepared By:

V. P. Sazonov

Experimental Data

Critical solution temperatures of mixtures of nitromethane and cycloalkane

Cycloalkane	B. p. cycloalkane/°C	t/°C	T/K (compiler)
Cyclohexane; C_6H_{12} ; [110-82-7]	80.8	79	352
Methylcyclohexane; C_7H_{14} ; [108-87-2]	100.8	90	363
Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]	194.6	116	389

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.

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Alkadienes; $C_6H_{10}-C_{11}H_{20}$

Original Measurements:

S. P. Mulliken and R. L. Wakeman, Rec. Trav. Chim. **54**, 366–72 (1935).

Variables:

T/K=264–355

Prepared By:

V. P. Sazonov

Experimental Data

Solubility temperatures of mixtures with equal volumes of nitromethane and alkadiene

Alkadiene	B. p. alkadiene/°C	t/°C	T/K (compiler)
2,4-Hexadiene*; C_6H_{10} ; [592-46-1]	81–84	−9	264
4-Methyl-1,3-pentadiene*; C_6H_{10} ; [926-56-7]	75–76.5	−2	271
1,5-Hexadiene*; C_6H_{10} ; [592-42-7]	59.6	52	278
2,4-Heptadiene; C_7H_{12} ; [628-72-8]	107.5–108.0	17	290
5,5-Dimethyl-2,3-hexadiene; C_8H_{14} ; [36382-08-6]	107.6–108.0	20	293
2,4-Octadiene; C_8H_{14} ; [13643-08-8]	133.5–134.0	36	309
4-Methyl-1,5-heptadiene; C_8H_{14} ; [998-94-7]	110.5–110.9	53	326
4-Propyl-1,5-heptadiene; $C_{10}H_{18}$	156.2–156.6	77	350
4,5-Dimethyl-2,6-octadiene; $C_{10}H_{18}$; [18476-57-8]	152.9–153.8	78	351
4-Propen-2-yl-2-octene; $C_{11}H_{20}$	178–179	82	355

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Miscibility was determined in a glass-stoppered tube of 4 mm inside diameter. Equal volumes (0.1 mL) of (1) and (2) were measured into the tube which was then strapped to a thermometer, warmed to 5 or 10 °C above the solubility temperature, mixed well by shaking, and then allowed to cool slowly, still shaking, in a bath of white oil, water or (below 0 °C) nonfreezing mixture.

Source and Purity of Materials;

(1) Not specified.
(2) Some alkadienes (*) were obtained from Dr. F. Cortese; others were purest commercial samples available from BDH.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Alkynes; C_7H_{12}, C_8H_{14}, C_9H_{16}, and $C_{16}H_{30}$

Original Measurements:

S. P. Mulliken and R. L. Wakeman, Rec. Trav. Chim. **54**, 366–72 (1935).

Variables:

T/K=270–365

Prepared By:

V. P. Sazonov

Experimental Data

Miscibility temperatures of mixtures with equal volumes of nitromethane and alkyne

Alkyne	B. p. alkyne/°C	t/°C	T/K (compiler)
2-Octyne; C_8H_{14} ; [2809-67-8]	138.0–138.4	−4	270
3-Heptyne; C_7H_{12} ; [2586-89-2]	105.3–106.7	24	297
4-Nonyne; C_9H_{16} ; [20184-91-2]	155.1–156.1	45	318
1-Hexadecyne; $C_{16}H_{30}$; [629-74-3]	280	92	365

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Miscibility was determined in a glass-stoppered tube of 4 mm inside diameter. Equal volumes (0.1 mL) of (1) and (2) were measured into the tube which was then strapped to a thermometer, warmed to 5 or 10 °C above the solubility temperature, mixed well by shaking, and then allowed to cool slowly, still shaking, in a bath of white oil (above 30 °C), water (below 30 °C), or nonfreezing mixture (below 0 °C).

Source and Purity of Materials:

(1) Not specified.
(2) 1-hexadecyne synthesized in the Research Laboratory of Organic Chemistry, Massachusetts Institute of Technology; others alkynes were purest commercial samples available from the British Drug Houses.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Cycloalkanes; C_8H_{16} and $C_{11}H_{22}$

Original Measurements:

S. P. Mulliken and R. L. Wakeman, Rec. Trav. Chim. **54**, 366–72 (1935).

Variables:

T/K = 346 and 380

Prepared By:

V. P. Sazonov

Experimental Data

Solubility temperatures of mixtures with equal volumes of nitromethane and cycloalkane

Cycloalkane	B.p. cycloalkane/°C	t/°C	T/K (compiler)
(3-Methylbutyl)cyclohexane; $C_{11}H_{22}$; [54105-76-9]	191–192	73	346
Dimethylcyclohexane; C_8H_{16} ; [27195-67-1]	120	107	380

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Miscibility was determined in a glass-stoppered tube of 4 mm inside diameter. Equal volumes (0.1 mL) of (1) and (2) were measured into the tube which was then strapped to a thermometer, warmed to 5 or 10 °C above the solubility temperature, mixed well by shaking, and then allowed to cool slowly, still shaking, in a bath of white oil.

Source and Purity of Materials:

(1) Not specified.
(2) Dimethylcyclohexane synthesized in the Research Laboratory of Organic Chemistry, Massachusetts Institute of Technology; the other cycloalkane was the purest commercial sample available.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Alkanes; C_8H_{18}, $C_{10}H_{22}$, $C_{12}H_{26}$, $C_{14}H_{30}$, $C_{16}H_{34}$, and $C_{18}H_{38}$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372–81 (1965).

Variables:

T/K = 384–432

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane + alkane

Alkane	t/°C	T/K (compiler)
Octane; C_8H_{18} ; [111-65-9]	110.5	383.7
Decane; $C_{10}H_{22}$; [124-18-5]	122.5	395.7
Dodecane; $C_{12}H_{26}$; [112-40-3]	132.5	405.7
Tetradecane; $C_{14}H_{30}$; [629-59-4]	142.0	415.2
Hexadecane; $C_{16}H_{34}$; [544-76-3]	151.0	424.2
Octadecane; $C_{18}H_{38}$; [593-45-3]	159.0	432.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Riechert 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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Aromatic hydrocarbons; C_8H_{10}–$C_{20}H_{28}$

Original Measurements:
A. W. Francis, Ind. Eng. Chem, **36**, 1096–104 (1944).

Variables:
T/K=242–368

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+aromatic hydrocarbon

Aromatic hydrocarbon	B. p. hydrocarbon/°C	t/°C	T/K (compiler)
Ethylbenzene*; C_8H_{10} ; [100-41-4]	136	−31	242
(1-Methylethyl)benzene; C_9H_{12} ; [98-82-8]	152	−28	245
1-Methyl-4-ethylbenzene*; C_9H_{12} ; [622-96-8]	162	−25	248
(1,1-Dimethylethyl)benzene; $C_{10}H_{14}$; [98-06-6]	169	−19	254
1-Methyl-3-(1-methylethyl)benzene; $C_{10}H_{14}$; [535-77-3]	176	−8	265
1,3-Diethylbenzene; $C_{10}H_{14}$; [141-93-5]	181	−4	269
(1-Methylethyl)naphthalene; $C_{13}H_{14}$; [29253-36-9]	264	−2	271
(1-Methylpropyl)benzene; $C_{10}H_{14}$; [135-98-8]	173	0	273
1,2,4-Trimethylbenzene; C_9H_{12} ; [95-63-6]	169	1	274
1-Ethyl-4-(1-methylethyl)benzene; $C_{11}H_{16}$; [4218-48-8]	195	9	282
1-Methyl-3,5-diethylbenzene; $C_{11}H_{16}$; [2050-24-0]	203	11	284
Bis(1-methylethyl)benzene; $C_{12}H_{18}$; [25321-09-9]	205	22	295
(1-Methylbutyl)benzene; $C_{11}H_{16}$; [2719-52-0]	192	25	298
1,3,5-Triethylbenzene; $C_{12}H_{18}$; [102-25-0]	216	26	299
(1-Methylethyl)naphthalene; $C_{15}H_{18}$	300	27	300
1,2,3,4-Tetrahydro-2-(1-methylethyl)naphthalene; $C_{13}H_{18}$; [33451-66-0]	261	34	307
1-Methyl-2,4-bis(1-methylethyl)benzene; $C_{13}H_{20}$; [1460-98-6]	217	34	307
Bis(1-methylethyl)naphthalene; $C_{16}H_{20}$; [38640-62-9]	310	35	308
1,2-Dipentylbenzene; $C_{16}H_{26}$; [635-89-2]	265	85	358
Dipentylnaphthalene; $C_{20}H_{28}$; [71784-99-1]	360	95	368

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) Some aromatic hydrocarbons (*) were available from the Socony-Vacuum Oil Co.; others were made by alkylation of benzene, toluene, ethylbenzene, naphthalene or tetralin with ethene, propene, 2-butene, isobutene or pentene, using aluminum chloride as catalyst.

Estimated Error:
Temperature: ±1 K.

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Aromatic hydrocarbons; $C_{10}H_{12}$–$C_{20}H_{18}$

Original Measurements:
S. P. Mulliken and R. L. Wakeman, Rec. Trav. Chim. **54**, 366–72 (1935).

Variables:
T/K=257–349

Prepared By:
V. P. Sazonov

Experimental Data:

Miscibility temperatures of mixtures with equal volumes of nitromethane and aromatic hydrocarbon

Aromatic hydrocarbon	B.p. Hydrocarbon/°C	t/°C	T/K (compiler)
1,2,3,4-Tetrahydronaphtalene; $C_{10}H_{12}$; [119-64-2]	203	−16	257
1,4-Diethylbenzene; $C_{10}H_{14}$; [105-05-5]	182	−5	268
1-Methyl-4-(1-methylethyl)benzene; $C_{10}H_{14}$; [99-87-6]	176.5	−4	269
1,3-Diethylbenzene; $C_{10}H_{14}$; [141-93-5]	181	−3	270
(1-Methylpropyl)benzene; $C_{10}H_{14}$; [135-98-8]	174	−1	272
Butylbenzene; $C_{10}H_{14}$; [104-51-8]	182	4	277
(1,1-Dimethylpropyl)benzene; $C_{11}H_{16}$; [2049-95-8]	190	14	287
1,1′,1″-(1-Ethenyl-2-ylidene)trisbenzene; $C_{20}H_{16}$; [58-72-0]	220/1.87 kPa	21	294
Cyclohexylbenzene; $C_{12}H_{16}$; [827-52-1]	238	24	297
1,8-Diphenyl-1,3,5,7-octatetraene; $C_{20}H_{18}$; [3029-40-1]	197/1.07 kPa	27	300
2,4-Dimethyl-3-benzylidenepentane*; $C_{14}H_{20}$	111 to 113/1.5 kPa	34	307
[1,3-Dimethyl-2-(1-methylethyl)-1-butenyl]-benzene*; $C_{15}H_{22}$; [100649-45-4]	109 to 111/0.4 kPa	49	322
2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0]	261	62	335
4,4′-Dimethyl-1,1′-diphenyl; $C_{14}H_{14}$; [613-33-2]	295	69	342
Octahydroanthracene; $C_{14}H_{18}$; [1079-71-6]	292	76	349

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Miscibility was determined in a glass-stoppered tube of 4 mm inside diameter. Equal volumes (0.1 mL) of (1) and (2) were measured into the tube which was then strapped to a thermometer, warmed to 5 or 10 °C above the solubility temperature, mixed well by shaking, and then allowed to cool slowly, still shaking, in a bath of white oil (above 30 °C), water (below 30 °C), or nonfreezing mixture (below 0 °C).

Source and Purity of Materials:

(1) Not specified.
(2) Some aromatic hydrocarbons (*) obtained from J. B. Conant, Harvard University; others were purest commercial samples.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Cycloalkenes; C_9H_{16}, $C_{10}H_{10}$ and $C_{10}H_{18}$

Original Measurements:
S. P. Mulliken and R. L. Wakeman, Rec. Trav. Chim. **54**, 366–72 (1935).

Variables:
T/K=333–352

Prepared By:
V. P. Sazonov

Experimental Data

Solubility temperatures of mixtures with equal volumes of nitromethane and cycloalkene

Cycloalkene	B. p. cycloalkene/°C	t/°C	T/K (compiler)
Bicyclo[4,2,2]deca-2,4,7,9-tetraene; $C_{10}H_{10}$; [15677-13-1]	170	60	333
(1-Methylethenyl)cyclohexane; C_9H_{16} ; [2157-18-8]	154.0–154.4	75	348
1-Methyl-4-(1-methylethyl)cyclohexene; $C_{10}H_{18}$; [5502-88-5]	175	79	362

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Miscibility was determined in a glass-stoppered tube of 4 mm inside diameter. Equal volumes (0.1 mL) of (1) and (2) were measured into the tube which was then strapped to a thermometer, warmed to 5 or 10 °C above the solubility temperature, mixed well by shaking, and then allowed to cool slowly, still shaking, in a bath of white oil.

Source and Purity of Materials:

(1) Not specified.
(2) (1-methylethenyl)cyclohexane synthesized in the Research Laboratory of Organic Chemistry, Massachusetts Institute of Technology; other cycloalkenes were purest available commercial samples.

Estimated Error:

Not reported.

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Terpenes; $C_{10}H_{16}$–$C_{15}H_{24}$

Original Measurements:
S. P. Mulliken and R. L. Wakeman, Rec. Trav. Chim. **54**, 366–72 (1935).

Variables:
T/K=310–358

Prepared By:
V. P. Sazonov

Experimental Data

Miscibility temperatures of mixtures with equal volumes of nitromethane and terpene

Terpene	B. p. terpene/°C	t/°C	T/K (compiler)
2-Methyl-5-(1-methylethyl)-1,3-cyclohexadiene (phellandrene); $C_{10}H_{16}$; [99-83-2]	175	37	310
1-Methyl-4-(1-methylethenyl)cyclohexene (d-limonene); $C_{10}H_{16}$; [138-86-3]	176	50	323
4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane (sabinene); $C_{10}H_{16}$; [3387-41-5]	163	52	325
(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene (1-α-pinene); $C_{10}H_{16}$; [7785-70-9]	156	68	341
(1S)-6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane (1-β-pinene); $C_{10}H_{16}$; [18172-67-3]	163	70	343
2,2-Dimethyl-3-methylenebicyclo[2.2.1]heptane (camphene); $C_{10}H_{16}$; [79-92-5]	160	77	350
(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene (d-α-pinene); $C_{10}H_{16}$; [7785-26-4]	156	78	351
4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene (caryophyllene); $C_{15}H_{24}$; [87-44-5]	259	85	358

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Miscibility was determined in a glass-stoppered tube of 4 mm inside diameter. Equal volumes (0.1 mL) of (1) and (2) were measured into the tube which was then strapped to a thermometer, warmed to 5 or 10 °C above the solubility temperature, mixed well by shaking, and then allowed to cool slowly, still shaking, in a bath of white oil or water.

Source and Purity of Materials:

(1) Not specified.
(2) Schimmel & Co.; purity not specified.

Estimated Error:

Not reported.

7. Nitromethane+Halogenated Hydrocarbons

Components:
(1) Tetrachloromethane; CCl_4 ; [56-23-5]
(2) Nitromethane; CH_3NO_2 ; [75-52-5]

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

Variables:
$T/\mathrm{K}=275$; $P/\mathrm{kPa}=3141-12412$

Prepared By:
V. P. Sazonov and A. V. Morozov

Experimental Data

The UCST was reported to be 1.10 °C (274.55 K, compilers). A value of $\mathrm{d}T_c/\mathrm{d}P$ of 0.0025 $\mathrm{K\cdot kPa^{-1}}$ was reported in the above pressure range.

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. The observations were carried out in sealed tubes in the presence of the vapor phase. A Cailletet 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) Tetrachloromethane; CCl_4; [56-23-5]
(2) Nitromethane; CH_3NO_2; [75-52-5]

Original Measurements:
A. Dorby, Makromol. Chem. **18/19**, 317–21 (1956).

Variables:
$T/\mathrm{K}=277$

Prepared By:
V. P. Sazonov

Experimental Data

The UCST was reported to be 3.5 °C (276.7 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) Diiodomethane; CH_2I_2; [75-11-6]
(2) Nitromethane; CH_3NO_2; [75-52-5]

Original Measurements:

V. P. Sazonov, I. N. Zhilyaeva, and L. V. Gudkina, Zh. Prikl. Khim. (Leningrad) **48**, 1953–7 (1975).

Variables:

T/K=284–321

Prepared By:

N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of diiodomethane and nitromethane

		Nitromethane-rich phase		Diiodomethane-rich phase	
t/°C	T/K (compilers)	100 w_1	x_1 (compilers)	100 w_1	x_1 (compilers)
11.00	284.15	30.02	0.0891	97.02	0.8812
29.22	302.37	42.42	0.1438	—	—
36.40	309.55	—	—	91.59	0.7128
36.57	309.72	49.81	0.1844	—	—
43.81	316.96	59.63	0.2518	—	—
46.32	319.47	—	—	84.99	0.5634
46.57	319.72	65.00	0.2974	—	—
47.52	320.67	70.00	0.3472	79.97	0.4764
47.87	321.02	—	—	74.96	0.4056

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method of Alekseev was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; analytical purity; fractionally distilled at about 0.27 kPa; $d(20\ °C)=3321.4\ g\cdot L^{-1}$.
(2) Source not specified; pure grade reagent; distilled over a column of 15 theoretical plates; $n(20\ °C,D)=1.3819$, $d(20\ °C)=1130\ g\cdot L^{-1}$.

Estimated Error:

Not specified.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Tetrachloroethene; C_2Cl_4; [127-18-4]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, May, 1996.

Critical Evaluation

Solubilities in the system comprising nitromethane and tetrachloroethene have been reported in three publications. Cornish *et al.*[1] determined the upper critical solution temperature by the synthetic method. Schuberth and Kranke[2] carried out measurements of the mutual solubilities of the components at 293, 303, and 313 K by the synthetic and the titration methods. Sazonov and Chernysheva[3] studied mutual solubility of (1) and (2) between 293 and 315 K by the synthetic method.

Values obtained by the graphical interpolation or extrapolation from the data sheets are presented in the table. Data are ''recommended'' if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Recommended values for the mutual solubility of nitromethane and tetrachloroethane

	Tetrachloroethene-rich phase		Nitromethane-rich phase	
T/K	100 w_1	x_1	100 w_2	x_2
293	5.3	0.132	33.5	0.156
303	8.1	0.193	41.8	0.209
313	17.7	0.369	58.5	0.342

The upper critical solution temperature has been reported as 314.2 K,[1] 314.35 K,[3] and 314.5 K.[2] The three reported values of UCST vary over a range of 0.3 K. Thus, the recommended value is: (314.35±0.15) K.

The numerical values reported in the above table have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.897\ 68$, $a_2=-0.110\ 82$, $b_1=8.719\ 62$, $b_2=-7.014\ 96$ (mean standard error of estimate was 0.0062).

For approximation $x_{c1}=0.538$ and recommended value of UCST have been used. This relationship is presented in Fig. 21 together with experimental data reported in Schuberth and Kranke[2] and Sazonov and Chernysheva.[3]

Components: (1) Nitromethane; CH_3NO_2; [75-52-5] (2) Tetrachloroethene; C_2Cl_4; [127-18-4]	**Original Measurements:** R. E. Comish, R. C. Archibald, E. A. Murphy, and H. M. Evans, Ind. Eng. Chem. **26**, 397–406 (1934).
Variables: T/K=314	**Prepared By:** V. P. Sazonov

Experimental Data

The upper critical solution temperature was reported to be 41 °C (314 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) Source not specified; commercial high-grade reagent.
(2) Source not specified; commercial high-grade reagent.

Estimated Error:

Not reported.

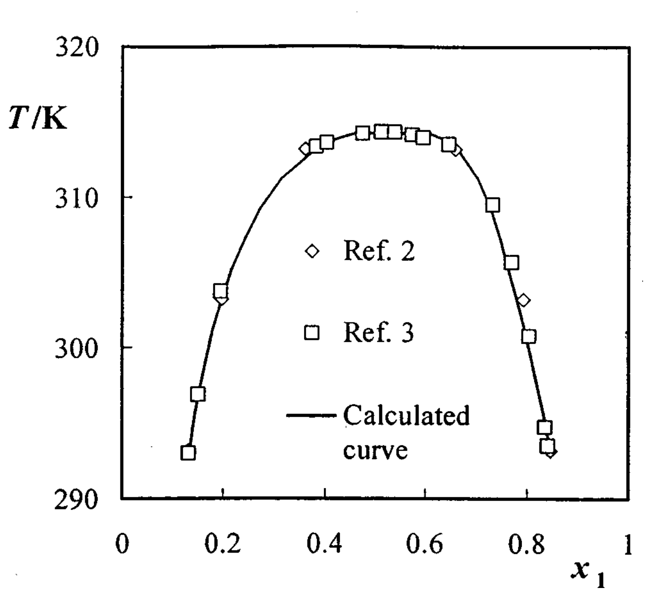

FIG. 21. Mutual solubility of nitromethane and tetrachloroethene.

References:

[1] R. E. Comish, R. C. Archibald, E. A. Murphy, and H. M. Evans, Ind. Eng. Chem. **26**, 397 (1934).
[2] H. Schuberth and P. Kranke, Z. Phys. Chem. (Leipzig) **245**, 49 (1970).
[3] V. P. Sazonov and M. F. Chernysheva, Zh. Obshch. Khim. **55**, 2440 (1985).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Tetrachloroethene; C_2Cl_4; [127-18-4]

Original Measurements:
H. Schuberth and P. Kranke, Z. Phys. Chem. (Leipzig) **245**, 49–67 (1970).

Variables:
T/K = 293–315

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and tetrachloroethene

t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
20.0	293.2	0.131	5.26	0.845	66.7
30.0	303.2	0.197	8.28	0.793	58.5
40.0	313.2	0.361	17.2	0.658	41.5
41.3	314.5	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic and the titration methods were used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; purity not specified; distilled; b.p. = 100.9 °C, $n(20\ °C,D) = 1.38195$, $d(20\ °C) = 1137.9\ g \cdot L^{-1}$.
(2) Source not specified; distilled; b.p. = 120.8 °C, $n(20\ °C,D) = 1.50545$, $d(20\ °C) = 1622.8\ g \cdot L^{-1}$.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Tetrachloroethene; C_2Cl_4; [127-18-4]

Original Measurements:
V. P. Sazonov and M. F. Chernysheva, Zh. Obshch. Khim. **55**, 2440–6 (1985).

Variables:
T/K = 293–315

Prepared By:
N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and tetrachloroethene

		Tetrachloroethene-rich phase		Nitromethane-rich phase	
T/K	t/°C (compilers)	100 w_1	x_1 (compilers)	100 w_1	x_1 (compilers)
293.05	19.90	5.2	0.130	—	—
293.55	20.40	—	—	66.0	0.841
294.80	21.65	—	—	65.1	0.835
296.95	23.80	6.0	0.148	—	—
300.80	37.65	—	—	60.0	0.803
303.75	30.60	8.1	0.193	—	—
305.70	32.55	—	—	55.0	0.769
309.55	36.40	—	—	50.0	0.731
313.30	40.15	18.5	0.381	—	—
313.55	40.40	—	—	40.0	0.644
313.65	40.50	20.0	0.404	—	—
313.99	40.84	—	—	35.0	0.594
314.10	40.95	—	—	33.0	0.572
314.20	41.05	25.0	0.475	—	—
314.30	41.15	27.9	0.513	—	—
314.31	41.16	30.0	0.538	—	—
314.35	41.20	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method of Alekseev was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled over a column of 20 theoretical plates; 99.9 mass % purity.
(2) Source not specified; pure grade reagent; distilled with glass packed fractionating column.

Estimated Error:
Not specified.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Hydropentadecafluoroheptane; C_7HF_{15}; [375-83-7]

Original Measurements:

J. O. Konecky and C. H. Deal, J. Phys. Chem. **67**, 504–6 (1963).

Variables:

$T/\mathrm{K}=312-373$

Prepared By:

V. P. Sazonov

Experimental Data

The mutual solubility of nitromethane and 1-hydropentadecafluoroheptane in volume fractions are presented over the temperature range in graphical form. The data in the following table were extracted by the compiler from the reported graphs.

Mutual solubility of nitromethane and 1-hydropentadecafluoroheptane

		Fluorohydrocarbon-rich phase			Nitromethane-rich phase		
$t/°\mathrm{C}$	T/K (compiler)	$100\,\varnothing_1$	$100\,w_1$ (compiler)	x_1 (compiler)	$100\,\varnothing_1$	$100\,w_1$ (compiler)	x_1 (compiler)
38.5	311.7	8.9	6.0	0.279	—	—	—
67.3	340.5	—	—	—	90.6	86.4	0.975
72.8	346.0	—	—	—	88.3	83.2	0.968
77.3	350.5	19.3	13.6	0.488	—	—	—
91.5	364.7	—	—	—	79.3	71.6	0.939
92.4	365.6	29.6	21.7	0.627	—	—	—
98.2	371.4	—	—	—	69.0	59.4	0.899
98.5	371.7	38.9	29.5	0.717	—	—	—
99.4	372.6	—	—	—	58.9	48.5	0.851
99.7	372.9	50.0	39.7	0.800	—	—	—
99.7	372.9	—	—		—	—	— (UCST)

Auxiliary Information

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 further details were reported.

Source and Purity of Materials:

(1) Source not specified; distilled on a ten plate microhelipod column at a reflux ratio of 5/1; b.p.$=101$ °C/101.6 kPa.
(2) Prepared by the decarboxylation of perfluorooctanoic acid; dried over phosphorus pentoxide and distilled on a ten plate microhelipod column at a reflux ratio of 5/1; b.p. $=95$ °C/100.1 kPa, $d(25\ °\mathrm{C})=1718\ \mathrm{g\cdot L^{-1}}$.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Bromides; $C_8H_{17}Br$, $C_{10}H_{21}Br$, $C_{12}H_{25}Br$, $C_{14}H_{29}Br$, $C_{16}H_{33}Br$, and $C_{18}H_{37}Br$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372–81 (1965).

Variables:

$T/\mathrm{K}=311-397$

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+1-bromide

1-Bromide	$t/°\mathrm{C}$	T/K (compiler)
1-Bromooctane; $C_8H_{17}Br$; [111-83-1]	38.0	311.2
1-Bromodecane; $C_{10}H_{21}Br$; [112-29-8]	63.0	336.2
1-Bromododecane; $C_{12}H_{25}Br$; [143-15-7]	82.5	355.7
1-Bromotetradecane; $C_{14}H_{29}Br$; [112-71-0]	98.0	371.2
1-Bromohexadecane; $C_{16}H_{33}Br$; [112-82-3]	111.0	384.2
1-Bromooctadecane; $C_{18}H_{37}Br$; [112-89-0]	123.5	396.7

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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °\mathrm{C,D})=1.3820$, $d(20\ °\mathrm{C})=1134\ \mathrm{g\cdot L^{-1}}$.
(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

8. Nitromethane+Alcohols (mono- and poly-)

Components:	**Evaluator:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	V. P. Sazonov, Technical University, Samara, Russia, May, 1996.

Critical Evaluation

Quantitative solubility data for the system nitromethane+1,2-ethanediol have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system nitromethane+1,2-ethanediol

Reference	T/K	Solubility	Method
Francis[1]	273–313	Mutual	Synthetic
Markuzin and Nikanorova[2]	301, 313	Mutual	Titration
Schmid *et al.*[3]	312	UCST	Synthetic
Burdykina and Zhuravlev[4]	278–314	Mutual	Synthetic
Zhuravleva *et al.*[5]	289–314	Mutual	Synthetic
Sazonov and Filippov[6]	297–313	Mutual	Synthetic
Salvi and Van Hook[7]	309–314[a]	Mutual	Synthetic

[a] At $0.9 \leq p/\text{MPa} \leq 50$.

Apart from Schmid *et al.*,[3] which did not contain sufficient information to justify its inclusion, all the original data are given in the data sheets following this Critical Evaluation.

In the tables that follow, values obtained by the evaluators by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). ''Best'' values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be 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 (±5% relative) agreement. All other data are regarded as tentative only.

Table 2 summarizes the available data for the solubility of nitromethane in 1,2-ethanediol, with the exception of the data of Markuzin and Nikanorova[2] whose glycol-rich phase data disagree markedly from all other studies and are rejected.

TABLE 2. Tentative and recommended (R) values for the solubility of nitromethane (1) in 1,2-ethanediol (2)

	Solubility, 100 w_1		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_1	x_1
273	20.0 (Ref. 1)	20.0	0.203
278	21.5* (Ref. 1), 23.1* (Ref. 4)	22.3±0.8 (R)	0.226
283	23.0 (Ref. 1), 23.2* (Ref. 5)	23.1±0.1 (R)	0.234
288	24.7* (Ref. 1)	24.7	0.250
293	27.0 (Ref. 1), 28.1* (Ref. 4), 27.1* (Ref. 5)	27.4±0.5 (R)	0.277
298	29.6* (Ref. 1), 29.8* (Ref. 6)	29.7±0.1 (R)	0.301
303	33.3* (Ref. 1), 34.3* (Ref. 4), 33.4* (Ref. 5), 33.3* (Ref. 6)	33.6±0.6 (R)	0.340
308	40.0* (Ref. 1), 38.7* (Ref. 6)	39.4±0.6 (R)	0.398
311	48.0* (Ref. 1), 45.0* (Ref. 6), 49.2* (Ref. 7)	47±2 (R)	0.47
313	59.0* (Ref. 2), 59.7* (Ref. 6), 59.6* (Ref. 7)	59.4±0.3 (R)	0.598

TABLE 3. Tentative and recommended (R) values for the solubility of 1, 2-ethanediol (2) in nitromethane (1)

	Solubility, 100 w_1		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_2	x_2
273	3.0 (Ref. 1)	3.0	0.029
278	3.5* (Ref. 1), 3.1* (Ref. 4)	3.3±0.2	0.032
283	4.0* (Ref. 1)	4.0	0.039
288	4.8* (Ref. 1)	4.8	0.047
293	6.0* (Ref. 1), 5.9* (Ref. 4), 5.8* (Ref. 5)	5.9±0.1 (R)	0.058
298	7.6* (Ref. 1), 7.9* (Ref. 6)	7.8±0.2 (R)	0.077
303	10.8* (Ref. 1), 9.3* (Ref. 4), 10.6* (Ref. 6)	10.2±0.6	0.101
308	18.0 (Ref. 1), 14.6* (Ref. 6)	16±2	0.16
311	25.0* (Ref. 1), 19.4* (Ref. 6), 21.3* (Ref. 7)	22±2	0.22
313	34.1 (Ref. 6), 35.5* (Ref. 7)	34.8±0.7 (R)	0.344

The numerical values reported in the tables above have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1 = 0.780\,77$, $a_2 = 0.006\,02$, $b_1 = -0.239\,90$, $b_2 = -0.058\,08$ (mean standard error of estimate was 0.0275).

For approximation the recommended values of UCST and x_{c1} have been used. The calculated compositions are inside declared in the tables inaccuracy at the each point. The calculated relationship is presented in Fig. 22 together with the ''best'' values from the above tables.

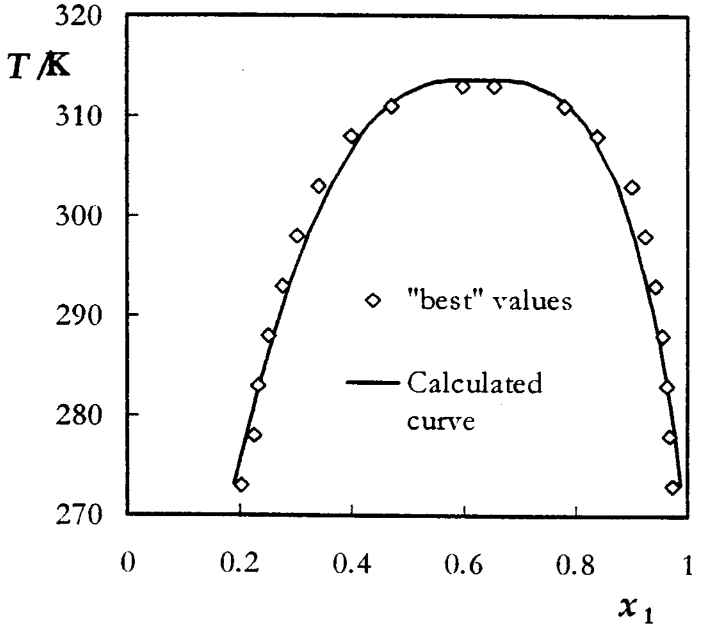

FIG. 22. Mutual solubility of nitromethane and 1,2-ethanediol.

The upper critical solution temperature has been reported as 312.2 K,[3] 312.9 K,[1] 313.17 K,[6] 314.2 K,[5] and 314.5 K.[4] The UCST of Schmid *et al.*[3] is rejected. The remaining values give an average recommended value of: UCST = 313.7 ± 0.6 K.

The corresponding critical solution composition has been reported as $x_{c1} = 0.624$,[1,6], $x_{c1} = 0.6309$, and $x_{c1} = 0.644$.[5] The average of these values, $x_{c1} = 0.633 \pm 0.008$, ($100\,w_1 = 62.9$) has a spread which is equal to the estimated error given by Sazonov[6] and is recommended.

References:

[1] A. W. Francis, J. Phys. Chem. **60**, 20 (1956).

[2] N. P. Markuzin and L. A. Nikanorova, Zh. Obshch. Khim **32**, 3469 (1962).

[3] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **11**, 376 (1966).

[4] P. I. Burdykina and E. F. Zhuravlev, Zh. Fiz. Khim. **42**, 1925 (1968).

[5] I. K. Zhuravleva, E. F. Zhuravlev, and N. M. Cherkasova, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **14**, 1010 (1971).

[6] V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222 (1975).

[7] M. V. Salvi and W. A. Van Hook, J. Phys. Chem. **94**, 7812 (1990).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	A. W. Francis, J. Phys. Chem. **60**, 20–7 (1956).
Variables: T/K = 273–313	**Prepared By:** V. P. Sazonov

Mutual solubility of nitromethane and 1,2-ethanediol

		Glycol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	$100\,w_1$	x_1 (compiler)	$100\,w_1$	x_1 (compiler)
0.0	273.2	20.0	0.203	97.0	0.970
10.0	283.2	23.0	0.233	96.0	0.961
16.0	289.2	25.0	0.253	95.0	0.951
20.0	293.2	27.0	0.273	94.0	0.941
22.0	295.2	28.0	0.284	94.0	0.941
23.4	296.6	29.0	0.293	93.0	0.931
26.0	299.2	30.0	0.303	92.0	0.921
28.0	301.2	32.0	0.324	91.0	0.911
29.0	302.2	31.0	0.314	90.0	0.901
35.0	308.2	40.0	0.404	82.0	0.822
39.7	312.9	62.0	0.624	62.0	0.624 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Eastman Kodak Co.; distilled with 30 cm column; b.p. = 101.25 °C, m.p. = −30.5 °C, n(20 °C,D) = 1.3820, d(25 °C) = 1129.8 $g \cdot L^{-1}$.
(2) Source not specified; purified by crystallization; m.p. = −13.3 °C, n(20 °C,D) = 1.4315, d(20 °C) = 1110.1 $g \cdot L^{-1}$.

Estimated Error:
Not reported.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

Original Measurements:

N. P. Markuzin and L. A. Nikanorova, Zh. Obshch. Khim. **32**, 3469–73 (1962).

Variables:

T/K=301 and 313

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1,2-ethanediol

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
28.0	301.2	37.7	0.381	91.9	0.920
40.0	313.2	25.3	0.256	59.0	0.594

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Solutions were mixed by stirring. The mixtures were weighed before and after the test to find the amount of added substance.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled over a column of 20 theoretical plates; $n(20\ °C,D)=1.3820$, $d(20\ °C)=1137.9\ g \cdot L^{-1}$.
(2) Source not specified; pure grade reagent; purified by vacuum distillation; $n(20\ °C,D)=1.4318$, $d(20\ °C)=1113.4\ g \cdot L^{-1}$.

Estimated Error:

Temperature: control to ±0.03 K.
Solubility: 1% (relative error).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

Original Measurements:

P. I. Burdykina and E. F. Zhuravlev, Zh. Fiz. Khim. **42**, 1925–9 (1968).

Variables:

T/K=278–314

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1,2-ethanediol

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
5.0	278.2	23.1	0.234	96.9	0.970
20.0	293.2	28.1	0.285	94.1	0.942
30.0	303.2	34.3	0.347	90.7	0.908
41.3	314.5	64.0	0.644	64.0	0.644 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and N. M. Cherkasova, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **14**, 1010–3 (1971).

Variables:
T/K=289–314

Prepared By:
V. P. Sazonov

Experimental Data

The mutual solubility of nitromethane and 1,2-ethanediol in mass percent over the specified temperature range were presented in graphical form in the original publication. The numerical data in the table below were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and 1,2-ethanediol

		Glycol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
15.7	288.9	25.0	0.253	—	—
25.3	298.5	30.0	0.303	—	—
31.5	304.7	35.0	0.305	—	—
32.4	305.6	—	—	90.0	0.902
35.4	308.6	40.0	0.404	—	—
37.5	310.7	—	—	85.0	0.852
38.2	311.4	45.0	0.454	—	—
40.4	313.6	50.0	0.504	—	—
40.6	313.8	—	—	80.0	0.802
40.9	314.1	60.0	0.604	75.0	0.753
41.0	314.2	65.0	0.654	70.0	0.704
41.0	314.2	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled; b.p. = 101 °C, n(24 °C,D) = 1.3800.
(2) Source not specified; analytical purity; distilled at vacuum; b.p. = 198 °C, n(24 °C,D) = 1.4300.

Estimated Error:
Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

Original Measurements:
V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222–5 (1975).

Variables:
T/K=297–313

Prepared By:
N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1,2-ethanediol

		Glycol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
24.15	297.30	—	—	92.50	0.9262
25.45	298.60	30.00	0.3035	—	—
29.33	302.48	—	—	90.00	0.9015
31.65	304.80	35.04	0.3542	—	—
35.58	308.73	—	—	85.00	0.8521
35.88	309.03	40.00	0.4040	—	—
37.98	311.13	44.98	0.4539	—	—
38.31	311.46	—	—	79.99	0.8025
39.21	312.36	50.03	0.5045	—	—
39.59	312.74	—	—	74.95	0.7526
39.79	312.94	54.99	0.5540	—	—
39.90	313.05	—	—	70.02	0.7037
40.01	313.16	60.00	0.6040	—	—
40.02	313.17	—	—	64.97	0.6535
40.02	313.17	62.70	0.6309	62.70	0.6309 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method of Alekseev[1] was used. Close to the phase transition temperature, heating and cooling of mixtures were accomplished in steps at a rate of 0.02 K/h.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled over a column of 15 theoretical plates; n(20 °C,D) = 1.3819, d(20 °C) = 1138.1 g·L^{-1}.
(2) Source not specified; analytical purity; fractionally distilled at about 260 Pa; n(20 °C,D) = 1.4318, d(20 °C) = 1113.5 g·L^{-1}.

Estimated Error:
Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	M. V. Salvi and W. A. Van Hook, J. Phys. Chem. **94**, 7812–20 (1990).
Variables:	**Prepared By:**
T/K=308–314, P/MPa=0.1–50	V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1,2-ethanediol

			Glycol-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	P/MPa	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
308.409	35.259	0.880	0.4371	43.30	—	—
309.416	36.266	0.180	—	—	0.8369	83.46
309.950	36.800	0.120	0.4663	46.21	—	—
310.630	37.480	0.110	0.4894	48.52	—	—
311.505	38.355	0.150	—	—	0.7749	77.20
311.781	38.631	0.140	0.5113	50.71	—	—
311.923	38.773	0.100	—	—	0.7397	73.65
311.991	38.841	0.570	0.5172	51.50	—	—
312.489	39.339	0.130	—	—	0.7143	71.09
312.498	39.348	0.140	0.5671	56.30	—	—
312.947	39.797	0.160	—	—	0.6782	67.45
312.975	39.825	0.110	—	—	0.6555	65.17
313.084	39.934	0.120	0.6298	62.59	—	—
313.098	39.948	0.130	0.6068	60.28	—	—
308.422	35.272	2.51	0.4371	43.30	—	—
309.443	36.293	2.51	—	—	0.8369	83.46
309.972	36.822	2.50	0.4663	46.21	—	—
311.536	38.386	2.52	—	—	0.7749	77.20
311.691	38.541	2.50	0.4894	48.52	—	—
311.832	38.682	2.51	0.5113	50.71	—	—
311.957	38.807	2.50	0.5192	51.50	—	—
312.025	38.875	2.51	—	—	0.7397	73.65
312.386	39.236	2.51	—	—	0.7143	71.09
312.515	39.365	2.51	0.5671	56.30	—	—
312.900	39.750	2.50	—	—	0.6782	67.45
312.988	39.838	2.50	—	—	0.6555	65.17
312.998	39.848	2.50	0.6068	60.28	—	—
313.097	39.947	2.50	0.6298	62.59	—	—
309.477	36.327	5.00	—	—	0.8369	83.46
309.972	36.822	5.00	0.4663	46.21	—	—
310.963	37.813	5.25	0.4894	48.52	—	—
311.614	38.464	5.00	—	—	0.7749	77.20
311.863	38.713	5.03	0.5113	50.71	—	—
312.066	38.916	4.85	0.5192	51.50	—	—
312.191	39.041	5.00	—	—	0.7397	73.65
312.426	39.276	5.00	—	—	0.7143	71.09
312.621	39.471	5.00	0.5671	56.30	—	—
312.914	39.764	5.00	—	—	0.6782	67.45
313.018	39.868	5.00	—	—	0.6555	65.17
313.115	39.965	5.00	0.6298	62.59	—	—
313.130	39.980	5.00	0.6068	60.28	—	—
309.554	36.404	10.26	—	—	0.8369	83.46
310.091	36.941	10.06	0.4663	46.21	—	—
310.780	37.630	8.430	0.4894	48.52	—	—
311.653	38.503	10.00	—	—	0.7749	77.20
311.881	38.731	10.00	0.5113	50.71	—	—
312.280	39.130	10.10	—	—	0.7397	73.65
312.601	39.451	10.00	—	—	0.7143	71.09
312.658	39.508	10.00	0.5671	56.30	—	—
313.035	39.885	10.00	—	—	0.6782	67.45
313.079	39.929	10.00	—	—	0.6555	65.17
313.191	40.041	10.03	0.6068	60.28	—	—
313.211	40.061	9.740	0.6298	62.59	—	—
309.607	36.457	15.04	—	—	0.8369	83.46
310.182	37.032	15.02	0.4663	46.21	—	—
311.786	38.636	15.00	—	—	0.7749	77.20
311.906	38.756	15.00	0.5113	50.71	—	—
312.013	38.863	13.27	0.5192	51.50	—	—
312.440	39.290	14.65	—	—	0.7397	73.65
312.685	39.535	14.98	0.5671	56.30	—	—
312.788	39.638	15.00	—	—	0.7143	71.09
313.103	39.953	15.00	—	—	0.6782	67.45
313.158	40.008	15.02	—	—	0.6555	65.17
313.281	40.131	15.00	0.6298	62.59	—	—
313.340	40.190	15.00	0.6068	60.28	—	—
309.664	36.514	20.06	—	—	0.8369	83.46
310.442	37.292	20.00	0.4663	46.21	—	—
311.902	38.752	20.00	0.5113	50.71	—	—
311.907	38.727	19.96	—	—	0.7749	77.20
312.090	38.940	20.36	0.5192	51.50	—	—
312.453	39.303	20.03	—	—	0.7397	73.65
312.748	39.598	20.00	0.5671	56.30	—	—
312.823	39.673	20.22	—	—	0.7143	71.09
313.175	40.025	20.00	—	—	0.6782	67.45
313.240	40.090	20.00	—	—	0.6555	65.17
313.268	40.118	20.00	0.6068	60.28	—	—
313.380	40.230	19.98	0.6298	62.59	—	—
310.606	37.456	25.00	0.4371	43.30	—	—
311.102	37.952	25.00	0.5113	50.71	—	—
311.997	38.847	25.06	—	—	0.7749	77.20
312.033	38.883	24.25	0.5192	51.50	—	—
312.551	39.401	25.01	—	—	0.7397	73.65
312.854	39.704	25.00	—	—	0.7143	71.09
313.160	40.010	24.89	0.5671	56.30	—	—
313.262	40.112	25.01	—	—	0.6782	67.45
313.313	40.163	25.04	—	—	0.6555	65.17
313.343	40.193	25.00	0.6068	60.28	—	—
313.448	40.298	25.00	0.6298	62.59	—	—
309.832	36.682	30.00	—	—	0.8369	83.46
311.997	38.847	30.00	0.5113	50.71	—	—
312.114	38.964	29.98	—	—	0.7749	77.20
312.222	39.072	30.00	0.5192	51.50	—	—
312.551	39.401	30.11	—	—	0.7397	73.65
312.987	39.837	30.00	—	—	0.7143	71.09
313.072	39.922	30.00	0.5671	56.30	—	—
313.333	40.183	30.00	—	—	0.6782	67.45
313.375	40.225	30.00	—	—	0.6555	65.17
313.450	40.300	30.00	0.6068	60.28	—	—

313.474	40.324	29.97	0.6298	62.59	—	—
309.904	36.754	35.14	—	—	0.8369	83.46
310.243	37.093	34.93	0.4663	46.21	—	—
312.951	39.801	35.00	—	—	0.7397	73.65
313.048	39.898	35.00	0.5113	50.71	—	—
313.050	39.900	35.00	—	—	0.7143	71.09
313.105	39.955	34.82	0.5671	56.30	—	—
313.431	40.281	35.04	—	—	0.6782	67.45
313.460	40.310	35.00	—	—	0.6555	65.17
313.548	40.398	35.03	0.6068	60.28	—	—
313.632	40.482	35.00	0.6298	62.59	—	—
309.978	36.828	40.00	—	—	0.8369	83.46
312.019	38.869	39.98	0.5113	50.71	—	—
312.305	39.155	40.00	—	—	0.7749	77.20
313.081	39.931	40.00	—	—	0.7397	73.65
313.333	40.183	40.00	0.5671	56.30	—	—
313.506	40.356	39.90	—	—	0.6555	65.17
313.521	40.371	40.00	—	—	0.6782	67.45
313.657	40.507	40.00	0.6068	60.28	—	—
313.708	40.558	40.00	0.6298	62.59	—	—
310.053	36.903	45.04	—	—	0.8369	83.46
312.132	38.982	45.00	0.5113	50.71	—	—
312.431	39.281	45.00	—	—	0.7749	77.20
313.147	39.997	45.00	—	—	0.7397	73.65
313.163	40.013	44.93	—	—	0.7143	71.09
313.426	40.276	45.06	0.5671	56.30	—	—
313.587	40.437	45.00	—	—	0.6555	65.17
313.702	40.552	45.00	0.6068	60.28	—	—
313.819	40.669	45.00	0.6298	62.59	—	—
312.211	39.061	50.00	0.5113	50.71	—	—
312.515	39.365	50.00	—	—	0.7749	77.20
313.194	40.044	50.06	—	—	0.7397	73.65
313.246	40.096	50.00	—	—	0.7143	71.09
313.649	40.499	50.00	—	—	0.6555	65.17
313.700	40.550	49.71	0.5671	56.30	—	—
313.782	40.632	49.96	0.6068	60.28	—	—
313.895	40.745	50.00	0.6298	62.59	—	—

UCST is 313.10 K at $x_1 = 0.640$ (100 $w_1 = 63.6$, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Measurements were made using techniques and apparatus described in Ref. 1 with minor modification. Mixtures of (1) and (2) were prepared gravimetrically. The solutions were degassed with a series of freeze–pump (≤0.1 Pa)–thaw cycles. After transfer to the apparatus (previously warmed above the CST) the demixing was determined by allowing the mixture to cool to the transition temperature at a rate of 3–5 mK/min while stirring. Temperature was measured by platinum resistance thermometry.

Source and Purity of Materials:

(1) Mallinkrodt; analytical grade; dried over anhydrous $CaCl_2$ and twice distilled in a spinning band column below 343 K.
(2) Mallinkrodt; analytical grade; dried over molecular sieve and twice distilled in a spinning band column at 16 kPa.

Estimated Error:

Temperature: ±0.3 mK.
Pressure: ±0.01 MPa.

References:

[1] R. R. Singh and W. A. Van Hook, J. Chem. Phys. **87**, 6097 (1987).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2-Ethanediol-d_2 ; $C_2D_2H_4O_2$; [7782-39-0]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
G. T. Hefter, Murdoch University, Perth, Australia, August 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 1,2-ethanediol-d_2 have been reported in two publications. Tsvetkov and Rabinovich[1] determined the upper critical solution temperature by the synthetic method. Salvi and Van Hook[2] reported extensive measurements of the mutual solubility of components (1) and (2) between 313 and 315 K and 0.1–50 MPa also by the synthetic method.

The upper critical solution temperature has been reported as 320.7 K (Ref. 1) and 315.04 K.[2] The latter result is preferred, and hence is classified as tentative, because of the higher quality, precision, and number of measurements reported in Ref. 2.

The corresponding critical solution composition has been reported as $x_{c1} = 0.642$ (100 $w_1 = 63.1$),[2] which can also be regarded as tentative.

The interested user is referred to the relevant data sheet[2] for values of the mutual solubilities of (1) and (2).

References:

[1] V. G. Tsvetkov and I. B. Rabinovich, Zh. Fiz. Khim. **47**, 2403 (1973).
[2] M. V. Salvi and W. A. Van Hook, J. Phys. Chem. **94**, 7812 (1990).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2-Ethanediol-d_2 ; $C_2D_2H_4O_2$; [7782-39-0]

Original Measurements:
V. G. Tsvetkov and I. B. Rabinovich, Zh. Fiz. Khim. **47**, 2403 (1973).

Variables:
T/K = 321

Prepared By:
V. P. Sazonov

Experimental Data

The upper critical solution temperature was reported to be 47.5 °C (320.7 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; purity not specified; purified.
(2) Obtained by method described in Ref. 1. The O.D. group of the product had a deuterium content of 97 at.%.

Estimated Error:

Temperature: ±0.1 K.

References:

[1] A. V. Nikolaev, Yu. A. Dyadin, and I. I. Yakovlev, Dokl. Akad. Nauk SSSR **170**, 110 (1966).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2-Ethanediol-d_2 ; $C_2D_2H_4O_2$; [7782-39-0]

Original Measurements:
M. V. Salvi and W. A. Van Hook, J. Phys. Chem. **94**, 7812–20 (1990)

Variables:
T/K = 313–316, P/MPa = 0.1–50

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1,2-ethanediol-d_2

			Glycol-rich phase		Nitromethane-rich phase	
T/K	t/°C (compiler)	P/MPa	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
313.109	39.959	0.1400	0.4981	48.60	—	—
313.384	40.234	0.1100	—	—	0.7844	77.61
313.651	40.501	0.1100	0.5181	50.60	—	—
314.631	41.481	0.1200	—	—	0.7041	69.31
314.703	41.553	0.5700	0.5992	58.75	—	—
315.031	41.881	0.1200	—	—	0.6539	64.28
313.150	40.000	2.510	0.4981	48.60	—	—
313.424	40.274	2.690	—	—	0.7844	77.61
313.694	40.544	2.520	0.5181	50.60	—	—
314.649	41.499	1.700	—	—	0.7041	69.31
315.071	41.921	2.500	0.6354	62.41	—	—
314.576	41.426	5.810	0.5992	58.75	—	—
314.704	41.554	5.030	—	—	0.7041	69.31
315.110	41.960	5.070	0.6354	62.41	—	—
313.212	40.062	10.11	0.4981	48.60	—	—
313.548	40.398	10.07	—	—	0.7844	77.61
313.748	40.598	9.880	0.5181	50.60	—	—
314.625	41.475	10.98	0.5992	58.75	—	—
314.760	41.610	10.10	—	—	0.7041	69.31
315.161	42.011	9.930	0.6354	62.41	—	—
313.300	40.150	14.74	0.4981	48.60	—	—
313.634	40.484	14.74	—	—	0.7844	77.61
313.720	40.570	15.03	—	—	0.7041	69.31
313.310	40.160	20.01	0.4981	48.60	—	—
313.830	40.680	20.01	0.5181	50.60	—	—
314.730	41.580	20.03	0.5992	58.75	—	—
314.886	41.736	20.02	—	—	0.7041	69.31
313.434	40.284	29.98	0.4981	48.60	—	—
313.867	40.717	30.31	—	—	0.7844	77.61
313.988	40.838	31.32	0.5181	50.60	—	—
314.894	41.744	30.04	0.5992	58.75	—	—
315.016	41.866	30.05	—	—	0.7041	69.31
313.945	40.795	35.06	—	—	0.7844	77.61
313.539	40.289	40.05	0.4981	48.60	—	—
314.074	40.924	40.93	0.5181	50.60	—	—
315.143	41.993	40.00	—	—	0.7041	69.31
315.203	42.053	40.13	0.5992	58.75	—	—
315.334	42.184	40.11	—	—	0.6539	64.28
313.583	40.433	44.86	0.4981	48.60	—	—
314.107	40.957	45.03	—	—	0.7844	77.61
313.660	40.510	50.08	0.4981	48.60	—	—
314.224	41.074	50.05	0.5189	50.60	—	—
315.283	42.133	50.01	—	—	0.7041	69.31
315.335	42.185	50.16	0.5992	58.75	—	—
315.505	42.355	50.03	—	—	0.6539	64.28

UCST at $P = 0.1$ MPa is 315.04 K at $x_1 = 0.642$ (100 $w_1 = 63.1$, compiler).
$(\mathrm{d}T_c/\mathrm{d}P) = (1.60 \pm 0.04) \cdot 10^{-2}$ K·MPa^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Measurements were made using techniques and apparatus described in Ref. 1 with minor modification. Mixtures of (1) and (2) were prepared gravimetrically. The solutions were degassed with a series of freeze–pump (≤0.1 Pa)–thaw cycles. After transfer to the appa ratus (previously warmed above the CST) the demixing was determined by allowing the mixture to cool to the transition temperature at a rate of 3–5 mK/min while stirring. Temperature was measured by platinum resistance thermometry

Source and Purity of Materials:

(1) Mallinkrodt; analytical grade; dried over anhydrous $CaCl_2$ and twice distilled in a spinning band column below 343 K.
(2) Prepared by refluxing reagent grade 99.8% D_2O/ethanediol $=2.5/1$ and removing the water by fractional distillation at reduced pressure; the deuterated glycol fraction was collected, dried again over molecular sieve, and redistilled.

Estimated Error:

Temperature: ±0.3 mK.
Pressure: ±0.01 MPa.

References:

[1] R. R. Singh and W. A. Van Hook, J. Chem. Phys. **87**, 6097 (1987).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2,3-Propanetriol; $C_3H_8O_3$; [56-81-5]

Original Measurements:

I. K. Zhuravleva, E. F. Zhuravlev, and N. A. Rudakova, Zh. Obshch. Khim. **46**, 2178–86 (1976).

Variables:

T/K$=296$–406

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1,2,3-propanetriol

		Glycerol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
23.5	296.7	—	—	92.6	0.950
24.5	297.7	0.4	0.006	—	—
30.5	303.7	—	—	92.0	0.946
44.0	317.2	—	—	91.3	0.941
50.0	323.2	1.2	0.018	—	—
57.0	330.2	—	—	90.4	0.934
63.0	336.2	—	—	88.9	0.924
70.5	343.7	2.4	0.036	—	—
91.5	364.7	5.0	0.074	—	—
94.5	367.7	—	—	84.9	0.895
108.5	381.7	—	—	80.0	0.858
117.5	390.7	13.2	0.187	—	—
117.5	390.7	25.0	0.335	—	—
125.0	398.2	—	—	70.0	0.779
128.0	401.2	35.0	0.448	—	—
131.0	404.2	28.2	0.372	—	—
131.5	404.7	45.0	0.552	—	—
132.0	405.2	—	—	65.0	0.737
133.0	406.2	50.3	0.604	—	—
133.0	406.2	56.0	0.657	56.0	0.657 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled; $n(20\ °C,D)=1.3820$, $d(20\ °C)=1132\ g\cdot L^{-1}$.
(2) Source not specified; pure grade reagent; distilled; $n(20\ °C,D)=1.4740$, $d(20\ °C)=1264\ g\cdot L^{-1}$.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz. -Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

Original Measurements:

I. K. Zhuravleva and E. F. Zhuravlev, Zh. Fiz. Khim. **49**, 778–81 (1975).

Variables:

T/K=266–289

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2-methyl-1-propanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	X_1 (compiler)
−7.0	266.2	—	—	90.0	0.916
−2.5	270.7	17.0	0.200	—	—
8.5	281.7	23.0	0.266	—	—
9.0	282.2	—	—	80.0	0.829
14.0	287.2	30.0	0.342	—	—
14.5	287.7	—	—	70.3	0.742
15.0	288.2	40.0	0.447	—	—
15.5	288.7	50.0	0.548	—	—
16.0	289.2	—	—	60.0	0.646
16.0	289.2	52.5	0.573	52.5	0.573 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled; b.p. =101.3 °C/101.33 kPa, n(20 °C,D)=1.3820, d(20 °C) =1132 g·L^{-1}.

(2) Source not specified; pure grade reagent; distilled; b.p. =106 °C/99.66 kPa, n(20 °C,D)=1.3960, d(20 °C) =801 g·L^{-1}.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, August 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 1-butanol have been reported in four publications. Mel'nikova and Zhuravlev[1] measured the mutual solubilities of the components between 275 and 291 K by the synthetic method. Sazonov and Filippov[2] studied mutual solubilities of (1) and (2) between 285 and 291 K, also using the synthetic method. Bittrich *et al.*[3] determined the upper critical solution temperature and critical solution composition. Battler and Rowley[4] reported the mutual solubility of the two components at 291.15 K.

Values obtained by the graphical interpolation or extrapolation from the data sheets are presented in Table 1. Data are ''recommended'' if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

TABLE 1. Recommended and tentative values for the mutual solubilities of nitromethane and l-butanol

	Alcohol-rich phase			Nitromethane-rich phase		
T/K	$100w_1$	x_1		$100w_2$	x_2	
278	18.8	0.219	Tentative	13.5	0.114	Tentative
283	23.4	0.271	Recommended	17.8	0.151	Recommended
288	32.1	0.365	Recommended	26.0	0.224	Recommended
290	40.5	0.453	Recommended	35.7	0.314	Tentative

The upper critical solution temperature has been reported as 290.5 K,[1] 291.14 K,[2] and 291.2 K.[3] Thus, the recommended value is: (290.9±0.3) K.

The corresponding critical solution composition has been reported as $x_{c1}=0.578$,[1] $x_{c1}=0.580$,[3] and $x_{c1}=0.587$.[2] The average value, $x_{c1}=(0.582\pm0.004)$, is therefore recommended.

The recommended UCST and critical solution composition are consistent with the values calculated from the respective relationships in the nitromethane–alcohol series, discussed at the beginning of this volume (these calculated values are: UCST=290.8 K and x_{c1} =0.587). The tentative and recommended values for the mutual solubility reported in the above tables have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.846\,74$, $a_2=0.469\,31$, $b_1=3.017\,49$, $b_2=-2.940\,53$ (mean standard error of estimate was 0.0101).

For approximation, recommended values of UCST and x_{c1} have been used. This relationship is presented in Fig. 23 together with experimental data reported in Refs. 1 and 2.

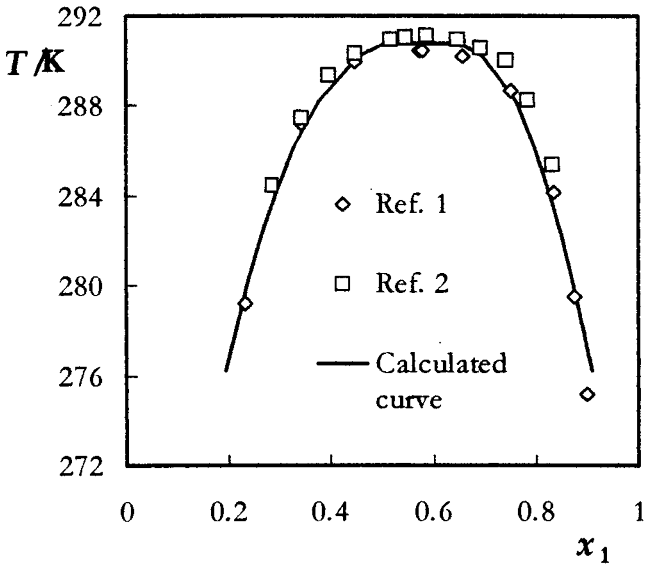

FIG. 23. Mutual solubility of nitromethane and 1-butanol.

References:

[1] I. K. Mel'nikova, Dissertation, Voronezh University, 1966; E. F. Zhuravlev and I. K. Mel'nikova, Zh. Fiz. Khim. **41**, 1580 (1967).

[2] V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222 (1975).

[3] H.-J. Bittrich, R. Eckert, and R. Kirsche, Z. Phys. Chem. (Leipzig) **268**, 457 (1987).

[4] J. R. Battler and R. L. Rowley, J. Chem. Eng. Data **35**, 334 (1990).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:

*I. K. Mel'nikova, Dissertation, Voronezh University, 1966.
E. F. Zhuravlev and I. K. Mel'nikova, Zh. Fiz. Khim. **41**, 1580–4 (1967).

Variables:

T/K = 275–291

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-butanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
2.0	275.2	—	—	87.9	0.898
6.0	279.2	20.0	0.233	—	—
6.3	279.5	—	—	85.0	0.873
11.0	284.2	—	—	80.4	0.833
14.0	287.2	30.0	0.342	—	—
15.5	288.7	—	—	71.3	0.751
16.8	290.0	40.0	0.447	—	—
17.0	290.2	—	—	61.2	0.657
17.3	290.5	52.5	0.573	—	—
17.3	290.5	53.0	0.578	53.0	0.578 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled; b.p = 101.3 °C at 101.33 kPa, n(20 °C,D) = 1.3820, d(20 °C) = 1132 g·L^{-1}.
(2) Source not specified; pure grade reagent; distilled.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol **18**, 222–5 (1975).

Variables:
T/K=284 to 291

Prepared By:
V. P. Sazonov and N. V. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-butanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
11.30	284.45	24.97	0.2878	—	—
12.25	285.40	—	—	80.08	0.8300
14.32	287.47	30.01	0.3424	—	—
15.14	288.29	—	—	74.93	0.7840
16.25	289.40	35.15	0.3969	—	—
16.77	290.02	—	—	69.98	0.7389
17.20	290.35	39.98	0.4471	—	—
17.43	290.58	—	—	64.93	0.6921
17.79	290.94	46.77	0.5162	—	—
17.83	290.98	—	—	60.01	0.6457
17.93	291.08	49.96	0.5480	—	—
17.99	291.14	53.93	0.5870	53.93	0.5870 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method of Alekseev was used. Close to the phase transition temperature, heating and cooling of the mixture were accomplished in steps at a rate of 0.02 K·h^{-1}.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled over a column of 15 theoretical plates; n(20 °C,D)=1.3819, d(20 °C)=1138.1 g·L^{-1}.
(2) Source not specified; analytical purity; distilled with glass packed fractionating column; n(20 °C,D)=1.3993, d(20 °C) =809.6 g·L^{-1}.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
H.-J. Bittrich, R. Eckert, and R. Kirsche, Z. Phys. Chem. (Leipzig) **268**, 457 (1987).

Variables:
T/K=291

Prepared By:
V. P. Sazonov

Experimental Data

The upper critical solution temperature was reported to be 18.0 °C at x_1=0.58 (291.2 K and 100 w_1=53.2, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
No further details were reported.

Source and Purity of Materials:
(1) Source not specified; purity more than 99 mole %.
(2) Source not specified; purity more than 99 mole %.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
J. R. Battler and R. L. Rowley, J. Chem. Eng. Data **35**, 334 (1990).

Variables:
T/K=291

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-butanol

t/°C (compiler)	T/K	100 w_1 (compiler)	x_1	100 w_1 (compiler)	x_1
18.00	291.15	48.0	0.53	68.0	0.72

Auxiliary Information

Method/Apparatus/Procedure:
No further details were reported.

Source and Purity of Materials:
(1) Source not specified; spectrophotometric grade; purity 99.9 mole %.
(2) Source not specified; spectrophotometric grade; purity 99.9 mole %.

Estimated Error:
Not specified.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and L. N. Salamatin, Zh. Fiz. Khim. **49**, 2609–14 (1975).

Variables:
T/K=271–297

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 3-methyl-1-butanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
−2.5	270.7	10.0	0.138	—	—
−2.0	271.2	—	—	90.0	0.929
14.5	287.7	20.0	0.265	—	—
17.5	290.7	—	—	80.0	0.852
21.0	294.2	30.0	0.383	—	—
21.5	294.7	—	—	70.0	0.771
23.0	296.2	—	—	60.0	0.684
23.5	296.7	40.0	0.491	—	—
23.5	296.7	50.0	0.591	—	—
23.5	296.7	51.0	0.601	51.0	0.601 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled; $n(20\ °C,D)=1.3820$, $d(20\ °C)=1132\ g\cdot L^{-1}$.
(2) Source not specified; pure grade reagent; distilled; $n(20\ °C,D)=1.4085$, $d(20\ °C)=812.9\ g\cdot L^{-1}$.

Estimated Error:
Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
G. T. Hefter, Murdoch University, Perth, Australia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, July, 1999.

Critical Evaluation

Quantitative solubility data for the nitromethane+1-pentanol have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system nitromethane+1-pentanol

Reference	T/K	Solubility	Method
Mel'nikova and Zhuravlev[1]	282–298	Mutual	Synthetic
Anisimov and Shakhparonov[2]	286–301	Mutual	Not stated
Khabibullaev *et al.*[3]	288–301	Mutual	Not stated
Zhuravleva *et al.*[4]	276–299	Mutual	Synthetic
Labowski and Hornowski[5]	281–301	Mutual	Synthetic

All the original data are compiled in the data sheets immediately following this Critical Evaluation. Among the available data, the values of Anisimov and Shakhparonov[2] were excluded from further consideration as only a graphical presentation was given. Some individual points in the alcohol-rich phase, in otherwise satisfactory studies, are in marked disagreement with other studies and have been rejected: Ref. 3 (298 K) and Ref. 5 (288 K). All other reported data are included in the tables below.

Values obtained by the Evaluators by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). ''Best'' values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits.

It will be noted from the tables following that there are serious disagreements among the solubility data reported by independent workers for the system nitromethane+1-pentanol. This is reflected in the large σ_n values. No one study or any of the averaged values can be singled out for recommendation and clearly this system requires a careful and thorough reinvestigation over the entire temperature range. The values given in Tables 2 and 3 should be regarded as tentative only until further independent studies can be made.

TABLE 2. The solubility nitromethane (1) in 1-pentanol (2)

	Solubility, 100 w_1		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_1	x_1
278	15.2*(Ref. 1), 13.2*(Ref. 4)	14±1	0.19
283	17.5 (Ref. 1), 15.1 (Ref. 4)	16±1	0.22
288	21.3*(Ref. 1), 19.*(Ref. 4)	20±1	0.27
293	27.4*(Ref. 1), 23.4*(Ref. 3), 24.3*(Ref. 4), 22.3*(Ref. 5)	24±2	0.31
298	35.4*(Ref. 4), 34.7*(Ref. 5)	35.1±0.4	0.439

TABLE 3. The solubility of 1-pentanol (2) in nitromethane (1)

	Solubility, 100 w_2		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_2	x_2
283	13.0*(Ref. 1), 11.1 (Ref. 4)	12±1	0.086
288	15.8*(Ref. 1), 13.6*(Ref. 3), 13.8*(Ref. 4)	14±1	0.10
293	21.2*(Ref. 1), 18.6*(Ref. 3), 17.6*(Ref. 4)	19±2	0.14
298	26.5*(Ref. 1), 30.0*(Ref. 4)	28±2	0.21

The upper critical solution temperature has been reported as 298.2 K,[1] 299.2 K,[4] 300.9 K,[2] 300.93 K,[3] and 301.0 K.[5] The UCSTs reported in both Refs. 1 and 4 are rather lower than the remaining data and are therefore rejected. The values of Refs. 2, 3, and 5 are in excellent agreement and their averaged value UCST=(300.9±0.1) K is recommended.

The corresponding critical solution composition has been reported as $x_{c1}=0.614$,[2] $x_{c1}=0.615$,[5] $x_{c1}=0.616$,[3] $x_{c1}=0.624$,[4] and $x_{c1}=0.629$.[1] Again the values of Refs. 1 and 4 are rejected and the average of the remaining three references, $x_{c1}=0.615\pm0.001$, (100 $w_1=52.5$) is recommended. It is noteworthy that the critical solution composition (even including the rejected data) does not appear to suffer from the uncertainties seen in the solubilities at other temperatures (Tables 2 and 3).

The recommended UCST and critical solution composition are consistent with the values calculated from the respective relationships in the nitromethane–alcohol series, discussed at the beginning of this volume (the calculated values are: UCST=300.9 K and $x_{c1}=0.615$).

The ''best'' values for the mutual solubility reported in the above tables have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.851\,56$, $a_2=0.126\,63$, $b_1=0.722\,13$, $b_2=-1.059\,05$ (mean standard error of estimate was 0.0106).

For approximation, recommended values of UCST and x_{c1} have been used. This relationship is presented in Fig. 24 together with experimental data reported in Refs. 1, 3, 4, and 5.

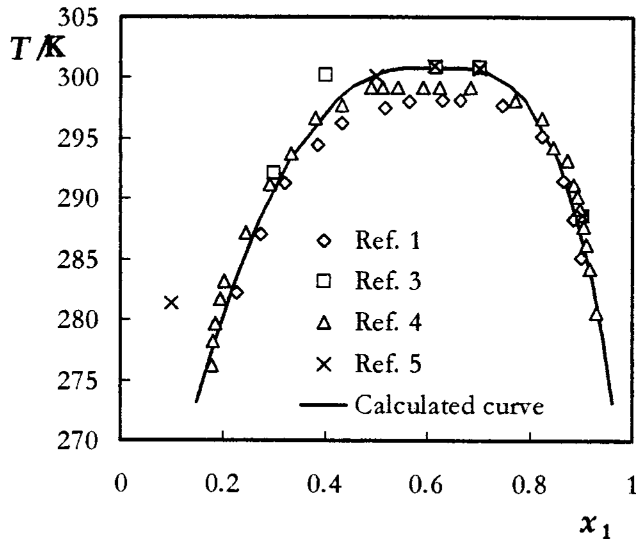

FIG. 24. Mutual solubility of nitromethane and 1-pentanol.

References:

[1] I. K. Mel'nikova and E. F. Zhuravlev, Zh. Fiz. Khim. **39**, 664 (1965); I. K. Mel'nikova, Dissertation, Voronezh University, 1966.

[2] M. A. Anisimov and M. I. Shakhparonov, Zh. Fiz. Khim. **40**, 2330 (1996).

[3] P. K. Khabibullaev, S. S. Aliev, M. I. Shakhparonov, and L. E. Kvasova, *Fizika I Fiziko-Khimiya Zhidkostei* (Nauka, Moskva, 1972), p. 94.

[4] I. K. Zhuravleva, E. F. Zhuravlev, and N. G. Lomakina, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 499 (1975); Deposited Doc., VINITI 1566 (1974).

[5] M. Labowski and T. Hornowski, J. Acoust. Soc. Am. **81**, 1421 (1987).

Components:
(1) Nitromethane CH_3NO_2; [75-52-5]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Original Measurements:
I. K. Mel'nikova and E. F. Zhuravlev, Zh. Fiz. Khim. **39**, 664–71 (1965).
*I. K. Mel'nikova, Dissertation, Voronezh University, 1966.

Variables:
T/K=282–298

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-pentanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	$100w_1$	x_1 (compiler)	$100w_1$	x_1 (compiler)
9.0	282.2	17.0	0.228	—	—
12.0	285.2	—	—	85.9	0.898
13.9	287.1	20.7	0.274	—	—
15.1	288.3	—	—	84.0	0.883
18.1	291.3	24.8	0.323	—	—
18.3	291.5	—	—	81.3	0.863
21.3	294.5	30.3	0.386	—	—
22.0	295.2	—	—	76.0	0.821
23.0	296.2	34.6	0.433	—	—
24.3	297.5	42.6	0.517	—	—
24.5	297.7	—	—	67.0	0.746
24.8	298.0	47.2	0.564	—	—
25.0	298.2		—	57.7	0.663
25.0	298.2	54.0	0.629	54.0	0.629 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled.
(2) Source not specified; pure grade reagent; distilled.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Original Measurements:
M. A. Anisimov and M. I. Shakhparonov, Zh. Fiz. Khim. **40**, 2330–2 (1966).

Variables:
T/K=301

Prepared By:
V. P. Sazonov

Experimental Data

The upper critical solution temperature was reported to be 27.7 °C at 100 $w_1=52.4$ ($x_1=0.614$; 300.9 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
No further 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:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Original Measurements:
P. K. Khabibullaev, S. S. Aliev, M. I. Shakhparonov, and L. E. Kvasova, *Fizika i Fiziko-Khimiy Zhidkostej* (Nauka, Moskva, 1966), pp. 94–120.

Variables:
T/K = 289–301

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-pentanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
15.50	288.65	—	—	0.900	86.2
19.00	292.15	0.300	22.9	—	—
27.11	300.26	0.400	31.6	—	—
27.70	300.85	—	—	0.700	61.8
27.78	300.93	0.616	52.6	0.616	52.6 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
No further 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: ±0.01 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and N. G. Lomakina, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 499 (1975). *Deposited Doc., VINITI 1566 (1974).

Variables:
T/K = 276–299

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-pentanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
3.0	276.2	13.0	0.178	—	—
5.0	278.2	13.2	0.180	—	—
6.5	279.7	13.6	0.185	—	—
7.5	280.7	—	—	90.0	0.929
8.5	281.7	14.4	0.195	—	—
10.0	283.2	15.1	0.204	—	—
11.0	284.2	—	—	88.4	0.917
13.0	286.2	—	—	87.3	0.908
14.0	287.2	18.4	0.246	—	—
14.5	287.7	—	—	86.7	0.904
16.0	289.2	—	—	85.7	0.896
17.0	290.2	—	—	85.1	0.892
18.0	291.2	22.3	0.293	84.1	0.884
20.0	293.2	—	—	82.4	0.871
20.5	293.7	25.7	0.333	—	—
21.0	294.2	—	—	79.0	0.844
23.5	296.7	30.0	0.382	76.0	0.821
24.5	297.7	34.7	0.434	—	—
25.0	298.2	—	—	70.0	0.771
26.0	299.2	40.0	0.491	60.0	0.684
26.0	299.2	42.1	0.512	—	—
26.0	299.2	45.0	0.542	—	—
26.0	299.2	50.0	0.591	—	—
26.0	299.2	53.5	0.624	53.5	0.624 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; purity not specified; distilled; b.p. = 101.3 °C, $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1132.0\ g \cdot L^{-1}$.
(2) Source not specified; purity not specified; distilled; b.p. = 138 °C, $n(20\ °C,D) = 1.4100$, $d(20\ °C) = 814.4\ g \cdot L^{-1}$.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Original Measurements:
M. Labowski and T. Hornowski, J. Acoust. Soc. Am. **81**, 1421 (1987).

Variables:
T/K=281–301

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-pentanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	x_1	100 w_1 (compiler)	x_1	100 w_1 (compiler)
8.2	281.4	0.100	7.1	—	—
15.5	288.7	—	—	0.900	86.2
26.9	300.1	0.500	40.9	—	—
27.6	300.8	—	—	0.700	61.8
27.8	301.0	0.615	52.5	0.615	52.5 (UCST)

Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; CP reagent; distilled; $n(29.2\ °C,D)=1.3776$, $d(29.2\ °C)=1124.1\ g\cdot L^{-1}$.
(2) Source not specified; CP reagent; distilled; $n(29.2\ °C,D)=1.4104$, $d(29.2\ °C)=814.8\ g\cdot L^{-1}$.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cyclohexanol; $C_6H_{12}O$; [108-93-0]

Original Measurements:
L. F. Erofeeva and N. V. Yunnikova, Sb. Nauch. Tr., Kuzbas. Polytekh. Inst. **26**, 1–6 (1971).

Variables:
T/K=275–291

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and cyclohexanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C (compiler)	T/K (compiler)	100 w_1 (compiler)	x_1 (compiler)	100 w_1 (compiler)	x_1 (compiler)
1.8	275.0	—	—	87.5	0.920
2.3	275.5	30.8	0.422	—	—
4.2	277.4	33.3	0.450	—	—
6.3	279.5	35.9	0.479	85.0	0.903
8.6	281.8	39.2	0.514	—	—
8.7	281.9	—	—	84.0	0.896
12.0	285.2	45.2	0.575	—	—
13.8	287.0	49.2	0.614	—	—
14.9	288.1	51.4	0.634	—	—
15.4	288.6	—	—	75.9	0.838
15.6	288.8	54.6	0.664	—	—
16.5	289.7	59.2	0.704	—	—
16.8	290.0	—	—	71.3	0.803
16.9	290.1	62.9	0.736	—	—
16.9	290.1	65.7	0.759	—	—
17.5	290.7	66.0	0.761	66.0	0.761 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled.
(2) Source not specified; pure grade reagent; dried and distilled under vacuum.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	V. P. Sazonov, Technical University, Samara, Russia. A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, July, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 1-hexanol have been reported in three publications. Sazonov and Filippov[1] and Zhuravleva *et al.*[2,3] determined the mutual solubility of the components between 293 and 309 K and between 282 and 309 K, respectively, using the synthetic method. Values obtained by the graphical interpolation or extrapolation from the data sheets are presented in Table 1. Data are ''recommended'' if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

TABLE 1. Recommended and tentative values for the mutual solubilities of nitromethane and 1-hexanol

	Alcohol-rich phase			Nitromethane-rich phase		
T/K	100 w_1	x_1		100 w_2	x_2	
283	11.2	0.174	Tentative	9.1	0.056	Tentative
288	13.3	0.204	Tentative	9.8	0.061	Tentative
293	16.0	0.242	Tentative	11.9	0.075	Tentative
298	20.1	0.296	Recommended	15.2	0.097	Recommended
303	25.6	0.365	Recommended	20.1	0.131	Recommended
308	46	0.59	Recommended	34	0.24	Recommended

The upper critical solution temperature has been reported as 308.2 K,[3] 308.7 K,[1] and 308.8 K.[2] The averaged value, 308.5 ±0.3 K, is recommended.

The corresponding critical solution composition has been reported as $x_{c1}=0.649^{2,3}$ and $x_{c1}=0.6740.^3$ The average, $x_{c1}=(0.657 \pm 0.010)$, is also recommended.

The recommended and tentative values for the mutual solubility reported in Table 1 have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.921\,15$, $a_2=-0.095\,61$, $b_1=3.173\,04$, $b_2=-3.321\,41$ (mean standard error of estimate was 0.0158).

For approximation, recommended values of UCST and x_{c1} have been used. This relationship is presented in Fig. 25 together with experimental data reported in Refs. 1, 2 and 3.

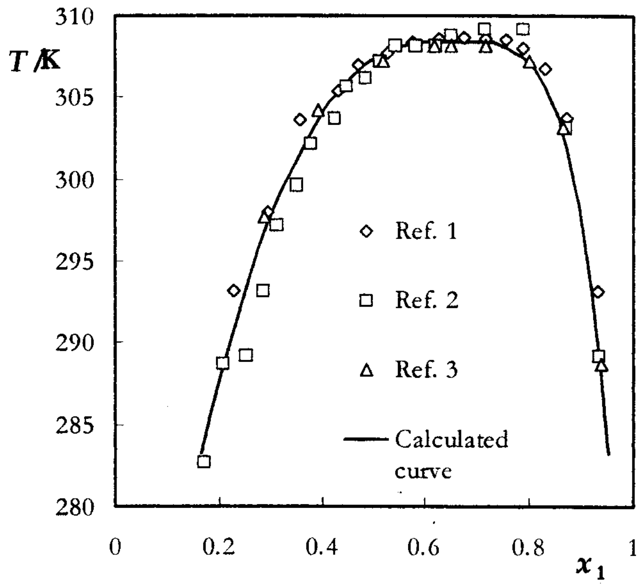

FIG. 25. Mutual solubility of nitromethane and 1-hexanol.

References:

[1] V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222 (1975).
[2] I. K. Zhuravleva, E. F. Zhuravlev, and N. A. Rudakova, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 333 (1975); Deposited Doc., VINITI 1587 (1974).
[3] I. K. Zhuravleva, E. F. Zhuravlev, and N. A. Rudakova, Zh. Obshch. Khim. **46**, 2178 (1976).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

Original Measurements:
V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222–5 (1975).

Variables:
T/K = 293–309

Prepared By:
N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-hexanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compilers)	100 w_1	x_1 (compilers)	100 w_1	x_1 (compilers)
20.00	293.15	15.00	0.2280	88.90	0.9306
24.83	297.98	20.03	0.2954	—	—
30.40	303.55	24.91	0.3570	—	—
30.63	303.78	—	—	79.99	0.8700
32.25	305.40	31.14	0.4308	—	—
33.60	306.75	—	—	74.38	0.8294
33.87	307.02	34.63	0.4700	—	—
34.54	307.69	40.00	0.5274	—	—
34.84	307.99	—	—	69.02	0.7886
35.25	308.40	44.84	0.5764	—	—
35.36	308.51	—	—	64.78	0.7548
35.45	308.60	49.99	0.6259	—	—
35.48	308.63	—	—	60.25	0.7173
35.50	308.65	52.43	0.6485	—	—
35.50	308.65	55.26	0.6740	55.26	0.6740 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method of Alekseev was used. Close to the phase transition temperature heating and cooling of mixture were accomplished in steps at a rate of 0.02 $K \cdot h^{-1}$.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled through a column of 15 theoretical plates; $n(20\ °C,D) = 1.3819$, $d(20\ °C) = 1138.1\ g \cdot L^{-1}$.
(2) Source not specified; pure grade reagent; distilled through a glass-packed fractionating column; $n(20\ °C,D) = 1.4182$, $d(20\ °C) = 819.7\ g \cdot L^{-1}$.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and N. A. Rudakova, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 333 (1975). *Deposited Doc., VINITI 1587 (1974).

Variables:
T/K = 283–309

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-hexanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
9.5	282.7	11.0	0.171	—	—
15.5	288.7	13.5	0.207	—	—
16.0	289.2	—	—	89.3	0.933
20.0	293.2	16.6	0.250	—	—
24.0	297.2	19.3	0.286	—	—
26.5	299.7	21.3	0.312	—	—
29.0	302.2	24.3	0.350	—	—
30.0	303.2	—	—	79.9	0.869
30.5	303.7	26.6	0.378	—	—
32.5	305.7	30.5	0.424	—	—
33.0	306.2	32.5	0.446	—	—
34.0	307.2	36.0	0.485	—	—
35.0	308.2	38.5	0.512	—	—
35.0	308.2	41.4	0.542	—	—
35.0	308.2	45.2	0.580	—	—
35.0	308.2	49.4	0.620	—	—
36.0	309.2	—	—	69.1	0.789
36.0	309.2	—	—	59.9	0.714
35.6	308.8	52.5	0.649	52.5	0.649 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; purity not specified; distilled; b.p. = 101.3 °C, $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1132.0\ g \cdot L^{-1}$.
(2) Source not specified; purity not specified; distilled; b.p. = 157.2 °C, $n(20°C,D) = 1.4190$, $d(20\ °C) = 818.6\ g \cdot L^{-1}$.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and N. A. Rudakova, Zh. Obshch. Khim. **46**, 2178–86 (1976).

Variables:
T/K=289–308

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-hexanol

		Alcohol-rich phase		Nitromethane-rich phase	
$t/°C$	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
15.5	288.7	—	—	90.0	0.938
24.5	297.7	19.4	0.287	—	—
30.0	303.2	—	—	79.3	0.865
31.0	304.2	27.7	0.391	—	—
34.0	307.2	39.1	0.518	70.3	0.799
35.0	308.2	49.0	0.617	60.1	0.716
35.0	308.2	52.5	0.649	52.5	0.649 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; purity not specified; distilled; $n(20\ °C,D)=1.3820$, $d(20°C)=1132.0\ g \cdot L^{-1}$.
(2) Source not specified; purity not specified; distilled; $n(20\ °C,D)=1.4135$, $d(20\ °C)=818.6\ g \cdot L^{-1}$.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, August 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 1-heptanol have been reported in two publications. Quinn and Smyth[1] determined the solubility of nitromethane in 1-heptanol at 294 K. Sazonov[2] measured the mutual solubilities of components (1) and (2) between 288 and 317 K by the synthetic method. The UCST=316.1 K and critical solution composition $x_{c1}=0.686$ (Ref. 2) may be treated as tentative. They are consistent with the values calculated from the respective relationships in the nitromethane–alcohol series, discussed at the beginning of this volume (the calculated values are: UCST=315.8 K and $x_{c1}=0.685$). The experimental data reported in Refs. 1 and 2 have been approximated (with the same weighing factor) by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.923\ 71$, $a_2=-0.068\ 18$, $b_1=6.954\ 67$, $b_2=-6.272\ 50$ (mean standard error of estimate was 0.0198).

For approximation x_{c1} and UCST from Ref. 2 have been used. In the opinion of the evaluators, the smoothed mutual solubilities, calculated by this equation, may be treated as tentative. The results of calculations for the selected temperatures are presented in Table I. This relationship together with experimental points[1,2] are also presented in Fig. 26.

TABLE 1. Mutual solubility of nitromethane and 1-heptanol

	Alcohol-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
288.2	0.1703	9.73	0.9833	96.86
293.2	0.2016	11.71	0.9650	93.55
298.2	0.2399	14.22	0.9456	90.12
303.2	0.2882	17.54	0.9235	86.39
308.2	0.3534	22.30	0.8958	81.87
313.2	0.4574	30.70	0.8493	74.76
314.2	0.4909	33.62	0.8324	72.29
315.2	0.5380	37.96	0.8055	68.51
315.7	0.5757	41.61	0.7808	65.18

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]

Original Measurements:
R. G. Quinn and C. P. Smyth, J. Chem. Phys. **41**, 2037–41 (1964).

Variables:
T/K=294

Prepared By:
V. P. Sazonov

Experimental Data

The solubility of nitromethane in 1-heptanol at 21.1 °C (294.3 K, compiler) was reported to be 100 $w_1=11.1$. The corresponding mole fraction, x_1, calculated by the compiler is 0.192.

Auxiliary Information

Method/Apparatus/Procedure:
The dielectric dispersion of a mixture of (1) and (2) having an upper critical solution temperature was measured over a range of 40 °C to the temperature of phase separation. No further experimental details are given.

Source and Purity of Materials:
(1) Eastman Organic Chemical Co.; spectro-grade; n(20 °C,D) =1.3812.
(2) Eastman Organic Chemical Co.; reagent-grade; n(20 °C,D) =1.4242.

Estimated Error:
Not specified.

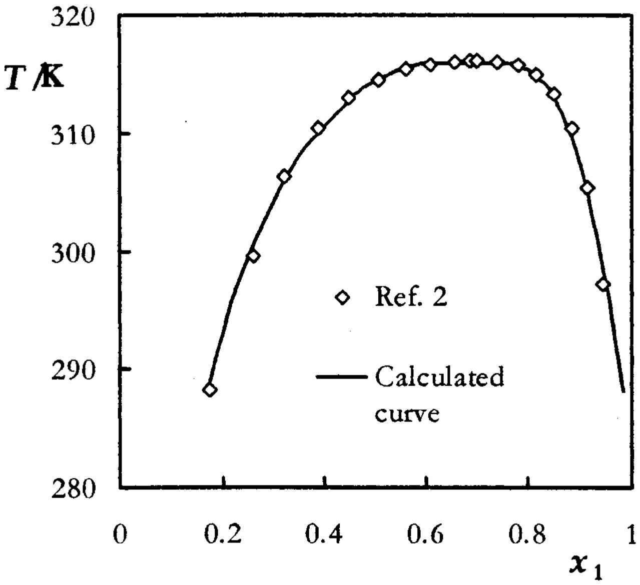

FIG. 26. Mutual solubility of nitromethane and 1-heptanol.

References:

[1] R. G. Quinn and C. P. Smyth, J. Chem. Phys. **41**, 2037 (1964).
[2] V. P. Sazonov, Zh. Obshch. Khim. **59**, 2431 (1989).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]

Original Measurements:

V. P. Sazonov, Zh. Obshch. Khim. **59**, 2431–5 (1989).

Variables:

T/K=288–316

Prepared By:

N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-heptanol

T/K	t/°C (compilers)	Alcohol-rich phase 100 w_1	Alcohol-rich phase x_1 (compiler)	Nitromethane-rich phase 100 w_1	Nitromethane-rich phase x_1 (compiler)
288.30	15.15	10.0	0.175	—	—
297.25	24.10	—	—	90.0	0.945
299.65	26.50	15.0	0.251	—	—
305.40	32.25	—	—	85.0	0.915
306.40	33.25	20.0	0.322	—	—
310.45	37.30	25.0	0.388	80.0	0.884
313.00	39.85	30.0	0.449	—	—
313.30	40.15	—	—	75.0	0.851
314.55	41.40	35.0	0.506	—	—
315.00	41.85	—	—	70.0	0.816
315.45	42.30	40.0	0.559	—	—
315.75	42.60	—	—	65.0	0.780
315.85	42.70	45.0	0.609	—	—
316.00	42.85	—	—	60.0	0.741
316.05	42.90	50.0	0.656	—	—
316.10	42.95	—	—	55.0	0.699
316.10	42.95	53.4	0.686	53.4	0.686 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The apparatus with visual indication of turbidity was described in Ref. 1. No additional details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; fractionally distilled; 99.85 mass % purity; $n(20\ °\mathrm{C,D})=1.3819$, $d(20\ °\mathrm{C})=1138.0\ \mathrm{g \cdot L^{-1}}$.
(2) Source not specified; pure grade reagent; purified by vacuum distillation; 99.7 mass % purity.

Estimated error:

Not reported.

References:

[1] V. P. Sazonov and M. F. Chernysheva, Zh. Obshch. Khim. **57**, 46 (1987).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Science, Warsaw, Poland, August 1999.

Critical Evaluation

Quantitative solubility data in the system comprising nitromethane and 1-octanol have been reported in the four publications.

Schmid *et al.*[1] determined the upper critical solution temperature by synthetic method. Zhuravieva *et al.*[2,3] carried out measurements of the mutual solubilities of (1) and (2) between 294 and 322 K by the synthetic method. Dewan and Menta[4] defined the mutual solubility of components (1) and (2) at 303 K. Apart from the work of Schmid *et al.*[1] which did not contain sufficient information to justify its inclusion, all the available data are listed in the data sheets following this Critical Evaluation.

Values obtained by the graphical interpolation or extrapolation from the data sheets are presented in Table 1. Data are ‘‘recommended’’ if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

TABLE 1. Recommended and tentative values for the mutual solubilities of nitromethane and 1-octanol

T/K	Alcohol-rich phase 100 w_1	Alcohol-rich phase x_1		Nitromethane-rich phase 100 w_2	Nitromethane-rich phase x_2	
298	11.0	0.209	Tentative	—	—	
303	13.5	0.250	Recommended	10.5	0.052	Recommended
308	16.1	0.290	Tentative	13.8	0.070	Recommended
313	21.3	0.366	Tentative	16.9	0.087	Recommended
318	29	0.47	Recommended	23.5	0.126	Recommended

The upper critical solution temperature has been reported as 319.7 K (Ref. 1) and 322.2 K.[2,3] The UCST values reported by Schmid *et al.*[1] for many other systems are significantly lower than other data and have generally been rejected. Accordingly, the value of 322.2 K reported by Zhuravleva *et al.*[2,3] is likely to be more realistic. The corresponding critical solution composition has been reported as $x_{c1}=0.706$.[2]

They were verified by the relationship of UCST in the nitromethane–alcohol series discussed at the beginning of this volume. This calculated UCST was equal to 321.9 K and may be treated as tentative. Critical solution composition has been reported in Ref. 2 as $x_{c1}=0.706$, while the value calculated on the basis of relationship in the series was equal to 0.711 and it may be also be treated as tentative. The recommended and tentative values for the mutual solubility reported in Table 1 have been approximated by the equation based on scaling law (described in the Introduction to this volume) and the following parameters have been adjusted: $a_1=0.867\,25$, $a_2=0.091\,86$, $b_1=6.543\,36$, $b_2=-6.195\,73$ (mean standard error of estimate was 0.0047). For approximation these tentative values of UCST and x_{1c}, consistent in the series have been used. This relationship is presented in Fig. 27 together with experimental data reported in Refs. 2, 3, and 4.

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	I. K. Zhuravleva, E. F. Zhuravlev, and N. A. Rudakova, Zh. Obshch, Khim. **46**, 2178–86 (1976).
Variables: T/K=294–322	**Prepared By:** V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-octanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
21.0	294.2	10.1	0.193	—	—
30.5	303.7	—	—	89.5	0.948
38.5	311.7	20.0	0.348	—	—
43.0	316.2	—	—	79.5	0.892
45.0	318.2	29.8	0.475	—	—
47.0	320.2	—	—	69.9	0.832
48.0	321.2	39.7	0.584	—	—
49.0	322.2	49.5	0.677	59.6	0.759
49.0	322.2	53.0	0.706	53.0	0.706 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; freshly distilled; $n(20\ °C,D)=1.3820$, $d(20\ °C)=1132.0\ g\cdot L^{-1}$.
(2) Source not specified; pure grade reagent; freshly distilled; $n(20\ °C,D)=1.4295$, $d(20\ °C)=824.6\ g\cdot L^{-1}$.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

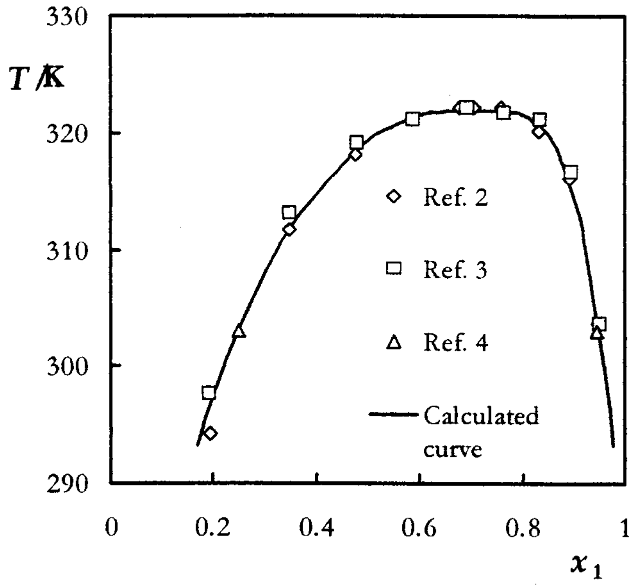

FIG. 27. Mutual solubility of nitromethane and 1-octanol.

References:

[1] H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).
[2] I. K. Zhuravleva, E. F. Zhuravlev, and N. A. Rudakova, Zh. Obshch. Khim. **46**, 2178 (1976).
[3] I. K. Zhuravleva, E. F. Zhuravlev, and N. G. Lomakina, Zh. Fiz. Khim. **51**, 1700 (1977).
[4] R. K. Dewan and S. K. Menta, J. Chem. Thermodyn. **18**, 101 (1986).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Original Measurements:
I. K. Zhuravlev, E. F. Zhuravlev, and N. G. Lomakina, Zh. Fiz. Khim. **51**, 1700–7 (1977).

Variables:
T/K = 298–322

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-octanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
24.5	297.7	10.0	0.192	—	—
30.5	303.7	—	—	90.0	0.950
40.0	313.2	20.0	0.348	—	—
43.5	316.7	—	—	80.0	0.895
46.0	319.2	30.0	0.478	—	—
48.0	321.2	40.0	0.587	70.0	0.833
48.5	321.7	—	—	60.0	0.762
49.0	322.2	51.0	0.690	—	—
49.0	322.2	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; purity not specified; $n(20\ °\mathrm{C,D}) = 1.3820$, $d(20\ °\mathrm{C}) = 1133.0^a\ \mathrm{g \cdot L^{-1}}$.
(2) Source not specified; purity not specified; $n(20\ °\mathrm{C,D}) = 1.4395$, $d(20\ °\mathrm{C}) = 824\ \mathrm{g \cdot L^{-1}}$.
[a] Recorded as 1330.0 in original. Value corrected by compiler.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Original Measurements:
R. K. Dewan and S. K. Menta, J. Chem. Thermodyn. **18**, 101–6 (1986).

Variables:
T/K = 303

Prepared By:
V. P. Sazonov

Experimental Data

The mole fraction of nitromethane in the (2)-rich phase at 303.15 K (30.00 °C, compiler) was reported to be $x_1 = 0.2500$, corresponding to 100 $w_1 = 13.51$ (compiler).

The mole fraction of nitromethane in the (1)-rich phase at 303.15 K (30.00 °C, compiler) was reported to be $x_1 = 0.9450$, corresponding to 100 $w_1 = 88.95$ (compiler).

Auxiliary Information

Method/Apparatus/Procedure:
Excess volumes of 1-octanol and nitro-methane were measured using a continuous-dilution dilatometer. No further details were reported.

Source and Purity of Materials:
(1) J. T. Baker Chemicals; fractionally distilled; $d(30\ °\mathrm{C}) = 1123.5\ \mathrm{g \cdot L^{-1}}$.
(2) Fluka AG Buchs; fractionally distilled; $d(30\ °\mathrm{C}) = 818.7\ \mathrm{g \cdot L^{-1}}$.

Estimated Error:
Not reported.

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1-Nonanol; $C_9H_{20}O$; [143-08-8]	V. P. Sazonov, Technical University, Samara, Russia, G. T. Hefter, Murdoch University, Perth, Australia. A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation:

Solubilities in the system comprising nitromethane and 1-nonanol have been reported in three publications. Schmid *et al.*[1] determined the upper critical solution temperature by the synthetic method. Both Sazonov and Chernysheva,[2] between 295 and 328 K, and Zhuravleva and Zhukova,[3] between 298 and 328 K, measured the mutual solubilities of (1) and (2) using the synthetic method.

The upper critical solution temperature has been reported as 325 K,[1] 327.7 K,[3] and 327.96 K.[2] The UCST of Schmid *et al.*[1] is, as in many systems investigated by these authors, considerably lower than other reported values and is therefore rejected. The remaining data[2,3] are in reasonable agreement and thus their average value: $T_c=(327.8\pm0.2)$ K is recommended. The corresponding critical solution composition has been reported in as $x_{c1}=0.743$ (Sazonov and Chernysheva[2]) and $x_{c1}=0.727$.[3]

All experimental values reported in Sazonov and Chernysheva[2] and Zhuravleva dn Zhukova[3] (treated with the same weighing factor) have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.868\,65$, $a_2=-0.056\,41$, $b_1=8.210\,78$, $b_2=-7.570\,06$ (mean standard error of estimate was 0.0244).

For approximation x_{c1} and UCST from Sazonov and Chernysheva[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 1. This relationship together with experimental points reported in Sazonov and Chernysheva[2] adn Zhuravleva and Zhukova[3] are also presented in Fig. 28.

TABLE 1. Mutual solubility of nitromethane and 1-nonanol

	1-Nonanol-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
293.2	0.1799	8.49	0.9926	98.26
298.2	0.2069	9.94	0.9803	95.47
303.2	0.2389	11.72	0.9682	92.79
308.2	0.2772	13.96	0.9557	90.12
313.2	0.3245	16.89	0.9422	87.34
318.2	0.3855	20.98	0.9260	84.11
323.2	0.4730	27.53	0.9013	79.44
324.2	0.4969	29.48	0.8936	78.03
325.2	0.5250	31.87	0.8837	76.27
326.2	0.5600	35.01	0.8697	73.85
326.7	0.5821	37.09	0.8597	72.17
327.2	0.6102	39.85	0.8455	69.84
327.7	0.6536	44.39	0.8191	65.71

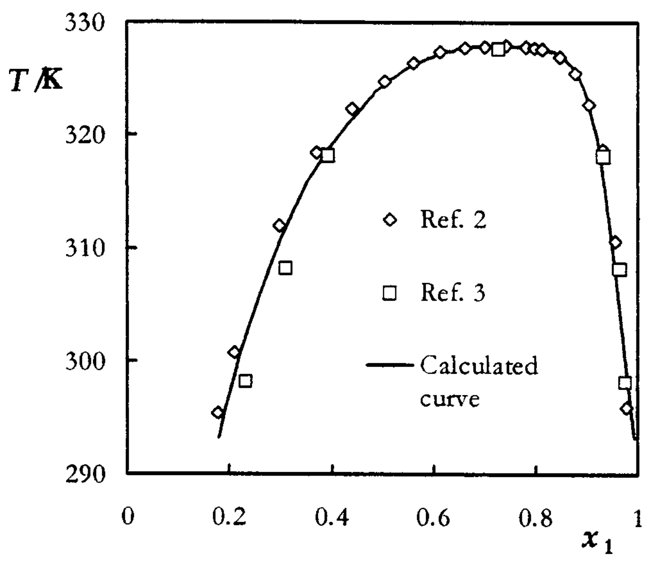

FIG. 28. Mutual solubility of nitromethane and 1-nonanol.

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).
[2] V. P. Sazonov and M. F. Chernysheva, Zh. Obshch. Khim. **46**, 997 (1976).
[3] I. K. Zhuravleva and L. M. Zhukova, Zh. Obshch. Khim. **47**, 1942 (1977).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Nonanol; $C_9H_{20}O$; [143-08-8]

Original Measurements:

V. P. Sazonov and M. F. Chernysheva, Zh. Obshch. Khim. **46**, 997–1000 (1976).

Variables:

T/K=295–328

Prepared By:

N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-nonanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compilers)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
22.32	295.47	8.4	0.178	—	—
22.86	296.01	—	—	95.0	0.978
27.69	300.84	10.0	0.208	—	—
37.56	310.71	—	—	90.0	0.955
38.90	312.05	15.2	0.298	—	—
45.24	318.39	20.0	0.371	—	—
45.61	318.76	—	—	85.1	0.931
49.19	322.34	25.0	0.441	—	—
49.61	322.76	—	—	80.2	0.905
51.67	324.82	30.1	0.504	—	—
52.44	325.59	—	—	75.0	0.876
53.34	326.49	35.0	0.560	—	—
53.86	327.01	—	—	70.0	0.847
54.22	327.37	40.0	0.612	—	—
54.52	327.67		—	65.0	0.814
54.63	327.78	45.1	0.660	62.5	0.798
54.76	327.91	49.8	0.701	60.2	0.781
54.81	327.96	55.0	0.743	55.0	0.743 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled through a glass packed fractionating column.
(2) Source not specified; pure grade reagent; fractionally distilled at about 267 Pa; purity 99.5 mass %.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Nonanol; $C_9H_{20}O$; [143-08-8]

Original Measurements:

I. K. Zhuravleva and L. M. Zhukova, Zh. Obshch. Khim. **47**, 1942–5 (1977).

Variables:

T/K=298–328

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-nonanol

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
25.0	298.2	11.2	0.230	94.5	0.976
35.0	308.2	16.0	0.310	91.6	0.963
45.0	318.2	21.4	0.392	84.9	0.930
54.5	327.7	53.0	0.727	53.0	0.727 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; purified; b.p.=101.3 °C, n(20 °C,D) =1.3820.
(2) Source not specified; purified; b.p.=213 °C, n(20 °C,D) =1.4310.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Quantitative solubility data for the nitromethane+1-decanol have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Francis[1]	273–299	Mutual	Synthetic
Schmid *et al.*[2]	330	UCST	Synthetic
Zhuravleva *et al.*[3]	300–331	Mutual	Synthetic
Sazonov[4]	298–333	Mutual	Synthetic

Apart from the publication by Schmid *et al.*,[2] which did not contain sufficient information to justify its inclusion, all the original data are given in the data sheets following this Critical Evaluation.

From the relationship of UCST in the nitromethane–alcohol series, discussed at the beginning of this volume in the Introduction material ''Relations of Solubility Data in Binary Systems Containing Nitromethane,'' the nitromethane–1-decanol UCST calculated value is 332.5 K. The most realistic experimental UCST=332.9 K was measured by Sazonov[4]—one of the evaluators of this system. The other experimentally measured UCST are: 329.5,[1] 330.2,[2] and 330.7.[3]

The value of critical solution composition calculated from similar relationship of the nitromethane–alcohol series is 0.758, while the experimentally measured values are 0.753 (Ref. 1) and 0.760.[4] These calculated values of UCST and critical solution composition, consistent in the series, may be treated as tentative. The solubility data reported in Refs. 1, 2, and 3 have been rejected. Therefore only experimental data reported in Ref. 4 could have been approximated by the equation based on scaling law and discussed at the beginning of this volume. (For the consistent description all used values were those reported in Ref. 4.) The following parameters have been adjusted: $a_1=0.849\,95$, $a_2=0.032\,69$, $b_1=8.370\,36$, $b_2=-7.847\,48$ (mean standard error of estimate was 0.0195).

In the opinion of the evaluators, 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 all experimental points[1,3,4] is also presented in Fig. 29.

TABLE 2. Mutual solubility of nitromethane and 1-decanol

	1-Decanol-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
298.2	0.1746	7.54	0.9925	98.07
303.2	0.2053	9.06	0.9816	95.37
308.2	0.2409	10.91	0.9709	92.79
313.2	0.2831	13.22	0.9600	90.24
318.2	0.3342	16.22	0.9482	87.59
323.2	0.3992	20.40	0.9339	84.48
328.2	0.4909	27.11	0.9114	79.86
329.2	0.5158	29.12	0.9042	78.44
330.2	0.5448	31.58	0.8948	76.63
331.2	0.5810	34.84	0.8813	74.11
332.2	0.6331	39.95	0.8571	69.82
332.7	0.6802	45.07	0.8285	65.07

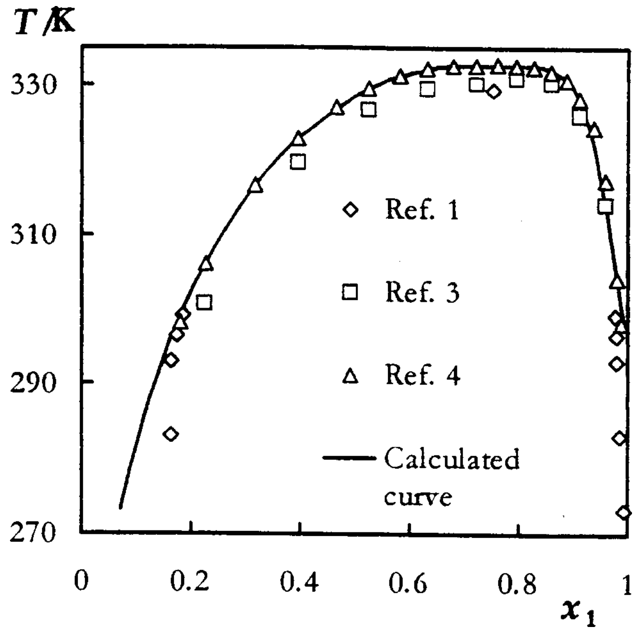

FIG. 29. Mutual solubility of nitromethane and 1-decanol.

References:
[1] A. W. Francis, J. Phys. Chem. **60**, 20 (1956).
[2] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).
[3] I. K. Zhuravleva, E. F. Zhuravlev, and N. G. Lomakina, Zh. Fiz. Khim. **51**, 1700 (1977).
[4] V. P. Sazonov, Zh. Obshch. Khim. **59**, 2431 (1989).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

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

Variables:
T/K=273–330

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-decanol

		Alcohol-rich phase		Nitromethane-rich phase	
°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
0.0	273.2	—	—	98.0	0.992
10.0	283.2	7.0	0.164	96.0	0.984
20.0	293.2	7.0	0.164	95.0	0.980
23.4	296.6	7.5	0.174	94.5	0.978
26.0	299.2	8.0	0.184	94.0	0.976
56.3	329.5	54.0	0.753	54.0	0.753 (UCST)

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) Eastman Kodak Co.; distilled through a 30 cm column; b.p.=101.25 °C, m.p.=−30.5 °C, $n(20\ °\mathrm{C,D})=1.3820$, $d(25\ °\mathrm{C})=1129.8\ \mathrm{g\cdot L^{-1}}$.
(2) Source not specified; purified by crystallization; m.p. =6.8 °C, $n(20\ °\mathrm{C,D})=1.4372$, $d(20\ °\mathrm{C})=831.8\ \mathrm{g\cdot L^{-1}}$.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and N. G. Lomakina, Zh. Fiz. Khim. **51**, 1700–7 (1977).

Variables:
T/K=301–331

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-decanol

		Hydrocarbon-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
27.5	300.7	10.0	0.224	—	—
41.0	314.2	—	—	90.0	0.959
46.5	319.7	20.0	0.393	—	—
53.0	326.2	—	—	80.0	0.912
53.5	326.7	30.0	0.526	—	—
56.5	329.7	40.0	0.633	—	—
57.0	330.2	50.0	0.722	70.0	0.858
58.0	331.2	—	—	60.0	0.796
57.5	330.7	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; purity not specified; $n(20\ °\mathrm{C,D})=1.3820$, $d(20\ °\mathrm{C})=1133.0\ \mathrm{g\cdot L^{-1}}$.[a]
(2) Source not specified; purity not specified; $n(20\ °\mathrm{C,D})=1.4370$, $d(20\ °\mathrm{C})=830\ \mathrm{g\cdot L^{-1}}$.
[a] Recorded as 1330.0 in original. Value corrected by compiler.

Estimated Error:
Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

Original Measurements:
V. P. Sazonov, Zh. Obshch. Khim. **59**, 2431–5 (1989).

Variables:
T/K=298–333

Prepared By:
N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-decanol

		Hydrocarbon-rich phase		Nitromethane-rich phase	
T/K	t/°C (compilers)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
298.2	25.0	7.7	0.178	96.5	0.986
304.2	31.0	—	—	95.0	0.980
306.2	33.0	10.1	0.226	—	—
316.6	43.4	15.0	0.314	—	—
317.5	44.3	—	—	90.0	0.959
322.9	49.7	20.0	0.393	—	—
324.5	51.3	—	—	85.0	0.936
327.1	53.9	25.0	0.464	—	—
328.4	55.2	—	—	79.9	0.912
329.7	56.5	30.0	0.526	—	—
330.7	57.5	—	—	75.0	0.886
331.3	58.1	35.0	0.583	—	—
331.9	58.7	—	—	70.0	0.858
332.3	59.1	40.0	0.633	—	—
332.6	59.4	—	—	65.0	0.828
332.7	59.5	45.0	0.680	—	—
332.8	59.6	50.0	0.722	60.0	0.796
332.9	59.7	55.0	0.760	55.0	0.760 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The apparatus with visual indication of turbidity was described in Sazonov and Chernysheva.[1] No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; fractionally distilled; 99.85 mass % purity; $n(20\,°C, D)=1.3819$, $d(20\,°C)=1138.0\ g \cdot L^{-1}$.
(2) Source not specified; pure grade reagent; purified by vacuum distillation; 99.3 mass % purity.

Estimated Error:

Not reported.

References:

[1] V. P. Sazonov and M. F. Chernysheva, Zh. Obshch. Khim. **57**, 46 (1987).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Undecanol; $C_{11}H_{24}O$; [112-42-5]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland September, 1999

Critical Evaluation

Solubilities in the system comprising nitromethane and 1-undecanol have been reported in three publications. Schmid *et al.*[1] determined the upper critical solution temperature by the synthetic method and the data have been reported in the table titled ''Nitromethane–1-Alcohols.'' Zhuravleva and Mukhametshin[2] carrier out measurements of the mutual solubilities of (1) and (2) between 292 and 336 K also by the synthetic method and these data were presented in graphical form only. Zhuravleva[3] studied the mutual solubility of (1) and (2) at 293.2, 303.2, 313.2, and 318.2 K by the synthetic method. These data were presented in graphical form only and are not presented as a compilation table. Monotectic equilibrium is realized at 250.0 K.[2,3]

From the relationship of UCST in the nitromethane–alcohol series, discussed at the beginning of this volume, the calculated UCST value for this system is 337.2 K. The experimental UCST=336.2 K measured by Zhuravleva *et al.*[2,3] does not differ very much and is treated as tentative, while the result of Schmid *et al.*,[1] reported as 334.7 K, have to be rejected. The value of critical solution composition, calculated from similar relationship of the nitromethane–alcohol series is 0.779, while the experimentally measured value is 0.784.[2] Only experimental data reported in Zhuravleva and Mukhametshin[2] could have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.772\,61$,$a_2=0.233\,05$,$b_1=8.388\,37$,$b_2=-7.955\,68$ (mean standard error of estimate was 0.0242).

For approximation x_{c1} and UCST from Zhuravleva and Mukhametshin[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 1. This relationship, together with experimental points reported in Zhuravleva and Mukhametshin,[2] are also presented in Fig. 30.

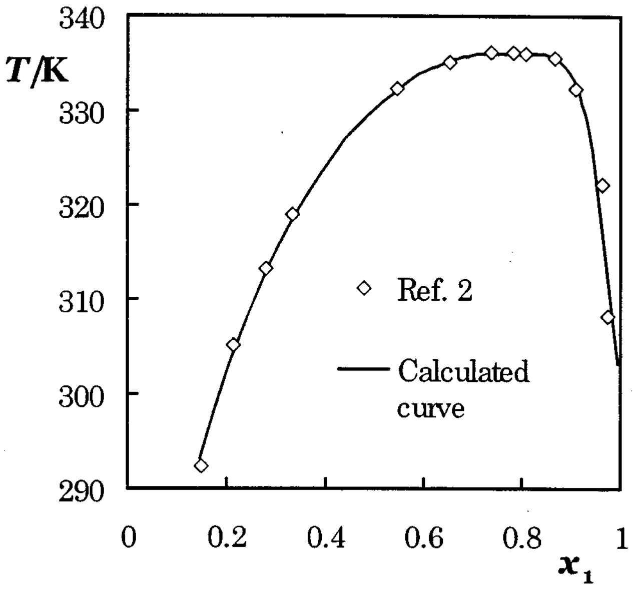

FIG. 30. Mutual solubility of nitromethane and 1-undecanol.

TABLE 1. Mutual solubility of nitromethane and 1-undecanol

	1-Undecanol-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
293.2	0.1459	5.71	—	—
298.2	0.1739	6.94	—	—
303.2	0.2053	8.38	0.9933	98.14
308.2	0.2410	10.11	0.9824	95.20
313.2	0.2819	12.21	0.9717	92.41
318.2	0.3299	14.85	0.9608	89.68
323.2	0.3877	18.32	0.9491	86.85
328.2	0.4616	23.30	0.9344	83.45
333.2	0.5713	32.07	0.9078	77.71
334.2	0.6043	35.10	0.8972	75.56
335.2	0.6483	39.50	0.8799	72.19
335.7	0.6805	43.00	0.8640	69.24

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).

[2] I. K. Zhuravleva and N. P. Mukhametshin, Zh. Obshch. Khim. **49**, 1217 (1979).

[3] I. K. Zhuravleva, Zh. Obshch. Khim. **54**, 982 (1984).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1-Undecanol; $C_{11}H_{24}O$; [112-42-5]	I. K. Zhuravleva and N. P. Mukhametshin, Zh. Obshch. Khim. **49**, 1217–22 (1979).
Variables: T/K=292–336	**Prepared By:** V. P. Sazonov

Experimental Data

The mutual solubility of nitromethane and 1-undecanol in mass percent over the specified temperature range were presented in graphical form in the original publication. The numerical data in the table below were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and 1-undecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
19.1	292.3	5.8	0.148	—	—
32.0	305.2	8.8	0.214	—	—
35.0	308.2	—	—	93.5	0.976
40.0	313.2	12.1	0.280	—	—
45.7	318.9	15.0	0.332	—	—
49.0	322.2	—	—	90.0	0.962
59.1	332.3	30.0	547	80.0	0.919
61.9	335.1	40.0	0.653	—	—
62.4	335.6	—	—	70.0	0.868
62.9	336.1	—	—	60.0	0.809
63.0	336.2	50.0	0.738	—	—
63.0	336.2	56.3	0.784	56.3	0.784 (UCST)

Monotectic equilibrium is realized at 11.8 °C (285.0 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled; b.p. $=101.3$ °C, $n(20\ °C, D)=1.3820$, $d(20\ °C)=1132\ g\cdot L^{-1}$.

(2) Source not specified; pure grade reagent; distilled; b.p. $=144$ °C/2.67 kPa, m.p$=15.1$ °C, $n(20\ °C, D)=1.4392$, $d(20\ °C)=833.0\ g\cdot L^{-1}$.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Quantitative solubility data for the system nitromethane+1-dodecanol have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system nitromethane+1-dodecanol

Reference	T/K	Solubility	Method
Francis[1]	289–336	Mutual	Synthetic
Markuzin and Nikanorova[2]	301 and 313	Mutual	Titration
Schmid *et al.*[3]	339	UCST	Synthetic
Zhuravleva *et al.*[4]	295–340	Mutual	Synthetic
Sazonov and Filippov[5]	291–341	Mutual	Synthetic

Apart from the publication of Schmid *et al.*,[3] which did not contain sufficient information to justify its inclusion, all the original data are given in the data sheets following this Critical Evaluation.

The following individual points in the alcohol-rich phase, in otherwise satisfactory studies, are in marked disagreement with other studies and have been rejected: 295 K (Ref. 1) and 322 K.[5] All other data are included in Tables 2 and 3 below.

In the tables that follow, values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). ''Best'' values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these ''best'' values do not have statistical significance and should be regarded only as a convenient representation of the spread of the values and not as error limits. The letter (R) indicates ''recommended'' data. Data are ''recommended'' if two or more apparently reliable studies are in reasonable (±5 % relative) agreement. All other data are regarded as tentative only.

TABLE 2. Tentative values for the solubility of nitromethane (1) in 1-dodecanol (2)

	Solubility, 100 w_1		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_1	x_1
293	4.5*(Ref. 5)	4.5	0.13
298	5.5*(Ref. 5)	5.5	0.15
303	7.3*(Ref. 1), 7.9*(Ref. 2), 6.9*(Ref. 5)	7.4±0.4	0.20
308	10.2*(Ref. 2), 9.8*(Ref. 4), 8.4*(Ref. 5)	9.5±0.8	0.24
313	12.8*(Ref. 2), 13.3*(Ref. 4), 10.2*(Ref. 5)	12±1	0.29
318	14.3*(Ref. 4), 12.3*(Ref. 5)	13±1	0.31
323	17.5*(Ref. 4), 15.0*(Ref. 5)	16±1	0.37
328	21.2*(Ref. 4), 18.4*(Ref. 5)	20±1	0.43
333	26.5*(Ref. 4), 22.5*(Ref. 5)	25±2	0.50
338	38.6*(Ref. 4), 29.5*(Ref. 5)	34±4	0.61

TABLE 3. Tentative and recommended (R) values for the solubility of 1-dodecanol (2) in nitromethane (1)

	Solubility, 100 w_1		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_2	x_2
293	2.6*(Ref. 1)	2.6	0.0087
298	3.5*(Ref. 1), 2.5*(Ref. 4)	3.0±0.5	0.010
303	3.1*(Ref. 2), 3.5*(Ref. 4)	3.3±0.2	0.011
308	4.2*(Ref. 2), 4.4*(Ref. 4), 3.4*(Ref. 5)	4.0±0.4	0.014
313	5.4*(Ref. 2), 5.3*(Ref. 4), 4.7*(Ref. 5)	5.1±0.4	0.017
318	6.9*(Ref. 4), 6.3*(Ref. 5)	6.3±0.3 (R)	0.022
323	8.8*(Ref. 4), 8.5*(Ref. 5)	8.7±0.2 (R)	0.030
328	10.1*(Ref. 4), 9.9*(Ref. 5)	10.0±0.1 (R)	0.0351
333	15.0*(Ref. 4), 14.8*(Ref. 5)	14.9±0.1 (R)	0.0542
338	23.0*(Ref. 4), 21.4*(Ref. 5)	22.2±0.8 (R)	0.0855

It will be noted from Table 2 that the agreement is only fair among the solubility data reported for the alcohol-rich phase by independent workers. This is reflected in the large σ_n values. On the other hand in the nitromethane-rich phase (Table 3), even though the solubilities are lower, the agreement is much better and a number of values have been recommended.

The upper critical solution temperature has been reported as 336.2 K,[1] 339 K,[3] 340.1 K,[4] and 341.33 K.[5] In well characterized systems, the UCST values reported by both Francis[1] and Schmid *et al.*[3] are generally lower than those reported in other studies. Accordingly, their data for the present system are rejected.

From the relationships of UCST and critical solution composition in the nitromethane–alcohol series, discussed at the beginning of this volume, the calculated values are 341.5 K and 0.799, respectively. The most realistic experimental UCST=341.3 K was measured by Sazonov and Filippov[5] (one of them is the evaluator of this system).

Critical solution composition, reported as $x_1=0.775$,[1] $x_1=0.794$,[5] and $x_1=0.808$,[4] are close to the value estimated in the series. This calculated values consistent in the series and experimental data[5] are recommended and they have been used for approximation of model parameters. The ''best'' values for the mutual solubility reported in the above tables have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.693\,82$, $a_2=0.351\,14$, $b_1=4.381\,92$, $b_2=-4.889\,36$ (mean standard error of estimate was 0.0061).

This relationship is presented in Fig. 31 together with experimental data reported in Markuzin and Nikanorova,[2] Zhuravleva *et al.*,[4] and Sazonov and Filippov.[5]

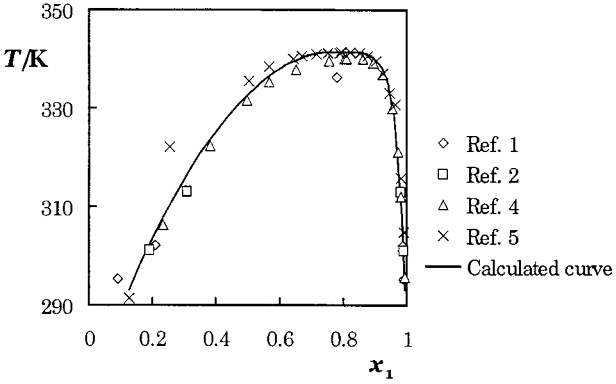

FIG. 31. Mutual solubility of nitromethane and 1-dodecanol.

References:

[1] A. W. Francis, J. Phys. Chem. **60**, 20 (1956).

[2] N. P. Markuzin and L. A. Nikanorova, Zh. Obshch. Khim. **32**, 3469 (1962).

[3] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).

[4] I. K. Zhuravleva, E. F. Zhuravlev, and R. S. Islamova, Zh. Fiz. Khim. **48**, 1863 (1974); Deposited Doc., VINITI 873 (1974).

[5] V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222 (1975).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

Original Measurements:

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

Variables:

T/K = 289–336

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-dodecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
16.0	289.2	—	—	98.0	0.993
22.0	295.2	3.0	0.09	97.0	0.990
28.0	301.2	7.0	0.19	96.0	0.987
29.0	302.2	8.0	0.21	96.0	0.987
63.0	336.2	53.0	0.78	53.0	0.78 (UCST)

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) Eastman Kodak Co.; distilled through a 30 cm column; b.p. = 101.25 °C, m.p. = −30.5 °C, n(20 °C, D) = 1.3820, d(25 °C) = 1129.8 g·L^{-1}.

(2) Source not specified; purified by crystallization; m.p. = 22.7 °C, n(24 °C, D) = 1.4410, d(24 °C) = 832 g·L^{-1}.

Estimated Error:

Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

Original Measurements:
N. P. Markuzin and L. A. Nikanorova, Zh. Obshch. Khim. **32**, 3469–73 (1962).

Variables:
T/K=301 and 313

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-dodecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
28.0	301.2	7.0	0.19	97.3	0.991
40.0	313.2	12.8	0.310	94.6	0.982

Auxiliary Information

Method/Apparatus/Procedure:
The titration method was used. The solutions were mixed by stirring. The mixture was weighed before and after the test to find the amount of added substance.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled through a column of 20 theoretical plates; $n(20\ °C,D)=1.3820$, $d(20\ °C)=1137.9\ g\cdot L^{-1}$.
(2) Source not specified; purified by vacuum distillation; m.p. $=22.2$ °C.

Estimated Error:
Temperature; control to ±0.05 K.
Solubility: 1% (relative error).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and R. S. Islamova, Zh. Fiz. Khim. **48**, 1863 (1974).
*Deposited Doc., VINITI 873 (1974).

Variables:
T/K=296–340

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-dodecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
22.4	295.6	—	—	98.0	0.993
33.0	306.2	9.0	0.232	—	—
39.0	312.2	—	—	94.8	0.982
48.0	321.2	—	—	92.0	0.972
49.2	322.4	17.0	0.383	—	—
57.8	330.0	—	—	87.3	0.955
58.4	331.6	24.5	0.498	—	—
62.0	335.2	30.0	0.567	—	—
63.7	336.9	—	—	79.6	0.923
64.7	337.9	38.0	0.652	—	—
66.0	339.2	—	—	73.2	0.893
66.4	339.6	50.2	0.755	—	—
66.8	340.0	57.4	0.804	67.0	0.861
66.8	340.0	58.0	0.808	58.0	0.808 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; freshly distilled.
(2) Source not specified; pure grade reagent; freshly distilled.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

Original Measurements:

V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222–5 (1975).

Variables:

T/K = 291–341

Prepared By:

N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-dodecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
18.20	291.35	4.50	0.1258	—	—
31.75	304.90	—	—	97.23	0.9907
42.75	315.90	—	—	94.62	0.9817
48.95	322.10	10.00	0.2533	—	—
57.60	330.75	—	—	89.61	0.9634
60.02	333.17	—	—	84.96	0.9452
62.25	335.40	25.00	0.5044	—	—
63.95	337.10	—	—	79.97	0.9242
65.25	338.40	29.99	0.5667	—	—
66.37	339.52	—	—	75.04	0.9018
66.77	339.92	36.94	0.6413	—	—
67.37	340.52	40.00	0.6705	—	—
67.52	340.67	—	—	70.05	0.8772
67.77	340.92	44.99	0.7140	—	—
67.97	341.12	49.97	0.7530	—	—
68.02	341.17	54.97	0.7884	—	—
68.03	341.18	—	—	65.01	0.8501
68.17	341.32	—	—	60.02	0.8208
68.18	341.33	55.80	0.7940	55.80	0.7940 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic (Alekseev) method was used. Close to the phase transition temperature, heating and cooling of mixtures were accomplished in steps at a rate of 0.02 K·h^{-1}.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled through a column of 15 theoretical plates; $n(20\ °C,D) = 1.3819$, $d(20\ °C) = 1138.1$ g·L^{-1}.
(2) Source not specified; pure grade reagent; fractionally distilled at about 400 Pa.

Estimated Error:

Not reported.

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) 1-Tridecanol; $C_{13}H_{28}O$; [112-70-9]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
G. T. Hefter, Murdoch University, Perth, Australia, September, 1999.

Critical Evaluation

Quantitative solubility data for the system nitromethane + 1-tridecanol have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system nitromethane + 1-tridecanol

Reference	T/K	Solubility	Method
Schmid *et al.*[1]	343	UCST	Synthetic
Zhuravleva *et al.*[2]	303–345	Mutual	Synthetic
Zhuravleva and Mukhametshin[3]	307–343	Mutual	Synthetic
Zhuravleva and Yamshanova[4]	304–345	Mutual	Synthetic

Apart from the publication Schmid *et al.*,[1] which did not contain sufficient information to justify its inclusion, all the original data are given in the data sheets following this Critical Evaluation. In the tables that follow, values obtained by the evaluators by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). ‘‘Best’’ values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these ‘‘best’’ values do not have statistical significance and should be regarded only as a convenient representation of the spread of the values and not as error limits.

The data in Tables 2 and 3 are generally in good agreement. However, as they have all been obtained by the same group they cannot be considered fully independent and thus must be classified as tentative only, pending future independent studies.

TABLE 2. Tentative values for the solubility of nitromethane (1) in 1-tridecanol (2)

	Solubility, 100 w_1		
		‘‘Best’’ values ($\pm\sigma_n$)	
T/K	Reported values	100 w_1	x_1
308	8.8* (Ref. 2), 5.5* (Ref. 3), 7.4* (Ref. 4)	7.2±1.2	0.20
313	10.3 (Ref. 2), 6.8* (Ref. 3), 8.8* (Ref. 4)	8.6±1.3	0.24
318	12.4 (Ref. 2), 8.8* (Ref. 3), 11.7* (Ref. 4)	11.0±1.5	0.287
323	14.6 (Ref. 2), 11.0* (Ref. 3), 14.5* (Ref. 4)	13.4±1.6	0.337
328	17.4 (Ref. 2), 14.4* (Ref. 3), 17.3* (Ref. 4)	16.4±1.3	0.392
333	20.5* (Ref. 2), 19.8* (Ref. 3), 20.3* (Ref. 4)	20.2±0.3	0.454
338	26.7* (Ref. 2), 25.9* (Ref. 3), 26.5* (Ref. 4)	26.4±0.3	0.541
340	30.7* (Ref. 2), 30.5* (Ref. 3), 29.1* (Ref. 4)	30.1±0.7	0.586

TABLE 3. Tentative values for the solubility of 1-tridecanol (2) in nitromethane (1)

	Solubility, 100 w_2		
		‘‘Best’’ values ($\pm\sigma_n$)	
T/K	Reported values	100 w_2	x_2
308	2.7* (Ref. 2)	2.7	0.0084
313	3.5 (Ref. 2), 5.4* (Ref. 3)	4.5±1	0.014
318	4.9 (Ref. 2), 6.5* (Ref. 3)	5.7±0.8	0.018
323	6.6 (Ref. 2), 7.7* (Ref. 3), 6.4* (Ref. 4)	6.9±0.5	0.022
328	6.6 (Ref. 2), 7.7* (Ref. 3), 6.4* (Ref. 4)	8.3±0.5	0.027
333	8.4 (Ref. 2), 8.9* (Ref. 3), 7.6* (Ref. 4)	12.0±0.2	0.0399
338	11.8* (Ref. 2), 12.0* (Ref. 3), 12.2* (Ref. 4)	16.7±0.7	0.0576
340	19.0* (Ref. 2), 21.0* (Ref. 3), 17.6* (Ref. 4)	19.2±1.2	0.0675

The upper critical solution temperature has been reported as 342.7 K,[3] 343.2 K,[1] 344.5 K,[4] and 344.7 K.[2] As the UCST values of Schmid *et al.*[1] in well characterized systems are generally lower than other reports it is possible that all of these values are somewhat low. From the relationship of UCST in the nitromethane–alcohol series, discussed at the beginning of this volume, the nitromethane–1-tridecanol UCST calculated value is 345.5 K.

The corresponding critical solution composition has been reported as $x_{c1}=0.796$,[4] $x_{c1}=0.807$,[2] and $x_{c1}=0.812$,[3] while the value calculated on the basis of similar relationship in the series was equal 0.818 has a small uncertainty but, in view of the comments above, it seems best to regard this value as tentative only at this stage. These calculated UCST and critical solution composition values, consistent in the series, are recommended and they have been used for approximation of model parameters. The ''best'' values for the mutual solubility reported in the above tables have been approximated by the equation based on scaling law (described in the Introduction to this volume) and the following parameters have been adjusted: $a_1=0.624\,09$, $a_2=0.619\,47$, $b_1=5.334\,51$, and $b_2=-5.782\,92$ (mean standard error of estimate was 0.0037). This relationship is presented in Fig. 32 together with experimental data reported in Zhuravleva *et al.*[2–4] Monotectic equilibrium[2,3] has been reported to occur at 301.2 K.

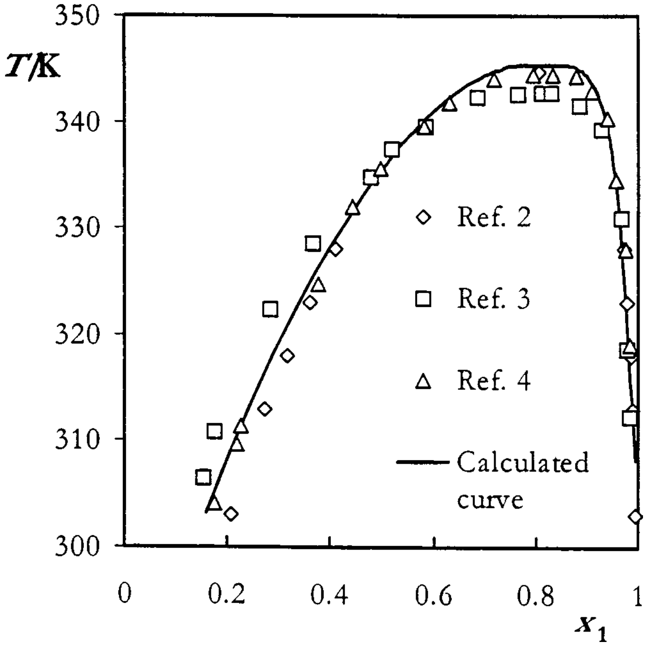

FIG. 32. Mutual solubility of nitromethane and 1-tridecanol.

References:

[1]H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).
[2]I. K. Zhuravleva, E. F. Zhuravlev, V. B. Mukhametshina, and Z. Z. Khisametdinova, Zh. Obshch. Khim. **47**, 1686 (1977).
[3]I. K. Zhuravleva and N. P. Mukhametshin, Zh. Obshch. Khim. **49**, 1217 (1979).
[4]I. K. Zhuravleva and N. M. Yamshanova, Termicheskij analiz i phazovye ravnovesiya, Perm' 109, 1985.

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1-Tridecanol; $C_{13}H_{28}O$; [112-70-9]	I. K. Zhuravleva, E. F. Zhuravlev, V. B. Mukhametshina, and Z. Z. Khisametdinova, Zh. Obshch. Khim. **47**, 1686–90 (1977).
Variables: T/K=303–345	**Prepared By:** V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and 1-tridecanol in mass percent over the specified temperature range were presented in graphical form in the original publication. The numeric data, in the table below, were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and 1-tridecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1 (compiler)	x_1 (compiler)	100 w_1 (compiler)	x_1 (compiler)
30	303	7.4	0.208	98.0	0.994
40	313	10.3	0.274	96.5	0.989
45	318	12.4	0.317	95.1	0.985
50	323	14.6	0.360	93.4	0.979
55	328	17.4	0.409	91.6	0.973
71.5	344.7	56.0	0.807	56.0	0.807 (UCST)

Monotectic equilibrium is realized at 28.0 °C (301.2 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled; b.p.=101.3 °C, n(20 °C,D)=1.3820, d(20 °C)=1132 g·L^{-1}.
(2) Source not specified; pure grade reagent; distilled; b.p.=117.3 °C/67 Pa, m.p=30.5 °C, d(34 °C)=822.3 g·L^{-1}.

Estimated Error:

Not reported.

References:

[1]V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
1-Tridecanol; $C_{13}H_{28}O$; [112-70-9]

Original Measurements:

I. K. Zhuravleva and N. P. Mukhametshin, Zh. Obshch. Khim. **49**, 1217–22 (1979).

Variables:

T/K=307–343

Prepared By:

V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and 1-tridecanol in mass percent over the specified temperature range were presented in graphical form in the original publication. The numeric data, in the table below, were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and 1-tridecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
33.3	306.5	5.2	0.153	—	—
37.7	310.9	6.1	0.176	—	—
39.1	312.3	—	—	94.6	0.983
45.4	318.6	—	—	93.3	0.979
49.1	322.3	10.8	0.284	—	—
55.4	328.6	15.0	0.367	—	—
57.8	331.0	—	—	90.0	0.967
61.6	334.8	21.9	0.479	—	—
64.2	337.4	24.8	0.520	—	—
66.1	339.3	—	—	80.0	0.929
66.3	339.5	30.0	0.585	—	—
68.3	341.5	—	—	70.0	0.884
69.1	342.3	40.0	0.686	—	—
69.4	342.6	50.0	0.766	—	—
69.5	342.7	—	—	60.0	0.831
69.5	342.7	56.8	0.812	56.8	0.812 (UCST)

Monotectic equilibrium is realized at 28.0 °C (301.2 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled; b.p.=101.3 °C, n(20 °C,D)=1.3820, d(20 °C)=1132 g·L^{-1}.
(2) Source not specified; pure grade reagent; distilled; b.p. =117.3 °C/67 Pa, m.p=30.5 °C, n(40 °C,D)=1.4373, d(34 °C)=822.3 g·L^{-1}.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Tridecanol; $C_{13}H_{28}O$; [112-70-9]

Original Measurements:

I. K. Zhuravleva and N. M. Yamshanova, Termicheskij analiz i phazovye ravnovesiya, Perm,’ 1985, pp. 109–15.

Variables:

T/K=304–345

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 1-tridecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
30.9	304.1	6.1	0.175	—	—
36.4	309.6	8.0	0.219	—	—
38.2	311.4	8.2	0.226	—	—
45.8	319.0	—	—	94.8	0.984
51.6	324.8	15.6	0.376	—	—
54.8	328.0	—	—	92.4	0.975
58.8	332.0	19.6	0.443	—	—
61.3	334.5	—	—	86.9	0.956
62.4	335.6	23.3	0.498	—	—
66.4	339.6	29.8	0.581	—	—
67.1	340.3	—	—	82.8	0.940
68.6	341.8	34.4	0.631	—	—
69.6	342.8	—	—	75.4	0.909
70.9	344.1	43.9	0.719	—	—
71.1	344.3	—	—	69.2	0.880
71.2	344.4	—	—	60.5	0.833
71.3	344.5	54.4	0.796	54.4	0.796 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

Solubility temperatures of the liquid phases were determined by the synthetic method.[1] No further experimental details given.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; purified; n(20 °C,D)=1.3820, d(20 °C)=1132.0 g·L^{-1}.
(2) Source not specified; purified; n(40 °C,D)=1.4373, d(40 °C)=822.3 g·L^{-1}.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1-Pentadecanol; $C_{15}H_{32}O$; [629-76-5]	V. P. Sazonov, Technical University, Samara, Russia. A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland. G. T. Hefter, Murdoch University, Perth, Australia, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 1-pentadecanol have been reported in three publications. Schmid *et al.*[1] determined the upper critical solution temperature by synthetic method. Zhuravleva *et al.*[2,3] studied the mutual solubility of (1) and (2) between 312 and 353 K using the synthetic method.

At the UCST, the only temperature where direct comparison is possible, the two studies are in rather poor agreement: [Schmid *et al.*[1] (351.2 K) and Zhuraleva *et al.*[2,3] (352.7 K).] However, it may be noted that the UCST values of Schmid *et al.*[1] in well characterized systems are generally lower than other reports and thus the value from Zhuravleva *et al.*[2,3] is more realistic.

The results of experimental measurements[2,3] have been verified by the calculated UCST=352.8 K obtained from the relationship of UCST in the nitromethane–alcohol series and discussed at the beginning of this volume. Critical solution composition was reported in Zhuravleva *et al.*[2,3] as $x_{c1}=0.849$, while the value calculated on the basis of relationship in the series was equal 0.854. These experimental values[2,3] of UCST and critical solution composition are treated as recommended because they are consistent with the respective values calculated in the series. They have been used further for approximation of model parameters.

The experimental data reported in Zhuravleva *et al.*,[2,3] measured in the same laboratory, have been approximated (with the same weighing factor) by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.651\,86$, $a_2=0.357\,69$, $b_1=5.609\,22$, and $b_2=-6.023\,27$ (mean standard error of estimate was 0.0428). 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 all experimental points,[2,3] is also presented in Fig. 33. Monotectic equilibrium[2,3] is reported to occur at 311.7 K.

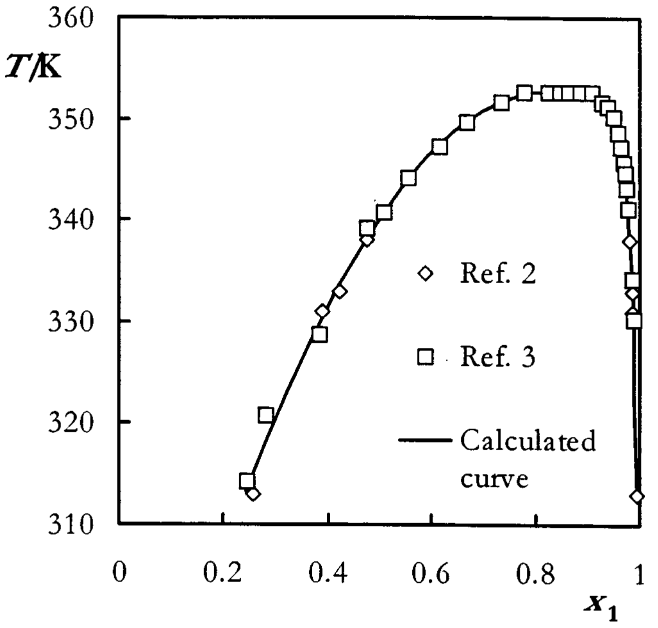

FIG. 33. Mutual solubility of nitromethane and 1-pentadecanol.

Mutual solubility of nitromethane and 1-pentadecanol

	Alcohol-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
313.2	0.2435	7.92	0.9944	97.94
318.2	0.2814	9.47	0.9923	97.17
323.2	0.3224	11.28	0.9902	96.41
328.2	0.3673	13.43	0.9879	95.61
333.2	0.4173	16.06	0.9851	94.65
338.2	0.4743	19.43	0.9813	93.35
343.2	0.5423	24.05	0.9750	91.25
348.2	0.6316	31.42	0.9612	86.89
350.2	0.6813	36.36	0.9490	83.26
351.2	0.7141	40.03	0.9382	80.22
352.2	0.7625	46.18	0.9163	74.52

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).
[2] I. K. Zhuravleva, E. F. Zhuravlev, and R. R. Faizulova, Zh. Obshch. Khim. **45**, 1929 (1975).
[3] I. K. Zhuravleva, E. F. Zhuravlev, V. B. Mukhametshina, and Z. Z. Khisametdinova, Zh. Fiz. Khim. **51**, 1003 (1977); Deposited Doc., VINITI 4286 (1976).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Pentadecanol; $C_{15}H_{32}O$; [629-76-5]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and R. R. Faizulova, Zh. Obshch. Khim. **45**, 1929–33 (1975).

Variables:
T/K = 313–353

Prepared By:
V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and 1-pentadecanol in mass percent over the specified temperature range were presented in graphical form in the original publication. The numeric data, in the table below, were provided by the authors at the request of the compiler

Mutual solubility of nitromethane and 1-pentadecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
40	313	4.0[a]	0.135	—	—
40	313	8.4	0.256	97.9	0.994
58	331	14.6	0.390	95.0	0.986
60	333	16.3	0.422	94.8	0.985
65	338	19.5	0.476	92.9	0.980
79.5	352.7	60.0	0.849	60.0	0.849 (UCST)

[a] Solid–liquid equilibrium.

Monotectic equilibrium is realized at 38.5 °C (311.7 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
Solubility temperatures of the liquid or solid phase were determined by the synthetic method.[1] No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; purified; b.p. = 101.3 °C; $n(20\ °\mathrm{C,D}) = 1.3820$, $d(20\ °\mathrm{C}) = 1132.0\ \mathrm{g \cdot L^{-1}}$.
(2) Source not specified; purified; b.p. = 174.0 °C/0.8 kPa; m.p. = 43.0 °C; $n(50\ °\mathrm{C,D}) = 1.4390$.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Pentadecanol; $C_{15}H_{32}O$; [629-76-5]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, V. B. Mukhametshina, and Z. Z. Khisametdinova, Zh. Fiz. Khim. **51**, 1003 (1977).
*Deposited Doc., VINITI 4286 (1976).

Variables:
T/K = 312–353

Prepared By:
V. P. Sazonov

Experimental Data

Solubility of nitromethane and 1-pentadecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
39.0[a]	312.2	6.5	0.206	—	—
40.0[a]	313.2	4.8	0.159	—	—
40.5[a]	313.7	3.8	0.129	—	—
41.0[a]	314.2	2.5	0.088	—	—
41.0	314.2	8.0	0.246	—	—
42.0[a]	315.2	1.0	0.036	—	—
47.5	320.7	9.5	0.282	—	—
55.5	328.7	12.5	0.384	—	—
57.0	330.2	—	—	95.5	0.988
61.0	334.2	—	—	94.6	0.985
66.0	339.2	19.5	0.475	—	—
67.5	340.7	21.7	0.509	—	—
68.0	341.2	—	—	92.5	0.979
70.0	343.2	—	—	91.5	0.976
71.0	344.2	25.0	0.555	—	—
71.5	344.7	—	—	90.5	0.973
72.5	345.7	—	—	89.5	0.970
74.0	347.2	30.0	0.616	87.5	0.963
75.5	348.7	—	—	86.0	0.958
76.6	349.7	35.0	0.668	—	—
77.0	350.2	—	—	83.5	0.950
78.0	351.2	—	—	80.5	0.939
78.5	351.7	42.5	0.734	77.5	0.928
79.5	352.7	48.5	0.779	73.0	0.910
79.5	352.7	56.0	0.826	68.0	0.888
79.5	352.7	—	—	63.0	0.864
79.5	352.7	60.0	0.849	60.0	0.849 (UCST)

[a] Solubility of the solid phase.

Monotectic equilibrium is realized at 38.5 °C (311.7 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled; b.p. = 101.3 °C/102 kPa, $n(20\ °\mathrm{C,D}) = 1.3820$, $d(20\ °\mathrm{C})$ $d(20\ °\mathrm{C}) = 1132.0\ \mathrm{g \cdot L^{-1}}$.
(2) Source not specified; pure grade reagent; distilled; b.p. = 162 °C/67 Pa, m.p. = 43.0 °C, $n(50\ °\mathrm{C,D}) = 1.4390$.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:	Evaluators:
(1) Nitromethane; CH_3NO_2; [75-52-5]	V. P. Sazonov, Technical University, Samara, Russia.
(2) 1-Hexadecanol; $C_{16}H_{34}O$; [36653-82-4]	A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland.
	G. T. Hefter, Murdoch University, Perth, Australia, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 1-hexadecanol have been reported in three publications. Schmid *et al.*[1] determined the upper critical solution temperature by the synthetic method. Zhuravleva *et al.*[2,3] measured the mutual solubilities of (1) and (2) between 318 and 357 K also using the synthetic method.

At the UCST, the only temperature where direct comparison of independently measured data is possible, the reported values are in rather poor agreement: Schmid *et al.*[1] (354.7 K) and Zhuravleva *et al.*[2,3] (356.7 K). Accordingly, in the absence of confirmatory studies, all data must be regarded as tentative. However, it may be noted that the UCST values of Schmid *et al.*[1] in well characterized systems are generally lower than other reports and thus the value from Zhuravleva *et al.*[2,3] is probably more realistic. The corresponding critical solution composition has been reported[2,3] as $x_{c1}=0.885$, $100\ w_1=66.0$. Monotectic equilibrium has been reported to occur at 316.7 K (Zhuravleva *et al.*[2,3]).

From the relationship of UCST and critical solution composition in the nitromethane–alcohol series, discussed at the beginning of this volume, the calculated values are 356.2 K and 0.871, respectively. These calculated values, consistent in the series, are recommended and they have been used further for approximation of model parameters. The experimental data reported in Zhuravleva *et al.*,[2,3] measured in the same laboratory, have been approximated (with the same weighing factor) by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.567\ 47$, $a_2=0.451\ 99$, $b_1=4.417\ 44$, and $b_2=-5.068\ 24$ (mean standard error of estimate was 0.0355). In the opinion of the evaluators, the mutual solubilities calculated by this equation may be treated as tentative.

The calculated solubilities, for the selected temperatures, are given in the following table, while the graphical representation of this relationship, together with all experimental points,[2,3] is presented in Fig. 34.

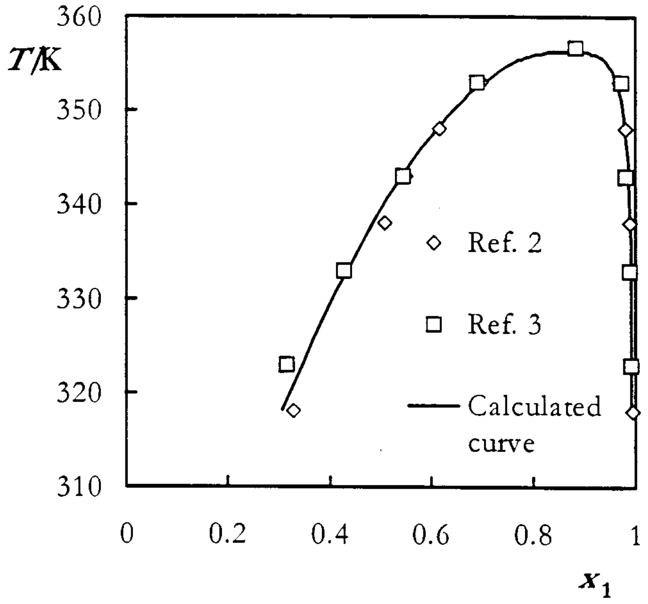

FIG. 34. Mutual solubility of nitromethane and 1-hexadecanol.

Mutual solubility of nitromethane and 1-hexadecanol

	Alcohol-rich phase		Nitromethane-rich phase	
T/K	x_1	$100\ w_1$	x_1	$100\ w_1$
318.2	0.3078	10.07	0.9929	97.25
323.2	0.3475	11.82	0.9924	97.04
328.2	0.3901	13.87	0.9917	96.79
333.2	0.4364	16.31	0.9907	96.40
338.2	0.4875	19.32	0.9890	95.75
343.2	0.5454	23.20	0.9858	94.60
348.2	0.6145	28.64	0.9794	92.30
353.2	0.7086	37.98	0.9625	86.59
354.2	0.7351	41.13	0.9549	84.20
355.2	0.7692	45.63	0.9422	80.40
356.2	0.8439	57.64	0.8961	68.46
357.2	0.8439	57.64	0.8961	68.46

References

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).
[2] I. K. Zhuravleva, E. F. Zhuravlev, and P. P. Faizulova, Zh. Obshch. Khim. **45**, 1929 (1975).
[3] I. K. Zhuravleva, E. F. Zhuravlev, I. A. Sukhova, and Z. Z. Khisametdinova, Zh. Fiz. Khim. **50**, 405 (1976).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Hexadecanol; $C_{16}H_{34}O$; [36653-82-4]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and R. R. Faizulova, Zh. Obshch. Khim. **45**, 1929–33 (1975).

Variables:
T/K = 318–357

Prepared By:
V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and 1-hexadecanol in mass percent over the specified temperature range were presented in graphical form in the original publication. The numeric data, in the following table, were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and 1-hexadecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
45	318	11.0	0.329	98.0	0.995
65	338	20.6	0.508	95.4	0.988
70	343	23.5	0.550	94.0	0.984
75	348	28.8	0.616	92.5	0.980
80	353	37.0	0.700	89.0	0.970
83.5	356.7	66.0	0.885	66.0	0.885 (UCST)

Monotectic equilibrium is realized at 43.5 °C (316.7 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
Solubility temperatures of the liquid or solid phase were determined by the synthetic method.[1] No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; distilled; b.p. = 101.3 °C, n(20 °C,D) = 1.3820, d(20 °C) = 1132 g·L^{-1}.
(2) Source not specified; pure grade reagent; distilled; b.p. = 206.0 °C/1.47 kPa, m.p = 49.5 °C, n(50 °C,D) = 1.4400, d(50 °C) = 817.6 g·L^{-1}.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Hexadecanol; $C_{16}H_{34}O$; [36653-82-4]

Original Measurements:
1. K. Zhuravleva, E. F. Zhuravlev, I. A. Sukhova, and Z. Z. Khisametdinova, Zh. Fiz. Khim. **50**, 405–10 (1976).

Variables:
T/K = 323–357

Prepared By:
V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and 1-hexadecanol in mass percent over the specified temperature range were presented in graphical form in the original publication. The numeric data, in the table below, were provided by the authors at the request of the compiler.

Mutual solubility of nitromethane and 1-hexadecanol

		Alcohol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1 (compiler)	x_1 (compiler)	100 w_1 (compiler)	x_1 (compiler)
50.0	323.2	10.4	0.316	97.2	0.993
60.0	333.2	15.9	0.429	96.0	0.990
70.0	343.2	23.1	0.544	92.9	0.981
80.0	353.2	36.0	0.691	89.8	0.972
83.5	356.7	66.0	0.885	66.0	0.885 (UCST)

Monotectic equilibrium is realized at 43.5 °C (316.7 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
Solubility temperatures of the liquid or solid phase were determined by the synthetic method.[1] No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; freshly distilled.
(2) Source not specified; pure grade reagent; freshly distilled.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) 1-Alcohols; $C_8H_{18}O$–$C_{20}H_{42}O$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:
T/K = 320–370

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+1-alcohol

1-Alcohol	t/°C	T/K (compiler)
1-Octanol; $C_8H_{18}O$; [111-87-5]	46.5	319.7
1-Nonanol; $C_9H_{20}O$; [143-08-8]	52.0	325.2
1-Decanol; $C_{10}H_{22}O$; [112-30-1]	57.0	330.2
1-Undecanol; $C_{11}H_{24}O$; [112-42-5]	61.5	334.7
1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]	66.0	339.2
1-Tridecanol; $C_{13}H_{28}O$; [112-70-9]	70.0	343.2
1-Tetradecanol; $C_{14}H_{30}O$; [112-72-1]	74.0	347.2
1-Pentadecanol; $C_{15}H_{32}O$; [629-76-5]	78.0	351.2
1-Hexadecanol; $C_{16}H_{34}O$; [124-29-8]	81.5	354.7
1-Heptadecanol; $C_{17}H_{36}O$; [1454-85-9]	85.5	358.7
1-Octadecanol; $C_{18}H_{38}O$; [112-92-5]	89.0	362.2
1-Nonadecanol; $C_{19}H_{40}O$; [1454-84-8]	93.0	366.2
1-Eicosanol; $C_{20}H_{42}O$; [629-96-9]	96.5	369.7

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 *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(2) Some alcohols obtained from the Hormel 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, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) 2-Alcohols; $C_9H_{20}O$–$C_{19}H_{40}O$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:
T/K = 316–362

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+2-alcohol

2-Alcohol	t/°C	T/K (compiler)
2-Nonanol; $C_9H_{20}O$; [628-99-9]	43.0	316.2
2-Decanol; $C_{10}H_{22}O$; [1120-06-5]	49.0	322.2
2-Undecanol; $C_{11}H_{24}O$; [1653-30-1]	54.5	327.7
2-Dodecanol; $C_{12}H_{26}O$; [10203-28-8]	59.0	332.2
2-Tridecanol; $C_{13}H_{28}O$; [1653-31-2]	63.5	336.7
2-Tetradecanol; $C_{14}H_{30}O$; [4706-81-4]	67.5	340.7
2-Pentadecanol; $C_{15}H_{32}O$; [1653-34-5]	71.5	344.7
2-Hexadecanol; $C_{16}H_{34}O$; [34019-44-8]	76.5	349.7
2-Heptadecanol; $C_{17}H_{36}O$; [16813-18-6]	80.0	353.2
2-Nonadecanol; $C_{19}H_{40}O$; [26533-36-8]	89.0	362.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described in Schmid *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(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, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Unsaturated 1-alcohols; $C_{18}H_{32}O$, $C_{18}H_{34}O$, and $C_{18}H_{36}O$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:

T/K=322–348

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+unsaturated 1-alcohol

Unsaturated 1-Alcohol	t/°C	T/K (compiler)
1-Octadecatrienol; $C_{18}H_{32}O$; [506-44-5]	48.5	321.7
1-Octadecadienol; $C_{18}H_{34}O$; [506-43-4]	62.0	335.2
1-Octadecenol; $C_{18}H_{36}O$; [143-28-2]	74.5	347.7

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 *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(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:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Unsaturated 2-Alcohols; $C_{19}H_{34}O$, $C_{19}H_{36}O$, and $C_{19}H_{38}O$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:

T/K=321–348

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+unsaturated 2-alcohol

Unsaturated 2-Alcohol	t/°C	T/K (compiler)
2-Nonadecatrienol; $C_{19}H_{34}O$	48.0	321.2
2-Nonadecadienol; $C_{19}H_{36}O$	62.0	335.2
2-Nonadecenol; $C_{19}H_{38}O$	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 in Schmid *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(2) Prepared by reduction of the respective α-chloroketones 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, J. Am. Oil Chem. Soc. **42**, 372 (1965).

9. Nitromethane+Aldehydes C16–C18

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Aldehydes; $C_{16}H_{32}O$, $C_{18}H_{34}O$, and $C_{18}H_{36}O$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **11**, 376–83 (1966).

Variables:
T/K=297–322

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+aldehyde

Aldehyde	t/°C	T/K (compiler)
cis-9-Octadecenal; $C_{18}H_{34}O$; [2423-10-1]	24.0	297.2
Hexadecanal; $C_{16}H_{32}O$; [629-80-1]	28.0	301.2
Octadecanal; $C_{18}H_{36}O$; [638-66-4]	49.0	322.2

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. As described in Schmid *et al.*,[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) Fisher Scientific Co.
(2) Not specified.

Estimated Error:
Not reported.

References:
[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

10. Nitromethane+Ethers

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Dialkyl ethers; $C_{12}H_{26}O$, $C_{14}H_{30}O$, $C_{16}H_{34}O$, $C_{18}H_{38}O$ and $C_{20}H_{42}O$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:
T/K=328–404

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+dialkyl ether

Dialkyl ether	t/°C	T/K (compiler)
1-Methoxyundecane (methyl-undecyl ether); $C_{12}H_{26}O$; [7289-53-4]	55.0	328.2
1-Ethoxydecane (ethyl-decyl ether); $C_{12}H_{26}O$; [16976-29-6]	66.5	339.7
1-Methoxytridecane (methyl-tridecyl ether); $C_{14}H_{30}O$; [7289-55-9]	75.0	348.2
1-Butoxyoctane (butyl-octyl ether); $C_{12}H_{26}O$; [53839-23-9]	77.5	350.7
1-Hexoxyhexane (dihexyl ether); $C_{12}H_{26}O$; [112-58-3]	78.0	351.2
1-Ethoxydodecane (ethyl-dodecyl ether); $C_{14}H_{30}O$; [7289-37-4]	85.0	358.2
1-Methoxypentadecane (methyl-pentadecyl ether); $C_{16}H_{34}O$	91.5	364.7
1-Butoxydecane (butyl-decyl ether); $C_{14}H_{30}O$; [111082-32-7]	93.5	366.7
1-Heptoxyheptane (diheptyl ether); $C_{14}H_{30}O$; [629-64-1]	94.5	367.7
1-Ethoxytetradecane (ethyl-tetradecyl ether); $C_{16}H_{34}O$; [4813-58-5]	100.0	373.2
1-Methoxyheptadecane (methyl-heptadecyl ether); $C_{18}H_{38}O$	105.0	378.2
1-Butoxydodecane (butyl-dodecyl ether); $C_{16}H_{34}O$; [7289-38-5]	108.0	381.2
1-Octoxyoctane (dioctyl ether); $C_{16}H_{34}O$; [629-82-3]	109.0	382.2
1-Ethoxyhexadecane (ethyl-hexadecyl ether); $C_{18}H_{38}O$; [13933-61-4]	112.5	385.7
1-Methoxynonadecane (methyl-nonadecyl ether); $C_{20}H_{42}O$	117.5	390.7
1-Butoxytetradecane (butyl-tetradecyl ether); $C_{18}H_{38}O$; [111082-34-9]	119.0	392.2
1-Hexoxydodecane (hexyl-dodecyl ether); $C_{18}H_{38}O$	120.5	393.7
1-Octoxydecane (octyl-decyl ether); $C_{18}H_{38}O$; [17088-93-6]	120.5	393.7
1-Ethoxyoctadecane (ethyl-octadecyl ether); $C_{20}H_{42}O$; [62435-06-7]	123.5	396.7
1-Butoxyhexadecane (butyl-hexadecyl ether); $C_{20}H_{42}O$; [18302-77-7]	129.0	402.2
1-Decoxydecane (didecyl ether); $C_{20}H_{42}O$; [2456-28-2]	131.0	404.2

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described in Schmid *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:
(1) Fisher Scientific Co.; certified, No. N-98; n(20 °C,D) =1.3820, d(20 °C)=1134 g·L^{-1}.
(2) Symmetrical dialkyl ethers from Lachat Chemicals Co.; other ethers prepared by reacting 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:
[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Alkyl glyceryl ethers; $C_{13}H_{28}O_3$–$C_{24}H_{50}O_3$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, Microchem. J. **11**, 306–14 (1966).

Variables:
T/K=326–369

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+alkyl glyceryl ether

Ether	t/°C	T/K (compiler)
1-(cis, cis, cis-9,12,15-Octadecatrienoxy)-2,3-propanediol; $C_{21}H_{38}O_3$	52.5	325.7
1-Decoxy-2,3-propanediol; $C_{13}H_{28}O_3$; [92219-12-0]	55.0	328.2
1-Undecoxy-2,3-propanediol; $C_{14}H_{30}O_3$; [126923-57-7]	61.5	334.7
1-(cis,cis-9,12-Octadecadienoxy)-2,3-propanediol; $C_{21}H_{40}O_3$; [70518-62-6]	62.0	335.2
1-Dodecoxy-2,3-propanediol; $C_{15}H_{32}O_3$; [1561-07-5]	66.5	339.7
1-(cis-9-Hexadecenoxy)-2,3-propanediol; $C_{19}H_{38}O_3$	68.0	341.2
1-Tridecoxy-2,3-propanediol; $C_{16}H_{34}O_3$; [126923-58-8]	70.5	343.7
1-Tetradecoxy-2,3-propanediol; $C_{17}H_{36}O_3$; [92219-13-1]	74.0	347.2
1-(cis-9-Octadecenoxy)-2,3-propanediol; $C_{21}H_{42}O_3$; [2929-07-9]	75.0	348.2
1-(trans-9-Octadecenoxy)-2,3-propanediol; $C_{21}H_{42}O_3$; [593-31-7]	77.0	350.2
1-Pentadecoxy-2,3-propanediol; $C_{18}H_{38}O_3$; [124770-96-3]	77.5	350.7
1-Hexadecoxy-2,3-propanediol; $C_{19}H_{40}O_3$; [506-03-6]	81.0	354.2
1-Heptadecoxy-2,3-propanediol; $C_{20}H_{42}O_3$; [113817-63-3]	84.0	357.2
1-Octadecoxy-2,3-propanediol; $C_{21}H_{44}O_3$; [544-62-7]	87.5	360.7
1-Nonadecoxy-2,3-propanediol; $C_{22}H_{46}O_3$; [10431-03-5]	90.5	363.7
1-Eicosoxy-2,3-propanediol; $C_{23}H_{48}O_3$; [158850-88-5]	93.0	366.2
1-Heneicosoxy-2,3-propanediol; $C_{24}H_{50}O_3$; [158789-24-3]	95.5	368.7

Auxiliary Information

Method/Apparatus/Procedure:
A microscope equipped with a heating stage[1] was employed for determining UCST values. No further experimental details are given.

Source and Purity of Materials:
(1) Fisher Scientific Co.; certified, No. N-98.
(2) Synthesized as in Baumann and Mangold.[2]

Estimated Error:
Not specified.

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

[2] W. J. Baumann and H. K. Mangold, J. Org. Chem. **29**, 3055 (1964).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2-Dialkyl glyceryl ethers; $C_{33}H_{68}O_3$–$C_{41}H_{84}O_3$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, Microchem. J. **11**, 306–14 (1966).

Variables:
T/K=396–427

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+1,2-dialkyl glyceryl ether

Ether	t/°C	T/K (compiler)
2-(Dodecyloxy)-3-(octadecyloxy)-1-propanol; $C_{33}H_{68}O_3$; [6076-36-4]	123.0	396.2
2,3-Bis(9-octadecenyloxy)-(Z,Z)-1-propanol; $C_{39}H_{76}O_3$; [6076-41-1]	126.0	399.2
3-(Octadecyloxy)-2-(tetradecyloxy)-1-propanol; $C_{35}H_{72}O_3$; [6076-37-5]	131.5	404.7
2,3-Bis(hexadecyloxy)-1-propanol; $C_{35}H_{72}O_3$; [6076-35-3]	132.0	405.2
3-(Octadecyloxy)-2-(cis-9-octadecenyloxy)-1-propanol; $C_{39}H_{78}O_3$	136.0	409.2
3-(cis-9-Octadecenyloxy)-2-(octadecyloxy)-1-propanol; $C_{39}H_{78}O_3$	136.5	409.7
3-(Octadecyloxy)-2-(trans-9-octadecenyloxy)-1-propanol; $C_{39}H_{78}O_3$	136.5	409.7
3-(Hexadecyloxy)-2-(octadecyloxy)-1-propanol; $C_{37}H_{76}O_3$; [6110-57-2]	139.5	412.7
2-(Hexadecyloxy)-3-(octadecyloxy)-1-propanol; $C_{37}H_{76}O_3$; [6110-58-3]	139.5	412.7
2,3-Bis(octadecyloxy)-1-propanol; $C_{39}H_{80}O_3$; [6076-38-6]	147.0	420.2
2-(Eicosyloxy)-3-(octadecyloxy)-1-propanol; $C_{41}H_{84}O_3$; [6068-26-4]	154.0	427.2

Auxiliary Information

Method/Apparatus/Procedure:
A microscope equipped with a heating stage[1] was employed for determining UCST values. No further experimental details are given.

Source and Purity of Materials:
(1) Fisher Scientific Co.; certified, No. N-98.
(2) Synthesized as in Baumann and Mangold.[2]

Estimated Error:
Not specified.

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

[2] W. J. Baumann and H. K. Mangold, J. Org. Chem. **29**, 3055 (1964).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2,3-Trialkyl glyceryl ethers; $C_{47}H_{96}O_3$–$C_{57}H_{116}O_3$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, Microchem. J. **11**, 306–14 (1966).

Variables:
T/K=450–469

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+1,2,3-trialkyl glyceryl ether

Ether	t/°C	T/K (compiler)
(Z,Z,Z)-1,2,3-Tris(9-octadecenyloxy)propane; $C_{57}H_{110}O_3$; [10431-15-9]	176.5	449.7
1-(Dodecyloxy)-2,3-bis(hexadecyloxy)propane; $C_{47}H_{96}O_3$; [6076-43-3]	178.0	451.2
1-(Dodecyloxy)-2-(hexadecyloxy)-3-(octadecyloxy)propane; $C_{49}H_{100}O_3$; [6068-27-5]	182.5	455.7
(Z,Z)-1,2-Bis(9-octadecenyloxy)-3-(octadecyloxy)propane; $C_{57}H_{112}O_3$; [10431-14-8]	183.0	456.2
1-(Dodecyloxy)-2,3-bis(octadecyloxy)propane; $C_{51}H_{104}O_3$; [5896-48-0]	185.5	458.7
1,2,3-Tris(hexadecyloxy)propane; $C_{51}H_{104}O_3$; [6110-59-4]	186.0	459.2
(Z)-1-(9-Octadecenyloxy)-2,3-bis(octadecyloxy)propane; $C_{57}H_{114}O_3$; [13166-06-8]	188.5	461.7
1,2,3-Tris(octadecyloxy)propane; $C_{57}H_{116}O_3$; [6076-42-2]	196.0	469.2

Auxiliary Information

Method/Apparatus/Procedure:
A microscope equipped with a heating stage[1] was employed for determining UCST values. No further experimental details are given.

Source and Purity of Materials:
(1) Fisher Scientific Co.; certified, No. N-98.
(2) Synthesized as in Baumann and Mangold.[2]

Estimated Error:
Not specified.

References:
[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).
[2] W. J. Baumann and H. K. Mangold, J. Org. Chem. **29**, 3055 (1964).

---

11. Nitromethane+Acids

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexanoic acid; $C_6H_{12}O_2$; [142-62-1]

Original Measurements:
G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685–9 (1936).

Variables:
T/K=264–270

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and hexanoic acid

		Acid-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
−8.90	264.25	32.89	0.4826	—	—
−8.05	265.10	34.00	0.4950	—	—
−7.20	265.95	—	—	77.26	0.8661
−6.20	266.95	—	—	74.98	0.8508
−5.85	267.30	—	—	74.64	0.8485
−5.25	267.90	40.71	0.5665	—	—
−4.20	268.95	44.60	0.6051	—	—
−3.85	269.30	—	—	66.25	0.7888
−3.80	269.35	47.40	0.6317	—	—
−3.65	269.50	49.21	0.6484	—	—
−3.65	269.50	49.42	0.6503	—	—
−3.55	269.60	—	—	63.17	0.7655
−3.50	269.65	53.04	0.6825	—	—
−3.45	269.70	—	—	61.05	0.7489
−3.40	269.75	56.04	0.7081	58.65	0.7297
−3.40	269.75	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, as described in Broughton,[1] was used. Liquid were pipetted into glass tubes. Temperatures at which complete miscibility occured were measured by thermometers standardized against thermometers having NPL certificates.

Source and Purity of Materials:
(1) Prepared from sodium monochloroacetate with sodium nitrite; distilled; $n(25\ °C,D)=1.3796$, $d(25\ °C)=1130.8\ g\cdot L^{-1}$.
(2) Eastman Kodak Co.; purified according to Jones and Betts[2] (fractionated in an all-glass apparatus at 1.46 kPa); m.p. $=-4.25$ °C, $n(25\ °C,D)=1.4149$.

Estimated Error:
Temperature: ± 0.05 K.

References:
[1] G. Broughton, Trans. Faraday Soc. **30**, 367 (1934).
[2] D. C. Jones and H. F. Betts, J. Chem. Soc. 1177 (1928).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octanoic acid; $C_8H_{16}O_2$; [124-07-2]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, August 1999.

Critical Evaluation

Quantitative solubility data for the system nitromethane+octanoic acid have been reported in the publications listed in Table 1.

TABLE 1. Summary of solubility data for the system nitromethane+octanoic acid

Reference	T/K	Solubility	Method
Broughton and Jones[1]	295–308	Mutual	Synthetic
Schmid *et al.*[2]	306	UCST	Synthetic
Sazonov and Filippov[3]	283–309	Mutual	Synthetic

Apart from the publication by Schmid *et al.*[2] which did not contain sufficient information to justify its inclusion, all the original data are given in the data sheets following this Critical Evaluation. In Tables 2 and 3, values obtained by the Evaluators by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). ''Best'' values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these ''best'' values do not have statistical significance and should be regarded only as a convenient representation of the spread of values and not as error limits. Where comparison is possible, the results reported by Broughton and Jones[1] and Sazonov and Filippov[3] are in excellent agreement for both phases, enabling their averages to be recommended over a range of temperatures. This suggests that the values of Sazonov and Filippov[3] at other temperatures are also likely to be reliable although in the absence of confirmatory studies they must at present be classified as tentative.

TABLE 2. Solubility nitromethane (1) in octanoic acid (2)

	Solubility, 100 w_1		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_1	x_1
283	8.8*(Ref. 3)	18.8	0.354
288	21.2*(Ref. 3)	21.2	0.389
293	24.2*(Ref. 3)	24.2	0.430
298	27.8*(Ref. 1), 28.8*(Ref. 3)	28.3±0.5	0.483
303	34.6*(Ref. 1), 35.0*(Ref. 3)	34.8±0.2	0.558
305	39.1*(Ref. 1), 39.7*(Ref. 3)	39.4±0.3	0.606

TABLE 3. Solubility of octanoic acid (2) in nitromethane (1)

	Solubility, 100 w_2		
		''Best'' values ($\pm\sigma_n$)	
T/K	Reported values	100 w_2	x_2
283	7.3*(Ref. 3)	7.3	0.032
288	9.0*(Ref. 3)	9.0	0.040
293	12.0*(Ref. 1), 11.4*(Ref. 3)	11.7±0.3	0.0531
298	15.0*(Ref. 1), 14.5*(Ref. 3)	14.8±0.3	0.0685
303	20.0*(Ref. 1), 19.2*(Ref. 3)	19.6±0.4	0.0935
305	22.8*(Ref. 1), 22.0*(Ref. 3)	22.4±0.4	0.109

The upper critical solution temperature has been reported as 305.7 K,[2] 308.00 K,[1] and 308.18 K.[3] The UCST of Schmid *et al.*[2] is much lower than the other reported values and is therefore rejected. The numeric values reported in the above tables, as the ''best,'' have been approximated by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.642\,60$, $a_2=0.223\,02$, $b_1=3.448\,69$, and $b_2=-3.645\,44$ (mean standard error of estimate was 0.0031).

An an approximation, the recommended value of UCST and $x_{c1}=0.77$ (estimated from Sazonov and Filippov[3]) have been used. These UCST and x_{c1} values are consistent with the data in Broughton and Jones[1] and Schmid *et al.*,[2] but inconsistent with the values calculated in the series (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane''). Therefore the final recommendation is to treat all values in the above tables as tentative. This relationship is presented in Fig. 35 together with experimental data reported in Broughton and Jones[1] and Sazonov and Filippov.[3]

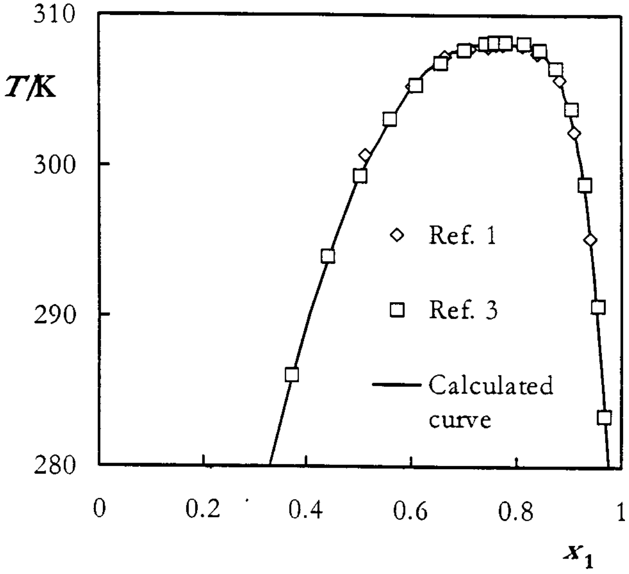

FIG. 35. Mutual solubility of nitromethane and octanoic acid.

References:
[1] G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685 (1936).
[2] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287 (1963).
[3] V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222 (1975).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octanoic acid; $C_8H_{16}O_2$; [124-07-2]

Original Measurements:
G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685–9 (1936).

Variables:
T/K = 295–308

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and octanoic acid

		Acid-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
22.00	295.15	—	—	86.85	0.9398
27.55	300.70	30.89	0.5136	—	—
29.10	302.25	—	—	81.00	0.9097
32.15	305.30	39.22	0.6039	—	—
32.55	305.70	—	—	75.96	0.8819
34.05	307.20	45.71	0.6655	—	—
34.30	307.45	—	—	69.11	0.8409
34.64	307.79	51.39	0.7141	—	—
34.72	307.87	55.68	0.7480	—	—
34.80	307.95	—	—	64.72	0.8125
34.85	308.00	57.63	0.7627	59.53	0.7766
34.85	308.00	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described in Groughton[1] was used. Liquids were pipetted into glass tubes. Temperatures at which complete miscibility occurred were measured by thermometers standardized against thermometers having NPL certificates.

Source and Purity of Materials:

(1) Prepared from sodium monochloroacetate with sodium nitrite; distilled; $n(25\ °C,D) = 1.3796$, $d(25\ °C) = 1130.8\ g \cdot L^{-1}$.
(2) Hopkins and Williams; purified according to Jones and Betts[2] (fractionated in an all-glass apparatus at 400 Pa); m.p.m.p. = 16.3 °C, $n(25\ °C,D) = 1.4263$.

Estimated Error:
Temperature: ±0.05 K.

References:

[1] G. Broughton, Trans. Faraday Soc. **30**, 367 (1934).
[2] D. C. Jones and H. F. Betts, J. Chem. Soc. 1177 (1928).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octanoic acid; $C_8H_{16}O_2$; [124-07-2]

Original Measurements:
V. P. Sazonov and V. V. Filippov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 222–5 (1975).

Variables:
T/K = 283–308

Prepared By:
N. V. Sazonov and V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and octanoic acid

		Acid-rich phase		Nitromethane-rich phase	
t/°C	T/K (compilers)	100 w_1	x_1 (compilers)	100 w_1	x_1 (compilers)
10.25	283.40	—	—	92.51	0.9669
12.90	286.05	19.99	0.3712	—	—
17.50	290.65	—	—	90.00	0.9551
20.78	293.93	25.01	0.4407	—	—
25.65	298.80	—	—	84.98	0.9304
26.12	299.27	30.00	0.5031	—	—
29.97	303.12	35.00	0.5599	—	—
30.65	303.80	—	—	80.02	0.9045
32.23	305.38	39.99	0.6116	—	—
33.28	306.43	—	—	74.99	0.8763
33.62	306.77	44.97	0.6588	—	—
34.52	307.67	—	—	70.01	0.8465
34.56	307.71	49.98	0.7025	—	—
34.92	308.07	55.02	0.7429	—	—
34.94	308.09	—	—	65.01	0.8145
35.02	308.17	—	—	59.99	0.7799
35.03	308.18	57.50	0.7617	—	—
35.03	308.18	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method of Alekseev was used. Close to the phase transition temperature heating and cooling of mixture were accomplished in steps at a rate of $0.02\ K \cdot h^{-1}$.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; distilled through a column of 15 theoretical plates; $n(20\ °C,D) = 1.3819$, $d(20\ °C) = 1138.1\ g \cdot L^{-1}$.
(2) Source not specified; pure grade reagent; fractionally distilled at about 267 Pa; $n(20\ °C,D) = 1.4279$, $d(20\ °C) = 909\ g \cdot L^{-1}$.

Estimated Error:
Not reported.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Nonanoic acid; $C_9H_{18}O_2$; [112-05-0]

Variables:
T/K=314–322

Original Measurements:
G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685–9 (1936).

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and nonanoic acid

		Acid-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
40.85	314.00	30.72	0.5348	—	—
43.80	317.95	—	—	80.29	0.9135
46.30	319.45	—	—	75.79	0.8903
46.55	319.70	40.64	0.6396	—	—
47.60	320.75	45.17	0.6811	—	—
48.05	321.20	—	—	70.04	0.8584
48.50	321.65	—	—	64.86	0.8271
48.55	321.70	52.59	0.7420	58.90	0.7879
48.55	321.70	—	—	57.90	0.7810
48.60	321.75	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, as described in ones and Betts,[1] was used. Liquids were pipetted into glass tubes. Temperatures at which complete miscibility occurred were measured by thermometers standardized against thermometers having NPL certificates.

Source and Purity of Materials:
(1) Prepared from sodium monochloroacetate with sodium nitrite; distilled; $n(25\ °\mathrm{C,D})=1.3796$, $d(25\ °\mathrm{C})=1130.8\ \mathrm{g \cdot L^{-1}}$.
(2) Not specified.

Estimated Error:
Temperature: ±0.05 K.

References:
[1] D. C. Jones and H. F. Betts, J. Chem. Soc. 1177 (1928).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Decanoic acid; $C_{10}H_{20}O_2$; [344-48-5]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
G. T. Hefter, Murdoch University, Perth, Australia, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and decanoic acid have been reported in two publications. Hoerr *et al.*[1] measured the mutual solubility of (1) and (2) between 285 and 328 K by the synthetic method. Schmid *et al.*[2] determined the upper critical solution temperature also using the synthetic method.

At the UCST, the only temperature where direct comparison is possible, the two studies are in rather poor agreement: Hoerr *et al.*[1] (328 K) and Schmid *et al.*[2] (331.7 K). The UCST equal to 330.7 1 K calculated on the basis of relationship in the series nitromethane–acids (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') may be treated as tentative UCST of this system. However, it may be noted that the UCST values of Hoerr *et al.*[1] in well characterized nitromethane–acid systems are generally lower than other reports and thus the value from Schmid *et al.*[2] is probably more realistic. Nevertheless, in the absence of confirmatory studies, all data must be regarded as tentative.

The numerical solubility values are given in the following data sheet.

References:
[1] C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603 (1946).
[2] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134 (1965).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Decanoic acid; $C_{10}H_{20}O_2$; [344-48-5]

Original Measurements:

C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603–9 (1946).

Variables:

T/K=285–328

Prepared By:

V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and decanoic acid, in mass percent, including the region of solubility of the solid phase, were presented in graphical form and in a table.

Mutual solubility of nitromethane and decanoic acid

		Acid-rich phase		Nitromethane-rich phase		
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	$g(2)/100\,g(1)$	100 w_1	x_1 (compiler)
11.9*	285.1	—	—	—	97.9[a]	0.993
16.3*	289.5	—	—	—	97.0[a]	0.989
20.0	293.2	—	—	4.6	95.6[a]	0.984
20.6*	293.8	—	—	—	95.1[a]	0.982
23.7*	296.9	—	—	—	93.2[a]	0.975
24.2*	297.4	17.8[a]	0.379	—	—	—
25.0*	298.2	14.2[a]	0.318	—	—	—
25.7*	298.9	11.8[a]	0.274	—	—	—
27.0*	300.2	7.4[a]	0.184	—	—	—
27.4*	300.6	20.7[b]	0.424	—	—	—
29.4*	302.6	2.6[a]	0.070	—	—	—
30.0	303.2	—	—	9.4	91.4[b]	0.968
31.6*	304.8	—	—	—	91.0[b]	0.966
37.6*	310.8	—	—	—	88.7[b]	0.957
40.0	313.2	—	—	14.3	87.5[b]	0.952
40.4*	313.6	—	—	—	87.2[b]	0.951
40.6*	313.8	24.8[b]	0.482	—	—	—
47.0*	320.2	29.7[b]	0.544	—	—	—
48.3*	321.5	—	—	—	81.9[b]	0.927
50.0	323.2	—	—	25.6	79.6[b]	0.917
50.6*	323.8	35.5[b]	0.608	—	—	—
53.0*	326.2	—	—	—	73.5[b]	0.887
53.7*	326.9	45.0[b]	0.698	—	—	—
54.5*	327.7	52.3[b]	0.756	—	—	—
54.6*	327.8	—	—	—	62.2[b]	0.823
54.8	328.0	—	—	—	—	— (UCST)

*These data were extracted by the compiler from the graphical information presented in the paper.
[a] Solid–liquid equilibrium.
[b] Liquid–liquid equilibrium.

Monotectic is 297.4 K.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described by Hoerr *et al.*,[1] was used. No additional details were reported.

Source and Purity of Materials:

(1) Source not specified; best grade of commercial product; twice distilled.
(2) Obtained by vacuum fractionation of Armour Neo-Fat 15 in a Stedman packed column; f.p.=31.35 °C.

Estimated Error:

Not reported.

References:

[1] C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Dodecanoic acid; $C_{12}H_{24}O_2$; [143-07-7]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and dodecanoic acid have been reported in three publications. Broughton and Jones[1] carried out measurements of the mutual solubilities of (1) and (2) between 342 and 353 K by the synthetic method. Hoerr *et al.*[2] studied solubility of (1) and (2) between 293 and 345 K by the synthetic method. Schmid *et al.*[3] determined the upper critical solution temperature by the synthetic method. The upper critical solution temperature has been reported as 345.2 K,[2] 349.7 K,[3] and 352.1 K.[1]

The experimental data, reported in Broughton and Jones[1] and Hoerr *et al.*,[2] differed significantly in the measured UCST influences on the temperatures of mutual solubility. The UCST equal to 349.6 K calculated on the basis of the relationship in the series nitromethane–acids (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') was treated as a tentative UCST for this system. Then the UCST and temperatures in each data set[1,2] have been normalized according to the formula:

$$T_{\text{new}}=(T/T_c)_{\text{exp}}\cdot T_{\text{c+sensitive}}.$$

Those transformed data have been approximated by the equation based on scaling law (described also in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1=0.515\,56$, $a_2=0.460\,80$, $b_1=2.658\,38$, and $b_2=-3.175\,72$ (mean standard error of estimate was 0.0157).

As an approximation, $x_{c1}=0.823$ and UCST$=349.6$ K have been used. The mutual solubilities calculated by this equation may be treated as tentative in the opinion of evaluators. The results of calculations for the selected temperatures are presented in the following table. This relationship, together with all experimental points,[1,2] is also presented in Fig. 36.

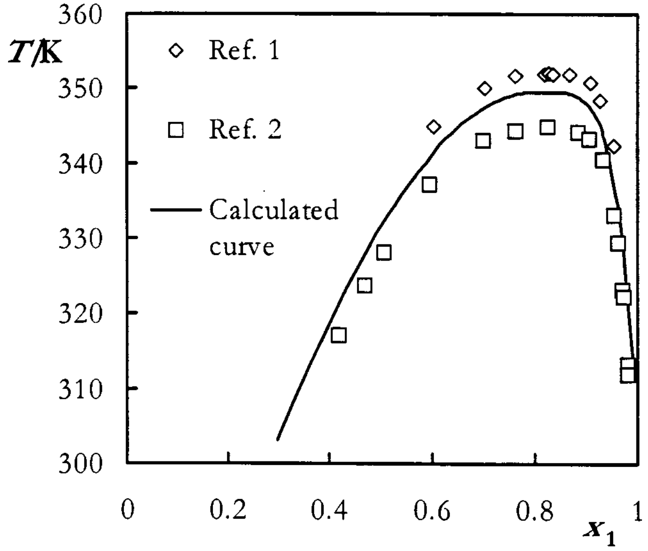

FIG. 36. Mutual solubility of nitromethane and dodecanoic acid.

Mutual solubility of nitromethane and dodecanoic acid

	Acid-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
323.2	0.4306	18.73	0.9796	93.61
333.2	0.5142	24.39	0.9640	89.09
343.2	0.6264	33.82	0.9364	81.76
344.2	0.6412	35.26	0.9317	80.61
345.2	0.6573	36.89	0.9263	79.29
346.2	0.6753	38.79	0.9196	77.71
347.2	0.6960	41.10	0.9111	75.74
348.2	0.7217	44.14	0.8989	73.04
349.2	0.7612	49.27	0.8756	68.20

References:

[1] G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685 (1936).
[2] C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603 (1946).
[3] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Dodecanoic acid; $C_{12}H_{24}O_2$; [143-07-7]

Original Measurements:
G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685–9 (1936).

Variables:
T/K=342–352

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and dodecanoic acid

		Acid-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
69.10	342.25	—	—	86.52	0.9547
71.85	345.00	31.77	0.6044	—	—
75.20	348.35	—	—	79.82	0.9285
76.95	350.10	41.88	0.7028	—	—
77.65	350.80	—	—	74.99	0.9077
78.60	351.75	49.56	0.7633	—	—
78.70	351.85	—	—	66.71	0.8680
78.80	351.95	57.90	0.8186	60.66	0.8350
78.90	352.05	—	—	59.28	0.8269
78.90	352.05	—	—	—	— UCST

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described in Broughton,[1] was used. Liquids were pipetted into glass tubes. Temperatures at which complete miscibility occurred were measured by thermometers standardized against thermometers having NPL certificates.

Source and Purity of Materials:

(1) Prepared from sodium monochloroacetate with sodium nitrite; distilled; $n(25\ °C,D)=1.3796$, $d(25\ °C)=1130.8\ g\cdot L^{-1}$.
(2) Source not specified; purified according to Jones and Betts[2] (recrystallized from petrol ether, m.p.=39 °C, recrystallized from petrol ether and acetone, m.p.=43.4 °C).

Estimated Error:

Temperature: ±0.05 K.

References:

[1] G. Broughton, Trans. Faraday Soc. **30**, 367 (1934).
[2] D. C. Jones and H. F. Betts, J. Chem. Soc. 1177 (1928).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Dodecanoic acid; $C_{12}H_{24}O_2$; [143-07-7]

Original Measurements:
C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603–9 (1946).

Variables:
T/K=293–345

Prepared By:
V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and dodecanoic acid, in mass percent, including the region of solubility of the solid phase, were presented in graphical form and in a table.

Mutual solubility of nitromethane and dodecanoic acid

		Acid-rich phase		Nitromethane-rich phase		
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	$g(2)/100\ g(1)$	100w_1	x_1 (compiler)
20.0	293.2	—	—	1.1	98.9[a]	0.997
21.4*	294.6	—	—	—	98.5[a]	0.995
28.3*	301.5	—	—	—	97.7[a]	0.993
30.0	303.2	—	—	2.8	97.3[a]	0.992
32.0*	305.2	—	—	—	96.7[a]	0.990
34.5*	307.7	—	—	—	95.6[a]	0.986
37.2*	310.4	15.3[a]	0.372	—	—	—
37.7*	310.9	11.9[a]	0.307	—	—	—
38.7*	311.9	—	—	—	94.1[b]	0.981
38.9*	312.1	8.3[a]	0.229	—	—	—
40.0	313.2	—	—	6.6	93.8[b]	0.980
40.4*	313.6	4.5[a]	0.134	—	—	—
43.9*	317.1	18.0[b]	0.419	—	—	—
49.0*	322.2	—	—	—	91.7[b]	0.973
50.0	323.2	—	—	9.7	91.2[b]	0.971
50.6*	323.8	21.3[b]	0.470	—	—	—
55.0*	328.2	23.9[b]	0.508	—	—	—
56.2*	329.4	—	—	—	88.7[b]	0.963
60.0	333.2	—	—	15.7	86.4[b]	0.954
64.0*	337.2	30.9[b]	0.595	—	—	—
67.2*	340.4	—	—	—	80.9[b]	0.933
69.9*	343.1	41.7[b]	0.701	—	—	—
70.0	343.2	—	—	34.1	74.6[b]	0.906
71.0*	344.2	—	—	—	70.0[b]	0.885
71.1*	344.3	49.7[b]	0.764	—	—	—
71.7*	344.9	—	—	—	59.0[b]	0.825
72.0	345.2	—	—	—	—	— (UCST)

*These data were extracted by the compiler from the graphical information presented in the paper.
[a] Solid–liquid equilibrium.
[b] Liquid–liquid equilibrium.

Monotectic is at 37.0 °C (310.2 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described in Hoerr *et al.*,[1] was used. No additional details were reported.

Source and Purity of Materials:

(1) Source not specified; best grade of commercial product; twice distilled.
(2) Prepared and purified as in Pool and Ralston;[2] f.p.=43.92 °C.

Estimated Error:

Not reported.

References:

[1] C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2] W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Tetradecanoic acid; $C_{14}H_{28}O_2$; [544-63-8]	V. P. Sazonov, Technical University, Samara, Russia. G. T. Hefter, Murdoch University, Perth, Australia, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and tetradecanoic acid have been reported in two publications. Hoerr *et al.*[1] studied the mutual solubility of (1) and (2) between 293 and 361 K by the synthetic method. Schmid *et al.*[2] determined the upper critical solution temperature, also using the synthetic method.

At the UCST, the only temperature where direct comparison is possible, the two studies are in rather poor agreement: Hoerr *et al.*[1] (361.0 K) and Schmid *et al.*[2] (364.7 K). However, it may be noted that the UCST values of Schmid *et al.*[2] in well characterized systems are generally lower than other reports. The UCST=364.7 K (Schmid *et al.*[2]) is consistent with the UCST calculated on the basis of critical evaluation of all experimental critical solution temperatures in the series nitromethane–carboxylic acids and discussed at the beginning of this volume. Therefore this UCST is recommended. For the numeric values of mutual solubility, the interested user is referred to the following data sheet, which may be treated as tentative.

References:

[1] C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603 (1946).
[2] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Tetradecanoic acid; $C_{14}H_{28}O_2$; [544-63-8]

Original Measurements:
C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603–9 (1946).

Variables:
T/K=293–361

Prepared By:
V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and tetradecanoic acid in mass percent, including the region of solubility of the solid phase, were presented in graphical form and in a table.

Mutual solubility of nitromethane and tetradecanoic acid

		Acid-rich phase		Nitromethane-rich phase		
t/°C	T/K (compiler)	100 w_1	x_1 (complier)	$g(2)/100\ g(1)$	100 w_1	x_1 (compiler)
20.0	293.2	—	—	0.7	99.3^a	0.998
30.0	303.2	—	—	1.3	98.7^a	0.997
33.0*	306.2	—	—	—	98.4^a	0.996
40.0	313.2	—	—	2.3	97.8^a	0.994
45.4*	318.6	—	—	—	96.7^a	0.991
48.1*	321.3	13.6^a	0.371	—	—	—
49.3*	322.5	8.9^a	0.268	—	—	—
50.0	323.2	—	—	4.7	95.5^b	0.988
51.1*	324.3	4.5^a	0.150	—	—	—
52.6*	325.8	16.7^b	0.429	—	—	—
60.0	333.2	—	—	7.1	93.4^b	0.981
62.6*	335.8	20.1^b	0.485	—	—	—
67.7*	340.9	—	—	—	91.3^b	0.975
70.0	343.2	—	—	11.1	90.0^b	0.971
73.0*	346.2	25.5^b	0.562	—	—	—
78.3*	351.5	—	—	—	85.4^b	0.956
80.0	353.2	—	—	19.2	83.9^b	0.951
81.4*	354.6	33.7^b	0.655	—	—	—
85.0*	358.2	—	—	—	76.8^b	0.925
85.5*	358.7	43.4^b	0.742	—	—	—
87.2*	360.4	52.5	0.805	—	—	—
87.8	361.0	—	—	—	—	— (UCST)

*These data were extracted graphically by the compiler.
[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

A monotectic was reported at 47.7 °C (320.9 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, as described by Hoerr *et al.*,[1] was used. No additional details were reported.

Source and Purity of Materials:
(1) Source not specified; best grade of commercial product; twice distilled.
(2) Prepared and purified as in Pool and Ralston;[2] f.p.=54.15 °C.

Estimated Error:
Not reported.

References:
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexadecanoic acid; $C_{16}H_{32}O_2$; [57-10-3]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and hexadecanoic acid have been reported in three publications: Broughton and Jones,[1] between 365 and 378 K, and Hoerr *et al.*,[2] between 293 and 371 K, measured the mutual solubility of the two components using the synthetic method. Schmid *et al.*[3] determined the upper critical solution temperature also by the synthetic method. The upper critical solution temperature has been reported as 377 K by Schmid *et al.*[3] and 377.70 K by Broughton and Jones.[1]

The experimental data reported in Broughton and Jones[1] and Hoerr *et al.*[2] differed significantly in measured UCST on what influenced the description of mutual solubility. The UCST equal to 376.6 K, calculated on the bases of relationship in the series nitromethane–acids, discussed at the beginning of this volume, was treated as a tentative UCST for this system. Then the UCST and temperatures in Broughton and Jones[1] have been normalized according to the formula:

$$T_{\text{new}}=(T/T_c)_{\text{exp}}\cdot T_{c\ \text{tentative}}\,.$$

These transformed data of Broughton and Jones[1] and data reported in Hoerr *et al.*[2] have been approximated by the equation based on scaling law (described in the Introduction material to this volume ‘‘Relations of Solubility Data in Binary Systems Containing Nitromethane’’) and the following parameters have been adjusted: $a_1=0.481\ 78$, $a_2=0.163\ 58$, $b_1=2.832\ 52$, $b_2=-3.151\ 04$ (mean standard error of estimate was 0.0114).

As an approximation, $x_{c1}=0.860$ and UCST=376.6 K have been used. In the opinion of 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 all experimental points[1,2] are also presented in Fig. 37.

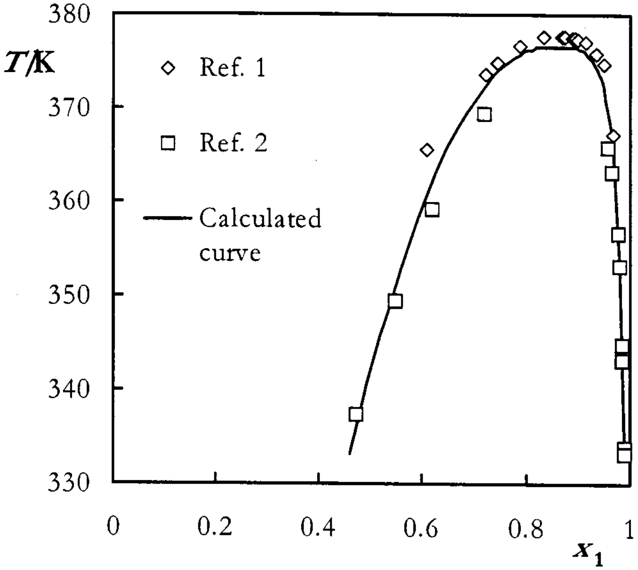

FIG. 37. Mutual solubility of nitromethane and hexadecanoic acid.

Mutual solubility of nitromethane and hexadecanoic acid

	Acid-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
333.2	0.4619	16.97	0.9898	95.85
338.2	0.4838	18.24	0.9878	95.05
343.2	0.5073	19.69	0.9855	94.17
348.2	0.5328	21.35	0.9829	93.18
353.2	0.5607	23.31	0.9797	91.99
358.2	0.5920	25.67	0.9756	90.51
363.2	0.6279	28.66	0.9700	88.51
368.2	0.6715	32.74	0.9613	85.52
373.2	0.7321	39.42	0.9435	79.90
374.2	0.7493	41.57	0.9368	77.92
375.2	0.7708	44.46	0.9269	75.11
376.2	0.8047	49.52	0.9071	69.92

References:

[1] G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685 (1936).
[2] C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603 (1946).
[3] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexadecanoic acid; $C_{16}H_{32}O_2$; [57-10-3]

Original Measurements:
G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685–9 (1936).

Variables:
T/K=366–378

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and hexadecanoic acid

		Acid-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
92.40	365.55	27.16	0.6104	—	—
94.05	367.20	—	—	87.86	0.9682
100.05	373.65	38.20	0.7220	—	—
101.60	374.75	—	—	81.55	0.9489
101.65	374.80	41.07	0.7454	—	—
102.75	375.90	—	—	77.10	0.9340
103.55	376.70	46.85	0.7874	—	—
103.95	377.10	—	—	71.56	0.9136
104.15	377.30	—	—	68.03	0.8994
104.30	377.45	—	—	66.64	0.8935
104.30	377.45	—	—	65.70	0.8895
104.45	377.60	54.23	0.8327	—	—
104.50	377.65	61.05	0.8682	—	—
104.55	377.70	62.52	0.8751	—	—
104.55	377.70	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described in Broughton,[1] was used. Liquids were pipetted into glass tubes. Temperatures at which complete miscibility occurred were measured by thermometers standardized against a set of thermometers having NPL certificates.

Source and Purity of Materials:

(1) Prepared from sodium monochloroacetate with sodium nitrite; distilled; $n(25\ °C,D)=1.3796$, $d(25\ °C)=1130.8\ g\cdot L^{-1}$.
(2) Source not specified; purified according to Jones and Betts[2] (recrystallized from petrol ether and ethanol, m.p.=62.6 °C).

Estimated Error:

Temperature: ±0.05 K.

References:

[1] G. Broughton, Trans. Faraday Soc. **30**, 367 (1934).
[2] D. C. Jones and H. F. Betts, J. Chem. Soc. 1177 (1928).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexadecanoic acid; $C_{16}H_{32}O_2$; [57-10-3]

Original Measurements:

C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603–9 (1946).

Variables:

T/K=293–369

Prepared By:

V. P. Sazonov

Experimental Data

The mutual solubilities of nitromethane and hexadecanoic acid in mass percent, including the region of immiscible solutions, over the temperature range were presented in graphical form and in a table.

Solubility of nitromethane and hexadecanoic acid

		Acid-rich phase		Nitromethane-rich phase		
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	$g(2)/100\ g(1)$	100 w_1	x_1 (compiler)
20.0	293.2	—	—	0.5	99.5^a	0.999
30.0	303.2	—	—	0.9	99.1^a	0.998
30.3*	303.5	—	—	—	99.0^a	0.998
40.0	313.2	—	—	1.4	98.6^a	0.997
42.4*	315.6	—	—	—	98.4^a	0.996
49.0*	322.2	—	—	—	98.1^a	0.995
50.0	323.2	—	—	2.2	97.9^a	0.995
53.8*	327.0	—	—	—	97.4^a	0.994
57.2*	330.4	12.3^a	0.371	—	—	—
58.3*	331.5	8.0^a	0.268	—	—	—
60.0	333.2	—	—	4.1	96.1^b	0.990
60.7*	333.9	—	—	—	96.0^b	0.990
64.2*	337.4	17.6^b	0.473	—	—	—
70.0	343.2	—	—	5.8	94.5^b	0.986
71.6*	344.8	—	—	—	94.3^b	0.986
76.3*	349.5	22.4^b	0.548	—	—	—
80.0	353.2	—	—	8.9	91.8^b	0.979
83.5*	356.7	—	—	—	91.3^b	0.978
85.9*	359.1	28.0^b	0.620	—	—	—
90.0	363.2	—	—	15.3	86.7^b	0.965
92.7*	365.9	—	—	—	84.5^b	0.958
96.3*	369.5	38.1^b	0.721	—	—	—

*These data were extracted graphically by the compiler.
[a] Solid–liquid equilibrium.
[b] Liquid–liquid equilibrium.

A monotectic was reported at 56.7 °C (329.9 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described in Hoerr *et al.*,[1] was used. No additional details were reported.

Source and Purity of Materials:

(1) Source not specified; best grade of commercial product; twice distilled.
(2) Prepared and purified as in Ref. 2; f.p.=62.82 °C.

Estimated Error:

Not reported.

References:

[1] C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2] W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) cis-9-Octadecenoic acid; $C_{18}H_{34}O_2$; [112-80-1]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
G. T. Hefter, Murdoch University, Perth, Australia, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and cis-9-octadecenoic acid have been reported in two publications. Hoerr *et al.*[1] studied the solubility of (2) in (1) between 233 and 393 K by the synthetic method. Schmid *et al.*[2] determined the upper critical solution temperature also using the synthetic method.

At the UCST, the only temperature where direct comparison is possible, the two studies are in rather poor agreement: Hoerr *et al.*[1] (367.7 K) and Schmid *et al.*[2] (369.7 K). Accordingly, in the absence of confirmatory studies, all data must be regarded as tentative. However, it may be noted that the UCST values of Schmid *et al.*[2] in well characterized systems are generally lower than other reports. Thus both the UCST values and the other available data[1] must be regarded with some scepticism. The tentative numeric data (but see comments above) are given in the following data sheet.

References:

[1] C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Phys. Chem. **56**, 1068 (1952).
[2] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) cis-9-Octadecenoic acid; $C_{18}H_{34}O_2$; [112-80-1]

Original Measurements:
C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Phys. Chem. **56**, 1068–73 (1952).

Variables:
T/K=233–368

Prepared By:
V. P. Sazonov

Experimental Data

Solubility of cis-9-octadecanoic acid in nitromethane

t/°C	T/K (compiler)	$g(2)/100\ g(1)$	100 w_2 (compiler)	x_2 (compiler)
−40.0	233.2	0.1	0.1	0.0002
−30.0	243.2	0.2	0.2	0.0004
−20.0	253.2	0.4	0.4	0.0009
−10.0	263.2	0.6	0.6	0.0013
0.0	273.2	0.8	0.8	0.0017
10.0	283.2	1.0	1.0	0.0022
20.0	293.2	1.1	1.1	0.0024
94.5	367.7	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method was used. Solubilities of acid were determined by weighing 2–5 g portions into 2×15 cm test tubes fitted with a Nichrome stirrer and thermocouple well. This tube was placed in a larger tube which served as an air bath. On addition of weighed amounts of solvent, solubilities were determined by measuring temperatures at which crystals precipitated or dissolved, with alternate heating and cooling of the system, in either an acetone dry ice or water bath.

Source and Purity of Materials:
(1) Source not specified; best grade reagent; dried and distilled.
(2) Prepared from high quality oil by saponification; purified by recrystallization and by vacuum distillation in a packed column; m.p.=16.30 °C, n(20 °C,D)=1.4599.

Estimated Error:
Temperature: ±0.1 K.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octadecanoic acid; $C_{18}H_{36}O_2$; [57-11-4]

Evaluators:

V. P. Sazonov, Technical University, Samara, Russia.
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, September, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and octadecanoic acid have been reported in three publications. Broughton and Jones[1] at 387 K and Hoerr *et al.*,[2] between 293 and 369 K studied the mutual solubilities of (1) and (2) using the synthetic method. Schmid *et al.*[3] determined the upper critical solution temperature also by the synthetic method.

At the UCST, the only temperature where direct comparison is possible, the two results available are in only fair agreement: Schmid *et al.*[3] (386.7 K) and Broughton and Jones[1] (387.2 K). Accordingly, in the absence of confirmatory studies, all data must be regarded as tentative. However, it may be noted that the UCST values of Schmid *et al.*[3] in well characterized systems are generally lower than other reports and thus the value from Broughton and Jones[1] is probably more realistic.

The measured UCST is not consistent with the values calculated from the respective relationships in the nitromethane–alcohol series, discussed at the beginning of this volume (the calculated value, UCST=386.5 K). The numeric values of liquid–liquid solubility, reported in Broughton and Jones[1] and Hoerr *et al.*,[2] have been approximated by the equation based on scaling law (described in the Introduction material to this volume ‘‘Relations of Solubility Data in Binary Systems Containing Nitromethane’’) and the following parameters have been adjusted: $a_1=0.340\ 23$, $a_2=0.508\ 66$, $b_1=-1.000\ 84$, $b_2=-0.033\ 78$ (mean standard error of estimate was 0.0754).

As an approximation, the UCST=387.2 (Ref. 1) and $x_{c1}=0.86$ have been used. This relationship together with all experimental points from liquid–liquid region[1,2] are presented in Fig. 38. The calculated results for the selected temperatures are presented in the following table. These mutual solubilities may to be treated as tentative.

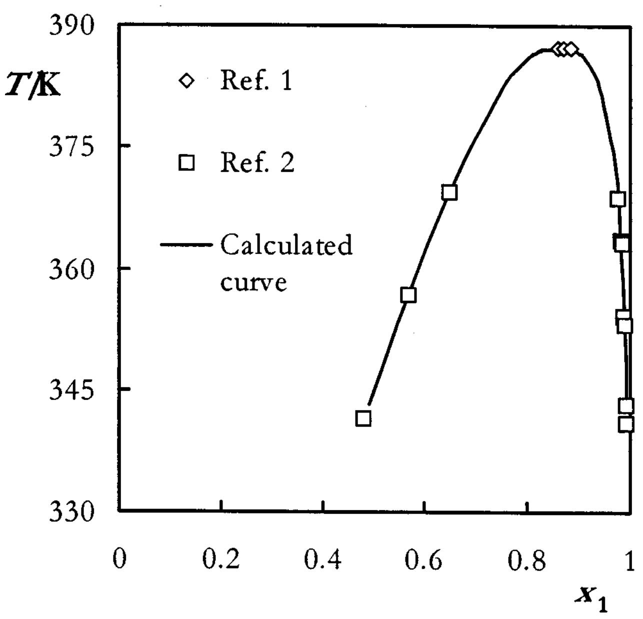

FIG. 38. Mutual solubility of nitromethane and octadecanoic acid.

Mutual solubility of nitromethane and octadecanoic acid

	Acid-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
341.2	0.4802	16.55	0.9918	96.30
343.2	0.4912	17.16	0.9916	96.20
348.2	0.5191	18.80	0.9906	95.75
353.2	0.5477	20.62	0.9888	94.97
358.2	0.5773	22.66	0.9861	93.82
363.2	0.6081	24.98	0.9821	92.18
368.2	0.6406	27.66	0.9766	89.94
373.2	0.6755	30.87	0.9686	86.89
378.2	0.7144	34.92	0.9567	82.59
383.2	0.7620	40.73	0.9362	75.88
384.2	0.7740	42.36	0.9296	73.91
385.2	0.7879	44.35	0.9212	71.48
386.2	0.8057	47.08	0.9088	68.13

References:

[1] G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685 (1936).
[2] C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Phys. Chem. **56**, 1068 (1952).
[3] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octadecanoic acid; $C_{18}H_{36}O_2$; [57-11-4]

Original Measurements:
C. W. Hoerr, R. S. Sedgwick, and A. W. Ralston, J. Org. Chem. **11**, 603–9 (1946).

Variables:
T/K=293–369

Prepared By:
V. P. Sazonov

Experimental Data

The solubilities of nitromethane and octadecanoic acid in mass percent, including the region of immiscible solutions, over the temperature range were presented in graphical form and in a table.

Solubility of nitromethane and octadecanoic acid

		Acid-rich phase		Nitromethane-rich phase		
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	$g(2)/100\ g(1)$	100 w_1	x_1 (compiler)
20.0	293.2	—	—	0.4	99.6[a]	0.999
30.0	303.2	—	—	0.7	99.3[a]	0.998
40.0	313.2	—	—	1.0	99.0[a]	0.998
50.0	323.2	—	—	1.3	98.7[a]	0.997
56.8*	330.0	—	—	—	98.3[a]	0.996
60.0	333.2	—	—	1.9	98.1[a]	0.996
62.3*	335.5	—	—	—	97.2[a]	0.994
63.9*	337.1	13.0[a]	0.411	—	—	—
65.0*	338.2	9.0[a]	0.316	—	—	—
66.4*	339.6	5.2[a]	0.204	—	—	—
67.8*	341.0	—	—	—	96.5[b]	0.992
68.2*	341.4	16.6[b]	0.481	—	—	—
70.0	343.2	—	—	3.6	96.5[b]	0.992
80.0	353.2	—	—	5.5	94.8[b]	0.988
80.9*	354.1	—	—	—	94.6[b]	0.987
83.5*	356.7	22.1[b]	0.569	—	—	—
90.0	363.2	—	—	8.1[c]	92.5[b]	0.983
90.3*	363.5	—	—	—	91.7[b]	0.981
95.6*	368.8	—	—	—	89.7[b]	0.976
96.3*	369.5	28.4[b]	0.649	—	—	—

*These data were extracted graphically by the compiler.
[a] Solid–liquid equilibrium.
[b] Liquid–liquid equilibrium.
[c] Recorded as 0.1 on original. Value estimated by compiler from the liquid–liquid curve.

A monotectic was reported at 63.5 °C (336.7 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method, as described in Hoerr *et al.*,[1] was used. No additional details were reported.

Source and Purity of Materials:
(1) Source not specified; best grade of commercial product; twice distilled.
(2) Prepared by repeated recrystallization of Armour Neo-Fat 1-65 from acetonitrile; f.p.=69.60 °C.

Estimated Error:
Not reported.

References:
[1] C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octadecanoic acid; $C_{18}H_{36}O_2$; [57-11-4]

Original Measurements:
G. Broughton and D. C. Jones, Trans. Faraday Soc. **32**, 685–9 (1936).

Variables:
T/K=387

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and octadecanoic acid

t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
114.0	387.2	56.67	0.8591	62.45	0.8857
114.0	387.2	59.39	0.8721	—	—
114.0	387.2	—	—	—	— (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, as described in Jones and Betts,[1] was used. Liquids were pipetted into glass tubes. Temperatures at which complete miscibility occurred were measured by thermometers standardized against a set of thermometers having NPL certificates.

Source and Purity of Materials:

(1) Prepared from sodium monochloroacetate with sodium nitrite; distilled; $n(25\ °C,D)=1.3796$, $d(25\ °C)=1130.8\ g\cdot L^{-1}$.
(2) Not specified.

Estimated Error:

Temperature: ±0.1 K.

References:

[1] D. C. Jones and H. F. Betts, J. Chem. Soc. 1177 (1928).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Saturated fatty acids; $C_8H_{16}O_2$–$C_{22}H_{44}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287–96 (1963).

Variables:
T/K=306–401

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the system nitromethane+saturated fatty acid

Acid	t/°C	T/K (compiler)
Octanoic acid; $C_8H_{16}O_2$; [124-07-2]	32.5	305.7
Decanoic acid; $C_{10}H_{20}O_2$; [344-48-5]	58.5	331.7
Undecanoic acid; $C_{11}H_{22}O_2$; [112-37-8]	68.0	341.2
Dodecanoic acid; $C_{12}H_{24}O_2$; [143-07-7]	76.5	349.7
Tridecanoic acid; $C_{13}H_{26}O_2$; [638-53-9]	84.0	357.2
Tetradecanoic acid; $C_{14}H_{28}O_2$; [544-63-8]	91.5	364.7
Pentadecanoic acid; $C_{15}H_{30}O_2$; [1002-84-2]	98.0	371.2
Hexadecanoic acid; $C_{16}H_{32}O_2$; [57-10-3]	104.0	377.2
Heptadecanoic acid; $C_{17}H_{34}O_2$; [506-12-7]	109.0	382.2
Octadecanoic acid; $C_{18}H_{36}O_2$; [57-11-4]	113.5	386.7
Eicosanoic acid; $C_{20}H_{40}O_2$; [506-30-9]	121.0	394.2
Docosanoic acid; $C_{22}H_{44}O_2$; [112-85-6]	128.0	401.2

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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D)=1.3820$, $d(20\ °C)=1134\ g\cdot L^{-1}$.
(2) Undecanoic, tridecanoic, pentadecanoic, and heptadecanoic acids obtained from Lachat Chemical Co.; other acids from the Hormel Foundation; purified by gas–liquid partition and thin-layer adsorption chromatography.

Estimated Error:

Temperature: ±0.5 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Unsaturated fatty acids; $C_{16}H_{26}O_2$–$C_{24}H_{46}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287–96 (1963).

Variables:
T/K=318–398

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+unsaturated fatty acid

Acid	t/°C	T/K (compiler)
Docosahexaenoic acid; $C_{22}H_{32}O_2$; [25167-62-8]	44.5	317.7
Hexadecatrienoic acid; $C_{16}H_{26}O_2$; [29428-96-4]	46.0	319.2
Eicosapentaenoic acid; $C_{20}H_{30}O_2$; [25378-27-2]	46.5	319.7
9,12,15-Octadecatrienoic acid; $C_{18}H_{30}O_2$; [463-40-1]	64.0	337.2
Eicosatetraenoic acid; $C_{20}H_{32}O_2$; [506-32-1]	64.5	337.7
Hexadecadienoic acid; $C_{16}H_{28}O_2$; [28933-88-2]	66.0	339.2
9, 12-Octadecadienoic acid; $C_{18}H_{32}O_2$; [60-33-3]	80.0	353.2
9-Hexadecenoic acid; $C_{16}H_{30}O_2$; [373-49-9]	84.0	357.2
6-Octadecenoic acid; $C_{18}H_{34}O_2$; [593-39-5]	96.0	369.2
cis-9-Octadecenoic acid; $C_{18}H_{34}O_2$; [112-80-1]	96.5	369.7
trans-9-Octadecenoic acid; $C_{18}H_{34}O_2$; [112-79-8]	100.0	373.2
11-Eicosenoic acid; $C_{20}H_{38}O_2$; [5561-99-9]	106.0	379.2
13-Docosenoic acid; $C_{22}H_{42}O_2$; [112-86-7]	116.0	389.2
15-Tetracosenoic acid; $C_{24}H_{46}O_2$; [506-37-6]	125.0	398.2

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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °\mathrm{C,D})=1.3820$, $d(20\ °\mathrm{C})=1134\ \mathrm{g \cdot L^{-1}}$.
(2) Obtained from the Hormel Foundation; purified by gas–liquid partition and thin-layer adsorption chromatography.

Estimated Error;
Temperature: ±0.5 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hydroxy acids; $C_{18}H_{34}O_3$ and $C_{18}H_{36}O_3$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **11**, 376–83 (1966).

Variables:
T/K=343 and 360

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+hydroxy acid

Hydroxy acid	t/°C	T/K (compiler)
12-Hydroxy-*cis*-9-octadecenoic acid; $C_{18}H_{34}O_3$; [141-22-0]	70.0	343.2
12-Hydroxyoctadecanoic acid; $C_{18}H_{36}O_3$; [106-14-9]	86.5	359.7

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. As described in Schmid *et al.*,[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) Fisher Scientific Co.
(2) Not specified.

Estimated Error:
Not reported.

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

12. Nitromethane+Two-Basic Acids and Salts

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Ethanedioic acid; $C_2H_2O_4$; [144-62-7]

Original Measurements:

H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:

T/K=273–308

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of ethanedioic acid in nitromethane

t/°C	T/K (compiler)	mol/L	100 w_2[a] (compiler)	x_2 (compiler)
0	273.2	0.014	0.11	0.0007
15.0	288.2	0.030	0.24	0.0016
25.0	298.2	0.063	0.50	0.0034
35.0	308.2	0.140	1.12	0.0076

[a] The densities of the solutions were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane and titrated against 0.07 N tetrabutylammonium hydroxide solution.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

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

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Propanedioic acid; $C_3H_4O_4$; [141-82-2]

Original Measurements:

H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:

T/K=273–308

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of propanedioic acid in nitromethane

t/°C	T/K (compiler)	mol/L	100 w_2[a](compiler)	x_2 (compiler)
0	273.2	0.012	0.11	0.0006
15.0	288.2	0.017	0.15	0.0009
25.0	298.2	0.040	0.37	0.0023
35.0	308.2	0.130	1.20	0.0071

[a] The densities of the solutions were taken to be by the compiler those of nitromethane (Ref. 1) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane, and titrated against 0.07 N tetrabutylammonium hydroxide solution.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

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

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Butanedioic acid; $C_4H_6O_4$; [110-15-6]

Original Measurements:

H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:

T/K=273–308

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of butanedioic acid (2) in nitromethane (1)

t/°C	T/K (compiler)	mol/L	100 w_2^a (compiler)	x_2 (compiler)
0	273.2	0.005	0.05	0.0002
15.0	288.2	0.007	0.07	0.0004
25.0	298.2	0.020	0.21	0.0011
35.0	308.2	0.072	0.75	0.0039

[a] The densities of the solution were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane, and titrated against 0.07 N tetrabutylammonium hydroxide solution.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

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

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Pentanedioic acid; $C_5H_8O_4$; [110-94-1]

Original Measurements:

H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:

T/K=273–308

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of pentanedioic acid (2) in nitromethane (1)

t/°C	T/K (compiler)	mol/L	100 w_2^a (compiler)	x_2 (compiler)
0	273.2	0.011	0.13	0.0005
15.0	288.2	0.013	0.15	0.0007
25.0	298.2	0.026	0.30	0.0014
35.0	308.2	0.086	1.01	0.0047

[a] The densities of the solutions were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane, and titrated against 0.07 N tetrabutylammonium hydroxide solution.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

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

Components:	**Evaluators:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Hexanedioic acid; $C_6H_{10}O_4$; [124-04-9]	V. P. Sazonov, Technical University, Samara, Russia. G. T. Hefter, Murdoch University, Perth, Australia, July, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and hexanedioic acid 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 the solubility of hexanedioic acid in nitromethane at 298 K. Smagowski[2] 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, differing by a factor of 2. Accordingly, all the available data (see the relevant data sheets) must be regarded as very tentative.

References:

[1] Z. S. Smolyan, G. N. Matveeva, V. K. Fukin, K. N. Korotaevskii, A. P. Ignat'eva, A. N. Kornilina, L. S. Zvereva, and A. S. Fomin, Khim. Prom-st (Moscow) **48**, 508 (1972).
[2] H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 53 (1974).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Hexanedioic acid; $C_6H_{10}O_4$; [124-04-9]	Z. S. Smolyan, G. N. Matveeva, V. K. Fukin, K. N. Korotaevskii, A. P. Ignat'eva, A. N. Kornilina, L. S. Zvereva, and A. S. Fomin, Khim. Prom-st (Moscow) **48**, 508–9 (1972).
Variables: $T/\mathrm{K}=298$	**Prepared By:** V. P. Sazonov

Experimental Data

The solubility of hexanedioic acid in nitromethane at 25 °C (298 K, compiler) was reported to be 100 $w_2=0.09$. The corresponding mole fraction x_2 calculated by the compiler is 0.0004.

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
No further details were reported.	(1) Source not specified; purity not specified. (2) Source not specified; purity not specified.
	Estimated Error: Temperature: ±1 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexanedioic acid; $C_6H_{10}O_4$; [124-04-9]

Original Measurements:
H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:
T/K=273–308

Prepared By:
V. P. Sazonov

Experimental Data

Solubility of hexanedioic acid in nitromethane

t/°C	T/K (compiler)	mol/L	100 w_2[a] (compiler)	x_2 (compiler)
0	273.2	0.005	0.06	0.0002
15.0	288.2	0.007	0.09	0.0004
25.0	298.2	0.012	0.16	0.0007
35.0	308.2	0.018	0.24	0.0010

[a] The densities of the solutions were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane and titrated against 0.07 N tetrabutylammonium hydroxide solution.

Source and Purity of Materials:
(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from ethyl acetate.

Estimated Error:
Not reported.

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

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Heptanedioic acid; $C_7H_{12}O_4$; [111-16-0]

Original Measurements:
H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:
T/K=273–308

Prepared By:
V. P. Sazonov

Experimental Data

Solubility of heptanedioic acid in nitromethane

t/°C	T/K (compiler)	mol/L	100 w_2[a] (compiler)	x_2 (compiler)
0	273.2	0.003	0.04	0.0002
15.0	288.2	0.005	0.07	0.0002
25.0	298.2	0.008	0.11	0.0004
35.0	308.2	0.014	0.20	0.0008

[a] The densities of the solutions were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane, and titrated against 0.07 N tetrabutylammonium hydroxide solution.

Source and Purity of Materials:
(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from ethyl acetate.

Estimated Error:
Not reported.

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

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Octanedioic acid; $C_8H_{14}O_4$; [505-48-6]

Original Measurements:

H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:

T/K=273–308

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of octanedioic acid in nitromethane

t/°C	T/K (compiler)	mol/L	100 w_2[a] (compiler)	x_2 (compiler)
0	273.2	0.002	0.03	0.0001
15.0	288.2	0.003	0.05	0.0002
25.0	298.2	0.006	0.09	0.0003
35.0	308.2	0.009	0.14	0.0005

[a] The densities of the solutions were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane, and titrated against 0.07 N tetrabutylammonium hydroxide solution.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported

References:

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

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Nonanedioic acid; $C_9H_{16}O_4$; [123-99-9]

Original Measurements:

H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:

T/K=273–308

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of nonanedioic acid in nitromethane

t/°C	T/K (compiler)	mol/L	100 w_2[a] (compiler)	x_2 (compiler)
0	273.2	0.002	0.03	0.0001
15.0	288.2	0.003	0.05	0.0002
25.0	298.2	0.005	0.08	0.0003
35.0	308.2	0.008	0.14	0.0004

[a] The densities of the solutions were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane, and titrated against 0.07 N tetrabutylammonium hydroxide solution by using bromothymol blue indicator.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

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

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Decanedioic acid; $C_{10}H_{18}O_4$; [111-20-6]

Original Measurements:

H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:

T/K=273–308

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of decanedioic acid (2) in nitromethane

t/°C	T/K (compiler)	mol/L	100 w_2[a] (compiler)	x_2 (compiler)
0	273.2	0.002	0.04	0.0001
15.0	288.2	0.003	0.05	0.0002
25.0	298.2	0.005	0.09	0.0003
35.0	308.2	0.008	0.15	0.0004

[a] The densities of the solutions were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane, and titrated against 0.07 N tetrabutylammonium hydroxide solution by using bromothymol blue indicator.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(2) Source not specified; purity not specified; purified by crystallization from water.

Estimated Error:

Not reported.

References:

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

Components:

(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Dicarboxylic acids monosodium salts; $C_2HNaO_4-C_{10}H_{17}NaO_4$

Original Measurements:

H. Smagowski, Zesz. Nauk. Wydz. Mat., Fiz. Chem., Univ. Gdanski, Chem. **3**, 45–53 (1974).

Variables:

T/K=298

Prepared By:

V. P. Sazonov

Experimental Data

Solubility of monosodium salts of dicarboxylic acids in nitromethane at 25.0 °C (298.2 K compiler)

Monosodium salt of dicarboxylic acid	mol/L	100 w_2 (compiler)	x_2 (compiler)
Ethanedioate; C_2HNaO_4 ; [1186-49-8]	0.003	0.03	0.0002
Propanedioate; $C_3H_3NaO_4$; [2922-55-6]	0.005	0.06	0.0003
Butanedioate; $C_4H_5NaO_4$; [2922-54-5]	0.007	0.09	0.0004
Pentanedioate; $C_5H_7NaO_4$; [3343-88-2]	0.006	0.08	0.0003
Hexanedioate; $C_6H_9NaO_4$; [18966-34-4]	0.008	0.12	0.0004
Heptanedioate; $C_7H_{11}NaO_4$; [6142-21-8]	0.006	0.10	0.0003
Octanedioate; $C_8H_{13}NaO_4$; [27796-70-9]	0.008	0.14	0.0004
Nonanedioate; $C_9H_{15}NaO_4$; [17356-30-8]	0.009	0.17	0.0005
Decanedioate; $C_{10}H_{17}NaO_4$; [19455-73-3]	0.005	0.10	0.0003

*The densities of the solutions were taken to be by the compiler those of nitromethane (Timmermans[1]) 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 into 50 mL volumetric flasks. The flasks were closed by ground stoppers and were 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 nitromethane, and titrated by 0.07 N $HClO_4$ by using crystal violet indicator.

Source and Purity of Materials:

(1) Source not specified; purity not specified; dried over P_2O_5 and distilled at reduced pressure.
(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:

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

13. Nitromethane+Esters

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Methyl-12-hydroxy-*cis*-9-octadecenoate; $C_{19}H_{36}O_3$; [141-24-2]

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **11**, 376–83 (1966).

Variables:

$T/\mathrm{K}=280$

Prepared By:

V. P. Sazonov

Experimental Data

The upper critical solution temperature of nitromethane with methyl-12-hydroxy-*cis*-9-octadecenoate was reported to be 7 °C (280 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. As described in Schmid *et al.*,[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) Fisher Scientific Co.
(2) Not specified.

Estimated Error:

Not reported.

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Esters; $C_{14}H_{28}O_2$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:

$T/\mathrm{K}=291-300$

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+ester

Ester	$t/°\mathrm{C}$	T/K (compiler)
Ethyldodecanoate; $C_{14}H_{28}O_2$; [106-33-2]	18.0	291.2
Undecylpropanoate; $C_{14}H_{28}O_2$; [5458-33-3]	18.0	291.2
Decylbutanoate; $C_{14}H_{28}O_2$; [5454-09-1]	22.0	295.2
Propylundecanoate; $C_{14}H_{28}O_2$	22.5	295.7
Butyldecanoate; $C_{14}H_{28}O_2$; [30673-36-0]	25.0	298.2
Octylhexanoate; $C_{14}H_{28}O_2$; [4887-30-3]	25.5	298.7
Hexyloctanoate; $C_{14}H_{28}O_2$; [1117-55-1]	27.0	300.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described in Schmid *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °\mathrm{C,D})=1.3820$, $d(20\ °\mathrm{C})=1134\ \mathrm{g\cdot L^{-1}}$.
(2) Ethyl and butyl esters purchased from Applied Science Laboratories, propyl and hexyl esters, propanoate 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, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Methyl esters saturated fatty acids; $C_{15}H_{30}O_2$–$C_{23}H_{46}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287–96 (1963).

Variables:
T/K=295–365

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+methyl ester saturated fatty acid

Methyl ester	t/°C	T/K (compiler)
Methyltetradecanoate; $C_{15}H_{30}O_2$; [124-10-7]	21.5	294.7
Methylpentadecanoate; $C_{16}H_{32}O_2$; [7132-64-1]	34.0	307.2
Methylhexadecanoate; $C_{17}H_{34}O_2$; [112-39-0]	44.0	317.2
Methylheptadecanoate; $C_{18}H_{36}O_2$; [1731-92-6]	53.5	326.7
Methyloctadecanoate; $C_{19}H_{38}O_2$; [112-61-8]	62.0	335.2
Methyleicosanoate; $C_{21}H_{42}O_2$; [1120-28-1]	78.5	351.7
Methyldocosanoate; $C_{23}H_{46}O_2$; [929-77-1]	91.5	364.7

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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(2) Pentadecanoate and heptadecanoate obtained from Lachat Chemical Co.; other esters from the Hormel Foundation; purified by gas–liquid partition and thin-layer adsorption chromatography.

Estimated Error:
Temperature: ±0.5 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Esters; $C_{16}H_{32}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:
T/K=297–323

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+ester

Ester	t/°C	T/K (compiler)
Pentadecylmethanoate; $C_{16}H_{32}O_2$; [66271-76-9]	23.5	296.7
Tetradecylethanoate; $C_{16}H_{32}O_2$; [638-59-5]	27.0	300.2
Methylpentadecanoate; $C_{16}H_{32}O_2$; [7132-64-1]	33.5	306.7
Ethyltetradecanoate; $C_{16}H_{32}O_2$; [124-06-1]	40.5	313.7
Tridecylpropanoate; $C_{16}H_{32}O_2$; [6271-77-0]	40.5	313.7
Dodecylbutanoate; $C_{16}H_{32}O_2$; [3724-61-6]	44.5	317.7
Propyltridecanoate; $C_{16}H_{32}O_2$; [88591-28-0]	45.0	318.2
Butyldodecanoate; $C_{16}H_{32}O_2$; [106-18-3]	47.0	320.2
Decylhexanoate; $C_{16}H_{32}O_2$; [52363-43-6]	47.5	320.7
Hexyldecanoate; $C_{16}H_{32}O_2$; [10448-26-7]	49.5	322.7
Octyloctanoate; $C_{16}H_{32}O_2$; [2306-88-9]	49.5	322.7

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 *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(2) Methyl, ethyl, and butyl esters purchased from Applied Science Laboratories; propyl and hexyl esters, formate, 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, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Methyl esters unsaturated fatty acids; $C_{17}H_{32}O_2$–$C_{25}H_{48}O_2$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287–96 (1963).

Variables:

T/K = 292–362

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane + methyl ester unsaturated fatty acid

Methyl ester	t/°C	T/K
Methyl-9-hexadecenoate; $C_{17}H_{32}O_2$; [3913-63-1]	19.0	292.2
Methyl-cis-9-octadecenoate; $C_{19}H_{36}O_2$; [112-62-9]	41.0	314.2
Methyl-cis-11-octadecenoate; $C_{19}H_{36}O_2$; [1937-63-9]	41.0	314.2
Methyl-cis-12-octadecenoate; $C_{19}H_{36}O_2$; [2733-86-0]	41.0	314.2
Methyl-cis-6-octadecenoate; $C_{19}H_{36}O_2$; [2777-58-4]	41.0	314.2
Methyl-trans-9-octadecenoate; $C_{19}H_{36}O_2$; [1937-62-8]	46.0	319.2
Methyl-11-eicosenoate; $C_{21}H_{40}O_2$; [2390-09-2]	58.5	331.7
Methyl-cis-13-docosenoate; $C_{23}H_{44}O_2$; [1120-34-9]	75.0	348.2
Methyl-15-tetracosenoate; $C_{25}H_{48}O_2$; [2733-88-2]	88.5	361.7

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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(2) Obtained from the Hormel Foundation; purified by gas–liquid partition and thin-layer adsorption chromatography.

Estimated Error:

Temperature: ±0.5 K.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Esters; $C_{18}H_{36}O_2$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:

T/K = 318–341

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane + ester

Ester	t/°C	T/K (compiler)
Heptadecylmethanoate; $C_{18}H_{36}O_2$; [66292-28-2]	44.5	317.7
Hexadecylethanoate; $C_{18}H_{36}O_2$; [629-70-9]	47.5	320.7
Methylheptadecanoate; $C_{18}H_{36}O_2$; [1731-92-6]	53.5	326.7
Ethylhexadecanoate; $C_{18}H_{36}O_2$; [628-97-7]	59.5	332.7
Pentadecylpropanoate; $C_{18}H_{36}O_2$	60.0	333.2
Propylpentadecanoate; $C_{18}H_{36}O_2$; [42232-08-6]	63.0	336.2
Tetradecylbutanoate; $C_{18}H_{36}O_2$; [6221-98-3]	63.5	336.7
Butyltetradecanoate; $C_{18}H_{36}O_2$; [110-36-1]	65.0	338.2
Dodecylhexanoate; $C_{18}H_{36}O_2$; [6938-60-9]	66.5	339.7
Hexyldodecanoate; $C_{18}H_{36}O_2$; [34316-64-8]	67.5	340.7
Octyldecanoate; $C_{18}H_{36}O_2$; [2306-92-5]	68.0	341.2
Decyloctanoate; $C_{18}H_{36}O_2$; [2306-89-0]	68.0	341.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described in Schmid *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(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:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Hexadecyl esters; $C_{18}H_{36}O_2$–$C_{34}H_{68}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372–81 (1965).

Variables:
T/K=321–426

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+hexadecyl ester

Hexadecyl ester	t/°C	T/K (compiler)
Hexadecylethanoate; $CH_{18}H_{36}O_2$; [629-70-9]	47.5	320.7
Hexadecylbutanoate; $C_{20}H_{40}O_2$; [6221-99-4]	79.0	352.2
Hexadecylhexanoate; $C_{22}H_{44}O_2$; [14331-11-4]	95.0	368.2
Hexadecyloctanoate; $C_{24}H_{48}O_2$; [29710-31-4]	108.0	381.2
Hexadecyldecanoate; $C_{26}H_{52}O_2$; [29710-34-7]	119.0	392.2
Hexadecyldodecanoate; $C_{28}H_{56}O_2$; [20834-06-4]	128.0	401.2
Hexadecyltetradecanoate; $C_{30}H_{60}O_2$; [2599-01-1]	136.5	409.7
Hexadecylhexadecanoate; $C_{32}H_{64}O_2$; [540-10-3]	145.0	418.2
Hexadecyloctadecanoate; $C_{34}H_{68}O_2$; [1190-63-2]	152.5	425.7

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 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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g\cdot L^{-1}$.
(2) Not specified.

Estimated Error:
Temperature: ±0.5 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Esters; $C_{20}H_{40}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:
T/K=336–357

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+ester

Ester	t/°C	T/K (compiler)
Nonadecylmethanoate; $C_{20}H_{40}O_2$; [66455-49-0]	62.5	335.7
Octadecylethanoate; $C_{20}H_{40}O_2$; [822-23-1]	65.0	338.2
Methylnonadecanoate; $C_{20}H_{40}O_2$; [1731-94-8]	70.0	343.2
Heptadecylpropanoate; $C_{20}H_{40}O_2$; [66455-48-9]	75.0	348.2
Ethyloctadecanoate; $C_{20}H_{40}O_2$; [111-61-5]	75.5	348.7
Propylheptadecanoate; $C_{20}H_{40}O_2$; [26718-84-3]	79.0	352.2
Hexadecylbutanoate; $C_{20}H_{40}O_2$; [6221-99-4]	79.0	352.2
Butylhexadecanoate; $C_{20}H_{40}O_2$; [111-06-8]	81.0	354.2
Tetradecylhexanoate; $C_{20}H_{40}O_2$; [71801-23-5]	82.0	355.2
Hexyltetradecanoate; $C_{20}H_{40}O_2$; [42231-99-2]	83.0	356.2
Dodecyloctanoate; $C_{20}H_{40}O_2$; [20292-09-5]	83.0	356.2
Octyldodecanoate; $C_{20}H_{40}O_2$; [5303-24-2]	83.5	356.7
Decyldecanoate; $C_{20}H_{40}O_2$; [1654-86-0]	83.5	356.7

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 *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:
(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g\cdot L^{-1}$.
(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:
[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Esters; $C_{22}H_{44}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:
T/K=351–370

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+ester

Ester	t/°C	T/K (compiler)
Heneicosylmethanoate; $C_{22}H_{44}O_2$	78.0	351.2
Eicosylethanoate; $C_{22}H_{44}O_2$; [822-24-2]	82.0	355.2
Methylheneicosanoate; $C_{22}H_{44}O_2$; [6064-90-0]	85.0	358.2
Ethyleicosanoate; $C_{22}H_{44}O_2$; [18281-05-5]	89.0	362.2
Nonadecylpropanoate; $C_{22}H_{44}O_2$; [66326-06-5]	89.0	362.2
Propylnonadecanoate; $C_{22}H_{44}O_2$; [27593-68-6]	92.5	365.7
Octadecylbutanoate; $C_{22}H_{44}O_2$; [13373-83-6]	93.0	366.2
Butyloctadecanoate; $C_{22}H_{44}O_2$; [123-95-5]	94.0	367.2
Hexadecylhexanoate; $C_{22}H_{44}O_2$; [14331-11-4]	95.0	368.2
Hexylhexadecanoate; $C_{22}H_{44}O_2$; [42232-25-7]	95.5	368.7
Tetradecyloctanoate; $C_{22}H_{44}O_2$; [16456-36-3]	96.0	369.2
Octyltetradecanoate; $C_{22}H_{44}O_2$; [16260-26-7]	96.5	369.7
Decyldodecanoate; $C_{22}H_{44}O_2$; [35528-28-6]	97.0	370.2
Dodecyldecanoate; $C_{22}H_{44}O_2$; [42231-50-5]	97.0	370.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described in Schmid *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D)=1.3820$, $d(20\ °C)=1134\ g\cdot L^{-1}$.
(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:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(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 $C_{32}H_{64}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **9**, 134–44 (1965).

Variables:
T/K=381–418

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+ester

Ester	t/°C	T/K (compiler)
Hexadecyloctanoate; $C_{24}H_{48}O_2$; [29710-31-4]	108.0	381.2
Octylhexadecanoate; $C_{24}H_{48}O_2$; [16958-85-3]	108.5	381.7
Decylhexadecanoate; $C_{26}H_{52}O_2$; [42232-27-9]	119.0	392.2
Hexadecyldecanoate; $C_{26}H_{52}O_2$; [29710-34-7]	119.0	392.2
Dodecylhexadecanoate; $C_{28}H_{56}O_2$; [42232-29-1]	128.0	401.2
Hexadecyldodecanoate; $C_{28}H_{56}O_2$; [20834-06-4]	128.0	401.2
Tetradecylhexadecanoate; $C_{30}H_{60}O_2$; [4536-26-9]	136.5	409.7
Hexadecyltetradecanoate; $C_{30}H_{60}O_2$; [2599-01-1]	136.5	409.7
Hexadecylhexadecanoate; $C_{32}H_{64}O_2$; [540-10-3]	145.0	418.2

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. A Reichert microscope, type RCH, equipped with a heating stage was used as described in Schmid *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D)=1.3820$, $d(20\ °C)=1134\ g\cdot L^{-1}$.
(2) Synthesized by transesterification of methyl esters and acetates using sodium methanoate as catalyst; purified by gas–liquid partition and thin-layer adsorption chromatography.

Estimated Error:
Temperature: ±0.5 K.

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Cholesteryl esters; $C_{39}H_{68}O_2$–$C_{49}H_{88}O_2$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372–81 (1965).

Variables:
T/K=441–471

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+cholesteryl ester

Cholesteryl ester	t/°C	T/K (compiler)
Cholest-5-en-3-yldodecanoate; $C_{39}H_{68}O_2$; [1908-11-8]	168.0	441.2
Cholest-5-en-3-yltetradecanoate; $C_{41}H_{72}O_2$; [1989-52-2]	175.0	448.2
Cholest-5-en-3-ylhexadecanoate; $C_{43}H_{76}O_2$; [601-34-3]	181.5	454.7
Cholest-5-en-3-yloctadecanoate; $C_{45}H_{80}O_2$; [35602-69-8]	187.0	460.2
Cholest-5-en-3-yleicosanoate; $C_{47}H_{84}O_2$; [2573-03-7]	192.0	465.2
Cholest-5-en-3-yldocosanoate; $C_{49}H_{88}O_2$; [61510-09-6]	197.5	470.7

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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

---

14. Nitromethane+Nitrogen Compounds

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2′-Iminobisethanol; $C_4H_{11}NO_2$; [111-42-2]

Evaluator:
V. P. Sazonov, Technical University, Samara, Russia, August 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and 2,2′-iminobisethanol have been reported in only two publications. Cherkasova *et al.*[1] carried out measurements of the mutual solubilities of the components between 288 and 338 K by the synthetic method. Zhuravleva *et al.*[2] studied the mutual solubilities of (1) and (2) between 291 and 339 K, also by the synthetic method.

Values obtained by the graphical interpolation or extrapolation from the data sheets are presented in the following table. Data are ‘‘recommended’’ if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Tentative values for the mutual solubilities of nitromethane and 2,2′-iminobisethanol

	Alcohol-rich phase		Nitromethane-rich phase	
T/K	100 w_1	x_1	100 w_2	x_2
293	25	0.37	1.8	0.011
303	28	0.40	2.1	0.013
313	31	0.44	3.5	0.020
323	38	0.51	5.8	0.034
333	46	0.60	11.8	0.072

The upper critical solution temperature has been reported as 337.7 K (Cherkasova *et al.*[1]) and 339.2 K (Zhuravleva *et al.*[2]). Thus, the tentative value is: 338.5±0.8 K. The corresponding critical solution composition has been reported as $x_{c1} = 0.770$ (Cherkasova *et al.*[1]) and $x_{c1} = 0.789$ (Zhuravleva *et al.*[2]), giving a tentative average $x_{c1} = 0.78 \pm 0.01$.

The tentative values for the mutual solubility reported in the above table have been approximated by the equation based on scaling law (described in the Introduction material to this volume ‘‘Relations of Solubility Data in Binary Systems Containing Nitromethane’’) and the following parameters have been adjusted: $a_1 = 0.675\ 85$, $a_2 = -0.194\ 28$, $b_1 = 0.768\ 81$, $b_2 = -1.230\ 84$ (mean standard error of estimate was 0.0052).

As an approximation, the tentative values of UCST and x_{c1} have been used. This relationship is presented in Fig. 39 together with experimental data.[1,2]

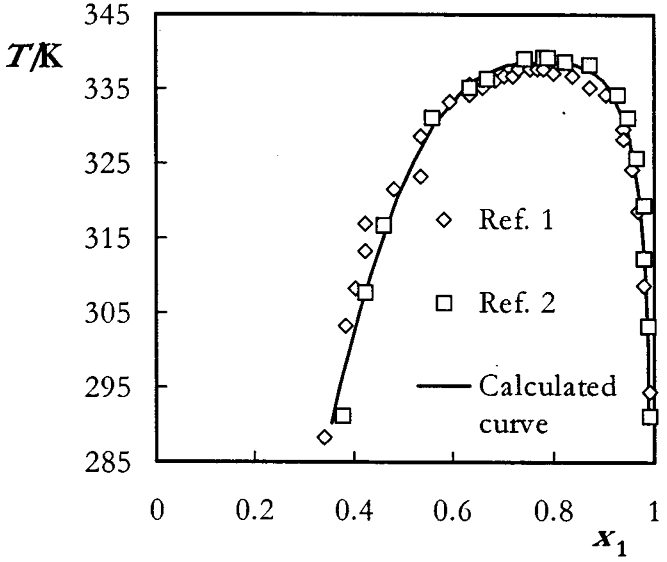

FIG. 39. Mutual solubility of nitromethane and 2,2′-iminobisethanol.

References:

[1] N. M. Cherkasova, I. K. Zhuravleva, E. F. Zhuravlev, and V. B. Mukhametshina, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **17**, 1602 (1974). Deposited Doc., VINITI 1181 (1974).

[2] I. K. Zhuravleva, E. F. Zhuravlev, and R. S. Islamova, Zh. Fiz. Khim. **48**, 1863 (1974). Deposited Doc., VINITI 873 (1974).

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2′-Iminobisethanol; $C_4H_{11}NO_2$; [111-42-2]

Original Measurements:

N. M. Cherkasova, I. K. Zhuravleva, E. F. Zhuravlev, and V. B. Mukhametshina, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **17**, 1602 (1974).
*Deposited Doc., VINITI 1181 (1974).

Variables:

T/K = 288–338

Prepared By:

V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2′-iminobisethanol

		Iminobisethanol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
15.0	288.2	23.0	0.340	—	—
21.2	294.4	—	—	98.6	0.992
30.0	303.2	26.5	0.383	—	—
35.0	308.2	28.2	0.404	—	—
35.5	308.7	—	—	96.5	0.979
40.0	313.2	30.0	0.425	—	—
43.8	317.0	30.0	0.425	—	—
45.5	318.7	—	—	94.5	0.967
48.3	321.5	35.0	0.481	—	—
50.0	323.2	40.0	0.535	—	—
51.0	324.2	—	—	93.0	0.958
55.0	328.2	—	—	90.0	0.939
55.5	328.7	40.0	0.535	—	—
56.5	329.7	—	—	90.0	0.939
60.0	333.2	46.0	0.595	—	—
61.0	334.2	50.0	0.633	84.5	0.904
62.0	335.2	53.0	0.660	80.0	0.873
62.3	335.5	50.0	0.633	—	—
63.0	336.2	56.0	0.687	—	—
63.5	336.7	58.0	0.704	75.0	0.838
63.5	336.7	60.0	0.721	—	—
64.0	337.2	—	—	70.0	0.801
64.5	337.7	61.5	0.733	67.5	0.781
64.5	337.7	64.0	0.754	—	—
64.5	337.7	66.0	0.770	66.0	0.770 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:

(1) Source not specified; pure grade reagent; freshly distilled; b.p. = 101.3 °C, $n(20\ °\mathrm{C,D}) = 1.3816$.
(2) Source not specified; pure grade reagent; freshly distilled; $n(20\ °\mathrm{C,D}) = 1.4770$, $d(20\ °\mathrm{C}) = 1097\ \mathrm{g \cdot L^{-1}}$.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 2,2′-Iminobisethanol; $C_4H_{11}NO_2$; [111-42-2]

Original Measurements:
I. K. Zhuravleva, E. F. Zhuravlev, and R. S. Islamova, Zh. Fiz. Khim. **48**, 1863 (1974).
*Deposited Doc., VINITI 873 (1974).

Variables:
T/K=291–339

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and 2,2′-iminobisethanol

		Iminobisethanol-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
18.0	291.2	26.0	0.377	98.5	0.991
30.0	303.2	—	—	98.0	0.988
34.5	307.7	30.0	0.425	—	—
39.2	312.4	—	—	96.7	0.981
43.5	316.7	33.3	0.462	—	—
46.5	319.5	—	—	96.4	0.979
52.5	325.7	—	—	94.2	0.966
58.0	331.2	42.5	0.560	91.5	0.949
61.0	334.2	—	—	88.3	0.929
61.9	335.1	50.0	0.633	—	—
63.2	336.4	54.0	0.669	—	—
65.0	338.2	—	—	80.0	0.873
65.5	338.7	—	—	73.3	0.825
65.8	339.0	62.7	0.743	—	—
66.0	339.2	67.5	0.782	—	—
68.5	341.7	68.5	0.789	68.5	0.789 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; pure grade reagent; freshly distilled.
(2) Source not specified; pure grade reagent; freshly distilled.

Estimated Error:
Not reported.

References:
[1] V. F. Alekseev. Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 6-(Hydroxyimino)-6-nitrohexanoic acid; $C_6H_{10}N_2O_{15}$; [1069-46-1]

Original Measurements:
Z. S. Smolyan, G. N. Matveeva, V. K. Fukin, K. N. Korotaevskii, A. P. Ignat'eva, A. N. Kornilina, L. S. Zvereva, and A. S. Fomin, Khim. Prom-st (Moscow) **48**, 508–9 (1972).

Variables:
T/K=298

Prepared By:
V. P. Sazonov

Experimental Data

The solubility of 6-(hydroxyimino)-6-nitrohexanoic acid in nitromethane at 25 °C (298 K, compiler) was reported to be 100 w_2 =2.8. The corresponding mole fraction, x_2, calculated by the compiler, is 0.0092.

Auxiliary Information

Method/Apparatus/Procedure:
No further 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) Nitromethane; CH_3NO_2; [75-52-5]
(2) N, N-Diethylethanamine; $C_6H_{15}N$; [121-44-8]

Evaluators:
V. P. Sazonov, Technical University, Samara, Russia.
G. T. Hefter, Murdoch University, Perth, Australia
A. Skrzecz, Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland, July, 1999.

Critical Evaluation

Solubilities in the system comprising nitromethane and N, N-diethylethanamine have been reported in three publications. Burdykina and Zhuravlev[1,2] determined the mutual solubility of (1) and (2) at 273 and 278 K and also the upper critical solution temperature by the synthetic method. Sinegubova *et al.*[3] measured the mutual solubilities of the two components at 263 K by the titration method. As might be expected, the data of Burdkykina and Zhuravlev[1,2] are self-consistent.

The experimental data reported in these three studies[1–3] have been approximated (with the same weighing factor) by the equation based on scaling law (described in the Introduction material to this volume ''Relations of Solubility Data in Binary Systems Containing Nitromethane'') and the following parameters have been adjusted: $a_1 = 0.650\,41$, $a_2 = 0.454\,78$, $b_1 = 6.209\,07$, $b_2 = -5.553\,74$ (mean standard error of estimate was 0.1106).

As an approximation, the UCST$=284.8$ K and $x_{c1} = 0.656$[1,2] have been used. In the opinion of the evaluators, in spite of the large estimation error, the estimated curve describes the solubility of the system and the calculated values reported in the following table for selected temperatures may be treated as tentative. This relationship together with all experimental points[1–3] are also presented in Fig. 40.

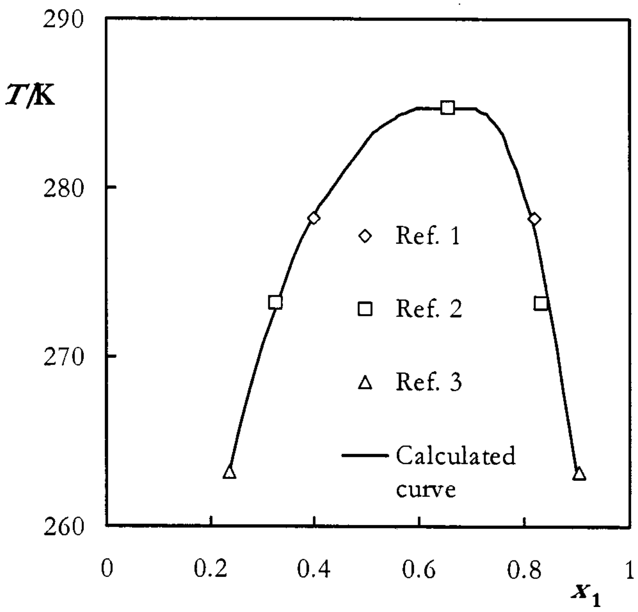

FIG. 40. Mutual solubility of nitromethane and N,N-diethylethanamine.

Mutual solubility of nitromethane and N, N-diethylethanamine

	Amine-rich phase		Nitromethane-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
263.2	0.2355	15.67	0.8995	84.38
268.2	0.2770	18.77	0.8738	80.68
273.2	0.3283	22.77	0.8462	76.84
278.2	0.3966	28.39	0.8137	72.49
279.2	0.4138	29.86	0.8059	71.47
280.2	0.4328	31.52	0.7973	70.35
281.2	0.4544	33.44	0.7875	69.09
282.2	0.4797	35.74	0.7757	67.60
283.2	0.5113	38.69	0.7602	65.66
284.2	0.5576	43.20	0.7344	62.52

References:

[1] R. I. Burdykina and E. F. Zhuravlev, Zh. Fiz. Khim. **42**, 1925 (1968).
[2] E. F. Zhuravlev and R. I. Burdykina, Zh. Fiz. Khim. **43**, 895 (1969).
[3] S. I. Sinegubova, A. G. Demakhin, V. M. Ovsyannikov, and Y. Shnarevich, Zh. Obshch. Khim. **58**, 1718 (1988).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) N,N-Diethylethanamine; $C_6H_{15}N$; [121-44-8]

Original Measurements:
E. F. Zhuravlev and P. I. Burdykina, Zh. Fiz. Khim. **43**, 895–900 (1969).

Variables:
T/K=273 and 285

Prepared By:
V. P. Sazonov

Experimental Data

Mutual solubility of nitromethane and N, N-diethylethanamine

		Amine-rich phase		Nitromethane-rich phase	
t/°C	T/K (compiler)	100 w_1	x_1 (compiler)	100 w_1	x_1 (compiler)
0.0	273.2	22.4	0.324	74.8	0.831
11.6	284.8	53.5	0.656	53.5	0.656 (UCST)

Auxiliary Information

Method/Apparatus/Procedure:
The synthetic method[1] was used. No further details were reported.

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

Estimated Error:
Not reported

References:
[1] V. F. Alekseev. Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) N,N-Diethylethanamine; $C_6H_{15}N$; [121-44-8]

Original Measurements:
S. I. Sinegubova, A. G. Demakhin, V. M. Ovsyannikov, and Y. Shnarevich, Zh. Obshch. Khim. **58**, 1718–1723 (1988).

Variables:
T/K=263

Prepared By:
V. P. Sazonov

Experimental Data

The solubility of nitromethane in N,-N-diethylethanamine at −10.0 °C (263.2 K, compiler) was reported to be 100 w_1=15.73. The corresponding mole fraction, x_1, calculated by the compiler is 0.2363.

The solubility of N,N-diethylethanamine in nitromethane at −10.0 °C (263.2 K, compiler) was reported to be 100 w_2=14.98. The corresponding mole fraction, x_2, calculated by the compiler is 0.0961.

Auxiliary Information

Method/Apparatus/Procedure:
The titration method[1] was used. No further details were reported.

Source and Purity of Materials:
(1) Source not specified; dried and twice distilled; b.p. =101 °C, $n(20\ °C,D)=1.3819$.
(2) Source not specified; dried and distilled; b.p. =(89.5 to 89.7) °C, $n(20\ °C,D)=1.4010$.

Estimated Error:
Not reported.

References:
[1] W. D. Bancroft, Phys. Rev. **3**, 21 (1896).

15. Nitromethane+Glycerides

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1-Monoglycerides; $C_{15}H_{30}O_4$, $C_{17}H_{34}O_4$, $C_{19}H_{38}O_4$ and $C_{21}H_{42}O_4$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372–81 (1965).

Variables:

$T/\mathrm{K}=315-343$

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+1-monoglyceride

1-Monoglyceride	$t/°\mathrm{C}$	T/K (compiler)
1-Dodecanoyloxy-2,3-propanediol; $C_{15}H_{30}O_4$; [142-18-7]	42.0	315.2
1-Tetradecanoyloxy-2,3-propanediol; $C_{17}H_{34}O_4$; [589-68-4]	54.0	327.2
1-Hexadecanoyloxy-2,3-propanediol; $C_{19}H_{38}O_4$; [542-44-9]	63.0	336.2
1-Octadecanoyloxy-2,3-propanediol; $C_{21}H_{42}O_4$; [123-94-4]	70.0	343.2

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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °\mathrm{C,D})=1.3820$, $d(20\ °\mathrm{C})=1134\ \mathrm{g \cdot L^{-1}}$.
(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

Components:

(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,3-Diglycerides; $C_{27}H_{52}O-C_{39}H_{76}O_5$

Original Measurements:

H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372–81 (1965)

Variables:

$T/\mathrm{K}=327-381$

Prepared By:

V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+1,3-diglyceride

1,3-Diglyceride	$t/°\mathrm{C}$	T/K (compiler)
1-Didodecanoyloxy-2-propanol; $C_{27}H_{52}O_5$; [539-93-5]	53.5	326.7
1,3-Ditetradecanoyloxy-2-propanol; $C_{31}H_{60}O_5$; [7770-09-4]	73.0	346.2
1,3-Dihexadecanoyloxy-2-propanol; $C_{35}H_{68}O_5$; [502-52-3]	92.0	365.2
1,3-Dioctadecanoyloxy-2-propanol; $C_{39}H_{26}O_5$; [504-40-5]	108.0	381.2

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 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) Fisher Scientific Co.; certified, No. N-98; $n(20\ °\mathrm{C,D})=1.3820$, $d(20\ °\mathrm{C})=1134\ \mathrm{g \cdot L^{-1}}$.
(2) Not specified.

Estimated Error:

Temperature: ±0.5 K.

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Triglycerides; $C_{27}H_{50}O_6$–$C_{69}H_{128}O_6$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 297–302 (1963).

Variables:
T/K=288–441

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+triglyceride

Triglyceride	t/°C	T/K (compiler)
1,2,3-Trioctanoyloxypropane (tricaprylin); $C_{27}H_{50}O_6$; [528-23-8]	15.0	288.2
1,2,3-Tridecanoyloxypropane (tricaprin); $C_{33}H_{62}O_6$; [621-71-6]	60.0	333.2
1,2,3-Tri(cis,cis,cis-9,12,15-octadecatrienoyloxy)propane (trilinolenin); $C_{57}H_{92}O_6$; [14465-68-0]	86.0	359.2
1,2,3-Tridodecanoyloxypropane (trilaurin); $C_{39}H_{74}O_6$; [538-24-9]	91.5	364.7
1,2,3-Tri(cis,cis,cis-9,12-octadecadienoyloxy)propane (trilinolein); $C_{57}H_{98}O_6$; [537-40-6]	107.0	380.2
1,2,3-Tri(cis-9-hexadecenoyloxy)propane (tripalmitolein); $C_{51}H_{92}O_6$; [20246-55-3]	110.5	383.7
1,2,3-Tritetradecanoyloxypropane (trimyristin); $C_{45}H_{86}O_6$; [555-45-3]	115.5	388.7
1,2,3-Tri(cis-9-octadecenoyloxy)propane (triolein); $C_{57}H_{104}O_6$; [122-32-7]	130.0	403.2
1,2,3-Tri(cis-6-octadecenoyloxy)propane (tripetroselinin); $C_{57}H_{104}O_6$; [50650-45-8]	132.0	405.2
1-Hexadecanoyloxy-2,3-di(cis-9-octadecenoyloxy)propane (1-palmito-2,3-diolein); $C_{55}H_{102}O_6$; [27071-84-7]	132.0	405.2
2-Hexadecanoyloxy-1,3-di(cis-9-octadecenoyloxy)propane (2-palmito-1,3-diolein); $C_{55}H_{102}O_6$; [1716-07-0]	132.0	405.2
1,2,3-Tri(trans-9-octadecenoyloxy)propane (trielaidin); $C_{57}H_{104}O_6$; [537-39-3]	133.5	406.7
1,2,3-Trihexadecanoyloxypropane (tripalmitin); $C_{51}H_{98}O_6$; [555-44-2]	135.0	408.2
1,3-Dihexadecanoyloxy-2-(cis-9-octadecenoyloxy)propane (1,3-dipalmito-2-olein); $C_{53}H_{100}O_6$; [28409-94-1]	135.0	408.2
1-Octadecanoyloxy-2,3-di(cis-9-octadecenoyloxy)propane (1-stearo-2,3-diolein); $C_{57}H_{106}O_6$; [29590-02-1]	135.0	408.2
2-Octadecanoyloxy-1,3-di(cis-9-octadecenoyloxy)propane (2-stearo-1,3-diolein); $C_{57}H_{106}O_6$; [2410-29-9]	135.5	408.7
1-Hexadecanoyloxy-2-octadecanoyloxy-3-(cis-9-octadecenoyloxy)propane (1-palmito-2-stearo-3-olein); $C_{55}H_{104}O_6$; [26836-31-7]	140.0	413.2
1-Hexadecanoyloxy-3-octadecanoyloxy-2-(cis-9-octadecenoyloxy)propane (1-palmito-3-stearo-2-olein); $C_{55}H_{104}O_6$	140.0	413.2
1,3-Dioctadecanoyloxy-2-(cis-9-octadecenoyloxy)propane (1,3-distearo-2-olein); $C_{57}H_{108}O_6$; [28880-75-3]	144.5	417.7
1,2,3-Tri-11-eicosenoyloxypropane (tri-11-eicosenoin); $C_{63}H_{116}O_6$; [115936-00-0]	145.0	418.2
1,2,3-Trioctadecanoyloxypropane (tristearin); $C_{57}H_{110}O_6$; [555-43-1]	152.0	425.2
1,2,3-Tri(cis-13-docosenoyloxy)propane (trierucin); $C_{69}H_{128}O_6$; [2752-99-0]	160.0	433.2
1,2,3-Trieicosanoyloxypropane (triarachidin); $C_{63}H_{122}O_6$; [620-64-4]	167.5	440.7

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 *et al.*[1] The disappearance and reappearance of the interface between (1) and (2) could be observed without difficulty.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98; $n(20\ °C,D) = 1.3820$, $d(20\ °C) = 1134\ g \cdot L^{-1}$.
(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:
[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, Microchem. J. **7**, 287 (1963).

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) 1,2-Dialkoxy-glycerides; $C_{45}H_{90}O_4$–$C_{59}H_{118}O_4$

Original Measurements:
H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, Microchem. J. **11**, 306–14 (1966).

Variables:
T/K=426–458

Prepared By:
V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+1,2-dialkoxy-glyceride

Ether	t/°C	T/K (compiler)
2-(Dodecyloxy)-3-(octadecyloxy)propyl ester lauric acid; $C_{45}H_{90}O_4$; [10322-44-8]	153.0	426.2
(Z,Z,Z)-2,3-Bis(9-octadecenyloxy)propyl ester oleic acid; $C_{57}H_{108}O_4$; [10322-53-9]	159.0	432.2
2-(Hexadecyloxy)-3-(octadecyloxy)propyl ester lauric acid; $C_{49}H_{98}O_4$; [10322-47-1]	164.0	437.2
(Z,Z)-2-(9-octadecenyloxy)-3-(octadecyloxy)propyl ester oleic acid; $C_{57}H_{110}O_4$; [10322-52-8]	166.5	439.7
2,3-Bis(hexadecyloxy)propyl ester hexadecanoic acid; $C_{51}H_{102}O_4$; [10322-42-6]	168.5	441.7
2-(Dodecyloxy)-3-(octadecyloxy)propyl ester stearic acid; $C_{51}H_{102}O_4$; [10322-45-9]	169.0	442.2
2,3-Bis(octadecyloxy)propyl ester lauric acid; $C_{51}H_{102}O_4$; [10322-49-3]	170.0	443.2
3-(Octadecyloxy)-2-(tetradecyloxy)propyl ester stearic acid; $C_{53}H_{106}O_4$; [10322-46-0]	172.5	445.7
2,3-Bis(octadecyloxy)propyl ester (Z)-9-octadecenoic acid; $C_{57}H_{112}O_4$; [10322-51-7]	173.5	446.7
2-(Hexadecyloxy)-3-(octadecyloxy)propyl ester stearic acid; $C_{55}H_{110}O_4$; [10322-48-2]	177.0	450.2
3-(Hexadecyloxy)-2-(octadecyloxy)propyl ester stearic acid; $C_{55}H_{110}O_4$; [10322-43-7]	177.0	450.2
2,3-Bis(octadecyloxy)propyl ester octadecanoic acid; $C_{57}H_{114}O_4$; [10322-50-6]	181.0	454.2
2-(Eicosyloxy)-3-(octadecyloxy)propyl ester stearic acid; $C_{59}H_{118}O_4$; [10322-54-0]	185.0	458.2

Auxiliary Information

Method/Apparatus/Procedure:

A microscope equipped with a heating stage[1] was employed for determining UCST values. No further experimental details are given.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98.
(2) Synthesized as in Baumann and Mangold.[2]

Estimated Error:
Not specified.

References:
[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).
[2] W. J. Baumann and H. K. Mangold, J. Org. Chem. **29**, 3055 (1964).

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) 1-Alkoxy-diglycerides; $C_{45}H_{88}O_5$–$C_{61}H_{120}O_5$	H. H. O. Schmid, H. K. Mangold, W. O. Lundberg, and W. J. Baumann, Microchem. J. **11**, 306–14 (1966).
Variables:	**Prepared By:**
T/K=409–448	V. P. Sazonov

Experimental Data

Upper critical solution temperatures of the systems nitromethane+1-alkoxy-diglyceride

1-Alkoxy-diglyceride	t/°C	T/K (compiler)
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester lauric acid; $C_{45}H_{88}O_5$; [10322-28-8]	135.5	408.7
(Z)-[(9-Octadecenyloxy)methyl]-1,2-ethanediyl ester oleic acid; $C_{57}H_{106}O_5$; [10322-38-0]	144.0	417.2
1-[(Decyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{49}H_{96}O_5$; [10431-17-1]	146.0	419.2
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester tetradecanoic acid; $C_{49}H_{96}O_5$; [10322-29-9]	146.5	419.7
1-[(Undecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{50}H_{98}O_5$; [10322-31-3]	149.0	422.2
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester oleic acid; $C_{57}H_{108}O_5$; [10329-25-6]	151.0	424.2
1-[(Dodecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{51}H_{100}O_5$; [10322-32-4]	152.0	425.2
1-[(Tridecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{52}H_{102}O_5$; [10322-33-5]	155.0	428.2
1-[(Tetradecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{53}H_{104}O_5$; [10322-34-6]	157.5	430.7
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester palmitic acid; $C_{53}H_{104}O_5$; [10322-30-2]	158.0	431.2
(Z)-[(9-Octadecenyloxy)methyl]-ethanediyl ester stearic acid; $C_{57}H_{110}O_5$; [10322-37-9]	158.5	431.7
1-[(Pentadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{54}H_{106}O_5$; [10431-21-7]	160.0	433.2
1-[(Hexadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{55}H_{108}O_5$; [923-63-7]	162.0	435.2
1-[(Heptadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{56}H_{110}O_5$; [10322-27-7]	164.0	437.2
1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{57}H_{112}O_5$; [923-62-6]	166.5	439.7
1-[(Nonadecyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{58}H_{114}O_5$; [10322-39-1]	168.5	441.7
1-[(Eicosyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{59}H_{116}O_5$; [10322-40-4]	170.5	443.7
1-[(Heneicosyloxy)methyl]-1,2-ethanediyl ester stearic acid; $C_{60}H_{118}O_5$; [10322-41-5]	172.5	445.7
1-[(Octadecyloxy)methyl]-ethanediyl ester eicosanoic acid; $C_{61}H_{120}O_5$; [10322-36-8]	175.0	448.2

Auxiliary Information

Method/Apparatus/Procedure:

A microscope equipped with a heating stage[1] was employed for determining UCST values. No further experimental details are given.

Source and Purity of Materials:

(1) Fisher Scientific Co.; certified, No. N-98.
(2) Synthesized as in Baumann and Mangold.[2]

Estimated Error:

Not specified.

References:

[1] H. H. O. Schmid, H. K. Mangold, and W. O. Lundberg, J. Am. Oil Chem. Soc. **42**, 372 (1965).

[2] W. J. Baumann and H. K. Mangold, J. Org. Chem. **29**, 3055 (1964).

16. Nitromethane+Crude Compounds

Components:	**Original Measurements:**
(1) Nitromethane; CH_3NO_2; [75-52-5] (2) Oils	L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel **4**, 26–8 (1968).
Variables:	**Prepared By:**
T/K=415–538	V. P. Sazonov

Experimental Data

Solubility temperatures of nitromethane and oil mixtures in the ratio 3:1

Oil	f.p. oil/°C	Kinematic viscosity oil/cSt	t/°C	T/K (compiler)
Diesel fuel	−56	8.5 (20 °C)	142[a]	415
Distillate	−45.5	7.84 (50 °C)	200[a]	473
Distillate	−33	16.5 (50 °C)	235[a]	508
Distillate	−27	6.28 (100 °C)	245[a]	518
Residual	−18	20.55 (100 °C)	265[a]	538

[a] These data were determined by extrapolation of oil solubility curves in mixtures of nitromethane/toluene solvents.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described in Poole,[1] was used. No further experimental details were given.

Source and Purity of Materials:

(1) Not specified.
(2) Prepared from Tuimaza crude oil.

Estimated Error:

Not reported.

Rerferences:

[1] G. M. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

Components:
(1) Nitromethane; CH_3NO_2 ; [75-52-5]
(2) Paraffins

Original Measurements:
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel **4**, 26–8 (1968).

Variables:
T/K=276–331

Prepared By:
V. P. Sazonov

Experimental Data

Solubilities of paraffins in nitromethane over the below temperature ranges are presented graphically in the form of straight lines for temperature vs $g(2)/100\ g(1)$ in log coordinates.

Paraffin	f.p. paraffin/°C	Temperature range/°C	Temperature range/K (compiler)
Paraffin	13.2	3–43	276–316
Paraffin	28.0	8–40	281–313
Paraffin[a]	41.7	28–46	301–319
Paraffin[a]	50.7	26–58	299–331

[a] Obtained by separation of the third oil fraction of Tuimazin crude.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method, described in Poole,[1] was used. No further experimental details were given.

Source and Purity of Materials:

(1) Not specified.
(2) Obtained by separation of narrow fractions with b.p. =196–270 and 300–365 °C from a wide fraction of diesel fuel. The remainder were obtained by separation of the third oil fraction of Tuimazin crude.

Estimated Error:
Not reported.

References:
[1] G. M. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

---

17. Nitromethane+Polymers

Components:
(1) Nitromethane; CH_3NO_2; [75-52-5]
(2) Polymers

Original Measurements:
C. S. Marvel, J. Harkema, and M. J. Copley, J. Am. Chem. Soc. **63**, 1609 (1941).

Variables:
T/K=298 and 303

Prepared By:
V. P. Sazonov

Experimental Data

Solubility of polymers in nitromethane

Polymer	$g(2)/100\ g(1)$	100 w_2 (compiler)
Temperature: 25 °C (298 K, compiler)		
Poly(1-acetoxy-1,2-ethanediyl)* (polyvinylacetate); $(C_6H_6O_2)_n$; [9003-20-7]	93	48
Poly 1-(methylcarbonyl)1,2-ethanediyl* (polymethylvinyl ketone); $(C_4H_6O)_n$	35	26
Poly 1-(methoxycarbonyl)-1-methyl-1,2-ethanediyl (polymethyl methacrylate); $(C_5H_8O_2)_n$; [9011-14-7]	19	16
Temperature: 30 °C (303 K, compiler)		
Vinylite* (copolymer of vinyl chloride and vinyl acetate containing 34.1% Cl)	2.1	2.0
Cellulose acetate; [9004-35-7]	0.017	0.017
Poly(1-chloro-1,2-ethanediyl)* (polyvinylchloride); $(C_2H_3Cl)_n$; [25038-46-4]	0.004	0.004

Auxiliary Information

Method/Apparatus/Procedure:

The method described in Marvel *et al.*[1] was used. The solubility determinations were made by adding an excess of the polymer to the solvent in a glass-stoppered bottle. The stoppered bottle was placed in a rotating device in a thermostat at 30 °C for 48 h. The saturated solution was removed, weighed, evaporated, and the residue weighed. This method worked well in cases where the solubility was low. In other cases, a weighed amount of solvent was added to a weighed sample of polymer. The mixture was shaken and allowed to stand at 25 °C for 48 h to see whether it became homogeneous. It was impossible to make accurate measurements even by this procedure. Hence the values given in the table for these high solubilities are to be regarded as minimum values.

Source and Purity of Materials:

(1) Source not specified; laboratory sample; redistilled and collected over a 2 °C boiling range.
(2) Some polymers (*) obtained from Carbide and Carbon Chemicals Corp.; others from du Pont Co.; technical grade.

Estimated Error:
Temperature: ±1 K
Solubility: about 10% (relative error).

References:
[1] C. S. Marvel, F. C. Dietz, and M. J. Copley, J. Am. Chem. Soc. **62**, 2273 (1940).

18. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables

0047-2689/2000/29(5)/1338/190/$35.00

19. Registry Number Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

[112-39-0]	$C_{17}H_{34}O_2$	Methylhexadecanoate	1325
[112-40-3]	$C_{12}H_{26}$	Dodecane	E1244-E1245, 1245, 1251
[112-42-5]	$C_{11}H_{24}O$	1-Undecanol	E1286-E1287, 1287, 1298
[112-53-8]	$C_{12}H_{26}O$	1-Dodecanol	E1288-E1289, 1289-1291, 1298
[112-58-3]	$C_{12}H_{26}O$	1-Hexoxyhexane	1300
[112-61-8]	$C_{19}H_{38}O_2$	Methyloctadecanoate	1325
[112-62-9]	$C_{19}H_{36}O_2$	Methyl-*cis*-9-octadecenoate	1326
[112-70-9]	$C_{13}H_{28}O$	1-Tridecanol	E1291-E1292, 1292-1293, 1298
[112-71-0]	$C_{14}H_{29}Br$	1-Bromotetradecane	1258
[112-72-1]	$C_{14}H_{30}O$	1-Tetradecanol	1298
[112-79-8]	$C_{18}H_{34}O_2$	trans-9-Octadecenoic acid	1317
[112-80-1]	$C_{18}H_{34}O_2$	cis-9-Octadecenoic acid	E1313, 1313, 1317
[112-82-3]	$C_{16}H_{33}Br$	1-Bromohexadecane	1258
[112-85-6]	$C_{22}H_{44}O_2$	Docosanoic acid	1316
[112-86-7]	$C_{22}H_{42}O_2$	13-Docosenoic acid	1317
[112-89-0]	$C_{18}H_{37}Br$	1-Bromooctadecane	1258
[112-92-5]	$C_{18}H_{38}O$	1-Octadecanol	1298
[119-64-2]	$C_{10}H_{12}$	1,2,3,4-Tetrahydronaphthalene	1252
[121-44-8]	$C_6H_{15}N$	N,N-Diethylethanamine	E1332, 1333
[122-32-7]	$C_{57}H_{104}O_6$	1,2,3-Tri(*cis*-9-octadecenoyloxy)propane	1335
[123-51-3]	$C_5H_{12}O$	3-Methyl-1-butanol	1270
[123-94-4]	$C_{21}H_{42}O_4$	1-Octadecanoyloxy-2,3-propanediol	1334
[123-95-5]	$C_{22}H_{44}O_2$	Butyloctadecanoate	1328
[123-99-9]	$C_9H_{16}O_4$	Nonanedioic acid	1322
[124-04-9]	$C_6H_{10}O_4$	Hexanedioic acid	E1320, 1320-1321
[124-06-1]	$C_{16}H_{32}O_2$	Ethyltetradecanoate	1325
[124-07-2]	$C_8H_{16}O_2$	Octanoic acid	E1303, 1304, 1316
[124-10-7]	$C_{15}H_{30}O_2$	Methyltetradecanoate	1325
[124-11-8]	C_9H_{18}	1-Nonene	1249
[124-18-5]	$C_{10}H_{22}$	Decane	E1242-E1243, 1243, 1251
[127-18-4]	C_2Cl_4	Tetrachloroethene	E1255-E1256, 1256-1257
[135-98-8]	$C_{10}H_{14}$	(1-Methylpropyl)benzene	1252
[138-86-3]	$C_{10}H_{16}$	1-Methyl-4-(1-methylethyl)cyclohexene	1253
[141-22-0]	$C_{18}H_{34}O_3$	12-Hydroxy-*cis*-9-octadecenoic acid	1317
[141-24-2]	$C_{19}H_{36}O_3$	Methyl-12-hydroxy-*cis*-9-octadecenoate	1324
[141-82-2]	$C_3H_4O_4$	Propanedioic acid	1318
[141-93-5]	$C_{10}H_{14}$	1,3-Diethylbenzene	1252
[142-18-7]	$C_{15}H_{30}O_4$	1-Dodecanoyloxy-2,3-propanediol	1334
[142-29-0]	C_5H_8	Cyclopentene	1194
[142-62-1]	$C_6H_{12}O_2$	Hexanoic acid	1302
[142-82-5]	C_7H_{16}	Heptane	E1219-E1220, 1220-1223
[143-07-7]	$C_{12}H_{24}O_2$	Dodecanoic acid	E1307, 1308-1309, 1316
[143-08-8]	$C_9H_{20}O$	1-Nonanol	E1282, 1283, 1298
[143-15-7]	$C_{12}H_{25}Br$	1-Bromododecane	1258
[143-28-2]	$C_{18}H_{36}O$	1-Octadecenol	1299
[144-62-7]	$C_2H_2O_4$	Ethanedioic acid	1318
[287-92-3]	C_5H_{10}	Cyclopentane	1194
[291-64-5]	C_7H_{14}	Cycloheptane	1212
[292-64-8]	C_8H_{16}	Cyclooctane	1224
[334-48-5]	$C_{10}H_{20}O_2$	Decanoic acid	E1305, 1306, 1316
[373-49-9]	$C_{16}H_{30}O_2$	9-Hexadecenoic acid	1317
[375-83-7]	C_7HF_{15}	1-Hydropentadecafluoroheptane	1258
[463-40-1]	$C_{18}H_{30}O_2$	9,12,15-Octadecatrienoic acid	1317
[493-02-7]	$C_{10}H_{18}$	trans-Decahydronaphthalene	1242
[502-52-3]	$C_{35}H_{68}O_5$	1,3-Dihexadecanoyloxy-2-propanol	1334
[504-40-5]	$C_{39}H_{76}O_5$	1,3-Dioctadecanoyloxy-2-propanol	1334
[505-48-6]	$C_8H_{14}O_4$	Octanedioic acid	1322
[506-03-6]	$C_{19}H_{40}O_3$	1-Hexadecoxy-2,3-propanediol	1301
[506-12-7]	$C_{17}H_{34}O_2$	Heptadecanoic acid	1316
[506-30-9]	$C_{20}H_{40}O_2$	Eicosanoic acid	1316
[506-32-1]	$C_{20}H_{32}O_2$	Eicosatetraenoic acid	1317
[506-37-6]	$C_{24}H_{46}O_2$	15-Tetratacosenoic acid	1317
[506-43-4]	$C_{18}H_{34}O$	1-Octadecadienol	1299
[506-44-5]	$C_{18}H_{32}O$	1-Octadecatrienol	1299
[513-35-9]	C_5H_{10}	2-Methyl-2-butene	1197
[528-23-8]	$C_{27}H_{50}O_6$	1,2,3-Trioctanoyloxypropane	1335
[535-77-3]	$C_{10}H_{14}$	1-Methyl-3-(1-methylethyl)benzene	1252
[537-39-3]	$C_{57}H_{104}O_6$	1,2,3-Tri(*trans*-9-octadecenoyloxy)propane	1335

[1069-53-0]	C_9H_{20}	2,3,5-Trimethylhexane	1236
[1071-26-7]	C_9H_{20}	2,2-Dimethylheptane	1236
[1079-71-6]	$C_{14}H_{18}$	Octahydroanthracene	1252
[1117-55-1]	$C_{14}H_{28}O_2$	Hexyloctanoate	1324
[1186-49-8]	C_2HNaO_4	Ethanoic acid monosodium salt	1323
[1120-06-5]	$C_{10}H_{22}O$	2-Decanol	1298
[1120-21-4]	$C_{11}H_{24}$	Undecane	1244
[1120-28-1]	$C_{21}H_{42}O_2$	Methyleicosanoate	1325
[1120-34-9]	$C_{23}H_{44}O_2$	Methyl-cis-13-docosanoate	1326
[1190-63-2]	$C_{34}H_{68}O_2$	Hexadecyloctadecanoate	1327
[1454-84-8]	$C_{19}H_{40}O$	1-Nonadecanol	1298
[1454-85-9]	$C_{17}H_{36}O$	1-Heptedecanol	1298
[1460-98-6]	$C_{13}H_{20}$	1-Methyl-2,4-bis(1-methylethyl)benzene	1252
[1561-07-5]	$C_{15}H_{32}O_3$	1-Dodecoxy-2,3-propanediol	1301
[1653-30-1]	$C_{11}H_{24}O$	2-Undecanol	1298
[1653-31-2]	$C_{13}H_{28}O$	2-Tridecanol	1298
[1653-34-5]	$C_{15}H_{32}O$	2-Pentadecanol	1298
[1654-86-0]	$C_{20}H_{40}O_2$	Decyldecanoate	1327
[1716-07-0]	$C_{55}H_{102}O_6$	2-Hexadecanoyloxy-1,3-di(cis-9-octadecenoyloxy) propane	1335
[1731-92-6]	$C_{18}H_{36}O_2$	Methylheptadecanoate	1325, 1326
[1731-94-8]	$C_{20}H_{40}O_2$	Methylnonadecanoate	1327
[1908-11-8]	$C_{39}H_{68}O_2$	Cholest-5-en-3-yldodecanoate	1329
[1937-62-8]	$C_{19}H_{36}O_2$	Methyl-trans-9-octadecenoate	1326
[1937-63-9]	$C_{19}H_{36}O_2$	Methyl-cis-11-octadecenoate	1326
[1989-52-2]	$C_{41}H_{72}O_2$	Cholest-5-en-3-yltetradecanoate	1329
[2049-95-8]	$C_{11}H_{16}$	(1,1-Dimethylpropyl)benzene	1252
[2050-24-0]	$C_{11}H_{16}$	1-Methyl-3,5-diethylbenzene	1252
[2157-18-8]	C_9H_{16}	(1-Methylethyl)cyclohexane	1253
[2216-33-3]	C_9H_{30}	3-Methyloctane	1237
[2216-34-4]	C_9H_{30}	4-Methyloctane	1238
[2306-88-9]	$C_{16}H_{32}O_2$	Octyloctanoate	1325
[2306-89-0]	$C_{18}H_{36}O_2$	Decyloctanoate	1326
[2306-92-5]	$C_{18}H_{36}O_2$	Octyldecanoate	1326
[2390-09-2]	$C_{18}H_{36}O_2$	Methyl-11-eicosenoate	1326
[2410-29-9]	$C_{57}H_{106}O_6$	2-Octadecanoyloxy-1,3-di(cis-9-octadecenoyloxy) propane	1335
[2423-10-1]	$C_{18}H_{34}O$	cis-9-Octadecenal	1300
[2456-28-2]	$C_{20}H_{42}O$	1-Decoxydecane	1300
[2551-62-4]	SF_6	Sulfur hexafluoride	1193
[2573-03-7]	$C_{47}H_{84}O_2$	Cholest-5-en-3-yleicosanoate	1329
[2586-89-2]	C_7H_{12}	3-Heptyne	1250
[2599-01-1]	$C_{30}H_{60}O_2$	Hexadecyltetradecanoate	1327, 1328
[2719-52-0]	$C_{11}H_{16}$	(1-Methylbutyl)benzene	1252
[2733-86-0]	$C_{19}H_{36}O_2$	Methyl-cis-12-octadecenoate	1326
[2733-88-2]	$C_{25}H_{48}O_2$	Methyl-15-tetracosenoate	1326
[2752-99-0]	$C_{69}H_{128}O_6$	1,2,3-Tri(cis-13-docosenoyloxy)propane	1335
[2777-58-4]	$C_{19}H_{36}O_2$	Methyl-cis-6-octadecenoate	1326
[2809-67-8]	C_8H_{14}	2-Octyne	1250
[2922-55-6]	$C_3H_3NaO_4$	Propanedioic acid monosodium salt	1323
[2922-54-5]	$C_4H_5NaO_4$	Butanedioic acid monosodium salt	1323
[2929-07-9]	$C_{21}H_{42}O_3$	1-(cis-9-Octadecenoxy)-2,3-propanediol	1301
[3029-40-1]	$C_{20}H_{18}$	1,8-Diphenyl-1,3,5,7-octatetraene	1252
[3221-61-2]	C_9H_{20}	2-Methyloctane	1237
[3343-88-2]	$C_5H_7NaO_4$	Pentanedioic acid monosodium salt	1323
[3387-41-5]	$C_{10}H_{16}$	4-Methylene-1-(1-methylethyl)bicyclo [3.1.0] hexane	1253
[3404-56-6]	C_8H_{16}	4-Methyl-2-heptene	1249
[3404-61-3]	C_7H_{14}	3-Methyl-1-hexene	1216
[3404-72-6]	C_7H_{14}	2,3-Dimethyl-1-pentene	1214
[3522-94-9]	C_9H_{20}	2,2,5-Trimethylhexane	1235
[3524-73-0]	C_7H_{14}	5-Methyl-1-hexene	1217
[3724-61-6]	$C_{16}H_{32}O_2$	Dodecylbutanoate	1325
[3769-23-1]	C_7H_{14}	4-Methyl-1-hexene	1216
[3913-63-1]	$C_{17}H_{32}O_2$	Methyl-9-hexadecenoate	1326
[4218-48-8]	$C_{11}H_{16}$	1-Ethyl-4-(1-methylethyl)benzene	1252
[4536-26-9]	$C_{30}H_{60}O_2$	Tetradecylhexadecanoate	1328
[4706-81-4]	$C_{14}H_{30}O$	2-Tetradecanol	1298
[4813-58-5]	$C_{16}H_{34}O$	1-Ethoxytetradecane	1300
[4887-30-3]	$C_{14}H_{28}O_2$	Octylhexanoate	1324
[5303-24-2]	$C_{20}H_{40}O_2$	Octyldodecanoate	1327

[10322-48-2]	$C_{55}H_{110}O_4$	2-(Hexadecyloxy)-3-(octadecyloxy)propyl ester stearic acid	1335
[10322-49-3]	$C_{51}H_{102}O_4$	2,3-Bis(octadecyloxy)propyl ester lauric acid	1335
[10322-50-6]	$C_{57}H_{114}O_4$	2,3-Bis(octadecyloxy)propyl ester octadecanoic acid	1335
[10322-51-7]	$C_{57}H_{112}O_4$	2,3-Bis(octadecyloxy)propyl ester (Z)-9-octadecenoic acid	1335
[10322-52-8]	$C_{57}H_{110}O_4$	2-(9-Octadecenyloxy)-(Z,Z)-3-(octadecyloxy)propyl ester oleic acid	1335
[10322-53-9]	$C_{57}H_{108}O_4$	2,3-Bis(9-octadecenyloxy)-(Z,Z,Z)-propyl ester oleic acid	1335
[10322-54-0]	$C_{59}H_{118}O_4$	2-(Eicosyloxy)-3-(octadecyloxy)propyl ester stearic acid	1335
[10329-25-6]	$C_{57}H_{108}O_5$	1-[(Octadecyloxy)methyl]-1,2-ethanediyl ester oleic acid	1336
[10377-51-2]	ILi	Lithium iodide	1192
[10405-85-3]	C_9H_{18}	4-Nonene	1249
[10431-03-5]	$C_{22}H_{46}O_3$	1-Nonadecoxy-2,3-propanediol	1301
[10431-14-8]	$C_{57}H_{112}O_3$	1,2-Bis(9-octadecenyloxy)-(Z,Z)-3-(octadecyloxy)propane	1302
[10431-15-9]	$C_{57}H_{110}O_3$	1,2,3-Tris(9-octadecenyloxy)-(Z,Z,Z)-propane	1302
[10431-17-1]	$C_{49}H_{96}O_5$	1-[(Decyloxy)methyl]-1,2-ethanediyl ester stearic acid	1336
[10431-21-7]	$C_{54}H_{106}O_5$	1-[(Pentadecyloxy)methyl]-1,2-ethanediyl ester stearic acid	1336
[10448-26-7]	$C_{16}H_{32}O_2$	Hexyldecanoate	1325
[13031-32-8]	CD_3NO_2	Nitromethane-d_3	1201
[13166-06-8]	$C_{57}H_{114}O_3$	1-(9-Octadecenyloxy)-(Z)-2,3-bis(octadecyloxy)propane	1302
[13373-83-6]	$C_{22}H_{44}O_3$	Octadecylbutanoate	1328
[13466-78-9]	$C_{10}H_{16}$	3,7,7-Trimethylbicyclo [4.1.0] hept-3-ene	1241
[13520-83-7]	$UO_2(NO_3)_2 \cdot 6H_2O$	Uranium bis(nitrato-O)dioxohexahydrate	1193
[13643-08-8]	C_8H_{14}	2,4-Octadiene	1250
[13933-61-4]	$C_{18}H_{38}O$	1-Ethoxyhexadecane	1300
[14331-11-4]	$C_{22}H_{44}O_2$	Hexadecylhexanoate	1327-1328
[14465-68-0]	$C_{57}H_{92}O_6$	1,2,3-Tri(cis,cis,cis-9,12,15-octadecatrienoyoxy) propane	1335
[15677-13-1]	$C_{10}H_{10}$	Bicyclo [4.2.2] deca-2,4,7,9-tetraene	1253
[15870-10-7]	C_8H_{16}	2-Methyl-1-heptene	1225
[16260-26-7]	$C_{22}H_{44}O_3$	Octyltetradecanoate	1328
[16456-36-3]	$C_{22}H_{44}O_3$	Tetradecyloctanoate	1328
[16746-86-4]	C_8H_{16}	2,3-Dimethyl-1-hexene	1224
[16747-26-5]	C_9H_{20}	2,2,4-Trimethylhexane	1235
[16813-18-6]	$C_{17}H_{36}O$	2-Heptadecanol	1298
[16958-85-3]	$C_{24}H_{48}O_2$	Octylhexadecanoate	1328
[16976-29-6]	$C_{12}H_{26}O$	1-Ethoxydecane	1300
[17088-93-6]	$C_{18}H_{38}O$	1-Octoxydecane	1300
[17356-30-8]	$C_9H_{15}NaO_4$	Nonanedioic acid monosodium salt	1323
[18172-67-3]	$C_{10}H_{16}$	(1S)-6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane	1253
[18281-05-5]	$C_{22}H_{44}O_2$	Ethyleicosanoate	1328
[18302-77-7]	$C_{20}H_{40}O$	1-Butoxyhexadecane	1300
[18476-57-8]	$C_{10}H_{18}$	4,5-Dimethyl-2,6-octadiene	1250
[18966-34-4]	$C_6H_9NaO_4$	Hexanedioic acid monosodium salt	1323
[19455-73-3]	$C_{10}H_{17}NaO_4$	Decanedioic acid monosodium salt	1323
[20184-91-2]	C_9H_{16}	4-Nonyne	1250
[20246-55-3]	$C_{51}H_{92}O_6$	1,2,3-Tri(cis-9-hexadecenoyloxy)propane	1335
[20292-09-5]	$C_{20}H_{40}O_2$	Dodecyloctanoate	1327
[20834-06-4]	$C_{28}H_{56}O_2$	Hexadecyldodecanoate	1327-1328
[25038-46-4]	$(C_2H_3Cl)_n$	Poly(1-chloro-1,2-ethanediyl)	1337-1338
[25167-62-8]	$C_{22}H_{32}O_2$	Docosahexaenoic acid	1317
[25321-09-9]	$C_{12}H_{18}$	Bis(1-methylethyl)benzene	1252
[25378-27-2]	$C_{20}H_{30}O_2$	Eicosapentaenoic acid	1317
[26533-36-8]	$C_{19}H_{40}O$	2-Nonadecanol	1298
[26718-84-3]	$C_{20}H_{40}O_2$	Propylheptadecanoate	1327
[26836-31-7]	$C_{55}H_{104}O_6$	1-Hexadecanoyloxy-2-octadecanoyloxy-3-(cis-9-octadecenoyloxy)propane	1335
[26952-14-7]	$C_{16}H_{32}$	Hexadecene	1249
[27071-84-7]	$C_{55}H_{102}O_6$	1-Hexadecanoyloxy-2,3-di(cis-9-octadecenoyloxy) propane	1335
[27195-67-1]	C_8H_{16}	Dimethylcyclohexane	1251
[27593-68-6]	$C_{22}H_{44}O_2$	Propylnonadecanoate	1328
[27796-70-9]	$C_8H_{13}NaO$	Octanedioic acid monosodium salt	1323
[28409-94-1]	$C_{53}H_{100}O_6$	1,3-Dihexadecanoyloxy-2-(cis-9-octadecenoyloxy) propane	1335
[28880-75-3]	$C_{57}H_{108}O_6$	1,3-Dioctadecanoyloxy-2-(cis-9-octadecenoyloxy) propane	1335
[28933-88-2]	$C_{16}H_{28}O_2$	Hexadecadienoic acid	1317
[29253-36-9]	$C_{13}H_{14}$	(1-methylethyl)naphthalene	1252
[29428-96-4]	$C_{16}H_{26}O_2$	Hexadecatrienoic acid	1317
[29590-02-1]	$C_{57}H_{106}O_6$	1-Octadecanoyloxy-2,3-(*cis*-9-octadecenoyloxy)propane	1335
[29710-31-4]	$C_{24}H_{48}O_2$	Hexadecyloctanoate	1327, 1328
[29710-34-7]	$C_{26}H_{52}O_2$	Hexadecyldecanoate	1327, 1328
[29730-67-4]	$C_{22}H_{44}$	Docosene	1249

20. Author Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.