IUPAC-NIST Solubility Data Series. 79. Alkali and Alkaline Earth Metal Pseudohalides

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This volume presents solubility data of azides, cyanides, cyanates, and thiocyanates of alkali metals, alkaline earth metals, and ammonium. Covered are binary and ternary systems in all solvents. No solubility data have been found for some of the compounds of alkali metals, alkaline metals, and ammonium. These include beryllium and magnesium azides, lithium, rubidium cesium, ammonium, and alkaline earth cyanates and cyanides, and beryllium thiocyanate. Likewise, no solubility data seem to exist for selenocyanates of the mentioned metals and ammonium. The literature has been covered up to the middle of 2001, and there was a great effort to have the literature survey as complete as possible. The few documents which remained unavailable to the editor, and could not be included in the volume, are listed in the Appendix. For some compounds it was not possible to show the *Chemical Abstracts* registry numbers since these have not been assigned. For this reason, the registry number index is incomplete. *© 2004 American Institute of Physics.* [DOI: 10.1063/1.1563591]

Key words: alkali metals; alkaline earth metals; ammonia; azides; cyanides; cyanates; organic solvents; thiocyanates; solid-liquie equilibrium; solubility; water.

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1. Preface

This volume presents solubility data of azides, cyanides, cyanates, and thiocyanates of alkali metals, alkaline earth metals, and ammonium. Covered are binary and ternary systems in all solvents. No solubility data have been found for some of the compounds of alkali metals, alkaline metals, and ammonium. These include beryllium and magnesium azides, lithium, rubidium cesium, ammonium, and alkaline earth cyanates and cyanides, and beryllium thiocyanate. Likewise, no solubility data seem to exist for selenocyanates of the mentioned metals and ammonium. The literature has been covered up to the middle of 2001, and there was a great effort to have the literature survey as complete as possible. The few documents which remained unavailable to the compiler, and could not be included in the volume are listed in the Appendix. For some compounds it was not possible to show the *Chemical Abstracts* registry numbers since these have not been assigned. For this reason, the registry number index is incomplete.

In addition to documents that published numerical data, some papers that presented data in graphical form only were included as well. They were considered for the volume either if no other data were available for the system, or if the data were published in difficult to obtain older literature. These criteria led the compiler to include sometimes papers in which the authors failed to specify conditions such as temperature, equilibrium time, or methods of analysis. Phase diagrams have been included for some of the ternary systems. For binary eutonic systems, phase diagrams were included only if no numerical data were reported in the original documents and the diagrams were the sole source of information. Of the many systems covered by the volume, relatively few were studied by more than one laboratory. Thus the opportunity to carry out evaluations has been limited, and only 20 systems have been evaluated. However, because of some uncertainty in most of the evaluated systems, only tentative solubility values could usually be recommended.

Only those published results that report meaningful data were considered for the volume. Papers that reported qualitative results with statements like ‘‘sparingly soluble’’ or ‘‘insoluble,’’ etc., were not considered. However, some documents reported solubility data which, although not included in the volume for one reason or other (e.g., single values of uncertain quality without any supporting information, sketches of phase diagrams), may nevertheless be of some informative value to the potential user of this volume in case they represent the only information available for a given system. For this reason, a list of systems for which only such data exist has been included in the Appendix.

The editor wishes to express his thanks to the following colleagues from IUPAC for their effort in proving copies of publications, which would otherwise not be available to him: Professor H. Akaiwa, Gunma, Japan (also for translating the Japanese papers); D. J. J. Counioux, Lyon, France; Dr. P. G. T. Fogg, London, U.K.; Professor Fu Jufu, Beijing, China; Dr. H. J. M. Grünbauer, Amsterdam, The Netherlands; Dr. A. Maczynski, Warsaw, Poland; Professor P. Paoletti, Florence, Italy; Professor V. M. Valyashko, Moscow, Russia; and Professor B. A. Wolf, Mainz, Germany. Without their help the volume would not be complete.

2. Introduction to the Solubility Data Series: Solubility of Solids 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 independent sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values, and compiled data sheets are published on consecutive pages.

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. Normally, 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;
(c) solvents.

In each of (a), (b) or (c), the 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.

The same order is followed in arranging the compilation sheets within a given volume.

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 Data

Components are described as (1), (2), etc., as defined in the ‘‘Components’’ box. Data are reported in the units used in the original publication, with the exception that modern names for units and quantities are used; e.g., mass percent for weight percent; mol dm^{-3} for molar; etc. 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 concentrations to mole fractions are included, but otherwise this is done in the evaluation, with the values and sources of the densities 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, compilers note that numerical data have been obtained from published graphs using digitizing techniques. In these cases, the precision of the data can be determined by the quality of the original graph and the limitations of the digitizing technique. In some cases graphs have been included, either to illustrate data more clearly, or if this is the only information in the original. Full grids are not usually inserted as it is not intended that users should read data from the graphs.

Method

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

Source and Purity of Materials

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

Estimated Error

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

Comments and/or Additional Data

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

References

The format for these follows the format for the Original Measurements box, except that final page numbers are omitted. References (usually cited in the original paper) are given where relevant to interpretation of the compile 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, patents and reports) 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 error. 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 accurately converted.

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

2.3.1. Mixtures, Solutions and Solubilities

A *mixture*[5] 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] 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.[6]

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

Either point of view, mixture or solution, may be taken in describing solubility. The two points of view find their expression in the reference states used for definition of activities, activity coefficients and osmotic coefficients.

Note that the composition of a saturated mixture (or solution) can be described in terms of any suitable set of thermodynamic components. Thus, the solubility of a salt hydrate in water is usually given as the relative proportions of anhydrous salt in solution, rather then the relative proportions of hydrated salt and water.

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, IUPAC Green Book.[3] A few quantities follow the ISO standards[7] or the German standard;[8] see a review by Cvitaš[9] 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 100 x_1.

2. *Ionic mole fractions* of salt i, x_{i+}, x_{i-}: For mixture of s binary salts i, each of which ionizes completely into n_{i+} cations and υ_{i-} anions, with $\upsilon_i = \upsilon_{i+} + \upsilon_{i-}$ and a mixture of p nonelectrolytes k, of which some may be considered as solvent components, a generalization of the definition in Robinson and Stokes[10] gives:

$$x_{+i} = \frac{\upsilon_{+i} x_{+i}}{1 + \sum_{j=1}^{s} (\upsilon_j - 1) x_j}, \quad x_{-i} = \frac{\upsilon_{-i} x_{+i}}{\upsilon_{+i}} \quad i = 1 \ldots s \tag{2}$$

$$x_{ok} = \frac{x_j}{1 + \sum_{j=1}^{s} (\upsilon_j - 1) x_j}, \quad k = (s+1) \ldots c. \tag{3}$$

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

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

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

$$x_1 = \frac{\upsilon_{+2} x_{o1}}{\upsilon_{+2} - (\upsilon_2 - 1) x_{+2}} \quad x_2 = \frac{x_{+2}}{\upsilon_{+2} - (\upsilon_2 - 1) x_{+2}}. \tag{5}$$

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

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)/100g solution* are no longer used.

4. *Solute mole fraction* of substance 1, $x_{\upsilon,1}$:

$$x_{s,1} = m_1 \Big/ \sum_{s=1}^{c'} m_s = x_1 \Big/ \sum_{s=1}^{c'} x_s \tag{7}$$

where c' is the number of solutes in the mixture. These quantities are sometimes called Jänecke mole (mass) fractions.[11,12] *Solute mass fraction* of substance 1, $w_{s,1}$, is defined analogously.

5. *Solvent mole fraction* of substance 1, $x_{\upsilon,1}$:

$$x_{\upsilon,1} = x_1 \Big/ \sum_{s=1}^{p} x_s. \tag{8}$$

Here, p is the number of solvent components in the mixture. *Solvent mass fraction* of substance 1, $w_{\upsilon,1}$, is defined analogously.

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

$$m_1 = n_1 / n_2 M_2 \tag{9}$$

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

7. *Aquamolality, Solvomolality* of substance 1 in a mixed solvent with components 2, 3,[13] $m_1^{(3)}$:

$$m_1^{(3)} = m_1 \overline{M} / M_3 \tag{10}$$

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

$$\overline{M} = x_{\upsilon,2} M_2 + (1 - \upsilon_{\upsilon,2}) M_3 \tag{11}$$

and x_υ, 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.

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

$$c_1 = [\text{formula of solute}] = n_1 / V \tag{12}$$

SI base units: mol cm^{-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.

9. *Mass concentration* of solute 1 in a solution of volume V, ρ_1:

$$\rho_1 = g_1 / V = c_1 M_1 / V \tag{13}$$

SI base units: kg m^{-3}.

10. *Mole ratio*, $r_{\mathrm{A,B}}$ (dimensionless):[9]

$$r_{n,12} = n_1 / n_2\,. \tag{14}$$

Mass ratio, symbol $\zeta_{\mathrm{A,B}}$, may be defined analogously.[9]

11. *Ionic strength*, I_m (molality basis), or I_c (concentration basis):

$$I_m = \frac{1}{2} \sum_i m_i z_i^2, \quad I_c = \frac{1}{2} \sum_i c_i z_i^2 \tag{15}$$

where z_i is the charge number of ion i. While these quantities are not used generally to express solubilities, they are used to express the compositions of nonsaturating components. For a single salt i with ions of charge numbers z_+ and z_-,

$$I_m = |z_+ z_-| \upsilon m_i, \quad I_c = |z_+ z_-| \upsilon c_i. \tag{16}$$

Mole and mass fractions and mole ratios are appropriate to either the mixture of 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 equation 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.

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

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

Salt hydrates are generally not considered to be saturating components since most solubilities are expressed in terms of the anhydrous salt. The existence of hydrates or solvates is noted carefully in the critical evaluation.

Mineralogical names are also quoted, along with their CA Registry Numbers, again usually in the text and CA Registry Numbers (where available) are given usually in the critical evaluation.

In addition to the quantities defined above, the following are useful in conversions between concentrations and other quantities.

12. *Density*, ρ:

$$\rho=g/V=\sum_{s=1}^{c}\rho_s \qquad (17)$$

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

13. *Relative density*, $d=\rho/\rho°$: 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 aims 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 this 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 Publications, Oxford, U.K., 1993).
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[12] H. L. Friedman, J. Chem. Phys. **32**, 1351 (1960).
[13] J. W. Lorimer, in *Alkali Metal and Ammonium Chlorides in Water and Heavy Water (Binary Systems)*, edited by R. Cohen-Adad, and J. W. Lorimer, IUPAC Solubility Data Series, Vol. 47 (Pergamon, Oxford, U.K., 1991), p. 495.

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3. The Solubility of Azides

3.1. Lithium Azide

Components:	Original Measurements:
(1) Lithium azide; LiN_3; [19597-69-4] (2) Solvents	T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261–309 (1898).

Variables:	Prepared By:
T/K: 283–289	J. Hála

Experimental Data

Solubility of LiN_3 in water or ethanol at different temperatures[a]

Solvent	Temperature (t/°C)	LiN_3 (g/100 g solvent)	LiN_3 (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	10	36.12	7.377
	15.5	62.07	12.68
	16	66.41	13.56
Ethanol; C_2H_6O; [64-17-5]	16	20.26	4.14

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: Saturated solutions of LiN_3 in water showed alkaline reaction.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish, and dried in a dessicator until constant weight was attained.

Source and Purity of Materials:

LiN_3 was prepared from Li_2SO_4 and $Ba(N_3)_2$ as colorless hygroscopic crystals. The product was recrystallized from water, and analyzed after prolonged drying over concentrated H_2SO_4 in a vacuum desiccator. Found/calculated for LiN_3(%):N 85.67–86.02/85.71, Li 14.09–14.18/14.29. The barium azide used was prepared by dissolving $Ba(OH)_2$ in 8% aqueous solution of HN_3. The latter was obtained by distillation with dilute H_2SO_4 of either $Pb(N_3)_2$ or NH_4N_3 according to Curtius.[1] Purity of water not specified. Absolute ethanol was used.

Estimated Error:

Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] T. Curtius, Ber. **24**, 3341 (1891).

Components:	Original Measurements:
(1) Lithium azide; LiN_3; [19597-69-4] (2) Water; H_2O; [7732-18-5]	A. P. Rollet and J. Wohlgemuth, Compt. Rend. **199**, 1772–4 (1934).

Variables:	Prepared By:
Temperature and composition.	J. Hála

Experimental Data

Phase diagram of the LiN_3-H_2O system[a]

Significant point	Temperature (t/°C)	LiN_3 (100 w_1/mass %)	LiN_3 (m_1/mol kg^{-1})[b]	Solid phase[c]
E	−47.5±0.5	26.0±0.4	7.176	A+B
T_1	−31.0±0.5	33.5±0.3	10.29	B+C
T_2	68.2±0.1	48.0±0.3	18.85	C+D

[a] Results were presented in graphical form (Fig. 1). Numerical values were reported for three significant points in the phase diagram.
[b] Calculated by compiler.
[c] A: Ice; H_2O; [7732-18-5]; B: $LiN_3 \cdot 4H_2O$; [ ]; C: $LiN_3 \cdot H_2O$; [34204-05-2]; D: LiN_3; [19597-69-4].

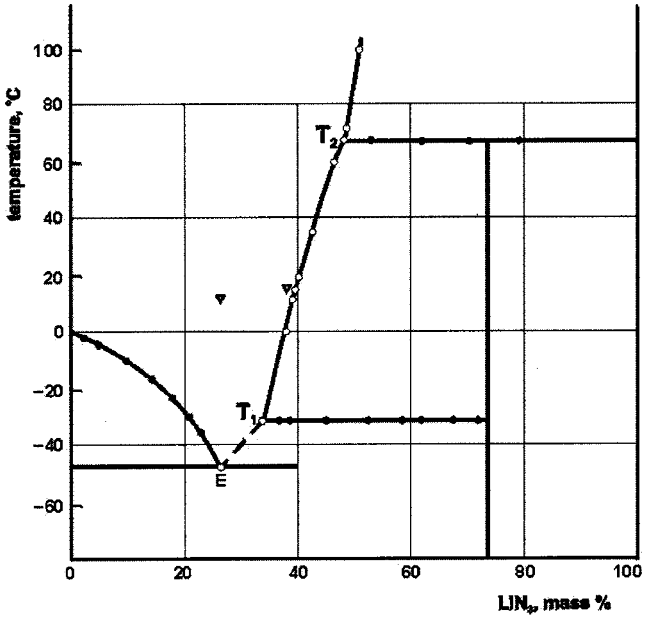

FIG. 1. Phase diagram of the LiN_3-H_2O system [(full circles) polythermal measurements, (open circles) isothermal measurements, (triangles) data from Curtius and Rissom,[1] included by authors].

Auxiliary Information

Method/Apparatus/Procedure:

Freezing curve was obtained by polythermal method. The solubility curve was obtained by isothermal method. Excess salt was equilibrated with water in a thermostat for 1 day in closed vessels. In the saturated solutions, azide was precipitated with $AgNO_3$, and subsequently determined gravimetrically as AgCl, lithium was determined gravimetrically as Li_2SO_4. Cooling curves were obtained by polythermal method, the time necessary to reach equilibrium was not specified. It was stated that equilibrium was attained very slowly, and that the systems showed considerable tendency to supersaturation even when inoculated.

Source and Purity of Materials:

No details reported.

Estimated Error:

Temperature: ±0.1–0.5 K (authors).
Solubility: 100 w_1: ±0.3%–0.4% (authors).

References:

[1] T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261 (1898).

3.2. Sodium Azide

Components:

(1) Sodium azide; NaN_3; [26628-22-8]
(2) Solvents

Original Measurements:

T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261–309 (1898).

Variables:

T/K: 283–290

Prepared By:

J. Hála

Experimental Data

Solubility of NaN_3 in water or ethanol at different temperatures[a]

Solvent	Temperature (t/°C)	NaN_3 (g/100 g solvent)	NaN_3 (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	10	40.16	6.178
	15.2	40.7	6.261
	17	41.7	6.414
Ethanol; C_2H_6O; [64-17-5]	16	0.3153	0.0485

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: Saturated solutions of NaN_3 in water showed alkaline reaction.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish, and dried in a desiccator until constant weight was attained.

Source and Purity of Materials:

NaN_3 was prepared by neutralizing 8% aqueous solution of HN_3 with NaOH. The solution of the acid was obtained by distillation with dilute H_2SO_4 of either $Pb(N_3)_2$ or NH_4N_3 according to Curtius.[1] NaN_3 was recrystallized from water, and dried over concentrated H_2SO_4 in a vacuum dessicator. Analysis, found/calculated for NaN_3 (%): Na 35.31–35.35/35.38. Purity of water not specified. Absolute ethanol was used.

Estimated Error:

Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] T. Curtius, Ber. **24**, 3341 (1891).

Components: (1) Sodium azide; NaN_3; [26628-22-8] (2) Water; H_2O; [7732-18-5]	**Original Measurements:** J. Wohlgemuth, Compt. Rend. **198,** 601–3 (1934).
Variables: Temperature	**Prepared By:** J. Hála

Experimental Data

Temperature (t/°C)	NaN_3 (100 w_1/mass %)	NaN_3 (m_1/mol kg^{-1})[c]	Note
−20	26.8	5.63	metastable eutectic point (ice+NaN_3)
−15.1	21.6	4.24	eutectic point
−2.1	27.8	5.92	transition point
0	28	5.98	
100	35.6	8.50	

[a] Results were presented in graphical form (Fig. 2). Numerical values were reported for five significant points in the phase diagram.

[b] Solid phases were reported to be $NaN_3 \cdot 3H_2O$, [ ], between −15.1 °C and −2.1 °C, and NaN_3, [26628-22-8], above −2.1 °C.

[c] Calculated by compiler.

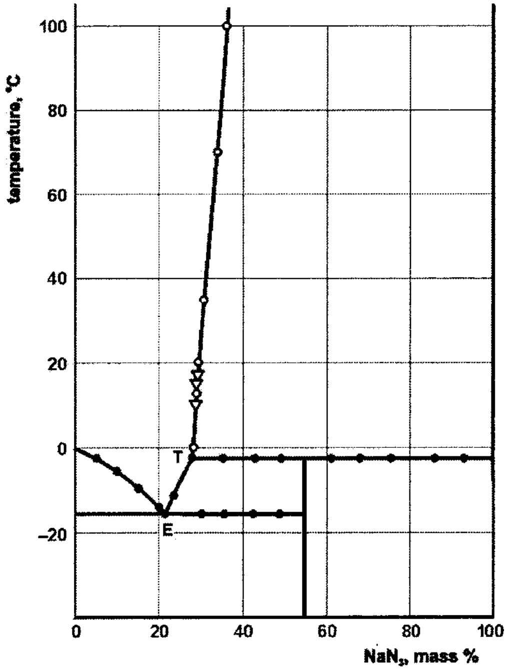

FIG. 2. Phase diagram of the NaN_3–H_2O system [(full circles) polythermal measurements; (open circles) isothermal measurements; (triangles) data from Curtius and Rissom,[1] included by the author].

Auxiliary Information

Method/Apparatus/Procedure:

The freezing curve was obtained by polythermal method. The solubility curve was obtained by isothermal method. Excess salt was equilibrated with water in a thermostat for 1 day in closed vessels. In samples of the saturated solutions, azide was precipitated with $AgNO_3$, and subsequently determined gravimetrically as AgCl, sodium was determined gravimetrically as Na_2SO_4. Cooling curves were obtained by polythermal method. Equilibrium time was not specified.

Source and Purity of Materials:

No details reported.

Estimated Error:

Insufficient data reported to allow for error estimate.

References:

[1] T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261 (1898).

Components:
(1) Sodium azide; NaN_3; [26628-22-8]
(2) Ethanol; C_2H_6O; [64-17-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
E. Lieber, C. N. R. Rao, H. E. Dingle, and J. Teetsow, J. Chem. Eng. Data **11**, 105 (1966).

Variables:
T/K: 298
Concentration of ethanol/% (v/v): 0–95.5

Prepared By:
J. Hála

Experimental Data

Solubility at 25 °C of NaN_3 in water–ethanol solutions[a]

C_2H_6O (%,v/v)	NaN_3 (g/100 g solvent)		NaN_3 (m_1/mol kg^{-1})[d]
0	43.60[b]		6.707
40	17.95[b]	18.19[c]	
60	11.17[b]	10.48[c]	
80		4.21[c]	
95.5	0.81[b]	1.05[c]	

[a] Solid phases were not investigated.
[b] Synthetic method.
[c] Isothermal method.
[d] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
The solubilities were determined by synthetic and isothermal methods. In the synthetic method,[1] the solutions of known compositions were prepared, and their saturation points were determined by varying the temperature. In the isothermal method, samples of the saturated solutions were evaporated, and the residue was dried and weighed. The authors considered the results obtained by isothermal method as more accurate and reliable.

Source and Purity of Materials:
No details reported.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] O. Flaschner and B. MacEwen, J. Chem. Soc. **93**, 1000 (1908).

Components:
(1) Sodium azide; NaN_3; [26628-22-8]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
J. A. Cranston and A. Y. Livingstone, J. Chem. Soc. 501–3 (1926).

Variables:
T/K: 273

Prepared By:
J. Hála

Experimental Data

The solubility of NaN_3 was reported to be 0.22 g salt in 100 g solvent at 0 °C. From this value the compiler calculated $m_1 = 0.0338$ mol kg^{-1}.

Additional information: The authors also reported the solubility of NaN_3 in boiling ethanol to be 0.46 g salt in 100 g solvent. Boiling point of the saturated solution and atmospheric pressure at which the measurement was conducted were not reported.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, details were not reported. Analysis of the saturated solutions was carried out by titrating azide[1] in weighed samples.

Source and Purity of Materials:
No information on NaN_3 reported. Ethanol used had density of 0.799 g cm^{-3} at 17 °C.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] F. Raschig, Chem. Ztg. 1203 (1908).

Components:
(1) Sodium azide; NaN_3; [26628-22-8]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
F. Hudswell, J. S. Nairn, and K. R. Gadsby, J. Appl. Chem., Suppl. Issue. No. **2**, S137–8 (1951).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

The solubility of NaN_3 was reported to be 2.491 or 2.486 g salt in 100 cm^3 of the saturated solution at 25 °C, as determined from weight of the residue or titration, respectively. Using the solubility of NaN_3 in water of 40.8 g salt per 100 g water at 20 °C,[1] and the density of the saturated solution of NaN_3 in methanol of 0.8083 g cm^{-3}, the authors corrected the experimentally determined solubility in methanol for the contribution from 0.035 mass % water in methanol used, and obtained the solubility of NaN_3 as 3.16±0.01 g NaN_3 in 100 g anhydrous methanol, or 2.48 NaN_3 in 100 cm^3 of the saturated solution. From the former value the compiler obtained $m_1 = 0.486$ mol kg^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess solid was shaken mechanically with the solvent for 5 min, and then kept in a thermostat for 1 h. This procedure was repeated three times which was sufficient to reach equilibrium. Twenty mL of the saturated solution was withdrawn with a pipette through a sintered/glass filter, and the solvent was evaporated below 50 °C in a weighed beaker. The residue was dried at 50 °C to constant weight, and corrected for blank experiment. The residue was then analyzed for NaN_3 by reacting it with excess $(NH_4)_2Ce(NO_3)_6$ and back-titrating excess Ce(IV) with $FeSO_4$ using the o-phenanthroline–Fe(II) complex as indicator.

Source and Purity of Materials:

NaN_3, source not specified, contained 99.9% NaN_3 after drying to constant weight at 50 °C. It was used without further purification. Methanol, boiling point 65 °C, was of high-grade purity. It contained 0.035 mass % water.

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.2% (authors, based on three measurements; individual results not reported).

References:

[1] T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261 (1898).

Components:
(1) Sodium azide; NaN_3; [26628-22-8]
(2) Solvents

Original Measurements:
R. Alexander, E. C. F. Ko, Y. C. Mac, and A. J. Parker, J. Am. Chem. Soc. **89**, 3703–12 (1967).

Variables:
T/K: 273 or 298

Prepared By:
J. Hála

Experimental Data

Solubility product of NaN_3 in three solvents[a]

Solvent	Temperature (t/°C)	K_{sp}[b]	NaN_3 (c_1/mol dm^{-3})[c]
Methanol; CH_4O; [67-56-1]	0	$10^{-0.9}$	0.355
Sulfinyl-bis methane;[d] C_2H_6OS; [67-68-5]	25	$10^{-0.64}$	0.479
N,N-dimethylformamide; C_3H_7NO; [68-12-2]	25	$10^{-1.9}$	0.112

[a] Solid phase was NaN_3, [26628-22-8], in all solvents.
[b] $K_{sp} = [Na^+][N_3^-]$
[c] Calculated by compiler.
[d] Dimethylsulfoxide.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Saturated solutions were prepared by shaking the solid with the solvent in a stoppered flask at 35 °C for 24 h, and then for further 24 h at 0 °C (methanol) or at 25 °C (other two solvents). The liquid phases were analyzed by potentiometric titration with $AgNO_3$. The solid phases were analyzed after drying at 1 mm Hg for 48 h at room temperature.

Source and Purity of Materials:

NaN_3, Analar grade product, source not specified. Methanol was purified according to Clare *et al.*[1] Dimethylsulfoxide was a product of Crown Zellerbach Corp. N,N-dimethylformamide (source not specified) was dried with type 4A molecular sieve, and fractionated twice under reduced pressure of dry nitrogen.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

1. B. W. Clare, D. Cook, E. C. F. Ko, Y. C. Mac, and A. J. Parker, J. Am. Chem. Soc. **88**, 1911 (1966).

Components:

(1) Sodium azide; NaN_3; [26628-22-8]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:

T. Kawakami and S. Moroto, Nagoya Kogyo Gijutsu Shkensho Hokoku **8**, 793–8 (1959).

Variables:

T/K: 231.7–263.9

Prepared By:

H. Akaiwa and J. Hála

Experimental Data

Solubility of NaN_3 in liquid ammonia as a function of temperature

Temperature (t/°C)	NaN_3 (g/100 g NH_3)	NaN_3 (m_1/mol kg^{-1})[a]	Solid phase[b]
−9.3	51.45	7.91	A
−18.0	52.51	8.08	A
−27.9	52.23	8.03	[c]
−28.9	50.40	7.75	[c]
−32.8	44.69	6.78	[c]
−36.0	39.25	6.03	B
−37.0	38.60	5.94	B
−41.5	32.14	4.94	B

[a] Calculated by compiler (J.H.).
[b] A: NaN_3; [26628-22-8]; B: $NaN_3 \cdot 6NH_3$, [ ].
[c] Not reported.

Auxiliary Information

Method/Apparatus/Procedure:

Dried NaN_3 (2.984 g) and excess of dried liquid ammonia were introduced into a pressure bottle. The mixture was transferred into a Dewar flask and cooled with acetone/dry ice coolant. The solubility of NaN_3 was determined by the cloud method. At temperatures below −35 °C the solutions showed a tendency toward supersaturation.

Source and Purity of Materials:

NaN_3, commercially available product (source not specified), was recrystallized from liquid ammonia.

Estimated Error:

Temperature: ±0.2 K (authors).
Solubility: precision not reported.

Components:

(1) Sodium azide; NaN_3; [26628-22-8]
(2) Sodium amide; $NaNH_2$; [7782-92-5]
(3) Ammonia; NH_3; [7664-41-7]

Original Measurements:

T. Kawakami and S. Moroto, Nagoya Kogyo Gijutsu Shkensho Hokoku **8**, 793–8 (1959).

Variables:

T/K: 273–303
m_2/mol kg^{-1}: 0–0.13

Prepared By:

H. Akaiwa and J. Hála

Experimental Data

Solubility in the NaN_3–$NaNH_2$–liquid ammonia system

Temperature (t/°C)	$NaNH_2$ (g/100 g NH_3)	$NaNH_2$ (m_2/mol kg^{-1})[b]	NaN_3 (g/100 g NH_3)	NaN_3 (m_1/mol kg^{-1})[b]	Solid phase[a]
0	0.91	0.0233	50.5	7.77	A
	0.92	0.0231	48.5	7.46	A
	2.69	0.0690	51.4	7.91	A+B
	2.32	0.0595	43.4	6.68	B
	1.98	0.0508	34.4	5.29	B
	1.70	0.0436	34.7	5.34	B
	1.24	0.0318	22.1	3.40	B
	0.78	0.0200	12.6	1.94	B
	0.77	0.0197	11.4	1.75	B
10	0	0	48.6	7.48	A
	1.51	0.0387	48.5	7.46	A
	3.10	0.0795	49.1	7.55	A+B
	3.16	0.0810	50.1	7.71	A+B
	2.73	0.0700	42.5	6.54	B
	2.11	0.0541	31.5	4.85	B
	1.58	0.0405	22.3	3.43	B
	0.98	0.0251	12.3	1.89	B
20	0.80	0.0205	48.1	7.40	A
	2.31	0.0509	49.5	7.62	A
	3.68	0.0943	48.4	7.45	A+B
	2.70	0.0692	35.8	5.51	B
	2.48	0.0636	31.2	4.80	B
	1.97	0.0505	25.7	3.95	B
	1.87	0.0479	23.1	3.55	B
	1.51	0.0387	19.9	3.06	B
	1.52	0.0390	19.3	2.97	B
	1.11	0.0285	12.4	1.91	B
	0.74	0.0190	7.57	1.16	B
	0.51	0.0131	5.05	0.777	B
30	1.59	0.0408	47.2	7.26	A
	3.39	0.0869	48.6	7.48	A+B
	5.07	0.130	46.0	7.08	B
	4.40	0.113	39.8	6.12	B
	3.44	0.0882	31.9	4.91	B
	2.72	0.0697	24.8	3.82	B
	2.32	0.0595	21.1	3.25	B

[a] A: NaN_3, [266628-22-8]; B: $NaNH_2$, [7782-92-5].
[b] Calculated by compiler (J.H.).

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess of solids were equilibrated with liquid ammonia at the desired temperature in a pressure bottle immersed in a thermostated Dewar flask. In samples of the saturated solutions, ammonia was determined from weight loss after allowing it to evaporate from a weighed sample. The content of $NaNH_2$ in the residue was determined alkalimetrically after decomposing the amide by adding carbonate-free water. The NH_3 liberated was absorbed in excess standard H_2SO_4 solution, and excess acid was back-titrated against NaOH solution. The method for NaN_3 determination was not reported.

Source and Purity of Materials:

NaN_3, source not specified, was a product of 99.45%–99.65% purity. $NaNH_2$ was prepared by reduction of NaN_3 with sodium metal in liquid ammonia, using iron powder as a catalyst. Purity of the product was not reported.

Estimated Error:

Temperature: precision ±0.2 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Sodium azide; NaN_3; [26628-22-8]
(2) 6,7,9,10,17,18,20,21-octahydro-dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin; $C_{20}H_{24}O_6$; [14187-32-7] (18-dibenzo-crown-6)
(3) Solvents

Original Measurements:

L. N. Yastrebov, T. M. Shuvaeva, and L. N. Kravchenko, Zh. Prikl. Khim. **50**, 2107–8 (1977).

Variables:

c_2/mol dm^{-3}: 0–0.15

Prepared By:

J. Hála

Experimental Data

Solubility of NaN_3 in various solvents as a function of 18-dibenzo-crown-6 concentration

Solvent	Temperature (t/°C)	$C_{20}H_{24}O_6$ (c_2/mol dm^{-3})	NaN_3 (c_1/mol dm^{-3})
Sulfinyl-bis(methane);[a] C_2H_6OS; [67-68-5]	80	0	1.1
		0.05	1.1
		0.10	1.19
		0.15	1.66
N,N-dimethylformamide; C_3H_6NO; [68-12-2]	80	0	0.18
		0.05	0.19
		0.10	0.21
		0.15	0.26
Ethanol; C_2H_6O; [64-17-5]	75	0	0.11
		0.05	0.12
		0.10	0.17
		0.15	0.31
Acetone; C_3H_6O; [67-64-1]	55	0	0.0024
		0.05	0.0058
		0.10	0.0104
		0.15	0.0139
2-Butanone; C_4H_8O; [78-93-3]	75	0	0.0019
		0.05	0.0028
		0.10	0.0070
		0.15	0.0115
Cyclohexanone; $C_6H_{10}O$; [108-94-1]	80	0.15	0.0038
Acetonitrile; C_2H_3N; [75-05-8]	80	0.15	0.0092

[a] Dimethylsulfoxide.

Auxiliary Information

Method/Apparatus/Procedure:

No information reported.

Source and Purity of Materials:

No information reported.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Sodium azide; NaN_3; [26628-22-8]
(2) 6,7,9,10,17,18,20,21-octahydro-dibenzo[b,k][1,4,7,10,13,16] hexaoxacyclooctadecin; $C_{20}H_{24}O_6$; [14187-327] (18-dibenzo-crown-6)
(3) Methanol; CH_4O; [67-56-1]
(4) Solvents

Original Measurements:
L. N. Yastrebov, T. M. Shuvaeva, and L. N. Kravchenko, Zh. Prikl. Khim. **50**, 2107–8 (1977).

Variables:
Concentration of CH_4O/v/v %: 1–3
For each solvent measurements were carried out at one temperature and one 18-dibenzo-Crown-6 concentration.

Prepared By:
J. Hála

Experimental Data

Solubility of NaN_3 in various solvents in the presence of 18-dibenzo-crown-6 as a function of methanol concentration

Solvent	Temperature (t/°C)	$C_{20}H_{24}O_6$ (c_2/mol dm^{-3})	Methanol (v/v %)	NaN_3 (c_1/mol dm^{-3})
Sulfinyl-bis methane; C_2H_6OS; [67-68-5][a]	80	0.15	1	1.66
			2	1.71
			3	2.17
N,N-dimethylformamide; C_3H_6NO; [68-12-2]	80	0.05	1	0.19
			2	0.22
			3	0.39
Acetone; C_3H_6O; [67-64-1]	55	0.1	1	0.012
			2	0.023
			3	0.068
2-Butanone; C_4H_8O; [78-93-3]	75	0.5[b]	1	0.018
			2	0.021
			3	0.038
Cyclohexanone; $C_6H_{10}O$; [108-94-1]	80	0.15	1	0.0053
			2	0.014
			3	0.026
Acetonitrile; C_2H_3N; [75-05-8]	80	0.15	1	0.011
			2	0.015
			3	0.025
Heptane; C_7H_{16}; [142-82-5]	80	0.15	3	0.0053
Tetrahydrofurane; C_4H_8O; [109-99-9]	65	0.15	3	0.0021
1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	80	0.15	3	0.0042
Benzene; C_6H_6; [71-43-2]	80	0.15	3	0.0064

[a] Dimethylsulfoxide.
[b] Based on the effect of methanol on the solubility of NaN_3, the compiler assumed this figure could be a misprint. The correct value could be either 0.15 or 0.05.

Auxiliary Information

Method/Apparatus/Procedure:
Nothing specified.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
Solubility: insufficient data given to allow for error estimate.

3.3. Potassium Azide

3.3.1. Evaluation of the KN_3–H_2O System

Components:
(1) Potassium azide; KN_3; [20762-60-1]
(2) Water; H_2O; [7732-18-5]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, June 2001

Critical Evaluation

The solubility of KN_3 in water was measured by isothermal method in two documents. Curtius and Rissom[1] reported three values between 283.6 and 290.1 K, while Wohlgemuth[2] reported the phase diagram of the KN_3–H_2O system, and numerical data only at 273.1 and 373.1 K. Although the two sets of data were obtained under different equilibration conditions and with unknown precision of temperature measurement the data seem to be in good agreement since they fall on a straight line. Least square treatment of the data between 273.1 and 290.1 K yielded an equation for the solubility of KN_3 in water as a function of temperature as

$$m_1/\text{mol kg}^{-1} = 0.0594\,T - 11.11,$$

which can be used to obtain tentative solubilities in the mentioned temperature range.

References:

[1] T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261 (1898).
[2] J. Wohlgemuth, Compt. Rend. **198**, 601 (1934).

Components:	**Original Measurements:**
(1) Potassium azide; KN_3; [20762-60-1] (2) Solvents	T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261–309 (1898).

Variables:	**Prepared By:**
T/K: 283–290	J. Hála

Experimental Data

Solubility of KN_3 in water or ethanol at different temperatures[a]

Solvent	Temperature (t/°C)	KN_3 (g/100 g solvent)	KN_3 (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	10.5	46.5	5.73
	15.5	48.9	6.03
	17	49.6	6.12
Ethanol; C_2H_6O; [64-17-5]	16	0.1375	0.0169

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior to withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish, and dried in a dessicator until constant weight was attained.

Source and Purity of Materials:

KN_3 was prepared by reacting stoichiometric amount of KOH with either NH_4N_3, or an aqueous solution of HN_3. Both NH_4N_3 and the HN_3 solution were obtained according to Curtius,[1] the latter by distillation with dilute H_2SO_4 of either $Pb(N_3)_2$ or NH_4N_3. Purity of water not specified. Absolute ethanol was used.

Estimated Error:

Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] T. Curtius, Ber. **24**, 3341 (1891).

Components:	**Original Measurements:**
(1) Potassium azide; KN_3; [20762-60-1] (2) Water; H_2O; [7732-18-5]	J. Wohlgemuth, Compt. Rend. **198**, 601–3 (1934).

Variables:	**Prepared By:**
Temperature	J. Hála

Experimental Data

Temperature (t/°C)	KN_3[a] (100 w_1/mass %)	KN_3 (m_1/mol kg^{-1})[b]
−12.9	26.2	4.38[c]
0	29.3	5.11
100	51.4	13.04

[a] Above eutectic point, KN_3, [20762-60-1], was the equilibrium solid phase (see Fig. 3).
[b] Calculated by compiler.
[c] Eutectic point.

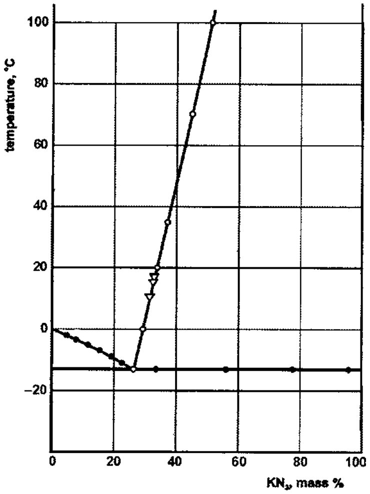

FIG. 3. Phase diagram of the KN_3–H_2O system.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility curve was obtained by the isothermal method. Excess salt was equilibrated with water in a thermostat for 1 day in closed vessels. In samples of the saturated solutions, azide was precipitated with $AgNO_3$, and subsequently determined gravimetrically as AgCl, potassium was determined gravimetrically as K_2SO_4. Cooling curves were obtained by polythermal method. Equilibrium time was not specified.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Solubility: insufficient data reported to allow for error estimate.

Components:
(1) Potassium azide; KN_3; [20762-60-1]
(2) Ethanol; C_2H_6O; [64-17-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
J. A. Cranston and A. Y. Livingstone, J. Chem. Soc. 501–3 (1926).

Variables:
T/K: 273
ethanol concentration: 80% and 100% (v/v)

Prepared By:
J. Hála

Experimental Data

Solubility of KN_3 at 0 °C in ethanol and one ethanol–water system[a]

Ethanol (% (v/v))	KN_3 (g/100 g solvent)	KN_3 (m_1/mol kg^{-1})[b]
80	1.8	
100	0.16	0.020

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: Also reported were the solubilities of KN_3 at boiling points of the saturated solutions as 5.9 and 0.54 g KN_3 per 100 g solvent for 80% and 100% (v/v) ethanol, respectively. The boiling points temperatures and atmospheric pressure at which the measurements were performed were not reported.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Equilibration time was not specified. In weighed samples of the saturated solutions the azide content was determined titrimetrically.[1]

Source and Purity of Materials:
Source and purity of KN_3 use were not specified. Ethanol used had density of 0.799 g cm^{-3} at 17 °C.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] F. Raschig, Chem. Ztg. 1203 (1908).

3.4. Rubidium Azide

Components:
(1) Rubidium azide; RbN_3; [22756-36-1]
(2) Solvents (water and ethanol)

Original Measurements:
T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261–309 (1898).

Variables:
T/K: 289 and 290

Prepared By:
J. Hála

Experimental Data

Solubility of RbN_3 in water or ethanol at two temperatures[a]

Solvent	Temperature (t/°C)	RbN_3 (g/100 g solvent)	RbN_3 (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	16	107.1	8.40
Water; H_2O; [7732-18-5]	17	114.1	8.95
Ethanol; C_2H_6O; [64-17-5]	16	0.182	0.0143

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior to withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish, and dried in a desiccator until constant weight was attained.

Source and Purity of Materials:
RbN_3 was prepared by double decomposition from Rb_2SO_4 and $Ba(N_3)_2$. The product was recrystallized from water, and analyzed after prolonged drying over concentrated H_2SO_4 in a vacuum dessicator. Found/calculated for RbN_3 (%): N 33.10–33.20/33.02, Rb 66.73–66.89/66.98. The barium azide used was prepared by dissolving $Ba(OH)_2$ in 8% aqueous solution of HN_3. The latter was obtained by distillation with dilute H_2SO_4 of either $Pb(N_3)_2$ or NH_4N_3 according to Curtius.[1] Purity of water not specified. Absolute ethanol was used.

Estimated Error:
Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

References:
[1] T. Curtius, Ber. **24**, 3341 (1891).

3.5. Cesium Azide

Components:
(1) Cesium azide; CsN_3; [22750-57-8]
(2) Solvents (water and ethanol)

Original Measurements:
T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261–309 (1898).

Variables:
T/K: 273 and 289

Prepared By:
J. Hála

Experimental Data

Solubility of CsN_3 in water or ethanol at two temperatures[a]

Solvent	Temperature (t/°C)	CsN_3 (g/100 g solvent)	CsN_3 (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	0	224.2	12.82
Water; H_2O; [7732-18-5]	16	307.4	17.57
Ethanol; C_2H_6O; [64-17-5]	16	1.0366	0.0593

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior to withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish, and dried in a desiccator until constant weight was attained.

Source and Purity of Materials:

CsN_3 was prepared by double decomposition from Cs_2SO_4 and $Ba(N_3)_2$. The product was recrystallized from water, and analyzed after prolonged drying over concentrated H_2SO_4 in a vacuum dessicator. Found/calculated for CsN_3 (%): N 23.95–24.13/24.04, Cs 75.82–75.83/75.96. The barium azide used was prepared by dissolving $Ba(OH)_2$ in 8% aqueous solution of HN_3. The latter was obtained by distillation with dilute H_2SO_4 of either $Pb(N_3)_2$ or NH_4N_3 according to Curtius.[1] Purity of water not specified. Absolute ethanol was used.

Estimated Error:
Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] T. Curtius, Ber. **24**, 3341 (1891).

3.6. Ammonium Azide

Components:
(1) Ammonium azide; NH_4N_3; [12164-94-2]
(2) Solvents

Original Measurements:
W. S. Frost, J. C. Cothran, and A. W. Browne, J. Am. Chem. Soc. **55**, 3516–8 (1933).

Variables:
T/K: 273; 293; 313

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4N_3 in five solvents at different temperatures[a]

Solvent	Temperature (t/°C)	ρ[b] (g cm^{-3})	NH_4N_3 (g/100 g)[c]	NH_4N_3 (c_1/mol dm^{-3})[d]	NH_4N_3 (m_1/mol kg^{-1})[d]
Water; H_2O; [7732-18-5]	0	1.0435	13.80	2.30	2.54
	20	1.0473	20.16	3.36	3.97
	40	1.0554	27.07	4.51	5.74
Methanol; CH_4O; [67-56-1]	20	0.8166	3.268	0.544	0.694
	40	0.7986	3.984	0.663	0.874
Ethanol; C_2H_6O; [64-17-5]	20	0.7972	1.060	0.176	0.224
	40	0.7803	1.325	0.221	0.288
Benzene; C_6H_6; [71-42-3]	20	0.8778	0.0032	0.000 532	0.000 607
	40	0.8609	0.0078	0.00130	0.00151
Diethylether; $C_4H_{10}O$; [60-29-7]	20	0.7129	0.0063	0.00105	0.00147

[a] Solid phases were not investigated.
[b] Density of the saturated solutions.
[c] Grams NH_4N_3 per 100 g saturated solution.
[d] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Experiments were performed in an apparatus designed for systems consisting of volatile both solvents and solutes. Details of the apparatus or analytical methods used were not reported.

Source and Purity of Materials:

NH_4N_3 was prepared by refluxing an ether solution of HN_3 over $CaCl_2$, redistilling the solution from the desiccant, and neutralizing it with NH_3 gas until complete precipitation of NH_4N_3 occurred. The salt was freed from ether by storage over H_2SO_4. The ether solution of HN_3 was obtained by the reaction of NaN_3 with H_2SO_4 in the presence of ether. Source and purity of the solvents used were not reported.

Estimated Error:
Temperature: precision not reported.
Solubility: the authors stated that each solubility value was the average of at least two satisfactorily concordant determinations. Individual results were not reported.

Components:	**Original Measurements:**
(1)Ammonium azide; NH_4N_3; [12164-94-2] (2) Ammonia; NH_3; [7664-41-7]	D. H. Howard, F. Friedrichs, and A. W. Browne, J. Am. Chem. Soc. **56**, 2332–40 (1934).
Variables:	**Prepared By:**
T/K: 195–280	J. Hála

Experimental Data

Composition of saturated solutions as a function of temperature

Temperature (t/°C)	NH_4N_3 ($100\ w_1$/mass %)[a]	NH_4N_3 (m_1/mol kg^{-1})[b]	Solid phase[c]	Temperature (t/°C)	NH_4N_3 ($100\ w_1$/mass %)[a]	NH_4N_3 (m_1/mol kg^{-1})[b]	Solid phase[c]
−77.7	0						
−82.5	14.98	2.934	A	−44.85	38.71	10.52	C
−83.0	16.03	3.179	A	−41.2	39.19	10.73	C
−83.8	17.79	3.603	A	−7.7	39.76	10.99	C
−84.4	18.80	3.855	A	−35.65	40.16	11.17	C
−85.2	20.48	4.288	A	−32.7	40.74	11.45	C
−86.0	22.40	4.806	A	−30.25	41.29	11.71	C
−86.1	24.52	5.409	B	−27.1	41.82	11.97	C
−85.4	25.49	5.696	B	−24.0	42.66	12.39	C
−82.9	27.58	6.341	B	−21.35	43.28	12.70	C
−80.9	29.20	6.867	B	−18.65	44.02	13.09	C
−78.5	30.39	7.269	B	−16.3	44.78	13.50	C
−78.0	30.98	7.474	B	−13.4	45.59	13.95	C
−76.8	31.80	7.764	B	−12.5	45.85	14.10	C
−76.0	32.41	7.984	B	−11.3	46.17	14.28	C
−75.4	32.91	8.168	B	−10.7	46.42	14.43	C
−73.0	34.38	8.724	B	−10.2	46.56	14.51	C
−72.0	35.71	9.248	B	−9.4	46.82	14.66	C
−73.15	35.70	9.244	B	−28.4[d]	46.16	14.28	D
−71.4	35.86	9.309	B	−20.2[d]	46.46	14.45	D
−68.0	36.04	9.382	C	−13.6[d]	46.86	14.68	D
−65.8	36.23	9.460	C	−9.0	47.00	14.77	D
−63.8	36.43	9.542	C	−8.9	47.03	14.78	D
−60.5	36.73	9.666	C	−8.4	47.15	14.85	D
−57.25	36.99	9.775	C	−5.0	47.30	14.94	D
−54.7	37.33	9.918	C	−0.4	47.60	15.13	D
−51.3	37.73	10.09	C	+6.9	48.10	15.43	D
−47.4	38.23	10.31	C				

[a] Calculated by compiler from authors' mass % NH_3 data.

[b] Calculated by compiler.

[c] A: NH_3, [7664-41-7]; B: $NH_4N_3\cdot 5NH_3$, [ ]; C: $NH_4N_3\cdot 2NH_3$, [ ]; D: NH_4N_3, [12164-94-2].

[d] Metastable system.

The solid phases in equilibrium with saturated solutions along the various branches of the curve are, respectively, as follows: MN–NH_3, NO–$NH_4N_3\cdot 5NH_3$, OP–$NH_4N_3\cdot 2NH_3$, PQ–NH_4N_3 (PP′-metastable) (see Fig. 4). The eutectic point occurs at −87 °C and 24 mass % NH_4N_3. Transition points of conversion of $NH_4N_3\cdot 5NH_3$ to $NH_4N_3\cdot 2NH_3$, and of $NH_4N_3\cdot 2NH_3$ to NH_4N_3 are at −71 and −9 °C, respectively.

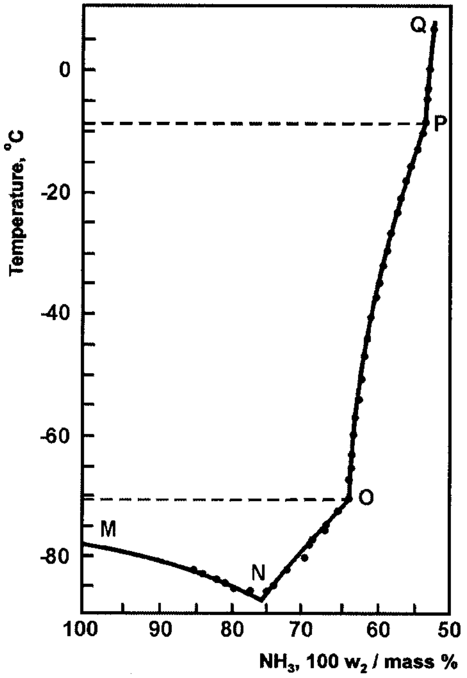

FIG. 4. Phase diagram of the NH_4N_3–NH_3 system.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Measurements were performed in an all-glass vacuum line. NH_3 gas was condensed on a weighed amount of the salt in the reaction cell connected to manometer. The temperature of the cell was controlled through a suitable bath. Equilibrium was attained by stirring of the bath, and by agitation of the reaction cell. The system showed a strong tendency toward the formation of supersaturated solutions and metastable solids. This was overcome by bringing the system for a short time to the temperature of either liquid air or solid CO_2. The method of the determination of the composition of the saturated solutions was not described. The composition of the solid phases was inferred from the pressure–concentration measurements.

Source and Purity of Materials:

NH_4N_3 was prepared according to Frost *et al.*[1] by neutralizing an ethereal solution of HN_3 by NH_3 gas. The product was sublimed in a sealed tube at 130 °C and stored over concentrated H_2SO_4. The HN_3 solution was obtained by the reaction of NaN_3 with H_2SO_4 in the presence of ether. NH_3 gas used was passed through a series of tubes filled with soda lime and sodium metal.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

References:

[1] W. S. Frost, J. C. Cothran, and A. W. Browne, J. Am. Chem. Soc. **55**, 3516 (1933).

3.7. Calcium Azide

Components:	**Original Measurements:**
(1) Calcium azide; $Ca(N_3)_2$; [19465-88-4] (2) Solvents (water and ethanol)	T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261–309 (1898).
Variables:	**Prepared By:**
T/K: 273; 288.2; 289	J. Hála

Experimental Data

Solubility of $Ca(N_3)_2$ in water or ethanol at different temperatures[a]

Solvent	Temperature (t/°C)	$Ca(N_3)_2$ (g/100 g solvent)	$Ca(N_3)_2$ (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	0	38.1	3.07
	15.2	45.0	3.63
Ethanol; C_2H_6O; [64-17-5]	16	0.211	0.0170

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish, and dried in a desiccator until constant weight was attained.

Source and Purity of Materials:

$Ca(N_3)_2$ was prepared by dissolving $Ca(OH)_2$ in 8% aqueous solution of HN_3, or by boiling freshly precipitated $Ca(OH)_2$ with NH_4N_3 solution. Excess $Ca(OH)_2$ was removed by precipitation as $CaCO_3$ with CO_2 gas, and the salt was obtained by evaporating the filtrate. After recrystallization from water the product contained, in mass %, 31.97–32.16 Ca and 67.54–67.59 N. Calculated for $Ca(N_3)_2$: 32.26 Ca, 67.74 N. The HN_3 solution was obtained according to Curtius.[1] Purity of water not specified. Absolute ethanol was used.

Estimated Error:

Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] T. Curtius, Ber. **24**, 3341 (1891).

Components:	**Original Measurements:**
(1) Calcium azide; $Ca(N_3)_2$; [19465-88-4] (2) Water; H_2O; [7732-18-5]	K. Torkar, H. Kirschner, and G. Ernst, Monatsh. Chem. **100**, 203–12 (1969).
Variables:	**Prepared By:**
T/K: 253.5–348.6	J. Hála

Experimental Data

Solubility of $Ca(N_3)_2$ in water as a function of temperature

Temperature (t/°C)	$Ca(N_3)_2$ (g/100 g H_2O)	$Ca(N_3)_2$ (100 w_1/mass %)	$Ca(N_3)_2$ (m_1/mol kg^{-1})[a]	Temperature (t/°C)	$Ca(N_3)_2$ (g/100 g H_2O)	$Ca(N_3)_2$ (100 w_1/mass %)	$Ca(N_3)_2$ (m_1/mol kg^{-1})[a]
−19.6	39.78	28.46	3.205	24.8	59.74	37.40	4.813
−16.2	42.32	29.74	3.410	26.6	59.64	37.36	4.805
−12.6	42.77	29.96	3.446	29.2	59.61	37.35	4.803
−9.6	44.19	30.65	3.560	29.6	63.07	38.29	5.081
−1.6	48.50	32.88	3.908	32.1	60.00	37.50	4.834
−0.5	50.00	33.33	4.028	33.4	60.77	37.80	4.896
1.7	49.80	33.24	4.012	36.8	63.71	38.92	5.133
3.0	50.90	33.73	4.101	40.1	67.14	40.17	5.409
8.5	51.00	33.80	4.109	41.5	67.41	40.21	5.431
13.4	52.92	34.61	4.264	42.3	68.06	40.50	5.484
16.4	54.51	35.28	4.392	42.9	71.85	41.81	5.789
20.0	55.44	35.67	4.467	43.7	66.61	39.98	5.367
22.3	57.35	36.45	4.621	53.9	66.97	40.11	5.396
23.2	60.82	37.82	4.900	75.5	75.90	43.15	6.115

[a] Calculated by compiler.

Additional information: Existence regions of the equilibrium solid phases were obtained by the authors by combining isothermal data with freezing point determinations, as follows: $Ca(N_3)_2$, [19465-88-4], above 41.5 °C; $Ca(N_3)_2 \cdot 0.5H_2O$, [22119-71-7], from 25±1 °C to 41.5 °C; $Ca(N_3)_2 \cdot 1.5H_2O$, [22119-72-8], from 0±2 to 25 °C; and $Ca(N_3)_2 \cdot 4H_2O$, [22119-73-9], from −20.8 to 0 °C. Cryohydratic point was at −20.8±0.5 °C, and at 28.3 mass % $Ca(N_3)_2$. Also reported were heats of solution, vapor pressures, and standard enthalpies of $Ca(N_3)_2$ and its hydrates.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Systems were equilibrated for 2 weeks in a thermostat. Samples of the saturated solutions were withdrawn with a filtering rod, weighed, and the calcium content determined titrimetrically with EDTA solution. Solid phases were identified by x-ray diffraction measurements.[1]

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] H. Krischner, Monatsh. Chem. **98**, 2134 (1968).

Components:

(1) Calcium azide; $Ca(N_3)_2$; [19465-88-4]
(2) Potassium azide; KN_3; [20762-60-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

H. Kirschner and H. E. Maier, Z. Anorg. Allgem. Chem. **460**, 217–20 (1980).

Variables:

T/K: 298
100 w_2/mass %: 0–36.2
100 w_1/mass %: 0–37.2

Prepared By:

J. Hála

Experimental Data

Solubility in the $Ca(N_3)_2-KN_3-H_2O$ system at 25 °C

KN_3 (100 w_2/mass %)	KN_3 (m_2/mol kg^{-1})[a]	$Ca(N_3)_2$ (100 w_1/mass)	$Ca(N_3)_2$ (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	37.2	4.772	A
5.2	1.054	34.0	4.505	A
6.0	1.130	28.6	3.522	B
8.5	1.547	23.8	2.833	B
10.8	1.946	20.8	2.450	B
13.1	2.374	18.9	2.239	B
18.5	3.398	14.3	1.714	B
21.0	3.859	11.9	1.428	B
26.6	4.960	7.3	0.899	B
31.7	5.153	4.9	0.622	B
32.2	5.270	4.5	0.572	B+C
33.0	5.405	3.5	0.444	C
36.2	5.991	0	0	C

[a] Calculated by compiler.
[b] A: $Ca(N_3)_2 \cdot 1.5H_2O$, [22119-71-7]; B: $K_2Ca(N_3)_4 \cdot 4H_2O$, [ ]; C: KN_3, [20762-60-1].

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Both salts were dissolved in different mole ratios in water acidified with HN_3, and the solution was slowly evaporated by passing through it a stream of CO_2-free air, until solid phase precipitated. The systems were stirred for several days since equilibrium was attained very slowly. Identical results were obtained by stirring excess solids with small amount of water for several days. Samples, approx. 0.5 g, of the saturated solutions were withdrawn with a filtering rod, and analyzed for potassium gravimetrically with $NaB(C_6H_5)_4$, for calcium titrimetrically with EDTA, and for azide by conductometric titration with $AgNO_3$ solution. Wet solid phases were characterized by x-ray diffraction.

Source and Purity of Materials:

$Ca(N_3)_2$ and KN_3 were prepared by passing a stream of wet HN_3 gas into a suspension of $CaCO_3$, or into a solution of KOH, respectively. Analysis of the products was not reported.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

3.8. Strontium Azide

3.8.1. Evaluation of the $Sr(N_3)_2-H_2O$ System

Components:

(1) Strontium azide; $Sr(N_3)_2$; [19465-89-5]
(2) Water; H_2O; [7732-18-5]

Evaluator:

J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, June 2001.

Critical Evaluation

The solubility of $Sr(N_3)_2$ in water has been reported in two documents. Curtius and Rissom[1] reported a single solubility value at 289.1 K without specifying the composition of the equilibrium solid phase, while Kirschner *et al.*[2] carried out an extensive study of the solubility of $Sr(N_3)_2$ as a function of temperature. They also noted a strong tendency of $Sr(N_3)_2$ hydrates to crystallize as metastable phases. It appears that the solubility reported in Ref. 1, i.e., $m_1 = 2.67$ mol kg^{-1}, although in excellent agreement with the value reported in Kirschner *et al.*,[2] refers in fact to the solubility of metastable $Sr(N_3)_2 \cdot 4H_2O$, and as such should not be used as the equilibrium solubility of $Sr(N_3)_2$ at this temperature. According to Kirschner *et al.*,[2] the equilibrium solid phase at 289.1 K is $Sr(N_3)_2 \cdot 2H_2O$ with an interpolated solubility of $m_1 = 2.42$ mol kg^{-1} (evaluator). The data of Kirschner *et al.*[2] can be recommended as tentative solubility values.

References:

[1] T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261 (1989).
[2] H. Kirschner, K. Torkar, and H. E. Roth, Z. Anorg. Allgem. Chem. **405**, 119 (1974).

Components:
(1) Strontium azide; $Sr(N_3)_2$; [19465-89-5]
(2) Solvents

Original Measurements:
T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261–309 (1898).

Variables:
T/K: 289

Prepared By:
J. Hála

Experimental Data

Solubility of $Sr(N_3)_2$ in water or ethanol at 16 °C[a]

Solvent	$Sr(N_3)_2$ (g/100 g solvent)	$Sr(N_3)_2$ (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	45.83	2.67
Ethanol; C_2H_6O; [64-17-5]	0.095	0.005 53

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish, and dried in a desiccator until constant weight was attained.

Source and Purity of Materials:

$Sr(N_3)_2$ was prepared by dissolving $Sr(OH)_2$ in 8% aqueous solution of HN_3, or by boiling $Sr(OH)_2$ with NH_4N_3 solution. Excess $Sr(OH)_2$ was removed by precipitation as $SrCO_3$ with CO_2 gas, and the salt was obtained by evaporating the filtrate. After recrystallization from water the product contained, in mass %, 50.85 Sr and 48.55–48.64 N. Calculated for $Sr(N_3)_2$: 51.02 Sr, 48.98 N. The HN_3 solution was obtained according to Curtius.[1] Purity of water not specified. Absolute ethanol was used.

Estimated Error:
Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

References:
[1] T. Curtius, Ber. **24**, 3341 (1891).

Components:
(1) Strontium azide; $Sr(N_3)_2$; [19465-89-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Kirschner, K. Torkar, and H. E. Roth, Z. Anorg. Allgem. Chem. **405**, 119–28 (1974).

Variables:
T/K: 263.5–338

Prepared By:
J. Hála

Experimental Data

Solubility of $Sr(N_3)_2$ in water as a function of temperature

Temperature (t/°C)	$Sr(N_3)_2$ (100 w_1/mass %)	$Sr(N_3)_2$ (m_1/mol kg^{-1})[a]	Solid phase[b]	Temperature (t/°C)	$Sr(N_3)_2$ (100 w_1/mass %)	$Sr(N_3)_2$ (m_1/mol kg^{-1})[a]	Solid phase[b]
−9.6	23.9	1.830	A[c]	−2.0	25.5	1.944	C[c]
−9.0	24.1	1.850	A[c]	10.0	28.1	2.277	C
−7.0	24.9	1.932	A[c]	15.0	29.2	2.403	C
−6.0	25.3	1.973	A[c]	17.0	29.6	2.449	C
−5.0	25.6	2.005	A[c]	20.0	30.2	2.521	C
−3.0	26.1	2.057	A[c]	21.0	30.4	2.545	C
−9.2	23.2	1.760	B	23.0	30.8	2.593	C
−8.0	23.4	1.780	B	24.0	31.0	2.617	C
−6.0	23.9	1.830	B	26.0	31.5	2.679	C
−2.0	24.9	1.932	B	27.0	31.7	2.704	C
−1.0	25.4	1.984	B	30.0	32.5	2.805	C[c]
0.0	25.7	2.015	B	31.0	32.7	2.831	C[c]
1.0	26.0	2.047	B	15.5	31.2	2.642	D[c]
3.0	26.7	2.122	B	19.0	31.5	2.679	D[c]
5.0	27.4	2.199	B[c]	20.0	31.5	2.679	D[c]
7.5	28.5	2.322	B[c]	22.0	31.6	2.691	D[c]
10.0	29.3	2.414	B[c]	24.0	31.6	2.691	D[c]
12.0	29.7	2.461	B[c]	25.0	31.7	2.704	D[c]
13.0	30.2	2.521	B[c]	30.0	32.0	2.741	D
15.0	30.8	2.593	B[c]	40.0	32.2	2.767	D
16.0	31.2	2.642	B[c]	50.0	32.1	2.754	D
17.0	31.6	2.691	B[c]	65.0	32.2	2.767	D
18.0	32.4	2.792	B[c]				
19.0	33.2	2.895	B[c]				

[a] Calculated by compiler.
[b] A: $Sr(N_3)_2 \cdot 6H_2O$, [52075-71-5]; the hydrate was formed easily but was metastable since the temperature of transition from hexahydrate to tetrahydrate was deduced by the authors to be at −79 °C, i.e., deep below the eutectic point; B: $Sr(N_3)_2 \cdot 4H_2O$, [52214-22-9], stable between −9.2 and 3 °C, metastable from 3 to 19 °C; C: $Sr(N_3)_2 \cdot 2H_2O$, [52075-72-6], stable from 3 to 28 °C, metastable from −2 to 3 °C, and from 28 to 31 °C; D: $Sr(N_3)_2$; [19465-89-5], stable above 28 °C, metastable from 15 to 28 °C.
[c] Metastable.

Additional information: Eutectic point (ice–$Sr(N_3)_2 \cdot 4H_2O$) was at −9.2 °C and 23.2 mass % $Sr(N_3)_2$.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Mixtures of water with excess of the corresponding hydrate of the salt were equilibrated by stirring for several days in a thermostated vessel. Solid phases were identified by x-ray diffraction using a low-temperature diffractometer. The system showed a strong tendency towards the formation of supersaturated solutions and metastable solid phases. The latter were stable for up to several weeks. Whenever doubts arose as to the true equilibrium solid phase, the system containing both hydrates in question was equilibrated for several days, and the conclusion was drawn from the change of the contents of the hydrates in the solid phase after equilibration. Water content of the hydrates was also verified by using thermostated autorecording scales on which the hydrates were dried to constant weight by passing over them a stream of gas with equilibrium water pressure corresponding to the temperature used.

Source and Purity of Materials:

$Sr(N_3)_2$ was prepared by reacting a solution of $Sr(OH)_2$ with dilute HN_3 gas. The solid salt was then obtained by either evaporation of by precipitation with acetone.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Strontium azide; $Sr(N_3)_2$; [19465-89-5]
(2) Potassium azide; KN_3; [20762-60-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. Paar and H. Kirschner, Z. Anorg. Allgem. Chem. **479**, 212–8 (1981).

Variables:

T/K: 268
100 w_2/mass %: 0–27.5
100 w_1/mass %: 0–25.2

Prepared By:

J. Hála

Experimental Data

Solubility in the $Sr(N_3)_2-KN_3-H_2O$ system at −5 °C

KN_3 (100 w_2/mass %)	KN_3 (m_2/mol kg^{-1})[a]	$Sr(N_3)_2$ (100 w_1/mass)	$Sr(N_3)_2$ (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	25.2	1.962	A
3.5	0.595	24.0	1.929	B
5.0	0.860	23.4	1.903	B+C
4.7	0.773	20.4	1.586	D
5.2	0.823	17.0	1.272	D
6.9	1.045	11.8	0.845	D
10.2	1.525	7.4	0.523	D
12.7	1.911	5.4	0.384	D
15.1	2.292	3.7	0.265	D
16.4	2.511	3.1	0.224	D+F
19.5	3.058	1.9	0.140	D+F
27.5	4.699	0.2	0.0151	D+F
27.2	4.605	0	0	E

[a] Calculated by compiler.

[b] A: $Sr(N_3)_2 \cdot 5H_2O$, [ ]; B: $Sr(N_3)_2 \cdot 4H_2O$, [52214-22-9]; C: $K_{1.34}Sr_{1.67}(N_3)_{4.69}(H_2O)_{6.62}$; D: stable mixed crystals with the composition varying from $K_{2.08}Sr_{1.30}(N_3)_{4.69}(H_2O)_{6.62}$ to that of the compound C; E: KN_3, [20762-60-1]; F: $K_2Sr(N_3)_4 \cdot 4H_2O$, [ ].

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Both salts were dissolved in different mole ratios in water, the solutions were acidified with HN_3 gas to pH 6, placed in jacketed thermostated vessels, and isothermally evaporated by passing through them a stream of CO_2-free air, until solid phases precipitated. The systems were stirred for 6 days to reach equilibrium. Approximately 1 g samples of the saturated solutions were withdrawn with a filtering rod, and analyzed for potassium gravimetrically with $NaB(C_6H_5)_4$, for strontium titrimetrically with EDTA, and for azide by conductometric titration with $AgNO_3$ solution. Solid phases were characterized by x-ray diffraction using a low-temperature chamber. The compositions of mixed solid solutions and of the mixed salt were confirmed by chemical analysis.

Source and Purity of Materials:

$Sr(N_3)_2$ and KN_3 were prepared by passing a stream of wet HN_3 gas into a suspension of $SrCO_3$, or into a solution of KOH, respectively. Analysis of the products was not reported.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data given to allow for error estimate.

3.9. Barium Azide

3.9.1. Evaluation of the $Ba(N_3)_2$–H_2O System

Components:	**Evaluator:**
(1) Barium azide; $Ba(N_3)_2$; [18810-58-7] (2) Water; H_2O; [7732-18-5]	J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, June 2001.

Critical Evaluation

The solubility of $Ba(N_3)_2$ in water has been reported in two documents. Curtius and Rissom[1] reported the results of four measurements in the temperature range from 273.1 to 291.1 K without identifying the solid phases, while Torkar *et al.*[2] performed solubility measurements over a wide temperature range, and identified two hydrates of $Ba(N_3)_2$, in addition to the anhydrous salt. The data in Curtius and Rissom[1] are systematically lower by 2.5%–4.4% than those reported in Torkar *et al.*,[2] the reason of which is not clear from the published information. In view of the existence of $Ba(N_3)_2$ hydrates, the gravimetric determination of barium as $BaSO_4$ in the saturated solutions used in Torkar *et al.*[2] seems to be more reliable than weighing the residues obtained by evaporation of the saturated solutions because the temperature of evaporation was not specified. However, it is not clear if, or to what extent, this could account for the differences in the solubilities. It is, therefore, recommended to use the data of Torkar *et al.*[2] as tentative solubility data.

References:

[1] T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261 (1898).
[2] K. Torkar, H. Kirschner, and K. H. Radl, Monatsh. Chem. **97**, 313 (1966).

Components:	**Original Measurements:**
(1) Barium azide; $Ba(N_3)_2$; [18810-58-7] (2) Solvents (water and ethanol)	T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261–309 (1898).
Variables:	**Prepared By:**
T/K: 273–290	J. Hála

Experimental Data

Solubility of $Ba(N_3)_2$ in water or ethanol at different temperatures[a]

Solvent	Temperature (t/°C)	$Ba(N_3)_2$ (g/100 g solvent)	$Ba(N_3)_2$ (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	0	12.5	0.565
	10.5	16.2	0.732
	15	16.7	0.754
	17	17.3	0.782
Ethanol; C_2H_6O; [64-17-5]	16	0.0172	7.77×10^{-4}

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish and dried in a desiccator until constant weight was attained.

Source and Purity of Materials:

$Ba(N_3)_2$ was prepared by dissolving $Ba(OH)_2$ in 8% aqueous solution of HN_3, or by boiling $Ba(OH)_2$ with NH_4N_3 solution. Excess $Ba(OH)_2$ was removed by precipitation as $BaCO_3$ with CO_2 gas, and the salt was obtained by evaporating the filtrate. After recrystallization from water the product contained, in mass %, 37.86–38.32 N and 61.55–62.03 Ba. Calculated for $Ba(N_3)_2$: 38.04 N, 61.96 Ba. Purity of water not specified. Absolute ethanol was used.

Estimated Error:

Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Barium azide; $Ba(N_3)_2$; [18810-58-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
K. Torkar, H. Kirschner, and K. H. Radl, Monatsh. Chem. **97**, 313–21 (1966).

Variables:
T/K: 273–358

Prepared By:
J. Hála

Experimental Data

Solubility of $Ba(N_3)_2$ in water as a function of temperature[a]

Temperature (t/°C)	$Ba(N_3)_2$ (g/100 g water)	$Ba(N_3)_2$ (100 w_1/mass %)	$Ba(N_3)_2$ (m_1/mol kg^{-1})[b]	Temperature (t/°C)	$Ba(N_3)_2$ (g/100 g water)	$Ba(N_3)_2$ (100 w_1/mass %)	$Ba(N_3)_2$ (m_1/mol kg^{-1})[b]
0	13.00	11.50	0.5873	34.5	22.92	18.66	1.035
1.9	13.20	11.67	0.5963	39.5	24.85	19.90	1.123
2.0	13.38	11.75	0.6044	45.0	26.90	21.20	1.215
4.5	13.67	12.03	0.6175	49.8	28.50	22.20	1.287
6.0	14.04	12.28	0.6342	52.1	29.42	22.73	1.329
11.0	16.78	14.38	0.7580	53.0	29.90	23.00	1.351
13.6	17.35	14.80	0.7838	55.0	30.18	23.20	1.363
15.7	17.62	14.98	0.7960	62.5	31.70	24.08	1.432
17.7	17.76	15.09	0.8023	70.0	32.90	24.75	1.486
20.0	18.13	15.36	0.8190	75.8	34.02	25.39	1.537
25.0	19.35	16.20	0.8741	85.0	35.90	26.42	1.622
28.0	20.70	17.15	0.9351				

[a] The authors combined the solubility data with freezing point measurements to obtain the following existence regions of the solid phases: $Ba(N_3)_2 \cdot 1.5H_2O$, [22208-76-0], below 11±1 °C; $Ba(N_3)_2 \cdot H_2O$, [12047-22-2], from 11±1 °C to 52.5 °C; $Ba(N_3)_2$, [18810-58-7], above 52.2 °C.

[b] Calculated by compiler.

Additional information: The cryohydratic point was at −2.6 °C and 11.2 mass % $Ba(N_3)_2$.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. A nearly saturated solution of the salt was isothermally evaporated in a thermostated flask by passing a stream of dry, CO_2-free nitrogen gas over the solution. When sufficient amount of the solid phase precipitated, nitrogen gas was disconnected, and the mixture was stirred for several more hours. Samples of the saturated solutions were then withdrawn with a filtering rod, and barium was determined gravimetrically as $BaSO_4$ in a weighed sample. Solid phases were identified by x-ray diffraction and optical microscopy.

Source and Purity of Materials:
No details reported.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

4. The Solubility of Cyanides

4.1. Lithium Cyanide

Components:
(1) Lithium cyanide; LiCN; [2408-36-8]
(2) Tetraethylammonium perchlorate; $C_8H_{20}ClNO_4$; [2567-83-1]
(3) 4-methyl-1,3-dioxalan-2-one; propylene carbonate; [108-32-7]

Original Measurements:
T. Nakamura and K. Izutsu, Anal. Sci. **7**, 1677–9 (1991).

Variables:
T/K: 298
c_2/mol dm^{-3}: 0.01

Prepared By:
J. Hála

Experimental Data

The solubility product of LiCN in propylene carbonate containing 0.01 mol dm^{-3} $(C_2H_5)_4NClO_4$ was determined as $K_{sp} = [Li^+] \times [CN^-] = 10^{-9.5}$ mol^2 dm^{-6}.

Additional information: The procedure for analyzing experimental results to obtain the solubility product was not reported; it was described by the authors in Nakamura *et al.*[1]

Auxiliary Information

Method/Apparatus/Procedure:
The solubility product of LiCN was obtained by potentiometric titration of a solution of $(C_2H_5)_4NCN$ with a solution of $LiClO_4$, both in propylene carbonate. An ion-selective electrode, prepared by coating a platinum disk with a polyacrylamide membrane coupled to the tetraaminophthalocyanine Co complex, according to Nakamura *et al.*[1] was used.

Source and Purity of Materials:
$(C_2H_5)_4NCN$ was a product of Fluka Co. Ltd. Source and purity of other chemicals were described in Nakamura *et al.*[1–4]

Estimated Error:
Temperature: precision not reported.
Solubility product: precision not reported.

References:
[1] T. Nakamura, Y. Tsukamoto, and K. Izutsu, Bunseki Kagaku **39**, 689 (1990).
[2] T. Nakamura, H. Higuchi, and K. Izutsu, Bull Chem. Soc. Jpn **61**, 1988 (1988).
[3] T. Nakamura, M. Komai, S. Hosono, and K. Izutsu, Anal. Chim. Acta **238**, 351 (1990).
[4] T. Nakamura, Y. Nakamura, T. Kojima, and K. Izutsu, Bull Chem. Soc. Jpn. **63**, 2615 (1990).

4.2. Sodium Cyanide

4.2.1. Evaluation of the NaCN–H_2O System

Components:
(1) Sodium cyanide; NaCN; [143-33-9]
(2) Water; H_2O; [7732-18-5]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, February 2001.

Critical Evaluation

Data on the solubility of NaCN in water are contained in several documents. Frost[1] reported solubility in mass %, obtained in the binary system NaCN–H_2O, further data, also in mass %, have been reported in the studies of ternary systems NaCN–NaCl–H_2O (Yajima and Odanaka[2]) and NaCN–NaOH–H_2O (Oliver and Johnson[3]). The following table summarizes data from these three documents as obtained in the temperature range of 288–308 K.

Temperature (T/K)	NaCN (100 w_1/mass %)	NaCN (m_1/mol kg^{-1})	Method	Temperature error (T/K)	Reference
288.1	34.2	10.61	Polythermal	±0.2	1
293.5	37.02	11.99	Polythermal	±0.2	1
294.1	37.14	12.06	Isothermal	±1	2
298.1	39.0	13.05	Isothermal	not reported	1
298.1	38.8	12.93	Isothermal	±0.05	3
298.5	39.1	13.10	Polythermal	±0.2	1
302.5	41.56	14.51	Polythermal	±0.2	1
307.1	44.82	16.57	Polythermal	±0.2	1
308.1	45.0	16.70	Isothermal	not reported	1
308.1	45.0	16.70	Isothermal	±0.05	3

The data from Frost[1] and Oliver and Johnson[3] agree in that the solubility of NaCN in water increases with temperature up to the point of transition of NaCN·$2H_2O$ to NaCN at 34.5 °C,[1] and that further on the solubility of anhydrous NaCN varies very little with temperature. Of the data in the table, those at 298.1 and 308.1 K from Frost[1] and Oliver and Johnson[3] can be compared, and very good agreement is observed. The evaluator recommends these data, recalculated to mol kg^{-1}, be used as tentative values, i.e., $m_1 = 13.0 \pm 0.1$ mol kg^{-1} at 298.1 K, and 16.7 ± 0.1 mol kg^{-1} at 308.1 K. In the temperature range of 288–308 K, the solubility of NaCN in water as a function of temperature could be fitted to a third order polynomial

$$m_1 = -6858.43 + 70.588\,(T/\mathrm{K}) - 0.242548\,(T/\mathrm{K})^2 + 0.27870 \times 10^{-3}\,(T/\mathrm{K})^3,$$

where m_1 is the solubility of NaCN in mol kg^{-1}, and T is temperature in Kelvin. Kireev and Vagranskaya[4] reported the solubility of NaCN in water in grams per dm^3. Since densities of the saturated solutions were not reported, comparison of their data with those of Frost[1] and Oliver and Johnson[3] is not possible. In a paper devoted to the measurement of vapor pressure over NaCN–H_2O solutions,[5] two values were reported for the solubility of NaCN in water, i.e., 36.16 mass % at 298.1 K, and 42.50 mass % at 313.1 K. Since no details were reported as to the method used, these data have not been considered for compilation or evaluation.

References:

[1] O. I. Frost, Zh. Obsh. Khim. **6**, 1910 (1936).
[2] K. Yajima and S. Odanaka, Kogyo Kagaku Zasshi **71**, 460 (1968).
[3] G. D. Oliver and S. E. J. Johnson, J. Am. Chem. Soc. **76**, 4721 (1954).
[4] V. A. Kireev and L. I. Vagranskaya, Zh. Obsh. Khim. **5**, 963 (1935).
[5] G. I. Voinilovich, L. K. Akhrap, and L. S. Mai, Zh. Prikl. Khim. **8**, 589 (1935).

Components:
(1) Sodium cyanide; NaCN; [143-33-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
O. I. Frost, Zh. Obsh. Khim. **6**, 1910–2 (1936).

Variables:
T/K: 245–308

Prepared By:
J. Hála

Experimental Data

Solubility of NaCN in water as a function of temperature

Temperature (t/°C)	NaCN (100 w_1/mass %)	NaCN (m_1/mol kg^{-1})[a]	Temperature (t/°C)	NaCN (100 w_1/mass %)	NaCN (m_1/mol kg^{-1})[a]
−4.0	5.56	1.203	−18.1	25.90	7.132
−9.2	11.03	2.530	−14.8	26.5	7.357
−12.5	13.90	3.294	−7.6	27.9	7.896
−13.8	14.56	3.477	−4.0	28.9	8.294
−15.2	16.01	3.900	10.0	32.5	9.825
−19.5	19.11	4.821	12.6	33.3	10.19
−23.4	21.23	5.500	15.0	34.2	10.61
−23.8	21.90	5.722	20.4	37.02	11.99
−24.2	22.0	5.755	25.0[c]	39.0	13.05
−25.4	22.6	5.958	25.4	39.1	13.10
−26.4	23.46	6.254	29.5	41.56	14.51
−27.8[b]	23.75	6.356	34.0	44.86	16.57
−21.4	24.84	6.744	35.0[c]	45.0	16.70

[a] Calculated by compiler.
[b] Eutectic point. The author considered NaCN·$2H_2O$, [25178-25-0], to be the equilibrium solid phase above the temperature of the eutectic point.
[c] Obtained by isothermal method.

Additional information: The point of transition from NaCN·$2H_2O$ to NaCN was reported to be at 34.5 °C.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. Solutions of known composition were placed in a test tube equipped with a platinum stirrer and a thermometer graduated to 0.2 °C. The system was cooled in a Dewar flask in liquid air until first crystals appeared. Then the tube was warmed up slowly, and the temperature of disappearance of last crystals was noted. To eliminate errors caused by hydrolysis of NaCN, each measurement was carried out with a freshly prepared solution of the desired concentration. The NaCN content in the solutions was determined by titration with standard 0.1 mol dm^{-3} $AgNO_3$ solution against KI as indicator. Solid phases were not investigated. Details of the two measurements performed by isothermal procedure were not reported.

Source and Purity of Materials:

NaCN, source unspecified, was recrystallized as dihydrate under reduced pressure, and dried over H_2SO_4. The product contained less than 0.5% Na_2CO_3.

Estimated Error:

Temperature: precision ±0.2 K (the difference between temperatures of appearance and disappearance of crystals was reported to be within 0.4 °C).
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Sodium cyanide; NaCN; [143-33-9]
(2) Sulfur dioxide; SO_2; [7446-09-5]

Original Measurements:
G. Jander and W. Ruppolt, Z. Phys. Chem. **179**, 43–50 (1937).

Variables:
T/K: 273

Prepared By:
J. Hála

Experimental Data

The solubility of NaCN in liquid sulfur dioxide was reported to be 0.018 g salt in 100 g solvent at 0 °C. From this value the compiler calculated $m_1/\text{mol kg}^{-1} = 0.003\,67$.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. About 10 g SO_2, carefully dried, was equilibrated with excess solid at 0 °C in water-ice bath in a three-compartment glass vessel in which equilibrating and sampling compartments were separated by a compartment containing glass/wool filter. Equilibration was performed for unspecified, prolonged period of time under frequent shaking. After equilibrium had been attained, the vessel was turned upside down, and the saturated solution was filtered into the empty sampling compartment, which was subsequently cooled and sealed off. After weighing the compartment with the sample, SO_2 was allowed to evaporate, the residue was weighed, dissolved in water, and the content of the salt was determined. Method of analysis was not specified.

Source and Purity of Materials:
NaCN, source not specified, was carefully dried before use. Commercially available SO_2 was purified by passing it through concentrated H_2SO_4 and over asbestos wool, and dried by using P_2O_5. Specific conductivity of the product was reported as 4.5 $\times 10^{-7}$ S/cm (Jander and Wickert[1]).

References:
[1] G. Jander and K. Wickert, Z. Phys. Chem. **178**, 57 (1936).

Components:
(1) Sodium cyanide; [143-33-9]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
B. B. Vasiliev, J. L. Ettinger, and M. P. Golovkov, Z. Anorg. Allgem. Chem. **219**, 341–7 (1934).

Variables:
T/K: 283–323

Prepared By:
J. Hála

Experimental Data

Solubility of NaCN in liquid ammonia as a function of temperature[a]

Temperature[b] (°C)	NaCN (g/kg NH_3)	NaCN (m_1/mol kg^{-1})[c]
10	403.0	8.223
20	494.0	10.08
30	585.0	11.94
40	676.0	13.79
50	767.0	15.65

[a] Equilibrium solid phase was NaCN, [143-33-9], in all measurements. Ammoniates of NaCN were reported to be stable below −40 °C.
[b] Freezing point temperature.
[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Polythermal methods were used. The apparatus was described in Akhumov and Vasiliev,[1] and was kept in an air thermostat.

Source and Purity of Materials:
No details reported.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:
[1] E. I. Akhumov and B. B. Vasiliev, Zh. Obsh. Khim. **2**, 271 (1932).

Components:
(1) Sodium cyanide; NaCN; [143-33-9]
(2) Solvents

Original Measurements:
M. R. Thompson, J. Res. Natl. Bur. Std. **6**, 1051–9 (1931).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of NaCN in methanol and ethanol at 25 °C[a]

Solvent	NaCN ($g\ dm^{-3}$ solvent)	NaCN (m_1/mol kg^{-1})
Methanol; CH_3OH; [67-56-1]	78.0	2.02[b]
Ethanol; C_2H_6O; [64-17-5]	9.7	0.252[c]

[a] Solid phases were not investigated.
[b] Calculated by compiler using density of methanol of 0.7865 g cm^{-3} at 25 °C.[1]
[c] Calculated by compiler using density of ethanol of 0.7852 g cm^{-3} at 25 °C.[1]

Additional information: The solubility of NaCN at 25 °C in 95% ethanol (v/v; 5% water) was reported to be 19.2 g salt in 1 dm^{-3} solvent.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The technique used and equilibrium time applied were not reported. The cyanide content in the saturated solutions was determined by a modified Liebig's method of titration against $AgNO_3$ solution in the presence of KI and NaOH.

Source and Purity of Materials:

NaCN in 99.13% purity was prepared by reacting a solution of sodium ethoxide in absolute ethanol with excess of liquid HCN. Absolute methanol and ethanol were used.

Estimated Error:

Temperature: precision not reported.
Solubility: Although the method of CN^- determination was reported to be accurate within ±0.2%–0.3%, the solubility values were reported as approximate. No reason for this was given.

References:

[1] *Handbook of Chemistry and Physics*, 38th ed. (Chemical Rubber, Cleveland, OH, 1956).

Components:
(1) Sodium cyanide; NaCN; [143-33-9]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
H. Henstock, J. Chem. Soc. 1340–3 (1934).

Variables:
T/K: 287; 340

Prepared By:
J. Hála

Experimental Data

Solubility of NaCN in methanol at two temperatures[a]

Temperature (°C)	NaCN (g/100 g solvent)[b]	NaCN (m_1/mol kg^{-1})[c]
15	6.44	1.314
67.4[d]	4.10	0.837

[a] Solid phases were not investigated.
[b] Average of three determinations, individual values not reported.
[c] Calculated by compiler.
[d] Boiling point of the saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Measurements at 15 °C were carried out in an apparatus described in Brönsted and Petersen,[1] immersed in a thermostat. At boiling point, the saturated solution was prepared under reflux. Portions of the saturated solutions were weighed at 15 °C in a graduated pipette,[2] using a thimble to separate the solid. Where crystallization occurred on cooling, the pipette was reheated until the solid dissolved, the contents being discharged into a weighing bottle, the pipette washed with boiling solvent, and the residue weighed after evaporation of the solvent and drying at 50 °C for 2 h.

Source and Purity of Materials:

NaCN, source not specified, was twice recrystallized and dried 4 h at 50 °C. Methanol was purified first from acetone and aldehyde by treatment with iodine.[3] It was then distilled with concentrated H_2SO_4 to remove basic substances, then from caustic soda to remove acidic substances, and finally distilled over sodium metal. The product boiled at 66 °C at 758 mm Hg pressure.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] J. N. Brönsted and A. Petersen, J. Am. Chem. Soc. **43**, 2265 (1921).
[2] F. D. Chattaway and W. J. Lambert, J. Chem. Soc. **107**, 1766 (1915).
[3] R. C. Menzies, J. Chem. Soc. **121**, 2790 (1922).

Components:
(1) Sodium cyanide; NaCN; [143-33-9]
(2) 2-furancarboxaldehyde (furfural); $C_5H_4O_2$; [98-01-1]

Original Measurements:
F. Trimble, Ind. Eng. Chem., Ind. Ed. **33**, 660–2 (1941).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

The solubility of NaCN is reported to be 0.02 mass % at 25 °C. From this value the compiler calculated $m_1 = 0.0041$ mol kg^{-1}. The composition of the solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess solid was agitated with furfural for 24 h in a constant temperature bath, which was sufficient for equilibrium to be reached. The mixture was filtered, and the NaCN content in the saturated solution was determined gravimetrically as Na_2SO_4. To this aim, 100 mL water was added to a weighed portion (about 40 g) of the saturated solution, and the mixture was evaporated until the total volume was reduced to about 10 mL. The solution was transferred to a weighed crucible, and evaporation continued to dryness. The residue was moistened with concentrated H_2SO_4, and ignited to about 700 °C.

Source and Purity of Materials:

NaCN was a C.P. product.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

4.2.2. Evaluation of the NaCN–NaOH–H_2O System

Components:
(1) Sodium cyanide; NaCN; [143-33-9]
(2) Sodium hydroxide; NaOH; [1310-73-2]
(3) Water; H_2O; [7732-18-5]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, March 2001.

Critical Evaluation

The solubility of NaCN in solutions of sodium hydroxide has been reported in two documents. Kireev and Vagranskaya[1] reported their data in grams per dm^3 at 273, 298, and 313 K, while Oliver and Johnson[2] reported the solubilities in mass % at 298, 308, and 328 K. Thus, comparison has been made possible only for four solubility values at 298 K, for which Kireev and Vagranskaya[1] reported densities of the saturated solutions. Compared with the respective data of Oliver and Johnson,[2] the value of $m_1 = 15.36$ mol kg^{-1}, recalculated by the evaluator from the data of Kireev and Vagranskaya[1] (see the compilation), is obviously too high, while the three other values are considerably lower. In addition, the data of Kireev and Vagranskaya[1] seem to be less accurate since the authors rounded their results to tens of grams per dm^3, due to unspecified errors in analysis. Therefore, the evaluator suggests the data of Oliver and Johnson[2] be given preference.

References:

[1] V. A. Kireev and L. I. Vagranskaya, Zh. Obsh. Khim. **5**, 963 (1935).
[2] G. D. Oliver and S. E. J. Johnson, J. Am. Chem. Soc. **76**, 4721 (1954).

Components:

(1) Sodium cyanide; NaCN; [143-33-9]
(2) Sodium hydroxide; NaOH; [1310-73-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. A. Kireev and L. I. Vagranskaya, Zh. Obsh. Khim. **5**, 963–6 (1935).

Variables:

T/K: 273–373
Concentration of NaOH (in g dm^{-3})

Prepared By:

J. Hála

Experimental Data

Solubility of NaCN in aqueous solutions of NaOH at 0–100 °C[a]

Temperature (°C)	NaOH (g dm^{-3})	NaOH (c_2/mol dm^{-3})[b]	NaCN (g dm^{-3})	NaCN (c_1/mol dm^{-3})[b]
0	10	0.25	370	7.55
	40	1.00	350	7.14
	40	1.00	347	7.10
	140	3.50	300	6.21
	160	4.00	280	5.71
5	0	0	380[c,d]	7.75
	10	0.25	370	7.55
10	0	0	395[c,d]	8.06
	6	0.15	390	7.96
20	0	0	465[c,d]	9.49
	6	0.15	460	9.38
25	0	0	530[c]	10.81
	45	1.125	490	10.0
	125	3.125	430	8.77
	130	3.25	425	8.67
	140	3.50	417	8.50
	160	4.00	400	8.16
	178	4.45	388	7.92
	210	5.25	365	7.45
	230	5.75	330	6.73
	288	7.20	300	6.12
	290	7.25	305	6.22
	420	10.5	220	4.49
	520	13.0	160	3.26
30	0	0	515[c,d]	10.51
	10	0.25	505	10.30
40	0	0	540[c]	11.02
	10	0.25	530	10.81
	20	0.50	525	10.71
	35	0.875	505	10.30
	90	2.25	460	9.39
	110	2.75	445	9.08
	164	4.10	400	8.16
	235	5.88	330	6.73
	260	6.50	325	6.63
	290	7.25	305	6.22
	340	8.50	280	5.71
	370	9.25	255	5.20
70	0	0	555[c,d]	11.32
	15	0.375	540	11.02
100	0	0	560[c,d]	11.47
	10	0.25	550	11.22

[a] Equilibrium solid phases were $NaCN \cdot 2H_2O$, [25178-25-0] at 20 °C and below, and NaCN, [143-33-9], at 25 °C and above.
[b] Calculated by compiler.
[c] Solubility of NaCN in water. Obtained by the authors by extrapolating to zero NaOH concentration of NaCN solubility in NaOH containing solutions. The authors used this approach in order to avoid the interfering influence of NaCN hydrolysis in water.
[d] The entire series of measurements of NaCN solubility as a function of NaOH concentration was not reported.

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared by slow isothermal evaporation of NaCN/NaOH solutions in a stream of dry air, freed from CO_2, in a thermostated bath under reduced pressure. When the solid phase appeared, it was filtered through a glass sinter in the same thermostat. The saturated solutions were analyzed for the NaCN and NaOH content titrimetrically, using the Deniges' method, and standard acid solution, respectively. The solid phases were analyzed for the NaCN content by the Deniges' method.

Source and Purity of Materials:

NaCN was prepared by adding excess anhydrous HCN to a 4% solution of NaOH in absolute ethanol.[1] The salt precipitated due to its low solubility in ethanol. It was washed with ethanol and dried in vacuum over P_2O_5. The entire procedure was carried out in an atmosphere of CO_2-free air.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: The authors rounded most of the results to tens of grams per dm^3, due to errors in analyses. The nature of the errors was not specified.

References:

[1] E. W. Goersney and M. S. Sherman, J. Am. Chem. Soc. **48**, 697 (1926).

Components:

(1) Sodium cyanide; NaCN; [143-33-9]
(2) Sodium hydroxide; NaOH; [1310-73-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

G. D. Oliver and S. E. J. Johnson, J. Am. Chem. Soc. **76**, 4721–4 (1954).

Variables:

T/K: 298; 308; 328
100 w_2/mass %: 0–49.2 at 298 K; 0–55 at 308 K; 0–61.4 at 328 K

Prepared By:

J. Hála

Experimental Data

Composition of saturated solutions in the NaCN–NaOH–H_2O system at three temperatures

Temperature (t/°C)	NaOH (100 w_2/mass %)	NaOH (m_2/mol kg^{-1})[a]	NaCN (100 w_1/mass %)	NaCN (m_1/mol kg^{-1})[a]	Solid phase[b]
25	0	0	38.8	12.93	A
	2.5	1.046	37.8	12.91	A
	6.4	2.758	35.6	12.52	A
	8.9	3.931	34.5	12.43	A
	9.5	4.318	35.5	13.17	A
	10.2	4.545	33.7	12.25	B
	11.5	5.152	32.7	11.95	B
	23.8	10.87	21.5	8.020	B
	38.7	20.49	14.1	6.095	B
	45.2	27.63	13.9	6.934	B
	46.2	28.45	13.2	6.604	C
	46.5	28.56	12.8	6.417	C
	46.8	27.72	11.0	5.318	C
	48.2	26.72	6.7	3.031	C
	49.2	26.11	3.7	1.602	C
35	0	0	45.0	16.70	B
	0.2	3.754	37.2	13.90	B
	16.8	7.650	28.3	10.51	B
	25.6	12.09	21.5	8.293	B
	26.7	12.50	19.9	7.604	B
	37.5	19.94	15.5	6.729	B
	43.7	26.26	14.7	7.210	B
	47.3	31.28	14.9	8.043	B
	48.2	31.38	13.4	7.120	D
	49.0	31.82	12.5	6.625	D
	49.6	31.71	11.3	5.897	D
	51.6	34.12	10.6	5.722	C
	51.8	34.17	10.3	5.545	C
	51.5	31.48	7.5	3.791	C
	52.5	32.01	6.5	3.234	C
	51.6	28.86	3.7	1.689	C
	52.3	28.86	2.4	1.081	C
	55.0	30.55	0	0	C
55	0	0	45.2	16.82	B
	7.6	8.499	38.1	14.31	B
	16.1	7.495	30.2	11.47	B
	32.9	17.03	18.8	7.942	B
	45.9	31.01	17.1	9.430	B
	46.8	32.50	17.2	9.749	B
	47.5	32.98	16.5	9.352	D
	48.5	38.96	15.8	9.030	D
	49.7	35.00	14.8	8.506	D
	52.6	37.79	12.5	7.388	D
	52.6	37.79	12.6	7.388	D
	56.0	41.54	10.3	6.236	D
	57.4	43.22	9.4	5.777	D
	58.3	44.98	9.3	5.857	D
	58.5	45.00	9.0	5.650	D
	58.2	43.82	8.6	5.285	C
	57.0	40.37	7.7	4.450	C
	57.2	39.61	6.7	3.787	C
	57.9	37.50	3.5	1.850	C
	61.4	39.76	0	0	C

[a] Calculated by compiler.

[b] A: NaCN·$2H_2O$, [25178-25-0]; B: NaCN, [143-33-9]; C: NaOH·H_2O, [ ]; D: NaCN·NaOH, [ ], incongruently saturating.

The composition of invariant points on solubility isotherms (authors):

Temperature (t/°C)	NaOH (100 w_2/mass %)	NaCN (100 w_2/mass %)	Notation in the phase diagram
25	9.8	34.2	k
	56.0	14.0	j
35	47.5	15.0	g
	51.5	10.5	f
55	47.0	17.0	h
	59.0	9.0	e

Note: See Fig. 5 and also reported were phase diagrams at 35 and 55 °C.

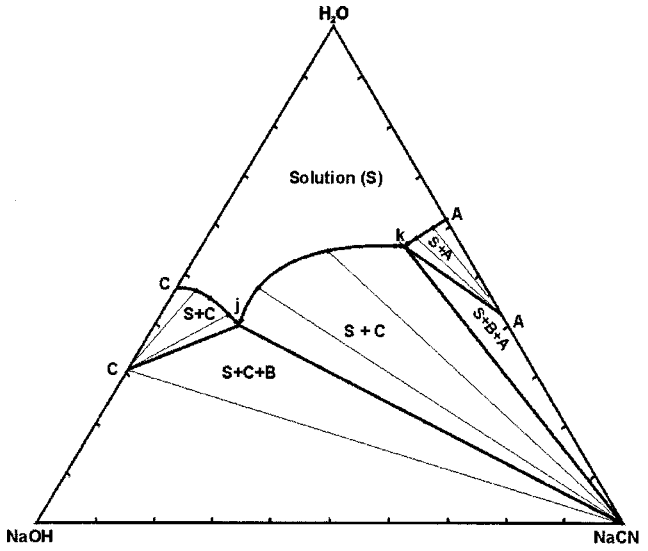

FIG. 5. Phase diagram of the NaCN–NaOH–H_2O system at 25 °C.

Components:

(1) Sodium cyanide; NaCN; [143-33-9]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

K. Yajima and S. Odanaka, Kogyo Kagaku Zasshi **71**, 460–1 (1968).

Variables:

T/K: 294; 313
100 w_2/mass %: 0–24.88 at 294 K; 0–26.44 at 313 K.

Prepared By:

H. Akaiwa and J. Hála

Experimental Data

Composition of the saturated solutions in the NaCN–NaCl–H_2O system at 21 and 40 °C

Temperature (t/°C)	NaCl (100 w_2/mass %)	NaCl (m_2/mol kg^{-1})[b]	NaCN (100 w_1/mass %)	NaCN (m_1/mol kg^{-1})[b]	Solid phase[a]
21	24.88	5.667	0	0	A
	24.12	5.555	1.58	0.434	A
	21.54	4.929	3.68	1.004	A
	22.49	5.225	3.86	1.069	A
	18.68	4.295	6.90	1.892	A
	16.99	3.993	10.21	2.862	A
	14.71	3.512	13.62	3.878	A
	12.91	3.114	16.15	4.645	A
	10.85	2.670	19.61	5.754	A
	5.14	1.354	29.90	9.392	A
	3.91	1.045	32.07	10.22	A
	3.07	0.837	34.18	11.11	A
	0	0	37.14	12.06	B
	0.99	0.269	36.11	11.71	B
	1.46	0.399	35.93	11.71	B
	2.49	0.685	35.33	11.59	B
	3.94	1.099	34.72	11.55	B
40	26.44	6.150	0	0	A
	19.83	4.627	6.84	1.903	A
	14.62	3.470	13.29	3.762	A
	10.96	2.687	19.25	5.628	A
	8.21	2.088	24.52	7.438	A
	5.46	1.445	29.89	9.434	A
	3.64	1.007	34.53	11.40	A
	0	0	43.69	15.83	[c]
	1.27	0.382	41.80	14.98	C
	2.49	0.762	41.61	15.19	C
	2.30	0.677	39.57	13.89	C
	2.71	0.791	38.69	13.47	C
	4.77	1.321	33.44	11.04	C
	6.20	1.651	29.56	9.389	C
	6.75	1.800	29.08	9.247	C

[a] A: NaCl, [7647-14-5]; B: $NaCN\cdot 2H_2O$, [25178-25-0]; C: solid solutions $NaCl_x(CN)_{1-x}$.

[b] Calculated by compiler (J.H.).

[c] Compiler's comment: NaCl stated as the solid phase, obviously by mistake. Above 25 °C, the equilibrium solid phase in the NaCN–H_2O system was reported to be NaCN, [143-33-9].[1]

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. A series of 100 g samples were prepared by weighing (to the nearest 0.1 g) the required amounts of salt and water into a flask. After heating to promote solution, the samples were filtered to remove the carbonate, and transferred to 200 mL glass tubes. Equilibrium was attained by agitating the tubes for 4–5 h in a thermostated bath. The saturated solutions were analyzed volumetrically for CN^- and OH^-. Each sample was first titrated with 0.1 N $AgNO_3$ to determine CN^-, and then with 0.1 N H_2SO_4 against phenol red to determine NaOH. The composition of the solid phases was determined by the method of wet residues.

Source and Purity of Materials:

NaCN, J. T. Baker reagent grade, contained 97.2% NaCN. NaOH, J. T. Baker reagent grade, contained 97.7% NaOH. The carbonate formed in strong NaOH solutions was removed by filtration.

Estimated Error:

Temperature: precision ±0.05 K (authors).
Solubility: insufficient data reported to allow for error estimate.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, details were not reported. Analytical methods used were the Liebig's method for NaCN, and Volhard's method for NaCl. NaCl was determined after decomposition of NaCN.

Source and Purity of Materials:
NaCN and NaCl were commercial, reagent grade products (source not reported), and were used without further purification.

Estimated Error:
Temperature: precision ±1 K at 294 K, ± 0.5 K at 313 K (authors).
Solubility: insufficient data reported to allow for error estimate.

References:

[1] V. A. Kireev and L. I. Vagranskaya, Zh. Obsh. Khim. **5**, 963 (1935).

4.3. Potassium Cyanide

Components:	**Original Measurements:**
(1) Potassium cyanide; KCN; [151-50-8] (2) Water; H_2O; [7732-18-5]	G. N. Lewis and T. B. Brighton, J. Am. Chem. Soc. **40**, 482–9 (1918).
Variables:	**Prepared By:**
T/K: 298	J. Hála

Experimental Data

Solubility of KCN in water at 25 °C

The solubility of KCN at 25 °C was reported to be 716 g KCN per 1000 g water ($m_1 = 10.996$ mol kg^{-1}; compiler). Also reported were freezing point temperatures for solutions containing 113.1–460.1 g KCN per 1000 g water. Cryohydric (eutectic) point was reported to at −29.61 °C, the composition at eutectic point was not reported. The equation describing the freezing point temperature as a function of KCN concentration was obtained by the compiler by least squares treatment of the data as

$$t\ (\text{f.p.})/°\text{C} = -5.497 \times 10^{-2} c + 0.555,$$

where c is the concentration of KCN in grams per 1000 g water. From this equation, the composition at the eutectic point was obtained by extrapolation as 548.5 g KCN per 1000 g water, or 8.42 mol kg^{-1} at −29.61 °C.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, details were not reported.

Source and Purity of Materials:
KCN, source not specified, contained small traces of carbonate. The salt was dried in a vacuum desiccator.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:	**Original Measurements:**
(1) Potassium cyanide; KCN; [151-50-8] (2) Water; H_2O; [7732-18-5]	L. A. Vasilevoy, Uch. Zap. Kazansk. Gos. Univ. (Sci. Papers Kazansk. Univ.) **85**, 81–2 (1925).
Variables:	**Prepared By:**
T/K: 243–288	J. Hála

Experimental Data

Solubility of KCN in water as a function of temperature[a]

Temperature (°C)	KCN (100 w_1/mass %)	KCN (100 x_1/mol %)	KCN (m_1/mol kg^{-1})[b]
−29.8	33.64	12.30	7.785
−28.1	34.73	12.83	8.172
−17.3	36.33	13.64	8.763
−14.1	37.06	14.01	9.043
−8.7	37.55	14.27	9.234
0	38.68	14.86	9.687
9.1	40.14	15.65	10.30
15.3	40.37	15.75	10.40

[a] Equilibrium solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Solutions containing excess KCN were equilibrated for an unspecified period of time and then filtered quickly through a precooled funnel. Saturated solutions were analyzed for potassium gravimetrically as K_2SO_4 after evaporating solution samples in a platinum crucible. Solubilities above 15 °C could not be determined because of the decomposition of KCN. No decomposition occurred below 0 °C.

Source and Purity of Materials:

KCN (Kahlbaum) contained about 3% of water, and traces of sulfates and chlorides. Distilled and boiled water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:	**Original Measurements:**
(1) Potassium cyanide; KCN; [151-50-8] (2) Solvents	M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).
Variables:	**Prepared By:**
T/K: 298	J. Hála

Experimental Data

Solubility of KCN in two solvents at 25 °C[a]

Solvent	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
Water; H_2O; [7732-18-5]	845	12.98
4-methyl-1,3-dioxalan-2-one (propylene carbonate); $C_4H_6O_3$; [108-32-7]	0.24	0.003 69

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The solvent was stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR (B.D.H.) material, and was used as supplied. In the course of the study, several batches of KCN were used. All gave consistent solubility results. Deionized water was used. Propylene carbonate (source not specified) was purified according to Gordon and Ford.[1]

Estimated Error:

Temperature: precision not reported
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:	Original Measurements:
(1) Potassium cyanide; KCN; [151-50-8] (2) Sulfur dioxide; SO_2; [7446-09-5]	G. Jander and W. Ruppolt, Z. Phys. Chem. **179**, 43–50 (1937).
Variables:	**Prepared By:**
T/K: 273	J. Hála

Experimental Data

The solubility of KCN in liquid sulfur dioxide was reported to be 0.017 g salt in 100 g solvent at 0 °C. From this value the compiler calculated m_1/mol kg^{-1} = 0.002 61.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. About 10 g SO_2, carefully dried, was equilibrated with excess solid at 0 °C in water–ice bath in a three-compartment glass vessel in which equilibrating and sampling compartments were separated by a compartment containing glass/wool filter. Equilibration was performed for unspecified, prolonged period of time under frequent shaking. After equilibrium had been attained, the vessel was turned upside down, and the saturated solution was filtered into the empty sampling compartment, which was subsequently cooled and sealed off. After weighing the compartment with the sample, SO_2 was allowed to evaporate, the residue was weighed, dissolved in water, and the content of the salt was determined. Method of analysis was not specified.

Source and Purity of Materials:

KCN, source not specified, was carefully dried before use. Commercially available SO_2 was purified by passing it through concentrated H_2SO_4 and over asbestos wool, and dried by using P_2O_5. Specific conductivity of the product was 4.5×10^{-7} Ω^{-1} (Jander and Wickert[1]).

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] G. Jander and K. Wickert, Z. Phys. Chem. **178**, 57 (1936).

Components:	Original Measurements:
(1) Potassium cyanide; KCN; [151-50-8] (2) Hydrogen cyanide; HCN; [74-90-8]	K. Fredenhagen and J. Dahmlos, Z. Anorg. Allgem. Chem. **179**, 77–88 (1929).
Variables:	**Prepared By:**
T/K: 273	J. Hála

Experimental Data

The solubility of KCN in liquid HCN was reported to be $c_1 = 0.10$ mol dm^{-3} at 0 °C.

Additional information: Specific conductivity of the saturated solution was reported to be 0.0085 Ω^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. HCN was distilled onto solid KCN in a special vessel. The salt was several times washed with fresh portions of HCN to remove eventual impurities that could increase the conductivity of the solution. The salt was then dissolved under agitation until the conductivity of the solution remained constant. Methods of analysis of the saturated solutions were not specified. Solid phases were not investigated.

Source and Purity of Materials:

KCN was a product of Kahlbaum (puriss.) and was dried before use. HCN gas was prepared from KCN and H_2SO_4 (1:2). The gas was dried with $CaCl_2$ and P_2O_5, and condensed. The liquid was repeatedly distilled to obtain a colorless product with specific conductivity of 0.6×10^{-6} Ω^{-1} at 0 °C.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

4.3.1. Evaluation of the KCN–NH_3 System

Components:
(1) Potassium cyanide; KCN; [151-50-8]
(2) Ammonia; NH_3; [7664-41-7]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, March 2001.

Critical Evaluation

Solubility of KCN in liquid ammonia has been reported in two documents. Johnson and Krumboltz[1] reported a single value at 239.3 K, while Schenk and Tulhoff[2] reported the solubility over the temperature range from 203 to 238 K. There is an obvious discrepancy between the two measurements, as seen from the solubilities reported at 239.3 and 238 K, i.e., 4.55 g KCN/100 g NH_3 or 0.7a0 mol kg^{-1} (Johnson and Krumboltz[1]), and 6.8 g KCN/100 g NH_3 or 1.044 mol kg^{-1} (Schenk and Tulhoff[2]), respectively. (Graphical extrapolation of the data in Schenk and Tulhoff[2] yielded an approximate KCN solubility of 1.035 mol kg^{-1} at 239.3 K.) The source of this discrepancy is not clear from the published information. It is clear, however, from the work of Schenk and Tulhoff[2] that the system needs thorough equilibration to attain equilibrium. Although the actual equilibration time was not reported in any of the two documents it can be assumed that true equilibrium might not have been obtained in Johnson and Krumboltz.[1] Moreover, since the data of Schenk and Tulhoff[2] were performed at more temperatures, and all the data consistently fell on a straight line, it is suggested that they be used as tentative solubility values.

References:

[1] W. C. Johnson and O. F. Krumboltz, J. Phys. Chem. **167**, 249 (1933).
[2] P. W. Schenk and H. Tulhoff, Ber. Bunsenges. Phys. Chem. **71**, 1158 (1967).

Components:
(1) Potassium cyanide; KCN; [151-50-8]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
W. C. Johnson and O. F. Krumboltz, Z. Phys. Chem. **167**, 249–59 (1933).

Variables:
T/K: 239

Prepared By:
J. Hála

Experimental Data

Solubility of KCN in liquid ammonia at −33.9 °C

Two measurements of the solubility of KCN in liquid ammonia at −33.9 °C were carried out, the composition of the saturated solutions being 0.0894 g KCN in 1.9523 g NH_3, and 0.0618 g KCN in 1.3600 g NH_3. From these values the authors obtained for the solubility of KCN the value of 4.55 g KCN in 100 g solvent ($m_1 = 0.699$ mol kg^{-1}; compiler) and, using the density of the saturated solution of 0.7048 g cm^{-3}, the value $c_1 = 0.471$ mol dm^{-3}. The authors assumed KCN, [151-50-8], to be the equilibrium solid phase.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess KCN was stirred with liquid NH_3 for 7 h in a closed apparatus, which made it possible to withdraw samples of the saturated solutions from the solubility vessel with exclusion of air. Temperature was controlled by keeping a constant NH_3 pressure over the solution. The ampoule with the sample was weighed, NH_3 allowed to evaporate, and the KCN content was determined by weighing the residue after drying it at 100 °C.

Source and Purity of Materials:

KCN, source not specified, was twice crystallized from distilled water. Commercially available anhydrous NH_3 was kept over sodium metal in steel containers.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:	**Original Measurements:**
(1) Potassium cyanide; KCN; [151-50-8] (2) Ammonia; NH_3; [7664-41-7]	P. W. Schenk and H. Tulhoff, Ber. Bunsenges. Phys. Chem. **71**, 1155–8 (1967).
Variables:	**Prepared By:**
T/K: 198–238	J. Hála

Experimental Data

Solubility of KCN in liquid ammonia as a function of temperature[a]

Temperature (t/°C)	KCN[b] (g/100 g NH_3)	KCN (m_1/mol kg^{-1})[c]
−70	10.9	1.674
−60	9.7	1.490
−50	8.6	1.321
−40	7.4	1.136
−35	6.8	1.044

[a] The solid phase was KCN, [151-50-8]. The authors stated that no solvates were observed.

[b] Obtained by the authors by interpolation from their experimental data.

[c] Calculated by compiler.

Additional information: The results of solubility measurements (g KCN per 100 g NH_3) taken at 15 different temperatures were presented in graphical form. The authors obtained the data shown in the table by interpolation.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method[1] was used. Measurements were carried out in a vessel connected to a vacuum line, and thermostated with methanol cooled in a cryostat. To a known amount of the solid salt, ammonia was gradually condensed until all solid dissolved. The mixture was intensely stirred during ammonia condensation. Toward the end of dissolution, additions of NH_3 were made small, and were added over sufficiently long time intervals to allow for equilibrium being attained and for keeping the temperature constant. The dissolution process was observed in side light. To ascertain that the point of saturation was not exceeded, the dissolution was stopped when a few very tiny crystals remained undissolved over a prolonged period of time. A small error introduced in this way by using large enough amount of the solid. The total amount of NH_3 condensed was calculated from the temperature, volume of the apparatus, and initial and final pressures of NH_3.

Source and Purity of Materials:

No details were reported as for KCN. Ammonia gas was dried by passing it through towers filled with NaOH, CaO, BaO, and sodium metal.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

References:

[1] P. W. Schenk and H. Tulhoff, Ber. Bunsenges. Phys. Chem. **71**, 206 (1967).

4.3.2. Evaluation of the KCN–Ethanol System

Components:	**Evaluator:**
(1) Potassium cyanide; KCN; [151-50-8] (2) Ethanol; C_2H_6O; [64-17-5]	J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, March 2001.

Critical Evaluation

The solubility of KCN in ethanol has been reported in three documents. The data are scarce and difficult to compare since they were obtained at different temperatures, and reported in different concentration units. The data are as follows: 6.87 g per dm^3 solvent at 292.5 K (de Bruyn[1]) (recalculated by evaluator from author's value of g salt per 100 g solvent); 1.9 g per dm^3 solvent at 298 K (Thompson[2]); and 8.4 g per dm^3 saturated solution at 298 K (Blandamer *et al.*[3]). Neglecting the differences in temperature and units, there could be two reasons for the discrepancy between the results of de Bruyn[1] and Blandamer *et al.*[3] on one hand, and of Thompson[2] on the other. Taking into consideration that the value of de Bruyn[1] is rather close to that of Thompson[2] for the solubility of KCN in 95% (v/v) ethanol, i.e., 6.1 g per dm^3 solvent, one might speculate that de Bruyn[1] did not use absolute ethanol (purity of ethanol used was not specified). However, it does not seem likely that this has also been the case in measurements of Blandamer and Burgess[3] (see compilation of their KCN–C_2H_6O–H_2O system), whose solubility value is, however, closer to that of de Bruyn.[1] The other reason could be in equilibration conditions which, however, have not been reported in the documents in sufficient detail to allow for an estimate of this effect to be made. Therefore, because of the uncertainty in the published solubility values, none of them can be recommended.

References:

[1] C. A. L. de Bruyn, Z. Phys. Chem. **10**, 782 (1892).
[2] M. R. Thompson, J. Res. Natl. Bur. Std. **6**, 1051 (1931).
[3] M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1 (1980).

Components:
(1) Potassium cyanide; KCN; [151-50-8]
(2) Solvents

Original Measurements:
C. A. L. de Bruyn, Z. Phys. Chem. **10**, 782–9 (1892).

Variables:
T/K: 292.5

Prepared By:
J. Hála

Experimental Data

Solubility of KCN in methanol and ethanol at 19.5 °C[a]

Solvent	KCN (g/100 g solvent)	KCN (m_1/mol kg^{-1})[b]	KCN (100 w_1/mass %)[b]
Methanol; CH_4O; [67-56-1]	4.91	0.754	4.68
Ethanol; C_2H_6O; [64-17-5]	0.875	0.134	0.867

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Excess solid was equilibrated with the solvent by frequent shaking in a glass vessel closed with rubber stopper. Equilibration was carried out in water bath for several days. The method of KCN analysis was not reported.

Source and Purity of Materials:
100% methanol was used. No other details reported.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium cyanide; KCN; [151-50-8]
(2) Solvents

Original Measurements:
M. R. Thompson, J. Res. Natl. Bur. Std. **6**, 1051–9 (1931).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of KCN in methanol and ethanol at 25 °C[a]

Solvent	KCN (g dm^{-3} solvent)	KCN (m_1/mol kg^{-1})
Methanol; CH_3OH; [67-56-1]	30.0	0.586[b]
Ethanol; C_2H_6O; [64-17-5]	1.9	0.0372[c]

[a] Solid phases were not investigated.
[b] Calculated by compiler using density of methanol[1] of 0.7865 g cm^{-3} at 25 °C.
[c] Calculated by compiler using density of ethanol[1] of 0.7852 g cm^{-3} at 25 °C.

Additional information: The solubility of KCN at 25 °C in 95% ethanol (v/v; 5% water) was reported to be 6.1 g salt in 1 dm^{-3} solvent.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. The technique used and equilibrium time applied were not reported. The cyanide content in the saturated solutions was determined by a modified Liebig's method of titration against $AgNO_3$ solution in the presence of KI and NaOH.

Source and Purity of Materials:
KCN was prepared by reacting a solution of KOH in absolute ethanol with a 10% excess of liquid HCN, during which reaction most of KCN precipitated. The product contained 99.74%–99.85% KCN. Absolute methanol and ethanol were used.

References:

[1] *Handbook of Chemistry and Physics*, 38th ed. (Chemical Rubber Co., Cleveland, OH, 1956).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) 1,2,3-Propanetriol (glycerol); $C_3H_8O_3$; [56-81-5]

Original Measurements:

A. M. Ossendowski, Zh. Russ. Fiz. Khim. Obsh. **38**, 1071–2 (1906).

Variables:

T/K: 288

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in glycerol at 15 °C.

The solubility of KCN in glycerol was reported to be 31.84 g salt in 100 g solvent at 15–15.6 °C ($m_1 = 4.90$ mol kg^{-1}; 100 $w_1 = 24.15$ mass %; compiler).

Auxiliary Information

Method/Apparatus/Procedure:

Nothing specified.

Source and Purity of Materials:

KCN, source and purity not specified, was twice recrystallized from water. Glycerol was prepared by saponification of soya bean oil. The product was distilled with steam and purified by distillation. The fraction used boiled at 284 °C, and had density of 1.2561 g cm^{-3} at 15 °C.

Estimated Error:

Temperature: precision not reported ±0.3 K (compiler).
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) Potassium hydroxide; KOH; [1310-58-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

H. Bassett and A. S. Corbet, J. Chem. Soc. **125**, 1660–75 (1924).

Variables:

T/K: 298
100 w_2/mass %: 0.16–23.57

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in aqueous solutions of KOH at 25 °C[a]

KOH (g/100 g solution)[b]	KOH (g/100 g solution)[c]	KOH (100 w_2/mass %)[c]	KOH (c_1/mol dm^{-3})[c]	KCN (g/100 g solution)	KCN (100 w_1/mass %)[c]	KCN (c_1/mol dm^{-3})[c]
0.11	0.095	0.163	0.1016	41.56	71.23	38.24
0.69	0.59	1.02	0.678	41.67	72.17	41.34
3.30	2.84	4.88	3.075	38.92	66.83	36.28
7.39	6.37	10.81	6.369	34.72	58.94	29.92
8.69	7.72	13.15	7.908	33.58	57.21	29.64
16.29	14.04	23.57	13.08	26.39	44.30	21.17

[a] Equilibrium solid phases were not investigated.
[b] Reported by the authors in terms of grams KCN.
[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Solutions containing excess KCN were equilibrated in a thermostated bath. KCN was determined in the saturated solutions by titration against standard $AgNO_3$ solution in the presence of ammonia and KI.

Source and Purity of Materials:

KCN was a commercial product (source not specified) containing as much as 3% KOH. Attempts to neutralize it with HCN were unsuccessful.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) Formamide; CH_3NO; [75-12-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:

T/K: 298
Volume % of formamide: 20–100

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in formamide–water mixtures at 25 °C[a]

CH_3NO (volume %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
20	720	11.06
40	540	8.29
60	420	6.45
80	310	4.76
100	250	3.84

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: The solubility of KCN in formamide at 25 °C, 146 g KCN per dm^{-3}, was reported by Colton and Brooker.[1] This document was compiled in the *Solubility Data Series*, Vol. 11, p. 47, B. Scrosati and C. A. Vincent, editors.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Formamide, source not specified, was purified according to Gordon and Ford.[2] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] E. Colton and R. E. Brooker, J. Phys. Chem. **62**, 1595 (1958).
[2] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) Methanol; CH_4O; [67-56-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans., 1–8 (1980).

Variables:

T/K: 298
volume % of methanol: 10–100 100 w_2/mass %: 10–40

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in methanol–water mixtures at 25 °C[a]

CH_4O (volume %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]	CH_4O (100 w_2/mass %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
10	810	12.44	10	780	11.98
20	760	11.67	20	720	11.06
30	700	10.75	30	610	9.37
40	600	9.21	40	540	8.29
50	450	6.91			
60	340	5.22			
70	230	3.53			
80	110	1.69			
90	51	0.783			
100	21	0.323			

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume or by weight. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Methanol, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) Acetonitrile; C_2H_3N; [75-05-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans., 1–8 (1980).

Variables:

T/K: 298
Volume % of C_2H_3N: 10–100

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in acetonitrile–water mixtures at 25 °C[a]

C_2H_3N (volume %)	KCN (g dm^{-3})	KCN (c_1 /mol dm^{-3})[b]
10	814	12.50
20	740	11.36
30	540	8.29
100	0.15	0.002 30

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: Phase separation occurred in mixtures containing 40–80 volume % acetonitrile in the presence of KCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Acetonitrile, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) Ethanol; C_2H_6O; [64-17-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:

T/K: 298
Volume % of C_2H_6O: 10–100

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in ethanol–water mixtures at 25 °C[a]

C_2H_6O (volume %)	KCN (g dm^{-3})	KCN (c_1 /mol dm^{-3})[b]
10	740	11.36
20	640	9.83
30	580	8.91
40	460	7.06
50	350	5.38
60	273	4.19
70	180	2.76
80	99	1.52
90	24	0.369
100	8.4	0.129

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Ethanol, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:
(1) Potassium cyanide; KCN; [151-50-8]
(2) 1,2-Ethanediol (ethyleneglycol); $C_2H_6O_2$; [107-21-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:
T/K: 298
Volume % of $C_2H_6O_2$: 30–100

Prepared By:
J. Hála

Experimental Data

Solubility of KCN in ethyleneglycol–water mixtures at 25 °C[a]

$C_2H_6O_2$ (volume %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
30	520	7.99
50	350	5.38
70	235	3.61
100	180	2.76

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:
KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Ethyleneglycol, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:
(1) Potassium cyanide; KCN; [151-50-8]
(2) Sulfinylbis(methane); dimethylsulfoxide; C_2H_6OS; [67-68-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:
T/K: 298
Volume % of C_2H_6OS: 10–100

Prepared By:
J. Hála

Experimental Data

Solubility of KCN in dimethylsulfoxide–water mixtures at 25 °C[a]

C_2H_6OS (volume %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
10	920	12.59
20	730	11.21
30	550	8.45
40	400	6.14
50	300	4.61
60	210	3.23
70	110	1.69
80	64	0.983
90	34	0.522
100	7.8	0.120

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:
KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Dimethylsulfoxide, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) 1,3-dioxolan-2-one (ethylenecarbonate); $C_3H_4O_3$; [96-49-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:

T/K: 298
100 w_2/mass %: 22–45

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in ethylenecarbonate–water mixtures at 25 °C[a]

$C_3H_4O_3$ (100 w_2/mass %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
22	440	6.76
33.5	320	4.91
45	300	4.61

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by weight. The solvent mixtures were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Ethylenecarbonate, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) Acetone; C_3H_6O; [67-64-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:

T/K: 298
Volume % of C_3H_6O: 20–100

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in acetone–water mixtures at 25 °C[a]

C_3H_6O (volume %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
20	700	10.75
30	580	8.91
50	360	5.53
70	100	1.54
80	5.8	0.0891
90	1.9	0.0292
100	0.03	0.000 461

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Acetone, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) N,N-Dimethylformamide; C_3H_7NO; [68-12-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:

T/K: 298
Volume % of C_3H_7NO: 20–100

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in N,N-dimethylformamide–water mixtures at 25 °C[a]

C_3H_7NO (volume %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
20	612	9.40
40	310	4.76
60	180	2.76
80	44	0.676
100	4.0	0.0614

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: The solubility of KCN in N,N-dimethylformamide was also reported in a booklet.[1] This document was compiled in *Solubility Data Series*, Vol. 11, p. 205, B. Scrosati and C. A. Vincent, editors.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. N,N-dimethylformamide, source not specified, was purified according to Gordon and Ford.[2] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] *Properties and Uses of Dimethylformamide*, DuPont Information Booklet (1976).
[2] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) 1,2,3-Propanetriol (glycerol); $C_3H_8O_3$; [56-81-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:

T/K: 298
100 w_2/mass %: 20–80

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in glycerol–water mixtures at 25 °C[a]

$C_3H_8O_3$ (100 w_2/mass %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
20	680	10.44
33.3	550	8.45
50	420	6.45
60	340	5.22
80	260	3.99

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by weight. The solvent mixtures were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Glycerol, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) 1,4-Dioxane; $C_4H_8O_2$; [1234-91-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:

T/K: 298
Volume % of $C_4H_8O_2$: 10–100

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in 1,4-dioxane–water mixtures at 25 °C[a]

$C_4H_8O_2$ (volume %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
10	750	11.52
30	580	8.91
40	490	7.53
90	7.2	0.111
100	0.9	0.0138

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: Phase separation occurred in mixtures containing 50–80 volume % 1,4-dioxane in the presence of KCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. 1,4-dioxane, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

Components:

(1) Potassium cyanide; KCN; [151-50-8]
(2) 2-Methyl-2-propanol (tert-butanol); $C_4H_{10}O$; [75-65-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. J. Blandamer, J. Burgess, and A. J. Duffield, J. Chem. Soc., Dalton Trans. 1–8 (1980).

Variables:

T/K: 298
Volume % of $C_4H_{10}O$: 10–100

Prepared By:

J. Hála

Experimental Data

Solubility of KCN in tert-butanol–water mixtures at 25 °C[a]

$C_4H_{10}O$ (volume %)	KCN (g dm^{-3})	KCN (c_1/mol dm^{-3})[b]
5	794	12.19
10	700	10.75
95	13	0.200
100	0.1	0.00154

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: Phase separation occurred in mixtures containing 20–90 volume % tert-butanol in the presence of KCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The binary aqueous/solvent mixtures were made up by volume. The solvent mixtures or the neat organic solvent were stirred or agitated with excess solid in a sealed, thermostated vessel until equilibrium had been attained. This was checked by analyzing aliquots taken at intervals. Immediately after withdrawal, samples of the saturated solutions were appropriately diluted and analyzed for K^+ and CN^- ions. Potassium was determined by flame photometry against standard K_2SO_4 solutions. Cyanide was titrated against standard $AgNO_3$ solution.

Source and Purity of Materials:

KCN was AnalaR material (B.D.H.) and was used as supplied. In the course of the study, several batches of KCN were used, and all gave consistent solubility results. Tert-butanol, source not specified, was purified according to Gordon and Ford.[1] De-ionized water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. J. Gordon and R. A. Ford, *The Chemist's Companion* (Wiley, New York, 1972).

5. The Solubility of Cyanates

5.1. Sodium Cyanate

5.1.1. Evaluation of the NaOCN–NH_3 System

Components:	**Evaluator:**
(1) Sodium cyanate; NaOCN; [917-61-3] (2) Ammonia; NH_3; [7664-41-7]	J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, April 2001.

Critical Evaluation

The solubility of NaOCN in liquid ammonia has been reported in two documents.[1,2] In both of them, the solubilities were obtained by isothermal method, and reported as a function of temperature. Both sets of data are in excellent agreement, as seen from Fig. 6. The agreement is particularly seen clearly from the two results at 273.2 K, i.e., 0.208 (Ariizumi *et al.*[1]) and 0.212 (Abe and Okabe[2]) mol kg^{-1}. The two sets of data were computer smoothed by linear regression of the data, and found to fit the equation

$$m_1\ (\text{mol kg}^{-1}) = 0.2122 - 2.321\times10^{-3}t,$$

where t is temperature in °C. The standard deviations of the constants are 1.53×10^{-3} and 6.71×10^{-5}, respectively.

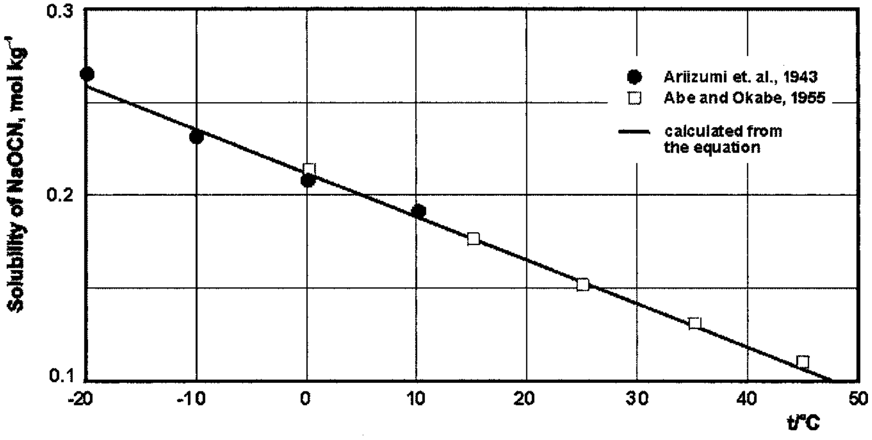

FIG. 6. Solubility of NaOCN in liquid NH_3 as a function of temperature.

References:

[1] M. Ariizumi, S, Kumoa, and R. Hara, Kogyo Kagaku Zasshi **46**, 237 (1943).

[2] S. Abe and T. Okabe, Kogyo Kagaku Zasshi **58**, 242 (1955).

Components:	**Original Measurements:**
(1) Sodium cyanate; NaOCN; [917-61-3] (2) Ammonia; NH_3; [7664-41-7]	M. Ariizumi, S. Kumoa, and R. Hara, Kogyo Kagaku Zasshi **46**, 237–40 (1943).
Variables:	**Prepared By:**
T/K: 253–283	H. Akaiwa

Experimental Data

Solubility of NaOCN in liquid ammonia as a function of temperature[a]

Temperature (°C)	NaOCN (g/100 g NH_3)	NaOCN (m_1/mol kg^{-1})[b]
10.2	1.24 ± 0.005^b ($n=3$)	0.191
0	1.35 ± 0.030^b ($n=4$)	0.208
−10.1	1.50 ± 0.025^b ($n=3$)	0.231
−19.8	1.72 ± 0.012^b ($n=3$)	0.265

[a] Solid phases were not investigated.

[b] Calculated by compiler. Standard deviations were calculated for the indicated number of measurements.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. From the samples of the saturated solutions, ammonia was allowed to evaporate and its content was determined from the difference in weight. NaOCN was determined from the weight of the residue, and by titration. The solubility was obtained by dissolving the residue in water, precipitating AgOCN, dissolution of the latter in excess of standard HNO_3, and back-titrating excess acid.

Source and Purity of Materials:

NaOCN, source not specified, was of 99.25% purity. It contained trace amounts of Na_2CO_3 and NaCl.

Estimated Error:

Temperature: precision not reported.
Solubility: see above.

Components:
(1) Sodium cyanate; NaOCN; [917-61-3]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
S. Abe and T. Okabe, Kogyo Kagaku Zasshi **58**, 242–7 (1955).

Variables:
T/K: 273–318

Prepared By:
H. Akaiwa

Experimental Data

Solubility of NaOCN in liquid ammonia as a function of temperature[a]

Temperature (t/°C)	NaOCN (g/100 g NH_3)	NaOCN (m_1/mol kg^{-1})[b]
0	1.39 1.39 1.38 1.37	
	1.38±0.008[b]	0.212
15	1.15 1.15 1.15 1.15	
	1.15	0.177
25	0.98 0.98 0.96 0.98	
	0.98±0.009[b]	0.151
35	0.87 0.85 0.85 0.84 0.85	
	0.85±0.010[b]	0.131
45	0.72 0.73 0.71 0.70 0.73	
	0.72±0.012[b]	0.111

[a] Solid phases were not investigated.
[b] Molalities and standard deviations calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. A sufficient amount of NaOCN was placed in the equilibration vessel, and liquid ammonia was introduced. The vessel was connected through a side-arm with a filtration setup and a sampling vessel. The equilibration vessel was kept in a thermostat for 2–8 h under constant stirring. After saturation had been attained, the mixture was filtered into the sampling vessel, and the content of NaOCN in the saturated solutions was determined titrimetrically using Volhard's method.

Source and Purity of Materials:
NaOCN was prepared by extracting the raw material (source not specified) with liquid NH_3 containing NH_4NO_3, and washing several times with methanol. Purity of the product was assumed to be 100%.

Estimated Error:
Temperature: precision not reported.
Solubility: see above.

Components:
(1) Sodium cyanate; NaOCN; [917-61-3]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
J. A. Cranston and A. Y. Livingstone, J. Chem. Soc. 501–3 (1926).

Variables:
T/K: 273

Prepared By:
J. Hála

Experimental Data

The solubility of NaOCN was reported to be 0.22 g salt in 100 g solvent at 0 °C. From this value the compiler calculated $m_1 = 0.0338$ mol kg^{-1}.

Additional information: The authors also reported the solubility of NaOCN in boiling ethanol to be 0.52 g salt in 100 g solvent. Boiling point of the saturated solution and atmospheric pressure at which the measurement was taken were not reported.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Details were not reported. Analysis of the saturated solutions was carried out by weighing samples of the saturated solutions, and determining the cyanate content volumetrically according to Mason.[1]

Source and Purity of Materials:
No information on NaOCN reported. Ethanol used had density of 0.799 g cm^{-3} at 17 °C.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] Mason, Chem. News **90**, No. 5, 17 (1906).

Components:

(1) Sodium cyanate; NaOCN; [917-61-3]
(2) 18-dibenzo-crown-6; $C_{20}H_{24}O_6$; [14187-32-7];
or 18-dicyclohexyl-crown-6; $C_{20}H_{36}O_6$;[ ]
(3) N,N-dimethylformamide; C_3H_7NO; [68-12-2];
or o-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]

Original Measurements:

V. A. Zlobin and A. K. Tarasov, Izv. VUZ, Khim. Khim. Tekhnol. **40**, No. 5, 134–5 (1997)

Variables:

T/K: 293; 363
c_2 /mol dm^{-3}: 0.04–0.10 ($C_{20}H_{24}O_6$); 0.02–0.10 ($C_{20}H_{36}O_6$)

Prepared By:

J. Hála

Experimental Data

Solubility of NaOCN in two solvents in the presence of crown ethers at 20 and 90 °C

Solvent	Temperature (t/°C)	$C_{20}H_{24}O_6$ (c_2 /mol dm^{-3})	NaOCN (g l^{-1})	NaOCN (10^2 c_1 /mol dm^{-3})	$C_{20}H_{36}O_6$ (c_2 /mol dm^{-3})	NaOCN (g l^{-1})	NaOCN (10^2 c_1 /mol dm^{-3})
C_3H_7NO	20	—	0.50	0.77	0.02	0.57	0.88
		0.04	0.55	0.85	0.06	0.78	1.20
		0.08	0.68	1.04	0.10	1.09	1.35
		0.10	1.09	1.35			
	90	—	0.75	1.15			
		0.10	1.21	1.86			
$C_6H_4Cl_2$	20	—	0.0157	0.025			
		0.10	0.0616	0.095			

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, details reported only on analytical methods used. The concentration of OCN^- in C_3H_7NO was determined chronocon-ductometrically by titrating an aliquot of the saturated solution against 0.1 mol dm^{-3} $AgNO_3$ solution in CH_3CN, which was delivered into the titration vessel via a capillary tube at a constant rate by a peristaltic pump. The apparatus was calibrated by titrating a 0.1 mol dm^{-3} HCl solution in isoamylalcohol. In $C_6H_4Cl_2$, OCN^- was determined chronopotentiometrically using Ag/AgCl electrodes.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Sodium cyanate; NaOCN; [917-61-3]
(2) Ammonium chloride; NH_4Cl; [12125-02-9]
(3) Ammonia; NH_3 ; [7664-41-7]

Original Measurements:

S. Abe and T. Okabe, Kogyo Kagaku Zasshi **58**, 242–7 (1955).

Variables:

T/K: 273
Concentration of (2)/g per 100 g NH_3 : 2.16–64.0

Prepared By:

H. Akaiwa

Experimental Data

Solubility at 0 °C of NaOCN in liquid ammonia in the presence of NH_4Cl[a]

NH_4Cl (g/100 g NH_3)	NH_4Cl (m_2 /mol kg^{-1})[b]	NaOCN (g/100 g NH_3)	NaOCN (m_1 /mol kg^{-1})[b]
2.16	0.3964	3.20	0.4923
4.32	0.7928	4.21	0.6476
9.37	1.720	6.18	0.9507
12.7	2.331	7.16	1.101
18.6	3.413	7.94	1.221
28.6	5.248	8.43	1.297
40.2	7.377	8.42	1.295
54.4	9.983	6.82	1.049
64.0	11.75	5.89	0.9061

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. A sufficient amount of the two salts was placed in the equilibration vessel, and liquid ammonia was introduced. The vessel was connected through a side arm with a filtration setup and a sampling vessel. The equilibration vessel was kept in a thermostat for 2–8 h under constant stirring. After saturation had been attained, the mixture was filtered into the sampling vessel, and the content of NaOCN in the saturated solutions was determined titrimetrically using Volhard's method.

Source and Purity of Materials:

NaOCN was prepared by extracting the raw material (source not specified) with liquid ammonia, containing NH_4NO_3 , and washing several times with methanol. The product was assumed to be 100% pure.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Sodium cyanate; NaOCN; [917-61-3]
(2) Ammonium nitrate; NH_4NO_3; [6484-52-2]
(3) Ammonia; NH_3; [7664-41-7]

Original Measurements:
S. Abe and T. Okabe, Kogyo Kagaku Zasshi **58**, 242–7 (1955).

Variables:
T/K: 273
Concentration of (2)/g per 100 g NH_3: 2.35–66.6

Prepared By:
H. Akaiwa

Experimental Data

Solubility at 0 °C of NaOCN in liquid ammonia in the presence of NH_4NO_3[a]

NH_4NO_3 (g/100 g NH_3)	NH_4NO_3 (m_2/mol kg^{-1})[b]	NaOCN (g/100 g NH_3)	NaOCN (m_1/mol kg^{-1})[b]
2.35	0.2936	3.05	0.4692
6.84	0.8545	4.94	0.7599
8.70	1.087	5.39	0.8291
11.6	1.449	6.11	0.9400
19.9	2.486	7.51	1.155
28.3	3.536	8.11	1.248
35.4	4.423	8.47	1.303
42.2	5.272	8.50	1.308
45.3	5.659	8.41	1.294
52.2	6.521	8.11	1.248
56.7	7.084	7.90	1.215
66.6	8.320	6.94	1.068

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. A sufficient amount of the two salts was placed in the equilibration vessel, and liquid ammonia was introduced. The vessel was connected through a side-arm with a filtration setup and a sampling vessel. The equilibration vessel was kept in a thermostat for 2–8 h under constant stirring. After saturation had been attained, the mixture was filtered into the sampling vessel, and the content of NaOCN in the saturated solutions was determined titrimetrically using Volhard's method.

Source and Purity of Materials:
NaOCN was prepared by extracting the raw material (source not specified) with liquid ammonia, containing NH_4NO_3, and washing several times with methanol. The product was assumed to be 100% pure.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Sodium cyanate; NaOCN; [917-61-3]
(2) Diethylether; $C_4H_{10}O$; [60-29-7]
(3) Methanol; CH_4O; [67-56-1]

Original Measurements:
H. Yashio, J. Takeshita, A. Okuwaki, and T. Okabe, Nippon Kagaku Kaishi 1473–5 (1984).

Variables:
T/K: 298
Volume fraction of (2): 0–0.5

Prepared By:
H. Akaiwa

Experimental Data

The solubility of NaOCN, in grams of salt per 100 g solvent, in mixtures of diethylether and methanol at 25 °C was reported in graphical form (Fig. 7).

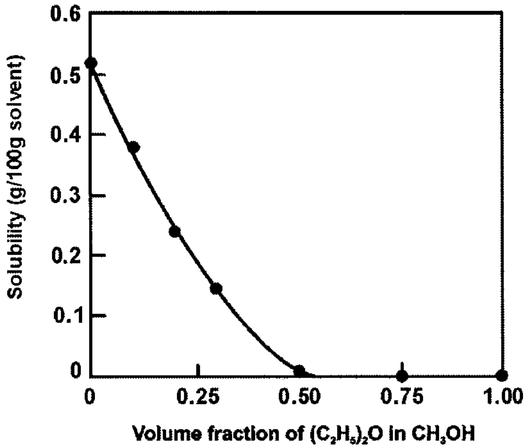

FIG. 7. Solubility of NaOCN in diethylether/methanol mixtures at 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. NaOCN was added to the solvent mixture containing the solvents in the desired volume ratio, and stirred first at 30 °C for 6 h, and then for at least 6 h at 25 °C in a sealed vessel in a thermostat. A sample of the saturated solution (30–50 cm^3) was withdrawn, weighed, the solvents were evaporated under reduced pressure, and NaOCN was determined in the residue by the Volhard's method.

Source and Purity of Materials:
NaOCN, source not specified, was dissolved in distilled water at 50 °C, and neutralized by glacial acetic acid. The solution was filtered, and NaOCN was allowed to crystallize in a refrigerator.

Estimated Error:
Temperature: precision not reported.

5.2. Potassium Cyanate

Components:
(1) Potassium cyanate; KOCN; [590-28-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
G. N. Lewis and T. B. Brighton, J. Am. Chem. Soc. **40**, 482–9 (1918).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

The solubility of KOCN in water at 25 °C was reported to be 750 g KOCN per 1000 g water ($m_1 = 9.246$ mol kg^{-1}; compiler).

Additional information: Also reported were freezing point temperatures for solutions containing 98.4–320 g KOCN/1000 g water. The cryohydric point was reported to be at −18.14 °C. The composition at the cryohydric point was not reported. Compiler smoother the freezing point data by linear regression of the data to a fifth order polynomial, from which the composition at the cryohydric point was obtained by extrapolation as 352.3 g KOCN/1000 g water.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Due to rapid decomposition of KOCN in the solutions, reproducible results were obtained by violent shaking in a thermostat for a short time.

Source and Purity of Materials:
KOCN, source not reported, contained unspecified small trace of carbonate. It was dried in a vacuum desiccator.

Estimated Error:
Temperature: precision not reported.
Solubility: ±0.3% (authors, from four determinations).

Components:
(1) Potassium cyanate; KOCN; [590-28-3]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
H. Hunt, J. Am. Chem. Soc. **54**, 3509–12 (1932).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

The solubility of KOCN was reported to be 1.70 g in 100 g solvent at 25 °C, or, using the density of liquid ammonia of 0.604 g cm^{-3} at 25 °C, 1.02 g KOCN in 100 cm^3 solvent. Compiler calculated $m_1 = 0.2096$ mol kg^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Ammonia (10–25 g) was equilibrated with the salt in the bottom part of a sealed, two/compartment Pyrex tube. The compartments were separated from each other with a narrow neck. The salt was introduced into the tube before sealing it off in a small cup closed with a very closely woven cotton cloth. The latter permitted the salt to dissolve the salt holding back the solid at the same time. The system was equilibrated for 1–3 weeks with occasional shaking. Then the tube was inverted in the bath and all the solution drained into the empty compartment, which was cooled and sealed off. When it reached room temperature it was dried and weighed, the ammonia allowed to boil off, the tube with the salt warmed until all odor of NH_3 was gone, and the salt was weighed.

Source and Purity of Materials:
KOCN, Baker C. P. product, was recrystallized and carefully dried. Commercially available anhydrous NH_3 was allowed to stand over metallic sodium for several weeks before use.

Estimated Error:
Temperature: ±0.025 K (author).
Solubility: 5% (author).

Components:

(1) Potassium cyanate; KOCN; [590-28-3]
(2) 18-dibenzo-crown-6; $C_{20}H_{24}O_6$; [14187-32-7];
or 18-dicyclohexyl-crown-6; $C_{20}H_{36}O_6$; [ ]
(3) N,N-dimethylformamide; C_3H_7NO; [68-12-2]

Original Measurements:

V. A. Zlobin and A. K. Tarasov, Izv. VUZ, Khim. Khim. Tekhnol. **40**, No. 5, 134–5 (1997).

Variables:

T/K: 293; 363
c_2 /mol dm^{-3}: 0.02–0.10 ($C_{20}H_{24}O_6$); 0.02–0.10 ($C_{20}H_{36}O_6$)

Prepared By:

J. Hála

Experimental Data

Solubility of KOCN in N,N-dimethylformamide in the presence of crown ethers at 20 and 90 °C

Temperature (t/°C)	$C_{20}H_{24}O_6$ (c_2 /mol dm^{-3})	KOCN (g l^{-1})	KOCN (10^2 c_1 /mol dm^{-3})	$C_{20}H_{36}O_6$ (c_2 /mol dm^{-3})	KOCN (g l^{-1})	KOCN (10^2 c_1 /mol dm^{-3})
20	—	0.87	1.08	0.02	1.03	1.27
	0.02	0.94	1.16	0.04	1.10	1.36
	0.04	1.13	1.39	0.08	1.59	1.97
	0.08	1.59	1.97	0.10	1.62	2.00
	0.10	2.96	3.65			
90	—	0.79	0.97			
	0.10	2.83	3.50			

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, details reported only on analytical methods used. The concentration of OCN$^-$ in C_3H_7NO was determined chronoconductometrically by titrating an aliquot of the saturated solution against 0.1 mol dm^{-3} $AgNO_3$ solution in CH_3CN, which was delivered into the titration vessel via a capillary tube at a constant rate by a peristaltic pump. The apparatus was calibrated by titrating a 0.1 mol dm^{-3} HCl solution in isoamylalcohol.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Potassium cyanate; KOCN; [590-28-3]
(2) Ethanol; C_2H_6O; [64-17-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

J. A. Cranston and A. Y. Livingstone, J. Chem. Soc. 501–3 (1926).

Variables:

T/K: 273
ethanol concentration: 80% and 100% (v/v)

Prepared By:

J. Hála

Experimental Data

Solubility of KOCN at 0 °C in ethanol and one ethanol—water system[a]

Ethanol (%, v/v)	KOCN (g/100 g solvent)	KOCN (m_1 /mol kg^{-1})[b]
80	1.9	
100	0.16	0.020

[a] Solid phases were not investigated.
[b] Value calculated by compiler.

Additional information: Also reported were the solubilities of KOCN at boiling points of the saturated solutions as 6.2 and 0.53 g KOCN per 100 g solvent for 80% and 100% (v/v) ethanol, respectively. The boiling points temperatures and atmospheric pressure at which the measurements were performed were not reported.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibration time was not specified. The saturated solutions were analyzed by weighing definite volume of the solution, and determining the cyanate content volumetrically.[1]

Source and Purity of Materials:

Source and purity of KOCN use were not specified. Ethanol used had density of 0.799 g cm^{-3} at 17 °C.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] Masson, Chem. News. **90**, 5, 17 (1906).

6. The Solubility of Thiocyanates

6.1. Lithium Thiocyanate

6.1.1. Evaluation of the LiSCN–H_2O System

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Water; H_2O; [7732-18-5]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, April 2001.

Critical Evaluation

The data on the LiSCN–water system have been reported in three documents. Iwase[1] reported the solubilities of LiSCN obtained by isothermal method in the temperature range from 293 to 313 K, while in the other two documents,[2,3] the system was studied by polythermal method. Except for the value at 305.6 K, which seems to be too low, the polythermal data of Schimmel[3] are in good agreement with those of Iwase[1] at 293–313 K, while the data of Nikolaev[2] are considerably higher in the same temperature range. This may have been caused by the tendency of LiSCN solutions to supersaturation, though explicitly this has been reported[2] only for highly concentrated LiSCN solutions.

Although Iwase[1] did not report the error of temperature measurement, he reported three consistent measurements at each temperature, and his data can be suggested as tentative values in the temperature range of 293–313 K.

There is some inconsistency in the published data as for the existence regions and the composition of the solid phases. Iwase[1] reported the eutectic point at −33 °C as that of the ice/LiSCN·$2H_2O$ pair, while Schimmel[3] reported the eutectic point at −92 °C for the ice/LiSCN·$5H_2O$ pair. In addition, Iwase[1] and Nikolaev[2] reported the transition of LiSCN·$2H_2O$ to LiSCNH_2O to occur at 34–35 °C, while Schimmel[3] described the dihydrate as the equilibrium solid phase up to 43.3 °C. Contrary to Iwase[1] and Nikolaev,[2] he also observed the trihydrate and pentahydrate, but not the monohydrate.

References:
[1] E. Iwase, Bull. Inst. Phys. Chem. Research (Tokyo) **9**, 541 (1930).
[2] V. I. Nikolaev, Zh. Russ. Fiz.-Khim. Obsh. **61**, 939 (1929).
[3] F. A. Schimmel, J. Chem. Eng. Data **5**, 519 (1960).

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. Iwase, Bull. Inst. Phys. Chem. Res. (Tokyo) **9**, 541–3 (1930).

Variables:
T/K: 293–313

Prepared By:
H. Akaiwa and J. Hála

Experimental Data

Solubility of LiSCN in water as a function of temperature[a]

Temperature (t/°C)	LiSCN (100 w_1/mass %)				LiSCN (m_1/mol kg^{-1})
20	53.16	53.11	53.25	53.2±0.06	17.48
25	54.75	54.24		54.5±0.3	18.42
30	55.97	56.75	56.65	56.6±0.3	20.14
35	58.99	58.49	58.76	58.7±0.2	21.95
40	60.54	60.20	60.43	60.4±0.1	23.46

[a] Average values, standard deviations, and molalities calculated by the compiler (J.H.). The results were reported also in graphical form (Fig. 8) showing the equilibrium solid phases.

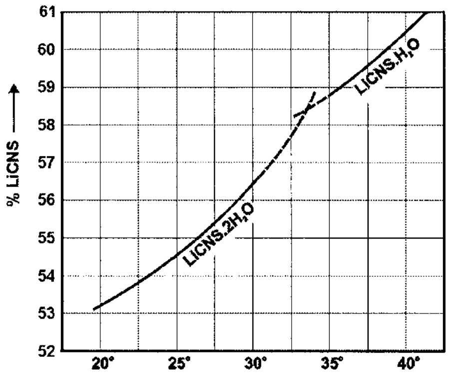

FIG. 8. Solubility curves of lithium thiocyanate hydrates in water.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Measurements were performed according to Findlay.[1]

Source and Purity of Materials:
LiSCN was prepared by double decomposition from Ba$(SCN)_2$ and Li_2SO_4, and crystallized as LiSCN·$2H_2O$.

Estimated Error:
Temperature: precision not reported.
Solubility: see the table above.

References:
[1] A. Findlay, *Practical Physical Chemistry* (1923), p. 269.

Components:

(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. I. Nikolaev, Zh. Russ. Fiz-Khim. Obsh. **61**, 939–45 (1929).

Variables:

T/K: 240–533

Prepared By:

J. Hála

Experimental Data

Freezing points and solubility in the LiSCN–H_2O system

Solidus temperature (t/°C)	LiSCN (100 x_1/mol %)	LiSCN (100 w_1/mass %)[a]	LiSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	0	0	A
−4.0	3.09	10.32	1.770	A
−10.8	4.86	15.57	2.836	A
−13.7	5.50	17.36	3.231	A
−18.0	7.04	21.47	4.205	A
−33.0	11.91	32.80	7.507	A+B
0	21.15	49.19	14.89	B
5.0	22.53	51.21	16.14	B
10.0	23.81	53.01	17.35	B
11.5	24.32	53.70	17.84	B
17.6	24.80	54.34	18.30	B
18.5	25.00	54.61	18.50	B
19.5	25.13	54.78	18.63	B
27.5	29.57	60.24	23.30	B
34.0	33.34	64.35	27.76	B
38.5	35.09	66.12	30.01	C
44.5	37.31	68.23	33.03	C
55.5	45.25	74.89		C
58	47.40	76.48		C
60.5	50.00	78.30		C
102	51.55	79.34		D
144	53.19	80.40		D
201.5	58.13	83.36		D
260[c]	83.34	94.75		D

[a] Calculated by compiler.
[b] A: Ice, H_2O [7732-18-5]; B: $LiSCN\cdot 2H_2O$ [84372-58-7]; C: $LiSCN\cdot H_2O$ [97034-69-8]; D: LiSCN [556-65-0].
[c] Melting under decomposition.

Additional information: One isothermal measurement was performed at 17 °C, yielding 100 w_1=63.3 mass % (m_1=26.35 mol kg^{-1}; compiler). In systems containing 12–21 mol % LiSCN, glasses with no distinct melting points were formed. Solutions with the LiSCN/H_2O ratio greater than 2 showed strong tendency to supersaturation.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. The systems were prepared from $LiSCN\cdot 2H_2O$ by either adding water to the salt (for LiSCN/H_2O ratios <2), or by drying the salt over H_2SO_4 of varying concentration in a desiccator (for LiSCN/H_2O ratios >2). Samples of LiSCN hydrated to the desired degree were sealed in thin-walled glass tubes, solidified by cooling, and the solidus temperatures were determined by the capillary method. Samples with LiSCN/H_2O ratios >2 were strongly hygroscopic and had to be prepared as quickly as possible. The composition of the samples was determined after the determination of solidus temperature. The tubes were weighed, broken, and the contents analyzed for SCN^-. Conditions used for the single isothermal measurement, and the method of identification of the solid phases were not reported.

Source and Purity of Materials:

$LiSCN\cdot 2H_2O$ was prepared by double decomposition from Li_2SO_4 and $Ba(SCN)_2$. Source and purity of these materials were not specified. Since solutions of LiSCN tend to form supersaturated solutions, crystallization of the dihydrate had to be induced by seeding.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

F. A. Schimmel, J. Chem. Eng. Data **5**, 519–20 (1950).

Variables:

T/K: 181–316

Prepared By:

J. Hála

Experimental Data

Composition of the saturated solutions in the LiSCN–H_2O system

Liquidus temperature (t/°C)	LiSCN (100 w_1/mass %)	LiSCN (m_1/mol kg^{-1})[a]	Solid phase[b]	Liquidus temperature (t/°C)	LiSCN (100 w_1/mass %)	LiSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
				−16.5	47.3	13.80	C
−7.5	10.19	1.745	A	−12.5	47.9	14.14	C
−17.9	18.00	3.376	A	−5.0	48.9	14.72	C
−25.0	21.34	4.172	A	0	50.0	15.38	C
−33.0	24.7	5.045	A	1	50.2	15.50	C+D
−62.5	33.0	7.575	A	3.0	50.3	15.56	D
−65.5	33.75	7.835	A	6.0	50.96	15.98	D
−92	38.2	9.506	A+B	12.0	51.68	16.45	D
−77	39.9	10.21	B	16.5	52.52	17.01	D
−68.5	40.9	10.64	B	24.5	54.1	18.13	D
−59.0	42.3	11.27	B	27.0	55.4	19.10	D
−56.0	43.0	11.60	B+C	28.0	55.5	19.18	D
−49.0	43.6	11.89	C	32.5	56.3	19.81	D
−42.0	44.4	12.28	C	40.3	60.5	23.56	D
−35.0	45.1	12.63	C	43.0	63.8	27.10	D
−28.0	45.8	13.00	C	43.3	64.3	27.70	D

[a] Calculated by compiler.
[b] A: Ice, H_2O [7732-18-5]; B: $LiSCN\cdot 5H_2O$ [ ]; C: $LiSCN\cdot 3H_2O$ [ ]; D: $LiSCN\cdot 2H_2O$ [84372-58-7].

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. The solubility was found by determining the temperature at which the solid phase disappeared. Each solution was first allowed to crystallize quickly by cooling it to low temperatures. Seeding with the proper hydrate was necessary because otherwise the entire system turned into a highly viscous or solid, glass-like substance which could not be crystallized. Very fine crystals were obtained. Temperature was then raised slowly. The rate of 1 °C per 15 min was sufficiently low to obtain reproducible values. Methods of analysis of the saturated solutions and of the solid phases were not reported.

Source and Purity of Materials:

LiSCN was prepared by reacting a LiOH solution with solid NH_4SCN. The solution was boiled until no ammonia could be detected. The solution was filtered and concentrated under vacuum. The salt obtained was recrystallized from water. The product was free from Fe, Ca, and sulfates. After drying over H_2SO_4, it contained 6.81% Li and 57.40% SCN. Calculated for the dihydrate: 6.87% Li, 57.47% SCN.

Estimated Error:

Temperature: ±0.25 and ±0.5 °C in the ranges of medium and very low temperatures, respectively (author).
Solubility: insufficient data reported to allow for error estimate.

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
G. C. Blytas, D. J. Kertesz, and F. Daniels, J. Am. Chem. Soc. **84**, 1083–5 (1962).

Variables:
T/K: 191–293

Prepared By:
J. Hála

Experimental Data

Composition of the saturated solutions in the LiSCN–NH_3 system[a]

Liquidus temperature (t/°C)	NH_3 (100 w_2/mass %)	Moles NH_3/mole LiSCN	LiSCN[b] (100 w_1/mass %)	LiSCN[b] (m_1/mol kg^{-1})
−75	96.55	106.8	3.45	0.5495
−82	79.75	15.04	20.25	3.905
−64	50.89	5.04	49.11	14.84
16	44.11	2.95	55.89	19.49
20	33.91	1.96	66.09	29.97

[a] Composition of the equilibrium solid phases not reported.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method[1] was used. The salt was quickly introduced into a glass tube, which was then sealed at one end, heated and evacuated for 24 h, and weighed. Then the volume of purified NH_3 necessary to give the desired salt concentration was distilled in, the tube was sealed off, and weighed again. Equilibrating and thermostating were carried out in different baths depending on the temperature range. Calibrated thermometers were used. Liquidus temperatures were recorded as those at which the last crystals disappeared with slow heating. This was preferred to observing temperatures of appearance of first crystals because of the tendency of the system to form supersaturated solutions on cooling. The solutions were viscous, and were difficult to work with. At higher LiSCN concentrations, the solutions were gel-like.

Source and Purity of Materials:

NH_3 used was stored over sodium metal.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] G. C. Blytas and F. Daniels, J. Am. Chem. Soc. **84**, 1075 (1926).

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) N,N-dimethylacetamide; C_4H_9NO; [127-19-5]

Original Measurements:
A. A. Fedorov, L. B. Sokolov, V. M. Savinov, M. A. Shlionskaya, and N. I. Filatova, Zh. Prikl. Khim. **44**, 2361–2 (1971).

Variables:
T/K: 295–298

Prepared By:
J. Hála

Experimental Data

The solubility of LiSCN in N,N-dimethylacetamide is reported to be $c_1 = 1.80$ mol dm^{-3} at 22–25 °C. The nature of the equilibrium solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:

The solvent was saturated with anhydrous salt. Then a part of the solvent was distilled off to remove water, and the saturated solution with excess solid was kept for 3 days in a dessicator in a paraffin-coated flask. The content of water in the saturated solution was $<0.1\%$. The saturated solution was analyzed for the content of sulfur by an unspecified method.

Source and Purity of Materials:

Anhydrous LiSCN was prepared according to Lee.[1] N,N-dimethylacetamide, source not specified, was freshly distilled before use.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] D. A. Lee, Inorg. Chem. **3**, 289 (1964).

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) N,N-dimethylacetamide; C_4H_9NO; [127-19-5]

Original Measurements:
N. A. Basanova, I. L. Krupatkin, and A. N. Basanov, *Fazovye Ravnovesiya* (Phase Equilibria) (Kalinin. Gosud. Univ., 1974), pp. 8–12.

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

The solubility of LiSCN in N,N-dimethylacetamide is reported to be $100\,x_1 = 28.4$ mol % at 25 °C (compiler: $m_1 = 4.55$ mol kg^{-1}). The nature of the equilibrium solid phase was not reported.

Additional information: Also reported was the phase diagram of the LiSCN–N,N-dimethylacetamide–n-decane system at 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:
No details reported.

Source and Purity of Materials:
Anhydrous LiSCN was prepared according to Lee.[1] Source and purity, in particular the content of water, of N,N-dimethylacetamide, was not reported.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] D. A. Lee, Inorg. Chem. **3**, 289 (1964).

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Tri-n-butyl(phosphate); $C_{12}H_{27}O_4P$; [126-73-8]

Original Measurements:
J. Hála and D. G. Tuck, Canad. J. Chem. **48**, 2843–6 (1970).

Variables:
T/K: 295

Prepared By:
J. Hála

Experimental Data

The solubility of LiSCN in tri-n-butyl(phosphate) is reported to be 12.0 g salt in 100 g solvent at 22 °C ($m_1 = 1.846$ mol kg^{-1}).

Additional information: Saturated solutions of LiSCN in the solvent were very viscous. The solvent/LiSCN mole ratio in the saturated solutions was found to be 2.03, indicating the existence of the disolvate, $LiSCN \cdot 2C_{12}H_{27}O_4P$.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. An excess of the salt was shaken overnight with 5 mL dry solvent. Preliminary experiments showed that this was sufficient for equilibrium to be reached. Samples of the saturated solutions were withdrawn through a sinter, diluted with acetone, and analyzed for the thiocyanate content by titration against $AgNO_3$ standard solution. Blank titrations showed that a small correction was required because of the presence of tri-n-butyl(phosphate).

Source and Purity of Materials:
LiSCN was prepared from lithium carbonate and a solution of thiocyanic acid. The latter was obtained by ion/exchange on a column of Dowex 50W-X8 resin in the H form. The solution of LiSCN was evaporated to dryness and then heated at 70–80 °C in a stream of dry nitrogen gas.[1] The final product contained approximately 85% LiSCN, the remainder of water could not be removed due to the decomposition of LiSCN above 80 °C. Tri-n-butyl(phosphate) (Fisher Scientific Co.) was purified by refluxing it with 0.5% caustic soda solution, followed by steam distillation. The product was dried first with anhydrous $MgSO_4$, and finally vacuum dried at 50 °C in a stream of dry nitrogen gas.[2]

Estimated Error:
Temperature: precision not reported.
Solubility: ±0.1 g salt/100 g solvent (authors).

References:
[1] J. E. Coates and E. J. Taylor, J. Chem. Soc. 1245 (1936).
[2] D. G. Tuck, J. Chem. Soc. 2783 (1958).

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Lithium chloride; LiCl; [7447-41-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
M. K. Khripun, A. Yu. Efimov, L. S. Lilis, and M. L. Kutuzova, Zh. Neorg. Khim. **31**, 2659–65 (1986).

Variables:
T/K: 298
m_2/mol kg^{-1}: 0–20.05

Prepared By:
J. Hála

Experimental Data

Solubility of LiSCN at 25 °C in aqueous solutions of LiCl

LiCl (m_2/mol kg^{-1})	LiCl (100 w_2/mass %)[a]	LiSCN (m_1/mol kg^{-1})	LiSCN (100 w_1/mass %)[a]	Solid phase[b]
0	0	19.70	56.16	A
1.58	2.95	18.50	53.00	A
3.65	6.80	17.25	49.27	A
4.26	8.03	16.45	47.53	A
6.50	12.03	15.60	44.30	A
7.00	13.02	15.10	43.09	A
8.80	16.20	14.30	40.38	A+B
8.80	16.25	14.20	40.21	A+B
8.70	16.09	14.20	40.28	A+B
8.60	15.93	14.20	40.36	A+B
8.55	16.13	13.60	39.36	A+B

[a] Calculated by compiler.
[b] A: LiSCN·$2H_2O$, [84372-58-7]; B: LiCl·H_2O, [16712-20-2].

Additional information: In addition to the data shown above, the authors reported also the compositions of 11 saturated solutions containing 10.40–20.05 mol kg^{-1} LiCl and 11.90–0 mol kg^{-1} LiSCN, where LiCl·H_2O was the equilibrium solid phase. These data are not shown here since they represent the solubility of LiCl in solutions of LiSCN.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Analysis of the solid and liquid phases was carried out by differential potentiometric titrations with standard $AgNO_3$ solution. The solid phases were also characterized by Schreinemakers' method.

Source and Purity of Materials:
No details reported.

Estimated Error:
Temperature: precision not reported.
Solubility: the error of the titrimetric method was reported as ±1.5%.

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Boric acid; H_3BO_3; [10043-35-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
V. G. Skvortsov, R. S. Tsekhanskii, Sh. V. Sadetdinov, and A. K. Molodkin, Zh. Neorg. Khim. **28**, 2677–9 (1983).

Variables:
T/K: 298
100 w_2/mass %: 0–5.6

Prepared By:
J. Hála

Experimental Data

Solubility of LiSCN at 25 °C in aqueous solutions of boric acid

H_3BO_3 (100 w_2/mass %)	H_3BO_3 (m_2/mol kg^{-1})[a]	LiSCN (100 w_1/mass %)	LiSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	52.94	17.30	A
1.97	0.701	52.58	17.79	A
1.96	0.697	52.55	17.77	A+B

[a] Calculated by compiler.
[b] A: LiSCN·$2H_2O$ [84372-58-7]; B: H_3BO_3 [10043-35-3].

Additional information: In addition to the data shown above, the authors also reported the compositions of six saturated solutions containing 1.98–5.6 mass % H_3BO_3 and 52.56–0 mass % LiSCN, where H_3BO_3 was the equilibrium solid phase. These data are not shown here since they represent the solubility of H_3BO_3 in solutions of LiSCN.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Solutions with excess solid were stirred for 20 h, which was sufficient for equilibrium to be reached. Borate and SCN$^-$ were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method. Solubility isotherms were also confirmed by refractometric measurements.

Source and Purity of Materials:
LiSCN and H_3BO_3 were chemically pure products, and were recrystallized before use.

Estimated Error:
Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Lithium borate; $LiBO_2$; [13453-69-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. G. Skvortsov, Sh. V. Sadetdinov, R. S. Tsekhanskii, and A. K. Molodkin, Zh. Neorg. Khim. **24**, 209–12 (1979).

Variables:

T/K: 298
100 w_2/mass %: 0–3.04

Prepared By:

J. Hála

Experimental Data

Solubility of LiSCN at 25 °C in aqueous solutions of lithium borate

$LiBO_2$ (100 w_2/mass %)	$LiBO_2$ (m_2/mol kg^{-1})[a]	LiSCN (100 w_1/mass %)	LiSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	52.94	17.30	A
1.07	0.461	52.24	17.21	A
1.08	0.465	52.20	17.18	A+B
1.05	0.452	52.23	17.19	B
1.10	0.417	45.89	13.13	B
1.27	0.411	36.60	9.060	B
1.38	0.394	28.18	6.153	B

[a] Calculated by compiler.
[b] A: $LiSCN \cdot 2H_2O$ [84372-58-7]; B: $(LiBO_2)_m \cdot (LiSCN)_n$, solid solutions of variable composition ($m > n$).

Additional information: In addition to the data shown above, the authors also reported the compositions of six saturated solutions containing 1.60–3.04 mass % $LiBO_2$ and 23.05–0 mass % LiSCN, where $LiBO_2 \cdot 8H_2O$ or $LiBO_2 \cdot 2H_2O$ were the equilibrium solid phases. These data are not shown here since they represent the solubility of $LiBO_2$ in solutions of LiSCN. Also reported were densities, viscosities, and refraction indexes of the saturated solutions.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibrium was reached within 24 h under constant shaking in a thermostat. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method and chemical analysis.

Source and Purity of Materials:

LiSCN and $LiBO_2$ were chemically pure products, and were recrystallized before use.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Lithium tetraborate; $Li_2B_4O_7$; [12007-60-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. G. Skvortsov, A. K. Molodkin, Sh. V. Sadetdinov, and R. S. Tsekhanskii, Zh. Neorg. Khim. **26**, 3164–6 (1981).

Variables:

T/K: 298
100 w_2/mass %: 0–2.42

Prepared By:

J. Hála

Experimental Data

Solubility of LiSCN at 25 °C in aqueous solutions of sodium tetraborate

$Li_2B_4O_7$ (100 w_2/mass %)	$Li_2B_4O_7$ (m_2/mol kg^{-1})[a]	LiSCN (100 w_1/mass %)	LiSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	52.94	17.30	A
0.35	0.0435	52.10	16.85	A+B

[a] Calculated by compiler.
[b] A: $LiSCN \cdot 2H_2O$ [84372-58-7]; B: $Li_2B_4O_7 \cdot 3H_2O$ [37195-62-3].

Additional information: In addition to the data shown above, the authors also reported the compositions of six saturated solutions containing 0.37–2.92 mass % $Li_2B_4O_7$ and 52.07–0 mass % LiSCN, where $Li_2B_4O_7 \cdot 3H_2O$ was the equilibrium solid phase. These data are not shown here since they represent the solubility of $Li_2B_4O_7$ in solutions of LiSCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibrium was reached within 20 h, which was checked by chemical analysis and refraction index of the saturated solutions. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method.

Source and Purity of Materials:

LiSCN and $Li_2B_4O_7$ were chemically pure products, and were recrystallized before use.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Lithium thiocyanate; LiSCN; [556-65-0]
(2) Urea; CH_4N_2O; [57-13-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
R. Turgunbekova, K. Nogoev, and K. Sulaimankulov, Zh. Neorg. Khim. **18**, 1119–22 (1973).

Variables:
T/K: 288, 303, and 318
100 w_2/mass %: 0–66.48 at 288 K, 0–72.50 at 303 K, 0–74.52 at 318 K

Prepared By:
J. Hála

Experimental Data

Composition of the saturated solutions in the LiSCN–urea–H_2O system at three temperatures

Temperature (t/°C)	Urea (100 w_2/mass %)	Urea (100 x_2/mol %)	LiSCN (100 w_1/mass %)	LiSCN (100 x_2/mol %)	Solid phase[a]
15	0	0	52.00	23.07	A
	3.32	1.64	51.51	23.32	A
	7.34	3.79	51.04	24.40	A
	9.88	5.26	50.86	25.03	A
	15.38	8.77	50.72	26.74	A
	20.19	12.43	50.41	29.25	A+B
	20.75	12.49	49.33	27.44	B
	23.32	13.59	44.55	23.99	B
	25.49	14.41	40.70	21.39	B
	29.09	16.49	36.99	19.38	B
	38.69	23.14	31.48	17.39	B
	49.41	31.33	25.04	14.67	B
	58.45	40.60	22.00	14.12	B
	65.92	50.78	20.63	14.68	B
	66.48	51.87	20.77	14.97	B+C
	66.49	51.97	20.86	15.06	C
	61.55	40.41	15.53	9.42	C
	59.92	37.21	13.49	7.74	C
	57.94	34.17	11.87	6.47	C
	56.06	31.28	6.69	4.99	C
	53.87	27.92	6.12	2.93	C
	49.00	22.38	0	0	C
30	0	0	56.70	26.60	A
	3.78	2.01	56.61	27.78	A
	7.09	3.92	56.53	28.89	A
	9.88	5.65	56.05	29.52	A
	10.01	5.80	57.02	30.49	A+D
	10.37	5.94	55.72	29.41	D
	13.79	8.06	54.24	29.35	D
	17.09	10.21	52.25	28.80	D
	25.65	17.06	51.00	31.25	D
	26.25	17.28	49.80	30.22	D+B
	24.88	15.95	49.44	29.21	B
	33.87	31.55	40.24	23.61	B
	46.23	31.15	31.94	19.84	B
	57.72	41.94	25.31	16.96	B
	64.09	49.54	22.57	16.09	B
	71.94	62.38	20.81	16.65	B
	72.50	61.07	18.86	14.66	C
	68.96	50.68	15.09	10.23	C
	68.12	46.92	12.13	7.77	C
	60.55	33.53	4.76	2.43	C
	57.50	28.87	0	0	C
45	20.47	13.43	55.26	33.46	D
	26.04	17.28	50.58	30.98	D
	28.96	19.61	48.96	30.57	D
	31.88	21.88	47.01	29.79	D
	31.81	21.98	47.47	30.28	B
	39.54	27.23	39.78	25.29	B
	46.22	32.03	33.70	21.55	B
	50.66	36.05	30.97	20.33	B
	56.10	41.54	27.96	19.10	B
	62.10	48.59	25.13	18.12	B
	65.10	52.42	23.74	17.63	B
	70.83	61.19	21.70	17.31	B
	74.52	67.65	20.44	17.10	B+C
	73.06	61.33	18.13	14.05	C
	69.84	50.74	13.59	9.11	C
	67.85	45.90	11.27	7.02	C
	66.39	42.19	8.72	5.11	C
	61.00	34.79	0	0	C

[a] A: $LiSCN\cdot 2H_2O$ [84372-58-7]; B: $LiSCN\cdot 2CO(NH_2)_2$ [41514-73-2]; C: $CO(NH_2)_2$ [57-13-6]; D: $LiSCN\cdot CO(NH_2)_2$ [41514-74-3].

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details reported.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:	**Original Measurements:**
(1) Lithium thiocyanate; LiSCN; [556-65-0] (2) Amines (3) Dichloromethane; CH_2Cl_2 ; [75-09-2]	G. Soula, Eur. Pat. Appl. 016673, 1979; Fr. Appl. 7905438.
Variables:	**Prepared By:**
T/K: unspecified ambient temperature c_2 /mol dm^{-3}: 0.1	J. Hála

Experimental Data

Solubility of LiSCN in 0.1 mol dm^{-3} solutions of two amines in dichloromethane[a]

Amine	LiSCN (mg dm^{-3})	LiSCN (c_1 /mol dm^{-3})[b]
2-(2-methoxyethoxy)-N,N-bis 2-(2-methoxyethoxy)ethyl ethanamine; (tris(dioxa-3,6-heptyl)amine); $C_{15}H_{33}NO_6$; [70384-51-9]	694	0.0106
2-methoxy-N,N-bis(methoxyethyl)ethanamine; (tris(oxa-3-butyl)amine); $C_9H_{21}NO_3$; [3235-51-6]	690	0.0106

[a] Solid phases were not investigated.

[b] Calculated by compiler.

Additional information: The solubility of LiSCN in neat CH_2Cl_2 was reported to be less than 1 mg dm^{-3}. The solubilization effect of tris(dioxa-3,6-heptyl)amine was explained by the author by the formation of a 1:1 adduct of LiSCN with the amine in the saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The salt, 0.001 mole, was equilibrated by stirring with 0.001 mole of the amine in 10 mL CH_2Cl_2 for 10 min. The content of the salt in the saturated solution was determined by flame photometry.

Source and Purity of Materials:

No details reported for LiSCN. Tris(dioxa-3,6-heptyl)amine was prepared by refluxing sodium methoxy-2-ethanolate in methoxy-2-ethanol for 12 h at 125 °C. The excess solvent was then distilled off, excess sodium methoxy-2-ethanolate decomposed with concentrated HCl, and the amine distilled at 165–180 °C at 0.5 mm Hg pressure. Tris(oxa-3-butyl)amine was obtained by a similar procedure using sodium methanolate, and methanol as the solvent. After treatment of the mixture with HCl, the amine was extracted into CH_2Cl_2 and distilled. Dichloromethane was dehydrated and purified from stabilizers.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

6.2. Sodium Thiocyanate

6.2.1. Evaluation of the NaSCN–H_2O System

Components:	**Evaluator:**
(1) Sodium thiocyanate; NaSCN; [540-72-7] (2) Water; H_2O; [7732-18-5]	J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, June 2001.

Critical Evaluation

The solubility of NaSCN in water as a function of temperature has been reported in Hughes and Mead,[1] Zhuravlev and Bychkova,[2] and Titova and Batura.[3] Partington[4] reported a single value at 298 K, and further data could be extracted from the studies of various ternary systems NaSCN–salt–H_2O.[5–13] All available data have been summarized in the following table and Fig. 9.

The solubility curve has two branches. Below 303 K, the equilibrium solid phase is the dihydrate,[2,5,7,12,13] NaSCN·2H_2O while above 303 K it is the anhydrous salt.[2,5,7] The dihydrate was confirmed as the solid phase by the method of wet residues and careful chemical analysis,[2] and it seems that the conclusions about NaSCN·H_2O (Hughes and Mead[1]) or anhydrous NaSCN (refer to four studies[8–11]) as the solid phases below 303 K were in error. The transition point from NaSCN·2H_2O to NaSCN has been reported to be at 30.3–30.5 °C (303.5–303.7 K)[1] or at 27.7 °C (300.9 K).[2] The transition point temperature of about 30 °C can also be estimated from the phase diagram of the NaSCN–H_2O system, reported by Darrin.[16] From this diagram, the ice–NaSCN·2H_2O eutectic point was estimated by the evaluator to appear at approximately −36 °C and 38.5 mass % NaSCN.

Summary of the solubility of NaSCN in water as a function of temperature

Temperature (t/°C)	Temperature (K)	NaSCN (m_1 /mol kg^{-1})	Ref.	Temperature (t/°C)	Temperature (K)	NaSCN (m_1 /mol kg^{-1})	Ref.
0	273.2	11.52	2	29.2	302.4	20.66	1
5.0	278.2	12.84	2	30.0	303.2	36.53	14
10.0	283.2	13.36	5	33.0	306.2	21.46	2
10.7	283.9	13.90	1			21.50	3
15.5	288.7	15.70	2	33.8	307.0	21.27	1
17.3	290.5	15.73	1	40.0	313.2	21.00	7
20.0	293.2	17.39	6			52.58	14
		20.43	14	40.5	313.7	21.59	3
21.3	294.5	17.18	1	46.1	319.3	21.96	1
24.0	297.2	18.12	2	50.0	323.2	22.41	2
25.0	298.2	15.21	4	53.0	326.2	22.71	2
		18.50	2			22.21	3
		17.39	7	65.0	338.2	23.45	3
		15.83	8	65.8	339.0	23.37	1
		17.58	9–11	73.8	347.0	24.20	1
		17.38	12	74.7	347.9	24.04	3
		17.89	5	81.8	355.0	24.92	1
		17.58	13	85.2	358.4	25.44	3

The graphical comparison of the solubility data (numbers in the graph refer to the corresponding references) shows a reasonable agreement between the polythermal[1] and analytical[2] methods below 303 K, and among three sets of data above 303 K.[1–3] The data below 303 K from Refs. 1 and 2, together with those from the studies of ternary systems,[5–7,9–13] have been computer smoothed by a linear regression of the data to a fifth order polynomial to obtain the solubility of NaSCN in water over the temperature range of 273–303 K as

$$m_1\ (\text{mol kg}^{-1}) = 0.1546\,99\times10^{6} - 0.129\,110\times10^{4}T - 0.784\,735\,T^{2} + 0.3677\,02\times10^{-1}\,T^{3} - 0.123\,204\times10^{-3}\,T^{4} + 0.126\,926\times10^{-6}\,T^{5}.$$

The solubility data of Partington and Sopher,[4] and Gode and Klyavina[8] at 298 K are obviously too low and were not considered for the smoothing procedure. Likewise, not considered was the solubility at 293.2 K reported in Lavrova *et al.*[14] It is too high, and obviously corresponds to the solubility of anhydrous NaSCN, which is metastable at this temperature.

Similarly, the data from Hughes and Mead,[1] Zhuravlev and Bychkova,[2] Titova and Batura,[3] and Golyand and Ludkovskaya[7] have been smoothed to obtain the solubility of NaSCN as a function of temperature in the range of 305–349 K as

$$m_1\ (\mathrm{mol\ kg^{-1}}) = -0.103\ 444\times10^{7} + 0.157\ 545\times10^{5}\ T - 0.958\ 919\times10^{2}\ T^2 + 0.291\ 578\ T^3 - 0.442\ 914\times10^{-3}\ T^4 + 0.268\ 887\times10^{-6}\ T^5.$$

The data of Lavrova *et al.*[14] are obviously unrealistically high, and were not included for the smoothing procedure. There is not straightforward explanation for these two measurements. The two equations can be suggested as yielding tentative solubility values in the respective temperature ranges.

It is noteworthy that solutions of NaSCN saturated at about 60 °C and cooled to room temperature show a very high tendency toward supersaturation.[15] The data reported by Bump[15] are shown in Fig. 9.

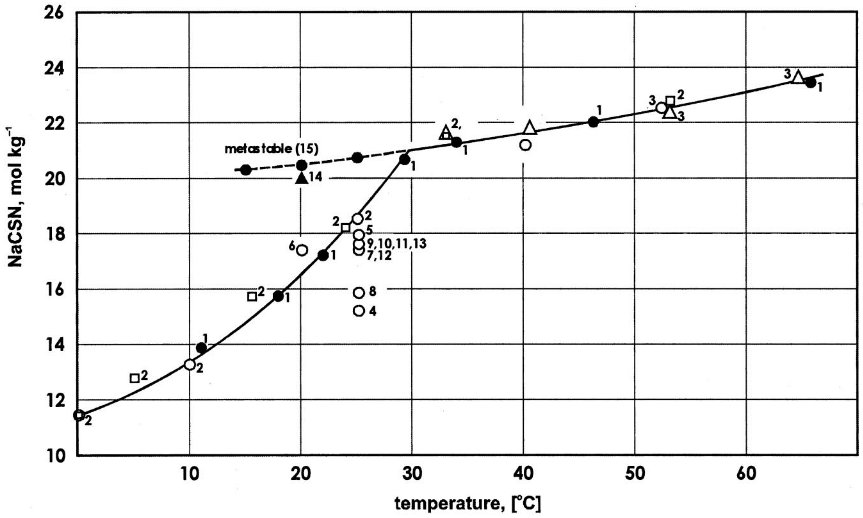

FIG. 9. Solubility of NaSCN in water as a function of temperature.

References:

[1] O. L. Hughes and T. H. Mead, J. Chem. Soc. 2282 (1929).

[2] E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367 (1959).

[3] V. A. Titova and Z. E. Batura, Zh. Neorg. Khim. **10**, 1711 (1965).

[4] J. R. Partington and W. E. Soper, Philos. Mag. **7**, 209 (1929).

[5] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

[6] E. Spacamella Marchetti, Atti. Acad. Sci. Torino, Clase. Fis. Mat. Nat. **94**, 353 (1960).

[7] S. M. Golyand and B. G. Ludkovskaya, Zh. Neorg. Khim. **11**, 1433 (1966).

[8] G. K. Gode and L. A. Klyavina, Zh. Neorg. Khim. **15**, 1147 (1970).

[9] V. G. Skvortsov, R. S. Tsekhanskii, Sh. V. Sadetdinov, and A. K. Molodkin, Zh. Neorg. Khim. **28**, 2677 (1983).

[10] V. G. Skvortsov, Sh. V. Sadetdinov, R. S. Tsekhanskii, and A. K. Molodkin, Zh. Neorg. Khim. **24**, 209 (1979).

[11] V. G. Skvortsov, A. K. Molodkin, Sh. V. Sadetdinov, R. S. Tsekhanskii, and V. M. Fedorov, Zh. Neorg. Khim. **26**, 3164 (1981).

[12] Z. G. Karov, I. N. Lepeshkov, and E. I. Kukulieva, Zh. Neorg. Khim. **17**, 509 (1972).

[13] A. K. Mc Kerrow, V. J. Occleshaw, and F. Drabble, J. Chem. Soc. 1 (1946).

[14] O. A. Lavrova, N. N. Mokosina, and O. S. Karchmarchik, Zh. Neorg. Khim. **29**, 1312 (1984).

[15] C. K. Bump, J. Phys. Chem. **36**, 1851 (1932).

[16] M. Darrin, U.S. Patent 1,570 047 (1925).

Components:	**Original Measurements:**
(1) Sodium thiocyanate; NaSCN; [540-72-7] (2) Water; H_2O; [7732-18-5]	O. L. Hughes and T. H. Mead, J. Chem. Soc. 2282–4 (1929).

Variables:	**Prepared By:**
T/K: 283–374	J. Hála

Experimental Data

Solubility of NaSCN in water as a function of temperature[a]

Temperature (t/°C)	NaSCN (g/100 g H_2O)	NaSCN (100 w_1/mass %)[b]	NaSCN (m_1/mol kg^{-1})[b]
10.7	112.7	52.99	13.90
17.3	127.5	56.04	15.73
21.3	139.3	58.21	17.18
29.2	167.5	62.62	20.66
33.8	172.4	62.30	21.27
46.1	178.0	64.03	21.96
65.8	189.5	65.46	23.37
73.8	196.2	66.24	24.20
81.8	202.0	66.89	24.92
101.4	225.6	69.29	27.83

[a] The equilibrium solid phases were reported to be NaSCN·H_2O and NaSCN at temperatures below and above 30.3–30.5 °C.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Polythermal method used. Solid NaSCN was heated with water in a sealed tube until one or two small crystals remained. Two temperatures were then recorded, one at which the sharpness of the crystal edges indicated that they were growing, and the other where the roundness of the crystals showed they were dissolving. Since these temperatures never differed by more than 0.5 °C, their mean was taken as the temperature of saturation. Owing to the deliquescence of NaSCN, the salt was introduced into the weighed tubes in an oven at 130 °C. The tube was allowed to cool in a dessicator, weighed with a rubber cap, the solvent quickly introduced, the tube sealed and weighed again. The thermometer, graduated in 0.2 °C, was standardized at the melting point of ice, temperature of the $Na_2SO_4\cdot10H_2O/Na_2SO_4$ transition, and the boiling point of water. The composition of the hydrated salt was determined by chemical analysis: calculated/found for the monohydrate, 20.4/20.0 and 20.6% H_2O.

Source and Purity of Materials:

NaSCN was prepared by heating A.R. NH_4SCN with equimolar amount of caustic soda in aqueous solution until no more ammonia was evolved. The solution was evaporated, and NaSCN recrystallized from alcohol, acetone, and again from alcohol. Conductivity grade water was used.

Estimated Error:

Temperature: ±0.5 K (compiler).

Solubility: insufficient data given to allow for error estimate.

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Solvents

Original Measurements:
J. R. Partington and W. E. Soper, Philos. Mag. **7**, 209–47 (1929).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data
Solubility of NaSCN in water and ethanol at 25 °C[a]

Solvent	NaSCN	NaSCN (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	14.6649 g salt in 11.8907 g solvent	15.21
Ethanol; C_2H_6O; [64-17-5]	2.6832 g salt in 12.7292 g solvent	2.60

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details reported.

Source and Purity of Materials:
NaSCN, analytical grade, source not specified, was recrystallized before use. Absolute ethanol was prepared from a 96% product in the following way. It was first kept over freshly burnt lime for some days with periodical shaking. It was then fractionated, the first and last runnings being rejected. It was then allowed to stand over freshly cleaned and turned metallic calcium, and was refractionated, the first and last runnings being again rejected. The product was free from aldehyde, and was stored in a vessel with a siphon attachment and a guard tube with P_2O_5.

Estimated Error:
Temperature: precision not reported.
Solubility: only one solubility measurement reported for each solvent.

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).

Variables:
T/K: 273–326

Prepared By:
J. Hála

Experimental Data
Solubility of NaSCN in water as a function of temperature

Temperature (t/°C)	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	48.3	11.52	A
5.0	51.0	12.84	A
15.5	56.0	15.70	A
24.0	59.5	18.12	A
33.0	63.5	21.46	B
53.0	64.8	22.71	B

[a] Calculated by compiler.
[b] A: $NaSCN \cdot 2H_2O$ [17032-40-5]; B: NaSCN [540-72-7].

Additional information: The point of transition from $NaSCN \cdot 2H_2O$ to NaSCN was reported to be at 27.7 °C.

Auxiliary Information

Method/Apparatus/Procedure:
The solubilities were obtained by graphical analytical method.[1,2] A series of mixtures of the salt and water covering the fields of unsaturated and saturated solutions were prepared by weighing. After equilibrium had been attained, refractive indexes of the solutions were measured. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The composition of $NaSCN \cdot 2H_2O$ as the solid phase was confirmed gravimetrically by drying the solid product, which was obtained by cooling the peritectic solutions. Calculated/found (mass %) for the dihydrate: 30.76/32.49.

Source and Purity of Materials:
NaSCN, source not specified, was recrystallized as dihydrate and then dehydrated at 120–130 °C to obtain the anhydrous salt.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:
[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
V. A. Titova and Z. E. Batura, Zh. Neorg. Khim. **10**, 1711–2 (1965).

Variables:
T/K: 306–425

Prepared By:
J. Hála

Experimental Data

Solubility of NaSCN in water as a function of temperature[a]

Temperature (t/°C)	NaSCN (g/100 g H_2O)	NaSCN (100 w_1/mass %)[b]	NaSCN (m_1/mol kg^{-1})[b]
33.0	174.3	63.54	21.50
40.5	175.0	63.64	21.59
53.0	180.0	64.29	22.21
65.0	190.1	65.53	23.45
74.7	194.9	66.09	24.04
85.2	206.3	67.35	25.44
99.3	226.1	69.34	27.90
122.1	252.9	71.66	31.19
139.9	282.2	73.83	34.82
152.0	301.1	75.07	37.14

[a] Solid phases were not investigated.
[b] Calculated by complier.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Samples of the saturated solutions were withdrawn by means of special filtration equipment. Care was taken to avoid condensation of water vapor in the filtration apparatus from the saturated solutions. The solutions were analyzed for the SCN^- content by potentiometric titration with $AgNO_3$ solution.

Source and Purity of Materials:

NaSCN, chemically pure grade, was recrystallized from water. Distilled water was used.

Estimated Error:
Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Sodium thiocyanate: NaSCN; [540-72-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
O. A. Lavrova, N. N. Mokosina, and O. S. Karchmarchik, Zh. Neorg. Khim. **29**, 1312–6 (1984).

Variables:
T/K: 293–313

Prepared By:
J. Hála

Experimental Data

Solubility of NaSCN in water at three temperatures[a]

Temperature (t/°C)	NaSCN (100 w_1/mass %)	NaSCN (100 x_1/mol %)	NaSCN (m_1/mol kg^{-1})[b]
20	62.4	26.9	20.43
30	77.0	42.6	36.53
40	81.0	48.6	52.58

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method[1] was used. Excess solid was stirred with water in a thermostated vessel until equilibrium was reached. The content of NaSCN in the saturated solutions was determined by titration against a standard $AgNO_3$ solution.

Source and Purity of Materials:

Nothing specified.

Estimated Error:
Temperature: ±0.05 K (authors).
Solubility: ±0.2–0.5 mol % (authors).

References:

[1] T. M. Lesteva and V. I. Chernaya, Zh. Neorg. Khim. **23**, 2556 (1978).

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Sulfur dioxide; SO_2; [7446-09-5]

Original Measurements:
G. Jander and W. Ruppolt, Z. Phys. Chem. **179**, 43–50 (1937).

Variables:
T/K: 273

Prepared By:
J. Hála

Experimental Data

The solubility of NaSCN in liquid sulfur dioxide was reported to be 0.652 g salt in 100 g solvent at 0 °C. From this value the compiler calculated m_1/mol kg^{-1}=0.0804.

Additional information: A bright-yellow equilibrium solid phase, NaSCN$\cdot 2SO_2$, was reported in Foote and Fleischer.[2]

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. About 10 g SO_2, carefully dried, was equilibrated with excess NaSCN at 0 °C in water–ice bath in a three-compartment glass vessel in which equilibrating and sampling compartments were separated by a compartment containing a glass/wool filter. Equilibration was performed for unspecified, prolonged period of time under frequent shaking. After equilibrium had been attained, the vessel was turned upside down, and the saturated solution was filtered into the empty sampling compartment, which was subsequently cooled and sealed off. After weighing the compartment with the sample, SO_2 was allowed to evaporate, the residue was weighed, dissolved in water, and the content of the salt was determined. Method of analysis was not specified.

Source and Purity of Materials:

NaSCN, source not specified, was carefully dried before use. Commercially available SO_2 was purified by passing it through concentrated H_2SO_4 and over asbestos wool, and dried by using P_2O_5. Specific conductivity of the product was 4.5×10^{-7} Ω^{-1} (Jander and Wickert[1]).

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] G. Jander and K. Wickert, Z. Phys. Chem. **178**, 57 (1936).
[2] H. W. Foote and J. Fleischer, J. Am. Chem. Soc. **54**, 3903 (1932).

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
H. Hunt, J. Am. Chem. Soc. **54**, 3509–12 (1932).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

The solubility of NaSCN was reported to be 205.50 g in 100 g solvent at 25 °C, or, using the density of liquid ammonia of 0.604 g cm^{-3} at 25 °C, 124.12 g NaSCN in 100 cm^3 solvent. Compiler calculated m_1=25.35 mol kg^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Ammonia (10–25 g) was equilibrated with the salt in the bottom part of a sealed, two/compartment Pyrex tube. The compartments were separated from each other with a narrow neck. The salt was introduced into the tube before sealing it off in a small cup closed with a very closely woven cotton cloth. The latter permitted the salt to dissolve the salt holding back the solid at the same time. The system was equilibrated for 1–3 weeks with occasional shaking. Then the tube was inverted in the bath and all the solution drained into the empty compartment, which was cooled and sealed off. When it reached room temperature it was dried and weighed, the ammonia allowed to boil off, the tube with the salt warmed until all odor of NH_3 was gone, and the salt was weighed.

Source and Purity of Materials:

NaSCN, Baker C. P. product, was recrystallized and carefully dried. Commercially available anhydrous NH_3 was allowed to stand over metallic sodium for several weeks before use.

Estimated Error:

Temperature: ±0.025 K (author).
Solubility: 5% (author).

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
G. C. Blytas and F. Daniels, J. Am. Chem. Soc. **84**, 1075–83 (1962).

Variables:
T/K: 192–578

Prepared By:
J. Hála

Experimental Data

Compositions at eutectic points and the phase diagram of the NaSCN–NH_3 system (see Fig. 10)

Temperature (t/°C)	NH_3 (100 w_2/mass %)	NaSCN (100 w_1/mass %)[b]	NaSCN (m_1/mol kg^{-1})[a]
−18.5	36	64	21.93
−81	73.5	26.5	4.447

[a] Calculated by compiler.

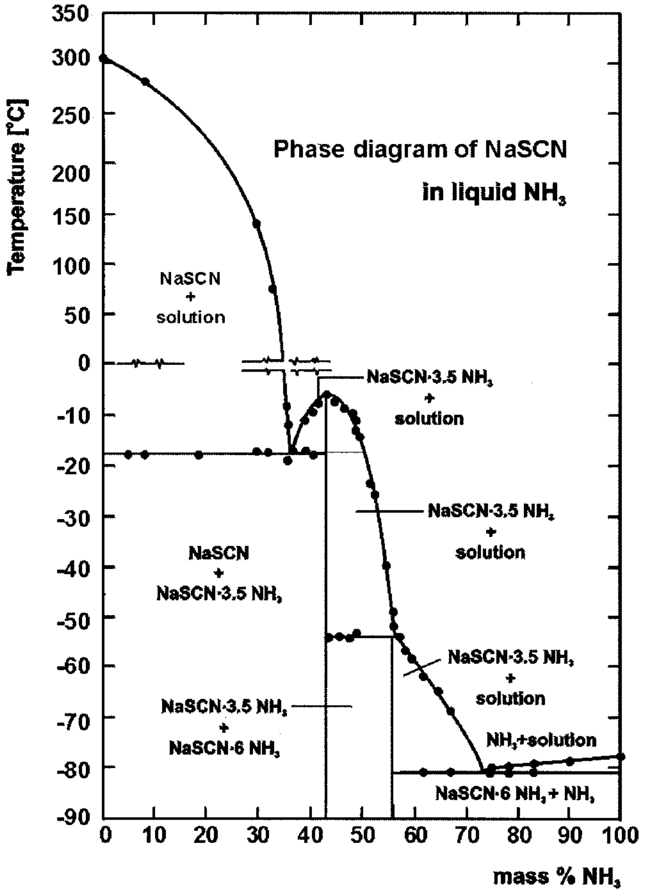

FIG. 10. Phase diagram of the NaSCN–NH_3 system.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method[1] was used. The salt was quickly introduced into a glass tube, which was then sealed at one end, heated and evacuated for 24 h, and weighed. Then the volume of purified NH_3 necessary to give the desired salt concentration was distilled in, the tube was sealed off, and weighed again. Equilibrating and thermostating were carried out in different baths depending on the temperature range. Calibrated thermometers were used. Liquidus temperatures were recorded as those at which the last crystals disappeared with slow heating. This was preferred to observing temperatures of appearance of first crystals because of the tendency of the system to form supersaturated solutions on cooling.

Source and Purity of Materials:

NaSCN, chemically pure, was heated and evacuated, pulverized, reheated, and re-evacuated. NH_3 used was stored over sodium metal.

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.01 mass % (authors).

References:

[1] G. C. Blytas and F. Daniels, J. Am. Chem. Soc. **84**, 1075 (1962).

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
O. L. Hughes and T. H. Mead, J. Chem. Soc. 2282–4 (1929).

Variables:
T/K: 289–325

Prepared By:
J. Hála

Experimental Data

Solubility of NaSCN in methanol as a function of temperature[a]

Temperature (t/°C)	NaSCN (g/100 g CH_4O)	NaSCN (100 w_1/mass %)[b]	NaSCN (m_1/mol kg^{-1})[b]
15.8	35.00	25.93	4.317
24.7	40.04	28.59	4.939
34.6	45.14	31.10	5.568
48.0	50.98	33.77	6.288
48.9	51.50	33.99	6.352
52.3	53.54	34.87	6.604

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. Solid NaSCN was heated with methanol in a sealed tube until one or two small crystals remained. Two temperatures were then recorded, one at which the sharpness of the crystal edges indicated that they were growing, and the other where the roundness of the crystals showed they were dissolving. Since these temperatures never differed by more than 0.5 °C, their mean was taken as the temperature of saturation. Owing to the deliquescence of NaSCN, the salt was introduced into the weighed tubes in an oven at 130 °C. The tube was allowed to cool in a dessicator, weighed with a rubber cap, the solvent quickly introduced, the tube sealed and weighed again. The thermometer, graduated in 0.2 °C, was standardized at the melting point of ice, temperature of the $Na_2SO_4 \cdot 10H_2O/Na_2SO_4$ transition, and the boiling point of water.

Source and Purity of Materials:

NaSCN was prepared by heating A.R. NH_4SCN with equimolar amount of caustic soda in aqueous solution until no more ammonia was evolved. The solution was evaporated, and NaSCN recrystallized from alcohol, acetone, and again from alcohol. Conductivity grade methanol was prepared according to Hartley and Raikes[1] and Woolcock and Hartley.[2]

Estimated Error:
Temperature: ±0.5 K (compiler).
Solubility: insufficient data given to allow for error estimate.

References:

[1] H. Hartley and H. R. Raikes, J. Chem. Soc. **127**, 524 (1925).
[2] J. W. Woolcock and H. Hartley, Philos. Mag. **5**, 1133 (1928).

6.2.2. Evaluation of the NaSCN–Ethanol System

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Ethanol; C_2H_6O; [64-17-5]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, June 2001.

Critical Evaluation

Available solubility data for NaSCN in ethanol are the isothermally obtained values of Partington and co-workers[1–3] at 298 K, and the polythermal data of Hughes and Mead.[4] The solubility at 298 K reported originally by Partington, i.e., 2.59 (King and Partington[1]) and 2.60 (Partington and Soper[2]) mol kg^{-1}, were later refined by the authors[3] to obtain $m_1 = 2.548$ mol kg^{-1}. The authors explained this difference by more thorough drying of the materials used in Partington and Winterton.[3] A value of 2.29 mol kg^{-1} can be obtained for the solubility of NaSCN in ethanol at 298 K by interpolation of the data of Hughes and Mead.[4] Partington and Winterton[3] analyzed the reasons for this discrepancy and came to the conclusion that the solutions of Hughes and Mead[4] were probably not saturated. They repeated the polythermal measurements, and their results were, however, inconsistent, and always lower than those obtained by isothermal measurements.

Recommended value for the solubility of NaSCN in ethanol at 298 K: 2.548 mol kg^{-1} or 17.12 mass %.

References:

[1] F. E. King and J. R. Partington, Trans. Faraday Soc. **23**, 522 (1927).
[2] J. R. Partington and W. E. Soper, Philos. Mag. **7**, 209 (1929).
[3] J. R. Partington and R. J. Winterton, Trans. Faraday Soc. **30**, 1104 (1934).
[4] O. L. Hughes and T. H. Mead, J. Chem. Soc. 2282 (1929).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:

O. L. Hughes and T. H. Mead, J. Chem. Soc. 2282–4 (1929).

Variables:

T/K: 292–344

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN in ethanol as a function of temperature[a]

Temperature (t/°C)	NaSCN (g/100 g C_2H_6O)	NaSCN (100 w_1/mass %)[b]	NaSCN (m_1/mol kg^{-1})[b]
18.8	18.37	15.52	2.266
35.8	19.05	16.00	2.350
39.6	19.34	16.21	2.386
52.8	21.05	17.39	2.596
59.6	22.20	18.17	2.738
61.8	22.60	18.43	2.788
70.9	24.43	19.63	3.013

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. Solid NaSCN was heated with ethanol in a sealed tube until one or two small crystals remained. Two temperatures were then recorded, one at which the sharpness of the crystal edges indicated that they were growing, and the other where the roundness of the crystals showed they were dissolving. Since these temperatures never differed by more than 0.5 °C, their mean was taken as the temperature of saturation. Owing to the deliquescence of NaSCN, the salt was introduced into the weighed tubes in an oven at 130 °C. The tube was allowed to cool in a dessicator, weighed with a rubber cap, the solvent quickly introduced, the tube sealed and weighed again. The thermometer, graduated in 0.2 °C, was standardized at the melting point of ice, temperature of the $Na_2SO_4 \cdot 10H_2O/Na_2SO_4$ transition, and the boiling point of water.

Source and Purity of Materials:

NaSCN was prepared by heating A.R. NH_4SCN with equimolar amount of caustic soda in aqueous solution until no more ammonia was evolved. The solution was evaporated, and NaSCN recrystallized from alcohol, acetone, and again from alcohol. Conductivity grade ethanol was prepared according to Hartley and Raikes[1] and Woolcock and Hartley.[2]

Estimated Error:

Temperature: ±0.5 K (compiler).
Solubility: insufficient data given to allow for error estimate.

References:

[1] H. Hartley and H. R. Raikes, J. Chem. Soc. **127**, 524 (1925).
[2] J. W. Woolcock and H. Hartley, Philos. Mag. **5**, 1133 (1928).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Alcohols

Original Measurements:

A: F. E. King and J. R. Partington, Trans. Faraday Soc. **23**, 522–31 (1927).
B: J. R. Partington and R. J. Winterton, Trans. Faraday Soc. **30**, 1104–5 (1934).
C: J. R. Partington and R. J. Winterton, Trans. Faraday Soc. **30**, 619–26 (1934).

Variables:

T/K: 298

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN in two alcohols at 25 °C[a]

Alcohol	NaSCN (g salt/100 g solvent)	NaSCN (m_1/mol kg^{-1})[b]	d^c (g cm^{-3})
Ethanol; C_2H_6O; [64-17-5] (source A)	20.99	2.589	0.882 502
Ethanol; C_2H_6O; [64-17-5] (source B)	20.66	2.548	
2-propen-1-ol (allylalcohol); C_3H_6O; [107-18-6] (source C)	12.40	1.530	0.904 65

[a] Solid phases were not investigated.
[b] Calculated by compiler.
[c] Density of the saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method[1] was used. The salt was equilibrated with the solvent in an atmosphere of hydrogen gas, first in an air thermostat at 25±0.05 °C until equilibrium was reached, and then left for 12 h in water thermostat at 25±0.015 °C. Samples of the saturated solutions were taken into an evaporating bottle, which was made to fit the equilibrium vessel through a ground joint. Analysis was carried out both by direct evaporation of the solution, and gravimetrically as AgCN.

Source and Purity of Materials:

NaSCN was prepared by decomposition of pure NH_4SCN with caustic soda, which, in turn, was prepared from sodium metal. NaSCN was recrystallized from distilled water and 96% ethanol, and dried at 120 °C over P_2O_5. Analysis of the product as AgSCN yielded the theoretical percentage of SCN, i.e., 71.64%. Ethanol was prepared from a 96% product. The latter was refluxed for 6 h over freshly burnt CaO, distilled, and again refluxed with CaO. It was then distilled onto 5 g dried $AgNO_3$, refluxed, and redistilled, again refluxed with Ca turnings and distilled. The product (density of 0.7851 g cm^{-3} at 25 °C) was stored in a bottle with a guard tube with P_2O_5. Allylalcohol (Kahlbaum) was fractionated through a 5 ft column. The fraction boiling at 96 °C was allowed to stand over $CuSO_4$ for 24 h and again fractionated. The final product boiled at 97.1 °C at 760 mm Hg pressure (density of 0.84572 g cm^{-3}) was stored in the dark with hydrogen above it in order to avoid the formation of aldehyde.

Estimated Error:

Temperature: ±0.015 K (authors).
Solubility: insufficient data reported to allow for error estimate.

References:

[1] F. S. Hawkins and J. R. Partington, Trans. Faraday Soc. **24**, 518 (1928).

6.2.3. Evaluation of the NaSCN–Acetone System

Components:	**Evaluator:**
(1) Sodium thiocyanate; NaSCN; [540-72-7] (2) 2-propanone (acetone); C_3H_6O; [67-64-1]	J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, June 2001.

Critical Evaluation

The solubility of NaSCN in acetone as a function of temperature has been reported in two documents.[1,2] Although the polythermal data[1] suffer from a temperature error of ±0.25 K, Fig. 11 shows a fairly good agreement between isothermal[2] and polythermal[1] results. The two sets of data have been computer smoothed by a linear regression to a second order polynomial. The equation for the temperature dependence of NaSCN solubility in acetone was obtained as

$$m_1\,/\text{mol kg}^{-1} = 49.157 - 0.355\,07\,(T/\text{K}) + 0.000\,649\,(T/\text{K})^2,$$

with standard deviations of the constants of 2.285, 0.0149, and 0.000 024, respectively. The equation can be suggested as yielding tentative data for the solubility of NaSCN in acetone over the temperature range of 280–340 K.

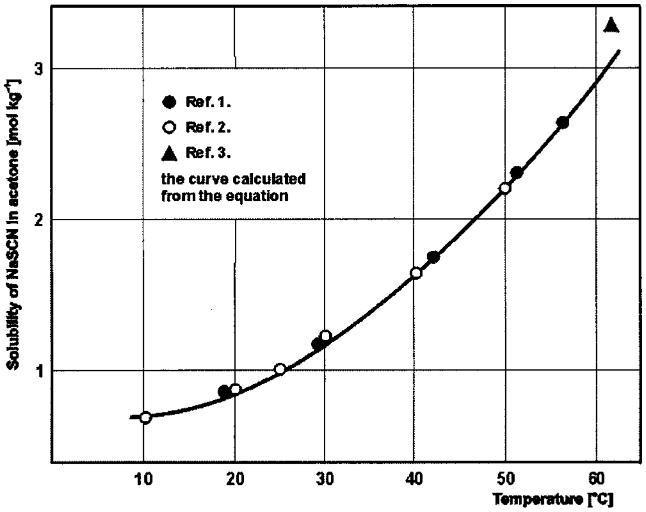

FIG. 11. Solubility of NaSCN in acetone as a function of temperature.

The single value of Dernini *et al.*[3] for the solubility of NaSCN at the boiling point of the saturated solution is also shown in the graph. Since the boiling point temperature was not reported by the authors this solubility value was not considered for the computer smoothing procedure.

There appears to be a disagreement as for the composition of the equilibrium solid phase. While Krumgalz *et al.*[2] reported the solid phase to be the anhydrous salt, Hughes and Mead[1] isolated the $NaSCN\cdot OC(CH_3)_2$ adduct from the saturated solution.

References:

[1] O. L. Hughes and T. H. Mead, J. Chem. Soc. 2282 (1929).
[2] B. S. Krumgalz, V. A. Smirnova, and Yu. I. Gerzhberg, Zh. Neorg. Khim. **17**, 1778 (1972).
[3] S. Dernini, R. DeSantis, and L. Marrelli, J. Chem. Eng. Data **21**, 170 (1976).

Components:	**Original Measurements:**
(1) Sodium thiocyanate; NaSCN; [540-72-7] (2) 2-Propanone (acetone); C_3H_6O; [67-64-1]	O. L. Hughes and T. H. Mead, J. Chem. Soc. 2282–4 (1929).
Variables: T/K: 292–329	**Prepared By:** J. Hála

Experimental Data

Solubility of NaSCN in acetone as a function of temperature[a]

Temperature (t/°C)	NaSCN (g/100 g C_3H_6O)	NaSCN (100 w_1/mass %)[b]	NaSCN (m_1/mol kg^{-1})[b]
18.8	6.85	6.41	0.8450
29.2	9.50	8.68	1.172
41.9	14.08	12.34	1.737
51.0	18.61	15.69	2.296
56.0	21.40	17.63	2.640

[a] The equilibrium solid phase was $NaSCN\cdot OC(CH_3)_2$ [ ] at all temperatures.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. Solid NaSCN was heated with acetone in a sealed tube until one or two small crystals remained. Two temperatures were then recorded, one at which the sharpness of the crystal edges indicated that they were growing, and the other where the roundness of the crystals showed they were dissolving. Since these temperatures never differed by more than 0.5 °C, their mean was taken as the temperature of saturation. Owing to the deliquescence of NaSCN, the salt was introduced into the weighed tubes in an oven at 130 °C. The tube was allowed to cool in a dessicator, weighed with a rubber cap, the solvent quickly introduced, the tube sealed and weighed again. The thermometer, graduated in 0.2 °C, was standardized at the melting point of ice, temperature of the $Na_2SO_4\cdot 10H_2O/Na_2SO_4$ transition, and the boiling point of water. The solid phases obtained from the saturated solutions were kept in a desiccator over anhydrous NaSCN for 1 day to remove any excess of acetone. Analysis found 45.3–45.8 mass % acetone; calculated for $NaSCN\cdot OC(CH_3)_2$, 45.0 mass %.

Source and Purity of Materials:

NaSCN was prepared by heating A.R. NH_4SCN with equimolar amount of caustic soda in aqueous solution until no more ammonia was evolved. The solution was evaporated, and NaSCN recrystallized from alcohol, acetone, and again from alcohol. Acetone (Poulenc) was dried over anhydrous K_2CO_3, fractionated twice, and distilled in a current of dry air.

Estimated Error:

Temperature: ±0.5 K (compiler).
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) 2-Propanone (acetone); C_3H_6O; [67-64-1]

Original Measurements:
B. S. Krumgalz, V. A. Smirnova, and Yu. I. Gerzhberg, Zh. Neorg. Khim. **17**, 1778–80 (1972).

Variables:
T/K: 283–323

Prepared By:
J. Hála

Experimental Data

Solubility of NaSCN in acetone as a function of temperature[a]

Temperature (t/°C)	NaSCN (m_1/mol kg^{-1})
10	0.680
20	0.860
25	1.000
30	1.210
40	1.644
50	2.190

[a] The equilibrium solid phase was NaSCN [540-72-7] at all temperatures.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method[1] was used. Excess solid was equilibrated with acetone by stirring in a closed, thermostated vessel. Attainment of equilibrium was checked by measuring electrical conductivity of the solution. To this aim, an electrolytic cell closed with a glass sinter was immersed in the solution throughout the measurement. At chosen time intervals, the measured solution was sucked in between two platinum electrodes, the conductivity was measured, and the solution was transferred back from the cell to the solubility vessel by applying overpressure of dry air. The procedure was repeated until steady conductivity of the solution was obtained. The equilibrium conductivity value was then used to read the concentration of NaSCN in the saturated solution from a calibration graph of conductivity plotted against NaSCN concentration in acetone.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.2% (error of conductivity measurements; authors).

References:

[1] B. S. Krumgalz, Yu. I. Gerzhberg, I. P. Nikitina, V. I. Derevskaya, G. F. Fedotova, and D. G. Traber, Zh. Prikl. Khim. **42**, 1414 (1969).

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Solvents

Original Measurements:
S. Dernini, R. DeSantis, and L. Marrelli, J. Chem. Eng. Data **21**, 170–3 (1976).

Variables:
Measurements at boiling points of the saturated solutions.

Prepared By:
J. Hála

Experimental Data

Solubility of NaSCN in two solvents at boiling points at 760 mm Hg pressure[a]

Solvent	NaSCN (g/100 g solvent)	NaSCN (m_1/mol kg^{-1})[b]	Boiling point of the saturated solution[c] (t/°C)
Acetone; C_3H_6O; [67-64-1]	26.5	3.27	61.7
Methanol; CH_4O; [67-56-1]	63.9	7.88	70.8

[a] Solid phases were not investigated.
[b] Calculated by compiler.
[c] Calculated by compiler using ebulioscopic constants of 1.7 and 0.8, and normal boiling points[1] of 56.15 and 64.51 °C for acetone and methanol, respectively, and assuming undissociated NaSCN in the saturated solutions.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Determination of the solubilities was performed by sampling 10 mL of the boiling liquid, and weighing first the sample, and then the residue after thorough evaporation of the solvent.

Source and Purity of Materials:

NaSCN was of 98.5 mass % purity. Acetone and methanol, source not specified, were both of 99.9 mass % purity.

Estimated Error:

Solubility: insufficient data given to allow for error estimate.

References:

[1] E. Hála and A. Reiser, *Physical Chemistry* (Czech ed.) (Academia, Prague, 1971), Vol. 1, p. 278.

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) 2-Butanone (methylethylketone); C_4H_8O; [78-93-3]

Original Measurements:

B. S. Krumgalz, V. A. Smirnova, and Yu. I. Gerzhberg, Zh. Neorg. Khim. **17**, 1778– 80 (1972).

Variables:

T/K: 283–323

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN in 2-butanone as a function of temperature[a]

Temperature (t/°C)	NaSCN (m_1/mol kg^{-1})
10	2.361
20	2.179
25	2.094
30	2.013
40	1.868
50	1.740

[a] The equilibrium solid phase was NaSCN [540-72-7] at all temperatures.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method[1] was used. Excess solid was equilibrated with 2-butanone by stirring in a closed, thermostated vessel. Attainment of equilibrium was checked by measuring electrical conductivity of the solution. To this aim, an electrolytic cell closed with a glass sinter was immersed in the solution throughout the measurement. At chosen time intervals, the measured solution was sucked in between two platinum electrodes, the conductivity was measured, and the solution was transferred back from the cell to the solubility vessel by applying overpressure of dry air. The procedure was repeated until steady conductivity of the solution was obtained. The equilibrium conductivity value was then used to read the concentration of NaSCN in the saturated solution from a calibration graph of conductivity plotted against NaSCN concentration in 2-butanone.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.2% (error of conductivity measurements; authors).

References:

[1] B. S. Krumgalz, Yu. I. Gerzhberg, I. P. Nikitina, V. I. Derevskaya, G. F. Fedotova, and D. G. Traber, Zh. Prikl. Khim. **42**, 1414 (1969).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Solvents

Original Measurements:

I. L. Krupatkin, L. D. Vorobeva, V. P. Maskhulia, and M. E. Veselova, Zh. Obsh. Khim. **45**, 985–90 (1975).

Variables:

T/K: 298

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN in furfural and methylethylketone at 25 °C[a]

Solvent	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[b]
2-furancarboxaldehyde (furfural); $C_5H_4O_2$; [98-01-1]	14.60	2.109
2-butanone (methylethylketone); C_4H_8O; [78-93-3]	11.40	1.587

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, no details reported.

Source and Purity of Materials:

NaSCN, source and purity not specified, was dried at 100 °C to constant weight before use. The solvents were purified by standard methods,[1] and their purity was checked through physical constants.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. Weisberger, E. Proskanzer, J. Riddick, and E. Toops, *Organic Solvents* (Russian translation of English ed.) (IL Publ. House, Moscow, 1958), pp. 351, 361.

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Methylacetate; $C_3H_6O_2$; [79-20-9]

Original Measurements:
J. Schroeder and M. Steiner, J. Prakt. Chem. **79**, 49–65 (1909).

Variables:
One measurement at boiling point temperature.

Prepared By:
J. Hála

Experimental Data

Solubility of NaSCN in boiling methylacetate

The solubility of NaSCN is reported to be $100\ w_1 = 12.00$ mass % at boiling point of the saturated solution (compiler: $m_1 = 1.682\ \text{mol kg}^{-1}$). The boiling point temperature was not reported. The solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:
Excess salt was boiled with methylacetate for a prolonged period of time in a flask closed with a stopper through which a short glass tube was protruding. The latter contained glass wool as a filter at the bottom end, and was made into a short capillary at the upper end. By turning the flask upside down, a portion of the saturated solution was allowed to pour out into a weighing flask. After more boiling, another two samples were taken in the same way. The samples were then evaporated, and the residue weighed.

Source and Purity of Materials:
NaSCN, source and purity not specified, was dried at 110 °C before use. Methylacetate was kept over anhydrous $CuSO_4$ for a prolonged period of time, and distilled. The fraction boiling at 56.2–56.7 °C was collected and stored in the dark.

Estimated Error:
Solubility: insufficient data reported to allow for error estimate.

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) 1,2-ethanediamine (ethylenediamine); $C_2H_8N_2$; [107-15-3]

Original Measurements:
H. S. Isbin and K. A. Kobe, J. Am. Chem. Soc. **67**, 464–5 (1945).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of NaSCN in ethylenediamine at 25 °C

The solubility of NaSCN is reported to be 93.5 g in 100 g solvent (compiler: $m_1 = 11.53\ \text{mol kg}^{-1}$). The composition of the solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. The solvent and excess solid were sealed in a glass test tube and rotated for at least 1 week in a water thermostat, which was found sufficient for equilibrium to be reached. Samples of the saturated solution were withdrawn with a weighing pipette, and analyzed for SCN^- content by titration against a standard $AgNO_3$ solution.

Source and Purity of Materials:
NaSCN, analytical grade, was dried at 150 °C before use. Ethylenediamine, source not specified, was dehydrated and purified according to Putnam and Kobe.[1]

Estimated Error:
Temperature: ±0.08 K (authors).
Solubility: ±0.5% (authors).

References:
[1] G. L. Putnam and K. A. Kobe, Trans. Electrochem. Soc. **74**, 609 (1938).

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Solvents

Original Measurements:
O. A. Lavrova, N. N. Mokosina, and O. S. Karchmarchik, Zh. Neorg. Khim. **29**, 1312–6 (1984).

Variables:
T/K: 293, 313, 333

Prepared By:
J. Hála

Experimental Data

Solubility of NaSCN in three solvents at two or three temperatures[a]

Solvent	Temperature (t/°C)	NaSCN (100 w_1/mass %)	NaSCN (100 x_1/mol %)	NaSCN (m_1/mol kg^{-1})[b]
N,N-dimethylformamide; C_3H_7NO; [68-12-2]	40	26.3	24.3	4.40
	60	32.4	30.2	5.91
N,N-dimethylacetamide; C_4H_9NO; [127-19-5]	20	17.8	18.9	2.67
	40	22.3	23.5	3.54
	60	30.4	31.9	5.39
N-methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	40	22.3	25.9	3.54
	60	26.7	30.9	4.49

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: Earlier data on the solubility of NaSCN in N,N-dimethylformamide[1] have been compiled in Lesteva and Chernaya.[2]

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method[3] was used. Excess solid was stirred with the solvent in a thermostated vessel until equilibrium was reached. The content of NaSCN in the saturated solutions was determined by titration against a standard $AgNO_3$ solution.

Source and Purity of Materials:
No details reported.

Estimated Error:
Temperature: ±0.05 K (authors).
Solubility: ±0.2–0.5 mol % (authors).

References:
[1] R. C. Paul, J. P. Singh, M. S. Lamba, D. S. Gill, and S. P. Narula, Indian J. Chem. **11**, 1024 (1973).
[2] *IUPAC Solubility Data Series*, edited by B. Scrosati and C. A. Vincent (Pergamon Press, Oxford), Vol. 11, pp. 181–185.
[3] T. M. Lesteva and V. I. Chernaya, Zh. Neorg. Khim. **23**, 2556 (1978).

Components:
(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) N,N-dimethylacetamide; C_4H_9NO; [127-19-5]

Original Measurements:
A. A. Fedorov, L. B. Sokolov, V. M. Savinov, M. A. Shlionskaya, and N. I. Filatova, Zh. Prikl. Khim. **44**, 2361–2 (1971).

Variables:
T/K: 295–298

Prepared By:
J. Hála

Experimental Data

The solubility of NaSCN in N,N-dimethylacetamide is reported to be $c_1 = 1.78$ mol dm^{-3} at 22–25 °C. The nature of the equilibrium solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:
The solvent was saturated with anhydrous salt. Then a part of the solvent was distilled off to remove water, and the saturated solution with excess solid was kept for 3 days in a desiccator in a paraffin-coated flask. The content of water in the saturated solution was $<0.1\%$. The saturated solution was analyzed for the content of sulfur by an unspecified method.

Source and Purity of Materials:
NaSCN was a chemically pure product, source was not specified N,N-dimethylacetamide, source not specified, was freshly distilled before use.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Tri-n-butyl(phosphate); $C_{12}H_{27}O_4P$; [126-73-8]

Original Measurements:

J. Hála and D. G. Tuck, Can. J. Chem. **48**, 2843–6 (1970).

Variables:

T/K: 295

Prepared By:

J. Hála

Experimental Data

The solubility of NaSCN in tri-n-butyl(phosphate) is reported to be 12.5 g salt in 100 g solvent at 22 °C ($m_1 = 1.542$ mol kg^{-1}; compiler).

Additional information: The solvent/NaSCN mole ratio in the saturated solutions was found to be 2.44, indicating the existence of the disolvate, $NaSCN \cdot 2C_{12}H_{27}O_4P$.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. An excess of the salt was shaken overnight with 5 mL dry solvent. Preliminary experiments showed that this was sufficient for equilibrium to be reached. Samples of the saturated solutions were withdrawn through a sinter, diluted with acetone, and analyzed for the thiocyanate content by titration against $AgNO_3$ standard solution. Blank titrations showed that a small correction was required because of the presence of tri-n-butyl(phosphate).

Source and Purity of Materials:

NaSCN, Fisher Scientific Co., was used without further purification. Tri-n-butyl(phosphate) (Fisher Scientific Co.) was purified by refluxing it with 0.5% caustic soda solution, followed by steam distillation. The product was dried first with anhydrous $MgSO_4$, and finally vacuum/dried at 50 °C in a stream of dry nitrogen gas.[1]

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.4 g salt/100 g solvent (authors).

References:

[1] D. G. Tuck, J. Chem. Soc. 2783 (1958).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) N,N-dimethylacetamide; C_4H_9NO; [127-19-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

O. A. Lavrova, N. N. Mokosina, and O. S. Karchmarcik, Zh. Neorg. Khim. **29**, 1312–6 (1984).

Variables:

T/K: 293
100 x_2/mol %: 0–0.81

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN in water–N,N-dimethylacetamide solutions at 20 °C

C_4H_9NO (100 x_2/mol %)	NaSCN (100 x_1/mol %)	Solid phase[a]
0	26.9	A
15.4	26.9	A
23.6	26.9	A
27.0	24.2	B
31.2	26.0	B
36.1	23.3	C
43.8	20.8	C
43.2	19.9	D
44.8	18.1	D
47.7	18.8	E
58.7	16.5	E
60.2	16.8	E
71.0	18.9	E
81.1	18.9	not reported

[a] A: NaSCN, [540-72-7]; B: $NaSCN \cdot C_4H_9NO$, [ ]; C: $3NaSCN \cdot 4C_4H_9NO$, [ ]; D: $NaSCN \cdot 2C_4H_9NO$, [ ]; E: $2NaSCN \cdot 5C_4H_9NO$, [ ].

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method[1] was used. Excess solid was stirred with the solvent in a thermostated vessel until equilibrium was reached. The content of NaSCN in the saturated solutions was determined by titration against standard $AgNO_3$ solution. Solid phases were characterized by the method of wet residues.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: ±0.05 K (authors).
Solubility: ±0.2–0.5 mol % (authors).

References:

[1] T. M. Lesteva and V. I. Chernaya, Zh. Neorg. Khim. **23**, 2556 (1978).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. A. Titova and Z. E. Batura, Zh. Neorg. Khim. **10**, 1711–2 (1965).

Variables:

100 w_2/mass % in the dry residue: 0–100

Prepared By:

J. Hála

Experimental Data

Composition of solutions saturated at boiling points[a]

NaCl (100 w_2/mass %)[b]	H_2O (g per 100 g dry residue)	Temperature (t/°C)[c]	NaCl[d] (100 w_2/mass %)	NaCl[d] (m_2/mol kg^{-1})	NaSCN[d] (100 w_1/mass %)	NaSCN[d] (m_1/mol kg^{-1})
0	33.2	152.0	0	0	75.08	37.15[f]
1.5	33.0	152.5	1.13	0.7793	74.06	36.82[f]
1.7[e]	32.3	153.0	1.29	0.9043	74.30	37.55[g]

[a] Atmospheric pressure of 745±5 mm Hg.
[b] In the dry residue.
[c] Boiling point of the saturated solution.
[d] Composition of the saturated solutions (calculated by compiler).
[e] Eutonic point.
[f] Solid phase: NaSCN, [540-72-7].
[g] Solid phases: NaSCN+NaCl, [7647-14-5].

Additional information: In addition to the data shown in the table, the authors reported also the results for another 11 saturated solutions containing 1.55–28.69 mass % NaCl and 69.07–0 mass % NaSCN, with NaCl as the equilibrium solid phase. The respective boiling points of these solutions decreased from 140.5 to 109.0 °C. These data were not included here since they refer to the solubility of NaCl in solutions of NaSCN.

Auxiliary Information

Method/Apparatus/Procedure:

Determinations were performed in a four-neck flask equipped with stirrer, condenser, thermometer, and a sampling device. The flask was thermostated in an oil bath. Atmospheric pressure was within 745±5 mm Hg throughout the measurements, and variations in solubility induced by these variations of pressure were found to be within the errors of the analytical methods used. Samples of the saturated solutions were first dried to constant weight and then analyzed for Cl^- and SCN^- content by potentiometric titration with $AgNO_3$ solution. Two titrations were performed. In one, the sum of SCN^- and Cl^- was determined, in the other Cl^- was titrated after decomposition of SCN^- with H_2O_2 in alkaline medium.

Source and Purity of Materials:

NaSCN and NaCl were chemically pure products, and were recrystallized before use. Distilled water was used.

Estimated Error:

Temperature: ±0.05 K (authors).
Solubility: ±0.015 mass % (authors).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).

Variables:

T/K: 278, 298, and 323
100 w_2/mass %: 0–26.2 at 278 K; 0–26.5 at 298 K; 0–26.9 at 323 K

Prepared By:

J. Hála

Experimental Data

Solubility in the NaSCN–NaCl–H_2O system at three temperatures

Temperature (t/°C)	NaCl (100 w_2/mass %)	NaCl (m_2/mol kg^{-1})[a]	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
5	0	0	51.0	12.88	B
	2.1	0.740	49.4	12.56	B+A
	4.4	1.354	40.0	8.873	A
	11.3	3.016	24.6	4.733	A
	19.7	4.878	11.2	1.999	A
	26.2	6.074	0	0	B
25	0	0	60.0	18.50	B+A
	1.9	0.820	58.5	18.22	A
	2.5	0.972	53.5	14.99	A
	4.8	1.492	39.8	8.861	A
	11.5	3.079	24.6	4.748	A
	19.9	4.941	11.2	2.005	A
	26.5	6.169	0	0	C
	0	0	64.5	22.41	C+A
50	2.0	1.118	62.5	21.90	A
	3.3	1.240	51.2	13.88	A
	5.2	1.614	39.7	8.887	A
	11.7	3.142	24.6	4.763	A
	20.1	5.005	11.2	2.010	A
	26.9	6.296	0	0	A

[a] Calculated by compiler.
[b] A: NaCl, [7647-14-5]; B: NaSCN. $2H_2O$, [17032-40-5]; C: NaSCN, [540-72-7].

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were obtained by graphical analytical method.[1,2] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions were prepared by weighing. After equilibrium had been attained, refractive indexes of the solutions were measured. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phases was not reported.

Source and Purity of Materials:

NaSCN, source not specified, was recrystallized as dihydrate and then dehydrated at 120–130 °C to obtain the anhydrous salt.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

S. M. Golyand and B. G. Ludkovskaya, Zh. Neorg. Khim. **11**, 1433–5 (1966).

Variables:

T/K: 298 and 313
100 w_2/mass %: 0 and 0.72 at 298 K; 0 and 0.51 at 313 K

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN in water, and compositions of eutonic points in the ternary NaSCN–NaCl–H_2O system at 25 and 40 °C

Temperature (t/°C)	NaCl (100 w_2/mass %)	NaCl (m_2/mol kg^{-1})[b]	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[b]	Solid phase[a]
25	0	0	58.5	17.39	A
	0.72	0.294	57.4	16.91	A+B
40	0	0	63.0	21.00	C
	0.51	0.235	62.3	20.66	D+B

[a] A: $NaSCN\cdot 2H_2O$, [17032-40-5]; B: NaCl, [7647-14-5]; C: NaSCN, [540-72-7]; D: solid solution of NaCl and NaSCN (of 1.85 mass % NaCl in the solid phase, 0.7 mass % was in the form of NaCl, and the rest in the form of the solid solution).
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Saturated solutions with equilibrium solid phases were prepared either by cooling saturated solutions prepared at 80 °C, or by warming from 20 °C solutions containing excess of solid salts. Intense stirring and seeding was applied. Both methods yielded identical results. Saturated solutions and the solid phases were analyzed titrimetrically for SCN^-, Cl^- (after decomposition of SCN^- by H_2O_2 in alkaline medium), and the sum of both ions. Solid phases were also investigated by x-ray diffraction. It was possible to identify as low as 0.5 mass % NaCl in mixtures of $NaSCN\cdot 2H_2O$ and NaCl. X-ray patterns of $NaSCN\cdot 2H_2O$ were recorded in dry atmosphere to avoid deliquescence of the salt.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Ammonium chloride; NH_4Cl; [12125-02-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).

Variables:

T/K: 278, 298, and 323
100 w_2/mass %: 0–23.8 at 278 K; 0–28.6 at 298 K; 0–33.5 at 323 K

Prepared By:

J. Hála

Experimental Data

Solubility in the NaSCN–NH_4Cl–H_2O system at three temperatures

Temperature (t/°C)	NH_4Cl (100 w_2/mass %)	NH_4Cl (m_2/mol kg^{-1})[a]	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
5	0	0	51.0	12.83	A
	2.1	0.797	49.6	12.66	A+B
	2.2	0.818	48.5	12.13	B
	6.6	2.155	37.2	8.164	B
	10.1	3.195	31.9	6.784	B
	15.7	4.826	24.6	5.082	B+C
	19.1	5.343	15.3	2.876	C
	21.3	5.505	7.7	1.337	C
	23.8	5.731	0	0	C
25	0	0	60.0	18.50	A
	1.9	0.884	58.7	18.37	A+B
	2.6	0.979	48.7	12.33	B
	7.0	2.302	37.2	8.223	B
	17.2	5.386	24.2	5.093	B
	20.1	6.251	20.9	4.369	B+C
	22.5	6.606	15.0	2.960	C
	25.0	6.796	7.5	1.370	C
	28.5	7.350	0	0	C
50	0	0	64.5	22.41	D
	2.3	1.219	63.1	22.49	D+B
	3.0	1.135	48.5	12.33	B
	7.8	2.588	36.9	8.230	B
	18.7	6.031	24.4	5.289	B
	26.1	8.373	16.7	3.601	B+C
	26.8	8.292	14.6	3.073	C
	29.7	8.610	7.0	1.364	C
	33.5	9.244	0	0	C

[a] Calculated by compiler.
[b] A: $NaSCN\cdot 2H_2O$, [17032-40-5]; B: NaCl, [7647-14-5]; C: NH_4Cl; [12125-02-9]; D: NaSCN, [540-72-7].

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were obtained by graphical analytical method.[1,2] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions were prepared by weighing. After equilibrium had been attained, refractive indexes of the solutions were measured. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phases was not reported.

Source and Purity of Materials:

NaSCN, source not specified, was recrystallized as dihydrate and then dehydrated at 120–130 °C to obtain the anhydrous salt.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Sodium sulfate; Na_2SO_4; [7757-82-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).

Variables:

T/K: 306 and 326
100 w_2/mass %: 0–33.0 at 306 K; 0–31.6 at 326 K

Prepared By:

J. Hála

Experimental Data

Solubility in the NaSCN–Na_2SO_4–H_2O system at two temperatures

Temperature (t/°C)	Na_2SO_4 (100 w_2/mass %)	Na_2SO_4 (m_2/mol kg^{-1})[a]	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
33	0	0	68.5	21.45	A
	0.4	0.0777	63.4	21.60	A+B
	1.0	0.118	39.6	8.223	B
	5.5	0.585	28.4	5.299	B
	13.3	1.349	17.3	3.074	B
	33.7	2.428	7.6	1.364	B
	33	3.467	0	0	B
53	0	0	64.8	22.70	A
	0.8	0.162	64.4	22.82	A+B
	1.0	0.118	39.6	8.223	B
	5.0	0.529	28.5	5.286	B
	12.7	1.280	17.5	3.092	B
	22.3	2.246	7.8	1.376	B
	31.6	3.252	0	0	B

[a] Calculated by compiler.
[b] A: NaSCN, [540-72-7]; B: Na_2SO_4; [7757-82-6].

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were obtained by graphical analytical method.[1,2] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions were prepared by weighing. After equilibrium had been attained, refractive indexes of the solutions were measured. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phases was not reported.

Source and Purity of Materials:

NaSCN, source not specified, was recrystallized as dihydrate and then dehydrated at 120–130 °C to obtain the anhydrous salt.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Potassium thicyanate; KSCN; [333-20-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549–52 (1968).

Variables:

T/K: 273–323
100 w_1/mass %: 0–48.3 at 273 K; 0–52 at 283 K; 0–59.2 at 298 K; 0–65 at 323 K
100 w_2/mass %: 0–64 at 273 K; 0–67.2 at 283 K; 0–70.9 at 298 K; 0–76.4 at 323 K

Prepared By:

J. Hála

Experimental Data

Solubility in the NaSCN–KSCN–H_2O system at four temperatures

Temperature (t/°C)	NaSCN (100 w_2/mass %)	NaSCN (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	0	64.0	18.29	A
	9.0	3.066	54.8	15.57	A
	23.6	8.223	41.0	11.91	A
	33.4	12.33	33.2	10.22	A+B
	35.2	13.56	32.8	10.54	B
	37.5	12.53	25.6	7.138	B
	40.6	12.03	17.8	4.403	B
	45.2	12.30	9.5	2.157	B
	48.3	11.52	0	0	B
10	0	0	67.2	21.08	A
	8.3	3.012	58.7	18.30	A
	21.7	8.235	45.8	14.50	A
	31.2	12.33	37.6	12.40	A
	38.3	16.17	32.5	11.45	A+B
	41.3	15.16	25.1	7.687	B
	44.5	14.14	16.7	4.429	B
	48.8	13.05	5.1	1.138	B
	52.0	13.36	0	0	B
25	0	0	70.9	25.07	A
	7.2	3.041	68.5	22.41	A
	19.0	8.252	52.6	19.05	A
	27.5	12.33	45.0	16.83	A
	36.5	18.52	39.2	16.59	A
	38.7	20.66	38.2	17.01	A+C
	46.2	21.18	26.9	10.29	C
	49.6	25.81	26.7	11.59	C
	54.8	21.39	13.6	4.428	B+C
	57.4	18.48	4.3	1.155	B
	59.2	17.89	0	0	B
50	0	0	76.4	33.31	
	5.5	2.962	71.6	32.17	
	14.6	8.185	63.4	29.65	
	21.5	12.33	57.0	27.28	
	29.3	18.53	51.2	27.01	
	33.2	23.00	49.0	28.32	
	36.5	23.69	44.5	24.10	
	48.5	23.27	25.8	10.33	
	51.8	22.49	19.8	7.174	
	56.5	22.92	13.1	4.434	
	62.0	22.36	3.8	1.143	
	65.0	22.90	0	0	

[a] Calculated by compiler.
[b] A: KSCN, [333-20-0]; B: NaSCN·$2H_2O$, [17032-40-5]; C: NaSCN, [540-72-7].

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were obtained by graphical analytical method.[1] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions were prepared by weighing. After equilibrium had been attained, refractive indexes of the solutions were measured. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phases was not reported.

Source and Purity of Materials:

NaSCN and KSCN (source not specified) were chemically pure products, and were dried over anhydrous $CaCl_2$.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Ammonium thicyanate; NH_4SCN; [1762-95-4]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).

Variables:

T/K: 278, 298, and 323
100 w_1/mass %: 0–51 at 278 K; 0–60 at 298 K; 0–64.5 at 323 K
100 w_2/mass %: 0–56.2 at 278 K; 0–64.4 at 298 K; 0–73.8 at 323 K

Prepared By:

J. Hála

Experimental Data

Solubility in the NaSCN–NH_4SCN–H_2O system at four temperatures

Temperature (t/°C)	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	NH_4SCN (100 w_2/mass %)	NH_4SCN (m_2/mol kg^{-1})[a]	Solid phase[b]
5	0	0	56.2	16.58	A
	7.7	2.193	49.0	14.86	A
	17.9	5.269	40.2	12.60	A
	26.8	8.223	33.0	10.78	A
	38.0	12.33	24.0	8.297	A
	39.4	12.95	23.1	8.092	A+B
	40.3	12.58	20.2	6.718	B
	45.0	12.33	10.0	2.919	B
	47.5	12.44	6.0	1.684	B
	51.0	12.83	0	0	B
25	0	0	64.4	23.76	A
	6.2	2.172	58.6	21.87	A
	14.6	5.296	51.4	19.86	A
	22.0	8.223	45.0	17.91	A
	31.2	12.29	37.5	15.73	A
	45.0	19.54	26.6	12.30	A+C
	48.3	19.21	20.7	8.772	C
	49.5	19.08	18.5	7.594	C+B
	53.3	18.16	10.5	3.810	B
	56.3	17.94	5.0	1.697	B
	58.0	18.25	2.8	0.938	B
	60.0	18.50	0	0	B
50	0	0	73.8	37.00	A
	4.6	2.182	69.4	35.06	A
	10.9	5.272	63.6	32.76	A
	16.6	8.256	58.6	31.04	A
	23.7	12.28	52.5	28.97	A
	35.1	19.67	42.9	25.61	A
	40.3	23.67	38.7	24.20	A+C
	43.0	23.26	34.2	19.70	C
	48.0	22.77	26.0	13.13	C
	53.8	22.12	16.2	7.094	C
	59.8	21.56	6.0	2.304	C
	64.5	22.41	0	0	C

[a] Calculated by compiler.
[b] A: NH_4SCN, [1762-95-4]; B: $NaSCN\cdot 2H_2O$, [17032-40-5]; C: NaSCN, [540-72-7].

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were obtained by graphical analytical method.[1,2] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions were prepared by weighing. After equilibrium had been attained, refractive indexes of the solutions were measured. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phases was not reported.

Source and Purity of Materials:

NaSCN and NH_4SCN (source not specified) were chemically pure products, and were dried over anhydrous $CaCl_2$.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Boric acid; H_3BO_3; [10043-35-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

G. K. Gode and L. A. Klyavina, Zh. Neorg. Khim. **15**, 1147 (1970).

Variables:

T/K: 298
100 w_2/mass %: 0–5.46

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN at 25 °C in aqueous solutions of boric acid

H_3BO_3 (100 w_2/mass %)	H_3BO_3 (m_2/mol kg^{-1})[a]	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	56.20	15.83	A
4.32	1.701	54.60	16.39	A+B

[a] Calculated by compiler.
[b] A: NaSCN, [540-72-7]; B: H_3BO_3, [10043-35-3].

Additional information: In addition to the data shown above, the authors also reported the compositions of nine saturated solutions containing 4.35–5.46 mass % H_3BO_3, and 49.75–0 mass % NaSCN, where H_3BO_3 was the equilibrium solid phase. These data are not shown here since they represent the solubility of H_3BO_3 in solutions of NaSCN. Also reported were densities of the saturated solutions.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Solutions with excess solid were stirred at 800 rpm for 1–2 days in a thermostated vessel. Saturated solutions were analyzed for H_3BO_3 alkalimetrically against naphtholphthaleine as the indicator, and for SCN^- by Volhard's method. The method used for identification of the solid phases was not specified.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Boric acid; H_3BO_3; [10043-35-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. G. Skvortsov, R. S. Tsekhanskii, Sh. V. Sadetdinov, and A. K. Molodkin, Zh. Neorg. Khim. **28**, 2677–9 (1983).

Variables:

T/K: 298
100 w_2/mass %: 0–5.6

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN at 25 °C in aqueous solutions of boric acid

H_3BO_3 (100 w_2/mass %)	H_3BO_3 (m_2/mol kg^{-1})[a]	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	58.77	17.58	A
3.40	1.425	58.01	18.54	A
3.41	1.429	57.99	18.53	A+B

[a] Calculated by compiler.
[b] A: NaSCN, [540-72-7]; B: H_3BO_3, [10043-35-3].

Additional information: In addition to the data shown above, the authors also reported the compositions of six saturated solutions containing 3.41–5.60 mass % H_3BO_3, and 57.98–0 mass % NaSCN, where H_3BO_3 was the equilibrium solid phase. These data are not shown here since they represent the solubility of H_3BO_3 in solutions of NaSCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Solutions with excess solid were stirred for 20 h, which was sufficient for equilibrium to be reached. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method. Solubility isotherms were also confirmed by refractometric measurements.

Source and Purity of Materials:

NaSCN and H_3BO_3 were chemically pure products, and were recrystallized before use.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Sodium borate; $NaBO_2$; [7775-19-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. G. Skvortsov, Sh. V. Sadetdinov, R. S. Tsekhanskii, and A. K. Molodkin, Zh. Neorg. Khim. **24**, 209–12 (1979).

Variables:

T/K: 298
100 w_2/mass %: 0–22

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN at 25 °C in aqueous solutions of sodium borate

$NaBO_2$ (100 w_2/mass %)	$NaBO_2$ (m_2/mol kg^{-1})[a]	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	58.77	17.58	A
2.85	1.092	57.48	17.87	A
2.84[c]	1.088	57.50	17.88	A+B

[a] Calculated by compiler.
[b] A: NaSCN, [540-72-7]; B: $NaBO_2 \cdot 4H_2O$, [10555-76-7].
[c] Eutonic point.

Additional information: In addition to the data shown above, the authors also reported the compositions of nine saturated solutions containing 2.87–21.99 mass % $NaBO_2$, and 57.46–0 mass % NaSCN, where $NaBO_2 \cdot 4H_2O$ was the equilibrium solid phase. These data are not shown here since they represent the solubility of $NaBO_2$ in solutions of NaSCN. Also reported were densities, viscosities, and refraction indexes of the saturated solutions.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibrium was reached within 24 h under constant shaking in a thermostat. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method and chemical analysis.

Source and Purity of Materials:

NaSCN and $NaBO_2$ were chemically pure products.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:	**Original Measurements:**
(1) Sodium thiocyanate; NaSCN; [540-72-7] (2) Sodium tetraborate; $Na_2B_4O_7$; [61088-24-8] (3) Water; H_2O; [7732-18-5]	V. G. Skvortsov, A. K. Molodkin, Sh. V. Sadetdinov, and R. S. Tsekhanskii, Zh. Neorg. Khim. **26**, 3164–6 (1981).
Variables:	**Prepared By:**
T/K: 298 100 w_2/mass %: 0–2.42	J. Hála

Experimental Data

Solubility of NaSCN at 25 °C in aqueous solutions of sodium tetraborate

$Na_2B_4O_7$ (100 w_2/mass %)	$Na_2B_4O_7$ (m_2/mol kg^{-1})[a]	NaSCN (100 w_1/mass %)	NaSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	58.77	17.58	A
0.16	0.0191	58.10	17.17	A+B

[a] Calculated by compiler.

[b] A: NaSCN, [540-72-7]; B: $Na_2B_4O_7 \cdot 10H_2O$, [1303-96-4].

Additional information: In addition to the data shown above, the authors also reported the compositions of seven saturated solutions containing 0.14–2.42 mass % $Na_2B_4O_7$, and 58.04–0 mass % NaSCN, where $Na_2B_4O_7 \cdot 10H_2O$ was the equilibrium solid phase. These data are not shown here since they represent the solubility of $Na_2B_4O_7$ in solutions of NaSCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibrium was reached within 20 h, which was checked by chemical analysis and refraction index of the saturated solutions. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method.

Source and Purity of Materials:

NaSCN and $Na_2B_4O_7 \cdot 10H_2O$ were chemically pure products, and were recrystallized before use.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:	**Original Measurements:**
(1) Sodium thiocyanate; NaSCN; [540-72-7] (2) Sodium molybdate; Na_2MoO_4; [7631-95-0] (3) Water; H_2O; [7732-18-5]	Z. G. Karov, I. N. Lepeshkov, and E. I. Kukulieva, Zh. Neorg. Khim. **17**, 509–13 (1972).
Variables:	**Prepared By:**
T/K: 298 100 w_2/mass %: 0–40	J. Hála

Experimental Data

Solubility in the NaSCN–Na_2MoO_4–H_2O system at 25 °C.

The phase diagram of the NaSCN–Na_2MoO_4–H_2O system at 25 °C was reported in graphical form. The only numerical data reported were those of the solubility of NaSCN in water as 100 w_1/mass % = 58.63 (m_1 = 17.38 mol kg^{-1}), and the composition of the eutonic solution: 100 w_1/mass % = 58.41 and 100 w_2/mass % = 0.38 (m_1 = 17.48 mol kg^{-1}; m_2 = 0.0448 mol kg^{-1}; compiler). The system is a simple eutonic one with equilibrium solid phases $NaSCN \cdot 2H_2O$, [17032-40-5] at 100 w_2/mass % < 0.38, and $Na_2MoO_4 \cdot 2H_2O$, [10102-40-6] at 100 w_2/mass % > 0.38.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibrium was attained within 5–6 h, samples for analysis were withdrawn after 2–3 days. In the saturated solutions and the wet residues, MoO_4^{2-} was determined titrimetrically by an unspecified reductometric method after decomposition of SCN^- in acidic solution of H_2O_2, and SCN^- was determined by the Volhard's method. Solid phases were characterized by the method of wet residues.

Source and Purity of Materials:

NaSCN was a chemically pure product, and was recrystallized twice before use. The product was 99.92% pure. Na_2MoO_4 was prepared by melting stoichiometric amounts of MoO_3 and NaOH. The product was recrystallized three times, its purity was 99.96%.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Methylthiocyanate; C_2H_3NS; [556-64-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. Spaccamela Marchetti, Atti. Acad. Sci. Torino, Clase Fis. Mat. Nat. **94**, 353–70 (1960).

Variables:

T/K: 293
Ratio of H_2O/CH_3CNS concentrations.

Prepared By:

J. Hála

Experimental Data

Solubility in the NaSCN–CH_3CNS–H_2O system at 20 °C

The phase diagram of the NaSCN–CH_3CNS–H_2O system at 20 °C was reported in Fig. 12.

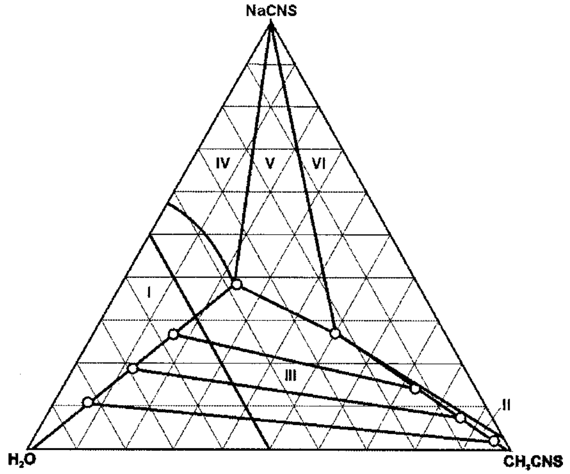

FIG. 12. Fields in the diagram: I and II—one liquid phase, III—two liquid phases, IV and VI—one liquid phase in equilibrium with solid NaSCN, and V—two liquid phases in equilibrium with solid NaSCN.

Numerical values were reported for the solubility of NaSCN in water-rich and CH_3CNS-rich CH_3CNS–H_2O mixtures (curves RP and QS in the phase diagram, respectively).

H_2O-rich region			CH_3CNS-rich region		
H_2O (100 w_3/mass %)	NaSCN (100 w_1/mass %)	CH_3CNS (100 w_2/mass %)	H_2O (100 w_3/mass %)	NaSCN (100 w_1/mass %)	CH_3CNS (100 w_2/mass %)
41.5	58.5[a]	0	13.9	16.3	69.8
39.3	55.8	4.9	8.0	9.2	82.8
38.4	54.5	7.1	4.9	4.9	90.2
37.7	52.9	9.4	0	1.9[b]	98.1
37.9	50.0	13.1			
36.7	47.3	16.0			
36.5	44.2	19.3			

[a] Solubility of NaSCN in water, $m_1 = 17.39$ mol kg^{-1} (compiler).
[b] Solubility of NaSCN in CH_3CNS, $m_1 = 0.239$ mol kg^{-1} (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

Solubility curves were obtained by titration of a mixture of two components with the third one in a thermostated bath. Burettes graduated by 0.01 cm^3 were used for titrations. Some of these measurements were verified by preparing the ternary system, and observing the temperature of homogenization. The solubility value corresponding to 20 °C was then obtained by interpolation.

Source and Purity of Materials:

NaSCN was dried at 110 °C before use. Source and purity of CH_3CNS not specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) 2-(2-methoxyethoxy)-N,N-bis-2-(2-methoxyethoxy)ethyl ethanamine {tris(dioxa-3,6-heptyl)amine}; $C_{15}H_{33}NO_3$; [70384-51-9]; or 2-methoxy-N,N-bis(methoxyethyl)ethan amine; {tris(oxa-3-butyl)amine}; $C_9H_{21}NO_3$; [3235-51-6]
(3) Dichloromethane; CH_2Cl_2 ; [75-09-2]

Original Measurements:

G. Soula, Eur. Pat. Appl. 016673, 1979; French Appl. 7905438.

Variables:

T/K: unspecified
c_2 /mol dm^{-3}: 0.1

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN in CH_2Cl_2 in the presence of amines[a]

Amine	NaSCN (mg dm^{-3})	NaSCN (c_1 /mol dm^{-3})[b]
$C_{15}H_{33}NO_3$	2300	0.0284
$C_9H_{21}NO_3$	2150	0.0265

[a] Measurements performed at an unspecified, ambient temperature. Solid phases were not investigated.

[b] Calculated by compiler.

Additional information: The solubility of NaSCN in neat CH_2Cl_2 was reported to be less than 1 mg dm^{-3}. The solubilization effect of $C_{15}H_{33}NO_3$ was explained by the authors in terms of the formation of a 1:1 adduct of NaSCN with the amine in the solution.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The salt (0.001 mole) was equilibrated with 0.001 mole amine in 10 mL CH_2Cl_2 by stirring. The content of the salt in the saturated solution was determined by flame photometry.

Source and Purity of Materials:

$C_{15}H_{33}NO_3$ was prepared by refluxing sodium methoxy-2-ethanoate with chlorohydrate of tris(chloro-2-ethyl) amine in methoxy-2-ethanol for 12 h at 125 °C. The excess of solvent was then distilled off, excess of sodium methoxy-2-ethanoate decomposed with concentrated HCl, and the amine was distilled at 165–180 °C at 0.5 mm Hg. $C_9H_{21}NO_3$ was obtained by a similar procedure using sodium methanoate and methanol as the solvent. After treatment of the mixture with HCl, the amine was extracted into CH_2Cl_2 , and distilled. Anhydrous CH_2Cl_2 was purified from stabilizers.

Estimated Error:

Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Sodium thiocyanate; NaSCN; [540-72-7]
(2) Acetic acid; $C_2H_4O_2$; [64-19-7]
(3) N,N-diethylethanamine (triethylamine); $C_6H_{15}N$; [121-44-8]; or N,N-dimethylbenzeneamine; (dimethyl-Aniline); $C_8H_{11}N$; [121-69-7]
(4) Solvents

Original Measurements:

T. Jasinski and R. Korewa, Rocz. Chem. (Warsaw) **39**, 963–8 (1965).

Variables:

T/K: 293

Prepared By:

J. Hála

Experimental Data

Solubility of NaSCN at 20 °C in solvents in the presence of amines and acetic acid[a]

Solvent	$C_2H_4O_2$ (c_2 /mol dm^{-3})	$C_6H_{15}N$ (c_3 /mol dm^{-3})	$C_8H_{11}N$ (c_3 /mol dm^{-3})	NaSCN (c_1 /mol dm^{-3})
Ethylacetate; $C_4H_8O_2$; [141-78-6]	0.05	0	0	0.0110
	0	0.05	0	0.0048
	0.05	0.05	0	0.0122[b]
	0	0	0.05	0.0020
	0.05	0	0.05	0.0050[b]
Dichloromethane; CH_2Cl_2 ; [75-09-2]	0.05	0	0	0.0016
	0	0.05	0	0.0002
	0.05	0.05	0	0.0030[b]
	0	0	0.05	0.0002
	0.05	0	0.05	0.0012[b]
Benzene; C_6H_6 ; [71-43-2]	0.05	0.05	0	0.0108[b]
Chlorobenzene; C_6H_5Cl; [108-90-7]	0.05	0.05	0	0.0120[b]
	0.05	0	0.05	0.0095[b]
Diethylether; $C_4H_{10}O$; [60-29-7]	0.05	0.05	0	0.0128[b]

[a] Solid phases were not investigated.

[b] Solubility of NaSCN in the presence of the corresponding ammonium acetate.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The salt was equilibrated in closed flasks for 5 days with 20 cm^3 portions of the solutions of the amine, acetic acid, or their mixture, as may be the case, in the desired solvent. Then a 10 cm^3 sample was withdrawn, added to water, and the salt was extracted into water by shaking. The SCN^- content was determined in the aqueous layer by potentiometric titration with 0.01 mol dm^{-3} $AgNO_3$ solution.

Source and Purity of Materials:

NaSCN, reagent grade, was twice recrystallized from water, and dried in an oven to constant weight. Acetic acid, source not specified, was purified by crystallization and distillation. The amines, source unspecified, were dried over KOH and distilled over zinc powder. CH_2Cl_2 , chlorobenzene, and ethylacetate were dried over P_2O_5 , and distilled over anhydrous Na_2CO_3 . Benzene and diethylether were dried with sodium metal, and distilled.

Estimated Error:

Temperature: ±0.5 K (authors).
Solubility: ±2% (authors).

6.3. Potassium Thiocyanate

6.3.1. Evaluation of the KSCN–H_2O System

Components:	**Evaluator:**
(1) Potassium thiocyanate; KSCN; [333-20-0] (2) Water; H_2O; [7732-18-5]	J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, June 2001.

Critical Evaluation

The solubility of KSCN in water has been reported in a number of papers. Measurements in the binary KSCN–H_2O system have been carried out by Kraczek[1] by a polythermal method over a wide temperature range of 305.7–450 K, and by Rüdorff[2] who reported isothermal measurements at three temperatures. In three documents,[3–5] the solubility has been obtained isothermally at 298.2 K. In addition, data on the KSCN–H_2O system could be extracted from the measurements on various ternary systems. All the data available for the temperature range from 243 to 330 K have been summarized in the following table and, in order to test how consistent they have also been plotted in the graph (Fig. 13). Fourteen data available for 298.2 K are represented in the graph as the bar, showing the range into which these data fall.

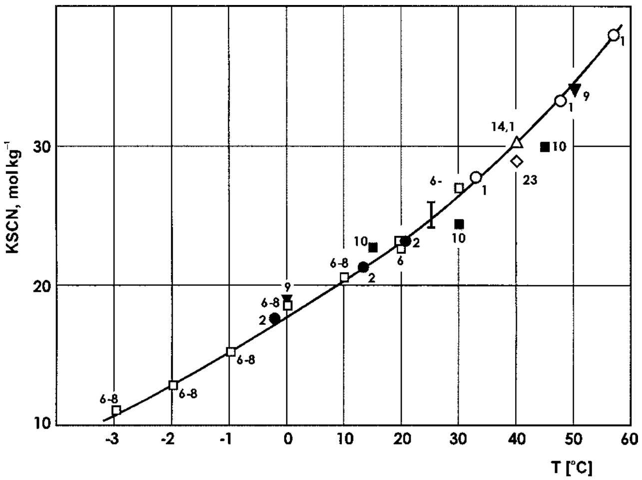

FIG. 13. Survey of the data on the solubility of KSCN in water.

Solubility of KSCN as a function of temperature

Temperature (t/°C)	Temperature (K)	KSCN (m_1/mol kg^{-1})	Ref.	Temperature (t/°C)	Temperature (K)	KSCN (m_1/mol kg^{-1})	Ref.
−30	243.2	11.15[a]	6–8	25	298.2	25.32[f]	12,13
−20	253.2	12.83[a]	6–8			24.98[g]	14
−10	263.2	15.24[a]	6–8			24.83[g]	15–17
−2.2	271.0	17.77[b]	2			25.07[c]	9
0	273.2	18.29[a]	6–8			24.59[g]	18–20
		18.62[c]	9			25.08[g]	21
10	283.2	20.43[a]	6–8			25.06[e]	26
12.9	286.1	20.97[b]	2	30	303.2	26.46[a]	6–8
15	288.2	22.18[d]	10			24.01[d]	10
20	293.2	22.90[a]	6–8	32.6	305.8	27.28[b]	1
		22.27[a]	7,11	40	313.2	29.87[f,g]	13,16
20.5	293.7	22.38[b]	2			28.75[d]	22
25	298.2	24.45,24.81[e]	3	45	318.2	30.22[d]	10
		23.96[d]	4	47.3	320.5	32.63[b]	1
		24.67,24.63,24.56,24.58[e]	5	50	323.2	33.31[c]	9
				57	330.2	36.90[b]	1

Experimental method used:

[a] Ternary system studied by visual polythermal method, isothermal data obtained graphically.
[b] Visual polythermal.
[c] Graphical method using refractive index of the solutions.
[d] Isothermal, analysis of the saturated solutions not reported.
[e] Isothermal, gravimetric analysis of the saturated solutions.
[f] Isothermal, saturated solutions analyzed by potentiometric titrations.
[g] Isothermal, saturated solutions analyzed by Volhard's method.

Irrespective of the variety of experimental methods used, the data show a remarkable consistency except, perhaps, for the data of Turgunbekova *et al.*[10] taken from their ternary system KSCN–urea–H_2O, and were computer smoothed by a linear regression of the data to a fifth order polynomial. The solubility value at 303.2 K (Ref. 10) was not considered for the smoothing procedure. The following equation has been obtained for the KSCN solubility as a function of temperature:

$$m_1\ (\mathrm{mol\ kg}^{-1}) = 0.140\,021\times10^{4} - 0.103\,192\times10^{2}\ T - 0.335\,259\times10^{-1}\ T^2 + 0.505\,469\times10^{-3}\ T^3 - 0.158\,237\times10^{-5}\ T^4 + 0.160\,181\,4\times10^{-8}\ T^5,$$

and can be recommended for obtaining tentative values of KSCN solubilities in water over the temperature range from 243 to 330 K.

Of numerous data reported at 298.2 K, those of Foote[3] and Chang[5] have been obtained by careful gravimetric analysis of the saturated solutions, and can be considered as being superior in precision to the data obtained by other methods. The data of Foote[3] and Chang[5] have been taken to obtain the solubility of KSCN in water at 298.2 K as 24.6±0.1 mol kg^{-1} (or 70.5±0.1 mass %), which is suggested as the recommended value.[11]

The following table summarizes the reported temperatures and compositions of the eutectic (cryohydric) point in the KSCN–H_2O system:

Temperature	KSCN concentration at the eutectic point			
(t/°C)	(100 w_1/mass %)	(m_1/mol kg^{-1})	(100 x_1/mol %)	Reference
−29.5	51.2	10.80[a]		23
−31.2	53.60[a]	11.89[a]	17.64	1
−31				24
−31.2	50.23	10.39[a]		25

[a] Calculated by evaluator.

References:

[1] F. C. Kraczek, J. Washington Acad. Sci. **26**, 307 (1936).
[2] F. Rüdorff, Ann. Phys. Chem. **136**, 276 (1869).
[3] H. W. Foote, Z. Phys. Chem. **46**, 79 (1903).

[4] J. R. Partington and W. E. Soper, Philos. Mag. **7**, 209 (1929).

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[11] A. M. Babenko and A. M. Andrianov, Zh. Neorg. Khim. **23**, 3123 (1978).

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[21] Z. G. Karov, I. N. Lepeshkov, and S. B. Semenova, Zh. Neorg. Khim. **16**, 2273 (1971).

[22] M. I. Bakeev and I. P. Akimova, Dep. Doc. VINITI, No. 1148-76 (1976).

[23] A. Chrétien and O. Hoffer, Compt. Rend. **201**, 1131 (1935).

[24] E. Kordes, Z. Anorg. Allgem. Chem. **167**, 97 (1927).

[25] A. M. Vassiliev, Zh. Russ. Fiz. Khim. Obsh. **42**, 423 (1910).

[26] V. J. Occleshaw, J. Chem. Soc. 55 (1931).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

F. Rüdorff, Ann. Phys. Chem. **136**, 276–84 (1869).

Variables:

T/K: 271–293

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN in water as a function of temperature[a]

Temperature (t/°C)	KSCN (g/100 g H_2O)	KSCN (m_1 /mol kg^{-1})[c]
−2.2	172.7	17.77
0[b]	177.2	18.23
12.9	203.8	20.97
20[b]	217.0	22.33
20.5	217.5	22.38

[a] Solid phases were not investigated.

[b] Interpolated values obtained by the author; reported also in Rüdorff.[1]

[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The salt was first shaken with water to obtain a solution saturated at a temperature slightly above the desired one. Then the solution was allowed to cool down, and stand at the desired temperature for 12 h. The KSCN content was determined in a weighed portion of the saturated solution by titration with standard $AgNO_3$ solution against K_2CrO_4 as the indicator.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] F. Rüdorff, Ber. Deutsch. Chem. Ges. **2**, 68–70 (1869).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. W. Foote, Z. Phys. Chem. **46**, 79–86 (1903).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Two measurements of the solubility of KSCN in water at 25 °C were reported, i.e., 100 $w_1 = 70.38$ and 70.68 mass % ($m_1 = 24.45$ and 24.805 mol kg^{-1}, respectively; compiler).

Auxiliary Information

Method/Apparatus/Procedure:
To an accurately weighed quantity of KSCN, a known amount of water was added in a glass tube so that the salt was in excess. The mixture was first heated till the salt dissolved, and then equilibrated at 25 °C. After equilibration, a small portion of the saturated solution was withdrawn, and the SCN^- content was determined gravimetrically as AgSCN.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. R. Partington and W. E. Soper, Philos. Mag. **7**, 209–47 (1929).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

The solubility of KSCN in water is reported to be 23.91 g KSCN in 10.27 g solvent at 25 °C ($m_1 = 23.96$ mol kg^{-1}; compiler).

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used.

Source and Purity of Materials:
KSCN, source not specified, was an analytical grade product, and was recrystallized before use.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:	**Original Measurements:**
(1) Potassium thiocyanate; KSCN; [333-20-0] (2) Water; H_2O; [7732-18-5]	A. Chrétien and O. Hoffer, Compt. Rend. **201**, 1131–3 (1935).
Variables:	**Prepared By:**
Temperature	J. Hála

Experimental Data

Phase diagram of the KSCN–H_2O system

The data were presented in graphical form (see Fig. 14).

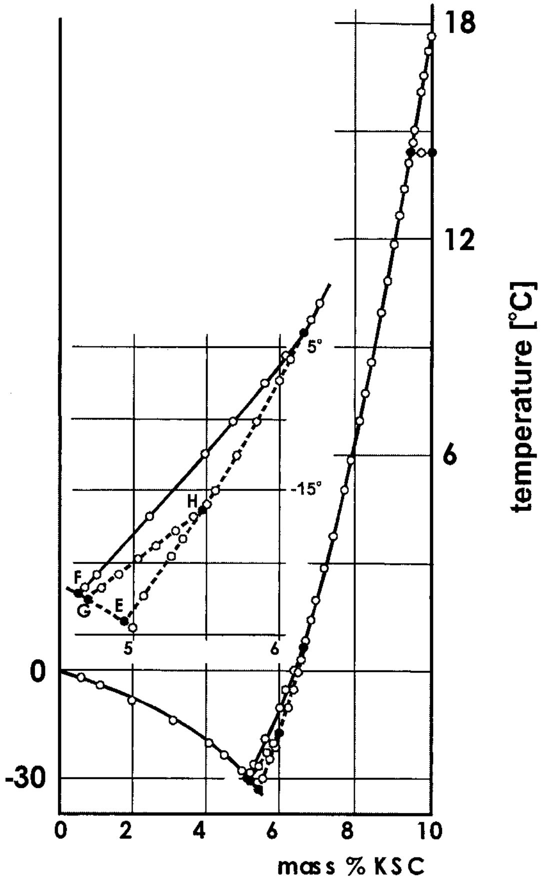

FIG. 14. Phase diagram of the KSCN–H_2O system.

Numerical data were given for the following significant points:

Temperature (t/°C)	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})^a	Significant point
−29.5	51.2	10.80	eutectic (F)
−33.2	54.4	12.28	eutectic–metastable (E)
−30.05	51.8	11.06	eutectic–metastable (G)
+6.8			transition (C)
−17.75	59.7	15.24	transition–metastable (H)

[a] Calculated by compiler.

Additional information: Anhydrous KSCN, [333-20-0], is the equilibrium solid phase over the temperature interval from 6.8 to 177.2 °C (melting point of KSCN). At 142.3 °C (point D in the diagram), transition between two forms of KSCN occurs. Below 6.8 °C, anhydrous KSCN is metastable (section CE). In the temperature interval from −29.5 to +6.8 °C, the equilibrium solid phase is KSCN·$0.5H_2O$ (section CF). At temperatures from −30.1 to −17.75 °C, a metastable phase KSCN·$0.8H_2O$ was observed (section GH).

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used, no details reported.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. C. Kraczek, J. Washington Acad. Sci. **26**, 307–13 (1936).

Variables:
T/K: 305.7–413.9

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in water as a function of temperature[a]

Temperature (t/°C)	KSCN (g/100 g H_2O)	KSCN (100 x_1/mole %)	KSCN (m_1/mol kg^{-1})[b]	Temperature (t/°C)	KSCN (g/100 g H_2O)	KSCN (100 x_1/mole %)
32.6	265.10	32.95	27.28	140.6	1825.6	77.19
47.3	317.05	37.02	32.63	142.7	1957.7	78.40
57.0	358.60	39.93	36.90	146.1	2188.2	80.23
66.7	408.45	43.09	42.03	149.4	2471.1	82.08
74.5	455.90	45.81	46.91	155.0	3116.2	85.25
84.2	526.9	49.42	54.22	157.4	3599.6	86.97
99.0	673.6	55.53	69.31	160.0	4185.8	88.59
108.4	802.9	59.82	82.62	164.5	5773	91.46
116.8	956.6	63.94	98.44	169.2	9342	94.55
124.6	1150.2	68.08		170.7	11961	95.69
130.7	1346.2	71.40		176.8[c]	—	—
133.9	1476.1	73.24				

[a] Solid phases were the two polymorphic forms of KSCN, labeled by the authors as KSCN I and KSCN II. They existed below and above 140.6 °C, which was the point of transition between the two forms.
[b] Calculated by compiler.
[c] Melting point of KSCN.

Additional information: The solubility of KSCN in water as a function of temperature was expressed by the author as

$$\lg(100\ x_1) = a + b(T/\mathrm{K}) + c\ \lg(T/\mathrm{K}) + d(T/\mathrm{K}),$$

where the coefficients a, b, c, and d are −20.71904, 892.459, 7.81532, and 0, respectively, for the temperature range where KSCN I was the equilibrium solid phase, and 31.855 76, −957.918, −12.278 25, and 0.010 8207 for the KSCN II region.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. Weighed quantities of KSCN and water were sealed in Pyrex tubes. The tubes were rotated in a thermostat until all the crystals dissolved, as judged by visual observation. Owing to the destruction of nuclei on complete dissolution, the equilibrium could not be approached from above. Solubility determinations consisted in establishing the temperature at which the last crystal disappeared. The thermostat was a copper-lined muffle furnace of rectangular cross section, open at both ends, and provided with an air propeller, and with a slowly revolving tube holder.

Source and Purity of Materials:

KSCN, reagent grade, was recrystallized, and dried in vacuum at a temperature above the transition point, but below the melting point. No decomposition was noticed.

Estimated Error:

Temperature: ±0.01 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Water-d_2; H_2O-d_2; [7789-20-0]

Original Measurements:
A. Selecki, B. Tyminski, and B. Marianowska, J. Chem. Eng. Data **15**, 130–4 (1970).

Variables:
T/K: 298–363

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in heavy water as a function of temperature[a]

Temperature (t/°C)	KSCN (100 x_1/mole %)	KSCN (m_1/mol kg^{-1})[b]
25	30.0	21.40
35	32.6	24.15
45	35.2	27.12
60	39.8	33.01
75.5	44.4	39.87
91	48.7	47.39

[a] Composition of equilibrium solid phases was not reported.
[b] Calculated by compiler using $M_r = 20.028$ for H_2O-d_2.

Additional information: Refractive indices for solutions of KSCN at various concentrations in heavy water were reported.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. A curve was plotted of refractive indices of KSCN solutions against concentration, at a constant temperature. At the saturation point the curve is broken, and runs horizontally above the saturation point. The saturation point was obtained graphically as the point of intersection of the two branches of the curve. The technique was checked by determining the solubility curve of NaBr in ordinary water with good agreement with published data. Refractive indices were measured by using a RL refractometer, PZO, Warsaw, equipped with Amici prisms. Precision of the refractometer was 0.0002.

Source and Purity of Materials:

KSCN, source not specified, was of analytical purity. H_2O-d_2, product of the USSR. Before solubility determinations, the isotopic composition of oxygen was normalized by electrolytic decomposition of water. The concentration of deuterium in the final product was determined by the picnometric method to be 99.8 mole %.

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.1 mole % (maximum deviation from arithmetic mean; authors).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Water; H_2O; [7732-18-5]; or Water-d_2; H_2O-d_2; [7789-20-0]

Original Measurements:
T. L. Chang and Y. Y. Hsieh, J. Chin. Chem. Soc. **16**, 65–71 (1949).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility at 25 °C of KSCN in water and heavy water

Solubility of KSCN in H_2O: The solubility was reported to be $m_1 = 24.6$ mol kg^{-1} at 25 °C. This value is the mean of four independent measurements, i.e., 24.67, 24.63, 24.56, and 24.58.

Solubility of KSCN in H_2O-d_2: Duplicate analysis of one saturated solution at 25 °C yielded the following compositions of the saturated solution: 0.4469 g KSCN in 0.2135 g solvent, and 0.4805 g KSCN in 0.2298 g solvent (m_1/mol kg^{-1} = 21.54 and 21.52, respectively; compiler).

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Saturated solutions were prepared by the method of supersaturation.[1] The supersaturated solutions, made by agitating excess salt with the solvent at 60 °C for 1 h, were agitated at 25 °C for 2–3 h in a water bath. A sample of the clear solution was delivered into a weighing bottle, the solvent was allowed to evaporate, and the residual salt was dried in vacuum at 100 °C and weighed.

Source and Purity of Materials:
KSCN was a cooling point product of Merck. H_2O-d_2 (Norsk Hydro-Electrisk Kvalstofaktieselskab, Oslo) contained 99.7 mole % deuterium oxide. The H_2O-d_2 content in the solvent was determined by density measurement before and after the measurement. The mole % data were calculated from the density according to Swift.[2]

Estimated Error:
Temperature: precision not reported.
Solubility: standard deviation of $m_1 = \pm 0.05$ mol kg^{-1} (compiler).

References:
[1] T. L. Chang and Y. Y. Hsieh, J. Chinese Chem. Soc. **16**, 10 (1949).
[2] E. Swift, J. Am. Chem. Soc. **61**, 198 (1939).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Sulfur dioxide; SO_2; [7446-09-5]

Original Measurements:
G. Jander and W. Ruppolt, Z. Phys. Chem. **179**, 43–50 (1937).

Variables:
T/K: 273

Prepared By:
J. Hála

Experimental Data

The solubility of KSCN in liquid sulfur dioxide was reported to be 4.87 g salt in 100 g solvent at 0 °C (m_1/mol kg^{-1} = 0.501; compiler). Solid phases were not investigated. However, the authors quoted the existence of the adducts $KSCN \cdot SO_2$ (Walden and Centnerszwer[1] and Ephraim and Kornblum[2]) and $KSCN \cdot 0.5SO_2$ (Ephraim and Kornblum[2]).

Additional information: High solubility of KSCN in liquid ammonia, though not properly specified, was reported in Shatenshtein and Viktorov[4] and Foote and Fleischer.[5] Saturated solutions were yellow in color, and the solid phase was red–orange. In Foote and Fleischer,[5] the composition of the solid phase was reported to be $KSCN \cdot 2SO_2$.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. About 10 g SO_2, carefully dried, was equilibrated with excess solid at 0 °C in water–ice bath in a three-compartment glass vessel in which equilibrating and sampling compartments were separated by a compartment containing glass/wool filter. Equilibration was performed for unspecified, prolonged period of time under frequent shaking. After equilibrium had been attained, the vessel was turned upside down, and the saturated solution was filtered into the empty sampling compartment, which was subsequently cooled and sealed off. After weighing the compartment with the sample, SO_2 was allowed to evaporate, the residue was weighed, dissolved in water, and the content of the salt was determined. The method of analysis was not specified.

Source and Purity of Materials:
KSCN, source not specified, but was carefully dried before use. Commercially available SO_2 was purified by passing it through concentrated H_2SO_4 and over asbestos wool, and dried by using P_2O_5. The specific conductivity of the product was 4.5×10^{-7} Ω^{-1} (Jander and Wickert[3]).

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:
[1] P. Walden and M. Centnerszwer, Z. Phys. Chem. **42**, 432 (1903).
[2] F. Ephraim and I. Kornblum, Ber. **49**, 2007 (1916).
[3] G. Jander and K. Wickert, Z. Phys. Chem. **178**, 57 (1936).
[4] A. I Shatenshtein and M. M. Viktorov, Acta Physicokhim. USSR **7**, 883 (1937).
[5] H. W. Foote and J. Fleischer, J. Am. Chem. Soc. **54**, 3903 (1932).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
G. C. Blytas and F. Daniels, J. Am. Chem. Soc. **84**, 1075–83 (1962).

Variables:
T/K: 214

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in liquid NH_3 at one temperature

The solution saturated at −59 °C (liquidus temperature) was reported to contain 51.38 mass % NH_3. From this, the compiler calculated the solubility of KSCN at −59 °C to be 100 w_1=48.62 mass %, or m_1=9.737 mol kg^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method[1] was used. The salt was quickly introduced into a glass tube, which was then sealed at one end, heated and evacuated for 24 h, and weighed. Then the volume of purified NH_3 necessary to give the desired salt concentration was distilled in, the tube was sealed off, and weighed again. Equilibrating and thermostating were carried out in different baths depending on the temperature range. Calibrated thermometers were used. Liquidus temperatures were recorded as those at which the last crystals disappeared with slow heating. This was preferred to observing temperatures of appearance of first crystals because of the tendency of the system to form supersaturated solutions on cooling.

Source and Purity of Materials:

NH_3 used was stored over sodium metal.

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.01 mass % (authors).

References:

[1] G. C. Blytas and F. Daniels, J. Am. Chem. Soc. **84**, 1075 (1962).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
P. W. Schenk and H. Tulhoff, Ber. Bunsenges. Phys. Chem. **71**, 1155–8 (1967).

Variables:
T/K: 198–259

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in liquid ammonia as a function of temperature

The solubility measurements were presented in graphical form (equilibrium solid phases are indicated in Fig. 15).

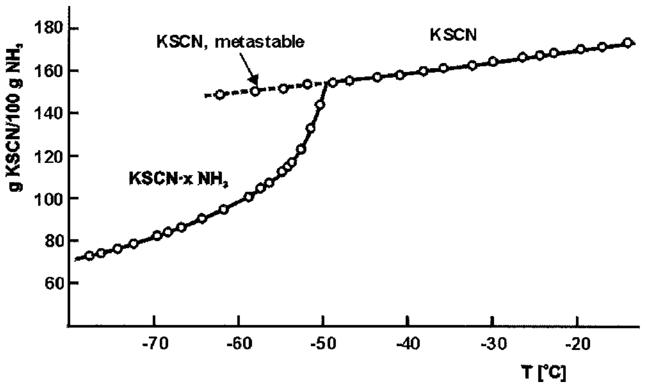

FIG. 15. Solubility of KSCN in liquid ammonia as a function of temperature.

From the graph, the authors obtained the following numerical data by interpolation:

Temperature (t/°C)	KSCN[a] (g/100 g NH_3)	KSCN (m_1/mol kg^{-1})[b]	Temperature (t/°C)	KSCN[a] (g/100 g NH_3)	KSCN (m_1/mol kg^{-1})[b]
−75	75.0	7.718	−60	149[c]	15.33
−70	81.2	8.356	−50	153[c]	15.74
−65	88.1	9.066	−40	157	16.16
−60	96.5	9.930	−30	162	16.67
−55	110	11.32	−20	168	17.29
−50	144	14.82			

[a] Expressed as unsolvated salt.
[b] Calculated by compiler.
[c] KSCN as metastable solid phase. Since the ammoniates crystallized with difficulty it was possible to determine the solubility of KSCN in the metastable range from −49 to −62 °C.

Tensimetric measurements of the solid residues obtained from the saturated solutions after evaporation of the solvent yielded the existence regions of the following ammoniates:

Temperature range, $t/°C$	Solid phase
<-69.7	$KSCN\cdot 5NH_3$
$-69.7--67.9$	$KSCN\cdot 5NH_3+\alpha$-$KSCN\cdot 4NH_3$
$-67.9--60.4$	α-$KSCN\cdot 4NH_3$
$-60.4--56.1$	α-$KSCN\cdot 4NH_3+\beta$-$KSCN\cdot 4NH_3$
$-56.1--53.1$	β-$KSCN\cdot 4NH_3$
$-53.1--52.0$	β-$KSCN\cdot 4NH_3+\gamma$-$KSCN\cdot 4NH_3$
$-52.0--49.1$	γ-$KSCN\cdot 4NH_3$
>-49.1	KSCN, [333-20-2]

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method[1] was used. Measurements were carried out in a vessel connected to a vacuum line, and thermostated with methanol cooled in a cryostat. To a known amount of the solid salt, ammonia was gradually condensed until all solid dissolved. The mixture was intensely stirred during ammonia condensation. Toward the end of dissolution, additions of NH_3 were made small, and were added over sufficiently long time intervals to allow for equilibrium being attained and for keeping the temperature constant. The dissolution process was observed in side light. To ascertain that the point of saturation was not exceeded, the dissolution was stopped when a few very tiny crystals remained undissolved over a prolonged period of time. A small error introduced in this way by using large enough amount of the solid. The total amount of NH_3 condensed was calculated from the temperature, volume of the apparatus, and initial and final pressures of NH_3 .

Source and Purity of Materials:

No details were reported as for KSCN. Ammonia gas was dried by passing it through towers filled with NaOH, CaO, BaO, and sodium metal.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] P. W. Schenk and H. Tulhoff, Ber. Bunsenges. Phys. Chem. **71**, 206 (1967).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Acetonitrile; C_2H_3N; [75-05-8]

Original Measurements:

A. Naumann, Ber. **47**, 247–56 (1914).

Variables:

T/K: 291

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN in acetonitrile at one temperature

The solubility of KSCN was reported to be 0.1131 g salt in 1 g solvent at 18 °C. From this value, the compiler calculated $100\ w_1=10.16$ mass %, or $m_1=1.164\ \mathrm{mol\ kg^{-1}}$.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess solid was shaken with the solvent in a water thermostat for 2–6 h. Attainment of equilibrium was checked by occasional analysis of the liquid phase. The saturated solutions were rapidly filtered into weighing vessels kept at 18 °C, and the content of SCN^- was determined titrimetrically (presumably by the Volhard's method).

Source and Purity of Materials:

KSCN, source and purity not specified, was dried in a vacuum dessicator before use. Acetonitrile (Kahlbaum) was purified from acetamide by allowing the solvent to stand for 3–4 weeks over P_2O_5 , and distilled. The product used boiling point at 81.6 °C.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate. The solubility value reported is the mean of two determinations (individual results not reported).

Components:	Original Measurements:
(1) Potassium thiocyanate; KSCN; [333-20-0] (2) 1,2-ethanediamine (ethylenediamine); $C_2H_8N_2$; [107-15-3]	H. S. Isbin and K. A. Kobe, J. Am. Chem. Soc. **67**, 464–5 (1945).
Variables:	**Prepared By:**
T/K: 298	J. Hála

Experimental Data

Solubility of KSCN in ethylenediamine at 25 °C

The solubility of KSCN is reported to be 83.0 g in 100 g solvent (compiler: $m_1 = 8.54$ mol kg^{-1}). The composition of the solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. The solvent and excess solid were sealed in a glass test tube and rotated for at least 1 week in a water thermostat, which was found sufficient for equilibrium to be reached. Samples of the saturated solution were withdrawn with a weighing pipette, and analyzed for SCN^- content by titration against a standard $AgNO_3$ solution.

Source and Purity of Materials:

KSCN, analytical grade, was dried at 150 °C before use. Ethylenediamine, source not specified, was dehydrated and purified according to Putnam and Kobe.[1]

Estimated Error:

Temperature: ±0.08 K (authors).
Solubility: ±0.5% (authors).

References:

[1] G. L. Putnam and K. A. Kobe, Trans. Electrochem. Soc. **74**, 609 (1938).

6.3.2. Evaluation of the KSCN–Ethanol System

Components:	Evaluator:
(1) Potassium thiocyanate; KSCN; [333-20-0] (2) Ethanol; C_2H_6O; [64-17-5]	J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, July 2001.

Critical Evaluation

The solubility of KSCN in ethanol has been reported in three documents. Nikitina *et al.*[1] reported the solubility as a function of temperature over the range from 283 to 323 K while Stepin and co-workers[2] reported a single value at 298 K. The other document[3] has not been available to the evaluator. Nikitina *et al.*[1] did not specify the concentration unit in which they expressed the solubility. Assuming they used molality, as they did in their later work,[4] their solubility value at 298 K can be compared to that of Stepin *et al.*,[2] the respective values being m_1 /mol kg^{-1} = 0.241 (Nikitina *et al.*[1]) and 0.530 (Stepin *et al.*[2]). This difference can presumably be ascribed to the purity of ethanol since for the solubility of KSCN in organic solvents, water content in the latter is of crucial importance due to the high solubility of KSCN in water. However, it has not been possible to draw any definite conclusion as for the purity of ethanol used in the two documents. Nikitina *et al.*[1] did not report any information on purity of the solvent, while the density of ethanol of 0.7987 g cm^{-3} reported by Stepin *et al.*[2] seems to correspond to approximately 98% purity of ethanol. Due to scarcity of information provided in the two documents, no data can be recommended.[5]

References:

[1] I. P. Nikitina, B. S. Krumgalz, D. G. Traber, and G. F. Fedotova, Zh. Neorg. Khim. **14**, 2593 (1969).
[2] B. D. Stepin, V. E. Plyushchev, and Yu. A. Ivanova, Khim. Prom. (Chem. Industry) 404 (1962).
[3] B. S. Krumgalz, Teoria Rastvorov (Theory of Solutions) 242 (1971); Chem. Abstr. **77**, abstract no. 157018 (1972).
[4] B. S. Krumgalz, V. A. Smirnova, and Yu. I. Gerzberg, Zh. Neorg. Khim. **17**, 1778 (1972).
[5] *Physico-Chemical Tables* (Publ. House Tech. Lit, Prague, 1953), Vol. 1, p. 320.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
I. P. Nikitina, B. S. Krumgalz, D. G. Traber, and G. F. Fedotova, Zh. Neorg. Khim. **14**, 2593–4 (1969).

Variables:
T/K: 283–323

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in ethanol as a function of temperature[a]

Temperature (t/°C)	KSCN (m_1/mol kg^{-1})[b]
10	0.188
15	0.205
20	0.222
25	0.241
30	0.260
35	0.281
40	0.301
45	0.322
50	0.342

[a] Solid phases were not investigated.

[b] Concentration unit not specified in the original document. The compiler assumed this to be molality, as in the authors' other work.[1]

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method[2] was used. Excess solid was equilibrated with ethanol by stirring in a closed, thermostated vessel. Attainment of equilibrium was checked by measuring electrical conductivity of the solution. To this aim, an electrolytic cell closed with a glass sinter was immersed in the solution throughout the measurement. At chosen time intervals, the measured solution was sucked in between two platinum electrodes, the conductivity was measured, and the solution was transferred back from the cell to the solubility vessel by applying overpressure of dry air. The procedure was repeated until steady conductivity of the solution was obtained. The equilibrium conductivity value was then used to read the concentration of KSCN in the saturated solution from a calibration graph of conductivity plotted against KSCN concentration in acetone.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.2% (error of conductivity measurements; authors).

References:

[1] B. S. Krumgalz, V. A. Smirnova, and Yu. I. Gerzberg, Zh. Neorg. Khim. **17**, 1778 (1972).
[2] B. S. Krumgalz, Yu. I. Gerzhberg, I. P. Nikitina, V. I. Derevskaya, G. F. Fedotova, and D. G. Traber, Zh. Prikl. Khim. **42**, 1414 (1969).

6.3.3. Evaluation of the KSCN–Acetone System

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 2-propanone (acetone); C_3H_6O; [67-64-1]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, July 2001.

Critical Evaluation

Two investigations of the solubility of KSCN in acetone have been reported. Laszczynski[1] reported the solubilities at 295 and 331 K, and Dernini *et al.*[2] reported the solubility at the boiling point of the saturated solution, but did not report the boiling point temperature. The latter has been calculated by the evaluator to be 331.8 K, using ebulioscopic constant and normal boiling point of acetone. Although this temperature is very close to that of 331 K used in Laszczynski,[1] the two respective solubility values differ considerably, i.e., m_1/mol kg^{-1}=2.10 (Laszczynski[1]) and 1.41 (Dernini *et al.*[2]). The reason for this discrepancy is not clear. Even though the solubility reported by Laszczynski[1] at 295 K coincides well with that for 293 K given graphically by Weitz and Grohrock[3] none of the solubility data can be recommended.

References:

[1] S. von Laszczynski, Ber. **27**, 2285 (1894).
[2] S. Dernini, R. DeSantis, and L. Marrelli, J. Chem. Eng. Data **21**, 170 (1976).
[3] E. Weitz and E. Grohrock **67**, 1085 (1934).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 2-Propanone (acetone); C_3H_6O; [67-64-1]

Original Measurements:
S. von Laszczynski, Ber. **27**, 2285–8 (1894).

Variables:
T/K: 295, 331

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in acetone at two temperatures[a]

Temperature (t/°C)	KSCN (g/100 g solvent)[b]	KSCN (m_1/mol kg^{-1})[c]	KSCN (100 w_1/mass %)[c]
22	20.75	2.135	17.2
58	20.40	2.099	16.9

[a] Solid phases were not investigated.
[b] Mean of at least two measurements, individual results not reported.
[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess solid was equilibrated with the solvent for a prolonged period of time in a flask equipped with a reflux condenser. The flask was kept in a water bath at the desired temperature. Samples of clear saturated solutions were withdrawn into small flasks, weighed, the solvent was allowed to evaporate, and the residue was weighed again.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; NaSCN; [333-20-0]
(2) Methylacetate; $C_3H_6O_2$; [79-20-9]

Original Measurements:
J. Schroeder and M. Steiner, J. Prakt. Chem. **79**, 49–65 (1909).

Variables:
One measurement at boiling point temperature.

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in boiling methylacetate

The solubility of KSCN is reported to be 100 $w_1 = 0.85$ mass % at boiling point of the saturated solution (compiler: $m_1 = 0.0882$ mol kg^{-1}). The boiling point temperature was not reported. The solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:

Excess salt was boiled with methylacetate for a prolonged period of time in a flask closed with a stopper through which a short glass tube was protruding. The latter contained glass wool as a filter at the bottom end, and was made into a short capillary at the upper end. By turning the flask upside down, a portion of the saturated solution was allowed to pour out into a weighing flask. After more boiling, another two samples were taken in the same way. The samples were then evaporated, and the residue weighed.

Source and Purity of Materials:

KSCN, source and purity not specified, was dried at 110 °C before use. Methylacetate was kept over anhydrous $CuSO_4$ for a prolonged period of time, and distilled. The fraction boiling at 56.2–56.7 °C was collected and stored in the dark.

Estimated Error:

Solubility: insufficient data reported to allow for error estimate.

6.3.4. Evaluation of the KSCN–2-Butanone System

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 2-Butanone; C_4H_8O; [78-93-3]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, July 2001.

Critical Evaluation

Two measurements of the solubility of KSCN in 2-butanone (methylethylketone) at 298 K have been reported.[1,2] The solubilities were obtained by isothermal method as $m_1/\text{mol kg}^{-1} = 0.180$ (Stepin *et al.*[1]) and 0.141 (Krupatkin *et al.*[2]), as calculated from the authors' mass % data. Since in both documents the solvent was purified before use, it is recommended to use the mean of the two values, 0.16 ± 0.02 mol kg^{-1}, as the tentative solubility at 298 K.

References:

[1] B. D. Stepin, V. E. Plyushchev, and Yu. A. Ivanova, Khim. Prom. (Chem. Industry) 404 (1962).
[2] I. L. Krupatkin, L. D. Vorobeva, V. P. Makhulia, and M. E. Veselova, Zh. Obsh. Khim. **45**, 985 (1975).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Ethylacetate; $C_4H_8O_2$; [141-78-6]

Original Measurements:
S. von Laszczynski, Ber. **27**, 2285–8 (1894).

Variables:
T/K: 273, 287, 352

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in ethylacetate at three temperatures[a]

Temperature (t/°C)	KSCN (g/100 g solvent)[b]	KSCN ($m_1/\text{mol kg}^{-1}$)[c]
0	0.44	0.0453
14	0.40	0.0412
79	0.20	0.0206

[a] Solid phases were not investigated.
[b] Mean of at least two measurements, individual results not reported.
[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Excess solid was equilibrated with the solvent for a prolonged period of time in a flask equipped with a reflux condenser. The flask was kept in a water bath at the desired temperature. Samples of clear saturated solutions were withdrawn into small flasks, weighed, the solvent was allowed to evaporate, and the residue was weighed again.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

6.3.5. Evaluation of the KSCN–1-Butanol System

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Evaluator:
J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, July 2001.

Critical Evaluation

Two measurements of the solubility of KSCN in 1-butanol have been reported.[1,2] In both documents, isothermal method was used, and the solvent was dried and distilled before use. Ionin *et al.*[1] reported the solubility of KSCN as a function of temperature over the range from 273 to 338 K, while Bakeev and Akimova[2] reported a single value at 313 K as $m_1 = 0.148$ mol kg^{-1}. The solubility value obtained by interpolation to 313 K from the data in Ionin *et al.*[1] is approximately 0.13 mol kg^{-1}. Since the two values agree reasonably, and the data of Ionin *et al.*[1] cover a wider temperature range, it is recommended to use the latter data as tentative values.

References:

[1] M. V. Ionin, Z. B. Kuznetsova, and T. I. Moleva, Zh. Neorg. Khim. **14**, 2850 (1969).
[2] M. I. Bakeev and I. P. Akimova, Dep. Doc. VINITI No. 1148–76 (1976).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
M. V. Ionin, Z. B. Kuznetsova, and T. I. Moleva, Zh. Neorg. Khim. **14**, 2850–3 (1969).

Variables:
T/K: 273–338

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in 1-butanol as a function of temperature[a]

Temperature (t/°C)	KSCN (m_1/mol kg^{-1})
0	0.050
10	0.047
15	0.070
20	0.077
25	0.090
35	0.114
45	0.146
55	0.173
65	0.219

[a] Solid phases were not investigated.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. No details reported except that the concentration of SCN^- in the saturated solutions was determined by titration with a standard $Hg(NO_3)_2$ solution against Fe(III) salt as an indicator.

Source and Purity of Materials:
KSCN, chemically pure, was recrystallized from water. 1-Butanol was dried and distilled on a column. The fraction boiling point at 117.5 °C was used.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Tetrahydro-1,1-thiophene dioxide (sulfolane); $C_4H_8O_2S$; [126-33-0]

Original Measurements:

P. Srivastava, M. M. Husain, and R. Gopal, J. Chem. Eng. Data **30**, 144–5 (1985).

Variables:

T/K: 313–328

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN in sulfolane as a function of temperature[a]

Temperature (t/°C)	KSCN (g/100 g solvent)	KSCN (m_1/mol kg^{-1})[b]
40	18.59	1.913
45	20.59	2.119
50	21.44	2.206
55	22.38	2.303

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. A sample of the saturated solution in a Petri dish was heated carefully in an oven, and finally on an electrical heater to expel the solvent completely. Too rapid heating was avoided to check spurting of the solution and charring of sulfolane. The dish was then cooled in dry nitrogen box and weighed. The procedure was repeated until constant weight of the residue was obtained.

Source and Purity of Materials:

KSCN, source and purity not specified, was recrystallized twice from conductivity water, and dried under vacuum before use. Sulfolane, Fluka puriss., was purified according to Pankaj and Gopal.[1] Melting point of the purified product was close to 27 °C, density at 40 °C was 1.2515 g cm^{-3}.

Estimated Error:

Temperature: precision not reported.
Solubility: ±1% (authors).

References:

[1] Pankaj and R. Gopal, Indian J. Chem. **21A**, 404 (1982).

6.3.6 Evaluation of the KSCN–Pyridine System

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Pyridine; C_5H_5N; [110-86-1]

Evaluator:

J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, July 2001.

Critical Evaluation

Two investigations[1,2] of the solubility of KSCN in pyridine have been reported. Both sets of data agree in that the solubility decreases with increasing temperature. However, the solubility data differ considerably, the data from the polythermal measurements[2] being 3–4 times lower than those obtained by the isothermal method.[1] It is not clear from the published information whether this is caused by deviations from the true equilibrium in the polythermal measurements,[2] or by insufficient drying of the solvent used in the isothermal study[1] since no details were reported about materials used. Due to the high solubility of KSCN in water, the purity of the solvent with respect to water content could affect the solubility of the salt in pyridine considerably. For these reasons, none of the two sets of data can be recommended, and the KSCN–pyridine system would need a reinvestigation.

References:

[1] S. von Laszczynski, Ber. **27**, 2285 (1894).
[2] K. L. Wagner and E. Zerner, Monatsh. Chem. **31**, 833 (1910).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Pyridine; C_5H_5N; [110-86-1]

Original Measurements:
S. von Laszczynski, Ber. **27**, 2285–8 (1984).

Variables:
T/K: 273–388

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in pyridine as a function of temperature[a]

Temperature (t/°C)	KSCN (g/100 g solvent)[b]	KSCN (m_1/mol kg^{-1})[c]	KSCN (100 w_1/mass %)[c]
0	6.75	0.695	6.32
20	6.15	0.633	5.96
58	4.97	0.511	4.73
95	3.88	0.399	3.74
115	3.21	0.330	3.11

[a] Solid phases were not investigated.
[b] Mean of at least two measurements, individual results not reported.
[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess solid was equilibrated with the solvent for a prolonged period of time in a flask equipped with a reflux condenser. The flask was kept in a water bath at the desired temperature. Samples of clear saturated solutions were withdrawn into small flasks, weighed, the solvent was allowed to evaporate, and the residue was weighed again.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Pyridine; C_5H_5N; [110-86-1]

Original Measurements:
K. L. Wagner and E. Zerner, Monatsh. Chem. **31**, 833–41 (1910).

Variables:
T/K: 230–390

Prepared By:
J. Hála

Experimental Data

Solubility in the KSCN–pyridine system

Liquidus temperature (t/°C)	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[e]
116–117	0.89	0.0924	A
70–71	1.23	0.128	A
10[b]	2.2	0.231	A
−43.3[c]	3.1	0.329	A+B
−42.8	2.4	0.253	B
−42.4	1.33	0.139	B
−42.1	0.5	0.0517	B
−42[d]	0		

[a] Calculated by compiler.
[b] Mean of several readings taken between 8 and 12 °C.
[c] Very close to eutectic point.
[d] Melting point of pyridine.
[e] A: KSCN; [333-20-0]; B: C_5H_5N; [110-86-1].

Additional information: At 172.8 °C, the homogeneous solution separated into two liquid phases containing approximately 0.6 mass % KSCN, and at least 92.7 mass % KSCN. The pyridine rich phase contained 0.4 mass % KSCN at 188.5 °C.

Auxiliary Information

Method/Apparatus/Procedure:

Sythetic polythermal method used. Measurements were carried out in sealed glass ampoules with volumes of 0.5–1.0 cm^3. First, KSCN was introduced, dried at 100 °C, and weighed. Then pyridine was added from a capillary pipette, the ampoule was sealed and weighed again. The ampoules were rotated in a thermostated bath of concentrated H_2SO_4. Liquidus temperatures were obtained as the mean of readings of disappearance of last crystals, and appearance of first crystals.

Source and Purity of Materials:

KSCN, Merck, p.a., was twice recrystallized from water, then precipitated by ethanol, and dried in vacuum over P_2O_5. Pyridine was refluxed for 3 h with CaO, and fractionated. The middle fraction was then three times fractionated, and the fraction boiling at 115.37 °C was used.

Estimated Error:

Temperature: ±2 K around 10 °C, ±0.5 K at higher temperatures (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) N,N-Dimethylacetamide; C_4H_9NO; [127-19-5]

Original Measurements:

A. A. Fedorov, L. B. Sokolov, V. M. Savinov, M. A. Shlionskaya, and N. I. Filatova, Zh. Prikl. Khim. **44**, 2361–2 (1971).

Variables:

T/K: 295–298

Prepared By:

J. Hála

Experimental Data

The solubility of KSCN in N,N-dimethylacetamide is reported to $c_1 = 1.10$ mol dm^{-3} at 22–25 °C. The nature of the equilibrium solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:

The solvent was saturated with anhydrous salt. Then a part of the solvent was distilled off to remove water, and the saturated solution with excess solid was kept for 3 days in a desiccator in a paraffine-coated flask. The content of water in the saturated solution was less than 0.1%. The saturated solution was analyzed for the content of sulfur by an unspecified method.

Source and Purity of Materials:

Anhydrous KSCN, source not specified, was dried at 120 °C for 6 h N,N-dimethylacetamide, source not specified, was freshly distilled before use.

Estimated Error:

Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Original Measurements:

S. von Laszczynski, Ber. **27**, 2285–8 (1894).

Variables:

T/K: 284–406

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN in 1-pentanol as a function of temperature[a]

Temperature (t/°C)	KSCN (g/100 g solvent)[b]	KSCN (m_1/mol kg^{-1})[c]	KSCN (100 w_1/mass %)[c]
13	0.18	0.0185	0.18
65	1.34	0.138	1.32
100	2.14	0.220	2.10
133.5	3.15	0.324	3.05

[a] Solid phases were not investigated.
[b] Mean of at least two measurements, individual results not reported.
[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess solid was equilibrated with the solvent for a prolonged period of time in a flask equipped with a reflux condenser. The flask was kept in a water bath at the desired temperature. Samples of clear saturated solutions were withdrawn into small flasks, weighed, the solvent was allowed to evaporate, and the residue was weighed again.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Tri-n-butyl(phosphate); $C_{12}H_{27}O_4P$; [126-73-8]

Original Measurements:
J. Hála and D. G. Tuck, Can. J. Chem. **48**, 2843–6 (1970).

Variables:
T/K: 295

Prepared By:
J. Hála

Experimental Data

The solubility of KSCN in tri-n-butyl(phosphate) is reported to be 6.96 g salt in 100 g solvent at 22 °C ($m_1 = 0.716$ mol kg^{-1}; compiler).

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. An excess of the salt was shaken overnight with 5 mL dry solvent. Preliminary experiments showed that this was sufficient for equilibrium to be reached. Samples of the saturated solutions were withdrawn through a sinter, diluted with acetone, and analyzed for the thiocyanate content by titration against $AgNO_3$ standard solution. Blank titrations showed that a small correction was required because of the presence of tri-n-butyl(phosphate).

Source and Purity of Materials:

KSCN, Fisher Scientific Co., was used without further purification. Tri-n-butyl(phosphate) (Fisher Scientific Co.) was purified by refluxing it with 0.5% caustic soda solution, followed by steam distillation. The product was dried first with anhydrous $MgSO_4$, and finally vacuum/dried at 50 °C in a stream of dry nitrogen gas.[1]

Estimated Error:

Temperature: precision not reported.
Solubility: ±0.1 g salt/100 g solvent (authors).

References:

[1] D. G. Tuck, J. Chem. Soc. 2783 (1958).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Solvents

Original Measurements:
S. Dernini, R. DeSantis, and L. Marrelli, J. Chem. Eng. Data **21**, 170–3 (1976).

Variables:
Measurements at boiling points of the saturated solutions.

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in two solvents at boiling points at 760 mm Hg pressure[a]

Solvent	KSCN (g/100 g solvent)	KSCN (m_1/mol kg^{-1})[b]	Boiling point of the saturated solution[c] (t/°C)
Acetone; C_3H_6O; [67-64-1]	13.7	1.41	58.6
Methanol; CH_4O; [67-56-1]	50.1	5.16	68.6

[a] Solid phases were not investigated.
[b] Calculated by compiler.
[c] Calculated by compiler using ebulioscopic constants of 1.7 and 0.8, and normal boiling points[1] of 56.15 and 64.51 °C for acetone and methanol, respectively, and assuming undissociated KSCN in the saturated solutions.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Determination of the solubilities was performed by sampling 10 mL of the boiling liquid, and weighing first the sample, and then the residue after thorough evaporation of the solvent.

Source and Purity of Materials:

KSCN was of 99.5 mass % purity. Acetone and methanol, source not specified, were both of 99.9 mass % purity.

Estimated Error:

Solubility: insufficient data given to allow for error estimate.

References:

[1] E. Hála and A. Reiser, *Physical Chemistry* (Czech Edition) (Academia, Prague, 1971), Vol. 1, p. 278.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Solvents

Original Measurements:
I. L. Krupatkin, L. D. Vorobeva, V. P. Maskhulia, and M. E. Veselova, Zh. Obsh. Khim. **45**, 985–90 (1975).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in furfural and methylethylketone at 25 °C[a]

Solvent	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[b]
2-furancarboxaldehyde (furfural); $C_5H_4O_2$; [98-01-1]	16.30	2.004
2-butanone (methylethylketone); C_4H_8O; [78-93-3]	1.35	0.141

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details reported.

Source and Purity of Materials:
KSCN, source and purity not specified, was dried at 100 °C to constant weight before use. The solvents were purified by standard methods,[1] and their purity was checked through physical constants.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] A. Weisberger, E. Proskanzer, J. Riddick, and E. Toops, *Organic Solvents*, Russian ed. (IL Publ. House, Moscow, 1958), pp. 351 and 361.

Components:
(3) Potassium thiocyanate; KSCN; [333-20-0]
(4) Solvents

Original Measurements:
B. D. Stepin, V. E. Plyushchev, and Yu. A. Ivanova, Khim. Prom. (Chem. Industry) 404–7 (1962).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN at 25 °C in five solvents[a]

Solvent	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[b]
Methanol; CH_4O; [67-56-1]	22.40	2.970
Ethanol; C_2H_6O; [64-17-5]	4.90	0.530
2-Butanone; C_4H_8O; [78-93-3]	1.72	0.180
Cyclohexanone; $C_6H_{10}O$; [108-94-1]	3.70	0.395
1-Phenylethanone; C_8H_8O; [98-86-2]	1.10	0.115

[a] Solid phases not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details reported.

Source and Purity of Materials:
Refractive indices and densities, respectively, both at 20 °C, of the solvents used were as follows: methanol, 1.3289, 0.7908; ethanol, 1.3609, 0.7987; 2-butanone, 1.3780, 0.8041; cyclohexanone, 1.4500, 0.9453; 1-phenylethanone (acetophenone), 1.5328, 1.0270.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Water; H_2O; [7732-18-5]
(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:

M. I. Bakeev and I. P. Akimova, Dep. Doc. VINITI, No. 1148–76 (1976).

Variables:

T/K: 313
100 w_2/mass %: 0–26.48

Prepared By:

J. Hála

Experimental Data

Composition of solutions saturated at 40 °C[a]

H_2O (100 w_2/mass %)	H_2O (m_2/mol kg^{-1})[b]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[b]
0	0	1.42	0.148
0.96	0.552	2.56	0.273
1.42	0.826	3.15	0.340
26.48		73.52[c]	28.75

[a] Solid phases were not investigated.
[b] Calculated by compiler.
[c] Solubility of KSCN in water.

Additional information: The phase diagram of the KSCN–$C_4H_{10}O$–H_2O system at 20 °C was also reported.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, no details reported.

Source and Purity of Materials:

KSCN, reagent grade, was recrystallized before use. Butanol, reagent grade, was dried and distilled before use.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium chloride; KCl; [7447-40-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. S. Bogoyavlenskii, and K. M. Syui, Zh. Strukt. Khim. **1**, 425–30 (1960).

Variables:

T/K: 298
100 w_2/mass %: 0–25.56

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN at 25 °C in water and one aqueous solutions of KCl

KCl (100 w_2/mass %)	KCl (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	71.10	25.32	A
1.62	0.755	69.59	24.87	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-2]; B: KCl, [7447-40-7].

Additional information: In addition to the data shown above, the authors also reported the compositions of 18 saturated solutions containing 2.00–26.56 mass % KCl, where KCl was the equilibrium solid phase. These data are not shown here since they refer to the solubility of KCl in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. No details reported except that the solid and liquid phases were analyzed for the content of Cl^- and SCN^- ions by potentiometric titration against standard $AgNO_3$ solution.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium chloride; KCl; [7447-40-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Babenko and A. M. Andrianov, Ukrain. Khim. Zh. **45**, 931–4 (1979).

Variables:

T/K: 242–299
100 w_2/mass %: 0–19.9

Prepared By:

J. Hála

Experimental Data

Solubility in the KSCN–KCl–H_2O system as measured by polythermal method

KCl (100 w_2/mass %)	KSCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]	KCl (100 w_2/mass %)	KSCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]
19.9	0	−10.8	A+B	1.662	44.4	−21.6	A+B+D
16.0	8.4	−10.0	A+B	3.0	53.35	−21.0	B+D
12.0	17.6	−13.0	A+B	2.5	58.5	−14.0	B+D
8.0	27.6	−15.6	A+B	0	63.9	0	C+D
6.8	32.0	−17.6	A+B	1.155	62.5	−11.5	B+C+D
4.0	38.56	−19.6	A+B	3.3	64.789	+15.0	B+C
2.0	47.04	−24.2	A+B	3.1	64.923	+26.0	B+C
1.56	48.0	−26.5	A+B+C	3.8	62.0	0	B+C
0	50.2	−31.2	A+B+D				

Solubility isotherms in the KSCN–KCl–H_2O system[b]

Temperature (t/°C)	KCl (100 w_2/mass %)	KCl (m_2/mol kg^{-1})[c]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[c]	Solid phase[a]
−20	0	0	55.5	12.83	D
−10	0	0	59.7	15.24	D
	3.4	1.049	53.13	12.58	D
0	0	0	64.0	18.29	D
	1.092	0.4148	63.6	18.54	D
10	0	0	66.5	20.43	C
	1.081	0.4431	66.2	20.82	C
	1.76	0.7059	64.8	19.94	C
20	0	0	69.0	22.90	C
	1.63	0.7059	67.4	22.39	C
	3.48	1.490	65.2	21.42	C
30	0	0	72.0	26.46	C
	0.864	0.4148	71.2	26.23	C
	3.2	1.490	68.0	24.30	C
	3.5	1.622	67.55	24.01	C

[a] A: Ice, H_2O, [7732-18-5]; B: KCl, [7447-40-7]; C: KSCN; [333-20-2]; D: KSCN· $0.5H_2O$, [ ].

[b] Solubility isotherms were obtained by the authors from polythermal measurements. Of numerous data reported, only those referring to the solubility of KSCN were included here. In systems containing higher KCl concentrations, the equilibrium solid phases were either ice or KCl.

[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Visual polythermal method used. In total, 12 sections of the KSCN–KCl–H_2O system were investigated, of which nine corresponded to 10, 20, 30, 40, 48, 55, 60, 67, and 70 mass % KSCN, and three to 3, 5, and 10 mass % KCl. Measurements were carried out in an apparatus described in Eraizer and Kaganskii.[1] The solubility vessel, equipped with a thermometer, was coated with a transparent semiconductor layer to which two heating silver electrodes were soldered. The vessel was placed inside a Dewar flask with transparent walls which, in measurements performed below room temperature, was filled to 1/5 of its volume with liquid nitrogen or solid CO_2. With the solubility vessel kept above the coolant, it was possible to control the rate of cooling or heating by moving the Dewar flask. The mixture in the solubility vessel was stirred by using two external electromagnets, and illuminated to observe disappearance or appearance of crystals.

Source and Purity of Materials:

KSCN and KCl were chemically pure products. They were recrystallized twice before use, and dried at 40–50 °C.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] L. N. Eraizer and I. M. Kaganskii, Zavodskaya Lab. **33**, 119 (1967).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium bromide; KBr; [7758-02-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. S. Bogoyavlenskii and K. M. Syui, Zh. Neorg. Khim. **6**, 469–73 (1961).

Variables:

T/K: 298, 313
100 w_2/mass %: 0–40.87 at 298 K
0–43.17 at 313 K

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN at 25 and 40 °C in water and aqueous solutions of KBr

Temperature (t/°C)	KBr (100 w_2/mass %)	KBr (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
25	0	0	71.10	25.32	A
	4.00	1.171	67.30	24.13	A+B
40	0	0	74.38	29.87	A
	1.98	0.647	72.32	28.96	A
	4.29	1.445	70.76	29.18	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-2]; B: KBr, [7758-02-3].

Additional information: In addition to the data shown above, the authors also reported the compositions of 12 (at 25 °C) and 20 (at 40 °C) saturated solutions containing 5.60–40.87 and 4.79–43.17 mass % KBr, respectively, where KBr was the equilibrium solid phase. These data are not shown here since they refer to the solubility of KBr in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. No details reported except that the solid and liquid phases were analyzed for the content of Br^- and SCN^- ions by potentiometric titration against standard $AgNO_3$ solution according to Mahr and Otterbein.[1] In one sample, the sum of both anions was determined, in another sample, the SCN^- was decomposed by action of H_2O_2, and Br^- was titrated.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] C. Mahr and H. Otterbein, Angew. Chem. **66**, 636 (1954).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium iodide; KI; [7681-11-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. S. Bogoyavlenskii and K. M. Syui, Zh. Strukt. Khim. **1**, 425–30 (1960).

Variables:

T/K: 298
100 w_2/mass %: 0–59.42

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN at 25 °C in water and aqueous solutions of KI

KI (100 w_2/mass %)	KI (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	71.10	25.32	A
4.72	1.008	67.06	24.45	A
6.72	1.463	65.61	24.40	A
9.38	2.080	63.45	24.03	A
12.87	2.907	60.46	23.33	A
15.55	3.592	58.37	23.03	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-2]; B: KI, [7681-11-0].

Additional information: In addition to the data shown above, the authors also reported the compositions of ten saturated solutions containing 16.97–59.42 mass % KI, where KI was the equilibrium solid phase. These data are not shown here since they refer to the solubility of KI in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. No details reported except that the solid and liquid phases were analyzed for the content of I^- and SCN^- ions by potentiometric titration against standard $AgNO_3$ solution.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium nitrite; KNO_2; [7758-09-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
P. S. Bogoyavlenskii and L. Kh. Van, Zh. Strukt. Khim. **1**, 431–6 (1960).

Variables:
T/K: 298
100 w_2/mass %: 0–76.16

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN at 25 °C in water and aqueous solutions of KNO_2

KNO_2 (100 w_2/mass %)	KNO_2 (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	70.83	24.90	A
3.68	1.531	68.08	24.80	A
8.41	3.723	65.05	25.22	A
13.22	6.319	62.20	26.03	A
18.12	9.197	58.73	26.10	A
22.44	11.86	55.34	25.62	A
27.85	16.09	51.82	26.22	A
32.46	20.49	48.93	27.95	A
40.17	29.87	43.87	28.28	A
45.21	37.22	40.52	29.21	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-2]; B: KNO_2, [7758-09-0].

Additional information: In addition to the data shown above, the authors also reported the compositions of seven saturated solutions containing 50.82–76.16 mass % KNO_2, where KNO_2 was the equilibrium solid phase. These data are not shown here since they refer to the solubility of KNO_2 in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. No details reported except that the solid and liquid phases were analyzed for the content of SCN^- and K^+ ions by potentiometric titration against standard $AgNO_3$ solution, and gravimetrically as K_2SO_4, respectively.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium nitrate; KNO_3; [7757-79-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
P. S. Bogoyavlenskii, Dokl. Akad. Nauk SSSR **101**, 865–8 (1955); Zh. Fiz. Khim. **32**, 2035–41 (1958).

Variables:
T/K: 298
100 w_2/mass %: 0–27.16

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN at 25 °C in water and aqueous solutions of KNO_3

KNO_3 (100 w_2/mass %)	KNO_3 (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	70.7	24.83	A
6.35	2.325	66.64	25.39	A
9.45	3.687	65.2	26.47	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-0]; B: KNO_3, [7757-79-1].

Additional information: In addition to the data shown above, the authors also reported the compositions of nine saturated solutions containing 9.94–27.16 mass % KNO_3, where KNO_3 was the equilibrium solid phase. These data are not shown here since they refer to the solubility of KNO_3 in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:
No details reported but the compiler assumes that the same procedure was adopted as in the authors previous work,[1] i.e., isothermal method and chemical analysis of the equilibrium solid phases, and identification of solid phases by optical microscopy.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] P. S. Bogoyavlenskii and G. V. Sukmanskaya, Zh. Obsh. Khim. **23**, 1092 (1953).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium nitrate; KNO_3; [7757-79-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Babenko and A. M. Andrianov, Zh. Neorg. Khim. **23**, 3123–6 (1978).

Variables:

T/K: 243–292
100 w_2/mass %: 0–10

Prepared By:

J. Hála

Experimental Data

Solubility in the KSCN–KNO_3–H_2O system as measured by polythermal method

KNO_3 (100 w_2/mass %)	KSCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]	KNO_3 (100 w_2/mass %)	KSCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]
10.0	0	−2.9	A+B	3.2	53.24	−23.0	B+C
7.36	8.0	−2.0	A+B	2.0	60.76	−10.0	B+C
6.0	9.4	−4.8	A+B	4.0	59.52	−10.2	B+D
4.0	19.2	−8.2	A+B	4.0	57.6	−14.2	B+D
4.0	28.8	−13.4	A+B	6.0	62.04	+4.0	B+D
3.2	38.72	−19.2	A+B	8.0	64.4	+19.0	B+D
3.0	48.5	−25.2	A+B+C	3.5	56.0	−21.0	B+C+D
0	52.0	−30.0	A+C	1.2	60.0	−16.0	C+D
1.44	52.0	−28.0	A+C	0	64.0	−0.8	C+D

Solubility isotherms in the KSCN–KNO_3–H_2O system[b]

Temperature (t/°C)	KNO_3 (100 w_2/mass %)	KNO_3 (m_2/mol kg^{-1})[c]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[c]	Solid phase[a]
−20	1.26	0.306	58.0	14.65	C
	3.64	0.860	54.5	13.40	C
−10	0	0	59.7	15.24	C
	1.17	0.306	61.0	16.59	C
0	0	0	64.0	18.29	D
	1.08	0.306	64.0	18.86	D
	3.08	0.860	61.5	17.87	D
10	0	0	66.5	20.43	D
	1.02	0.306	66.0	20.59	D
	2.88	0.860	64.0	19.88	D
20	0	0	68.4	22.27	D
	0.93	0.306	69.0	23.61	D
	2.72	0.860	66.0	21.71	D
30	0	0	72.0	26.46	D
	0.85	0.304	71.5	26.61	D
	2.48	0.860	69.0	24.90	D

[a] A: Ice, H_2O, [7732-18-5]; B: KNO_3, [7757-79-1]; C: $KSCN\cdot0.5H_2O$, [ ]; D: KSCN; [333-20-2].
[b] Solubility isotherms were obtained by the authors from polythermal measurements. Of numerous data reported, only those referring to the solubility of KSCN were included here. In systems containing higher KNO_3 concentrations, the equilibrium solid phases were either ice or KNO_3.
[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Visual polythermal method used. In total, 12 sections of the KSCN–KNO_3–H_2O system were investigated, of which ten corresponded to 10, 20, 30, 40, 50, 55, 60, 62, 66, and 70 mass % KSCN, and two to constant KNO_3 content (only one given numerically, i.e., 3.86 mass % KNO_3). Measurements were carried out in an apparatus described in Ref. 1. The solubility vessel, equipped with a thermometer, was coated with a transparent semiconductor layer to which two heating silver electrodes were soldered. The vessel was placed inside a Dewar flask with transparent walls which, in measurements performed below room temperature, was filled to 1/5 of its volume with liquid nitrogen or solid CO_2. With the solubility vessel kept above the coolant, it was possible to control the rate of cooling or heating by moving the Dewar flask. The mixture in the solubility vessel was stirred by using two external electromagnets, and illuminated to observe disappearance or appearance of crystals.

Source and Purity of Materials:

KSCN and KNO_3 were chemically pure products. They were recrystallized twice before use, and dried at 40 °C.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] L. N. Eraizer and I. M. Kaganskii, Zavodskaya Lab. **33**, 119 (1967).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium hydrogencarbonate; $KHCO_3$; [298-14-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. S. Bogoyavlenskii and E. D. Gashpar, Zh. Neorg. Khim. **17**, 3055–8 (1972).

Variables:

T/K: 298, 313
100 w_2/mass %: 0–26.72 at 298 K
0–31.98 at 313 K

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN at 25 and 40 °C in water and aqueous solutions of $KHCO_3$

Temperature (t/°C)	$KHCO_3$ (100 w_2/mass %)	$KHCO_3$ (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
25	0	0	70.70	24.83	A
	1.03	0.3464	69.27	24.00	A+B
40	0	0	74.38	29.87	A
	1.32	0.494	71.99	27.76	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-2]; B: $KHCO_3$, [289-14-6].

Additional information: In addition to the data shown above, the authors also reported the compositions of ten (at 25 °C) and 11 (at 40 °C) saturated solutions containing 1.07–26.72 and 1.36–31.98 mass % $KHCO_3$, respectively, where $KHCO_3$ was the equilibrium solid phase. These data are not shown here since they refer to the solubility of $KHCO_3$ in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. Solid phases were characterized by Schreinemaker's method. The saturated solutions and wet residues were analyzed for SCN^- ions by potentiometric titration against standard $AgNO_3$, and for HCO_3^- by titration against standard acid solution.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium hydrogencarbonate; $KHCO_3$; [298-14-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Babenko and A. M. Andrianov, Zh. Neorg. Khim. **23**, 2826–32 (1978).

Variables:

T/K: 243–305
100 w_2/mass %: 0–16.2

Prepared By:

J. Hála

Experimental Data

Solubility in the KSCN–$KHCO_3$–H_2O system as measured by polythermal method

$KHCO_3$ (100 w_2/mass %)	KSCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]	$KHCO_3$ (100 w_2/mass %)	KSCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]
16.2	0	−5.2	A+B	1.0	48.5	−27.0	A+B
14.25	5.0	−7.2	A+B	0.7	51.3	−29.2	A+B+C
12.0	8.8	−7.8	A+B	1.5	53.19	−24.6	B+C
8.38	16.2	−10.0	A+B	1.0	57.42	−21.0	B+C
8.0	18.4	−10.4	A+B	0.5	61.69	−9.0	B+C
4.0	28.8	−13.6	A+B	0.3	63.5	−4.8	B+C+D
4.0	33.6	−16.8	A+B	0	52.0	−30.0	A+D
3.30	34.0	−15.6	A+B	0	64.0	−0.8	C+D
2.0	39.2	−19.3	A+B	1.8	64.0	+31.6	B+D
1.5	44.32	−23.6	A+B				

Solubility isotherms in the KSCN–$KHCO_3$–H_2O system[b]

Temperature t/°C	$KHCO_3$ (100 w_2/mass %)	$KHCO_3$ (m_2/mol kg^{-1})[c]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[c]	Solid phase[a]
−10	0	0	59.7	15.24	C
0	0	0	64.0	18.29	D
10	0	0	66.5	20.43	D
20	0	0	69.0	22.90	D

[a] A: Ice, H_2O, [7732-18-5]; B: $KHCO_3$, [298-14-6]; C: KSCN·$0.5H_2O$, [ ]; D: KSCN; [333-20-0].
[b] Solubility isotherms were obtained by the authors from polythermal measurements. Of numerous data reported, only those referring to the solubility of KSCN were included here. In other systems, the equilibrium solid phases were either ice or $KHCO_3$.
[c] Calculated by compiler.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium carbonate; K_2CO_3; [584-08-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Babenko and A. M. Andrianov, Zh. Neorg. Khim. **23**, 2826–32 (1978).

Variables:

T/K: 238–361
$100\ w_2$/mass %: 0–51.5

Prepared By:

J. Hála

Experimental Data

Solubility in the KSCN–K_2CO_3–H_2O system as measured by polythermal method

K_2CO_3 ($100\ w_2$/mass %)	KSCN ($100\ w_1$/mass %)	Liquidus temperature (t/°C)	Solid phase[a]	K_2CO_3 ($100\ w_2$/mass %)	KSCN ($100\ w_1$/mass %)	Liquidus temperature (t/°C)	Solid phase[a]
41.4	0	−31.0	A+B	44.0	11.20	65.0	B+E
22.4	7.76	−13.0	A+B	40.0	18.0	76.5	B+E
16.0	16.8	−14.6	A+B	36.0	25.6	80.0	B+E
11.6	26.52	−18.3	A+B	36.0	28.8	54.6	B+E
5.4	37.84	−22.2	A+B	32.0	37.4	56.4	B+E
7.0	41.85	−28.6	A+B	28.0	43.2	54.5	B+E
15.88	20.6	−17.0	A+B	20.5	52.47	49.4	B+E
28.8	4.0	−13.0	A+B	16.0	58.8	52.2	B+E
0	52.0	−30.0	A+C	19.36	56.0	88.0	B+E
2.88	52.0	−34.0	A+C	8.0	64.4	33.0	B+D
5.2	48.0	−34.5	A+B+C	6.4	68.0	46.0	B+D
6.0	51.7	−26.0	B+C	9.6	68.0	64.0	B+D
4.0	57.6	−14.0	B+C	13.30	65.0	75.0	B+D
6.0	62.04	16.0	B+C+D	0	64.0	0.8	C+D
51.5	0	−4.0	B+E	21.6	64.0	8.0	C+D
48.0	5.2	63.0	B+E	3.6	64.0	13.0	C+D

Solubility isotherms in the KSCN–K_2CO_3–H_2O system[b,c]

Temperature (t/°C)	K_2CO_3 ($100\ w_2$/mass %)	K_2CO_3 (m_2/mol kg^{-1})[d]	KSCN ($100\ w_1$/mass %)	KSCN (m_1/mol kg^{-1})[d]
−30	0	0	55.5	12.83
	2.7	0.462	55.0	13.38
	2.83	0.462	52.8	12.25
	5.1	0.804	49.0	10.99
−10	0	0	59.7	15.24
	2.58	0.462	57.0	14.51
	4.7	0.804	53.0	12.89
0	0	0	64.0	18.29
	2.43	0.462	59.5	16.08
	4.5	0.804	55.0	13.97
10	0	0	66.5	20.43
	2.112	0.462	64.8	20.15
	4.1	0.804	59.0	16.45
20	0	0	68.4	22.27
	1.956	0.462	67.4	22.63
	3.4	0.804	66.0	22.19

[a] A: Ice, H_2O, [7732-18-5]; B: $K_2CO_3 \cdot 6H_2O$, [17033-98-6]; C: $KSCN \cdot 0.5H_2O$, [ ]; D: KSCN; [333-20-2]; E: $K_2CO_3 \cdot 1.5H_2O$, [6381-79-9]. See also Fig. 16.

[b] Solubility isotherms were obtained by the authors from polythermal measurements. Of numerous data reported, only those referring to

Auxiliary Information

Method/Apparatus/Procedure:

A visual polythermal method used. In total, 12 sections of the KSCN–$KHCO_3$–H_2O system were investigated, of which nine corresponded to 10, 20, 30, 40, 45, 49, 54, 58, and 62 mass % KSCN, and three to 5, 10, and 15 mass % $KHCO_3$. Measurements were carried out in an apparatus described in Eraizer and Kaganskii.[1] The solubility vessel, equipped with a thermometer, was coated with a transparent semiconductor layer to which two heating silver electrodes were soldered. The vessel was placed inside a Dewar flask with transparent walls which, in measurements performed below room temperature, was filled to 1/5 of its volume with liquid nitrogen or solid CO_2. With the solubility vessel kept above the coolant, it was possible to control the rate of cooling or heating by moving the Dewar flask. The mixture in the solubility vessel was stirred by using two external electromagnets, and illuminated to observe disappearance or appearance of crystals.

Source and Purity of Materials:

KSCN, chemically pure product, was recrystallized twice before use, and dried at 40 °C. $KHCO_3$ was purified according to Karyakhin and Angelov,[2] and dried at 40 °C.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] L. N. Eraizer and I. M. Kaganskii, Zavodskaya Lab. **33**, 119 (1967).
[2] Yu. V. Karyakhin and I. I. Angelov, *Pure Chemical Substances* Russian ed. (Khimiya, Moscow, 1974), p. 140.

the solubility of KSCN were included here. In other systems, the equilibrium solid phases were either ice or $K_2CO_3 \cdot 6H_2O$.

[c] Solid phase was $KSCN \cdot 0.5H_2O$ in all cases.

[d] Calculated by compiler.

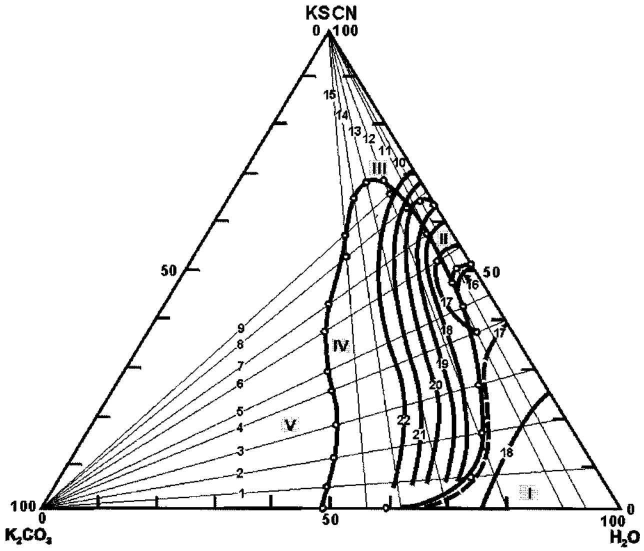

FIG. 16. Solubility polytherm of the $KSCN–K_2CO_3–H_2O$ system. Fields of crystallization: I: ice; II: $KSCN0.5H_2O$; III: KSCN; IV: $K_2CO_3 \cdot 6H_2O$; and V: $K_2CO_3 \cdot 1.5H_2O$.

Auxiliary Information

Method/Apparatus/Procedure:

Visual polythermal method used. In total, 15 sections of the $KSCN–K_2CO_3–H_2O$ system were investigated, of which nine corresponded to 10, 20, 30, 40, 45, 55, 60, 66, and 70 mass % KSCN, and six to 6, 10, 20, 30, 38, and 44 mass % K_2CO_3. Measurements were carried out in an apparatus described in Eraizer and Kaganskii.[1] The solubility vessel, equipped with a thermometer, was coated with a transparent semiconductor layer to which two heating silver electrodes were soldered. The vessel was placed inside a Dewar flask with transparent walls which, in measurements performed below room temperature, was filled to 1/5 of its volume with liquid nitrogen or solid CO_2. With the solubility vessel kept above the coolant, it was possible to control the rate of cooling or heating by moving the Dewar flask. The mixture in the solubility vessel was stirred by using two external electromagnets, and illuminated to observe disappearance or appearance of crystals.

Source and Purity of Materials:

KSCN and K_2CO_3 were chemically pure products, recrystallized twice, and dried at 40 and 105 °C, respectively, before use.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

References:

[1] L. N. Eraizer and I. M. Kaganskii, Zavodskaya Lab. **33**, 119 (1967).

Components:	**Original Measurements:**
(1) Potassium thiocyanate; KSCN; [333-20-0] (2) Potassium sulfate; K_2SO_4; [7778-80-5] (3) Water; H_2O; [7732-18-5]	P. S. Bogoyavlenskii and G. V. Sukmanskaya, Zh. Obsh. Khim. **23**, 1092–5 (1953).
Variables:	**Prepared By:**
T/K: 298, 313 100 w_2/mass %: 0–10.76 at 298 K 0–13.1 at 313 K	J. Hála

Experimental Data

Solubility of KSCN at 25 and 40 °C in water and aqueous solutions of K_2SO_4

Temperature (t/°C)	K_2SO_4 (100 w_2/mass %)	K_2SO_4 (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
25	0	0	70.70	24.83	A
	0.04	0.0078	70.60	24.74	A+B
40	0	0	74.31	29.77	A
	0.03	0.0067	74.24	29.69	A+B

[a] Calculated by compiler.

[b] A: KSCN, [333-20-2]; B: K_2SO_4, [7778-80-5].

Additional information: In addition to the data shown above, the authors also reported the compositions of 13 (at 25 °C) and 18 (at 40 °C) saturated solutions containing 0.10–10.76 and 0.13–13.10 mass % K_2SO_4, respectively, where K_2SO_4 was the equilibrium solid phase. These data are not shown here since they refer to the solubility of K_2SO_4 in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Saturated solutions were analyzed for SCN^- and sulfate ions (methods not specified), solid phases were characterized by optical microscopy. The time necessary to reach equilibrium increased with increasing KSCN concentration in the system, up to 24–30 h at KSCN concentration higher than 45 mass %.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium sulfate; K_2SO_4; [7778-80-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549–52 (1968).

Variables:
T/K: 273, 298, 323
100 w_2/mass %: 0–7.25 at 273 K; 0–10.9 at 298 K; 0–14.15 at 323 K

Prepared By:
J. Hála

Experimental Data

Solubility in the KSCN–K_2SO_4–H_2O system at two temperatures

Temperature (t/°C)	K_2SO_4 (100 w_2/mass %)	K_2SO_4 (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	0	64.40	18.62	A
	0.04	0.0064	64.35	18.60	A+B
25	0	0	70.90	25.07	A
	0.18	0.035	70.32	24.53	A+B
50	0	0	76.40	33.31	A
	0.34	0.0837	76.36	33.72	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-0]; B: K_2SO_4; [7778-80-5].

Additional information: In addition to the data shown above, the authors reported also compositions of 12 saturated solutions containing 0.90–7.25, 1.40–10.90, and 2.20–14.15 mass % K_2SO_4 at 0, 25, and 50 °C, respectively, where the equilibrium solid phase was K_2SO_4. These were not included here since they represent the solubilities of K_2SO_4 in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:
The solubilities were obtained by graphical analytical method.[1] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions, were prepared by weighing. After equilibrium had been attained, refractive indices of the solutions were measured, and plotted as a function of the composition of the mixtures. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phase was not reported.

Source and Purity of Materials:
KSCN, chemically pure product, was dried over anhydrous $CaCl_2$. Doubly distilled water was used.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:
[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Boric acid; H_3BO_3; [10043-35-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
V. G. Skvortsov, R. S. Tsekhanskii, Sh. V. Sadetdinov, and A. K. Molodkin, Zh. Neorg. Khim. **28**, 2677–9 (1983).

Variables:
T/K: 298
100 w_2/mass %: 0–5.6

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN at 25 °C in aqueous solutions of boric acid

H_3BO_3 (100 w_2/mass %)	H_3BO_3 (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	70.50	24.59	A
4.87	3.119	69.88	28.48	A
4.87	3.121	69.89	28.49	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-0]; B: H_3BO_3, [10043-35-3].

Additional information: In addition to the data shown above, the authors also reported the compositions of seven saturated solutions containing 4.89–5.60 mass % H_3BO_3, and 69.87–0 mass % KSCN, where H_3BO_3 was the equilibrium solid phase. These data are not shown here since they represent the solubility of H_3BO_3 in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:
Isothermal method used. Solutions with excess solid were stirred for 20 h, which was sufficient for equilibrium to be reached. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method. Solubility isotherms were also confirmed by refractometric measurements.

Source and Purity of Materials:
KSCN and H_3BO_3 were chemically pure products, and were recrystallized before use.

Estimated Error:
Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium borate; KBO_2; [13709-94-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
V. G. Skvortsov, Sh. V. Sadetdinov, R. S. Tsekhanskii, and A. K. Molodkin, Zh. Neorg. Khim. **24**, 209–12 (1979).

Variables:
T/K: 298
100 w_2/mass %: 0–18.42

Prepared By:
J. Hála

Experimental Data
Solubility of KSCN at 25 °C in aqueous solutions of potassium borate

KBO_2 (100 w_2/mass %)	KBO_2 (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	70.50	24.59	A
0.98[c]	0.407	69.64	24.39	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-0]; B: KBO_2, [13709-94-9].
[c] Eutonic point.

Additional information: In addition to the data shown above, the authors also reported the compositions of eight saturated solutions containing 1.06–18.42 mass % KBO_2, and 69.67–0 mass % KSCN, where KBO_2 was the equilibrium solid phase. These data are not shown here since they represent the solubility of KBO_2 in solutions of KSCN. Also reported were densities, viscosities, and refraction indexes of the saturated solutions.

Auxiliary Information

Method/Apparatus/Procedure:
Isothermal method used. Equilibrium was reached within 24 h under constant shaking in a thermostat. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method and chemical analysis.

Source and Purity of Materials:
KSCN was a chemically pure product, source not specified. KBO_2 was prepared from boric acid and KOH.

Estimated Error:
Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium tetraborate; $K_2B_4O_7$; [1332-77-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
V. G. Skvortsov, A. K. Molodkin, Sh. V. Sadetdinov, and R. S. Tsekhanskii, Zh. Neorg. Khim. **26**, 3164–6 (1981).

Variables:
T/K: 298
100 w_2/mass %: 0–18.03

Prepared By:
J. Hála

Experimental Data
Solubility of KSCN at 25 °C in aqueous solutions of potassium tetraborate

$K_2B_4O_7$ (100 w_2/mass %)	$K_2B_4O_7$ (m_2/mol kg^{-1})[a]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	70.50	24.59	A
0.85	0.124	69.73	24.39	A+B
0.84	0.122	69.75	24.40	A+B

[a] Calculated by compiler.
[b] A: KSCN, [333-20-0]; B: $K_2B_4O_7 \cdot 4H_2O$, [12045-78-2].

Additional information: In addition to the data shown above, the authors also reported the compositions of seven saturated solutions containing 0.87–18.03 mass % $K_2B_4O_7$, and 69.70–0 mass % KSCN, where $K_2B_4O_7 \cdot 4H_2O$ was the equilibrium solid phase. These data are not shown here since they represent the solubility of $K_2B_4O_7 \cdot 4H_2O$ in solutions of KSCN.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. Equilibrium was reached within 20 h, which was checked by chemical analysis and refraction index of the saturated solutions. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method.

Source and Purity of Materials:
KSCN and $K_2B_4O_7$ were chemically pure products, and were recrystallized before use.

Estimated Error:
Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Potassium molybdate; K_2MoO_4; [13446-49-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Z. G. Karov, I. N. Lepeshkov, and S. B. Semenova, Zh. Neorg. Khim. **16**, 2273–8 (1971).

Variables:

T/K: 298
100 w_2/mass %: 0–64.66

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN in solutions of K_2MoO_4 at 25 °C

K_2MoO_4 (100 w_2/mass %)	K_2MoO_4 (m_2/mol kg^{-1})[b]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[b]	Solid phase[a]
0	0	70.91	25.08	A
8.83	1.316	62.99	23.00	A
15.52	2.368	56.96	21.30	A
21.71	3.392	51.41	19.68	A
28.96	4.663	44.96	17.74	A+B
29.14	4.710	44.88	17.78	A+B
29.16	4.719	44.89	17.80	A+B
29.20	4.730	44.88	17.82	A+B
29.24	4.739	44.85	17.81	A+B

[a] A: KSCN, [333-20-0]; B: K_2MoO_4, [13446-49-6].
[b] Calculated by compiler.

Additional information:

(i) Composition of the saturation solution at the eutonic point was reported to be 100 $w_1 = 44.89$ mass % KSCN and 100 $w_2 = 29.61$ mass % K_2MoO_4. The solubility of KSCN in solutions of K_2MoO_4 at 25 °C was expressed by the authors as

$$S(\text{in mass }\%) = 70.91 - 0.924 \times (100\,w_2)^{0.99}.$$

(ii) In addition to the data given above, the authors also reported compositions of another six saturated solutions containing 29.69–64.66 mass % K_2MoO_4 and 44.25–0 mass % KSCN. These data were not included in the compilation since they represent the solubility of K_2MoO_4 in solutions of KSCN.

(iii) Also reported were densities, viscosities, refractive indexes, surface tensions, pH, and electrical conductivities of the KSCN–K_2MoO_4 solutions.

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. Solutions containing excess solid were stirred in thermostated vessels equipped with oil seal. Equilibrium was attained in 6–8 h, samples for analysis were withdrawn after 2–3 days equlibration. Saturated solutions and wet residues were analyzed for Mo by reductometric titration, and for SCN^- by Volhard method. Solid phases were identified by Schreinemakers method and by optical microscopy.

Source and Purity of Materials:

KSCN, chemically pure, was twice recrystallized. Analysis showed 99.86% purity. K_2MoO_4 was prepared from chemically pure MoO_3 and KOH. The product was three times recrystallized, and was 99.90% pure.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Urea; CH_4N_2O; [57-13-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. Turgunbekova, K. Nogoev, and K. Sulaimankulov, Zh. Neorg. Khim. **17**, 1455–7 (1972).

Variables:

T/K: 288, 303, and 318
100 w_2/mass %: 0–49 at 288 K, 0–57.5 at 303 K, 0–64.5 at 318 K

Prepared By:

J. Hála

Experimental Data

Composition of the saturated solutions in the KSCN–urea–H_2O system at three temperatures

Temperature (t/°C)	Urea (100 w_2/mass %)	Urea (100 x_2/mole %)	KSCN (100 w_1/mass %)	KSCN (100 x_1/mole %)	Solid phase[a]
15	0	0	68.31	28.56	A
	2.87	1.94	65.70	27.39	A
	8.55	6.08	63.48	27.87, 27.82[b]	A
	8.76	6.26	63.68	28.12	B
	9.15	6.43	62.30	26.96	B
	12.65	8.54	57.31	23.89	B
	14.15	9.06	53.01	20.95	B
	17.26	11.15	50.87	20.29	B
	22.89	14.95	46.64	18.79	B
	26.50	17.01	42.60	16.90	B
	33.46	21.95	37.84	15.34	B
	40.50	28.01	34.70	14.81	B
	43.00	31.27	35.14	15.79	B+C
30	0	0	70.00	30.21	A
	6.17	4.45	66.44	29.66	A
	8.00	5.79	65.00	29.09	A+B
	10.35	7.69	64.30	29.54	B
	14.00	9.73	57.75	24.82	B
	16.30	10.99	54.15	22.58	B
	21.00	13.63	48.00	19.27	B
	28.18	18.51	42.49	17.26	B
	35.00	23.35	37.50	15.48	B
	43.50	31.84	35.08	15.88	B
	45.00	33.21	34.20	15.61	B+C
45	0	0	74.60	35.25	A
	4.90	3.58	98.00	30.59	A
	8.70	6.42	65.40	29.85	A
	13.70	10.63	63.60	30.55	A
	14.20	11.22	63.89	31.16	A+BB
	15.50	12.30,12.40[b]	63.40	31.35	B
	22.06	16.60	54.82	25.48	B
	24.65	18.31	51.97	23.83	B
	32.70	24.25	45.00	20.61	B
	40.08	30.24	39.50	18.42	B
	43.00	33.13	38.00	18.07	B
	47.53	37.45	35.18	17.11	B
	51.00	42.42	34.65	18.81, 17.81[b]	B
	51.56	43.06	34.37	17.74	B+C

[a] A: KSCN, [333-20-0]; B: $KSCN\cdot CO(NH_2)_2$, [37604-15-2]; C: $CO(NH_2)_2$, [57-13-6].
[b] The authors' mole % data were computer recalculated by the compiler. Most of the data agreed within ±0.02 mole %, the differences being most likely caused by rounding errors. Those differing more are shown in the table as data marked with superscript [b].

Additional information: In addition to the data shown in the table, the authors also reported compositions of another seven saturated solutions at 15 °C containing 43.46–49.0 mass % urea and 29.89–22.38 mass % KSCN, six saturated solutions at 30 °C containing 44.48–57.50 mass % urea and 31.37–28.86 mass % KSCN, and seven saturated solutions at 45 °C containing 49.88–64.50 mass % urea and 38.63–35.28 mass % KSCN, where urea was the equilibrium solid phase. These data have not been included in the compilation since they represent the solubility of urea in solutions of KSCN. Also reported was the phase diagram of the KSCN–urea–H_2O system at 30 °C (see Fig. 17).

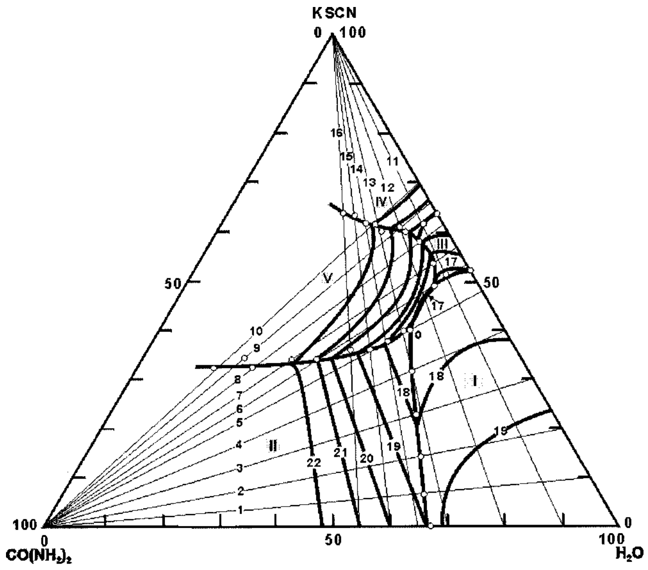

FIG. 17. Solubility polytherm of the KSCN–urea–H_2O system. Fields of crystallization: I: ice; II: urea; III: $KSCN\cdot 0.5H_2O$; IV: KSCN; and V: KSCN urea.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used; no details reported except that the composition of the $KSCN\cdot CO(NH_2)_2$ compound was confirmed by chemical analysis. Found (mass %): 61.89 urea, 37.22 KSCN; calculated (compiler): 38.20 urea, 61.80 KSCN. The authors' data were apparently confused by mistake.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Urea; CH_4N_2O; [57-13-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Babenko and A. M. Andrianov, Zh. Neorg. Khim. **23**, 1344–8 (1978).

Variables:

T/K: 241–316
100 w_2/mass %: 0–49.6

Prepared By:

J. Hála

Experimental Data

Solubility in the KSCN–CH_4N_2O–H_2O system as measured by polythermal method

CH_4N_2O (100 w_2/mass %)	KSCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]	CH_4N_2O (100 w_2/mass %)	KSCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]
33.0	0	−10.6	A+B	49.6	35.28	43.0	B+C
30.5	6.95	−14.7	A+B	18.0	40.0	−30.8	B+C
27.8	14.4	−17.7	A+B	21.7	38.0	−24.8	B+C
24.0	22.8	−21.0	A+B	25.6	36.0	−15.7	B+C
20.3	31.88	−26.4	A+B	28.8	36.0	−8.3	B+C
16.8	39.23	−31.8	A+B+C	0	64.0	−0.8	D+E
10.4	48.0	−30.8	A+C+D	3.8	62	−1.8	D+E
0	52.0	−30.0	A+D	8.0	60.72	2.6	C+E
4.81	52.0	−31.6	A+D	8.0	60.0	3.0	C+E
6.0	58.28	−8.0	C+D+E	11.94	60.2	12.0	C+E
36.0	33.92	9.5	A+B+C	12.0	61.6	14.5	C+E
40.0	34.2	19.2	B+C	13.16	62.4	26.0	C+E
43.6	34.96	27.6	B+C	14.4	64.0	36.0	C+E
47.6	34.58	37.6	B+C	16.2	64.0	41.6	C+E

Solubility isotherms in the KSCN–CH_4N_2O–H_2O system[b]

Temperature (t/°C)	CH_4N_2O (100 w_2/mass %)	CH_4N_2O (m_2/mol kg^{-1})[c]	KSCN (100 w_1/mass %)	KSCN (m_1/mol kg^{-1})[c]	Solid phase[a]
−30	0	0	52.0	11.15	D
	4.75	1.850	52.5	12.64	D
	10.36	4.163	48.2	11.97	C
	10.6	4.163	47.0	11.41	C
	13.0	4.785	41.76	9.499	A
	17.7	6.886	39.5	9.497	C
	17.97	7.136	40.1	9.841	C
	18.36	7.136	38.8	9.320	A
−20	0	0	38.8	6.524	A
	0	0	55.5	12.83	D
	4.42	1.850	55.8	14.43	D
	5.2	1.522	37.92	6.860	A
	6.38	1.850	36.2	6.487	A
	6.8	2.825	53.12	13.64	C
	10.2	4.024	47.59	11.60	C
	13.0	4.009	33.0	6.288	A
	17.58	7.136	41.4	10.39	C
	21.42	8.966	38.8	10.04	C
	22.44	7.136	25.2	4.953	A
	23.0	9.565	36.96	9.499	B
	23.8	8.668	30.48	6.860	B

	24.15	8.966	31.0	7.113	B
	24.6	7.761	22.62	4.410	B
−10	0	0	24.0	3.250	A
	0	0	59.7	15.24	C
	4.08	1.850	59.2	16.59	C,D[d]
	7.9	1.850	21.0	3.039	A
	9.6	2.210	18.08	2.573	A
	9.6	4.111	51.52	13.64	C
	13.5	5.529	45.84	11.60	C
	16.92	4.163	15.4	2.341	A
	17.16	7.136	42.8	11.00	C
	25.12	11.10	37.2	10.16	C
	28.2	12.58	34.46	9.497	B
	29.0	11.33	28.4	6.860	B
	30.0	10.19	21.0	4.410	B
	30.45	8.966	13.0	2.366	B
	31.8	9.705	13.64	2.573	B
	33.0	9.113	6.7	1.143	B
0	0	0	64.0	18.29	E
	3.75	1.850	62.5	19.06	E
	7.8	3.707	57.16	16.79	C
	8.8	4.163	56.0	16.37	C
	14.5	6.566	48.73	13.64	C
	16.38	7.136	45.4	12.22	C
	18.8	8.201	43.03	11.60	C
	20.19	8.963	42.3	11.60	C
	24.4	11.10	39.0	10.96	C
	28.03	13.62	37.7	11.32	C
	33.4	16.06	31.96	9.494	B
	34.2	14.42	26.32	6.860	B
	35.2	12.92	19.44	4.410	B
	37.0	12.22	12.6	2.573	B
10	0	0	66.5	20.43	E
	3.5	1.850	65.0	21.23	E
	7.6	4.163	62.0	20.99	E
	12.0	5.965	54.5	16.74	C
	13.68	7.136	54.4	17.54	C
	18.6	8.951	46.8	13.92	C
	22.5	11.22	44.1	13.59	C
	36.2	20.09	33.8	11.59	C
	38.6	20.13	29.47	9.497	B
	39.5	18.12	24.2	6.860	B
	40.4	16.09	17.8	4.382	B
	42.5	15.38	11.5	2.573	B
20	0	0	51.8	11.06	E[e]
	10.44	4.163	47.8	11.78	E[e]
	16.32	7.136	45.6	12.32	E[e]
	26.97	15.36	43.8	15.42	E[e]
	31.27	18.78	41.0	15.21	E[e]
	33.9	21.96	40.4	16.18	C
	46.6	26.42	24.03	8.419	C
	48.98	27.17	21.0	7.198	C
	50.0	27.75	20.0	6.860	C
	54.8	31.06	15.82	5.541	C
	55.57	32.32	15.8	5.679	C
	60.90	38.85	13.0	5.125	B[f]
	66.5	38.85	5.0	1.805	B[f]
	67.7	38.78	3.23	1.143	B[f]
	69.0	37.06	0	0	B[f]

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[a] A: Ice, H_2O, [7732-18-5]; B: CH_4N_2O, [57-13-6]; C: $KSCN \cdot CH_4N_2O$, [37604-15-2]; D: $KSCN \cdot 0.5H_2O$, [ ]; E: KSCN, [333-20-0].

[b] Solubility isotherms were obtained by the authors from polythermal measurements.

[c] Calculated by compiler.

[d] Two saturated solutions with identical compositions, but different solid phases were reported.

[e] In the original document, urea is reported as the solid phase in equilibrium with these solutions, evidently by mistake.

[f] In the original document, KSCN is reported as the solid phase in equilibrium with these solutions, evidently by mistake.

Auxiliary Information

Method/Apparatus/Procedure:

Visual polythermal method used. In total, 16 sections of the KSCN–urea–H_2O system were investigated, of which ten corresponded to 10, 20, 30, 40, 50, 53, 57, 62, 66, and 70 mass % KSCN, and six to 10, 20, 30, 35, 40, and 45 mass % urea. Measurements were carried out in an apparatus described in Eraizer and Kaganskii.[1] The solubility vessel, equipped with a thermometer, was coated with a transparent semiconductor layer to which two heating silver electrodes were soldered. The vessel was placed inside a Dewar flask with transparent walls which, in measurements performed below room temperature, was filled to 1/5 of its volume with liquid nitrogen or solid CO_2. With the solubility vessel kept above the coolant, it was possible to control the rate of cooling or heating by moving the Dewar flask. The mixture in the solubility vessel was stirred by using two external electromagnets, and illuminated to observe disappearance or appearance of crystals.

Source and Purity of Materials:

KSCN and urea were chemically pure products, twice recrystallized from water, and dried at 50 °C before use.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

References:

[1] L. N. Eraizer and I. M. Kaganskii, Zavodskaya Lab. **33**, 119 (1967).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Acetone; C_3H_6O; [67-64-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
E. Weitz and E. Grohrock, Ber. **67**, 1085–91 (1934).

Variables:
T/K: 293
Volume % acetone: 0–100

Prepared By:
J. Hála

Experimental Data

The solubility of KSCN in acetone–water solutions at 20 °C was reported in Fig. 18.

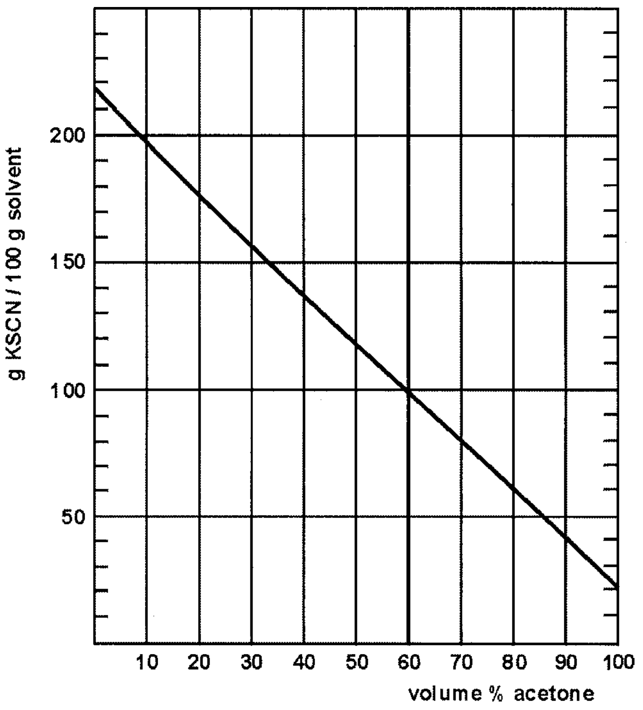

FIG. 18. Solubility of KSCN in water–acetone solutions.

Auxiliary Information

Method/Apparatus/Procedure:
Nothing specified.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 1,2-ethanediol (ethyleneglycol); $C_2H_6O_2$; [107-21-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
Z. Adamcová, Coll. Czech. Chem. Commun. **34**, 3149–53 (1969); **36**, 2338–41 (1971).

Variables:
T/K: 298
100 w_2/mass %: 20–100

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in H_2O–ethyleneglycol mixtures at 25 °C[a]

$C_2H_6O_2$ (100 w_2/mass %)[b]	KSCN (g/100 g mixed solvent)
20	220
40	178.7
60	136.2
80	95.4
90	78.1
95	72.7
100	66.7

[a] Equilibrium solid phase was KSCN, [333-20-0], in all solutions.
[b] Mass % ethyleneglycol in the initial solvent mixture.

Additional information: The solubility of KSCN, S, in grams salt per 100 g mixed solvent, as a function of solvent composition was obtained by least squares method as

$$S = 252.4 - 1.815(100\ w_2) - 0.00112(100\ w_2)^2.$$

Calculated and experimental solubilities agreed within ±2%.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. The glycol–water mixtures were prepared by weighing. Measurements were carried out in thermostated flasks equipped with a vertical stirrer. Equilibration time was 2 h. Samples of the saturated solutions were withdrawn by means of a pipette with a cotton wad, and KSCN content was determined by Volhard's method. The glycol was found not to affect the results. The composition of the solid phases was characterized by Schreinemakers' method.

Source and Purity of Materials:
KSCN, analytical grade (source not specified), was recrystallized from water and dried at 105 °C. Ethyleneglycol, source not specified, was purified by distillation at normal pressure. The product used showed the following properties: boiling point 197.3 °C at normal pressure, refractive index 1.4315, density 1.1151 g cm^{-3}.

Estimated Error:
Temperature: precision ±0.05 K (author).
Solubility: average experimental error was ±0.33 mass % relative (author).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 2,2′-oxybis-ethanol (diethyleneglycol); $C_4H_{10}O_3$; [111-46-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Z. Adamcová, Coll. Czech. Chem. Commun. **34**, 3149–53 (1969); **36**, 2338–41 (1971).

Variables:

T/K: 298
100 w_2/mass %: 20–100

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN in H_2O–diethyleneglycol mixtures at 25 °C[a]

$C_4H_{10}O_3$ (100 w_2/mass %)[b]	KSCN (g/100 g mixed solvent)
20	201.6
40	155.3
60	111.5
80	77.4
100	52.5

[a] Equilibrium solid phase was KSCN, [333-20-0], in all solutions.
[b] Mass % diethyleneglycol in the initial solvent mixture.

Additional information: The solubility of KSCN, S, in grams salt per 100 g mixed solvent, as a function of solvent composition was obtained by least squares method as

$$S = 251.6 - 2.748(100\, w_2) + 0.00742(100\, w_2)^2.$$

Calculated and experimental solubilities agreed within ±1.62%.

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. The glycol–water mixtures were prepared by weighing. Measurements were carried out in thermostated flasks equipped with a vertical stirrer. Equilibration time was 4 h. Samples of the saturated solutions were withdrawn by means of a pipette with a cotton wad, and KSCN content was determined by Volhard's method. The glycol was found not to affect the results. The composition of the solid phases was characterized by Schreinemakers' method.

Source and Purity of Materials:

KSCN, analytical grade (source not specified), was recrystallized from water and dried at 105 °C. Diethyleneglycol, source not specified, was purified by distillation at reduced pressure. The product used showed the following properties: boiling point 174.0 °C at 60 mm Hg pressure, refractive index 1.4469, density 1.1181 g cm^{-3}.

Estimated Error:

Temperature: precision ±0.05 K (author).
Solubility: average experimental error was ±0.33 mass % relative (author).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 2,2′-[1,2-ethanediyl bis(oxy)]bis-ethanol; (triethyleneglycol); $C_6H_{14}O_4$; [112-27-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Z. Adamcová, Coll Czech. Chem. Commun. **34**, 3149–53 (1969); **36**, 2338–41 (1971).

Variables:

T/K: 298
100 w_2/mass %: 20–100

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN in H_2O–triethyleneglycol mixtures at 25 °C[a]

$C_6H_{14}O_4$ (100 w_2/mass %)[b]	KSCN (g/100 g mixed solvent)
20	194.5
40	148.3
60	106.2
80	71.6
90	58.6
95	53.3
100	48.3

[a] Equilibrium solid phase was KSCN, [333-20-0], in all solutions.
[b] Mass % triethyleneglycol in the initial solvent mixture.

Additional information: The solubility of KSCN, S, in grams salt per 100 g mixed solvent, as a function of solvent composition was obtained by least squares method as

$$S = 250.2 - 2.955(100\, w_2) + 0.00925(100\, w_2)^2.$$

Calculated and experimental solubilities agreed within ±0.88%.

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. The glycol–water mixtures were prepared by weighing. Measurements were carried out in thermostated flasks equipped with a vertical stirrer. Equilibration time was 24 h. Samples of the saturated solutions were withdrawn by means of a pipette with a cotton wad, and KSCN content was determined by Volhard's method. The glycol was found not to affect the results. The composition of the solid phases was characterized by Schreinemakers' method.

Source and Purity of Materials:

KSCN, analytical grade (source not specified), was recrystallized from water and dried at 105 °C. Triethyleneglycol, source not specified, was purified by distillation at reduced pressure. The product used showed the following properties: boiling point 201.5 °C at 60 mm Hg pressure, refractive index 1.4556, density 1.1260 g cm^{-3}.

Estimated Error:

Temperature: precision±0.05 K (author).
Solubility: average experimental error was ±0.33 mass % relative (author).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Polyethyleneglycol (200)
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Z. Adamcová, Coll. Czech. Chem. Commun. **36**, 2338–41 (1971).

Variables:

T/K: 298
100 w_2/mass %

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN in H_2O–PEG-200 mixtures at 25 °C

The solubility at 25 °C of KSCN, S, in grams salt per 100 g mixed solvent, as a function of solvent composition was obtained by least squares method as

$$S = 246.7 - 3.200(100\ w_2) + 0.011\ 56(100\ w_2)^2,$$

where 100 w_2 is the concentration of PEG-200 in mass % in the initial solvent mixture. Numerical data and equilibrium solid phases were not reported. Average deviation of experimental solubilities from the calculated data was ±0.0167%.

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. To a mixture of the desired water–PEG ratio, the salt was added in excess, the mixture was sealed in an ampoule, and equilibrated in a thermostat for 72 h. Samples of the saturated solutions were withdrawn by means of a pipette with a cotton wad, and were analyzed for KSCN by Volhard's method, and for water by Fischer's method. The content of PEG-200 was obtained by difference.

Source and Purity of Materials:

KSCN, analytical grade (source not specified), was recrystallized from water and dried at 105 °C. Polyethyleneglycol PEG-200 was a product of Chemische Werke, Hüls, AG, Germany. Its mean molecular weight, as determined by vapor phase osmometry, was 182%±5%.

Estimated Error:

Temperature: precision ±0.05 K (author).
Solubility: not reported.

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Polyethyleneglycols
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Z. Adamcová, Sci. Papers Inst. Chem. Technol. Prague **B17**, 217–24 (1973).

Variables:

T/K: 298
composition

Prepared By:

J. Hála

Experimental Data

Ternary phase diagrams of the KSCN–H_2O–polyethyleneglycol (1500) and KSCN–H_2O–polyethyleneglycol (6000) at 25 °C were reported (see Figs. 19 and 20). Numerical data were not given. The solid phase in equilibrium with H_2O–polyethyleneglycol mixtures was KSCN, [333-20-0].

Regions in the diagrams are as follows: I and VI—one liquid phase; II—two liquid phases; III—two liquid phases in equilibrium with solid polyethyleneglycol; IV—one liquid phase in equilibrium with solid KSCN, [333-20-0] (solubility curve: QS); and V—one liquid phase in equilibrium with solid polyethyleneglycol.

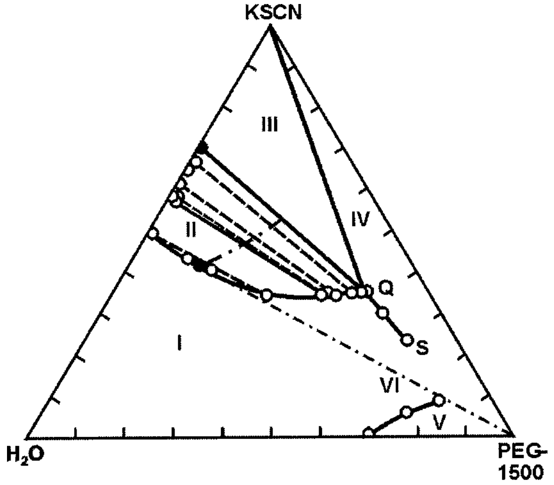

FIG. 19. Phase diagram of the KSCN–H_2O–polyethyleneglycol (1500).

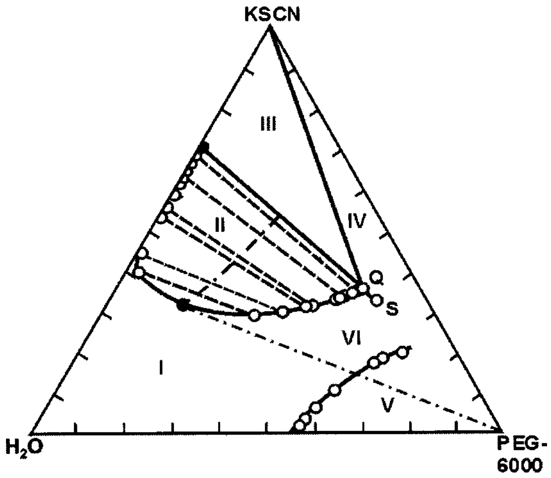

FIG. 20. Phase diagram of the KSCN–H_2O–polyethyleneglycol (6000).

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. To a mixture of the desired water–PEG ratio, the salt was added either in excess, when determining the solubility isotherm, or in calculated amount when salting/out was studied. The mixtures were sealed in ampoules, and equilibrated in a thermostat for 72 h. After the crystals had sedimented and the liquid phases separated, samples of the liquid phases for analysis were withdrawn by means of a syringe. The KSCN content was determined by Volhard's method, water content by Fischer's method. The content of PEG was obtained by difference.

Source and Purity of Materials:

KSCN, analytical grade (source not specified), was recrystallized from water and dried at 105 °C. PEG-1500 was a product of Chemische Werke, Hüls, AG, Germany. PEG-6000 was a product of Chemical Works, Novaky, Czechoslovakia. It contained 0.58 mass % water, melted in the range of 53–65 °C.

Estimated Error:

Temperature: precision ±0.05 K (author).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Methylthiocyanate; $C_2H_3NS(CH_3CNS)$; [556-64-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. Spaccamela Marchetti, Atti. Acad. Sci. Torino, Clase Fis. Mat. Nat. **94**, 353–70 (1960).

Variables:

T/K: 293
ratio of H_2O/C_2H_3NS concentrations

Prepared By:

J. Hála

Experimental Data

Phase diagram of the KSCN–C_2H_3NS–H_2O system at 20 °C

The ternary phase diagram of the KSCN–C_2H_3NS–H_2O system at 20 °C was reported (Fig. 21). The following fields were observed in the diagram: I and II—one liquid phase, III—two liquid phases, IV and VI—one liquid phase in equilibrium with solid KSCN, and V—two liquid phases in equilibrium with solid KSCN. Numerical data were reported for the solubility of KSCN in water-rich C_2H_3NS–H_2O mixtures (curve RP in the diagram) and in C_2H_3NS-rich C_2H_3NS–H_2O mixtures (curve QS in the diagram).

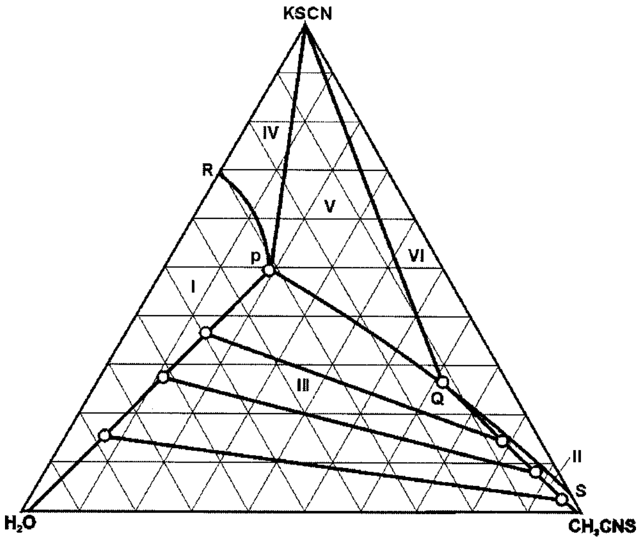

FIG. 21. Phase diagram of the KSCN–CH_3CNS–H_2O system at 20 °C.

Composition of the solutions saturated at 20 °C

H_2O-rich region			C_2H_3NS-rich region		
H_2O (100 w_3/mass %)	KSCN (100 w_1/mass %)	C_2H_3NS (100 w_2/mass %)	H_2O (100 w_3/mass %)	KSCN (100 w_1/mass %)	C_2H_3NS (100 w_2/mass %)
31.5	68.5[a]	0	0	0.9[b]	99.1
30.0	66.9	3.1	2.3	6.8	90.9
28.8	65.2	6.0	5.1	13.0	81.9
28.6	63.2	8.2	12.3	17.2	75.5
28.0	60.5	11.5			
27.9	58.2	13.9			

[a] Solubility of KSCN in water, $m_1 = 22.38$ mol kg^{-1} (compiler).
[b] Solubility of KSCN in C_2H_3NS, $m_1 = 0.0935$ mol kg^{-1} (compiler).

Components:

(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) Ethylthiocyanate; $C_3H_5NS(C_2H_5CNS)$; [542-90-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. Spaccamela Marchetti, Atti. Acad. Sci. Torino, Clase Fis. Mat. Nat. **94**, 353–70 (1960).

Variables:

T/K: 293
ratio of H_2O/C_3H_5NS concentrations

Prepared By:

J. Hála

Experimental Data

Phase diagram of the KSCN–C_3H_5NS–H_2O system at 20 °C

The ternary phase diagram of the KSCN–C_3H_5NS–H_2O system at 20 °C was reported (Fig. 22). The following fields were observed in the diagram: I and II—one liquid phase, III—two liquid phases, IV and VI—one liquid phase in equilibrium with solid KSCN, and V—two liquid phases in equilibrium with solid KSCN. Numerical data were reported for the solubility of KSCN in water-rich C_3H_5NS–H_2O mixtures (curve RP in the diagram) and in C_3H_5NS-rich C_3H_5NS–H_2O mixtures (curve QS in the diagram).

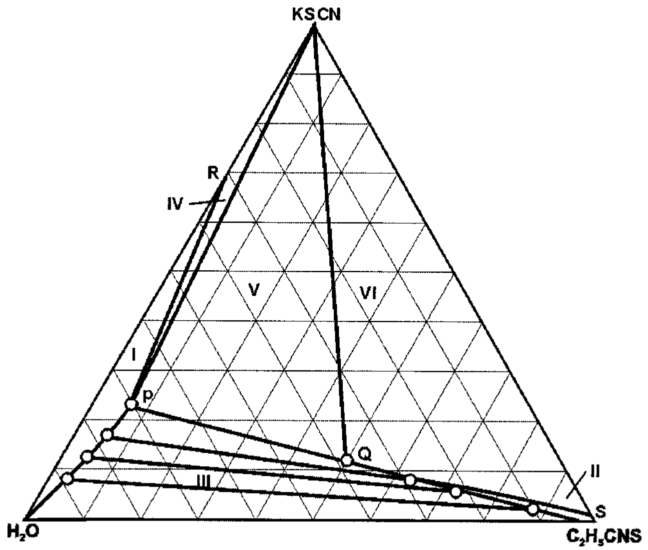

FIG. 22. Phase diagram of the KSCN–C_3H_5NS–H_2O system at 20 °C.

Auxiliary Information

Method/Apparatus/Procedure:

Solubility curves were obtained by titration a mixture of two components with the third one in a thermostated bath. Some of these measurements were verified by preparing the ternary systems, and observing the temperature of homogenization. The value corresponding to 20 °C was then obtained by interpolation. Burettes graduated by 0.01 cm^3 were used for titrations.

Source and Purity of Materials:

KSCN was dried at 110 °C before use. No details reported on C_2H_3NS.

Estimated Error:

Temperature: precision not reported.

Composition of the solutions saturated at 20 °C

H_2O-rich region			C_3H_5NS-rich region		
H_2O (100 w_3/mass %)	KSCN (100 w_1/mass %)	C_3H_5NS (100 w_2/mass %)	H_2O (100 w_3/mass %)	KSCN (100 w_1/mass %)	C_3H_5NS (100 w_2/mass %)
31.5	68.5[a]	0	0	0.9[b]	99.1
39.7	58.5	1.5	6.3	1.7	92.0
44.1	54.0	1.9	19.3	5.8	74.9
51.5	45.3	3.2			
63.3	31.8	4.9			
74.4	18.1	7.5			

[a] Solubility of KSCN in water, $m_1 = 22.38$ mol kg^{-1} (compiler).
[b] Solubility of KSCN in C_3H_5NS, $m_1 = 0.0935$ mol kg^{-1} (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

Solubility curves were obtained by titration a mixture of two components with the third one in a thermostated bath. Some of these measurements were verified by preparing the ternary systems, and observing the temperature of homogenization. The value corresponding to 20 °C was then obtained by interpolation. Burettes graduated by 0.01 cm^3 were used for titrations.

Source and Purity of Materials:

KSCN was dried at 110 °C before use. No details reported on C_3H_5NS.

Estimated Error:

Temperature: precision not reported.

Components:

(1) Potassium thiocyanate; KSCN; [540-72-7]
(2) Acetic acid; $C_2H_4O_2$; [64-19-7]
(3) N,N-diethylethanamine (triethylamine); $C_6H_{15}N$; [121-44-8]; or N,N-dimethylbenzeneamine; (dimethtyl-Aniline); $C_8H_{11}N$; [121-69-7]
(4) Solvents

Original Measurements:

T. Jasinski and R. Korewa, Rocz. Chem. (Warsaw) **39**, 963–8 (1965).

Variables:

T/K: 293

Prepared By:

J. Hála

Experimental Data

Solubility of KSCN at 20 °C in solvents in the presence of amines and acetic acid[a]

Solvent	$C_2H_4O_2$ (c_2/mol dm^{-3})	$C_6H_{15}N$ (c_3/mol dm^{-3})	$C_8H_{11}N$ (c_3/mol dm^{-3})	NaSCN (c_1/mol dm^{-3})
Ethylacetate; $C_4H_8O_2$; [141-78-6]	0.05	0	0	0.0020
	0	0.05	0	0.0016
	0.05	0.05	0	0.009[b]
	0	0	0.05	0.0026
	0.05	0	0.05	0.0034[b]
Dichloromethane; CH_2Cl_2; [75-09-2]	0.05	0	0	0.0004
	0	0.05	0	0.0010
	0.05	0.05	0	0.0026[b]
	0	0	0.05	0.0008
	0.05	0	0.05	0.0010[b]
Benzene; C_6H_6; [71-43-2]	0.05	0.05	0	0.0074[b]
Chlorobenzene; C_6H_5Cl; [108-90-7]	0.05	0.05	0	0.0080[b]
	0.05	0	0.05	0.0044[b]
Diethylether; $C_4H_{10}O$; [60-29-7]	0.05	0.05	0	0.0092[b]

[a] Solid phases were not investigated.
[b] Solubility of KSCN in the presence of the corresponding ammonium acetate.

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. The salt was equilibrated in closed flasks for 5 days with 20 cm^3 portions of the solutions of the amine, acetic acid, or their mixture, as may be the case, in the desired solvent. Then a 10 cm^3 sample was withdrawn, added to water, and the salt was extracted into water by shaking. The SCN^- content was determined in the aqueous layer by potentiometric titration with 0.01 mol dm^{-3} $AgNO_3$ solution.

Source and Purity of Materials:

KSCN, reagent grade, was twice recrystallized from water, and dried in an oven to constant weight. Acetic acid, source not specified, was purified by crystallization and distillation. The amines, source unspecified, were dried over KOH and distilled over zinc powder. CH_2Cl_2, chlorobenzene, and ethylacetate were dried over P_2O_5, and distilled over anhydrous Na_2CO_3. Benzene and diethylether were dried with sodium metal, and distilled.

Estimated Error:

Temperature: ±0.5 K (authors).
Solubility: ±2% (authors).

Components:
(1) Potassium thiocyanate; KSCN; [333-20-0]
(2) 2-(2-methoxyethoxy)-N,N-bis-2-(2-methoxyethoxy) ethyl ethanamine {tris(dioxa-3,6-heptyl)amine}; $C_{15}H_{33}NO_3$; [70384-51-9]; or
2-methoxy-N,N-bis(methoxyethyl)ethanamine; {tris(oxa-3-butyl)amine}; $C_9H_{21}NO_3$; [3235-51-6]
(3) Dichloromethane; CH_2Cl_2; [75-09-2]

Original Measurements:
G. Soula, Eur. Par. Appl. 016673 (1979); French Appl. 7905438.

Variables:
T/K: unspecified
c_2 /mol dm^{-3}: 0.1

Prepared By:
J. Hála

Experimental Data

Solubility of KSCN in CH_2Cl_2 in the presence of amines[a]

Amine	KSCN (mg dm^{-3})	KSCN (c_1 /mol dm^{-3})[b]
$C_{15}H_{33}NO_3$	3910	0.0402
$C_9H_{21}NO_3$	490	0.000504

[a] Measurements performed at an unspecified, ambient temperature. Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: The solubility of KSCN in neat CH_2Cl_2 was reported to be less than 1 mg dm^{-3}. The solubilization effect of $C_{15}H_{33}NO_3$ was explained by the authors in terms of the formation of a 1:1 adduct of KSCN with the amine in the solution.

Auxiliary Information

Method/Apparatus/Procedure:
Isothermal method used. The salt (0.001 mole) was equilibrated with 0.001 mole amine in 10 mL CH_2Cl_2 by stirring. The content of the salt in the saturated solution was determined by flame photometry.

Source and Purity of Materials:
$C_{15}H_{33}NO_3$ was prepared by refluxing sodium methoxy-2-ethanoate with chlorohydrate of tris(chloro-2-ethyl) amine in methoxy-2-ethanol for 12 h at 125 °C. The excess of solvent was then distilled off, excess of sodium methoxy-2-ethanoate decomposed with concentrated HCl, and the amine was distilled at 165–180 °C at 0.5 mm Hg. $C_9H_{21}NO_3$ was obtained by a similar procedure using sodium methanoate and methanol as the solvent. After treatment of the mixture with HCl, the amine was extracted into CH_2Cl_2, and distilled. Anhydrous CH_2Cl_2 was purified from stabilizers.

Estimated Error:
Solubility: insufficient data reported to allow for error estimate.

6.4. Rubidium Thiocyanate

Components:
(1) Rubidium thiocyanate; RbSCN; [3879-02-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. D. Stepin and I. N. Bykova, Trudy IREA (Moscow) No. **28**, 246–50 (1966).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of RbSCN in water at 25 °C

The solubility at 25 °C of RbSCN in water is reported to be 100 $w_1 = 69.2$ mass % ($m_1 = 15.65$ mol kg^{-1}; compiler).

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details reported.

Source and Purity of Materials:
RbSCN was prepared from Rb_2CO_3 and NH_4SCN (source and purity of starting materials not reported) according to Unmack *et al.*[1] The product was recrystallized from 70% ethanol and dried at 120–160 °C. It contained 99.5% RbSCN.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] A. Unmack, D. M. Rust, and H. Hartley, Proc. R. Soc., Ser. A **127**, 228 (1930).

Components:
(1) Rubidium thiocyanate; RbSCN; [3879-02-5]
(2) Solvents

Original Measurements:
B. D. Stepin, V. E. Plyushchev, and Yu. A. Ivanova, Khim. Prom. (Chem. Industry) 404–7 (1962).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of RbSCN at 25 °C in five solvents[a]

Solvent	RbSCN (100 w_1/mass %)	RbSCN (m_1/mol kg^{-1})[b]
Methanol; CH_4O; [67-56-1]	16.50	1.377
Ethanol; C_2H_6O; [64-17-5]	2.75	0.197
2-Butanone; C_4H_8O; [78-93-3]	1.10	0.0775
Cyclohexanone; $C_6H_{10}O$; [108-94-1]	0.86	0.0604
1-Phenylethanone; C_8H_8O; [98-86-2]	0.55	0.0385

[a] Solid phases not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, no details reported.

Source and Purity of Materials:

Refractive indices and densities, respectively, both at 20 °C, of the solvents used were as follows: methanol, 1.3289, 0.7908; ethanol, 1.3609, 0.7987; 2-butanone, 1.3780, 0.8041; cyclohexanone, 1.4500, 0.9453; 1-phenylethanone (acetophenone), 1.5328, 1.0270.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:
(1) Rubidium thiocyanate; RbSCN; [3879-02-5]
(2) Tri-n-butyl(phosphate); $C_{12}H_{27}O_4P$; [126-73-8]

Original Measurements:
J. Hála and D. G. Tuck, Canad. J. Chem. **48**, 2843–6 (1970).

Variables:
T/K: 295

Prepared By:
J. Hála

Experimental Data

The solubility of RbSCN in tri-n-butyl(phosphate) is reported to be 3.4 g salt in 100 g solvent at 22 °C ($m_1 = 0.237$ mol kg^{-1}; compiler).

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. An excess of the salt was shaken overnight with 5 mL, dry solvent. Preliminary experiments showed that this was sufficient for equilibrium to be reached. Samples of the saturated solutions were withdrawn through a sinter, diluted with acetone, and analyzed for the thiocyanate content by titration against $AgNO_3$ standard solution. Blank titrations showed that a small correction was required because of the presence of tri-n-butyl(phosphate).

Source and Purity of Materials:

RbSCN was prepared by neutralizing of RbOH (Alfa Inorganics) with thiocyanic acid solution obtained by ion-exchange of the sodium salt on a Dowex 50W-X8 column in H form. Tri-n-butyl(phosphate) (Fisher Scientific Co.) was purified by refluxing it with 0.5% caustic soda solution, followed by steam distillation. The product was dried first with anhydrous $MgSO_4$, and finally vacuum/dried at 50 °C in a stream of dry nitrogen gas.[1]

Estimated Error:
Temperature: precision not reported.
Solubility: ±0.05 g salt/100 g solvent (authors).

References:

[1] D. G. Tuck, J. Chem. Soc. 2783 (1958).

6.5. Cesium Thiocyanate

Components:
(1) Cesium thiocyanate; CsSCN; [3879-01-4]
(2) Tri-n-butyl(phosphate); $C_{12}H_{27}O_4P$; [126-73-8]

Original Measurements:
J. Hála and D. G. Tuck, Canad. J. Chem. **48**, 2843–6 (1970).

Variables:
T/K: 295

Prepared By:
J. Hála

Experimental Data

The solubility of CsSCN in tri-n-butyl(phosphate) is reported to be 0.57 g salt in 100 g solvent at 22 °C ($m_1 = 0.0298$ mol kg^{-1}; compiler).

Auxiliary Information

Method/Apparatus/Procedure:
Isothermal method used. An excess of the salt was shaken overnight with 5 mL dry solvent. Preliminary experiments showed that this was sufficient for equilibrium to be reached. Samples of the saturated solutions were withdrawn through a sinter, diluted with acetone, and analyzed for the thiocyanate content by titration against $AgNO_3$ standard solution. Blank titrations showed that a small correction was required because of the presence of tri-n-butyl(phosphate).

Source and Purity of Materials:
CsSCN was prepared by neutralizing of CsOH (Alfa Inorganics) with thiocyanic acid solution obtained by ion exchange of the sodium salt on a Dowex 50W-X8 column in H form. Tri-n-butyl(phosphate) (Fisher Scientific Co.) was purified by refluxing it with 0.5% caustic soda solution, followed by steam distillation. The product was dried first with anhydrous $MgSO_4$, and finally vacuum/dried at 50 °C in a stream of dry nitrogen gas.[1]

Estimated Error:
Temperature: precision not reported.
Solubility: ±0.02 g salt/100 g solvent (authors).

References:
[1] D. G. Tuck, J. Chem. Soc. 2783 (1958).

Components:
(1) Cesium thiocyanate; CsSCN; [3879-01-4]
(2) Urea; CH_4N_2O; [57-13-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
R. Turgunbekova and K. Nogoev, *Geterogennye Ravnovesia Sistem Neorg. Org. Soed.* (Heterogeneous Equilibria of Systems of Inorganic and Organic Compounds) (Akad. Nauk Kirgiz, SSR, 1971), pp. 34–35.

Variables:
T/K: 288, 303, and 318
100 w_2/mass %: 0–49 at 288 K, 0–57.5 at 303 K, 0–64 at 318 K

Prepared By:
J. Hála

Experimental Data

Composition of the saturated solutions in the CsSCN–urea–H_2O system at three temperatures

Temperature (t/°C)	Urea (100 w_2/mass %)	Urea (100 x_2/mole %)	CsSCN (100 w_1/mass %)	CsSCN (100 x_1/mole %)	Solid phase[a]
15	0	0	61.51	8.367	A
	7.08	3.329	57.51	8.504	A
	29.75	20.88	46.52	10.27	A
	29.98	21.46	46.76	10.53	A+B
	31.06	22.55	46.00	10.50	B
	45.26	16.11	7.95	0.889	B
	49.00	16.00	0	0	B
30	0	0	67.39	10.82	A
	6.97	3.922	63.44	11.23	A
	30.05	25.20	50.09	13.21	A
	30.55	26.10	49.96	13.42	A+B
	30.35	25.94	50.17	13.49	B
	53.95	22.99	6.98	0.9354	B
	57.50	22.53	0	0	A
45	0	0	67.75	11.00	A
	6.08	3.810	67.35	13.27	A
	30.38	32.26	53.94	18.01	A+B
	33.46	38.85	52.20	19.06	B
	33.00	37.08	52.18	18.44	B
	54.65	26.72	11.29	1.736	B
	64.00	29.60	0	0	B

[a] A: CsSCN, [3879-01-4]; B: CH_4N_2O, [57-13-6].
[b] The authors' mole % data were computer recalculated by the compiler. Most of the data agreed within ±0.02 mole %, the differences being most likely caused by rounding errors. Those differing more are shown in the table as data marked with superscript [b].

Additional information: Also reported were the solubility diagrams of the CsSCN–urea–H_2O system at 15, 30, and 45 °C.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details reported except that solid phases were characterized by Schreinemaker's method.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

6.6. Ammonium Thiocyanate

6.6.1. Evaluation of the NH_4SCN-H_2O System

Components:	**Evaluator:**
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4] (2) Water; H_2O; [7732-18-5]	J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, August 2001.

Critical Evaluation

The solubility in the binary NH_4SCN-H_2O system as a function of temperature has been reported in five documents. Isothermal method was used by Rüdorf,[1] polythermal method was used in three laboratories,[3–5] and one set of data was obtained by graphical analytical method.[2] In these documents, the solubility of NH_4SCN was reported over the temperature range of 271–344 K. In addition, additional data of the solubility of NH_4SCN in water at temperatures from 253 to 303 K could be extracted from the measurements on various ternary systems.[6–13] From the graph where all the data have been plotted (Fig. 23) a reasonable agreement is seen for the solubility data below 313 K. The data in this temperature range have been summarized in the following table. Except for the three values marked with an asterisk, the data have been computer smoothed by a linear regression to a fifth order polynomial.

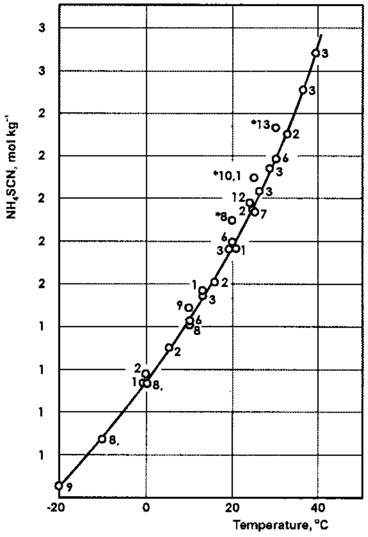

FIG. 23. Solubility of NH_4SCN in water as a function of temperature (numbers refer to the corresponding references).

Solubility of NH_4SCN as a function of temperature

Temperature (t/°C)	Temperature (T/K)	NH_4SCN (m_1/mol kg^{-1})	Ref.	Temperature (t/°C)	Temperature (T/K)	NH_4SCN (m_1/mol kg^{-1})	Ref.
−20	253.1	10.57	9	20	293.1	21.93	6
−10	263.1	12.77	8,9			22.95*	8
−2.2	270.9	15.42	1	20.8	293.9	21.65	1
0	273.1	15.74	2	25.0	298.1	23.46	2
		15.42	8,9			23.45	7
5.0	278.1	17.06	2			24.96*	10,11
10	283.1	18.31	6			23.69	12
		18.14	8	26.33	299.4	24.34	3
		18.90	9	28.82	301.9	25.42	3
12.9	286.0	19.69	1	30	303.1	25.80	6
13.0	286.1	19.36	3			27.28*	13
16.0	289.1	20.12	2	33.0	306.1	27.04	2
18.99	292.1	21.62	3	36.36	309.5	29.05	3
				39.44	312.5	30.73	3

To obtain the temperature dependence of the NH_4SCN solubility in water as

$$S/(\mathrm{mol\ kg^{-1}}) = 0.844\,625\times10^{5} - 0.148\,246\times10^{4}\,(T/\mathrm{K}) + 0.103\,815\times10^{2}\,(T/\mathrm{K})^2 - 0.362\,571\times10^{-1}\,(T/\mathrm{K})^3$$

$$+0.631\,477\times10^{-4}\,(T/\mathrm{K})^4 - 0.438\,662\times10^{-7}\,(T/\mathrm{K})^5.$$

This equation can be suggested as yielding tentative solubility values in the temperature range from 253 to 313 K.

At temperatures above 313 K, the agreement between solubility data from various sources[2–5] is not so good, presumably because at these temperatures the saturated solutions are rather concentrated, and even small errors in analysis may result in considerable deviations in the determined solubility. For this reason, these data have not been included in the smoothing procedure.

The composition at the eutectic (cryohydric) point in the NH_4SCN-H_2O system has been reported in other documents.[14,15] In both documents, the eutectic temperature was reported to be 248 K, the compositions at the eutectic point being $100\ w_1 = 41.95$ mass %[14] and $100\ x_1 = 15$ mole %[15] ($100\ w_1 = 42.7$ mass %; evaluator). For these two documents compilation sheets were not prepared since, except for eutectic points, no other data or details were reported.

References:

[1] F. Rüdorf, Ann. Phys. Chem. **136**, 276 (1869).
[2] E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367 (1959).
[3] L. Shnidman, J. Phys. Chem. **38**, 901 (1934).
[4] I. L. Krupatkin and L. D. Vorobeva, Zh. Obsh. Khim. **45**, 980 (1975).
[5] M. I. Ravich, V. Ya. Ketkovich, and I. S. Rassonskaya, Izv. Sektora Fiz. Khim. Anal. **17**, 254 (1949).
[6] H. W. Foote, J. Am. Chem. Soc. **43**, 1031 (1921).
[7] P. S. Bogoyavlenskii, Zh. Fiz. Khim. **32**, 2035 (1958).
[8] A. M. Babenko and A. M. Andrianov, Ukrain. Khim. Zh. **45**, 1177 (1979).
[9] A. M. Babenko and A. M. Andrianov, Zh. Neorg. Khim. **23**, 2819 (1978).
[10] V. G. Skvortsov, A. K. Molodkin, R. S. Tsekhanskii, Sh. V. Sadetdinov, and F. V. Nikonov, Zh. Neorg. Khim. **30**, 826 (1985).
[11] Sh. V. Sadetdinov, V. G. Skvortsov, and R. S. Tsekhanskii, Sb. Trudov Yaroslav. Gosud. Ped. Inst., No. 169, 72 (1978).
[12] V. J. Occleshaw, J. Chem. Soc. 1892 (1934).
[13] L. S. Bleshinskaya, K. Sulaimankulov, M. D. Davranov, and Z. Yu. Yunusova, Dep. Doc. VINITI, No. 120-83 (1983).
[14] A. M. Vasiliev, Zh. Russ. Fiz. Khim. Obsh. **42**, 423 (1910).
[15] E. Kordes, Z. Anorg. Allg. Chem. **167**, 97 (1927).

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. Rüdorff, Ann. Phys. Chem. **136**, 276–84 (1869).

Variables:
T/K: 271–293

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN in water as a function of temperature[a]

Temperature (t/°C)	NH_4SCN (g/100 g H_2O)	NH_4SCN (m_1/mol kg^{-1})[c]
−2.2	117.4	15.42
0[b]	122.1	16.04
12.9	149.9	19.69
20[b]	162.2	21.31
20.8	164.8	21.65

[a] Solid phases were not investigated.
[b] Interpolated values obtained by the author; reported also in Rüdorff.[1]
[c] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. The salt was first shaken with water to obtain a solution saturated at a temperature slightly above the desired one. Then the solution was allowed to cool down, and stand at the desired temperature for 12 h. The NH_4SCN content was determined in a weighed portion of the saturated solution by titration with standard $AgNO_3$ solution against K_2CrO_4 as the indicator.

Source and Purity of Materials:

Nothing specified.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] F. Rüdorff, Ber. Deutsch. Chem. Ges. **2**, 68–70 (1869).

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. Shnidman, J. Phys. Chem. **38**, 901–6 (1934).

Variables:
T/K: 286–344.5

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN in water as a function of temperature[a]

Temperature (t/°C)	NH_4SCN (100 w_1/mass %)	NH_4SCN (x_1)	NH_4SCN (m_1/mol kg^{-1})[b]
13.00	59.57	0.2588	19.36
18.99	62.20	0.2803	21.62
26.33	64.95	0.3043	24.34
28.82	65.93	0.3138	25.42
36.36	68.86	0.3435	29.05
39.44	70.05	0.3567	30.73
46.92	72.86	0.3885	35.27
51.37	74.53	0.4092	38.44
52.50	74.94	0.4154	39.35
57.23	76.63	0.4376	43.08
62.46	78.53	0.4637	48.05
67.21	80.18	0.4890	53.15
71.53	81.73	0.5145	58.77

[a] Solid phases were not investigated.
[b] Calculated by compiler from the author's mass % data.

Auxiliary Information

Method/Apparatus/Procedure:

Polythermal method used. Weighed quantities of the solvent and solute were heated in a sealed tube rotated in a water bath, and the temperature at which the solid phase had nearly disappeared was noted. The apparatus described in Sunier[1] was used. Care was taken in attaining true equilibrium conditions at the solubility temperature by slow heating, and ensuring the presence of small crystals.[2] In some cases, thermostating at the respective solubility temperature for about 2 h was employed. A thermometer certified by the Bureau of Standards was used.

Source and Purity of Materials:

NH_4SCN, Baker C. P. grade, was twice crystallized from methanol. A nonhygroscopic product with a melting point of 149.7 °C was obtained. It was analyzed for NH_3 and SCN^- by distillation and Volhard's methods, respectively, to yield 22.40% ± 0.06% NH_3 and 76.29% ± 0.05% SCN^-. Boiled distilled water was used.

Estimated Error:
Temperature: ±0.01 K (author).
Solubility: insufficient data given to allow for error estimate.

References:

[1] A. A. Sunier, J. Phys. Chem. **34**, 2582 (1930).
[2] L. Shnidman, J. Phys. Chem. **37**, 693 (1933).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. I. Ravich, V. Ya. Ketkovich, and I. S. Rassonskaya, Izv. Sektora Fiz. Khim. Anal. **17**, 254–85 (1949).

Variables:

T/K: 340–422.5

Prepared By:

J. Hála

Experimental Data

Solubility of NH_4SCN in water as a function of temperature and phase diagram of the NH_4SCN–H_2O system (see Fig. 24)

Temperature t/°C	H_2O (100 w_2/mass %)	H_2O (100 x_2/mol %)	NH_4SCN (100 w_2/mass %)	NH_4SCN[a] (100 x_2/mol %)	Solid phase[b]
67	19.89	51.22	80.11	52.91	A
71	18.53	49.00	81.47	57.76	A
72.5	17.56	47.36	82.44	61.68	A
76.5	16.34	45.21	83.66	67.26	A
80	15.39	43.35	84.61	72.22	A
84	13.93	40.61	86.07	81.17	A
86.5	13.06	38.82	86.94	87.45	A
89	12.31	37.23	87.31		B
91.5	11.65	35.78	88.35		B
93	11.40	35.22	88.60		B
96.5	10.69	33.59	89.31		B
103.5	8.79	28.81	91.21		B
110	7.34	25.07	92.66		B
119.5	5.35	19.27	94.65		B
123	4.71	17.27	95.29		C
135	2.57	10.02	97.43		C
149.5[c]	—	—	100		C

[a] Calculated by compiler.
[b] A: γ-NH_4SCN; B: β-NH_4SCN; C: α-NH_4SCN.
[c] Melting point of NH_4SCN.

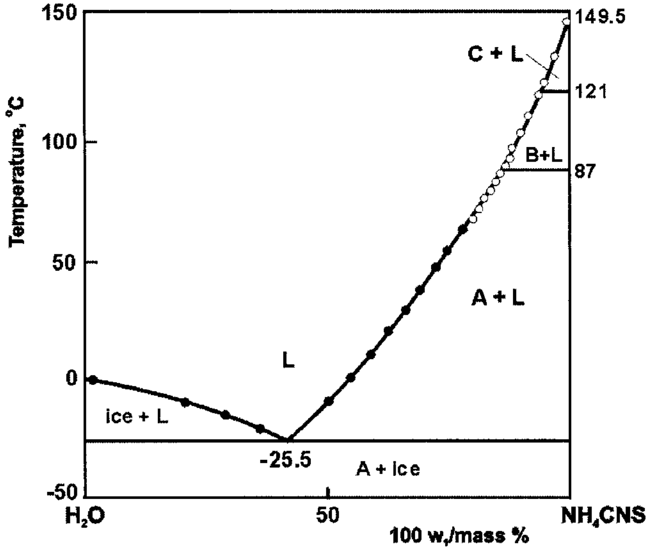

FIG. 24. Phase diagram of the NH_4SCN–H_2O system (α, β, and γ stand for the corresponding forms of NH_4SCN, L stands for solution).

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. No details were reported except that in measurements above 100 °C closed vessels were used to avoid evaporation of water. Separate experiments showed that at temperatures slightly above 100 °C only negligible fraction (about 10^{-2} %) of NH_4SCN was isomerized to thiourea, while 1%–1.5% thiourea was formed only at temperatures close to the melting point of the salt.

Source and Purity of Materials:

NH_4SCN, commercial, chemically pure product, was recrystallized, dried at 120 °C, and kept over P_2O_5 in a dessicator.

Estimated Error:

Temperature: precision ± 0.5 K (authors).

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).

Variables:
T/K: 273–326

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN in water as a function of temperature[a]

Temperature (t/°C)	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[b]
0	54.5	15.74
5.0	56.5	17.06
16.0	60.5	20.12
25.0	64.1	23.46
33.0	67.3	27.04
50.0	72.8	35.16
53.0	73.2	35.88

[a] Solid phase was NH_4SCN, [1762-95-4], in all solutions.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were obtained by graphical analytical method.[1,2] A series of mixtures of the salt and water covering the fields of unsaturated and saturated solutions were prepared by weighing. After equilibrium had been attained, refractive indexes of the solutions were measured. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition graph.

Source and Purity of Materials:

NH_4SCN, source not specified, was recrystallized and dried over anhydrous $CaCl_2$.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. L. Krupatkin and L. D. Vorobeva, Zh. Obsh. Khim. **45**, 980–4 (1975).

Variables:
T/K: 322.6–348.1

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN in water as a function of temperature[a]

Temperature (t/°C)	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[b]
49.50	74.80	38.99
60.25	78.50	47.97
63.75	79.45	50.79
64.50	79.75	51.74
65.50	80.25	53.38
66.00	80.43	53.99
66.80	80.97	55.90
68.50	81.42	57.57
71.00	82.03	59.97
75.00	83.52	66.58

[a] Solid phase was reported to be $NH_4SCN \cdot H_2O$, [ ], in all solutions.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used, no details reported.

Source and Purity of Materials:

NH_4SCN, source not specified, was dried at 70 °C before use. Doubly distilled water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Sulfur dioxide; SO_2; [7446-09-5]

Original Measurements:
G. Jander and W. Ruppolt, Z. Phys. Chem. **179**, 43–50 (1937).

Variables:
T/K: 273

Prepared By:
J. Hála

Experimental Data

The solubility of NH_4SCN in liquid sulfur dioxide was reported to be 46.8 g salt in 100 g solvent at 0 °C (m_1/mol kg^{-1} = 6.148; compiler).

Additional information: High, though unspecified solubility of NH_4SCN in liquid SO_2 was reported in Friedrichs[2] and Franklin.[3] Saturated solutions were reported to be yellow in color and very viscous.[2] Another liquid phase separated from the saturated solutions at 100 °C as a yellow oil.[3]

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method. About 10 g SO_2, carefully dried, was equilibrated with excess solid at 0 °C in water–ice bath in a three-compartment glass vessel in which equilibrating and sampling compartments were separated by a compartment containing glass/wool filter. Equilibration was performed for unspecified, prolonged period of time under frequent shaking. After equilibrium had been attained, the vessel was turned upside down, and the saturated solution was filtered into the empty sampling compartment, which was subsequently cooled and sealed off. After weighing the compartment with the sample, SO_2 was allowed to evaporate, the residue was weighed, dissolved in water, and the content of the salt was determined. Method of analysis was not specified.

Source and Purity of Materials:

NH_4SCN, source not specified, was carefully dried before use. Commercially available SO_2 was purified by passing it through concentrated H_2SO_4 and over asbestos wool, and dried by using P_2O_5. Specific conductivity of the product was 4.5×10^{-7} Ω^{-1} (Jander and Wickert).[1]

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] G. Jander and K. Wickert, Z. Phys. Chem. **178**, 57 (1936).
[2] F. Friedrichs, Z. Anorg. Allgem. Chemie **84**, 373 (1914).
[3] E. C. Franklin, J. Phys. Chem. **15**, 687 (1911).

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
W. P. Bradley and W. B. Alexander, J. Am. Chem. Soc. **34**, 15–24 (1912).

Variables:
T/K: 182–421

Prepared By:
J. Hála

Experimental Data

Solubility in the NH_4SCN–NH_3 system

NH_3 (100 w_2/mass %)	Freezing point (t/°C)	NH_4SCN^a (100 w_1/mass %)	NH_4SCN^a (m_1/mol kg^{-1})	NH_3 (100 w_2/mass %)	Freezing point (t/°C)	NH_4SCN^a (100 w_1/mass %)	NH_4SCN^a (m_1/mol kg^{-1})
0	148	100	—	56.18	79.8	43.82	10.25
9.89	77	90.11	119.7	56.63	−76.8	43.37	10.06
13.22	56	86.78	86.24	57.43	−75.8	42.57	9.738
16.55	32	83.45	66.24	57.77	−79	42.33	9.603
17.62	23	82.38	61.42	58.62	−79.8	41.38	9.274
19.40	10.3	80.60	54.58	59.22	−79.8	40.78	9.046
20.93	−0.3	79.07	49.63	59.29	−79.8	40.71	9.020
21.91	−5.8	78.09	46.82	60.07	−79.8	39.93	8.733
22.50	−13.8	77.50	45.25	60.73	−84.7	39.27	8.495
23.27	−18	76.73	43.32	61.53	−86.3	38.47	8.214
23.94	−20	76.06	41.74	61.63	−84.3	38.37	8.179
24.89	−22	75.11	39.64	62.33	−87	37.67	7.940
25.61	−24.3	74.39	38.16	63.05	−87.2	36.95	7.699
26.30	−25.8	73.70	36.81	64.55	−87.3	35.45	7.215
27.67	−29.8	72.33	34.34	65.60	−88.3	34.40	6.889
29.13	−34.8	70.78	31.96	66.11	−89.3	33.89	6.735
29.90	−39.8	70.10	30.80	66.40	−90.8	33.60	6.648
30.75	−42.8	69.25	29.59	66.41	−91.3	33.59	6.645
32.29	−39.8	67.71	27.55	66.79	−95	33.21	6.532
34.01	−39.2	65.99	25.49	67.30	−93	32.70	6.383
36.38	−38.8	63.62	22.97	67.93	−91.8	32.07	6.202
38.76	−38.8	61.24	20.76	68.25	−90.3	31.75	6.111
42.08	−41.3	57.92	18.08	68.84	−89	31.16	5.946
44.08	−42	55.92	16.67	69.65	−88	30.35	5.725
45.40	−44	54.60	15.80	71.00	−85.7	29.00	5.366
47.33	−47.2	52.67	14.62	73.77	−82.7	26.23	4.671
48.76	−52.2	51.24	13.81	76.18	−81.3	23.82	4.108
49.75	−57	50.25	13.27	78.75	−79	21.25	3.545
51.08	−60.6	48.92	12.58	79.38	−79.2	20.62	3.413
52.20	−65.2	47.80	11.98	83.18	−78.7	16.82	2.656
53.96	−70.8	46.04	11.21	86.78	−78	13.22	2.001
54.65	−72.8	45.35	10.90	90.01	−77	9.99	1.458
54.90	−73	45.10	10.79	93.50	−76.9	6.50	0.9133
55.13	−75.7	44.87	10.69	94.78	−76.8	5.22	0.7235
55.52	−77	44.48	10.52	94.90	−76.7	5.10	0.7060
55.91	−79.3	44.09	10.36	100	−76.2	—	—

[a] Calculated by compiler.

Equilibrium solid phases and their existence regions are shown in the phase diagram (Fig. 25) as A: $NH_4SCN \cdot NH_3$; B:$NH_4SCN \cdot 3NH_3$; C:$NH_4SCN \cdot 6NH_3$; D:$NH_4SCN \cdot 7NH_3$; E: $NH_4SCN \cdot 8NH_3$. The authors stated that their data were not conclusive about the heptaammoniate, as well as about $NH_4SCN \cdot 6.5NH_3$ or $2NH_4SCN \cdot 13NH_3$. Approximate values of melting points of ammoniates A, B, C, D, and E are −16 °C (metastable), −38 °C, −76 °C, −84 °C, and −87 °C, respectively.

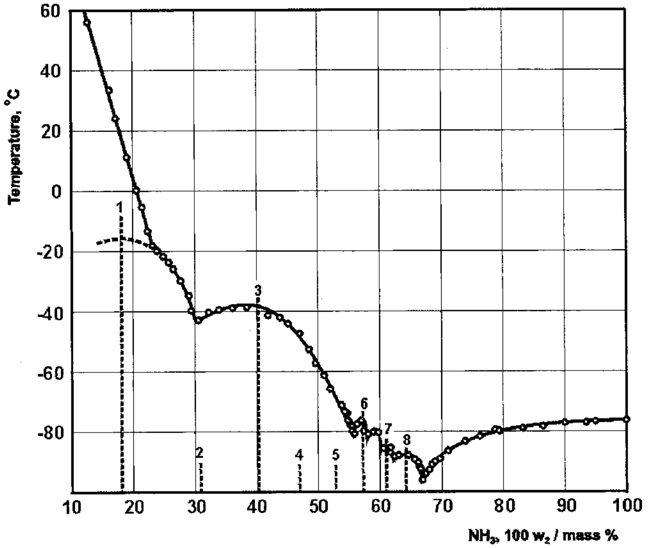

FIG. 25. Phase diagram of the NH_4SCN–NH_3 system.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method was used. Measurements were carried out in glass tubes containing weighed amounts of the salt and condensed NH_3. The tubes were closed with a special cap and cooled in an alcohol–ether mixture until the solution froze partly. (A bath of warm water was used at temperatures above room temperature.) Under effective stirring the bath and spinning the tube, the bath was allowed to warm up slowly and the temperature of disappearance of the last crystals was recorded, At least three readings were taken at each concentration. If the interval between disappearance and reappearance of crystals was brief, there was no evidence of supercooling in the solution. Temperature was read by means of a platinum resistance thermometer protected by a thin-walled glass tube. The thermometer was standardized by means of ice and CO_2–ether mixture.

Source and Purity of Materials:

NH_4SCN, Kahlbaum, was purified by several crystallizations from water, ground, and kept over concentrated H_2SO_4. The product melted at 148 °C. NH_3 gas was obtained from pure concentrated ammonium hydroxide. It was dried over caustic potash and by washing with its own liquid at its normal boiling temperature.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:

H. W. Foote and M. A. Hunter, J. Am. Chem. Soc. **42**, 69–78 (1920).

Variables:

T/K: 276–323

Prepared By:

J. Hála

Experimental Data

Freezing point measurements in the NH_4SCN–NH_3 system[a]

Temperature (t/°C)	NH_3 (100 w_2/mass %)	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[b]
2.8[c]	23.13	76.87	43.66
10.0[d]	22.51	77.49	45.22
20.0[d]	21.64	78.36	47.57
23.3[c]	21.48	78.52	48.02
30.0[d]	19.99	80.01	52.58
31.0[c]	19.86	80.14	53.01
33.0[c]	19.24	80.76	55.14
40.0[d]	18.50	81.50	57.87
49.8[c]	16.67	83.33	65.67

[a] Solid phases were not investigated.
[b] Calculated by compiler.
[c] Polythermal method.
[d] Vapor pressure measurement.

Auxiliary Information

Method/Apparatus/Procedure:

A polythermal method and vapor pressure measurements were used. In the polythermal method, a weighed quantity of a solution of the salt in ammonia, prepared by passing NH_3 gas over the solid salt, having a known composition, was sealed in a tube with weighed amount of NH_4SCN. The mixture was heated until all dissolved, then cooled rapidly to form small crystals. On heating the mixture slowly in a water bath, the temperature was determined at which the last of the crystals dissolved. Some solubility values were obtained during vapor pressure measurements where NH_3 gas at a known pressure was passed through a known amount of the salt in a thermostated U tube until no further change in weight occurred. The vapor pressure of the saturated solution was obtained by reducing the pressure until NH_4SCN crystals just began to appear, and then increasing it slightly until they just dissolved.

Source and Purity of Materials:

NH_4SCN, a C. P. product, was recrystallized and dried. Dry NH_3 gas was obtained by warming a concentrated aqueous solution of ammonia and passing the gas through towers containing quicklime and fused caustic potash.

Estimated Error:

Temperature: precision not reported.

Solubility: the authors stated that individual results were not without appreciable error which, however, was not specified, and that the two methods yielded results agreeing reasonably.

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonia; NH_3; [7664-41-7]

Original Measurements:
H. Hunt, J. Am. Chem. Soc. **54**, 3509–12 (1932).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Three results were reported for the solubility of NH_4SCN: 311.9, 312.4, and 311.6 g in 100 g solvent at 25 °C. From the mean value of 312.0 g salt/100 g solvent and the density of liquid ammonia of 0.604 g cm^{-3} at 25 °C, the author calculated the solubility to be 188.45 g NH_4SCN in 100 cm^3 solvent. Compiler calculated $m_1 = 40.99$ mol kg^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:
Isothermal method used. Ammonia (10–25 g) was equilibrated with the salt in the bottom part of a sealed, two-compartment Pyrex tube. The compartments were separated from each other with a narrow neck. The salt was introduced into the tube before sealing it off in a small cup closed with a very closely woven cotton cloth. The latter permitted the salt to dissolve the salt holding back the solid at the same time. The system was equilibrated for 1–3 weeks with occasional shaking. Then the tube was inverted in the bath and all the solution drained into the empty compartment, which was cooled and sealed off. When it reached room temperature it was dried and weighed, the ammonia allowed to boil off, the tube with the salt warmed until all odor of NH_3 was gone, and the salt was weighed.

Source and Purity of Materials:
NH_4SCN, Baker C. P. product, was recrystallized and carefully dried. Commercially available anhydrous NH_3 was allowed to stand over metallic sodium for several weeks before use.

Estimated Error:
Temperature: ±0.025 K (author).
Solubility: 5% (author).

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
L. Shnidman, J. Phys. Chem. **38**, 901–6 (1934).

Variables:
T/K: 298–338

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN as a function of temperature[a]

Temperature (t/°C)	NH_4SCN ($100\,w_1$/mass %)	NH_4SCN (x_1)	NH_4SCN (m_1/mol kg^{-1})[b]
24.58	37.11	0.1989	7.752
32.94	40.05	0.2194	8.776
44.80	44.70	0.2538	10.62
54.76	49.30	0.2904	12.77
64.55	54.55	0.3356	15.77

[a] Solid phases were not investigated.
[b] Calculated by compiler from the mass % data.

Auxiliary Information

Method/Apparatus/Procedure:
Polythermal method used. Weighed quantities of the solvent and salt were heated in a sealed tube rotated in a water bath, and the temperature at which the solid phase had nearly disappeared was noted. The apparatus described in Sunier[1] was used. Care was taken in attaining true equilibrium conditions at the solubility temperature by slow heating and ensuring the presence of small crystals.[2] In some cases thermostating at the respective solubility temperature for about 2 h was employed. A thermometer certified by the Bureau of Standards was used.

Source and Purity of Materials:
NH_4SCN, Baker C. P. grade, was twice crystallized from methanol. A nonhygroscopic product with melting point at 149.7 °C was obtained. It was analyzed for NH_3 and SCN^- by distillation and Volhard's method, respectively, to yield 22.40%±0.06% NH_3 and 76.29%±0.05% SCN^-. Methanol, Baker C. P., was purified according to Shnidman.[2] It was refluxed twice with lime over 6 h and then distilled through a six-bulb LeBel–Henniger column. The fraction boiling point within 64.63±0.01 °C was used.

Estimated Error:
Temperature: ±0.01 K (author).
Solubility: insufficient data given to allow for error estimate.

References:
[1] A. A. Sunier, J. Phys. Chem. **34**, 2582 (1930).
[2] L. Shnidman, J. Phys. Chem. **37**, 693 (1933).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Acetonitrile; C_2H_3N; [75-05-8]

Original Measurements:

A. Naumann, Ber. **47**, 247–56 (1914).

Variables:

T/K: 291

Prepared By:

J. Hála

Experimental Data

The solubility of NH_4SCN is reported to be 0.0752 g in 1 g solvent at 18 °C (compiler: $m_1 = 0.988$ mol kg^{-1}, $100\,w_1 = 7.00$ mass %).

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Excess solid was shaken with the solvent in a water thermostat for 2–6 h. Attainment of equilibrium was ascertained by occasional analysis of the liquid phase. The saturated solutions were rapidly filtered into weighing vessels kept at 18 °C, and the SCN^- content was determined titrimetrically.

Source and Purity of Materials:

NH_4SCN, source and purity not specified, was dried in a vacuum dessicator before use. Acetonitrile (Kahlbaum) was purified from acetamide by allowing the solvent to stand for 3–4 weeks over P_2O_5, and subsequent distillation. The fraction boiling point at 81.6 °C was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate. The reported solubility value is the mean of two determinations, individual results were not reported.

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:

L. Shnidman, J. Phys. Chem. **38**, 901–6 (1934).

Variables:

T/K: 291–337

Prepared By:

J. Hála

Experimental Data

Solubility of NH_4SCN in ethanol as a function of temperature[a]

Temperature (t/°C)	NH_4SCN ($100\,w_1$/mass %)	NH_4SCN (x_1)	NH_4SCN (m_1/mol kg^{-1})[b]
18.45	19.07	0.1247	3.096
33.25	21.54	0.1421	3.607
36.93	22.16	0.1469	3.740
43.36	23.46	0.1565	4.027
57.62	26.72	0.1807	4.790
64.20	28.63	0.1953	5.270

[a] Solid phases were not investigated.
[b] Calculated by compiler from the mass % data.

Additional information: Solutions of NH_4SCN in ethanol turned yellow on standing, on exposure to light, and in the heating period, indicating some reaction between the two components.

Auxiliary Information

Method/Apparatus/Procedure:

Polythermal method used. Weighed quantities of the solvent and salt were heated in a sealed tube rotated in a water bath, and the temperature at which the solid phase had nearly disappeared was noted. The apparatus described in Sunier[1] was used. When the work was carried out with small crystals they were so fine as to give a colloidal, turbid opalescent solution, and the solubility temperatures were overstepped by 1° or more. It was, therefore, necessary to cool the solutions slowly as to favor the formation of large crystals. True solubility temperatures could be obtained with large crystals with 10 min thermostating. A thermometer certified by the U. S. Bureau of Standards was used.

Source and Purity of Materials:

NH_4SCN, Baker C. P. grade, was twice crystallized from methanol. A nonhygroscopic product with melting point at 149.7 °C was obtained. It was analyzed for NH_3 and SCN^- by distillation and Volhard's method, respectively, to yield $22.40\% \pm 0.06\%$ NH_3 and $76.29\% \pm 0.05\%$ SCN^-. Ethanol was purified according to Shnidman.[2] It was refluxed twice with lime over 6 h and then distilled through a six-bulb LeBel–Henniger column. The fraction boiling point within 78.43±0.02 °C was used.

Estimated Error:

Temperature: ±0.01 K (author).
Solubility: insufficient data given to allow for error estimate.

References:

[1] A. A. Sunier, J. Phys. Chem. **34**, 2582 (1930).
[2] L. Shnidman, J. Phys. Chem. **37**, 693 (1933).

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) N,N-diethyl-ethanamine (triethylamine); $C_6H_{15}N$; [121-44-8]

Original Measurements:
L. D. Vorobeva and I. L. Krupatkin, *Fazovye Ravnovesia* (Phase Equilibria), (Kalinin. Gosud. Univ., Kalinin, 1974), pp. 18–25.

Variables:
T/K: 293–298

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN in triethylamine as a function of temperature[a]

Temperature (t/°C)	NH_4SCN ($100\,w_1$/mass %)	NH_4SCN (m_1/mol kg^{-1})[b]
20	53.45	15.08
23	55.60	16.45
25	57.50	17.77

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Additional information: When saturated solutions of NH_4SCN in triethyalmine were diluted with triethylamine, a narrow homogeneous region of unsaturated solutions was first observed. On further dilution, the system separated into two liquid phases, the corresponding NH_4SCN concentrations being 42.50, 44.50, and 46.00 mass % at 20, 23, and 25 °C, respectively. Based on infrared spectral measurements the authors assumed that a complex $[(C_2H_5)_3N...H_4N^+]SCN^-$ was being formed in the system.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details reported.

Source and Purity of Materials:
NH_4SCN, chemically pure, was dried to constant weight before use. Triethylamine, source not specified, was dried over anhydrous $MgSO_4$, and distilled twice. The product used boiling point at 89.2 °C, and showed d. of 0.7232 g cm^{-3} at 20 °C.

Estimated Error:
Temperature: ±0.1 K (authors).
Solubility: insufficient data reported to allow for error estimate.

Components:
(1) Amonnium thiocyanate; NH_4SCN; [1762-95-4]
(2) Tri-n-butyl(phosphate); $C_{12}H_{27}O_4P$; [126-73-8]

Original Measurements:
J. Hála and D. G. Tuck, Canad. J. Chem. **48**, 2843–6 (1970).

Variables:
T/K: 295

Prepared By:
J. Hála

Experimental Data

The solubility of NH_4SCN in tri-n-butyl(phosphate) is reported to be 11.6 g salt in 100 g solvent at 22 °C ($m_1 = 1.524$ mol kg^{-1}; compiler).

Additional information: From the ratio of the solvent and NH_4SCN concentrations of 2.46 in the saturated solutions the authors suggested that the saturated solution contained the disolvate of the salt, $NH_4SCN \cdot 2C_{12}H_{27}O_4P$, with some free solvent.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. An excess of the salt was shaken overnight with 5 mL dry solvent. Preliminary experiments showed that this was sufficient for equilibrium to be reached. Samples of the saturated solutions were withdrawn through a sinter, diluted with acetone, and analyzed for the thiocyanate content by titration against $AgNO_3$ standard solution. Blank titrations showed that a small correction was required because of the presence of tri-n-butyl(phosphate).

Source and Purity of Materials:
NH_4SCN, Fisher Scientific Co., was used without further purification. Tri-n-butyl(phosphate) (Fisher Scientific Co.) was purified by refluxing it with 0.5% caustic soda solution, followed by steam distillation. The product was dried first with anhydrous $MgSO_4$, and finally vacuum/dried at 50 °C in a stream of dry nitrogen gas.[1]

Estimated Error:
Temperature: precision not reported.
Solubility: ±0.1 g salt/100 g solvent (authors).

References:

[1] D. G. Tuck, J. Chem. Soc. 2783 (1958).

Components:
(1) Amonnium thiocyanate; NH_4SCN; [1762-95-4]
(2) Solvents

Original Measurements:
I. L. Krupatkin, L. D. Vorobeva, V. P. Maskhulia, and, M. E. Veselova, Zh. Obsh. Khim. **45**, 985–90 (1975).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN in furfural and methylethylketone at 25 °C[a]

Solvent	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[b]
2-furancarboxaldehyde (furfural); $C_5H_4O_2$; [98-01-1]	10.30	1.509
2-butanone (methylethylketone); C_4H_8O; [78-93-3]	10.70	1.574

[a] Solid phases were not investigated.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details reported.

Source and Purity of Materials:
NH_4SCN, source and purity not specified, was dried at 70 °C to constant weight before use. The solvents were purified by standard methods,[1] and their purity was checked through physical constants.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] A. Weisberger, E. Proskanzer, J. Riddick, and E. Toops, *Organic Solvents* (Russian translation of English ed.) (IL Publ. House, Moscow, 1958), pp. 351, 361.

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonia; NH_3 ; [7664-41-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
H. W. Foote, J. Am. Chem. Soc. **43**, 1031–8 (1921).

Variables:
T/K: 283–303
100 w_2/mass %: 0–22.70

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN in aqueous solutions of ammonia at three temperatures[a]

Temperature (t/°C)	NH_3 (100 w_2/ mass %)	NH_4SCN (100 w_1/ mass %)	NH_4SCN (m_1/mol kg^{-1})[b]	Temperature (t/°C)	NH_3 (100 w_2/ mass %)	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[b]
10	0	58.23	18.31	30	0	66.26	25.80
	3.49	59.40			2.85	67.28	
	6.86	61.03			5.79	68.30	
	9.23	62.61			8.38	69.48	
	12.33	65.29			12.18	71.84	
	14.53	66.67			14.46	74.00	
	17.12	69.70			17.04	76.63	
	19.78	72.84			20.01	79.99	52.52
	22.70	77.30	44.74				
20	0	62.54	21.93				
	3.53	63.57					
	6.23	64.99					
	8.57	66.20					
	11.19	67.57					
	12.54	69.06					
	15.65	71.89					
	18.07	74.15					
	21.35	78.65	48.40				

[a] NH_4SCN, [1762-95-4], was the equilibrium solid phase in all saturated solutions.
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method[1] was used. Measurements were carried out in thermostated glass-stoppered bottles. Equilibrium was reached after 1 h shaking. Samples for analysis were withdrawn through a plug of glass wool into a weighed specimen tube under cooling to avoid losses of NH_3. Ammonia was determined by titration using congored as indicator, SCN^- by Volhard's method. Solid phases were chemically analyzed.

Source and Purity of Materials:
NH_4SCN, source not specified, chemically pure, was recrystallized and dried until it showed no trace of moisture. Dry NH_3 gas was obtained by warming a concentrated aqueous solution of ammonia and passing the gas through towers containing quicklime and fused caustic potash.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] H. W. Foote and S. R. Brinkley, J. Am. Chem. Soc. **43**, 1081 (1921).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonium nitrate; NH_4NO_3; [6484-52-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. I. Ravich, V. Ya. Ketkovich, and I. S. Rassonskaya, Izv. Sektora Fiz. Khim. Anal. **17**, 254–85 (1949).

Variables:

T/K: 273–363
$100\ x_2$/mol %: 3.6–53.5

Prepared By:

J. Hála

Experimental Data

Solubility in the $NH_4SCN-NH_4NO_3-H_2O$ system as a function of temperature

Temperature (t/°C)	NH_4NO_3 ($100\ x_2$/mol %)	NH_4SCN ($100\ x_1$/mol %)	Solid phase[a]	Temperature (t/°C)	NH_4NO_3 ($100\ x_2$/mol %)	NH_4SCN ($100\ x_1$/mol %)	Solid phase[a]
0	3.6	20.8	A	80	8.6	52.8	A
	8.7	19.8	A		17.8	48.7	A
	12.0	18.4	A+B		24.3	47.1	A
	14.3	11.1	B		33.3	48.0	C
	16.4	5.6	B		35.1	48.0	C
30	8.4	28.5	A		38.5	44.1	C
	12.2	28.4	A		41.5	38.9	C
	22.1	26.4	A+B		43.9	36.9	C
	22.4	15.5	B		44.7	33.2	B
	25.1	10.7	B		45.8	23.5	B
	29.5	5.0	B		51.0	12.0	B
60	7.4	41.9	A	90	12.8	56.8	A
	14.1	40.8	A		22.2	52.7	A
	25.1	38.5	A		28.1	52.7	A
	27.3	37.9	A		30.4	51.5	C
	32.1	35.8	A		37.6	47.7	C
	34.0	35.5	A+B		40.5	42.6	C
	33.5	34.9	B		47.5	35.7	C
	33.8	28.4	B		47.8	30.6	B
	34.2	17.0	B		47.5	25.9	B
	39.6	10.0	B		53.5	16.7	B

Polythermal measurements for the ternary system corresponding to the section of 15.00 mol % NH_4NO_3 + 85.00 mol % NH_4SCN[b]

H_2O ($100\ x_3$/mol %)	Freezing point temperature (t/°C)	Solid phase[a]
80.51	−17.0	A
82.22	−21.9	A
83.35	−25.0	A
84.39	−27.3	A+D
85.26	−25.4	D
86.30	−24.0	D
92.33	−13.8	D
95.84	−7.2	D

Composition of invariant points

NH_4SCN ($100\ x_1$/mol %)	NH_4NO_3 ($100\ x_2$/mol %)	Temperature (t/°C)	Solid phases[a]
39.5	38.4	68	A+B+C
12.9	5.7	−30	A+B+D

[a] A: NH_4SCN, [1762-95-4] (monoclinic at 60 and 80 °C, rhomboedral at 90 °C; crystal form at 0 and 30 °C not reported; B: NH_4NO_3, [6484-52-2] (trigonal at 60 °C, α-rhomboedral at 80 and 90 °C; crystal form at 0 and 30 °C not reported; C: solid solutions of NH_4SCN and NH_4NO_3 of variable composition; D: Ice, [7732-18-5] (see Fig. 26).

[b] Cooling curves were also obtained for the section corresponding to 59.80 mol % NH_4NO_3 + 40.20 mol % NH_4SCN, where NH_4NO_3 and ice were identified as the solid phases.

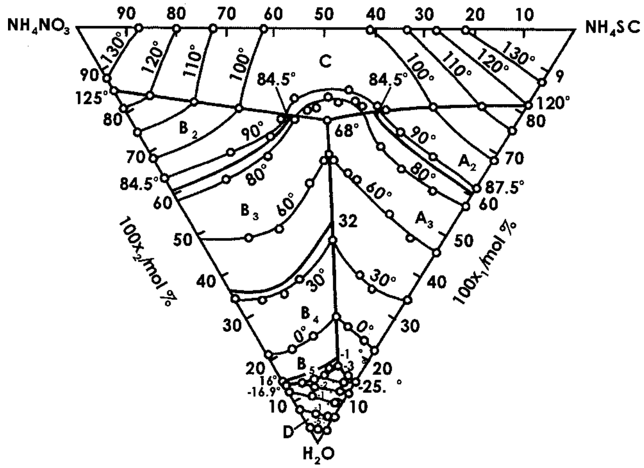

FIG. 26. Solubility polytherm for the $NH_4NO_3-NH_4SCN-H_2O$ system. (B_1: cubic NH_4NO_3; B_2: trigonal NH_4NO_3; B_3: α-rhomboedral NH_4NO_3; B_4: β-rhomoedral NH_4NO_3; B_5: hexagonal NH_4NO_3; A_2; rhomboedral NH_4SCN; A_3: monoclinic NH_4SCN; C: solid solutions; D: ice).

Auxiliary Information

Method/Apparatus/Procedure:

At 0 °C and above the system was studied isothermally. A mixture of solid salts (8–10 g) was dissolved in water completely at a temperature above the desired one, then the flask was placed in a thermostat and kept at the desired temperature to let equilibrium be established, and equilibrium solid phases to crystallize. This took 12 h at 0 °C, and 5 h above 0 °C. At 0 and 30 °C, samples of the saturated solutions were withdrawn with a pipette preheated and/or precooled to the corresponding temperature. A small glass U tube with a wad of glass wool inside was attached to the pipette. At 60 °C and above, samples were taken into a preheated glass tube. The samples were allowed to crystallize on cooling to room temperature and weighed in a weighing bottle. The samples were analyzed for NH_4^+ acidimetrically after distilling off ammonia in the presence of MgO, and for SCN^- by Volhard's method. The content of water was obtained by difference. Solid phases were identified by Schreinemaker's method.

Source and Purity of Materials:

NH_4NO_3 and NH_4SCN were commercial chemically pure products. They were recrystallized, dried at 120 °C, and kept in a dessicator over P_2O_5.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonium nitrate; NH_4NO_3; [6484-52-2]
(3) Ammonia; NH_3; [7664-41-7]

Original Measurements:
H. W.-Foote and S. R. Brinkley, J. Am. Chem. Soc. **43**, 1018–31 (1923).

Variables:
T/K: 273–293
100 w_2/mass %: 0–79.45

Prepared By:
J. Hála

Experimental Data

Solubility in the NH_4SCN–NH_4NO_3–NH_3 system at three temperatures

Temperature (t/°C)	NH_4NO_3 (100 w_2/mass %)	NH_4NO_3 (m_2/mol kg^{-1})[a]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[a]	NH_3 (100 w_3/mass %)	Solid phase[b]
0	0	0	77.12	44.28	22.88	A
	9.16	5.460	69.88	43.79	20.96	A
	15.45	9.848	64.95	43.53	19.60	A
	19.25	12.59	61.55	42.40	19.10	A+B
	19.20	12.62	61.80	42.73	19.00	A+B
10	0	0	77.30	44.74	22.70	A
	8.40	5.218	71.49	46.70	20.11	A
	17.49	12.24	64.66	47.59	17.85	A
	21.05	15.228	61.68	46.92	17.27	A+B
	21.09	15.23	61.61	46.79	17.30	A+B
20	0	0	78.65	48.40	21.35	A
	4.69	2.991	75.72	50.78	19.59	A
	11.64	8.025	70.24	50.93	18.12	A
	16.88	12.35	66.04	50.80	17.08	A
	24.73	20.30	60.05	51.83	15.22	A+B
	24.86	20.45	59.95	51.85	15.19	A+B

[a] Calculated by compiler.
[b] A: NH_4SCN, [1762-95-4]; B: NH_4NO_3, [6484-52-2].

Additional information: In addition to the data shown in the table, the authors also reported compositions of another nine saturated solutions at 0 °C, containing 20.06–76.87 mass % NH_4NO_3 and 59.97–0 mass % NH_4SCN, seven saturated solutions at 10 °C, containing 25.11–78.09 mass % NH_4NO_3, and 56.37–0 mass % NH_4SCN, and nine saturated solutions at 20 °C, containing 27.90–79.45 mass % $NH_4NO_3$and 54.37–0 mass % NH_4SCN, where NH_4NO_3 was the equilibrium solid phase. These data have not been included in the compilation since they represent the solubility of NH_4NO_3 in solutions of NH_4SCN.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility determinations were carried out in thermostated glass-stoppered bottles. Starting from the two-component solution saturated with NH_4SCN, the solubility of this salt was determined as a function of increasing amount of NH_4NO_3, and vice versa. Equilibrium was reached after 1 h shaking. Samples for analysis were withdrawn through a plug of glass wool into a weighed specimen tube under cooling to avoid losses of NH_3. Ammonia was determined by titration against congo red as indicator, SCN^- by Volhard method. The content of NH_4NO_3 was obtained by difference. Solid phases were analyzed chemically. Separate experiments were designed to confirm that no double salts were formed.

Source and Purity of Materials:

NH_4SCN and NH_4NO_3 were very pure chemicals, their source was not specified. They were recrystallized and dried until they showed no trace of moisture. Dry NH_3 gas was obtained by warming a concentrated solution of ammonia, and passing the gas through towers containing quicklime and fused caustic poptash.[1]

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] H. W. Foote and M. A. Hunter, J. Am. Chem. Soc. **42**, 69 (1920).

Components:
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonium nitrate; NH_4NO_3; [6484-52-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
P. S. Bogoyavlenskii, Zh. Fiz. Khim. **32**, 2035–41 (1958).

Variables:
T/K: 298
100 w_2/mass %: 0–68

Prepared By:
J. Hála

Experimental Data

Solubility of NH_4SCN at 25 °C in water and aqueous solutions of NH_4NO_3

NH_4NO_3 (100 w_2/mass %)	NH_4NO_3 (m_2/mol kg^{-1})[a]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	64.1	23.45	A
5.17	1.937	61.5	24.24	A
9.97	3.979	58.73	24.64	A
15.77	6.671	54.7	24.33	A
21.49	9.910	51.42	24.93	A
33.06	17.98	43.98	25.16	A
38.0	23.24	41.58	26.75	A
39.5	25.26	40.97	27.55	A+B

[a] Calculated by compiler.
[b] A: NH_4SCN, [1762-95-4]; B: NH_4NO_3; [6484-52-2].

Additional information: In addition to the data shown above, the authors also reported the compositions of seven saturated solutions containing 42.53–68.0 mass % NH_4NO_3 where NH_4NO_3 was the equilibrium solid phase. These data are not shown here since they refer to the solubility of NH_4NO_3 in solutions of NH_4SCN.

Auxiliary Information

Method/Apparatus/Procedure:

No details reported. The compiler assumed that the same procedure was adopted as in the author's previous work (Bogoyavlenskii and Sukmanskaya[1]), i.e., isothermal method with chemical analysis of the equilibrium liquid phases, and investigation of solid phases by means of optical microscopy.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] P. S. Bogoyavlenskii and G. V. Sukmanskaya, Zh. Obsh. Khim. **23**, 1092 (1953).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Potassium thiocyanate; KSCN; [333-20-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. I. Ravich, V. Ya. Ketkovich, and I. S. Rassonskaya, Izv. Sektora Fiz. Khim. Anal. **17**, 254–85 (1949).

Variables:

T/K: 273, 303, 333, and 363
Concentration ratio of NH_4SCN and KSCN

Prepared By:

J. Hála

Experimental Data

Solubility in the NH_4SCN–KSCN–H_2O system at four temperatures[a]

Temperature (t/°C)	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[b]	KSCN (100 w_2/mass %)	KSCN (m_2/mol kg^{-1})[b]
0	42.9	13.26	14.6	3.534
	35.7	11.75	24.4	6.292
	30.1	11.04	34.1	9.801
	29.7	11.21	35.5	10.49
	25.0	9.173	39.2	11.26
	19.9	7.261	44.1	12.60
	10.7	3.959	53.8	15.59
30	55.4	21.53	10.8	3.287
	47.8	19.08	19.3	6.086
	46.7	19.60	22.0	7.232
	41.0	18.13	29.3	10.15
	39.8	18.41	31.8	11.52
	29.1	13.27	42.1	15.04
	23.2	10.58	48.0	17.15
	13.1	5.893	57.7	20.33
60	71.5	41.19	5.7	2.572
	64.4	38.98	13.9	6.591
	61.8	38.11	16.9	8.164
	59.4	36.29	19.1	9.141
	59.2	37.03	19.8	9.702
	50.6	30.63	27.7	13.13
	36.0	21.30	41.8	19.37
	23.3	13.85	54.6	25.42
	14.0	8.322	63.9	29.75
90	74.6	65.77	10.5	7.251
	70.1	60.98	14.8	10.08
	61.4	54.50	23.8	16.54
	47.0	40.35	37.7	25.35
	29.9	26.90	55.5	39.11
	15.1	12.79	69.4	46.07

[a] The only solid phases observed were two types of solid solutions labeled as β and γ in Fig. 27. The γ solid solution contained more NH_4SCN than the salt residue of the corresponding liquid phase. In the range of crystallization of the β solid solutions the ratio of the concentrations of both salts was identical in the solid and liquid phases.
[b] Calculated by compiler.

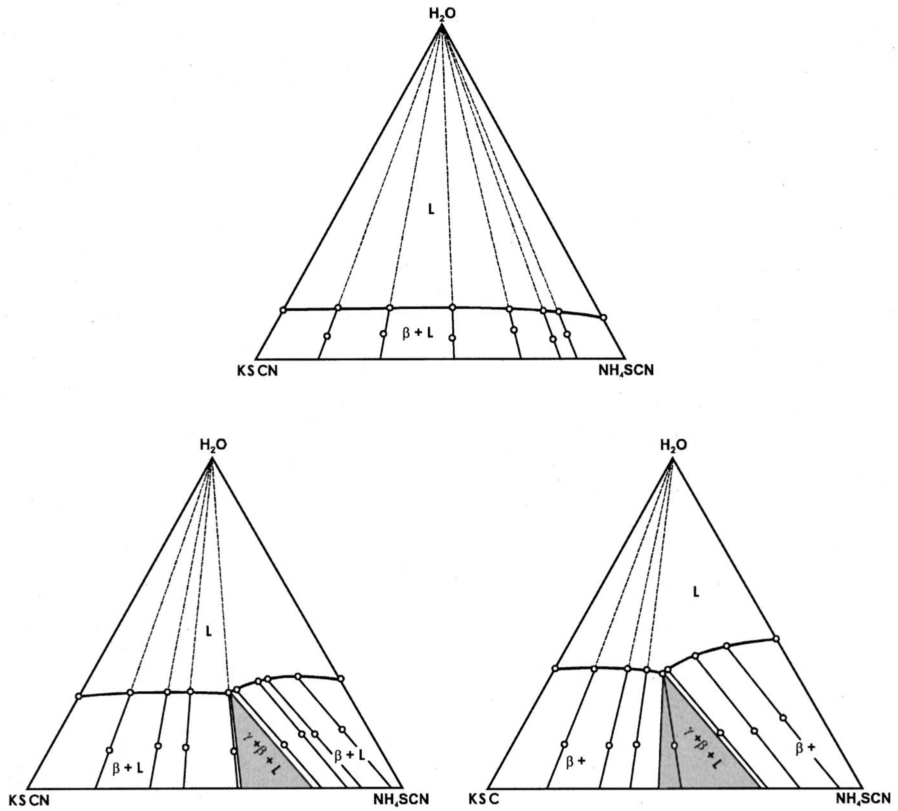

FIG. 27. Phase diagrams of the NH_4SCN–KSCN–H_2O at 90 °C (top), 30 °C (bottom left), and 0 °C (bottom right).

Additional information: Phase diagram for 60 °C and the solubility polytherm were also reported. In addition to the isothermal data, the authors reported also some polythermal measurements below 0 and above 100 °C. The results have not been included here since temperatures of crystallization differed in some cases depending on whether seeding was applied or not, which indicated the existence of both stable and metastable solid phases.

Auxiliary Information

Method/Apparatus/Procedure:

Isothermal method used. A mixture of solid salts, 8–10 g, was dissolved in water above the desired temperature, then the flask was placed in a thermostat at the desired temperature to allow equilibrium to be established. This took 6–7 h at 0, 30, and 60 °C, and 4–5 h at 90 °C. At 0 and 30 °C, samples of the saturated solutions were withdrawn with a pipette preheated and/or precooled to the corresponding temperature. A small glass U tube with a wad of glass wool inside was attached to the pipette. At 60 °C and above, samples were taken into a preheated glass tube. The samples were allowed to crystallize on cooling to room temperature, and weighed in a weighing bottle. Saturated solutions were analyzed for NH_4^+, SCN^-, and K^+ ions. NH_4^+ was determined acidimetrically after distilling ammonia off in the presence of MgO, SCN^- by Volhard's method, and K^+ gravimetrically as K_2SO_4 after evaporation of the sample with excess H_2SO_4, and ignition. Solid phases were identified by Schreinemakers' method.

Source and Purity of Materials:

NH_4SCN and KSCN were chemically pure products. They were recrystallized, dried at 120 °C, and kept over P_2O_5 in a dessicator.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Potassium thiocyanate; KSCN; [333-20-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Babenko and A. M. Andrianov, Ukrain. Khim. Zh. **45**, 1177–81 (1979); short abstract published in Zh. Prikl. Khim. **51**, 235 (1978).

Variables:

T/K: 240–325
100 w_1/mass %: 0–42
100 w_2/mass %: 0–70

Prepared By:

J. Hála

Experimental Data

Solubility in the $NH_4SCN–KSCN–H_2O$ system as measured by polythermal method

NH_4SCN (100 w_1/mass %)	KSCN (100 w_2/mass %)	Liquidus temperature (t/°C)	Solid phase[a]	NH_4SCN (100 w_1/mass %)	KSCN (100 w_2/mass %)	Liquidus temperature (t/°C)	Solid phase[a]
42.0	0	−25.3	A+B	5.22	47.8	−31.4	A+C
37.6	6.24	−24.7	A+B	0	52.0	−30.0	A+C
33.4	13.32	−26.0	A+B	10.0	51.3	−13.0	C+D
27.4	21.78	−28.0	A+B	4.0	60.0	2.4	C+E
21.0	31.6	−30.8	A+B	0	64.0	−0.8	C+E
19.74	34.2	−32.6	A+B	8.0	60.72	17.0	D+E
27.3	22.0	−27.8	A+B	8.0	64.4	31.4	D+E
36.0	10.0	−25.8	A+B	8.0	60.0	15.0	D+E
13.2	42.664	−32.6	A+B	9.0	70.0	52.0	D+E
11.44	42.8	−33.0	A+B+D	21.0	40.0	−9.7	B+D
11.0	47.17	−23.0	A+C+D	23.8	40.5	−1.2	B+D
5.0	58.9	−5.0	C+D+E	31.0	38.0	12.4	B+D

Solubility isotherms in the $NH_4SCN–KSCN–H_2O$ system[b]

Temperature (t/°C)	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[c]	KSCN (100 w_2/mass %)	KSCN (m_2/mol kg^{-1})[c]	Solid phase[a]
−30	20.0	5.473	32.0	6.860	A
	12.08	3.284	39.6	8.433	A
	10.0	2.807	43.2	9.498	A
	5.38	1.459	46.2	9.818	A
	21.4	5.961	31.44	6.860	B
	14.7	4.352	40.94	9.498	B
	11.2	3.284	44.0	10.10	B
	20.64	5.630	31.2	6.666	B
	19.26	5.630	35.8	8.197	B
	0	0	52.0	11.14	C
	5.17	1.459	48.3	10.68	C
−20	31.0	6.557	6.9	1.143	A
	24.9	5.415	15.04	2.572	A
	16.0	3.574	25.2	4.410	A
	6.4	1.497	37.44	6.860	A
	6.50	1.459	34.2	5.942	A
	0	0	38.8	6.500	A
	40.0	9.721	6.0	1.149	B
	36.2	9.317	12.76	2.572	B
	31.2	8.510	20.64	4.410	B
	26.5	7.394	29.4	6.960	B
	19.8	6.237	38.49	9.498	B

	18.0	5.630	40.0	9.800	B
	24.36	7.073	30.4	6.914	B
	12.6	4.029	46.32	11.60	D
	10.44	3.284	47.8	11.77	D
	4.78	1.459	52.2	12.48	C
	0	0	55.5	12.83	C
−10	20.5	3.387	0	0	A
	19.4	3.284	3	0.397	A
	8.34	1.459	16.6	2.275	A
	7.4	1.312	18.52	2.572	A
	0	0	24	3.249	A
	44.8	11.84	5.52	1.143	B
	41.0	11.41	11.8	2.572	B
	36.0	10.55	19.2	4.410	B
	31.6	10.11	27.36	6.860	B
	25.0	8.421	36	9.498	B
	20.79	7.073	40.6	10.82	B
	27.68	8.758	30.8	7.633	B
	49.3	12.77	0	0	B
	18	6.135	43.46	11.60	D
	11.8	4.086	50.27	13.63	D
	16.68	5.630	44.4	11.73	D
	0	0	59.7	15.24	C
	4.38	1.459	56.2	14.67	C
	9.68	3.284	51.6	13.71	C
0	54.0	15.42	0	0	B
	49.6	14.36	5.04	1.143	B
	45.8	13.87	10.84	2.572	B
	41.3	13.20	17.61	4.410	B
	36.5	12.58	25.4	6.860	B
	30	10.82	33.6	9.498	B
	23.2	8.443	40.70	11.60	B
	0	0	64	18.29	E
	4	1.459	60	17.15	E
	23.22	8.758	41.7	12.26	D
	19.25	7.073	45	12.95	D
	17.5	6.480	47.02	13.64	D
	15.36	5.630	48.8	14.01	D
	8.96	3.284	55.2	15.84	D
	7.8	2.924	57.16	16.78	D
10	58.8	18.14	0	0	B
	54.4	17.41	4.56	1.143	B
	46.4	16.24	16.08	4.410	B
	41.8	15.72	23.28	6.860	B
	35.2	13.69	31.04	9.461	B
	33	13.13	34	10.60	B
	28.4	11.08	37.94	11.59	B
	0	0	66.5	20.42	E
	3.72	1.459	62.8	19.30	E
	2.4	0.949	64.41	19.96	E
	23.2	9.229	43.77	13.64	D
	21.68	8.758	45.8	14.49	D
	17.71	7.160	49.8	15.77	D
	23.2	9.229	43.77	13.64	D
	14.1	5.630	53	16.57	D
	8.2	3.284	59	18.50	D
	13.2	5.256	53.81	16.78	D
20	68.6	22.95	0	0	B
	59.4	21.35	4.06	1.143	B
	55.4	20.39	8.92	2.572	B
	51.4	19.84	14.58	4.410	B
	47.0	19.41	21.2	6.860	B
	40.5	17.16	28.5	9.460	B
	33.6	13.70	24.19	10.92	B
	54.0	19.70	10.0	2.858	B
	0	0	69.0	22.90	E
	3.45	1.459	65.5	21.70	E
	7.56	3.284	62.2	21.16	E
	29.5	13.13	41.0	14.30	D
	28.6	12.23	40.69	13.64	D
	20.0	8.758	50.0	17.15	D
	18.6	7.943	50.64	16.91	D
	16.15	7.107	54.0	18.61	D
	12.9	5.630	57.0	19.48	D
	10.7	4.629	58.93	19.97	D

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[a] A: Ice, H_2O, [7732-18-5]; B: NH_4SCN, [1762-95-4]; C: $KSCN \cdot 0.5H_2O$, [ ]; D: solid solutions of $m NH_4SCN \cdot n KSCN$; E: KSCN, [333-20-2].

[b] Solubility isotherms were obtained by the authors from polythermal measurements (see Fig. 28).

[c] Calculated by compiler.

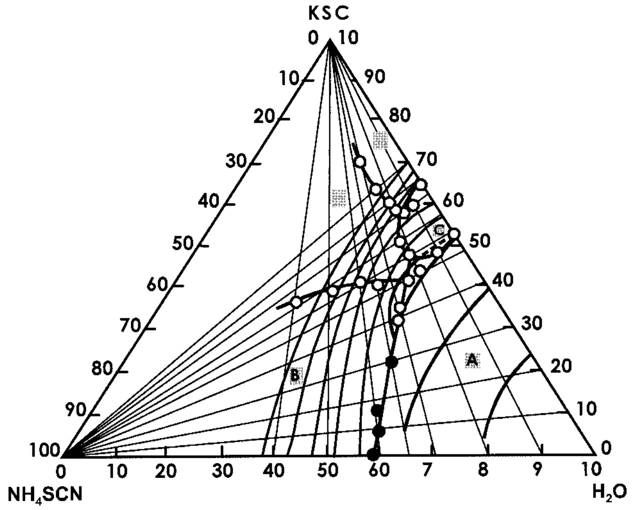

FIG. 28. Solubility polytherm of the NH_4SCN–KSCN–H_2O system. Fields of crystallization: A: ice; II: NH_4SCN; C: $KSCN \cdot 0.5H_2O$; IV: KSCN; and V: solid solutions $m NH_4SCN \cdot n KSCN$.

Components:	**Original Measurements:**
(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).
Variables:	**Prepared By:**
T/K: 278, 298, 323 100 w_2/mass %: 0–26.2 at 278 K; 0–26.5 at 298 K 0–26.9 at 323 K	J. Hála

Experimental Data

Solubility in the $NH_4SCN–NaCl–H_2O$ system at three temperatures

Temperature (t/°C)	NaCl (100 w_2/mass %)	NaCl (m_2/mol kg^{-1})[a]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[a]	Solid phase[b]
5	0	0	56.5	17.06	A
	2.3	0.923	55.1	16.99	A
	5.1	2.092	53.2	16.76	A+B
	5.5	2.214	52.0	16.07	B
	9.7	3.339	40.6	10.73	B
	13.4	4.131	31.1	7.361	B
	19.2	5.214	17.8	3.711	B
	22.0	5.836	13.5	2.749	B+C
	22.3	5.781	11.7	2.328	C
	26.2	6.074	0	0	C
25	0	0	64.1	23.45	A
	1.9	0.926	63.0	23.57	A
	4.6	2.301	61.2	23.50	A+B
	7.5	3.084	50.9	16.07	B
	11.5	4.040	39.8	10.73	B
	17.5	5.262	25.6	5.910	B
	20.6	5.914	19.8	4.364	B+C
	21.0	5.871	17.9	3.820	C
	22.6	5.876	11.6	2.315	C
	26.5	6.169	0	0	C
50	0	0	72.8	35.16	A
	1.4	0.907	72.2	35.92	A
	2.8	1.871	71.6	36.74	A
	3.8	2.580	71.0	37.01	A+B
	9.5	3.993	49.8	16.07	B
	13.6	4.888	38.8	10.70	B
	18.1	5.910	29.5	7.395	B+C
	21.5	6.060	17.8	3.852	C
	23.0	6.017	11.6	2.330	C
	26.9	6.296	0	0	C

[a] Calculated by compiler.

[b] A: NH_4SCN, [1762-95-4]; B: NH_4Cl, [12125-02-9]; C: NaCl, [7647-14-5].

Auxiliary Information

Method/Apparatus/Procedure:

Visual polythermal method used. In total, 19 sections of the $NH_4SCN–KSCN–H_2O$ system were investigated, of which 11 corresponded to 0, 10, 20, 30, 40, 50, 53, 57, 62, 66, and 70 mass % KSCN, and 8 to 0, 10, 20, 30, 35, 40, 50, and 60 mass % NH_4SCN. Measurements were carried out in an apparatus described in Eraizer and Kaganskii.[1] The solubility vessel, equipped with a thermometer, was coated with a transparent semiconductor layer to which two heating silver electrodes were soldered. The vessel was placed inside a Dewar flask with transparent walls which, in measurements performed below room temperature, was filled to 1/5 of its volume with liquid nitrogen or solid CO_2. With the solubility vessel kept above the coolant, it was possible to control the rate of cooling or heating by moving the Dewar flask. The mixture in the solubility vessel was stirred by using two external electromagnets, and illuminated to observe disappearance or appearance of last crystals.

Source and Purity of Materials:

KSCN and NH_4SCN were reagent grade products, and were twice recrystallized from water, and dried at 30–40 °C before use.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

References:

[1] L. N. Eraizer and I. M. Kaganskii, Zavodskaya Lab. **33**, 119 (1967).

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were obtained by graphical analytical method.[1] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions, were prepared by weighing. After equilibrium had been attained, a property (compiler assumed this to be refractive index, as in the authors' subsequent work[2]) of the solutions were measured, and plotted as a function of the composition of the mixtures. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phase was not reported.

Source and Purity of Materials:

NH_4SCN and NaCl were chemically pure products. They were recrystallized and dried over anhydrous $CaCl_2$. Doubly distilled water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonium chloride; NH_4Cl; [12125-02-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).

Variables:

T/K: 278, 298, 323
100 w_2/mass %: 0–23.8 at 278 K; 0–28.6 at 298 K
0–33.5 at 323 K

Prepared By:

J. Hála

Experimental Data

Solubility in the $NH_4SCN–NH_4Cl–H_2O$ system at three temperatures

Temperature (t/°C)	NH_4Cl (100 w_2/mass %)	NH_4Cl (m_2/mol kg^{-1})[a]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[a]	Solid phase[b]
5	0	0	56.5	17.06	A
	4.7	2.039	53.0	16.46	A
	5.9	2.546	52.4	16.46	A+B
25	0	0	64.1	23.45	A
	3.9	2.056	61.3	23.14	A
	5.8	2.880	60.2	22.99	A+B
50	0	0	72.8	35.16	A
	4.6	3.323	70.0	36.20	A+B

[a] Calculated by compiler.
[b] A: NH_4SCN, [1762-95-4]; B: NH_4Cl, [12125-02-9].

Additional information: In addition to the data shown above, the authors reported also compositions of 16 saturated solutions containing 10.6–23.8, 8.4–28.6, and 5.8–33.5 mass % NH_4Cl at 5, 25, and 50 °C, respectively, where the equilibrium solid phase was NH_4Cl. These were not included here since they represent the solubilities of NH_4Cl in solutions of NH_4SCN.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was obtained by graphical analytical method.[1] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions, were prepared by weighing. After equilibrium had been attained, a property (compiler assumed this to be refractive index, as in the authors' subsequent work[2]) of the solutions were measured, and plotted as a function of the composition of the mixtures. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phase was not reported.

Source and Purity of Materials:

NH_4SCN and NH_4Cl were chemically pure products. They were recrystallized and dried over anhydrous $CaCl_2$. Doubly distilled water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonium sulfate; $(NH_4)_2SO_4$; [7783-20-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Babenko and A. M. Andrianov, Zh. Neorg. Khim. **23**, 2819–25 (1978).

Variables:

T/K: 248–280
100 w_2/mass %: 0–39.8

Prepared By:

J. Hála

Experimental Data

Solubility in the $NH_4SCN-(NH_4)_2SO_4-H_2O$ system as measured by polythermal method

$(NH_4)_2SO_4$ (100 w_2/mass %)	NH_4SCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]	$(NH_4)_2SO_4$ (100 w_2/mass %)	NH_4SCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]
39.8	0	−19.0	A+B	6.2	38.0	−24.0	A+B+C
33.0	6.7	−18.2	A+B	8.0	41.4	−11.6	B+C
27.4	14.52	−20.0	A+B	6.0	47.0	−11.8	B+C
18.0	24.6	−23.6	A+B	5.0	52.25	+7.6	B+C
8.0	36.8	−19.6	A+B	0	42.0	−25.3	A+C
14.0	30.0	−23.0	A+B	3.0	40.0	−22.0	A+C
25.8	14.0	−18.8	A+B				

Solubility isotherms in the $NH_4SCN-(NH_4)_2SO_4-H_2O$ system[b,c]

Temperature (t/°C)	$(NH_4)_2SO_4$ (100 w_2/mass %)	$(NH_4)_2SO_4$ (m_2/mol kg^{-1})[d]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[d]
−20	0	0	44.6	10.57
	2.93	0.398	41.4	9.770
	7.0	0.949	37.2	8.758
−10	0	0	49.3	12.77
	2.68	0.395	46.4	11.76
	5.55	0.841	44.50	11.70
0	0	0	54.0	15.42
	2.44	0.398	51.2	14.51
	5.06	0.841	49.4	14.25
	6.5	1.052	46.75	13.14
10	0	0	59.0	18.90
	2.19	0.398	56.2	17.74
	4.6	0.841	54.0	17.14

---

[a] A: Ice, H_2O, [7732-18-5]; B: $(NH_4)_2SO_4$, [7783-20-2]; C: NH_4SCN; [1762-95-4].

[b] Solid phase NH_4SCN; [1762-95-4] in all solutions.

[c] Solubility isotherms were obtained by the authors from polythermal measurements (see Fig. 29). Of numerous data reported, only those referring to the solubility of NH_4SCN were included here. In systems containing higher $(NH_4)_2SO_4$ concentrations, the equilibrium solid phases were either ice or $(NH_4)_2SO_4$.

[d] Calculated by compiler.

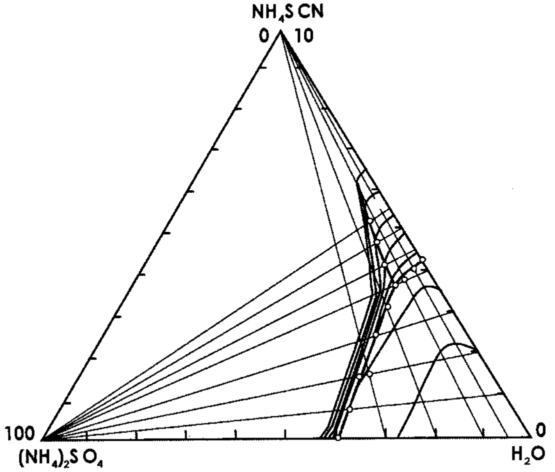

FIG. 29. Solubility polytherm of the $NH_4SCN-(NH_4)_2SO_4-H_2O$ system. Fields of crystallization: A: ice; B: $(NH_4)_2SO_4$; and C: NH_4SCN.

Auxiliary Information

Method/Apparatus/Procedure:

A visual polythermal method was used. In total, 11 sections of the $NH_4SCN-(NH_4)_2SO_4-H_2O$ system were investigated, of which seven corresponded to 10, 20, 30, 40, 45, 50, and 55 mass % NH_4SCN, and four to 5, 10, 20, and 30 mass % $(NH_4)_2SO_4$. Measurements were carried out in an apparatus described in Eraizer and Kaganskii.[1] The solubility vessel, equipped with a thermometer, was coated with a transparent semiconductor layer to which two heating silver electrodes were soldered. The vessel was placed inside a Dewar flask with transparent walls which, in measurements performed below room temperature, was filled to 1/5 of its volume with liquid nitrogen or solid CO_2. With the solubility vessel kept above the coolant, it was possible to control the rate of cooling or heating by moving the Dewar flask. The mixture in the solubility vessel was stirred by using two external electromagnets, and illuminated to observe disappearance or appearance of crystals.

Source and Purity of Materials:

NH_4SCN and $(NH_4)_2SO_4$ were chemically pure products. They were recrystallized twice before use, and dried at 40 °C.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] L. N. Eraizer and I. M. Kaganskii, Zavodskaya Lab. **33**, 119 (1967).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonium sulfate; $(NH_4)_2SO_4$; [7783-20-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. F. Zhuravlev and M. N. Bychkova, Zh. Neorg. Khim. **4**, 2367–75 (1959).

Variables:

T/K: 306, 326
100 w_2/mass %: 0–42.6 at 306 K; 0–45 at 326 K

Prepared By:

J. Hála

Experimental Data

Solubility in the $NH_4SCN-(NH_4)_2SO_4-H_2O$ system at two temperatures

Temperature (t/°C)	$(NH_4)_2SO_4$ (100 w_2/mass %)	$(NH_4)_2SO_4$ (m_2/mol kg^{-1})[a]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[a]	Solid phase[b]
33	0	0	67.3	27.03	A
	1.7	0.398	66.0	26.84	A
	2.7	0.640	65.4	26.93	A+B
	9.4	1.428	40.9	10.76	B
	21.0	2.873	23.7	5.630	B
	32.0	4.189	10.2	2.318	B
	42.6	5.616	0	0	B
53	0	0	73.8	37.00	A
	1.3	0.382	73.0	37.31	A
	1.5	0.445	73.0	37.60	A+B
	9.5	1.443	40.7	10.73	B
	22.9	3.195	23.2	5.644	B
	35.0	4.789	9.7	2.304	B
	45.0	6.191	0	0	B

[a] Calculated by compiler.
[b] A: NH_4SCN, [1762-95-4]; B: $(NH_4)_2SO_4$ [7783-20-2].

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was obtained by graphical analytical method.[1] A series of mixtures of the salts and water corresponding to a chosen section in the triangular diagram, running from one pure salt to the opposite leg of the triangle, thus covering the fields of unsaturated and saturated solutions, were prepared by weighing. After equilibrium had been attained, a property (compiler assumed this to be refractive index, as in the authors' subsequent work[2]) of the solutions were measured, and plotted as a function of the composition of the mixtures. The transition from unsaturated to saturated solutions, i.e., the corresponding solubility value, was obtained as a break on the refractive index versus composition plot. The method of identification of the solid phase was not reported.

Source and Purity of Materials:

NH_4SCN and $(NH_4)_2SO_4$ were chemically pure products. They were recrystallized and dried over anhydrous $CaCl_2$. Doubly distilled water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

References:

[1] E. F. Zhuravlev and A. D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).
[2] E. F. Zhuravlev and O. G. Nikitina, Zh. Neorg. Khim. **13**, 549 (1968).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Boric acid; H_3BO_3; [10043-35-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. G. Skvortsov, A. K. Molodkin, R. S. Tsekhanskii, Sh. V. Sadetdinov, and F. V. Nikonov, Zh. Neorg. Khim. **30**, 826–9 (1985).

Variables:

T/K: 298
100 w_2/mass %: 0–5.6

Prepared By:

J. Hála

Experimental Data

Solubility of NH_4SCN at 25 °C in aqueous solutions of boric acid

H_3BO_3 (100 w_2/mass %)	H_3BO_3 (m_2/mol kg^{-1})[a]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	65.52	24.96	A
3.01	1.515	64.86	26.52	A
3.02	1.519	64.82	26.48	A+B

[a] Calculated by compiler.
[b] A: NH_4SCN, [1762-95-4]; B: H_3BO_3, [10043-35-3].

Additional information: In addition to the data shown above, the authors also reported the compositions of six saturated solutions containing 2.99–5.60 mass % H_3BO_3, and 64.84–0 mass % NH_4SCN, where H_3BO_3 was the equilibrium solid phase. These data are not shown here since they represent the solubility of H_3BO_3 in solutions of NH_4SCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Solutions with excess solid were stirred for 7–8 h, which was sufficient for equilibrium to be reached. Solubility isotherms were confirmed by refractometric measurements of the liquid phases. Compiler assumes the solid phases were characterized by Schreinemakers' method, and that the saturated solutions were analyzed titrimetrically for borate and SCN^-, as in the authors' previous work.[1]

Source and Purity of Materials:

NH_4SCN and H_3BO_3 were chemically pure products, and were recrystallized before use.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

References:

[1] V. G. Skvortsov, R. S. Tsekhanskii, Sh. V. Sadetdinov, and A. K. Molodkin, Zh. Neorg. Khim. **28**, 2677 (1983).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonium tetraborate; $(NH_4)_2B_4O_7$; [12007-58-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Sh. V. Sadetdinov, V. G. Skvortsov, and R. S. Tsekhanskii, Sb. Trudov Yaroslav. Gos. Ped. Inst. No. **169**, 72–5 (1978).

Variables:

T/K: 298
100 w_2/mass %: 0–8.76

Prepared By:

J. Hála

Experimental Data

Solubility of NH_4SCN at 25 °C in water and one aqueous solution of ammonium tetraborate

$(NH_4)_2B_4O_7$ (100 w_2/mass %)	$(NH_4)_2B_4O_7$ (m_2/mol kg^{-1})[a]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	65.52	24.96	A
1.15	0.1794	65.34	25.62	A+B

[a] Calculated by compiler.
[b] A: NH_4SCN, [1762-95-4]; B: $(NH_4)_2B_4O_7 \cdot 4H_2O$, [12228-87-4].

Additional information: In addition to the data shown above, the authors also reported the compositions of seven saturated solutions containing 1.18–8.76 mass % $(NH_4)_2B_4O_7$, and 65.30–0 mass % NH_4SCN, where $(NH_4)_2B_4O_7 \cdot 4H_2O$ was the equilibrium solid phase. These data are not shown here since they represent the solubility of $(NH_4)_2B_4O_7 \cdot 4H_2O$ in solutions of NH_4SCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibrium was reached within 20 h, which was checked by chemical analysis and refraction index of the saturated solutions. Borate and SCN^- were determined in the saturated solutions titrimetrically (methods not specified), solid phases were characterized by Schreinemakers' method.

Source and Purity of Materials:

NH_4SCN and $(NH_4)_2B_4O_7$ were chemically pure products, and were recrystallized before use.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) N,N-diethyl-ethanamine (triethylamine); $C_6H_{15}N$; [121-44-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. D. Vorobeva and I. L. Krupatkin, *Fazovye Ravovesia* (Phase Equilibria), (Kalinin. Gosud. Univ., Kalinin, 1974), pp. 18–25.

Variables:

T/K: 296, 298

Prepared By:

J. Hála

Experimental Data

Phased diagrams of the ternary system NH_4SCN–triethylamine–H_2O at 23 and 25 °C were reported (Fig. 30). For 20 °C the phase diagram was reported to be identical with that at 23 °C. The crystallization line AB represents the solubility of NH_4SCN in triethalamine-H_2O mixtures (numerical data were not reported). Low NH_4SCN concentrations (1 mass % at 23 °C, 0.75 mass % at 20 °C) cause homogenization of the H_2O–triethalmine system. Further increase in the salt concentration results in strong salting-out of triethylamine and in reappearance of two liquid phases, of which one is pure triethylamine.

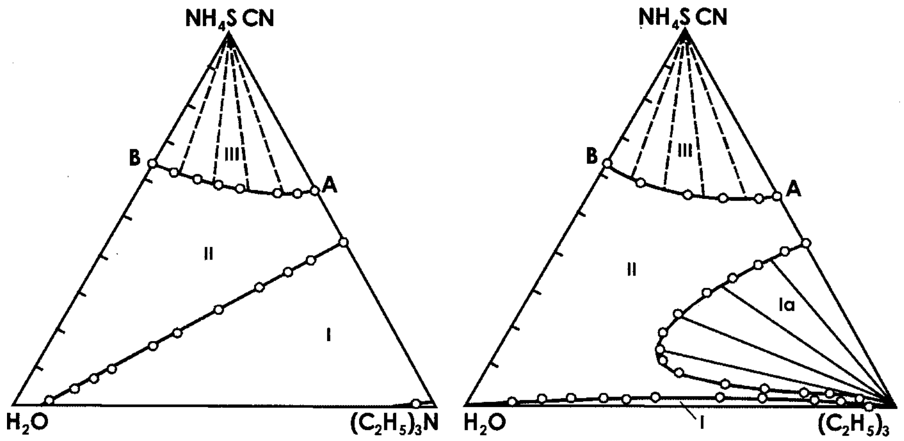

FIG. 30. Phase diagrams of the NH_4SCN–triethylamine–H_2O system at 23 °C (right) and 25 °C (left). Regions of existence: I, Ia: two liquid phases; II: unsaturated solutions; and III: solid and liquid phases.

Auxiliary Information

Method/Apparatus/Procedure:

Phase diagrams were obtained by isothermal phase titrations.

Source and Purity of Materials:

NH_4SCN, chemically pure, was dried to constant weight before use. Triethylamine, source not specified, was dried over anhydrous $MgSO_4$, and distilled twice. The product used boiling point at 89.2 °C, and showed d. of 0.7232 g cm^{-3} at 20 °C. Doubly distilled water was used.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Urea; CH_4N_2O; [57-13-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Babenko and A. M. Andrianov, Zh. Neorg. Khim. **23**, 2819–25 (1978).

Variables:

T/K: 241–266
100 w_2/mass %: 0–39

Prepared By:

J. Hála

Experimental Data

Solubility in the NH_4SCN–CH_4N_2O–H_2O system as measured by polythermal method

CH_4N_2O (100 w_2/mass %)	NH_4SCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]	CH_4N_2O (100 w_2/mass %)	NH_4SCN (100 w_1/mass %)	Liquidus temperature (t/°C)	Solid phase[a]
33.0	0	−10.6	A+B	0	42.0	−25.3	A+C
32.0	6.8	−14.0	A+B	6.0	40.0	−26.6	A+C
29.8	14.04	−17.4	A+B	12.4	38.0	−27.6	A+C
27.8	21.66	−19.8	A+B	19.2	36.0	−29.8	A+C
26.0	25.9	−22.3	A+B	23.17	33.8	−32.2	A+B+C
26.6	29.36	−27.8	A+B	24.96	38.0	−29.7	B+C
29.0	35.5	−29.8	A+B	28.8	36.0	−26.4	B+C
32.0	37.4	−20.6	A+B	35.2	36.0	−15.6	B+C
				39.0	40.0	−7.0	B+C

[a] A: Ice, H_2O, [7732-18-5]; B: CH_4N_2O, [57-13-6]; C: NH_4SCN, [1762-95-4].

Solubility isotherms in the NH_4SCN–CH_4N_2O–H_2O system[b,c]

Temperature (t/°C)	CH_4N_2O (100 w_2/mass %)	CH_4N_2O (m_2/mol kg^{-1})[d]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[d]
−20	0	0	44.6	10.58
	5.68	1.850	43.2	11.10
	11.68	4.163	41.6	11.70
	21.28	8.966	39.2	13.03
	21.0	8.853	39.5	13.14
	24.0	11.10	40.0	14.60
−10	0	0	49.3	12.77
	5.2	1.850	48.0	13.47
	10.76	4.163	46.2	14.10
	19.74	8.966	43.6	15.62
	21.0	9.836	43.45	16.06
	22.4	11.10	44.0	17.20
	25.92	13.62	42.4	17.58
0	0	0	54.0	15.42
	4.78	1.850	52.2	15.94
	9.84	4.163	50.8	16.96
	15.3	7.136	49.0	18.03
	18.2	8.966	48.0	18.66
	20.8	11.10	48.0	20.21
	24.3	13.63	46.0	20.35
	32.0	20.49	42.0	21.22
	40.0	24.67	33.0	16.06
10	0	0	58.8	18.75
	4.32	1.850	56.8	19.19
	9.12	4.163	54.4	19.59
	13.92	7.136	53.6	21.68
	16.1	8.966	54.0	23.73
	22.5	13.63	50.0	23.89
	29.0	20.12	47.0	25.77

[b] Solubility isotherms were obtained by the authors from polythermal measurements (see Fig. 31). Of the numerous data reported, only those were included here which refer to the solubility of NH_4SCN. In other systems the equilibrium solid phases were ice or urea.

[c] Solid phase was NH_4SCN, [1762-95-4] in all solutions.

[d] Calculated by compiler.

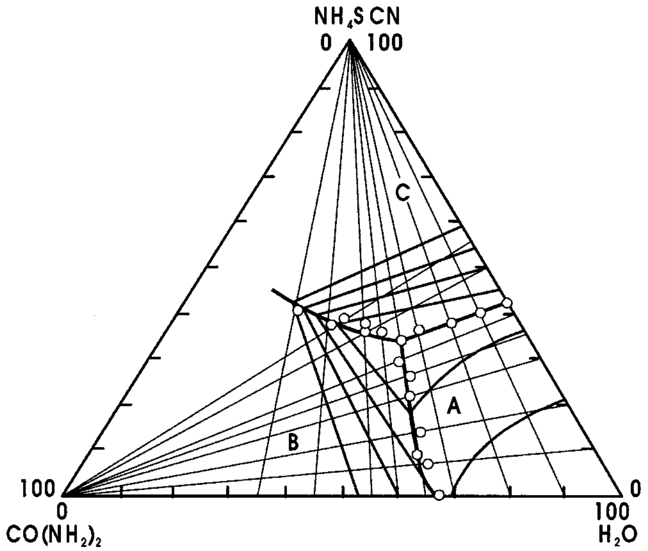

FIG. 31. Solubility polytherm of the NH_4SCN–urea–H_2O system. Fields of crystallization: A: ice; B: urea; and C: NH_4SCN.

Auxiliary Information

Method/Apparatus/Procedure:

A visual polythermal method was used. In total, 15 sections of the NH_4SCN–urea–H_2O system were investigated, of which eight corresponded to 10, 20, 30, 35, 40, 45, 55, and 65 mass % NH_4SCN, and seven to 10, 20, 30, 35, 40, 45, and 55 mass % urea. Measurements were carried out in an apparatus described in Ref. 1. The solubility vessel, equipped with a thermometer, was coated with a transparent semiconductor layer to which two heating silver electrodes were soldered. The vessel was placed inside a Dewar flask with transparent walls which, in measurements performed below room temperature, was filled to 1/5 of its volume with liquid nitrogen or solid CO_2. With the solubility vessel kept above the coolant, it was possible to control the rate of cooling or heating by moving the Dewar flask. The mixture in the solubility vessel was stirred by using two external electromagnets, and illuminated to observe disappearance or appearance of the last crystals.

Source and Purity of Materials:

NH_4SCN and urea were chemically pure products, twice recrystallized from water, and dried at 50 °C before use.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] L. N. Eraizer and I. M. Kaganskii, Zavodskaya Lab. **33**, 119 (1967).

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Imidodicarbonic diamide (biuret); $C_2H_5N_3O_2$; [108-19-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. S. Bleshinskaya, K. S. Sulaymankulov, M. D. Davranov, and Z. Yu. Yunusova, Dep. Doc. VINITI No. 120–83 (1983).

Variables:

T/K: 303
100 w_2/mass %: 0–3.78

Prepared By:

J. Hála

Experimental Data

Solubility of NH_4SCN in aqueous solutions of biuret at 30 °C

$HN(CONH_2)_2$ (100 w_2/mass %)	$HN(CONH_2)_2$ (m_2/mol kg^{-1})[a]	NH_4SCN (100 w_1/mass %)	NH_4SCN (m_1/mol kg^{-1})[a]	Solid phase[b]
0	0	67.50	27.28	A
0.62	0.1828	66.48	26.55	A
2.52	0.7269	63.85	24.94	A
3.78	1.082	62.32	24.15	A+B
3.61	0.9913	61.06	22.70	B
3.50	0.6488	44.17	11.09	B
2.62	0.3773	30.02	5.855	B
2.77	0.3259	14.78	2.355	B
3.08	0.3083	0	0	B

[a] Calculated by compiler.
[b] A: NH_4SCN, [1762-95-4]; B: $HN(CONH_2)_2$, [108-19-0].

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibration was carried out for 8–9 h, which was found sufficient to reach equilibrium. Solid phases were characterized by the method of wet residues. In the saturated solutions, SCN^- was precipitated with stoichiometric amount of $AgNO_3$, and the filtrates were analyzed for NH_4^+ titrimetrically by the formaldehyde method, and for total nitrogen by Kjeldahl method.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Methylthiocyanate; C_2H_3NS (CH_3CNS); [556-64-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. Spaccamela Marchetti, Atti. Acad. Sci. Torino, Clase Fis. Mat. Nat. **94**, 353–70 (1960).

Variables:

T/K: 293
ratio of H_2O/C_2H_3NS concentrations

Prepared By:

J. Hála

Experimental Data

Phase diagram of the $NH_4SCN–C_2H_3NS–H_2O$ system at 20 °C

The ternary phase diagram of the $NH_4SCN–C_2H_3NS–H_2O$ system at 20 °C was reported (Fig. 32). The following fields were observed in the diagram: I and II—one liquid phase, III—two liquid phases, IV and VI—one liquid phase in equilibrium with solid NH_4SCN, and V—two liquid phases in equilibrium with solid NH_4SCN. Numerical data were reported for the solubility of NH_4SCN in water-rich $C_2H_3NS–H_2O$ mixtures (curve RP in the diagram) and in C_2H_3NS-rich $C_2H_3NS–H_2O$ mixtures (curve QS in the diagram).

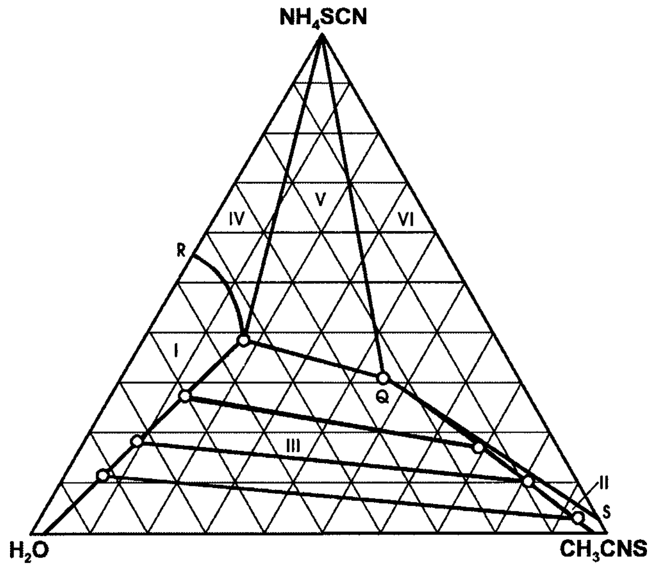

FIG. 32. Phase diagram of the $NH_4SCN–CH_3CNS–H_2O$ system at 20 °C.

Composition of the solutions saturated at 20 °C:

H_2O-rich region			C_2H_3NS-rich region		
H_2O (100 w_3/mass %)	NH_4SCN (100 w_1/mass %)	C_2H_3NS (100 w_2/mass %)	H_2O (100 w_3/mass %)	NH_4SCN (100 w_1/mass %)	C_2H_3NS (100 w_2/mass %)
44.2	55.8[a]	0	15.3	19.4	65.3
41.9	54.1	4.0	11.0	14.2	74.8
41.6	50.8	7.6	7.2	8.1	84.7
41.5	47.3	11.2	4.2	3.1	92.7
42.1	44.0	13.9	0	1.9[b]	98.1

[a] Solubility of NH_4SCN in water, $m_1 = 16.58$ mol kg^{-1} (compiler).

[b] Solubility of NH_4SCN in C_2H_3NS, $m_1 = 0.254$ mol kg^{-1} (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

Solubility curves were obtained by titration a mixture of two components with the third one in a thermostated bath. Some of these measurements were verified by preparing the ternary systems, and observing the temperature of homogenization. The value corresponding to 20 °C was then obtained by interpolation. Burettes graduated by 0.01 cm^3 were used for the titrations.

Source and Purity of Materials:

NH_4SCN was dried at 110 °C before use. No details reported on C_2H_3NS.

Estimated Error:

Temperature: precision not reported.

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Aniline; C_6H_7N; [62-53-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. D. Vorobeva and I. L. Krupatkin, *Phase Equilibria* (Russian edition), (Kalinin. Gosud. Univ., 1974), pp. 26–31.

Variables:

T/K: 298
aniline/water concentration ratio

Prepared By:

J. Hála

Experimental Data

Solubility in the NH_4SCN–aniline–H_2O system at 25 °C

Composition of systems corresponding to the crystallization curve in the NH_4SCN–aniline–H_2O phase diagram

C_6H_7N (100 w_2/mass %)	H_2O (100 w_3/mass %)	NH_4SCN (100 w_1/mass %)
0	35.50	64.50[a]
5.44	33.67	60.89
16.78	28.66	54.56
20.01	25.45	49.54
40.19	20.54	39.27
53.42	15.37	31.21
72.42	7.95	19.58
81.51	4.26	14.23
89.47	0	10.59[b]

[a] Solubility of NH_4SCN in water; $m_1 = 23.87$ mol kg^{-1} (compiler).

[b] Solubility of NH_4SCN in aniline; $m_1 = 1.556$ mol kg^{-1} (compiler).

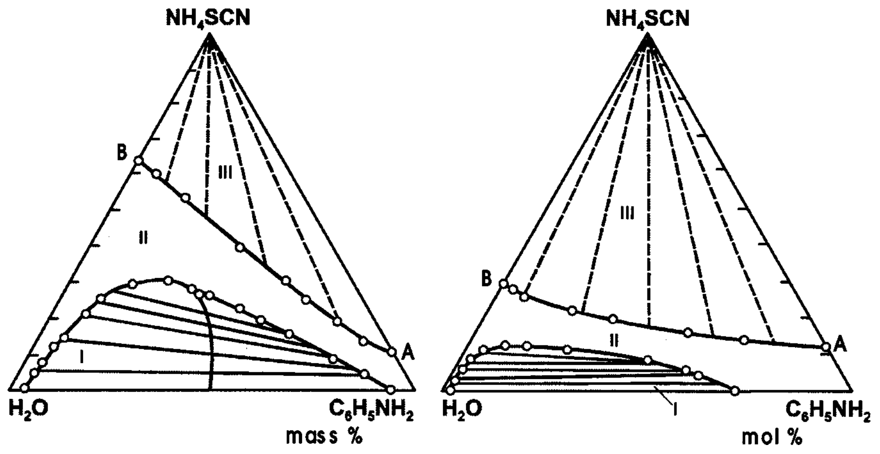

FIG. 33. Phase diagram of the NH_4SCN–aniline–H_2O system at 25 °C. I: two liquid phases; II: homogeneous region; and III: solid and liquid phases in equilibrium.

Auxiliary Information

Method/Apparatus/Procedure:

Phase diagram was obtained by isothermal phase titration (see Fig. 33)

Source and Purity of Materials:

NH_4SCN, chemically pure product, was dried to constant weight before use. Aniline was purified by distillation, and the fraction boiling point at 184.2 °C was used. The product had the density and refraction index of 1.0224 g cm^{-3} and 1.5862, respectively.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(2) Ammonium carbonate; $(NH_4)_2CO_3$; [506-87-6]
(3) Ammonia; NH_3; [7664-41-7]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

I. N. Belyayev and E. A. Grigoreva, Zh Neorg. Khim. **21**, 2866–8 (1976).

Variables:

T/K: 288
100 w_2/mass %: 0–44

Prepared By:

J. Hála

Experimental Data

Solubility of NH_4SCN in aqueous ammoniacal solutions of $(NH_4)_2CO_3$ at 15 °C

$(NH_4)_2CO_3$ (100 w_2/mass %)	NH_4SCN (100 w_1/mass %)	H_2O+NH_3[a] [100(w_3+w_4)/mass %]	Density (g cm^{-3})	Solid phase[b]
0	61.3	35.2	1.1354	A
7.2	57.9	31.9	1.1483	A
12.9	55.6	29.0	1.1754	A
14.8	55.0	28.2	1.1760	A
16.9	54.5	26.6	1.1850	A+B

[a] The sum of concentrations of all four components varied within 95.5–98 mass %. At the same time, the saturated solutions were reported to contain 2–4 mass % NH_3. The compiler assumed that the figures given in this column referred to the content of water only, while the difference from 100 mass % was the content of NH_3.

[b] A: NH_4SCN, [1762-95-4]; B: $(NH_4)_2CO_3\cdot 2NH_4HCO_3$, [ ].

Additional information: In addition to the data compiled, the authors also reported the compositions of another 13 saturated solutions containing 20.0–44.0 mass % $(NH_4)_2CO_3$ and 49–0 mass % NH_4SCN where the equilibrium solid phases were either $(NH_4)_2CO_3\cdot 2NH_4HCO_3$ or $(NH_4)_2CO_3\cdot H_2O$. These data were not included in the compilation since they refer to the solubility of $(NH_4)_2CO_3$ in solutions of NH_4SCN.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Samples were equilibrated in a thermostat by stirring in vessels equipped with hydrostatic seal. Under constant stirring equilibrium was attained within 8–10 h. All solutions contained 2–4 mass % of NH_3 in excess to the stoichiometry of $(NH_4)_2CO_3$ in order to prevent precipitation of NH_4HCO_3. Saturated solutions and the solid phases were analyzed for SCN^- by Volhard method, carbonate was determined by volumetric method, and NH_3 was titrated against standard HCl solution. Solid phases were characterized by the method of wet residues.

Source and Purity of Materials:

NH_4SCN and $(NH_4)_2CO_3$ were chemically pure products, the latter was recrystallized from a concentrated NH_3 solution.

Estimated Error:

Temperature: ±0.1 K (authors).
Solubility: insufficient data given to allow for error estimate. The sum of H_2O+NH_3 mass %: ±2.0–4.5.

6.7. Magnesium Thiocyanate

Components:

(1) Magnesium thiocyanate; $Mg(SCN)_2$; [306-61-6]
(2) Solvents

Original Measurements:

I. L. Krupatkin, E. M. Ostrovskaya, L. D. Vorobeva, and G. V. Kamyshnikova, Zh. Obsh. Khim. **48**, 957–60 (1978).

Variables:

T/K: 298

Prepared By:

J. Hála

Experimental Data

Solubility of $Mg(SCN)_2$ in three solvents at 25 °C[a]

Solvent	$Mg(SCN)_2$ ($100\,w_1$/mass %)	$Mg(SCN)_2$ (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	46.95	6.30
Aniline; C_6H_7N; [62-53-3]	8.72[c]	—
o-Toluidine; C_7H_9N; [95-53-4]	2.41[c]	—

[a] Solid phases were not investigated.
[b] Calculated by compiler for anhydrous salt.
[c] The authors did not specify whether this solubility value referred to the anhydrous or hydrated salt.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, no details were reported.

Source and Purity of Materials:

$Mg(SCN)_2 \cdot 4H_2O$, chemically pure, origin not specified. Aniline and *o*-toluidine were purified by standard methods.[1] Doubly distilled water was used.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:

[1] A. Weisberger, E. Proskauer, J. Riddick, and E. Toops, *Organic Solvents* (Russian edition), (IL Publ. House, Moscow, 1958), pp. 351, 361.

Components:

(1) Magnesium thiocyanate; $Mg(SCN)_2$; [306-61-6]
(2) Urea; CH_4N_2O; [57-13-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. Turgunbekova, K. Nogoev, and K. Sulaymankulov, Zh. Neorg. Khim. **17**, 2016–9 (1972).

Variables:

T/K: 288, 303, 318
$100\,w_2$/mass %: 0–55 at 288 K, 0–64 at 303 K, 0–66.5 at 318 K

Prepared By:

J. Hála

Experimental Data

Composition of the saturated solutions in the $Mg(SCN)_2$–urea–H_2O system at three temperatures

Temperature (t/°C)	Urea ($100\,w_2$/mass %)	Urea (m_2/mol kg^{-1})[b]	$Mg(SCN)_2$ ($100\,w_1$/mass %)	$Mg(SCN)_2$ (m_1/mol kg^{-1})[b]	Solid phase[a]
15	0	0	43.51	5.483	A
	3.52	1.090	42.69	5.650	A
	15.00	5.874	42.48	7.112	A
	15.24	6.025	42.64	7.207	A+B
	15.58	6.123	42.05	7.065	B
	19.00	7.432	38.43	6.427	B
	23.36	9.105	33.92	5.653	B
	27.03	10.77	31.16	5.306	B
	32.05	13.55	28.56	5.162	B
	36.76	16.50	26.15	5.019	B
	46.18	26.64	24.95	6.152	B
	48.20	29.73	24.80	6.539	B+C
	48.15	28.84	24.05	6.159	C
	51.00	30.43	21.09	5.380	C
	55.05	32.42	16.68	4.200	C
	54.20	30.06	15.78	3.742	D
	50.70	19.93	6.73	1.126	D
	49.00	16.00	0	0	D
30	0	0	45.51	5.946	A
	5.05	1.685	45.03	6.422	A
	8.85	3.152	44.39	6.758	A
	16.96	7.307	44.39	8.176	A
	20.09	9.485	44.64	9.010	A
	20.07	9.551	44.94	9.144	A+B
	19.49	9.137	44.99	9.017	B
	25.95	12.63	39.83	8.286	B
	32.97	17.01	34.75	7.664	B
	42.55	24.52	28.56	7.038	B
	49.13	33.53	26.47	7.723	B
	52.69	38.41	24.47	7.627	B
	54.70	43.66	24.44	8.341	B+C
	54.51	41.94	23.85	7.846	C
	59.13	45.94	19.44	6.458	C
	63.82	57.01	17.54	6.699	C
	64.00	55.16	16.68	6.146	C+D
	63.07	47.41	14.78	4.750	D
	59.25	27.92	5.41	1.090	D
	57.50	22.53	0	0	D
45	0	0	47.50	6.441	A
	4.85	1.642	45.96	6.652	A

12.46	4.866	44.90	7.496	A
26.06	14.96	44.94	11.03	A
27.33	16.65	45.34	11.81	A+B
27.59	16.51	44.59	11.41	A+B
28.17	17.03	44.29	11.45	B
39.09	22.76	32.31	8.043	B
44.12	28.39	30.00	8.252	B
48.04	32.18	27.10	7.761	B
55.67	46.63	24.45	8.756	B
56.07	49.06	24.90	9.315	B+C
55.33	45.01	24.20	8.416	C
58.40	44.79	19.89	6.522	C
63.50	55.45	17.43	6.507	C
66.47	71.68	18.09	8.341	C
65.96	66.93	17.63	7.648	C+D
66.11	64.53	16.83	7.023	D
63.54	35.93	7.01	1.695	D
64.00	29.60	0	0	D

[a] A: $Mg(SCN)_2 \cdot 4H_2O$, [ ]; B: $Mg(SCN)_2 \cdot 4CH_4N_2O$, [37954-71-5]; C: $Mg(SCN)_2 \cdot 8CH_4N_2O$, [37954-70-4]; D: CH_4N_2O, [57-13-6].

[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, no details reported. Composition of the adducts of $Mg(SCN)_2$ with urea was confirmed by chemical analysis of the solid phases.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Magnesium thiocyanate; $Mg(SCN)_2$; [306-61-6]
(2) Thiourea; CH_4N_2S; [62-56-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

K. S. Sulaymankulov, K. Abykeev, and S. Isakova, *Heterogen. Equil. Systems Inorg. Org. Compds*. (Russian edition) (Frunze, USSR, 1974), pp. 9–12.

Variables:

T/K: 303
100 w_2/mass %: 0–17.17

Prepared By:

J. Hála

Experimental Data

Solubility in the $Mg(SCN)_2$–thiourea–H_2O system at 30 °C

CH_4N_2S (100 w_2/mass %)	CH_4N_2S (m_2/mol kg^{-1})	$Mg(SCN)_2$ (100 w_1/mass %)	$Mg(SCN)_2$ (m_1/mol kg^{-1})	Solid phase[a]
0	0	45.5	5.943	A
4.28	1.455	42.05	6.934	A
10.21	2.738	40.8	5.929	A
10.21	2.766	41.30	6.063	A
11.75	3.284	41.25	6.248	A+B
10.40	2.785	40.54	5.883	B
10.45	2.519	35.06	4.581	B
10.49	2.255	28.4	3.308	B
10.48	2.019	21.34	2.228	B
13.12	2.270	10.94	1.026	B
15.42	2.545	4.97	0.444	B
17.71	2.827	0	0	B

[a] A: $Mg(SCN)_2 \cdot 4H_2O$, [ ]; B: CH_4N_2S, [62-56-6].

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Equilibrium was reached within 6–8 h, no details about equilibration method were reported. The saturated solutions were analyzed for the content of Mg and N. Magnesium was determined by complexometric titration against eriochrome black T as indicator. The content of thiourea was obtained from the content of N as determined by Kjeldahl method.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data given to allow for error estimate.

6.8. Calcium Thiocyanate

Components:
(1) Calcium thiocyanate; $Ca(SCN)_2$; [2092-16-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. K. McKerrow, V. J. Occleshaw, and F. Drabble, J. Chem. Soc. 1–5 (1946).

Variables:
T/K: 273–323

Prepared By:
J. Hála

Experimental Data

Solubility of $Ca(SCN)_2$ in water as a function of temperature

Temperature (t/°C)	$Ca(SCN)_2$ ($100\ w_1$/mass %)	$Ca(SCN)_2$ (m_1/mol kg^{-1})[b]	Solid phase[a]
0	55.44	7.963	A
8	56.11	8.182	A
16	57.90	8.802	A
20	59.00	9.210	A
23	59.80	9.521	A
25	60.20	9.681	B
27.5	60.26	9.705	B
30	60.54	9.820	B
35	60.94	9.986	B
41	61.69	10.31	B
45	62.37	10.68	B
50	63.27	11.03	B

[a] A: β-modification of $Ca(SCN)_2 \cdot 4H_2O$; B: α-modification of $Ca(SCN)_2 \cdot 4H_2O$.

Additional information: The point of transition from β- to α-modification of $Ca(SCN)_2 \cdot 4H_2O$ occurred at 23.7 °C.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used. The salt was shaken with water in hard/glass tubes until a sufficient excess of the salt remained, and rotated in a thermostat for a day. Inoculation was usually required to induce crystallization. The solid phases were characterized by optical microscopy. Saturated solutions were analyzed for Ca titrimetrically against a standard solution of $KMnO_4$ via precipitated Ca oxalate, and for SCN^- by Volhard method.

Source and Purity of Materials:
$Ca(SCN)_2$, source not specified, was recrystallized from water until the Ca/SCN ratio was satisfactory.

Estimated Error:
Temperature: ±0.05 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:
(1) Calcium thiocyanate; $Ca(SCN)_2$; [2092-16-2]
(2) Solvents

Original Measurements:
I. L. Krupatkin, E. M. Ostrovskaya, L. D. Vorobeva, and G. V. Kamyshnikova, Zh. Obsh. Khim. **48**, 957–60 (1978).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of $Ca(SCN)_2$ in three solvents at 25 °C[a]

Solvent	$Ca(SCN)_2$ ($100\ w_1$/mass %)	$Ca(SCN)_2$ (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	67.34	13.20
Aniline; C_6H_7N; [62-53-3]	7.72[c]	—
o-Toluidine; C_7H_9N; [95-53-4]	5.28[c]	—

[a] Solid phases were not investigated.
[b] Calculated by compiler for anhydrous salt.
[c] The authors did not specify whether this solubility value referred to the anhydrous or hydrated salt.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details were reported.

Source and Purity of Materials:
$Ca(SCN)_2 \cdot 3H_2O$ prepared according to Karyakin and Angelov.[1] Aniline and o-toluidine were purified by standard methods.[2] Doubly distilled water was used.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] Yu. B. Karyakin and I. I. Angelov, *Pure Chemical Substances* (Russian edition) (Khimia, Moscow, 1974), p. 137.
[2] A. Weisberger, E. Proskauer, J. Riddick, and E. Toops, *Organic Solvents* (Russian edition) (IL Publ. House, Moscow, 1958), pp. 351, 361.

Components:

(1) Calcium thiocyanate; $Ca(SCN)_2$; [2092-16-2]
(2) N,N-Dimethylacetamide; C_4H_9NO; [127-19-5]

Original Measurements:

A. A. Fedorov, L. B. Sokolov, V. M. Savinov, M. A. Shlionskaya, and N. I. Filatova, Zh. Prikl. Khim. **44**, 2361–2 (1971).

Variables:

T/K: 295–298

Prepared By:

J. Hála

Experimental Data

The solubility of $Ca(SCN)_2$ in N,N-dimethylacetamide is reported to $c_1 = 0.24$ mol dm^{-3} at 22–25 °C. The nature of the equilibrium solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:

The solvent was saturated with anhydrous salt. Then a part of the solvent was distilled off to remove water, and the saturated solution with excess solid was kept for 3 days in a desiccator in a paraffine-coated flask. The content of water in the saturated solution was less than 0.1%. The saturated solution was analyzed for the content of sulfur by an unspecified method.

Source and Purity of Materials:

Anhydrous $Ca(SCN)_2$, source not specified, was dried at 120 °C for 6 h. N,N-dimethylacetamide, source not specified, was freshly distilled before use.

Estimated Error:

Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Calcium thiocyanate; $Ca(SCN)_2$; [2092-16-2]
(2) Sodium thiocyanate; NaSCN; [540-72-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. K. McKerrow, V. J. Occleshaw, and F. Drabble, J. Chem. Soc. 1–5 (1946).

Variables:

T/K: 298
100 w_2/mass %: 0–59
100 w_1/mass %: 0–60.2

Prepared By:

J. Hála

Experimental Data

Solubility in the $Ca(SCN)_2$–NaSCN–H_2O system at 25 °C

NaSCN (100 w_2/mass %)	NaSCN (m_2/mol kg^{-1})[b]	$Ca(SCN)_2$ (100 w_1/mass %)	$Ca(SCN)_2$ (m_1/mol kg^{-1})[b]	Solid phase[a]
0	0	60.20	9.681	A
3.09	0.992	58.49	9.743	A
5.11	1.688	57.57	9.873	A
8.78	2.999	55.11	9.768	A
9.88	3.419	54.48	9.783	A+B
11.10	3.869	53.52	9.682	B
11.15	3.839	53.03	9.475	B
14.14	4.819	49.67	8.784	B
16.36	5.427	46.46	7.997	B
19.57	6.496	43.27	7.452	B
21.32	6.990	41.06	6.985	B
22.40	7.331	39.91	6.777	B
29.32	9.460	32.45	5.432	B
32.38	10.53	29.71	5.015	B
37.91	12.29	24.07	4.052	B
38.82	12.58	23.13	3.890	B
41.74	13.66	20.59	3.498	B
42.99	13.98	19.09	3.222	B+C
42.98	13.94	19.00	3.198	C
45.37	14.47	15.97	2.643	C
52.08	15.77	7.19	1.129	C
58.78	17.58	0	0	C

[a] A: $Ca(SCN)_2 \cdot 4H_2O$, [ ]; B: NaSCN, [540-72-7]; C: $NaSCN \cdot 2H_2O$, [17032-40-5].
[b] Calculated by compiler.

See Fig. 34 and note that the original document reported also the composition of four metastable systems. These have not been included in the compilation.

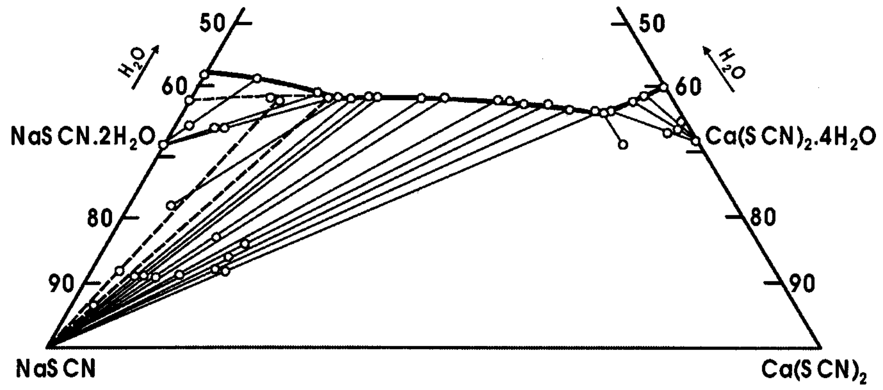

FIG. 34. Phase diagram of the Ca(SCN)$_2$−NaSCN−H$_2$O system at 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Known proportions of the salts were shaken with definite volumes of water in hard-glass tubes until a sufficient excess of solid remained. The mixtures were then heated until solution was complete, and finally rotated in a thermostat for 1 day. Suitable inoculation was usually required to induce crystallization. The nature of the solid phases was determined by the method of wet residues and by optical microscopy. Filtration of the saturated solutions was carried out at 25 °C. Saturated solutions and the wet residues were analyzed for Ca titrimetrically with a standard $KMnO_4$ solution via precipitated Ca oxalate, and for total SCN^- by Volhard method. The content of NaSCN was obtained by difference.

Source and Purity of Materials:

$Ca(SCN)_2$, source not specified, was recrystallized from water until the Ca/SCN ratio was satisfactory. NaSCN was prepared according to Occleshaw[1] by repeated crystallization from water of a commercial product (source not specified). The remaining Na_2CO_3 impurity was removed by crystallization from 96% ethanol and drying at 130 °C. The anhydrous salt contained the theoretical SCN^- percentage.

Estimated Error:

Temperature: ±0.05 K (authors).
Solubility: insufficient data given to allow for error estimate.

References:

[1] V. J. Occleshaw, J. Chem. Soc. **55** (1931).

Components:

(1) Calcium thiocyanate; $Ca(SCN)_2$; [2092-16-2]
(2) Potassium thiocyanate; KSCN; [333-20-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. K. McKerrow, V. J. Occleshaw, and F. Drabble, J. Chem. Soc. 1–5 (1946).

Variables:

T/K: 298
100 w_2/mass %: 0–70.7
100 w_1/mass %: 0–60.2

Prepared By:

J. Hála

Experimental Data

Solubility in the $Ca(SCN)_2$−KSCN−H_2O system at 25 °C

KSCN (100 w_2/mass %)	KSCN (m_2/mol kg^{-1})[b]	$Ca(SCN)_2$ (100 w_1/mass %)	$Ca(SCN)_2$ (m_1/mol kg^{-1})[b]	Solid phase[a]
0	0	60.20	9.681	A
2.13	0.563	58.99	9.710	A
5.23	1.452	57.71	9.966	A
7.90	2.294	56.67	10.23	A
10.46	3.178	55.68	10.52	A
13.81	4.468	54.39	10.94	A
17.54	6.166	53.19	11.63	A
17.77	6.294	53.18	11.71	A+B
18.62	6.481	51.82	11.22	B
24.00	8.414	46.65	10.17	B
26.55	9.489	44.66	9.928	B
32.56	12.29	40.17	9.428	B
35.39	13.65	37.95	9.110	B
36.28	14.22	37.47	9.136	B+C
36.89	14.63	37.18	9.177	C
39.06	15.62	35.22	8.764	C
40.22	16.19	34.22	8.568	C
41.12	16.79	33.69	8.560	C
42.07	17.23	32.81	8.359	C
42.84	17.59	32.11	8.204	C
43.56	18.08	31.66	8.177	[c]
43.77	18.75	32.21	8.582	C+D
43.75	18.10	31.39	8.081	D
44.09	16.96	29.16	6.977	D
45.57	16.85	26.61	6.122	D
49.34	17.35	21.41	4.684	D
53.38	18.40	16.78	3.599	D
59.32	20.23	10.51	2.229	D
66.16	22.82	4.01	0.860	D
70.76	24.90	0	0	D

[a] A: $Ca(SCN)_2 \cdot 4H_2O$, [ ]; B: $2KSCN \cdot Ca(SCN)_2 \cdot 3H_2O$, [ ]; C: $3KSCN \cdot Ca(SCN)_2 \cdot 3H_2O$, [ ]; D: KSCN, [333-20-0].

[b] Calculated by compiler.

[c] Solid phase not reported.

Additional information: The original document reported also the composition of eight metastable systems. These are not included here. In some of these systems, $Ca(SCN)_2 \cdot 2H_2O$, a solid solution with a composition approaching that of the double salt $4KSCN \cdot Ca(SCN)_2 \cdot 2H_2O$, and another modification of $Ca(SCN)_2 \cdot 4H_2O$, labeled as the β modification, were found as metastable solid phases (see Fig. 35).

Components:

(1) Calcium thiocyanate; $Ca(SCN)_2$; [2092-16-2]
(2) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. K. McKerrow, V. J. Occleshaw, and F. Drabble, J. Chem. Soc. 1–5 (1946).

Variables:

T/K: 298
100 w_2/mass %: 0–64.3
100 w_1/mass %: 0–60.2

Prepared By:

J. Hála

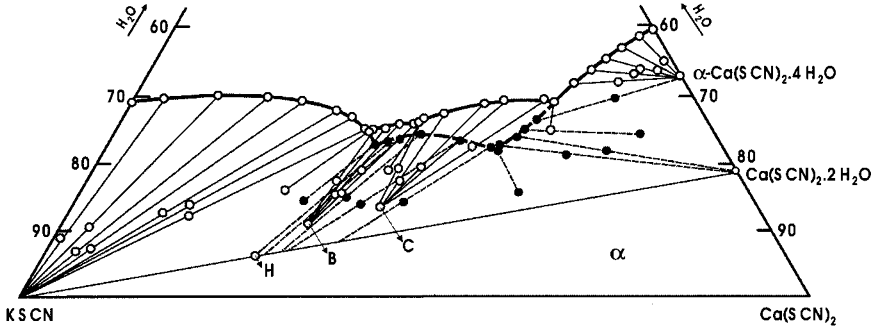

FIG. 35. Phase diagram of the $Ca(SCN)_2$–$KSCN$–H_2O system at 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Known proportions of the salts were shaken with definite volumes of water in hard-glass tubes until a sufficient excess of solid remained. The mixtures were then heated until solution was complete, and finally rotated in a thermostat for 1 day. Suitable inoculation was usually required to induce crystallization. The nature of the solid phases was determined by the method of wet residues and by optical microscopy. Filtration of the saturated solutions was carried out at 25 °C. Saturated solutions and the wet residues were analyzed for Ca titrimetrically with a standard $KMnO_4$ solution via precipitated Ca oxalate, and for total SCN^- by Volhard method. The content of KSCN was obtained by difference.

Source and Purity of Materials:

$Ca(SCN)_2$, source not specified, was recrystallized from water until the Ca/SCN ratio was satisfactory. KSCN, AnalaR quality, source not specified.

Estimated Error:

Temperature: ±0.05 K (authors).
Solubility: insufficient data given to allow for error estimate.

Experimental Data

Solubility in the $Ca(SCN)_2$–NH_4SCN–H_2O system at 25 °C

NH_4SCN (100 w_2/mass %)	NH_4SCN (m_2/mol kg^{-1})[b]	$Ca(SCN)_2$ (100 w_1/mass %)	$Ca(SCN)_2$ (m_1/mol kg^{-1})[b]	Solid phase[a]
0	0	60.20	9.681	A
9.29	3.635	57.14	10.89	A
15.23	6.745	55.11	11.89	A
17.32	8.414	55.64	13.17	A+B
18.40	8.742	53.95	12.48	B
20.55	10.30	53.26	13.01	B
21.38	10.96	52.76	13.05	B
23.31	12.21	51.62	13.17	B
24.45	13.07	50.99	13.28	B
25.55	13.80	50.13	13.19	B+C
25.50	13.61	49.89	12.97	B+C
25.95	13.64	49.07	12.57	C
26.87	13.66	47.39	11.71	C
28.15	14.44	46.34	11.55	C
29.04	14.88	45.33	11.31	C
31.37	16.26	43.29	10.93	C
31.48	16.34	43.22	10.93	C
32.89	16.92	41.58	10.42	C
34.13	17.45	40.19	10.01	C
34.35	17.25	39.49	9.661	C
35.24	17.75	39.04	9.640	C
36.98	18.83	37.36	9.318	C
37.67	19.54	37.01	9.355	C+D
37.84	17.65	34.00	7.727	D
40.38	16.52	27.52	5.487	D
42.72	16.67	23.62	4.491	D
49.18	18.93	16.70	3.132	D
57.85	21.80	7.29	1.338	D
64.23	23.96	0	0	D

[a] A: $Ca(SCN)_2 \cdot 4H_2O$, [ ]; B: $7NH_4SCN \cdot 6Ca(SCN)_2 \cdot 12H_2O$, [ ]; C: $4NH_4SCN \cdot Ca(SCN)_2 \cdot 2H_2O$, [ ]; D: NH_4SCN, [1762-95-4].
[b] Calculated by compiler.

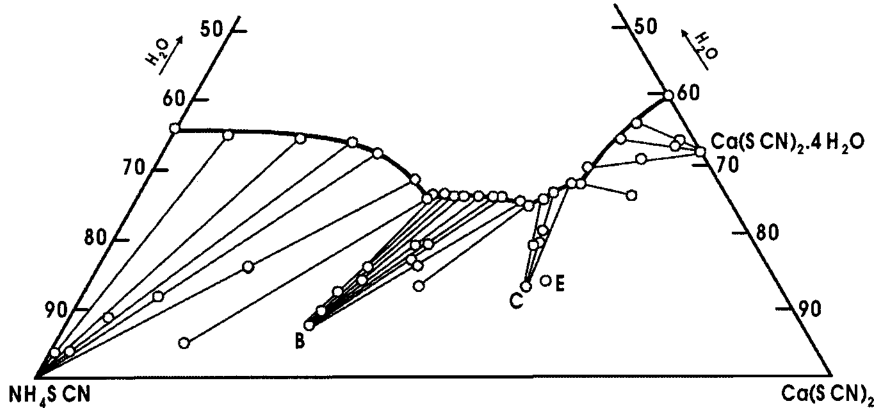

FIG. 36. Phase diagram of the $Ca(SCN)_2$–NH_4SCN–H_2O system at 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Known proportions of the salts were shaken with definite volumes of water in hard-glass tubes until a sufficient excess of solid remained. The mixtures were then heated until solution was complete, and finally rotated in a thermostat for 1 day. Suitable inoculation was usually required to induce crystallization. The nature of the solid phases was determined by the method of wet residues and by optical microscopy. Filtration of the saturated solutions was carried out at 25 °C. Saturated solutions and the wet residues were analyzed for Ca titrimetrically with a standard $KMnO_4$ solution via precipitated Ca oxalate, and for total SCN^- by Volhard method. The content of NH_4SCN was obtained by difference (see Fig. 36).

Source and Purity of Materials:

$Ca(SCN)_2$, source not specified, was recrystallized from water until the Ca/SCN ratio was satisfactory. NH_4SCN, AnalaR quality, source not specified.

Estimated Error:

Temperature: ±0.05 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Calcium thiocyanate; $Ca(SCN)_2$; [2092-16-2]
(2) Methylthiocyanate; $C_2H_3NS(CH_3CNS)$; [556-64-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. Spaccamela Marchetti, Atti. Acad. Sci. Torino, Clase Fis. Mat. Nat. **94**, 353–70 (1960).

Variables:

T/K: 293
ratio of H_2O/C_2H_3NS concentrations

Prepared By:

J. Hála

Experimental Data

Phase diagram of the $Ca(SCN)_2$–C_2H_3NS–H_2O system at 20 °C

The ternary phase diagram of the $Ca(SCN)_2$–C_2H_3NS–H_2O system at 20 °C was reported (Fig. 37). The following fields were observed in the diagram: I and II—one liquid phase, III—two liquid phases, IV and VI—one liquid phase in equilibrium with solid $Ca(SCN)_2$, and V—two liquid phases in equilibrium with solid $Ca(SCN)_2$. Numerical data were reported for the solubility of $Ca(SCN)_2$ in water-rich C_2H_3NS–H_2O mixtures (curve RP in the diagram) and in C_2H_3NS-rich C_2H_3NS–H_2O mixtures (curve QS in the diagram).

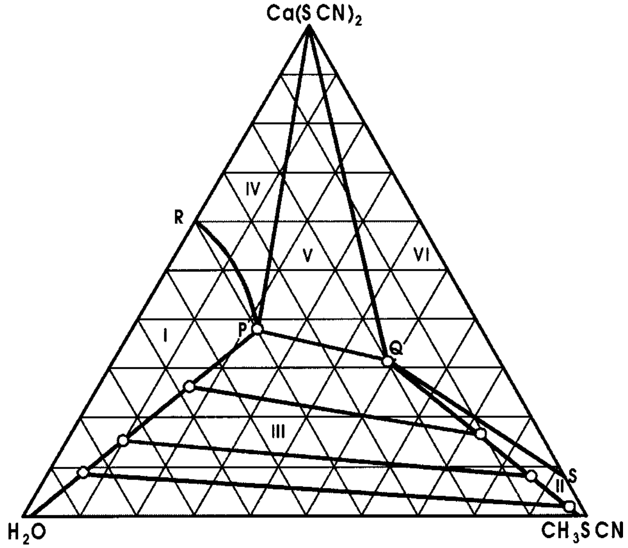

FIG. 37. Phase diagram of the $Ca(SCN)_2$–CH_3CNS–H_2O system at 20 °C.

Composition of the solutions saturated at 20 °C:

H_2O-rich region			C_2H_3NS-rich region		
H_2O (100 w_3/mass %)	$Ca(SCN)_2$ (100 w_1/mass %)	C_2H_3NS (100 w_2/mass %)	H_2O (100 w_3/mass %)	$Ca(SCN)_2$ (100 w_1/mass %)	C_2H_3NS (100 w_2/mass %)
40.2	59.8[a]	0	12.8	20.9	66.3
37.7	56.2	6.1	9.4	14.6	76.0
37.3	53.4	7.6	6.5	11.1	82.4
36.5	48.3	15.2	4.8	7.3	87.9
			0	7.3[b]	92.7

[a] Solubility of $Ca(SCN)_2$ in water, $m_1 = 9.52$ mol kg^{-1} (compiler).

[b] Solubility of $Ca(SCN)_2$ in C_2H_3NS, $m_1 = 0.504$ mol kg^{-1} (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

Solubility curves were obtained by titration a mixture of two components with the third one in a thermostated bath. Some of these measurements were verified by preparing the ternary systems, and observing the temperature of homogenization. The value corresponding to 20 °C was then obtained by interpolation. Burettes graduated by 0.01 cm^3 were used for the titrations.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.

Components:

(1) Calcium thiocyanate; $Ca(SCN)_2$; [2092-16-2]
(2) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(3) Ammonia; NH_3; [7664-41-7]

Original Measurements:

A. Stasiewicz, Ann. Univ. M. Curie/Sklodowska, Lublin, Poland **14**, Sect. AA, 49–57 (1959).

Variables:

T/K: 291

Prepared By:

J. Hála

Experimental Data

The solubility of $Ca(SCN)_2$ in liquid ammoniate of NH_4SCN is reported to be $c_1 = 1.80$ mol dm^{-3} or $100\ w_1 = 30.0$ mass % at 18 °C. The composition of the solvent corresponded to the molar ratio $NH_3/NH_4SCN = 2.7$.

Auxiliary Information

Method/Apparatus/Procedure:

The ammoniate of NH_4SCN, a clear liquid (density of 0.9345 g cm^{-3}), was obtained by action of NH_3 gas onto solid NH_4SCN at atmospheric pressure. The preparation of the solvent, and solubility measurements were carried out in a dry box under a stream of dry NH_3 gas.

Source and Purity of Materials:

$Ca(SCN)_2$ was prepared by the reaction of $Ca(OH)_2$ with NH_4SCN. The composition of the salt prepared was not specified. NH_4SCN, Argon-Lodz, was repeatedly recrystallized, and dried in a dessicator over concentrated H_2SO_4, first at normal pressure and then under vacuum for 1 month. Ammonia was dried with Na metal in a steel container.

Estimated Error:

Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

6.9. Strontium Thiocyanate

Components:
(1) Strontium thiocyanate; $Sr(SCN)_2$; [18807-10-8]
(2) Solvents

Original Measurements:
I. L. Krupatkin, E. M. Ostrovskaya, L. D. Vorobeva, and G. V. Kamyshnikova, Zh. Obsh. Khim. **48**, 957–60 (1978).

Variables:
T/K: 298

Prepared By:
J. Hála

Experimental Data

Solubility of $Sr(SCN)_2$ in three solvents at 25 °C[a]

Solvent	$Sr(SCN)_2$ (100 w_1/mass %)	$Sr(SCN)_2$ (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	56.43	6.356
Aniline; C_6H_7N; [62-53-3]	7.21[c]	—
o-Toluidine; C_7H_9N; [95-53-4]	1.73[c]	—

[a] Solid phases were not investigated.
[b] Calculated by compiler for anhydrous salt.
[c] The authors did not specify whether this solubility value referred to the anhydrous or hydrated salt.

Auxiliary Information

Method/Apparatus/Procedure:
An isothermal method was used, no details were reported.

Source and Purity of Materials:
$Sr(SCN)_2 \cdot 3H_2O$ prepared according to Karyakin and Angelov.[1] Aniline and *o*-toluidine were purified by standard methods.[2] Doubly distilled water was used.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

References:
[1] Yu. B. Karyakin and I. I. Angelov, *Pure Chemical Substances* (Russian edition) (Khimia, Moscow, 1974), p. 137.
[2] A. Weisberger, E. Proskauer, J. Riddick, and E. Toops, *Organic Solvents* (Russian edition) (IL Publ. House, Moscow, 1958), pp. 351, 361.

Components:
(1) Strontium thiocyanate; $Sr(SCN)_2$; [18807-10-8]
(2) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(3) Ammonia; NH_3; [7664-41-7]

Original Measurements:
A. Stasiewicz, Ann. Univ. M. Curie/Sklodowska, Lublin, Poland **14**, Sect. AA, 49–57 (1959).

Variables:
T/K: 291

Prepared By:
J. Hála

Experimental Data

The solubility of $Sr(SCN)_2$ in liquid ammoniate of NH_4SCN is reported to be $c_1 = 1.68$ mol dm^{-3} or 100 $w_1 = 36.5$ mass % at 18 °C. The composition of the solvent corresponded to the molar ratio $NH_3/NH_4SCN = 2.7$.

Auxiliary Information

Method/Apparatus/Procedure:
The ammoniate of NH_4SCN, a clear liquid (density of 0.9345 g cm^{-3}), was obtained by action of NH_3 gas onto solid NH_4SCN at atmospheric pressure. The preparation of the solvent, and solubility measurements were carried out in a dry box under a stream of dry NH_3 gas.

Source and Purity of Materials:
$Sr(SCN)_2$ was prepared by the reaction of $Sr(OH)_2$ with NH_4SCN. The composition of the salt prepared was not specified. NH_4SCN, Argon-Lodz, was repeatedly recrystallized, and dried in a dessicator over concentrated H_2SO_4, first at normal pressure and then under vacuum for a month. Ammonia was dried with Na Metal in a steel container.

Estimated Error:
Temperature: precision not reported.
Solubility: insufficient data reported to allow for error estimate.

6.10. Barium Thiocyanate

6.10.1. Evaluation of the $Ba(SCN)_2-H_2O$ System

Components: (1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3] (2) Water; H_2O; [7732-18-5]	**Evaluator:** J. Hála, Department of Inorganic Chemistry, Masaryk University, 61137 Brno, Czech Republic, April 2002.

Critical Evaluation

The solubility of $Ba(SCN)_2$ in water has been reported in four documents. Of these, measurements were performed at 298.1 K in three documents. The solubility reported by Occleshaw[1] (62.61 mass %; $m_1 = 6.606$ mol kg^{-1}, compiler) is in excellent agreement with that of Foote and Hickey[2] (62.63 mass %; $m_1 = 6.611$ mol kg^{-1}). Krupatkin *et al.*[3] reported a slightly higher value (63.04 mass %; $m_1 = 6.73$ mol kg^{-1}), but did not report any information on the method used. Therefore, the solubility of $Ba(SCN)_2$ of 6.61 mol kg^{-1} is recommended as a tentative value, based on the measurements in Occleshaw[1] and Foote and Hickey.[2] In the study of the $Ba(SCN)_2$–urea–H_2O system at 288.1, 303.1, and 318.1 K, Turgunbekova *et al.*[4] also reported the solubility of $Ba(SCN)_2$. Although it is difficult to determine the exact course of the solubility versus temperature function from the three measurements, interpolation of their data points to the solubility of $Ba(SCN)_2$ in water at 298.1 K to be between 6.9 and 7.0 mol kg^{-1}, a value considerably higher than those of Occleshaw[1] and Foote and Hickey.[2] The reason for this is not clear since no details were reported on the experimental method used. It could be related to the tendency of concentrated $Ba(SCN)_2$ solution to form metastable systems.

References:

[1] V. J. Occleshaw, J. Chem. Soc. 2282 (1931).

[2] H. W. Foote and F. C. Hickey, J. Am. Chem. Soc. **59**, 648 (1937).

[3] I. L. Krupatkin, E. M. Ostrovskaya, L. D. Vorobeva, and G. V. Kamyshnikova, Zh. Obsh. Khim. **48**, 957 (1978).

[4] R. Turgunbekova, K. Nogoev, and K. Sulaimankulov, Zh. Neorg. Khim. **18**, 2847 (1973).

Components: (1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3] (2) Water; H_2O; [7732-18-5]	**Original Measurements:** I. L. Krupatkin, E. M. Ostrovskaya, L. D. Vorobeva, and G. V. Kamyshnikova, Zh. Obsh. Khim. **48**, 957–60 (1978).
Variables: T/K: 298	**Prepared By:** J. Hála

Experimental Data

The solubility of $Ba(SCN)_2$ in water at 25 °C is reported to be 100 $w_1 = 63.04$ mass % ($m_1 = 6.73$ mol kg^{-1}; compiler).

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, details not reported.

Source and Purity of Materials:

$Ba(SCN)_2$ was prepared as dihydrate according to Karyakin and Angelov.[1] Doubly distilled water was used.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

References:

[1] Yu. B. Karyakin and I. I. Angelov, *Pure Chemical Substances* (Russian edition) (Khimiya, Moscow, 1974), p. 137.

Components:	**Original Measurements:**
(1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3] (2) N,N-Dimethylacetamide; C_4H_9NO; [127-19-5]	A. A. Fedorov, L. B. Sokolov, V. M. Savinov, M. A. Shlionskaya, and N. I. Filatova, Zh. Prikl. Khim. **44**, 2361–2 (1971).
Variables:	**Prepared By:**
T/K: 295–298	J. Hála

Experimental Data

The solubility of $Ba(SCN)_2$ in N,N-dimethylacetamide is reported to be $c_1 = 0.24$ mol dm^{-3} at 22–25 °C. The nature of the equilibrium solid phase was not investigated.

Auxiliary Information

Method/Apparatus/Procedure:

The solvent was saturated with anhydrous salt. Then a part of the solvent was distilled off to remove water, and the saturated solution with excess solid was kept for 3 days in a desiccator in a paraffine-coated flask. The content of water in the saturated solution was less than 0.1%. The saturated solution was analyzed for the content of sulfur by an unspecified method.

Source and Purity of Materials:

Anhydrous $Ba(SCN)_2$, source not specified, was dried at 120 °C for 6 h. N,N-dimethylacetamide, source not specified, was freshly distilled before use.

Estimated Error:

Solubility: insufficient data reported to allow for error estimate.

Components:	**Original Measurements:**
(1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3] (2) Sodium thiocyanate; NaSCN; [540-72-7] (3) Water; H_2O; [7732-18-5]	V. J. Occleshaw, J. Chem. Soc. 55–60 (1931).
Variables:	**Prepared By:**
T/K: 298 100 w_2/mass %: 0–58.8 100 w_1/mass %: 0–62.6	J. Hála

Experimental Data

Solubility in the $Ba(SCN)_2$–NaSCN–H_2O system at 25 °C[a]

NaSCN (100 w_2/mass %)	NaSCN (m_2/mol kg^{-1})[b]	$Ba(SCN)_2$ (100 w_1/mass %)	$Ba(SCN)_2$ (m_1/mol kg^{-1})[b]
0	0	62.61	6.606
12.96	4.296	49.83	5.283
19.93	6.728	43.53	4.700
24.64	8.530	39.73	4.399
31.11	11.30	34.93	4.058
39.33	16.32	30.94	4.105
41.52	16.80	27.99	3.621
41.60	16.87	27.99	3.631
46.03	16.60	19.77	2.280
54.14	17.22	7.07	0.719
58.78[c]	17.59	0	0

[a] Stable equilibrium solid phases in the system were $NaSCN \cdot 2H_2O$, [17032-40-5] and $Ba(SCN)_2 \cdot 3H_2O$, [68016-36-4] (see Fig. 38). No double salts exist in the system at 25 °C.

[b] Calculated by compiler.

[c] Solubility of NaSCN in water as the mean of four closely agreeing determinations (individual results not reported) on solutions shaken for between 2 days and 1 month.

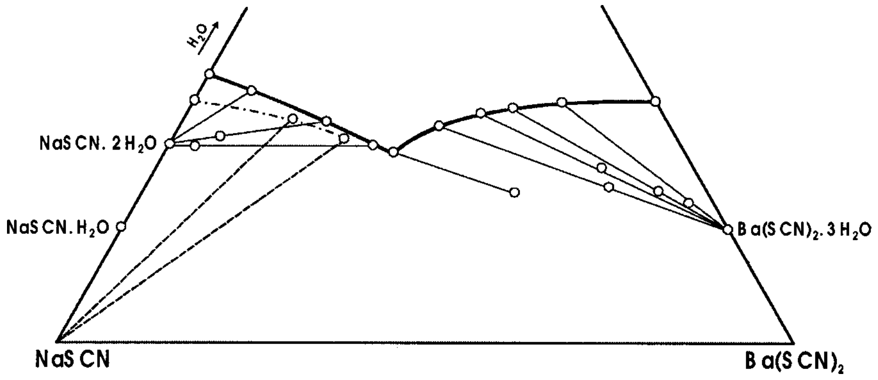

FIG. 38. Phase diagram of the $Ba(SCN)_2$–NaSCN–H_2O system at 25 °C.

Additional information: The composition of $NaSCN \cdot 2H_2O$ was characterized by chemical analysis (SCN found 48.56%–49.67%, calculated for the dihydrate 49.60%). The temperature of the transition from $NaSCN \cdot 2H_2O$ to anhydrous NaSCN was determined to be 30.4 °C dilatometrically, and 30.3 °C thermometrically.

Components:	**Original Measurements:**
(1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3] (2) Potassium thiocyanate; KSCN; [333-20-0] (3) Water; H_2O; [7732-18-5]	V. J. Occleshaw, J. Chem. Soc. 55–60 (1931).
Variables:	**Prepared By:**
T/K: 298 100 w_2/mass %: 0–70.9 100 w_1/mass %: 0–62.6	J. Hála

Experimental Data

Solubility in the $Ba(SCN)_2$–KSCN–H_2O system at 25 °C[a]

KSCN (100 w_2/mass %)	KSCN (m_2/mol kg^{-1})[b]	$Ba(SCN)_2$ (100 w_1/mass %)	$Ba(SCN)_2$ (m_1/mol kg^{-1})[b]
0	0	62.61	6.606
14.45	4.985	55.72	7.369
19.46	7.308	53.14	7.651
19.50	7.255	52.84	7.536
26.04	9.794	46.60	6.719
28.95	10.88	43.66	6.288
34.02	13.20	39.45	5.866
34.47	13.42	39.10	5.836
37.18	14.84	37.04	5.668
43.92	18.56	31.73	5.141
45.00	19.10	30.75	5.002
47.67	20.99	28.96	4.889
48.28	21.56	28.68	4.911
52.42	21.75	22.78	3.624
62.32	23.37	10.24	1.472
70.89	25.06	0	0

[a] Stable equilibrium solid phases in the system were KSCN, [333-20-0], $Ba(SCN)_2 \cdot 3H_2O$, [68016-36-4] (see Fig. 39), and the double salt $3KSCN \cdot 2Ba(SCN)_2 \cdot 5H_2O$, [ ].

[b] Calculated by compiler.

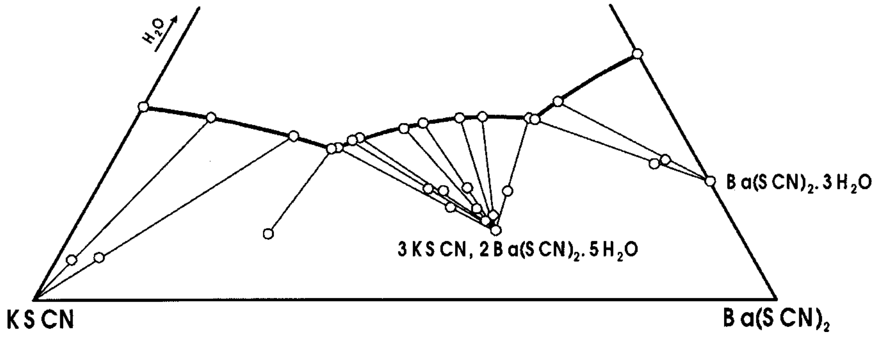

FIG. 39. Phase diagram of the $Ba(SCN)_2$–KSCN–H_2O system at 25 °C.

Additional information: The double salt $3KSCN \cdot 2Ba(SCN)_2 \cdot 5H_2O$ was prepared by crystallization at 25 °C from a solution containing the components in the stoichiometric ratio. The salt dried by suction in air contained, in mass %, 32.91–33.09 KSCN and 56.63–57.29 $Ba(SCN)_2$; calculated for $3KSCN \cdot 2Ba(SCN)_2 \cdot 5H_2O$:32.91 KSCN, 56.99 $Ba(SCN)_2$.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Since usual equilibration did not always give the stable solid phase, the mixtures were made up from weighed amounts of solids with sufficient water to give undersaturated solutions through which dry, filtered air at 25 °C was drawn until sufficient solid phase separated. The mixtures were then shaken in a thermostat for periods varying from 2 days to 4 weeks. Even so in most cases the mixtures had to be inoculated with solid $NaSCN \cdot 2H_2O$ to induce separation of the stable solid phase. Samples of the saturated solutions were withdrawn with a warmed pipette with a glass–wool filter, and analyzed gravimetrically for Ba and SCN as $BaSO_4$ and AgSCN, respectively. Solid phases were characterized by the method of wet residues.

Source and Purity of Materials:

$Ba(SCN)_2 \cdot 3H_2O$ was obtained from a commercial product (source not specified) by repeated crystallization and drying over fused $CaCl_2$. Small amount of ammonium salt was removed prior the final crystallization by boiling the solution with a slight excess of $Ba(OH)_2$, and removing the excess of the latter by passing through a cold solution of $Ba(SCN)_2$ a stream of CO_2. NaSCN was prepared by repeated crystallization from water of a commercial product (source not specified). The remaining Na_2CO_3 impurity was removed by crystallization from 96% ethanol and drying at 130 °C. The anhydrous salt obtained contained the theoretical SCN percentage (71.64%). Distilled water was used.

Estimated Error:

Temperature: ±0.05 K (author).

Solubility: insufficient data given to allow for error estimate.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Mixtures prepared from weighed amounts of the two salts and water were warmed to obtain a homogeneous solution. This was cooled to 25 °C, any solid separating was dissolved by the addition of a little water, and then rotated in a thermostat for 2–7 days at 25 °C. Samples of the saturated solutions were withdrawn with a warmed pipette with a glass–wool filter, and analyzed gravimetrically for Ba and SCN as $BaSO_4$ and AgSCN, respectively. Solid phases were characterized by the method of wet residues.

Source and Purity of Materials:

$Ba(SCN)_2 \cdot 3H_2O$ was obtained from a commercial product (source not specified) by repeated crystallization and drying over fused $CaCl_2$. Small amount of ammonium salt was removed prior the final crystallization by boiling the solution with a slight excess of $Ba(OH)_2$, and removing the excess of the latter by passing through a cold solution of $Ba(SCN)_2$ a stream of CO_2. KSCN was an A.R. quality product, source not specified. Distilled water was used.

Estimated Error:

Temperature: ±0.05 K (author).

Solubility: insufficient data given to allow for error estimate.

Components:

(1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3]

(2) Ammonium thiocyanate; NH_4SCN; [1762-95-4]

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

Original Measurements:

V. J. Occleshaw, J. Chem. Soc. 55–60 (1931).

Variables:

T/K: 298

100 w_2/mass %: 0–64.3

100 w_1/mass %: 0–62.6

Prepared By:

J. Hála

Experimental Data

Solubility in the $Ba(SCN)_2$–NH_4SCN–H_2O system at 25 °C

NH_4SCN (100 w_2/mass %)	NH_4SCN (m_2/mol kg^{-1})[b]	$Ba(SCN)_2$ (100 w_1/mass %)	$Ba(SCN)_2$ (m_1/mol kg^{-1})[b]	Solid phase[a]
0	0	62.61	6.606	A
15.48	7.010	55.51	7.548	A
20.75	11.02	54.51	8.692	A
24.70	14.86	53.47	9.663	A
24.69	14.97	53.65	9.771	A+B
25.64	16.05	53.37	10.03	B
26.73	16.79	52.36	9.878	B
27.41	17.18	51.63	9.717	B
28.85	18.23	50.36	9.556	B
29.52	18.72	49.76	9.474	B
29.64	18.83	49.68	9.477	B
30.78	19.96	48.96	9.533	B
31.00	19.89	48.52	9.346	B
31.52	20.65	48.43	9.529	B
31.85	21.11	48.33	9.619	B+C
34.73	19.33	41.66	6.961	C
38.95	19.35	34.60	5.160	C
42.72	19.76	28.88	4.012	C
52.36	21.28	15.31	1.868	C
57.72	22.37	8.38	0.9752	C
64.33	23.69	0	0	C

[a] A: $Ba(SCN)_2 \cdot 3H_2O$, [68016-36-4]; B: $Ba(SCN)_2 \cdot NH_4SCN \cdot H_2O$, [ ]; C: NH_4SCN, [1762-95-4].

[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Since the solutions were very concentrated and viscous, the mixtures were rotated in a thermostat for periods varying up to 7 days. Since the systems readily formed metastable mixtures, inoculation with the appropriate equilibrium solid phase was carried out in order to ensure the attainment of stable equilibrium. Samples of the saturated solutions and wet equilibrium solid phases were analyzed gravimetrically for Ba and SCN as $BaSO_4$ and AgSCN, respectively. Solid phases were characterized by the method of wet residues, and the double salt also by optical microscopy. The double salt could be isolated from solutions containing 31.85–24.69 mass % NH_4SCN and 48.33–53.65 mass % $Ba(SCN)_2$, and could be air/dried at lower temperatures. It was characterized by chemical analysis.

Source and Purity of Materials:

$Ba(SCN)_2 \cdot 3H_2O$ was obtained from a commercial product (source not specified) by repeated crystallization and drying over fused $CaCl_2$. Small amount of ammonium salt was removed prior the final crystallization by boiling the solution with a slight excess of $Ba(OH)_2$, and removing the excess of the latter by passing through a cold solution of $Ba(SCN)_2$ a stream of CO_2. NH_4SCN was an A.R. quality product, source not specified. Distilled water was used.

Estimated Error:

Temperature: ±0.05 K (author).

Solubility: insufficient data given to allow for error estimate.

Components:

(1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3]
(2) Barium hydroxide; $Ba(OH)_2$; [17194-00-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

H. W. Foote and F. C. Hickey, J. Am. Chem. Soc. **59**, 648–50 (1937).

Variables:

T/K: 298
100 w_2/mass %: 0–8.5

Prepared By:

J. Hála

Experimental Data

Solubility in the $Ba(SCN)_2$–$Ba(OH)_2$–H_2O system at 25 °C

$Ba(OH)_2$ (100 w_2/mass %)	$Ba(OH)_2$ (m_2/mol kg^{-1})[b]	$Ba(SCN)_2$ (100 w_1/mass %)	$Ba(SCN)_2$ (m_1/mol kg^{-1})[b]	Solid phase[a]
0	0	62.63	6.611	A
2.05	0.333	61.97	6.795	A
3.16	0.525	61.73	6.936	A+B
3.18	0.527	61.61	6.903	A+B
4.75	0.731	57.34	5.967	B
6.16	0.914	54.49	5.463	B
8.49	1.223	51.00	4.966	B+C
8.45	1.213	50.88	4.935	B+C
5.89	0.738	47.51	4.022	C
3.44	0.287	26.54	1.495	C
3.58	0.259	15.83	0.775	C
4.489	0.274	0	0	C

[a] A: $Ba(SCN)_2 \cdot 3H_2O$, [68016-36-4]; B: Ba(OH)SCN, [ ]; C: $Ba(OH)_2 \cdot 8H_2O$, [12230-71-6].
[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used. Mixtures of the three components in suitable proportions were rotated in a thermostat for several days. Equilibrium was reached in 2 days. Samples of the saturated solutions were withdrawn through asbestos or glass wool filters and weighed. $Ba(OH)_2$ was determined by titration with standard HCl solution using nitrazine yellow as indicator, SCN^- was determined by Volhard method. Solid phases were identified by Schreinemakers method.

Source and Purity of Materials:

$Ba(SCN)_2$ was a product of high purity (source not specified) and was used without further purification. $Ba(OH)_2 \cdot 8H_2O$ was recrystallized before use in an apparatus which excluded CO_2.

Estimated Error:

Temperature: ±0.03 K (authors).
Solubility: insufficient data given to allow for error estimate.

Components:

(1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3]
(2) Methylthiocyanate; $C_2H_3NS(CH_3CNS)$; [556-64-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. Spaccamela Marchetti, Atti. Acad. Sci. Torino, Clase Fis. Mat. Nat. **94**, 353–70 (1960).

Variables:

T/K: 293
Ratio of H_2O/C_2H_3NS concentrations

Prepared By:

J. Hála

Experimental Data

Phase diagram of the $Ba(SCN)_2$–C_2H_3NS–H_2O system at 20 °C

The ternary phase diagram of the $Ba(SCN)_2$–C_2H_3NS–H_2O system at 20 °C was reported (Fig. 40). The following fields were observed in the diagram: I and II—one liquid phase, III—two liquid phases, IV and VI—one liquid phase in equilibrium with solid $Ba(SCN)_2$, and V—two liquid phases in equilibrium with solid $Ba(SCN)_2$. Numerical data were reported for the solubility of $Ba(SCN)_2$ in water-rich C_2H_3NS–H_2O mixtures (curve RP in the diagram) and in C_2H_3NS-rich C_2H_3NS–H_2O mixtures (curve QS in the diagram).

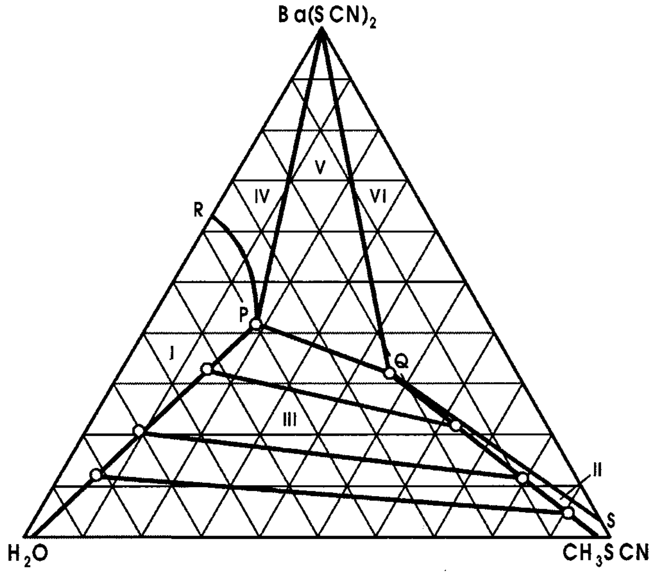

FIG. 40. Phase diagram of the $Ba(SCN)_2$–CH_3CNS–H_2O system at 20 °C.

Composition of the solutions saturated at 20 °C

H_2O-rich region			C_2H_3NS-rich region		
H_2O (100 w_3/mass %)	$Ba(SCN)_2$ (100 w_1/mass %)	C_2H_3NS (100 w_2/mass %)	H_2O (100 w_3/mass %)	$Ba(SCN)_2$ (100 w_1/mass %)	C_2H_3NS (100 w_2/mass %)
37.5	62.5[a]	0	15.0	23.2	61.8
35.8	59.2	5.0	9.4	16.1	74.5
35.0	55.9	9.1	4.7	10.0	85.3
			4.0	8.1	87.9
			0	3.8[b]	96.2

[a] Solubility of $Ba(SCN)_2$ in water, $m_1 = 6.575$ mol kg^{-1} (compiler).

[b] Solubility of $Ba(SCN)_2$ in C_2H_3NS, $m_1 = 0.156$ mol kg^{-1} (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

Solubility curves were obtained by titration a mixture of two components with the third one in a thermostated bath. Some of these measurements were verified by preparing the ternary systems, and observing the temperature of homogenization. The value corresponding to 20 °C was then obtained by interpolation. Burettes graduated by 0.01 cm^3 were used for the titrations.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.

Components:

(1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3]
(2) Urea; CH_4N_2O; [57-13-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. Turgunbekova, K. Nogoev, and K. Sulaimankulov, Zh. Neorg. Khim. **18**, 2847–9 (1973).

Variables:

T/K: 288, 303, and 318
100 w_2/mass %: 0–53.5 at 288 K, 0–57.5 at 303 K, 0–64.0 at 318 K

Prepared By:

J. Hála

Experimental Data

Composition of the saturated solutions in the $Ba(SCN)_2$–urea–H_2O system at three temperatures

Temperature (t/°C)	Urea (100 w_2/mass %)	Urea (100 m_2/mol kg^{-1})[b]	$Ba(SCN)_2$ (100 w_1/mass %)	$Ba(SCN)_2$ (100 m_1/mol kg^{-1})[b]	Solid phase[a]
15	0	0	62.32	6.525	A
	4.97	2.488	61.77	7.326	A
	9.43	5.390	61.44	8.320	A
	12.82	8.284	61.41	9.401	A
	13.81	9.348	61.59	9.877	A+B
	13.55	8.759	60.69	9.294	B
	16.03	10.08	57.50	8.569	B
	19.31	12.08	54.08	8.017	B
	25.94	18.16	50.28	8.341	B
	31.20	25.10	48.10	9.167	B
	35.18	31.78	46.39	9.930	B
	41.87	51.11	44.49	12.87	B
	48.10		43.04		B
	53.42		42.04		B
	53.53		40.61		C
	52.50		36.15		C
	50.68	42.15	29.30	5.774	C
	50.14	32.47	24.15	3.706	C
	49.00	25.90	19.50	2.442	C
	48.60	20.64	12.20	1.228	C
	48.50	17.71	5.90	0.510	C
	49.00	16.00	0	0	C
30	0	0	64.47	7.158	A
	4.72	2.513	64.00	8.071	A
	8.32	4.930	63.58	8.926	A
	11.47	7.824	64.12	10.36	A
	13.42	10.35	65.00	11.88	A+B
	12.82	9.367	64.39	11.15	B
	15.25	10.94	61.54	10.46	B
	20.15	14.81	57.20	9.962	B
	23.13	18.20	55.71	10.39	B
	26.39	23.34	54.78	11.48	B
	31.03	35.68	54.49	14.85	B
	32.02	40.15	54.70	16.25	D
	34.50	35.64	49.38	12.08	D
	39.57	41.10	44.40	10.93	D
	49.00		40.65		D
	54.84		39.68		D
	55.39		38.79		C
	53.65		28.58		C

	54.62	38.36	21.67	3.606	C
	54.96	29.97	14.50	1.873	C
	57.50	22.53	0	0	C
45	0	0	67.11	8.049	A
	6.35	3.730	65.30	9.086	A
	11.06	7.122	63.08	9.623	A
	20.59	18.45	60.83	12.92	A
	25.23	29.07	60.32	16.47	A
	29.59	46.48	59.81	22.26	A+D
	29.38	40.57	58.56	19.16	D
	31.61	39.37	55.02	16.23	D
	34.54	41.08	51.46	14.50	D
	42.30		47.84		D
	45.53		47.33		D
	50.98		47.48		C
	52.00		41.77		C
	53.03		35.81		C
	54.79		28.39		C
	58.48	44.12	19.45	3.477	C
	60.18	36.49	12.36	1.776	C
	64.00	29.60	0	0	C

[a] A: $Ba(SCN)_2 \cdot 3H_2O$, [68016-36-4]; B: $Ba(SCN)_2 \cdot 2CO(NH_2)_2$, [ ]; C: $CO(NH_2)_2$, [57-13-6]; D: $Ba(SCN)_2 \cdot 3CO(NH_2)_2$, [ ].

[b] Calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

An isothermal method was used, no details reported.

Source and Purity of Materials:

Nothing specified.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

Components:

(1) Barium thiocyanate; $Ba(SCN)_2$; [2092-17-3]
(2) Ammonium thiocyanate; NH_4SCN; [1762-95-4]
(3) Ammonia; NH_3; [7664-41-7]

Original Measurements:

A. Stasiewicz, Ann. Univ. M. Curie/Sklodowska, Lublin, Poland **14**, Sect. AA, 49–57 (1959).

Variables:

T/K: 291

Prepared By:

J. Hála

Experimental Data

The solubility of $Ba(SCN)_2$ in liquid ammoniate of NH_4SCN is reported to be $c_1 = 1.10$ mol dm^{-3} or 100 $w_1 = 29.6$ mass % at 18 °C. The composition of the solvent corresponded to the molar ratio $NH_3/NH_4SCN = 2.7$.

Auxiliary Information

Method/Apparatus/Procedure:

The ammoniate of NH_4SCN, a clear liquid (density of 0.9345 g cm^{-3}), was obtained by action of NH_3 gas onto solid NH_4SCN at atmospheric pressure. The preparation of the solvent, and solubility measurements were carried out in a dry box under a stream of dry NH_3 gas.

Source and Purity of Materials:

$Ba(SCN)_2$ was prepared by the reaction of $Ba(OH)_2$ with NH_4SCN. The composition of the salt prepared was not specified. NH_4SCN, Argon-Lodz, was repeatedly recrystallized, and dried in a dessicator over concentrated H_2SO_4, first at normal pressure and then under vacuum for 1 month. Ammonia was dried with Na metal in a steel container.

Estimated Error:

Temperature: precision not reported.

Solubility: insufficient data reported to allow for error estimate.

7. Appendix

List of systems for which the original documents were not available to the editor, and systems for which only data of uncertain quality exist.

NaN_3–chloroform, *n*-hexane, CCl_4, trichloroethylene, ethylacetate[1]
NaN_3 or KN_3–benzene[2]
NH_4N_3–SO_2[3,4] (two liquid phases separate at saturation)
NaOCN or KOCN–water[5]
NaOCN or KOCN–benzene[2]
KOCN, KCN, or KSCN–$POCl_3$[6]
NaCN–NaCl–NH_3[7]
NaCN–NaOH–Na_2CO_3–NH_3[8]
KCN–dimethylsulfoxide[9]
KCN–polyethyleneglycol(400)[9]
LiSCN, NaSCN, KSCN, or CsSCN–poly(methyl glycidyl ether)[25]
NaSCN–nitrobenzene[10]
NaSCN, KSCN, or NH_4SCN–CF_3COOH[11]
NaSCN or KSCN–acetone–water[12a]
NaSCN or KSCN–phenol–water[13]
NaSCN, KSCN, or NH_4SCN–cresols–water[14]
NaSCN–K_2SO_4–water[15]
NaSCN or RbSCN–1-butanol–water[16]
NaSCN, KSCN, or NH_4SCN–triethylamine–water[22]
NaSCN or KSCN–acetone–methanol[26]
KSCN–SO_2–H_2O[17]
KSCN–methylmetacrylate[18]
KSCN–furfural–water[19]
KSCN–CH_3CN–water[34]
KSCN–1-butanol[16,20,24]
KSCN–Na_2SO_4–H_2O[15]
KSCN–poly(ethylene oxide)[21]
KSCN, RbSCN, CsSCN, or NH_4SCN–1-butanol–water[23a]
CsSCN–1-butanol–water[16,32a]
NH_4SCN–SO_2–water[17,27]
NH_4SCN–SO_2–formamide[27]
NH_4SCN–phenol–water[28,35]
NH_4SCN–thiourea–water[36]
NH_4SCN–diethylether–water[37]
$Mg(SCN)_2$–acetamide–water[33a]
$Ba(SCN)_2$–SO_2[29]
$Ba(SCN)_2$–amines[30]
$Ba(SCN)_2$–methanol–propylene[31]
[a]Original document not available to the editor.

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8. System Index

Page numbers preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables. Diammonium, trisodium, etc. salts are indexed under ammonium, sodium, etc. The symbol (aq) stands for water as additional component in the respective system.

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9. Registry Number Index

Page numbers preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables.

10. Author Index

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