INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
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GUIDELINES FOR REPORTING OF PHASE EQUILIBRIUM MEASUREMENTS

(IUPAC Recommendations 2011)

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ABSTRACT

Recommendations are given for reporting in the primary scientific literature of measurements involving phase equilibrium. The focus is on documentation issues, and many of the recommendations may also be applied to the more general fields of thermodynamic and transport properties. The historical context of the work and specific plans for implementation of the recommendations are discussed.

INTRODUCTION

The critical importance of phase equilibrium properties in the development and optimization of numerous industrial processes is well established [1], particularly with regard to separation methods, such as distillation, extraction, and crystallization. This article reports the results of IUPAC (International Union of Pure and Applied Chemistry) Project 2007-024-2-100 with the objective of establishing recommendations for the reporting of measurements involving phase equilibrium with a focus on documentation issues. This work builds upon earlier related efforts that span approximately 60 years. The history of these efforts, which stem from the 1953 U. S. Calorimetry Conference, was summarized in 1972 in the report of the IUPAC Project *A Guide to Procedures for the Publication of Thermodynamic Data* (*1972 Guide*) chaired by Professor Stig Sunner [2]. The concern with careful and standardized representation of results in the archival literature is almost unique to the field of thermochemical and thermophysical property measurements. (One other field in which standardization has been implemented is that of crystallographic structure determination, as represented in the Cambridge Crystallographic Database [3] and Protein Data Bank [4].) As stated in the 1972 IUPAC report, “The highly interdependent nature of thermodynamic data imposes special obligations upon the author of papers reporting the results of thermodynamic investigations. He must give enough information about his experiment to allow readers to appraise the precision and accuracy of his results so they may be properly consolidated within the existing body of data in the literature.” Today organizations worldwide {DDBST Software & Separation Technology GmbH [5], NIST Thermodynamics Research Center [6], DECHEMA Gesellschaft für Chemische Technik und Biotechnologie e.V. [7]**,** the Design Institute for Physical Property Data (DIPPR$^{®}$) Project 801 [8], Korea Thermophysical Properties Data Bank [9], and AIST (National Institute of Advanced

Industrial Science and Technology of Japan), Network Database System for Thermophysical Property Data [10], and others} continue the work of compiling, archiving, analyzing, and disseminating property data based on an archival literature spanning more than a century. The most recent work in the area of documentation standards in this field, the *Guide for Reporting Experimental Data on Vapor-Liquid Equilibria of Mixtures at Low and Moderate Pressures*, was the work of a CODATA Task Group and was published in 1989 (*1989 Guide*) [11]. As noted in the title of the project, the scope of that work was narrow.

In the last 20 years, several important and inter-related developments make imperative revision of the guidelines published previously [2,11]. These developments include advances in the establishment of international standards for (1) evaluation and reporting of uncertainties (The *Guide for the Estimation of Uncertainty in Measurement*, known as the “GUM”, published in 1993) [12-14] (2) nomenclature in physical chemistry (*Quantities, Units, and Symbols in Physical Chemistry*, also known as “The Green Book” and published by IUPAC, most recently in 2007) [15]; and (3) storage and exchange of experimental, predicted, and critically evaluated thermophysical and thermochemical property data, ThermoML, an XML-based IUPAC standard established in 2006 [16]. As ThermoML was an IUPAC project, it was developed with full adherence to the recommendations of the Green Book and the GUM.

The present work is also motivated by major advances in electronic databases for thermophysical properties. In particular, procedures have been developed involving cooperation between the U. S. National Institute of Standards and Technology (NIST) and journal editors and publishers to allow data reported in key journals (*Journal of Chemical and Engineering Data*, *Fluid Phase Equilibria*, *The Journal of Chemical Thermodynamics*, *Thermochimica Acta*, and *International Journal of Thermophysics*) to be easily incorporated into electronic databases and process simulation software without significant manual intervention [17].To this end, the *NIST ThermoML Archive of Published Experimental Data* (NIST ThermoML Archive) was established on the Web with all data available for free download in ThermoML format [18].These files represent the experimental data as published. Consequently, the quality and clarity of data descriptions in the original publications, including those of the uncertainty evaluations, are transferred to the ThermoML files, and have direct impact on their value to the research and industrial communities.

A further need for the present work stems from the rate of publication of phase equilibrium and property data that annually continues to increase, more than doubling in the last ten years. This large volume of information is an enormous challenge to traditional labor-intensive critical data evaluation procedures and has led to more automated evaluation models, such as the NIST ThermoData Engine (TDE) [19-23], and mechanisms for incorporating newly published data directly into process simulation engines (e.g., Aspen Plus® [24], SimSci-Escessor® [25], and VMGSim® [26]) from the NIST ThermoML Archive [18]. These software applications, together with those for regression and analysis of experimental data (e.g., the TUV SUD NEL Physical Property Data Service (PPDS) software [27] or Dortmond Data Bank Software Package (DDBSP) [28]), as well as the recently discussed concept of chemical-process and product design on demand [29], are clearly enhanced with improvements in the data-reporting standards.

Following some background information, the main body of this article provides recommendations for content and the general reporting format for each of the typical sections of an article reporting thermodynamic and transport property data, with an emphasis on phase equilibrium results.

DEFINITIONS OF DATA

The interpretation of the term *data* depends strongly on the scientific audience. Before delineating recommendations for the reporting of property data, it is necessary to establish definitions for various data types that are commonly reported. The following are practical definitions adapted here from those formulated by Frenkel et al. [19].

True Data

True data (or *true values*) are exact property values for a chemical system of defined composition in a specified state. These data have the following characteristics. They are (1) unique and permanent, (2) independent of any experiment or sample, and (3) a hypothetical concept with no known values. The other property types that follow (*experimental*, *predicted*, and *critically evaluated*) may be considered approximations to the true values. The difference between these values and a true value is defined as the *error*. The *error* is never known; however, it is given that it is never zero. The measure of confidence in an experimental, predicted, or critically evaluated value is the *uncertainty* [12-14], which is a range of values believed to include the *true* value with a certain probability. All data types should always be published with associated estimated uncertainties. There are several properties for which values have been defined to be exact, such as the triple point of water [30] or the speed of light [31]. These are special cases and are not considered here.

Experimental Data

Experimental data are defined as those obtained as the result of a particular experiment on a defined sample. The feature that distinguishes *experimental* data from *predicted* and *critically* *evaluated* data is use of a chemical sample, including characterization of its origin and composition.

Derived Data

Derived data are values calculated by mathematical operations from other data, possibly including *experimental*, *predicted*, and *critically evaluated* data. Derived data include values calculated directly from experimental values, such as excess volumes derived from measured densities, as well as gas-phase compositions y derived from pressure p, temperature T, and liquid-phase composition x {i.e., (p, T, x) data} for a binary system, where the calculation requires additional values from the literature, such as vapor pressures of pure substances, activity coefficients at infinite dilution, enthalpies of mixing, etc. Derived data were addressed explicitly in the *1972 Guide* [2], "…derived (or secondary) results never should be published at the cost of omitting the primary results on which they were based," as well as in the *1989 Guide* [11], "All derived values should be distinguished clearly from the experimental values. The authors can mislead their audience if they report the derived results as if they were experimental values." The present recommendations are in accord with these earlier statements.

Predicted Data

Predicted data (or predicted values) are defined as those obtained through application of a predictive model or method, such as a corresponding-states or group-contribution method. There is no sample associated with this type of property data.

Critically Evaluated Data

Like predicted data, there is no sample involved with critically evaluated data. The feature that distinguishes *critically evaluated* data from *predicted* data is the involvement of the judgment of a data evaluator (cf. references 32 and 33) or evaluation system [21]. Critically evaluated data are recommended property values that may be generated through assessment of available *experimental* data, *predicted* data, *derived* data, or any combination of these.

THE GIBBS PHASE RULE

The Gibbs phase rule provides an unequivocal accounting basis to ensure that reported property values are fully defined. It also is the principle upon which the structure of the ThermoML data communication standard is based. The phase rule for non-reacting systems is

$$F = N - \Pi + 2 - \phi \qquad (1)$$

where F is the number of degrees of freedom, N is the number of components, Π is the number of phases in equilibrium, and ϕ is the number of constraints including special states, such as the liquid-vapor critical or liquid-liquid consolute states. Some succinct examples involving complex phase behavior are given by Bolz et al. [34] in the IUPAC Technical Report, *Nomenclature for Phase Diagrams with Particular Reference to Vapor-Liquid and Liquid-Liquid Equilibria*. It is essential that all property values are fully defined in a concise way through identification of all degrees of freedom (variables and constraints), phases present, and any special states. This topic is more fully addressed later in these guidelines in the section concerning tables of results.

UNCERTAINTIES

In a forward to the *Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results* [14] the then Director of NIST, Dr. John W. Lyons, wrote, “It is generally agreed that the usefulness of measurement results, and thus much of the information that we provide as an institution, is to a large extent determined by the quality of the statements of uncertainty that accompany them.” This statement is equally applicable to all reported measurement results. Historically, it is unfortunate that a large portion of reported estimates of uncertainty in the literature are poorly defined or inadequate, if done at all, as was discussed in a recent case study of uncertainty for critical temperatures of pure compounds [35]. That study found that the most commonly reported quantity was the repeatability, which is simply a lower limit for the needed combined standard uncertainty. The combined standard uncertainty includes consideration of all contributions to the uncertainty, including equipment design, apparatus quality, equipment calibrations, sample quality, and proper assessment of error propagation.

The expression of uncertainty requires clear definition of a variety of quantities and terms. Quantities recommended here for the expression of uncertainty conform to the *Guide to the Expression of Uncertainty in Measurement*, ISO (International Organization for Standardization), October, 1993 [12]. These ISO recommendations were adopted with minor editorial changes as the *U.S. Guide to the Expression of Uncertainty in Measurement* [13]. Reference 12 is commonly referred to by its abbreviation; the GUM. Reference 13 is assumed equivalent to ref 12, and includes a summary of the historical development of the recommendations beginning in 1977. The recommendations of the GUM have been summarized in *Guidelines for the Evaluation and Expression of Uncertainty in NIST Measurement Results* [14], which is available via free download from the Internet (http://physics.nist.gov/cuu/). The recommendations of the GUM with particular application to thermochemical and thermophysical property measurements were summarized by Chirico et al. [36].

The *1972 Guide* [2] and the *1989 Guide* [11] refer to the need for reporting of the *accuracy* and *precision* of results. Although these specific terms are now considered meaningful only in a general sense (*i.e.*, they do not have numerical values) [13,14], it is clear that high-quality estimates of uncertainty have been consistently requested. The *1972 Guide* [2] includes an excellent statement summarizing why this is essential; the author “must give enough information about the experiment to allow readers to appraise the precision and accuracy of the results so they may be properly consolidated within the existing body of data in the literature.” A discussion of the differences between accuracy and uncertainty is available online from the National Physical Laboratory of the United Kingdom [37].

An extensive discussion of uncertainty and its assessment is beyond the scope of this article. Readers of the present guidelines are strongly encouraged to consult the references given here (references 12, 13, 14, and 36) for additional information. Specific recommendations are also included later in these guidelines concerning the inclusion of uncertainties in tables of results.

REPORTING REQUIREMENTS 1: TITLE AND ABSTRACT

Article Title

The presence of new experimental data in the article should be made clear in the title. If possible, the properties measured and the chemical systems studied should be named explicitly with IUPAC systematic names for the substances.

Abstract

The abstract should include a summary of the chemical systems studied, the experimental methods employed, and the properties measured for each system, including ranges of temperature, pressure, and composition, as appropriate.

REPORTING REQUIREMENTS 2: CHEMICAL SAMPLE INFORMATION

IUPAC Systematic Name and Chemical Formula

An IUPAC systematic name and chemical formula is required for all chemical samples. Guides to IUPAC nomenclature for organic compounds [38,39] and inorganic compounds [40] are readily available. An abbreviation can be defined for general use in the text. Authors are encouraged to include structural drawings of complex molecules to avoid naming ambiguities.

Registry Numbers

The CASRN should be provided, if available; however, this should not be considered a substitute for an IUPAC systematic name. Additional registry numbers, such as those of PubChem [41], Cambridge Crystallographic Database [3], Protein Data Bank [4], can be included, but provision of the IUPAC name is the primary mode of compound identification.

An important development in the last ten years has been development of the IUPAC International Chemical Identifier (InChI) [42], a non-proprietary identifier for chemical substances for use in printed and electronic data sources. Subsequently, a fixed-length (25-character) condensed digital representation of the Identifier was developed: the InChIKey [43]. The primary advantage of the InChIKey is that it can be generated by any researcher based on the structure alone, and is independent of the scheduling priorities and inevitable human errors of other systems. The InChIKey is not often included as a chemical identifier in publications today, but its expanded use is encouraged.

Sample Source

The origin of all chemical samples must be stated. Some typical sample origins are commercial (with the name of the supplier), synthesized, loaned, etc. The numerical purity (mass fraction or mole fraction) of the supplied sample of a nominally pure substance should be indicated, as well as the method of purity determination, if known. Any subsequent purification of the sample, such as distillation, crystallization, drying, etc., should be described. Details should be provided concerning major impurities, if present. If the samples are chemically unstable, evidence should be provided to show that the sample did not significantly decompose, or otherwise change its chemical form, between analysis and measurement. Some discussion of the rate of decomposition is necessary. Additives utilized for increased chemical stability or proper storage, such as sodium wire, molecular sieves, polymerization inhibitors, etc., should be indicated, and any corrections to the results needed due to their presence should be described along with any experiments performed to determine the amounts present.

Numerical Sample Purity

The sample purity must be expressed in numerical form (mass fraction or mole fraction), while for solutions, molality may also be used. The sample purity must be determined by calibrated analytical means, such as gas-liquid chromatography, fractional melting in a calorimeter, mass spectrometry, high-performance liquid chromatography, proton nuclear magnetic resonance, etc. If no impurities are detected, the detection limit of the analytical methods must be stated.

Comparisons with literature values for common measured properties, such as density or index of refraction, may be used to help confirm compound identity, but cannot be used to establish chemical purity. The listing of a commercial grade of chemical, such as *analytical*, *technical*, *puriss*, etc., is not a substitute for provision of the numerical purity. The symbol % should not be used in numerical expressions for purity or chemical distributions. The uncertainty for the purity value should be expressed through proper use of significant figures. For example, mole fraction purity $x = 0.99$ implies $u(x) \approx 0.01$, and mole fraction purity $x = 0.990$ implies $u(x) \approx 0.001$. This does not preclude explicit inclusion of the uncertainty for the purity, if known, or if it is essential to the scientific purpose of the article.

Polymers

Sample descriptions for polymers should include numerical characterizations of the dispersions of distributions of molar masses and degrees of polymerization. The terms for dispersity $Đ$ recommended by IUPAC are the *molar-mass dispersity* $Đ_M$ and *degree-of-polymerization dispersity* $Đ_X$ [44]. $Đ_M$ is defined in terms of the ratio of the *mass-average molar mass* to the *number-average molar mass*. $Đ_X$ is defined as the *mass-average degree of polymerization* to the *number-average degree of polymerization*. The reader is referred to the IUPAC *Compendium of Polymer Terminology and Nomenclature* (the "Purple Book") [45] for a more complete discussion.

The ThermoML data communication standard [16] was established in 2006, prior to publication of the most recent IUPAC recommendations for polymer terminology [44,45]. Consequently, many of the terms recommended presently for polymers are not included. There is an active IUPAC project for the purpose of updating and extending the ThermoML standard

(IUPAC Project 2007-039-1-024) that will address these inconsistencies. Completion of that project is planned for 2011.

Chemical Sample Table

A tabular summary of sample descriptions is strongly encouraged. Systematic names must be given there. An example of a table for the summary of chemical sample information is given in Table 1. Variations in style and format between journals are expected, but the essential information should be provided.

REPORTING REQUIREMENTS 3: APPARATUS AND EXPERIMENTAL PROCEDURES

The *1972 Guide* [2] and the *1989 Guide* [11] gave similar and fairly complete recommendations for the description of experimental apparatus and procedures. These are adapted here with some extensions.

New Apparatus

Sufficient detail of new apparatus should be provided in order for a reader to judge the general methodology utilized and the anticipated quality of the measurements. The controlled environment and the measuring systems for temperature, pressure, composition, etc., should be well described with particular attention to contributions to the experimental uncertainty. Stability and control of the experimental conditions may be crucial to the attainment of high-quality results, and should be detailed as needed. Stability and control of temperature, pressure, and composition were discussed at length in the *1989 Guide* with regard to VLE measurements at low and moderate pressures [11]. Information concerning traceability of measured quantities to national measurement institutes (NMIs) should be provided. The identity of the temperature scale should be provided. At present, this is the International Temperature Scale of 1990 (ITS-90) [46].

The measurement of standard chemical systems for properties with established uncertainties is strongly encouraged to validate results for an apparatus. A complete report of the test measurements should be included with the apparatus description.

All data-reduction procedures should be described in detail in the text. Once provided in detail, the descriptions can be cited in future applications of the method.

Existing Apparatus

For existing apparatus, a summary of the method used must be provided, even if complete details have been published elsewhere. Particular aspects that affect the expected uncertainty should always be given. A short description and a reference to any previous validating measurements are adequate. Once published, tables of results for the validation experiments should not be duplicated in subsequent reports.

If the apparatus has been described previously, but has been modified, then a summary of the changes and the anticipated advantages should be described. Any new measurements used to validate the apparatus should be reported with complete descriptions of the chemicals used. Validation of analytical methods must always be done for the chemical system under investigation.

Commercial Apparatus

For commercial apparatus, a summary of the underlying principles of the measurements must be provided. The manufacturer and equipment identification information (e.g., model number) should be provided, but this is not an adequate description of the apparatus. Particular aspects that affect the expected uncertainty should always be given. Measurements should always be made on standard chemical systems to provide validation for the apparatus. Of course, any modifications to the commercial apparatus should be described together with the reasons for the modifications and impacts on uncertainty.

Establishment of Phase Equilibrium

Methods used to attain and confirm the establishment of equilibrium conditions must be described for all measurement results. Equilibration time periods should be discussed, particularly for studies involving solid-liquid and liquid-liquid equilibrium.

REPORTING REQUIREMENTS 4: NUMERICAL EXPERIMENTAL RESULTS

The Stand-Alone Table

Experimental results must be given in tabular numerical form in the body of the article or as supporting information, and not simply as graphs or fitted equation coefficients. Graphs and equation coefficients may be included, as needed, but not at the expense of the tabular results. Numerical experimental results should never be given as part of the text, but instead, should be given in tabular form, even if only a single value, such as a normal melting temperature, is reported.

Most journals that publish thermophysical property data instruct authors to create tables that *stand alone*; however, this approach is very rarely enforced. A reader is often forced to peruse the text for key information, such as the identities of phases, values for constrained variables (e.g., constant temperature or pressure), definitions of symbols, definitions of composition representations, and particularly uncertainties. Such dispersed reporting ensures that any attempt to incorporate the reported results into the existing body of knowledge is highly error-prone. The recommendations that follow are based on the goal of creating truly stand-alone tables from which the required information for modern archives of experimental data can be correctly interpreted and extracted.

Nomenclature

The names of all properties, variables, and constraints must be written out in full and formulated in accord with IUPAC (Green Book) recommendations [2]. SI units [47,48] must be used consistently. Archaic units, such as centipoise or “p.s.i.a.”, should not be used.

Reporting of all Properties, Variables, Constraints

The property values must be reported together with the values for all variables and constraints in accordance with the Gibbs phase rule. No values of variables or constraints, such as a laboratory pressure p near $p = 0.1$ MPa or a constant temperature stated in the text, should be implied. This includes explicit definition of common symbols, such as T for temperature or y for mole fraction of a component in the gas phase. Examples of stand-alone tables for the reporting of vapor-liquid equilibrium (VLE) (Tables 2 and 3) and liquid-liquid equilibrium (LLE) (Table 4) are provided.

Identification of Phases

All phases and phase boundaries present must be specified in the table, including the chemical identity of solid phases in results for solid-liquid equilibrium (SLE) experiments (solubility studies, phase diagram determinations, etc.). Identification of the solid phase as “crystal” in SLE experiments is inadequate. Examples of stand-alone tables for the reporting of solubility data (Table 5), SLE phase diagram determination (Table 6), and SLE phase diagram determination with compound formation (Table 7) are provided.

Reporting of Multiple Types of Phase Equilibrium in a Single Table (Complex Equilibria)

For studies involving multiple types of phase equilibrium for a single chemical system, authors have found it convenient to report results in a single table. Although convenient for the author, the resulting tables are often difficult for a user to interpret. If only one type of phase boundary is represented in a data table, the phases can be defined in the table heading, as shown in Tables 2 through 5. Similarly, Tables 6 and 7 show SLE data, where it is necessary only to include the identity of the solid phase in the body of the table.

More complex systems are shown in Tables 8, 9 and 10. These tables list results for several types of phase equilibrium in a single table. The symbol ↔ between phase groups is used to define the phase change associated with a particular boundary. For example, the notation $\mathrm{l,g} \leftrightarrow \mathrm{l_1,l_2,g}$ indicates a boundary between a region of (liquid + vapor) equilibrium (VLE) and one of (liquid + liquid + vapor) equilibrium (VLLE).

Experimental results listed in Table 8 include SLE, LLE, and three-phase (solid + liquid + liquid) SLLE data for the system (octan-1-ol + ethanonitrile) together with SLE for pure ethanonitrile. At constant pressure, a single-component system with two phases present and a binary system with three phases present have zero degrees of freedom. This invariance is indicated in the table. Table 9 lists SLE and (solid + solid) SSE results for a binary system of long-chain alkanes, which form a solid solution that undergoes a solid-to-solid phase transition from the crystal phase s(II) to the rotator phase s(I) for all compositions. The invariant values for the pure components are indicated. Table 10 shows results of phase equilibrium studies for several isopleths that undergo a variety of phase changes with temperature. The notation used for the phase changes (*e.g.*, $\mathrm{l_1,l_2} \leftrightarrow \mathrm{l_1,l_2,g}$) provides clear definition for the processes involved.

Reporting of Composition

Compositions should be reported as mole fraction x, mass fraction w, or molality m. For compositions expressed as molality, the solvent must be defined explicitly. All compositions must be defined completely in the table, even if they are defined separately in the text. As noted above, such information distributed throughout the text often leads to incorrect interpretations by data evaluators and users. In particular, with regard to molalities, it is common in the existing literature for the identity of the solvent not to be specified. This is not a serious problem for binary chemical systems, but for systems of three or more components, the meaning is often ambiguous.

Composition should not be expressed as amount concentration (formerly known as *molarity* [15]). Such compositions can be converted to mole fractions only if the temperature and pressure of solution preparation are known and the necessary density values are available. This places an unacceptable burden on users of the data. Similarly, volume fractions should never be used as variables for the reporting of experimental data.

Uncertainties

Uncertainties must be included in the table for all properties, variables, and constraints. The standard uncertainty $u(\phi)$ or relative standard uncertainty $u_r(\phi) = u(\phi)/|\phi|$ must be included, where ϕ represents a variable or constraint. The combined expanded uncertainty $U(\phi)$ or relative combined expanded uncertainty $U_r = U(\phi)/|\phi|$ (with confidence of 0.95) should be reported for properties. For phase equilibrium studies, it is not possible to specify a single property, so the standard uncertainty $u(\phi)$ should be given for all quantities. The relative standard uncertainty u_r must never be used for temperature because of ambiguities resulting from the definitions of the temperature scales, degree Celsius and kelvin. In addition, u_r should never be used for compositions that span wide ranges in mole fraction for any specific component. For example, if vapor-liquid equilibrium compositions are reported for a binary mixture with mole fraction x for each component varied between $x = 0$ and $x = 1$, the reporting of $u_r(x)$ is inappropriate, and $u(x)$ should be given. In contrast, $u_r(x)$ may be entirely appropriate for reporting uncertainties for a series of low concentrations, such as those commonly observed in solubility studies involving a solute in supercritical carbon dioxide.

The units for an uncertainty value must match exactly those of the corresponding property, variable, or constraint in tabulated data. Relative uncertainties do not have units.

Property Measurements for Pure Components

When practical, the properties of the pure components (such as vapor pressures, melting temperatures, etc.) should be measured in the same apparatus used for the studies of the mixtures. These measurements should be done under conditions as close as possible to those used for the studies of the mixtures. Such data are very useful in the assessment of measurement quality.

Derived Data

The reporting of derived data (defined earlier) together with primary experimental data in a single table should be limited to that which is required for the discourse in the article. If derived data are included, they must be labeled clearly as derived, and the method of derivation must be described fully in the text. The combined expanded uncertainty should be provided for all derived data. This can be a complex task, as derived data may include contributions from literature values of poorly defined quality. Nonetheless, proper accounting of the uncertainty of all adjuvant data must be made. Sources of all property values used from the literature must be provided.

An important case is the reporting of results for the measurement of vapor-liquid equilibrium, where pressure p, temperature T, and overall system composition z {*i.e.*, (p, T, z) data} are measured for a binary system and the compositions of the liquid and vapor phases are derived. The primary (p, T, z) data must be reported, and the compositions of the individual phase must be labeled clearly as derived. The method of derivation for the phase compositions must be described clearly in the text.

Data Validation and Model Fitting

Data validation through application of models and consistency checks, such as those based on the Gibbs-Duhem equation for VLE data, are strongly encouraged. Models can also be used to compare the new experimental data with literature values obtained at other conditions, and can reveal data quality issues related to composition or temperature dependence that, otherwise, would remain undetected [cf. 49] Recommendation of specific models for particular data scenarios is an extensive and complex subject that is beyond the scope of this project. Development of models, including computational methods, is an active area of modern research.

Other Notation Issues

Use of the symbol % is strongly discouraged and should not be used in expressions for uncertainty. The meaning of % is 0.01, but it is often misused. Misuse of this symbol in the literature, particularly when applied to uncertainties for compositions (and for that matter, composition itself), has resulted in a large body of data with poorly defined quality.

Graphical Representation of Experimental Data

Graphical representation of the experimental data in the body of the article is encouraged. However, a graph should never be provided at the expense of reporting the primary numerical data in tabular form. Graphs of experimental data are particularly useful for interpretation of results involving solid-liquid equilibrium, where inter-component compound formation, crystal-to-crystal phase transitions, or regions of immiscibility may occur. Figures 1 through 3 show the experimental SLE data listed in Tables 6 through 8, respectively.

REPORTING REQUIREMENTS 5: COMPARISONS WITH PREVIOUSLY PUBLISHED DATA

Authors are expected to complete a detailed literature search and provide comparisons with previously published values. When possible, comparisons should be shown graphically in the form of deviations from either a particular model or fitted equation.

IMPLEMENTATION OF RECOMMENDATIONS

Background

The publication and use of experimental property data involve far more stakeholders than authors alone. In addition, the process involves publishers, editors, reviewers, data evaluators, academic researchers, designers of software for industrial applications, etc., all of whom have somewhat different, and sometimes competing, motivations and goals. Consequently, in spite of good intentions and the high quality of previous work in this field [2,11,34], implementation of recommendations for documentation of experimental results has been slow to occur. For example, Dong et al. [35] demonstrated that, even in recent years, a large portion of reported "uncertainties" are, in fact, repeatabilities, which are only lower limits for standard uncertainties, and are of little value in subsequent applications. A further key impediment to full adoption of previous recommendations has been the absence of a mechanism for their broad and targeted distribution or for their consistent application.

The present recommendations were developed by a diverse team that includes representatives of the chemical industry, editors of major journals, leaders in the field of property data evaluation and distribution, industrial engineers, and developers of software applications of property data to research and industrial process analysis. Through cooperation within the present team, establishment of the new recommendations as policy across the major journals can be ensured. This is an important step, but without the necessary mechanisms or tools for communication of the recommendations to authors or for validation of newly submitted data, full adoption of the recommendations will be difficult to achieve.

Implementation Mechanism: New Global Validation and Review Process

Beginning in 2004, cooperation was established between the National Institute of Standards and Technology (Boulder, Colorado, U. S. A.) and five major journals in the field of thermophysical properties (*Journal of Chemical and Engineering Data*, *Fluid Phase Equilibria*, *The Journal of Chemical Thermodynamics*, *International Journal of Thermophysics*, and *Thermochimica Acta*) with the purpose of establishing a data validation and global communication process. This process and its impact on the quality of published experimental data were described by Frenkel et al. [17]. Co-authors of that work included publishers, journal editors, experimentalists, and software product developers for chemical process analysis. The NIST-Journal cooperation continues today and can serve as a focal point for communication of these recommendations to authors. To this end, websites specific to each participating journal have been established to provide easy access to the documentation recommendations given here, together with examples of chemical sample descriptions and properly formatted and complete data tables [50-54].

Support for Improved Literature Comparisons

A common problem is the failure of authors to do an adequate review of the literature, as required by all journals. In 2009, the editors of the five journals involved in the cooperation with NIST published the *Joint Statement of Editors of Journals Publishing Thermophysical Property Data* [55], which stated, "A requirement for submission of a manuscript describing properties is a literature search and comparison of the results with previously reported literature values. Often, reviewers cannot make informed decisions regarding the manuscript because the authors have made only a minimal literature review and comparisons. It is then an unacceptable burden to require reviewers to research previously published literature data to ensure a proper comparison has been made and hence determine the ultimate worth of the manuscript." NIST maintains an extensive database of experimental property data and sources (references). When an article is submitted that reports new experimental data, software tools are used to search this archive for relevant data sources and provide the results of this search to the journals for use by editors, authors, and reviewers.

Comparisons of new experimental property data with those in the existing literature are also supported within the NIST-Journal cooperation through application of the *NIST ThermoData Engine* (*TDE*) [19-23] technology. This technology applies the dynamic data evaluation approach implemented in the most current version of *TDE* to provide critically evaluated property values for comparison with those in the submitted manuscript. The dynamic data evaluation is based on the existing experimental literature combined with a variety of prediction methods and correlating models. Evaluated results are always generated with estimates of combined expanded uncertainties with level of confidence 0.95. Major inconsistencies are included in a *NIST Data Report* that is provided to the journal editors prior to acceptance for publication. This approach has been effective in identifying numerous typographical problems, as well as problems with sample purity and even instrument calibration, all in advance of publication, thus avoiding publication of awkward errata.

Validation for Studies of Vapor-Liquid Equilibrium (VLE)

Data checking capabilities of the *TDE* technology are enhanced continuously, and were most recently updated with a quality assessment algorithm for vapor-liquid equilibrium data in the sub-critical region for both components [56]. The approach used involves application of four widely used tests of consistency that are based on restrictions following from the Gibbs-Duhem equation (commonly known as the *Herington Test* [57,58], *Van Ness Test* [59,60], *Point Test* [58,61], *Infinite Dilution Test* [58,61]), as well as a test for consistency between the VLE data and evaluated vapor pressures of the pure components. This last test also a simple validity check for (T, p, x) vapor-liquid equilibrium data, where tests based on the Gibbs-Duhem equation do not apply. The results of the five tests are assigned numerical values, rather than the traditional pass/fail, and combined algebraically to yield an overall quality factor Q_{VLE}. Graphical summaries of the test results are provided to journal editors as part of the *NIST Data Report*.

These efforts in data validation for VLE in no way supplant the obligation of the authors to report appropriate data validation and consistency checks as part of their work.

SAMPLE TABLE AND DATA TABLE EXAMPLES

An example of a sample description table is shown in Table 1. Examples of stand-alone tables of experimental data are provided in Tables 2 through 9. (The experimental data listed in the example tables are a subset of that reported in the original source documents. Readers should never cite the present article as a source of experimental values. References are provided in the list of tables below with each example table.) Each journal has specific standards for style and format, but the essential information should be provided. The data represented in the tables are as follows:

Table 2: Pressure, Temperature, Liquid Composition (*p, T, x*) (Vapor + Liquid) Equilibrium Data [62].

Table 3: Pressure, Temperature, Liquid and Gas Composition (*p, T, x, y*) (Vapor + Liquid) Equilibrium Data [63].

Table 4: (Liquid + Liquid) Equilibrium Data; often termed "Tie-Line" data [64].

Table 5: (Solid + Liquid) Equilibrium Data; often termed "Solubility" data [65].

Table 6: (Solid + Liquid) Equilibrium Data; often termed "SLE Phase Diagram" data [66]. The experimental data are shown in Fig. 1.

Table 7: (Solid + Liquid) Equilibrium Data; a phase diagram determination with inter-component compound formation [67]. The experimental data are shown in Fig. 2.

Table 8: Equilibrium data involving multiple phase equilibrium types; (Solid + Liquid), (Liquid + Liquid), and (Solid + Liquid + Liquid); phase diagram determination with a region of liquid immiscibility [68]. The invariant values are indicated for the mixture and pure components. The experimental data are shown in Fig. 3.

Table 9: Equilibrium data involving multiple phase equilibrium types; (Solid + Liquid) and (Solid + Solid); phase diagram with solid solution formation and a solid-to-solid phase transformation across the composition range [69]. The invariant values for the pure components are indicated. The experimental data are shown in Fig. 4.

Table 10: Equilibrium data involving multiple phase-transition types; (Liquid + Vapor) Equilibrium Data with phase separation in the liquid phase [70].

SUMMARY CHECKLIST OF DOCUMENTATION REQUIREMENTS

The following is a summary of the major recommendations of this report in outline form. It is hoped that this will be of use to authors, editors, and reviewers as part of the peer-review process.

- **Article Title**
  - Presence of new experimental data in the article should be clear
  - Properties measured and the chemical systems should be named, if practical
- **Abstract**
  - Chemical systems and properties measured should be summarized
  - Include variable ranges
- **Chemical Sample Information**
  - IUPAC systematic name and chemical formula are required
  - Include structural drawings for complex molecules
  - Inclusion of registry numbers is optional but recommended
  - Sources of samples must be given
  - A numerical sample purity must be given
    - Purities of pure components must be based on analytical methods
    - Comparisons of property measurement results with literature values cannot be used as evidence of chemical purity
  - A Chemical Sample Table is encouraged
- **Apparatus and Experimental Procedures**
  - ***New Apparatus***
    - Provide sufficient detail for the reader to judge…
      - Appropriateness of the methodology
      - Quality of the anticipated results
    - Report details of the controlled environment and the measuring systems
    - Measurements should be traceable to NMI standards, where possible (temperature, pressure, voltage, resistance, etc.)
    - Report measurements for standard chemical systems to demonstrate performance
  - ***Existing Apparatus***
    - Summarize the experimental method with focus on uncertainty impacts
    - Provide a short description of validating experiments
  - ***Commercial Apparatus***
    - Summarize the underlying principles with focus on uncertainty impacts
    - The manufacturer and equipment model number should be provided, but this is not an adequate description of the apparatus
    - Provide a description of validating experiments
- **Numerical Experimental Results: Stand-Alone Tables**
  - ***Nomenclature***
    - Names of all properties, variables, and constraints should be written out (e.g., temperature T, rather than simply T)
    - IUPAC (Green Book) recommendations must be followed
    - SI units only must be used

  - ***Reporting of all Properties, Variables, Constraints***
    - All values must be reported in accord with the Gibbs phase rule
    - Values of variables should not be implied or reported in the text
  - ***Identification of Phases***
    - All co-existing phases must be identified, including chemical identification of crystalline phases
  - ***Reporting of Composition***
    - Mole fraction, mass fraction, or molality should be used
    - All compositions must be defined completely in the table
    - If molality is used, the solvent must be clearly identified
    - Amount concentration (formerly molarity) and volume fraction must not be used as expressions of composition
  - ***Uncertainties***
    - Uncertainties must be included in the table for all properties, variables, and constraints
    - The standard uncertainty $u(\phi)$ or relative standard uncertainty $u_r(\phi) = u(\phi)/|\phi|$must be included for all variables and constraints
    - The combined expanded uncertainty $U(\phi)$ or relative combined expanded uncertainty $U_r = U(\phi)/|\phi|$ (with level of confidence = 0.95) should be reported for properties
    - For phase equilibrium studies, the standard uncertainty $u(\phi)$ or relative standard uncertainty $u_r(\phi)$ only should be given for all quantities; however, u_r must not be used for temperature
    - Use of the symbol % is discouraged, particularly for expressions of uncertainty and composition
  - ***Derived Data***
    - Reporting of primary experimental data and derived data in a single table must be limited to that required for the scientific discourse of the article
    - Derived data must always be clearly labeled as derived
    - Uncertainties must be provided
      - Uncertainties for adjuvant data must be considered
- **Data Validation and Model Fitting**
  - Data validation through application of consistency checks and models is strongly encouraged
- **Comparisons with Previously Published Data**
  - Authors are expected to complete a detailed literature search
  - Comparisons must be provided with previously published values
    - Comparisons for properties with state variables should be shown graphically in the form of deviations from a particular model or fitted equation

ACKNOWLEDGMENTS

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Table 1. Sample Table

Chemical Name	Source	Initial Mole Fraction Purity	Purification Method	Final Mole Fraction Purity	Analysis Method
heptane	Aldrich	0.98	distillation	0.997	GC [a]
THA [b]	synthesis	-	recrystallization	0.9998	fractional melting
hydrogen	Air Liquide	0.998	none	-	-

[a] Gas-liquid chromatography

[b] THA = 1,2,3,4-tetrahydroanthracene

Table 2. Experimental (Vapor + Liquid) Equilibrium (VLE) Data for the System Benzylamine (1) + Water (2) at Temperature T, Pressure p, and Liquid Mole Fraction x [a,b]

T/K	x_1	p/kPa	$u(p)$/kPa	T/K	x_1	p/kPa	$u(p)$/kPa
283.15	0.0000	1.1995	0.0024	333.15	0.0000	19.616	0.039
283.15	0.0512	1.1815	0.0024	333.15	0.0512	19.865	0.040
283.15	0.1017	1.1835	0.0024	333.15	0.1017	19.547	0.039
283.15	0.2526	1.1214	0.0022	333.15	0.2526	18.604	0.037
283.15	0.3613	1.0264	0.0021	333.15	0.3613	16.526	0.033
283.15	0.5009	0.8109	0.0041	333.15	0.5009	13.179	0.026
283.15	0.6687	0.5809	0.0029	333.15	0.6687	7.896	0.016
283.15	0.8391	0.1238	0.0062	333.15	0.8391	3.8535	0.0077
283.15	1.0000	0.0285	0.0014	333.15	1.0000	0.9048	0.0045
303.15	0.0000	4.1478	0.0083	353.15	0.0000	47.074	0.094
303.15	0.0512	4.1576	0.0083	353.15	0.0512	47.678	0.095
303.15	0.1017	4.1026	0.0082	353.15	0.1017	47.209	0.094
303.15	0.2526	3.8862	0.0078	353.15	0.2526	45.167	0.090
303.15	0.3613	3.4829	0.0070	353.15	0.3613	40.275	0.081
303.15	0.5009	2.7661	0.0055	353.15	0.5009	32.152	0.064
303.15	0.6687	1.8306	0.0037	353.15	0.6687	18.214	0.036
303.15	0.8391	0.9973	0.0050	353.15	0.8391	6.252	0.013
303.15	1.0000	0.1351	0.0068	353.15	1.0000	2.5850	0.0052
313.15	0.0000	7.222	0.014	363.15	0.0000	70.10	0.14
313.15	0.0512	7.276	0.015	363.15	0.0512	70.91	0.14
313.15	0.1017	7.158	0.014	363.15	0.1017	70.54	0.14
313.15	0.2526	6.788	0.014	363.15	0.2526	67.69	0.14
313.15	0.3613	6.050	0.012	363.15	0.3613	60.60	0.12
313.15	0.5009	4.8136	0.0096	363.15	0.5009	48.385	0.097
313.15	0.6687	3.0747	0.0061	363.15	0.6687	26.718	0.053
313.15	0.8391	1.7867	0.0036	363.15	0.8391	7.488	0.015
313.15	1.0000	0.2678	0.0013	363.15	1.0000	4.1465	0.0083

[a] Standard uncertainties u are $u(T) = 0.01$ K and $u(x_1) = 0.0002$. The values of $u(p)$ are given in the table.

[b] The experimental data in this table were abstracted from reference 62.

Table 3. Experimental (Vapor + Liquid) Equilibrium (VLE) Data for the System Dimethylether (1) + Diisopropylether (2) at Temperature T, Pressure p, Liquid Mole Fraction x, and Gaseous Mole Fraction y [a,b]

T/K	p/MPa	x_1	y_1
293.04	0.560	0.4101	0.9705
293.04	0.467	0.3557	0.9636
293.04	0.400	0.3098	0.9561
293.04	0.335	0.2659	0.9468
293.04	0.263	0.2237	0.9366
312.93	0.768	0.4332	0.9511
312.93	0.656	0.3773	0.9392
312.93	0.525	0.3038	0.9199
312.93	0.447	0.2627	0.9087
312.93	0.335	0.2131	0.8834
332.90	0.935	0.3925	0.9033
332.90	0.823	0.3421	0.8898
332.90	0.666	0.2893	0.8678
332.90	0.459	0.2094	0.8203
332.90	0.374	0.1777	0.8010
352.70	1.130	0.3668	0.8544
352.70	1.001	0.3295	0.8385
352.70	0.840	0.2836	0.8092
352.70	0.670	0.2360	0.7775
352.70	0.498	0.1853	0.7366

[a] Standard uncertainties u are $u(T) = 0.05$ K, $u(p) = 0.0035$ MPa, and $u(x_1) = u(y_1) = 0.001$.

[b] The experimental data in this table were abstracted from reference 63.

Table 4. Experimental (Liquid + Liquid) Equilibrium Data for the System Cyclohexane (1) + Cyclohexanone (2) + Dimethylsulfoxide (3) for Mole Fractions x at the Temperature $T = 303.2$ K and Pressure $p = 0.1$ MPa [a,b]

Liquid Mixture 1		Liquid Mixture 2	
x_1	x_2	x_1	x_2
0.9628	0.0244	0.0542	0.0541
0.9021	0.0692	0.0807	0.1312
0.8450	0.1069	0.1110	0.1834
0.7795	0.1468	0.1554	0.2263
0.6705	0.2025	0.2129	0.2589
0.5632	0.2355	0.2799	0.2751
0.5175	0.2475	0.3450	0.2722

[a] Standard uncertainties u are $u(T) = 0.1$ K, $u(x) = 0.0005$, and $u(p) = 10$ kPa.

[b] The experimental data in this table were abstracted from reference 64.

Table 5. Experimental Mole Fraction Solubilities x of Dimethyl Fumarate (cr) in Liquid Solvents at Temperature T and Pressure $p = 0.1$ MPa [a,b]

Solvent	T/K	x	T/K	x
methanol	297.45	0.007489	319.37	0.02794
	301.00	0.009483	322.28	0.03346
	305.55	0.01216	325.93	0.03997
	309.17	0.01520	329.15	0.04912
	312.85	0.01886	332.30	0.05996
	316.45	0.02314	337.65	0.08096
ethanol	289.95	0.003277	314.75	0.01990
	294.45	0.004650	318.65	0.02532
	297.55	0.006074	322.55	0.03261
	303.15	0.009081	327.35	0.04312
	307.30	0.01218	331.85	0.05805
	311.10	0.01566	336.05	0.07513
propan-1-ol	295.20	0.005038	323.65	0.03692
	299.95	0.006683	328.95	0.05351
	304.35	0.009057	332.50	0.06857
	307.85	0.01136	335.65	0.08701
	310.70	0.01381	338.15	0.1064
	313.20	0.01736	341.30	0.1361
	318.70	0.02531		

[a] Standard uncertainties u are $u(T) = 0.05$ K, $u_r(p) = 0.05$, $u_r(x) = 0.005$.

[b] The experimental data in this table were abstracted from reference 65.

Table 6. Experimental (Solid + Liquid) SLE Data for the System 18-Crown-6 (1) + 2-Methylpropan-2-ol (2) at Liquid Mole Fraction x, Temperature T, and Pressure p = 0.1 MPa [a,b]

x_1	T/K	Solid phase	x_1	T/K	Solid phase
0.0000	298.15	2-Methylpropan-2-ol(cr)	0.3769	297.75	18-Crown-6(cr, II)
0.0225	294.40	2-Methylpropan-2-ol(cr)	0.4389	299.55	18-Crown-6(cr, II)
0.0508	290.70	2-Methylpropan-2-ol(cr)	0.4920	300.65	18-Crown-6(cr, II)
0.0658	288.70	2-Methylpropan-2-ol(cr)	0.5183	301.30	18-Crown-6(cr, II)
0.0826	287.10	2-Methylpropan-2-ol(cr)	0.5523	302.00	18-Crown-6(cr, II)
0.1022	286.30	18-Crown-6(cr, II)	0.6336	303.72	18-Crown-6(cr, I)
0.1241	287.80	18-Crown-6(cr, II)	0.7005	305.65	18-Crown-6(cr, I)
0.1498	289.15	18-Crown-6(cr, II)	0.7620	307.20	18-Crown-6(cr, I)
0.1810	291.30	18-Crown-6(cr, II)	0.8635	309.55	18-Crown-6(cr, I)
0.2234	293.20	18-Crown-6(cr, II)	0.9320	310.95	18-Crown-6(cr, I)
0.2850	295.05	18-Crown-6(cr, II)	1.0000	312.45	18-Crown-6(cr, I)
0.3249	296.25	18-Crown-6(cr, II)			

[a] Standard uncertainties u are $u(T)$ = 0.05 K, $u(x)$ = 0.0005, $u(p)$ = 5 kPa.

[b] The experimental data are shown in Figure 1 and were abstracted from reference 66.

Table 7. Experimental (Solid + Liquid) Equilibrium Temperatures T and Liquid Mole Fractions x for the System Octan-1-ol (1) + Decylamine (2) at Pressure p = 0.1 MPa [a,b,c]

x_1	T/K	Solid phase	x_1	T/K	Solid phase
0.0000	289.16	Decylamine(cr)	0.4901	277.96	AB(cr)
0.0310	288.63	Decylamine(cr)	0.5167	278.00	AB(cr)
0.0556	288.06	Decylamine(cr)	0.5382	277.95	AB(cr)
0.0811	287.44	Decylamine(cr)	0.5603	277.70	AB(cr)
0.1087	286.87	Decylamine(cr)	0.5850	277.25	AB(cr)
0.1389	286.30	Decylamine(cr)	0.6122	276.60	AB(cr)
0.1590	285.76	Decylamine(cr)	0.6529	275.61	AB(cr)
0.1816	285.27	Decylamine(cr)	0.6883	274.57	AB(cr)
0.2006	284.76	Decylamine(cr)	0.7232	273.17	AB(cr)
0.2375	283.81	Decylamine(cr)	0.7648	270.80	AB(cr)
0.2779	282.58	Decylamine(cr)	0.8124	267.85	AB(cr)
0.3080	281.41	Decylamine(cr)	0.8652	263.60	AB(cr)
0.3343	280.42	Decylamine(cr)	0.8790	262.35	AB(cr)
0.3587	279.36	Decylamine(cr)	0.9149	258.45	AB(cr)
0.3821	278.45	Decylamine(cr)	0.9333	256.16	AB(cr)
0.4049	277.89	Decylamine(cr)	0.9526	256.35	Octan-1-ol(cr)
0.4345	277.60	AB(cr)	0.9753	257.14	Octan-1-ol(cr)
0.4623	277.75	AB(cr)	1.0000	258.03	Octan-1-ol(cr)
0.4832	277.83	AB(cr)			

[a] Standard uncertainties u are $u(T)$ = 0.1 K, $u(x)$ = 0.0005, and $u(p)$ = 5 kPa

[b] AB(cr) represents the crystal of the compound formed for mole fraction 0.5 of component 1.

[c] The experimental data are shown in Figure 2 and were abstracted from reference 67.

Table 8. Experimental (Solid + Liquid) $\mathrm{cr,l} \leftrightarrow \mathrm{l}$ (Solid + Liquid + Liquid) $\mathrm{cr,l_1,l_2} \leftrightarrow \mathrm{l_1,l_2}$, and (Liquid + Liquid) $\mathrm{l_1,l_2} \leftrightarrow \mathrm{l}$ Equilibrium Temperatures T and Liquid Mole Fractions x for the System Octan-1-ol (1) + Ethanonitrile (2) at Pressure p = 0.1 MPa [a,b]

x_1	T/K	Phase Boundary	x_1	T/K	Phase Boundary
0.0000	230.42	cr(2),l; invariant	0.8733	256.02	cr(1),l ↔ l
0.0100	246.88	cr(1),l ↔ l	0.9119	256.41	cr(1),l ↔ l
0.0226	253.45	cr(1),l ↔ l	0.9458	256.93	cr(1),l ↔ l
0.0324	255.34	cr(1),l ↔ l	0.9677	257.42	cr(1),l ↔ l
0.0454	255.53	cr(1),l_1,l_2; invariant	1.0000	258.03	cr(1),l ↔ l
0.0661	255.53	cr(1),l_1,l_2; invariant	0.0454	262.13	l_1,l_2 ↔ l
0.0847	255.53	cr(1),l_1,l_2; invariant	0.0661	270.06	l_1,l_2 ↔ l
0.1025	255.53	cr(1),l_1,l_2; invariant	0.0847	273.89	l_1,l_2 ↔ l
0.1320	255.53	cr(1),l_1,l_2; invariant	0.1025	276.89	l_1,l_2 ↔ l
0.1586	255.53	cr(1),l_1,l_2; invariant	0.1320	278.80	l_1,l_2 ↔ l
0.1966	255.53	cr(1),l_1,l_2; invariant	0.1586	280.25	l_1,l_2 ↔ l
0.2315	255.53	cr(1),l_1,l_2; invariant	0.1966	281.31	l_1,l_2 ↔ l
0.2721	255.53	cr(1),l_1,l_2; invariant	0.2315	281.93	l_1,l_2 ↔ l
0.2953	255.53	cr(1),l_1,l_2; invariant	0.2721	282.07	l_1,l_2 ↔ l
0.3315	255.53	cr(1),l_1,l_2; invariant	0.2953	282.03	l_1,l_2 ↔ l
0.3611	255.53	cr(1),l_1,l_2; invariant	0.3315	281.83	l_1,l_2 ↔ l
0.3939	255.53	cr(1),l_1,l_2; invariant	0.3611	281.56	l_1,l_2 ↔ l
0.4220	255.53	cr(1),l_1,l_2; invariant	0.3939	281.08	l_1,l_2 ↔ l
0.4680	255.53	cr(1),l_1,l_2; invariant	0.4220	280.60	l_1,l_2 ↔ l
0.4842	255.53	cr(1),l_1,l_2; invariant	0.4680	279.59	l_1,l_2 ↔ l
0.5032	255.53	cr(1),l_1,l_2; invariant	0.4842	279.12	l_1,l_2 ↔ l
0.5242	255.53	cr(1),l_1,l_2; invariant	0.5032	278.37	l_1,l_2 ↔ l
0.5593	255.53	cr(1),l_1,l_2; invariant	0.5242	277.69	l_1,l_2 ↔ l
0.5848	255.53	cr(1),l_1,l_2; invariant	0.5593	276.33	l_1,l_2 ↔ l
0.6372	255.53	cr(1),l_1,l_2; invariant	0.5848	274.81	l_1,l_2 ↔ l
0.6752	255.53	cr(1),l_1,l_2; invariant	0.6372	272.25	l_1,l_2 ↔ l
0.6983	255.53	cr(1),l_1,l_2; invariant	0.6752	269.33	l_1,l_2 ↔ l
0.7357	255.53	cr(1),l_1,l_2; invariant	0.6983	267.62	l_1,l_2 ↔ l
0.7708	255.53	cr(1),l_1,l_2; invariant	0.7357	264.93	l_1,l_2 ↔ l
0.7948	255.53	cr(1),l_1,l_2; invariant	0.7708	260.70	l_1,l_2 ↔ l
0.8315	255.82	cr(1),l ↔ l	0.7948	257.40	l_1,l_2 ↔ l

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[a] Standard uncertainties u are $u(x)$ = 0.0005, $u(T)$ = 0.1 K, and $u(p)$ = 0.005 MPa

[b] The experimental data are shown in Figure 3 and were abstracted from reference 68.

Table 9. Experimental equilibrium temperatures T and mole fractions x for {solid (II) + solid (I)} equilibrium, s(II) ↔ s(I),s(II) and s(I) ↔ s(I),s(II); and {solid (I) + liquid} equilibrium, s(I) ↔ s(I),l and l ↔ s(I),l for the system heptadecane (1) + nonadecane (2) at pressure p = 0.1 MPa.[a,b]

x_1	T/K	$u(T)$/K	Phase Boundary	T/K	$u(T)$/K	Phase Boundary	T/K	$u(T)$/K	Phase Boundary	T/K	$u(T)$/K	Phase Boundary
0	283.9	0.6	s(II) ↔ s(I) ; invariant				294.8	0.7	s(I) ↔ l; invariant			
0.05	271.6	0.6	s(II) ↔ s(I),s(II)	273.7	0.6	s(I) ↔ s(I),s(II)	294.8	0.8	s(I) ↔ s(I),l	295.0	0.8	l ↔ s(I),l
0.16	269.5	0.6	s(II) ↔ s(I),s(II)	271.3	0.6	s(I) ↔ s(I),s(II)	294.9	0.8	s(I) ↔ s(I),l	295.2	0.6	l ↔ s(I),l
0.25	268.4	0.8	s(II) ↔ s(I),s(II)	268.4	0.8	s(I) ↔ s(I),s(II)	295.0	1.0	s(I) ↔ s(I),l	296.4	0.7	l ↔ s(I),l
0.51	269.2	0.7	s(II) ↔ s(I),s(II)	271.3	1.0	s(I) ↔ s(I),s(II)	296.6	1.3	s(I) ↔ s(I),l	299.4	0.7	l ↔ s(I),l
0.75	276.2	0.6	s(II) ↔ s(I),s(II)	278.3	0.6	s(I) ↔ s(I),s(II)	299.2	1.3	s(I) ↔ s(I),l	301.8	0.7	l ↔ s(I),l
0.90	285.2	1.0	s(II) ↔ s(I),s(II)	286.2	1.0	s(I) ↔ s(I),s(II)	301.0	1.3	s(I) ↔ s(I),l	303.2	0.7	l ↔ s(I),l
1	294.8	0.6	s(II) ↔ s(I) ; invariant				304.5	0.7	s(I) ↔ l; invariant			

[a] Standard uncertainties u are $u(x) = 0.01$, $u(T) = 0.1$ K, and $u(p) = 0.005$ MPa

[b] The experimental data are shown in Figure 4 and were abstracted from reference 69.

Table 10. Experimental bubble point (liquid to liquid + vapor) $l \leftrightarrow l,g$, phase boundary (liquid + vapor to liquid + liquid + vapor) $l,g \leftrightarrow l_1,l_2,g$, and phase boundary (liquid + liquid + vapor to liquid + liquid) $l_1,l_2,g \leftrightarrow l_1,l_2$, data at pressure p and temperature T for $[w_1\ CO_2 + (1 - w_1)\{w_2 \cdot \mathrm{HPG}(5700\ \mathrm{g/mol}) + w_3 \cdot CH_3OH\}]$ at mass fractions w_1 of CO_2, for $w_2 = 0.499$ and $w_3 = 0.501$.[a,b]

w_1	T/K	p/MPa	phase boundary	w_1	T/K	p/MPa	phase boundary	w_1	T/K	p/MPa	phase boundary	w_1	T/K	p/MPa	phase boundary
0.020	332.70	0.941	$l \leftrightarrow l,g$	0.050	332.66	2.218	$l \leftrightarrow l,g$	0.100	332.99	4.330	$l \leftrightarrow l,g$	0.150	333.00	5.281	$l,g \leftrightarrow l_1,l_2,g$
0.020	342.47	1.081	$l \leftrightarrow l,g$	0.050	342.41	2.523	$l \leftrightarrow l,g$	0.100	343.00	4.691	$l \leftrightarrow l,g$	0.150	343.01	5.917	$l,g \leftrightarrow l_1,l_2,g$
0.020	352.20	1.246	$l \leftrightarrow l,g$	0.050	352.12	2.867	$l \leftrightarrow l,g$	0.100	353.03	5.611	$l \leftrightarrow l,g$	0.150	353.04	6.517	$l,g \leftrightarrow l_1,l_2,g$
0.020	361.89	1.407	$l \leftrightarrow l,g$	0.050	352.17	2.848	$l \leftrightarrow l,g$	0.100	363.03	6.282	$l \leftrightarrow l,g$	0.150	363.05	7.058	$l,g \leftrightarrow l_1,l_2,g$
0.020	371.57	1.594	$l \leftrightarrow l,g$	0.050	361.82	3.202	$l \leftrightarrow l,g$	0.100	373.04	6.952	$l \leftrightarrow l,g$	0.150	373.07	7.518	$l,g \leftrightarrow l_1,l_2,g$
0.020	381.29	1.812	$l \leftrightarrow l,g$	0.050	361.89	3.183	$l \leftrightarrow l,g$	0.100	383.03	7.633	$l \leftrightarrow l,g$	0.150	383.05	7.899	$l,g \leftrightarrow l_1,l_2,g$
0.020	390.99	2.042	$l \leftrightarrow l,g$	0.050	371.57	3.552	$l \leftrightarrow l,g$	0.100	393.04	8.053	$l,g \leftrightarrow l_1,l_2,g$	0.150	393.18	8.179	$l,g \leftrightarrow l_1,l_2,g$
0.020	400.73	2.317	$l \leftrightarrow l,g$	0.050	371.57	3.539	$l \leftrightarrow l,g$	0.100	403.07	8.198	$l,g \leftrightarrow l_1,l_2,g$	0.150	403.13	8.340	$l,g \leftrightarrow l_1,l_2,g$
0.020	410.48	2.622	$l \leftrightarrow l,g$	0.050	381.29	3.914	$l \leftrightarrow l,g$	0.100	408.02	8.198	$l,g \leftrightarrow l_1,l_2,g$	0.150	333.00	6.271	$l_1,l_2 \leftrightarrow l_1,l_2,g$
0.020	420.26	2.978	$l \leftrightarrow l,g$	0.050	381.31	3.933	$l \leftrightarrow l,g$	0.100	413.02	8.239	$l,g \leftrightarrow l_1,l_2,g$	0.150	343.01	7.132	$l_1,l_2 \leftrightarrow l_1,l_2,g$
				0.050	390.88	4.398	$l \leftrightarrow l,g$	0.100	423.02	8.179	$l,g \leftrightarrow l_1,l_2,g$	0.150	353.04	8.012	$l_1,l_2 \leftrightarrow l_1,l_2,g$
				0.050	400.76	4.818	$l \leftrightarrow l,g$	0.100	433.05	8.059	$l,g \leftrightarrow l_1,l_2,g$	0.150	363.05	8.853	$l_1,l_2 \leftrightarrow l_1,l_2,g$
				0.050	410.51	5.268	$l \leftrightarrow l,g$	0.100	442.99	8.039	$l,g \leftrightarrow l_1,l_2,g$	0.150	373.07	9.684	$l_1,l_2 \leftrightarrow l_1,l_2,g$
				0.050	420.27	5.768	$l \leftrightarrow l,g$	0.100	452.85	7.799	$l_1,l_2 \leftrightarrow l_1,l_2,g$	0.150	393.18	11.239	$l_1,l_2 \leftrightarrow l_1,l_2,g$
				0.050	439.79	6.879	$l \leftrightarrow l,g$	0.100	403.02	8.873	$l_1,l_2 \leftrightarrow l_1,l_2,g$	0.150	403.13	11.855	$l_1,l_2 \leftrightarrow l_1,l_2,g$
				0.050	449.55	7.494	$l \leftrightarrow l,g$	0.100	408.02	9.134	$l_1,l_2 \leftrightarrow l_1,l_2,g$				
								0.100	413.02	9.439	$l_1,l_2 \leftrightarrow l_1,l_2,g$				
								0.100	423.02	9.974	$l_1,l_2 \leftrightarrow l_1,l_2,g$				
								0.100	433.05	10.505	$l_1,l_2 \leftrightarrow l_1,l_2,g$				
								0.100	443.00	11.050	$l_1,l_2 \leftrightarrow l_1,l_2,g$				
								0.100	452.87	11.476	$l_1,l_2 \leftrightarrow l_1,l_2,g$				
								0.100	393.04	9.454	$l \leftrightarrow l,g$				
								0.100	403.05	12.141	$l \leftrightarrow l,g$				
								0.100	408.02	13.461	$l \leftrightarrow l,g$				

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[a] $u(w) = 0.001$, $u(T) = 0.02$ K, and $u(p) = 0.005$ MPa.

[b] The experimental data were abstracted from reference 70.

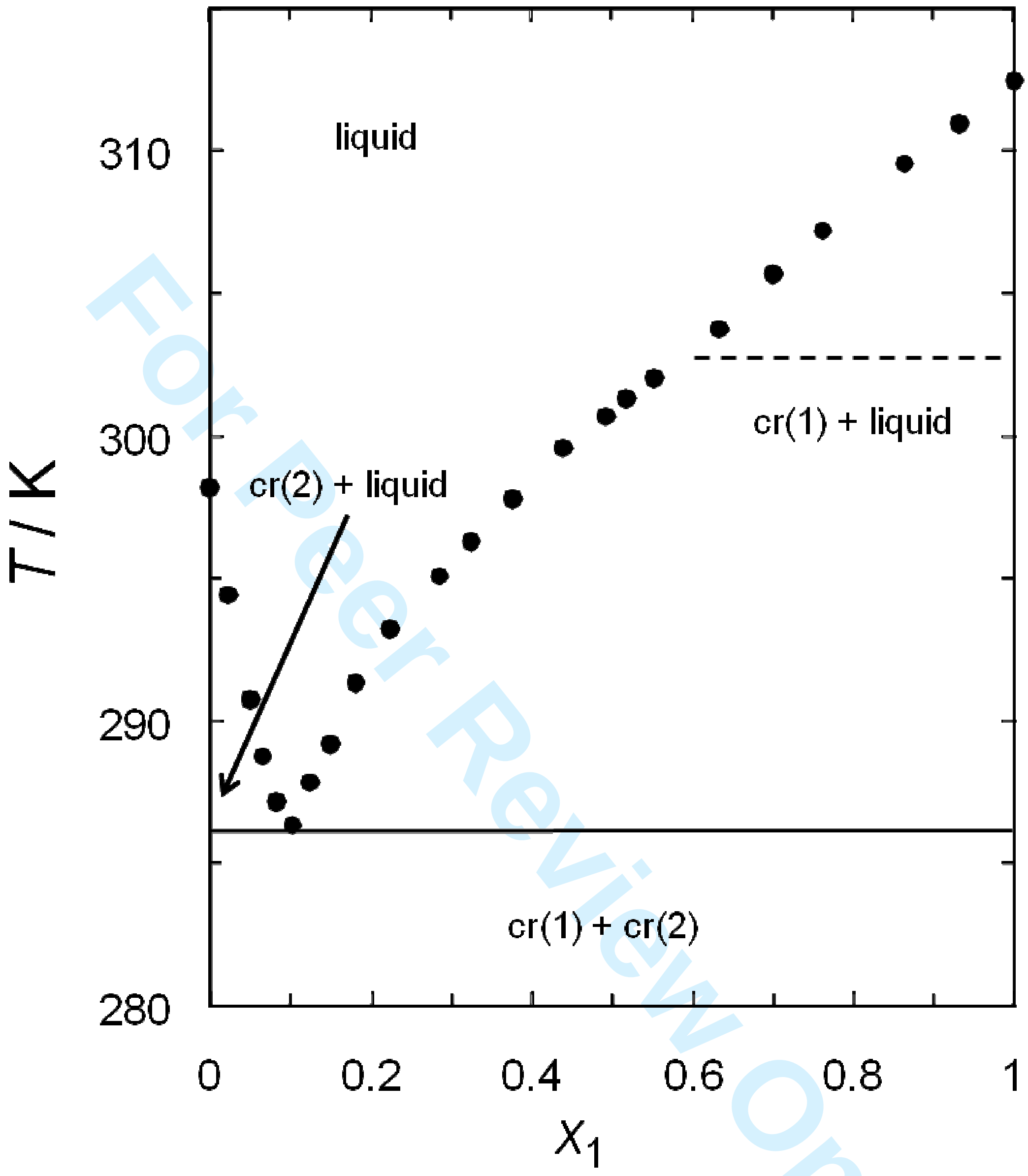

Figure 1. Experimental (solid + liquid) data for the system 18-Crown-6 (1) + 2-Methylpropan-2-ol (2) at mole fraction *x*, temperature *T*, and pressure *p* = 0.1 MPa. The uninterrupted line indicates the eutectic temperature. The dashed line indicates the temperature of the cr(I)-to-cr(II) phase transition in component 1.

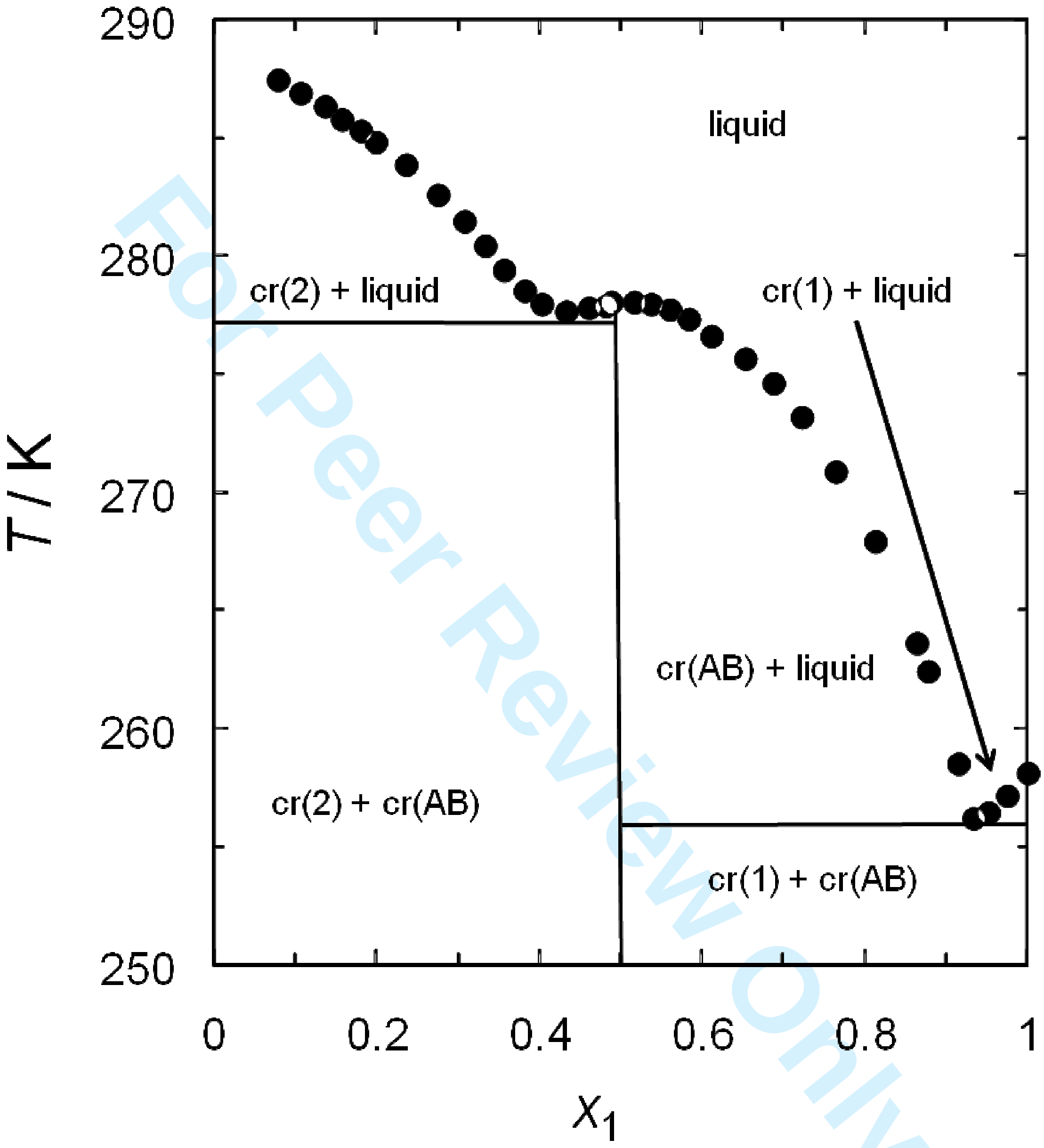

Figure 2. Experimental (solid + liquid) equilibrium temperatures *T* and mole fractions *x* for the system octan-1-ol (1) + decylamine (2) at pressure *p* = 0.1 MPa. The vertical line indicates the composition of the inter-component compound. The horizontal lines indicate eutectic temperatures.

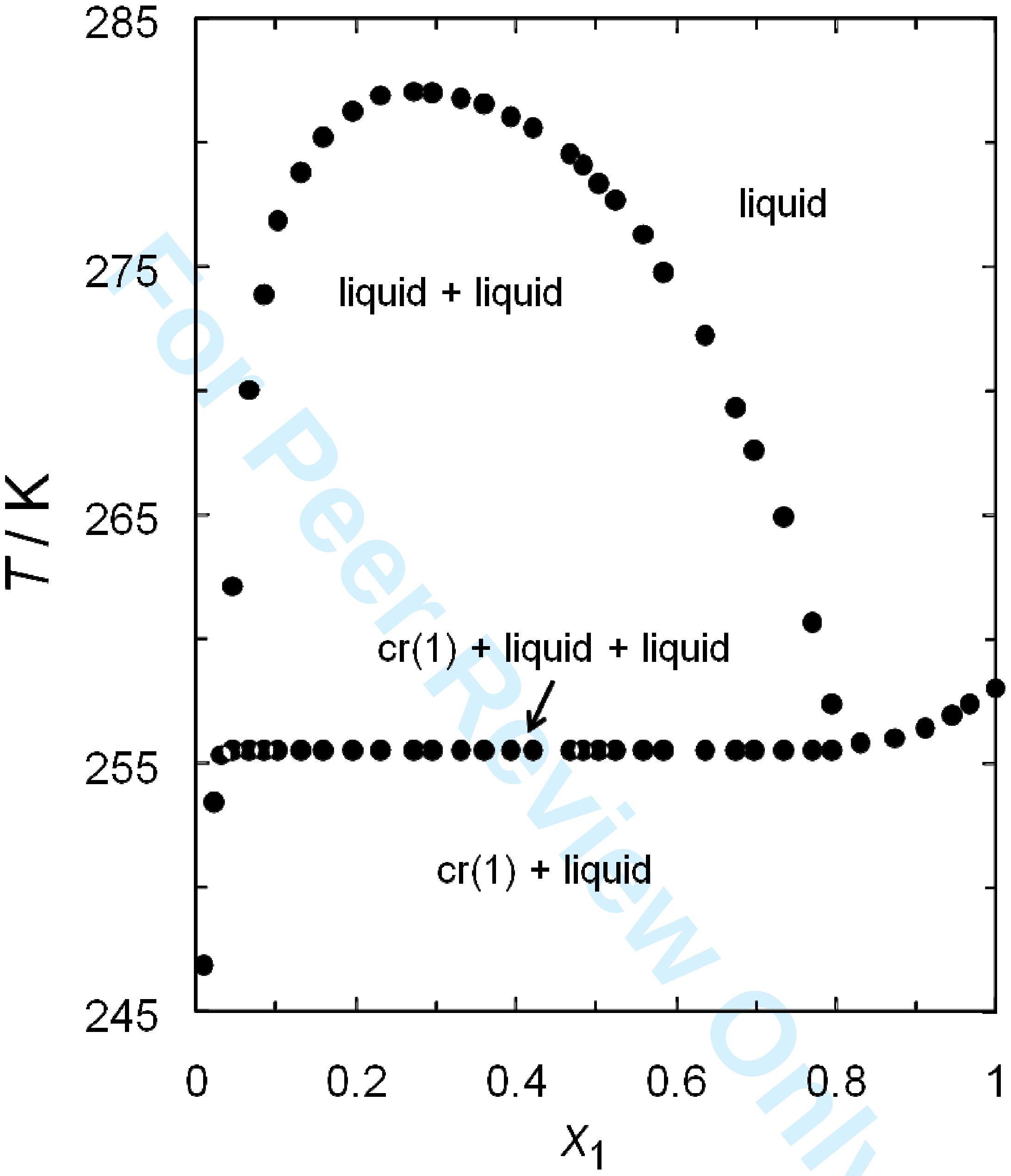

Figure 3. Experimental (solid + liquid), (solid + liquid + liquid), and (liquid + liquid) equilibrium temperatures T and mole fractions x for the system octan-1-ol (1) + ethanonitrile (2) at pressure p = 0.1 MPa.

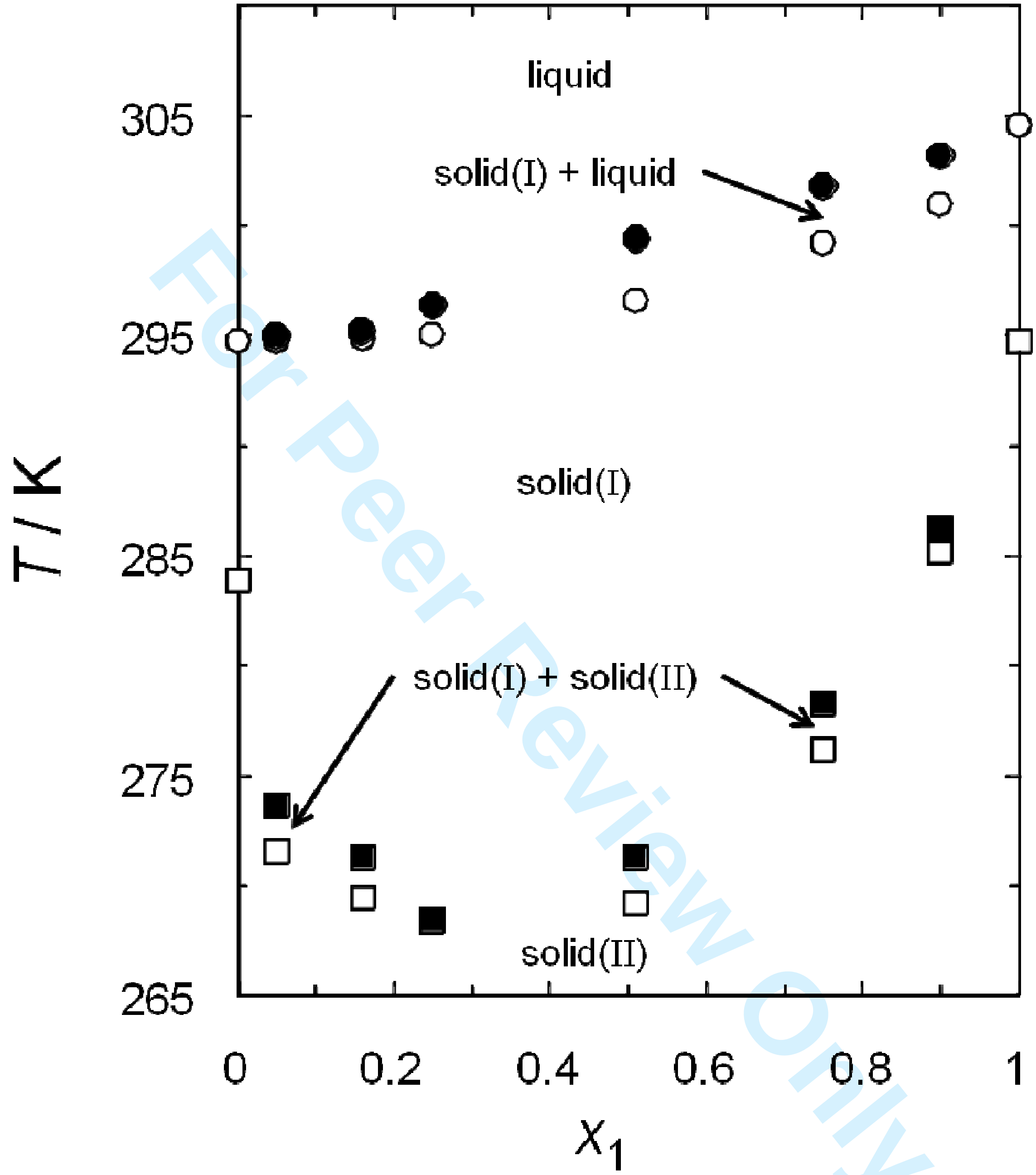

Figure 4. Experimental {solid(I) + liquid} and {solid (I) + solid (II)} equilibrium temperatures *T* and mole fractions *x* for the system heptadecane (1) + nonadecane (2) at pressure *p* = 0.1 MPa.