Errata Sheet to accompany NSRDS-NBS 61, Part II
Physical Properties Data Compilations Relevant to Energy Storage.
II. Molten Salts: Data on Single and Multi-Component Salt Systems
G. J. Janz, C. B. Allen, N. P. Bansal, R. M. Murphy, and R. P. T. Tomkins

Page 175: The heading for the third column of table 17.10 should be p_{O_2} (atm).

Page 187: Replace table 19.4 with the following:

Table 19.4. Parameters of equation (19.4) and precisions[a]

a x 10^{-3}	-b x 10^{-2}	c x 10^{2}	T range (K)	Precision
-14.9135	-0.3452	-	440-460	∿±11%
31.886_5	1.1359_1	10.121_2	466-533	∿±3.5%
9.312_5	0.3148	2.665_4	544-589	∿±2.9%

(a) for 330-420K, $\eta = 3.54642 \times 10^{-5} \exp(6305.9/RT)$, precision ~ ± 18%

Page 396: The missing tabular matter under the heading for table 45.1 is as follows:

a	b x 10^{7}	c x 10^{10}	Precision
2.06431	-4.76248	-5.60825	± 0.1%

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Foreword

The National Standard Reference Data System provides access to the quantitative data of physical science, critically evaluated and compiled for convenience and readily accessible through a variety of distribution channels. The System was established in 1963 by action of the President's Office of Science and Technology and the Federal Council for Science and Technology, and responsibility to administer it was assigned to the National Bureau of Standards.

NSRDS receives advice and planning assistance from a Review Committee of the National Research Council of the National Academy of Sciences-National Academy of Engineering. A number of Advisory Panels, each concerned with a single technical area, meet regularly to examine major portions of the program, assign relative priorities, and identify specific key problems in need of further attention. For selected specific topics, the Advisory Panels sponsor subpanels which make detailed studies of users' needs, the present state of knowledge, and existing data resources as a basis for recommending one or more data compilation activities. This assembly of advisory services contributes greatly to the guidance of NSRDS activities.

The System now includes a complex of data centers and other activities in academic institutions and other laboratories. Components of the NSRDS produce compilations of critically evaluated data, reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data. The centers and projects also establish criteria for evaluation and compilation of data and recommend improvements in experimental techniques. They are normally associated with research in the relevant field.

The technical scope of NSRDS is indicated by the categories of projects active or being planned: nuclear properties, atomic and molecular properties, solid state properties, thermodynamic and transport properties, chemical kinetics, and colloid and surface properties.

Reliable data on the properties of matter and materials are a major foundation of scientific and technical progress. Such important activities as basic scientific research, industrial quality control, development of new materials for building and other technologies, measuring and correcting environmental pollution depend on quality reference data. In NSRDS, the Bureau's responsibility to support American science, industry, and commerce is vitally fulfilled.

ERNEST AMBLER, *Director*

Preface

This series of publications is aimed at providing physical properties data on materials used in energy storage systems. It was inspired by a requirement in the Department of Energy's Division of Energy Storage Systems for materials property data needed by its contractors in the timely development of energy storage devices. As prime contractor for this program, the Lawrence Livermore Laboratory (LLL) has requested the Office of Standard Reference Data (OSRD) to manage the task of gathering the data, using its established network of data centers and other identified sources of expertise. The OSRD monitors the progress of work, reviews the results, and conveys the numerical data to LLL where the data are converted for entry into an automated data storage and retrieval system. Every effort is made to supply data which have been critically examined in light of the latest knowledge concerning theory and experiment. However it must be recognized that in a rapidly moving technology some of the data will be superseded rather quickly as new materials and techniques are introduced. Thus access to the data via computer terminal as well as publication in this series should help provide the practitioner with timely and useful data which he requires to solve his problems in energy storage. Funding for this series of projects from the Department of Energy, Division of Energy Storage, through the Lawrence Livermore Laboratory, is gratefully acknowledged.

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Physical Properties Data Compilations Relevant To Energy Storage

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The present work provides selected data with value judgements for a set of 49 salt systems of interest as candidate materials for thermal energy storage sub-systems and for electrochemical energy storage systems. The physical properties assessed are: melting points; phase diagrams; eutectic compositions; density; surface tension; viscosity; electrical conductivity; diffusion constants for ions; heat of fusion; heat capacity; volume change on fusion; vapor pressure; thermal conductivity (liquid and solid); and cryoscopic constant. The status of corrosion studies in the form of annotated bibliographic summaries, and salient observations on safety and hazards are also reported. A summarizing series of tables is provided as index to the data-gaps status for this set of candidate materials.

Key words: Corrosion; data compilation; electrochemical energy storage materials; molten salts; physical properties; safety and hazards; thermal energy storage materials; thermal properties; thermodynamic properties; transport properties.

1. Introduction

The present communication reports the results of some work undertaken, in part, to meet the need for an evaluated data file for salt systems to be stored in the LLL Data Banks for Energy Research at Livermore. [1,2,3][1] The situation encountered by the user (research scientist; design and development engineer) may be briefly illustrated by the following two examples.

The first point encountered is that the store of information on molten salts is considerable and is largely unevaluated. It exists partly as primary research literature and partly compiled in some of the emerging secondary and tertiary literature (numerical data projects, handbooks, bibliographies). An analysis of the 1974 publications [4] in this area of materials science may be summarized as follows.

- A total of more than 1300 research papers were published in 1974, in some 290 scientific and technical journals of some 16 different countries.
- Approximately 140 descriptors (keywords) were required to index these research papers by physical properties and/or subject matters.

Thus for an informed use of the accumulated knowledge in this relatively specialized area of materials science the user needs guidance, not only as to what is already established and how it can be accessed but, equally important, on the reliability, namely to what degree are the data adequate for "decision steps" in design and development applications.

The second point encountered is the diversified nature of the information required. For example, in thermal energy storage, the "data needs" that the user encounters include:

> melting point data; phase diagrams; heats of fusion; heat capacities; thermal conductivities; volume-changes on melting; viscosities; thermal diffusivity; expansion coefficients; vapor pressures; thermal stabilities; nucleation; corrosion; safety and hazards; interfacial properties; estimation methods,...

The present compilation was undertaken, thus, to provide a data base for the informed use of the accumulated knowledge on molten salts, particularly for applications to thermal energy storage and for energy storage electrochemically, as in advanced batteries.

The recommendations advanced by the Phase-Change Storage Systems Group [5] provide some guidelines and criteria for the selection of the candidate materials (salt systems). These, together with, the data requirements for electrochemical applications, and two practical considerations, from the viewpoint of economy, are summarized in table I.1. These principles and recent assessments of advanced batteries research, thermal and solar energy storage applications (see for example [5-10], for partial list) may be used to reduce the very large number of salt systems to a relatively short list, as summarized in table I.2. Specific examples of the systems thus included are:

- molten carbonates (Li_2CO_3, Na_2CO_3, K_2CO_3) and their mixtures; relevance: high temperature fuel cells technology; thermal energy storage - electric utilities load-levelling
- molten sodium polysulfides (Na_2S_x); relevance: sodium-sulfur advanced battery technology; transportation; load-levelling
- molten chlorides, and nitrates; for example: (a) LiCl-KCl eutectic; relevance: supporting electrolyte in ESB (advanced battery technology); (b) nitrate eutectics; relevance: thermal energy storage
- low melting mixtures; salt hydrates; $Na_2SO_4 \cdot 10H_2O$, m.pt. 32°C; relevance: thermal energy storage subsystems

The present communication reports the results of critical evaluations for some 26 single-salt systems and 23 mixtures (binary and ternary systems; including eutectics).

2. Systems and Properties Evaluated

A list of the salt systems for which results are reported herewith is in table I.3. The arrangement follows the Anion Classification used elsewhere for molten salts [see: 11,15]. Within an anion family the salts are ordered by cations. There are exceptions, e.g. the Na_2S-Sulfur system is listed as Na_2S_x since the concern is with polysulfide mixtures, and Sulfur, itself not a salt, has been included to complete this system. The physical properties are listed in table I.4.

[1] Figures in brackets indicate literature references.

Table I.1. Criteria for the selection of candidate materials

A. (For thermal energy storage systems (PCM)[a] and for electrochemical energy storage (ESB)[b]

1. Thermodynamic properties

(i) suitable melting point
(ii) high heat of fusion
(iii) congruent melting
(iv) small volume change on melting
(v) high thermal conductivity
(vi) heat capacity
(vii) density
(viii) surface tension

2. Chemical properties

(i) safety
(ii) stability
(iii) non-corrosive to container materials

3. Economy

(i) inexpensive
(ii) availability

B. Additional considerations for electrochemical energy storage (ESB)

(i) electrical conductivity
(ii) diffusion constants for ions
(iii) transport numbers for ions
(iv) cryoscopic constant
(v) emf series of metals
(vi) reference electrodes
(vii) thermodynamic activity coefficients

[a] (PCM); phase-change materials;
[b] (ESB); electrochemical storage batteries

Table I.2. Likely candidates list (salt systems)

A. Systems utilizing single salts (I.IIa and I.IIb)

I. Cations	II. Anions a	II. Anions b
lithium	chlorides	bromides
sodium	nitrates	iodides
potassium	carbonates	sulfates
magnesium	polysulfides	phosphates
calcium	fluorides	thiocyanates
barium	hydroxides	vanadates
	nitrites	borates
	sulfides	tungstates
		chromates
		formates
		acetates

B. Systems utilizing mixtures of salts

(a) Eutectics (2 or more salts from I.IIa)
(b) Eutectics (2 or more salts from I.IIb)
(c) Eutectics (2 or more salts from I.IIa, I.IIb)

C. Systems utilizing salt hydrates

Congruently melting salts with water of hydration

Table I.3. List of salt systems

System	Material	System	Material
Single salts		Salt mixtures	
1	LiF	27	LiCl-KCl
2	NaF	28	NaCl-KCl
3	KF	29	LiCl-$AlCl_3$
4	LiCl	30	NaCl-$AlCl_3$
5	NaCl	31	KCl-$AlCl_3$
6	KCl	32	NaCl-$CaCl_2$
7	$MgCl_2$	33	Na_2S_x
8	$CaCl_2$	34	NaF-KF
9	$AlCl_3$	35	LiF-LiCl
10	Li_2CO_3	36	NaCl-KCl-$AlCl_3$
11	Na_2CO_3	37	LiCl-KCl-$CaCl_2$
12	K_2CO_3	38	LiCl-NaCl-KCl
13	$LiNO_3$	39	LiF-LiCl-LiBr
14	$NaNO_3$	40	LiF-LiCl-LiI
15	KNO_3	41	Li_2CO_3-Na_2CO_3-K_2CO_3
16	Li_2SO_4	42	Li_2CO_3-Na_2CO_3
17	Na_2SO_4	43	Li_2CO_3-K_2CO_3
18	K_2SO_4	44	Na_2CO_3-K_2CO_3
19	Sulfur	45	$NaNO_3$-KNO_3
20	Na_2S	46	$LiNO_3$-$NaNO_3$-KNO_3
21	Na_2S_2	47	Li_2SO_4-K_2SO_4
22	Na_2S_3	48	Li_2SO_4-Na_2SO_4-K_2SO_4
23	Na_2S_4	49	NaCl-Li_2SO_4
24	Na_2S_5		
25	LiBr		
26	LiI		

Table I.4. List of physical properties

Physical property	Storage mode PCM	Storage mode ESB
1. melting temperatures	x	x
2. phase diagram (liquidus-solidus)	x	x
3. density of melt	x	x
4. surface tension (wetting)	x	x
5. viscosity	x	x
6. electrical conductivity		x
7. hazards (safety)	x	x
8. containment (corrosion)	x	x
9. diffusion constants for ions		x
10. heat of fusion	x	x
11. heat capacity	x	x
12. volume change on melting (%)	x	x
13. vapor pressure	x	x
14. thermal conductivity (melt)	x	x
15. thermal conductivity (solid)	x	x
16. cryoscopic constant	x	x

3. Fundamental Constants, Symbols and Units

The fundamental constants and glossary of symbols and units are in tables I.5 and I.6, respectively.

Table I.5. Fundamental constants

Symbol	Name	Value
N	Avogadro constant	$6.02252 \pm 0.00028 \times 10^{23}$ mol^{-1}
F	Faraday constant	96,487.0 ± 1.6 Coulombs mol^{-1} (23,060.9 ± 0.4 cal V^{-1} equiv.$^{-1}$)
e	Electronic charge	1.60210×10^{-19} Coulombs
R	Gas constant	8.3143 ± 0.0012 J K^{-1}mol^{-1} 1.98716 ± 0.00029 cal K^{-1}mol^{-1}

4. Treatment of Data

Statistical Analysis of Data

The recommended data values were selected based on the estimates of precision and uncertainty of the data surveyed in the literature. The Percent Departure also provided a guideline. The Percent Departure is defined as:

$$\text{Percent Departure} = \frac{\text{"compared value"} - \text{"tabulated value"}}{\text{"tabulated value"}} \times 100$$

Here "compared value" and "tabulated value" refer to the literature value and the value recommended in the present work. Both the "compared value" and the "tabulated value" were calculated from statistically derived equations since the results had to be interpolated to common temperatures and common compositions. Where the data sets from two or more studies were merged to provide the data base for the recommended values (either to extend the temperature range, or to fix the confidence level) this has been noted in the data tables. Unless otherwise noted, all values were recalculated to the Kelvin temperature scale and are thus reported throughout.

All calculations were made on the digital computer facilities at Rensselaer Polytechnic Institute. The data set of the recommended study were recalculated by a one-dimensional analysis, using the method of least squares, to establish equations indicating the variations of the physical quantities with temperature at the experimental compositions. If the data base was sufficient, calculations using a two-dimensional analysis, with a stepwise multiple regression routine were undertaken. In this way a physical property-temperature-composition matrix was developed. A result of this analysis is that it enables intercomparisions of property values at either common temperatures or at common compositions.

One-Dimensional Analysis

The criterion for choosing the equation of best fit in the one-dimensional analysis was the standard error of estimate.

Table I.6. Glossary of symbols and units

Symbol	Physical quantity	Units[a]
a	Thermodynamically defined activity	dimensionless
A	Pre-exponential factor	as in text
C	Concentration	mol %
C_p	Heat capacity	cal K^{-1}mol^{-1}
D	Diffusion coefficient	cm^{2}sec^{-1}
E	Energy of activation	cal mol^{-1}
ΔH_f°	Heat of fusion	kcal mol^{-1}
k_f	Cryoscopic constant	K mol^{-1} kg^{-1}
K_d	Equilibrium dissociation constant	atm.
M_1	Apparent molecular weight	g mol^{-1}
P_{vap}	Vapor pressure	mm Hg
t	Temperature (Celsius)	°C
T	Temperature (Kelvin)	K
T_m	Melting temperature	°C
T_o	Ideal glass transition temperature	K
V_s	Molar volume of solid	cm^{3}mol^{-1}
ΔV_f	Change in molar volume on fusion	cm^{3}mol^{-1}
$(\Delta V_f/V_s)\%$	Percent molar volume change	dimensionless
X	Mol fraction	dimensionless
γ	Surface tension	dyn cm^{-1}
η	Viscosity	cp or poise
κ	Electrical conductance	ohm^{-1} cm^{-1}
λ	Thermal conductivity[b]	cal cm^{-1}sec^{-1}K^{-1}
ρ	Density	g cm^{-3}

[a] For conversion to the SI system of units:

1 ohm^{-1}cm^{-1} = 1 x 10$^{-2}\Omega^{-1}$m^{-1}
1 g cm^{-3} = 1 x 10^{-3} Kg cm^{-3}
1 cp = 1 x 10^{-3}N s m^{-2}
1 dyn cm^{-1} = 1 x 10^{-3}N m^{-1}
1 cal mol^{-1} = 4.184 J mol^{-1}
sec = s

[b] For conversion

to:	multiply by:
mW m^{-1}K^{-1}	4.184×10^5
W m^{-1}K^{-1}	4.184×10^2
J cm^{-1}sec^{-1}K^{-1}	4.184
kcal m^{-1}hr^{-1}K^{-1}	3.600×10^2
BTU ft^{-1}hr^{-1}F^{-1}	2.419×10^2

This was defined by

$$s = \left[\frac{\sum^{n} (\gamma_e - \gamma)^2}{n - q}\right]^{\frac{1}{2}}$$

where γ_e = the experimental value at each temperature, γ = the value calculated from the least squares equation at the same temperature as γ_e, n = the number of experimental data points, and q = the number of coefficients in the least square equation (2 for linear, 3 for quadratic). The standard error of estimate was computed from the residuals in the least-squares routine.

Two-Dimensional Analysis

The computer programs consisted of the four routines, STPRG, CORRE, LOC and MSTR; the latter two are storage routines which have no effect on the accuracy of the results. In addition a subroutine STOUT was used to print the results of each regression step and the subroutine MATRIX, for printing a matrix of numerical values from the thus derived equation.

The abbreviated Doolittle method was used to select the variables entering the regression and for calculation of coefficients. The independent variable included in each step of the analysis was selected by computing the reduction of sums of squares of each variable. The variable causing the largest reduction was added to the equation and deleted from the table of sums of squares. The coefficients, intercept and statistical parameters for the new equation were computed and printed. This procedure was repeated until the maximum proportion of sums of squares to the total reduced was less than a limit set by the programmer.

The independent variables used in the initial selection were chosen from a generalized procedure, which generated 30 combinations of the input variables using powers, reciprocals, logarithmic and exponential quantities. It was found that the procedure consistently selected the equation $(T + C)^3$, so that the working program used nine independent variables. After the final equation was produced, it was transferred to the MATRIX routine, which recalculates values at rounded compositions and temperatures, within specified boundary conditions. In the presentation of the matrix, due cognizance is taken of the experimental range of investigation and of the phase relationships for the system so that values are always "interpolated" rather than "extrapolated". The final step in the procedure involves the residual analysis (giving the deviations of the original values from those computed from the "best-fit" equations).

In the programs used (vide infra), a summary of significant parameters is printed by the computer at each step in the regression analysis. These are: the sum of the squares reduced, S_i; the ratio S_i/D where D is defined below; and the cumulative sum of these variables, S_{cum} and P_{cum}. These quantities give an indication of the effect of each variable in the final equation. The programmers limit on P was always in the range $0.0001 < P_{cum} < 0.001$.

The standard error in the estimated y values adjusted for degrees of freedom, is then given by:

$$s = \left[\frac{D - S_{cum}}{n - q - 1} \right]^{\frac{1}{2}}$$

where $D = \sum (y - \bar{y})^2$, y = experimental values, $\bar{y}$ = average of all experimental values, and q = the number of independent variables in the equations.

An F value analysis of variance was used to determine if a particular model was acceptable. Tables of F values indicate that values greater than 2.0 are acceptable for the routine used here. In all cases values of F were greater than 1000. The F value is defined as:

$$F = \frac{S_{cum}/q}{(D - S_{cum})/(n - q - 1)}$$

where S_{cum}, q, D, and n are defined above.

5. Value Judgements

(a) Precision

Estimates of precision were based on standard error of estimate analysis. The standard error of estimate is the end result of a statistical analysis of the numerical data, and the statistical analysis depends on various factors, such as the number of data points, the nature of the concentration dependence and the temperature dependence of the particular physical property. The precision is the standard error expressed as a percent value. As a general guide, about 60% of the results lie within the estimate of precision, 95% within twice this value and approximately 99% within three times the value. Where the preceding approach was not possible, we refer to the published error estimates of the original authors.

(b) Accuracy

Accuracy estimates were based on assessments of experimental details including method of measurements, techniques, analytical characterization of chemicals, and intercomparisions with results from the same and/or different laboratories. The accuracy estimates are more subjective than the estimates of precision. The numerical values are reported to more significant figures than justified by the accuracy for internal consistency (i.e., the values fall within the limits of precision analysis).

For eutectic melting point data, values are reported without limits of

accuracy. This is largely because the experimental details (i.e., cooling/heating curves) are insufficient for accuracy estimates.

The various measurement techniques encountered are summarized in table I.7. The range is considerable and shows some aspects of the complexities and difficulties in this part of the task, i.e. firming up accuracy estimates. Descriptions of experimental details, particularly for molten salts studies, may be found in recent surveys [11-15], and it is sufficient to note some particular points encountered in the present task. The most widely used techniques appear to be: Archimedean (density), maximum bubble pressure (surface tension), capillary and oscillating sphere (viscosity), ac bridge (electrical conductance), chronopotentiometry (diffusion), drop calorimetry (heat of fusion; heat capacity), dilatometric (volume change on fusion) mass spectrometry-Knudsen cell (vapor pressure), hot wire (thermal conductivity), and heats of fusion (cryoscopic constants). The accuracy estimates based on these appear reasonably sound.

Concerning electrical conductivity, however, it is now apparent that the quartz capillary dipping cell technique leads to values as much as 3-5% too high at temperatures greater than 900°C [16].

Table I.7. High temperature experimental techniques

Density	**Cryoscopic constants**	**Thermal conductivity** (liquid, solid)
Archimedean	freezing point lowering (dilute solution)	hot wire - absolute and transient
dilatometric	freezing point depression (phase-rule)	modified hot wire
flotation	from heats of fusion	concentric cylinder - absolute and transient
maximum bubble	**Vapor pressure**	optical plane - absolute and transient
pycnometric	manometry (sickle or spoon gauge)	radial heat flux
Surface tension	dew point	linear heat flux
maximum bubble	boiling/reduced pressures	flat plate - steady state
Wilhelmy slide plate	vapor transpiration	comparative method
pin detachment	Knudsen effusion	others
capillary rise	Mass spectrometry and Knudsen effusion	**Diffusion**
sessible bubble	**Heat of fusion** **Heat capacity**	chronopotentiometry
pendant drop	isothermal calorimetry	linear sweep voltammetry
Viscosity	drop calorimetry	dc polarography
capillary	differential-scanning calorimetry (DSC)	oscillographic polarography
oscillating sphere	phase-rule (freezing point data)	faradaic impedance
oscillating cylinder	solution calorimetry	chronoamperometry
falling sphere	**Volume change on melting**	rotating disc electrode
Electrical conductance	gas manometry	porous frit
dc bridge	dilatometric	electrophoresis
ac bridge	pellet expansivity	wave-front interferometry
transformer bridge		capillary

A further point of some concern relative to conductance data is an error noted [17] in a USSR 1970 textbook of physical chemistry. In the English translation of Ya. Gerasimov's "Physical Chemistry", the composition of the conductance cell calibration standard 1 demal solution is specified as 74.1352 g KCl rather than the internationally accepted value, 71.1352 g KCl. This should not be overlooked as a possible contributing factor to discrepancies arising in published conductance data.

An emerging aspect relative to viscosity data is recognition [16] of the extreme care that must be given to features of experimental design/technique if the damped oscillation method (oscillating sphere) is to be used with confidence. As noted in the data sheets, it is apparent that the recommended viscosity values for NaCl may be as much as 25% too high at 900°C, even though the technique, as conventionally used, should be capable of an accuracy better than ±5%. An example selected from diffusion studies may be used to illustrate the situation encountered in analyzing the results from independently completed studies of the same systems. The results for various metal ions in the molten LiCl-KCl eutectic (500°) [18-23] are summarized in table I.8. Our critical evaluation places highest reliance to the results of Heus and Egan in this example. With reference to chronopotentiometry, it

Table I.8. Diffusion coefficients of metal ions in LiCl-KCl at 500°C

Metal ions	D X 10^5 ($cm^2 sec^{-1}$)				
	(a)	(b)	(c)	(d)	(e)
Pb^{2+}	2.18	1.3	1.7	1.75	1.29
Cd^{2+}	2.08,1.68	1.7	1.8	1.6	0.98
Co^{2+}	2.42			0.9	1.02
Ni^{2+}				1.8	1.26

a Chronopotentiometry at Pt electrodes
b Chronopotentiometry at Pt electrodes
c Polarography at dropping bismuth electrodes
d Linear sweep voltammetry at Pt electrodes
e Linear sweep voltammetry at glassy carbon electrodes

is of interest to note that applications to complex systems, such as the electrolytes of the Li/S battery systems and molten carbonate fuel cell systems now appear possible. Meaningful values for the derived diffusion coefficients should follow directly from the analysis advanced by Vallet and Braunstein [24] for electrochemical flux equations in binary mixtures of molten salts.

6. Data Tables

Values are reported throughout on the Kelvin temperature scale with the exception of the melting point data. The Celsius scale was retained for melting points for ease of reference to source materials. Information has been included relative to two aspects that do not lend themselves readily to critical assessments, namely Corrosion and Containment, and Safety and Hazards. For these two aspects the information is reported simply in an annotated bibliography format to provide ready access to the relevant source literature on a "need" basis.

A summary of systems for which no information is available has been prepared using a physical properties classification. This is in table I.9. From the latter, the data-gaps status is readily realized; for example, inspection shows that for the sodium polysulfides (Na/S battery; sulfur electrode) there is no information for heats of fusion, heat capacities, diffusion, and volume changes on melting.

Table I.9. Data gaps status

Melting point

No data gaps

Phase diagrams

No data gaps

Density

Na_2S
Na_2S_2
LiCl-KCl-$CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiI
$LiNO_3$-$NaNO_3$-KNO_3
Li_2SO_4-Na_2SO_4-K_2SO_4
NaCl-Li_2SO_4

Viscosity

Li_2SO_4
Na_2SO_4
K_2SO_4
Na_2S
Na_2S_2
Na_2S_3
Na_2S_4
Na_2S_5
LiCl-$AlCl_3$
KCl-$AlCl_3$
NaF-KF
LiF-LiCl
NaCl-KCl-$AlCl_3$
LiCl-KCl-$CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiBr
LiF-LiCl-LiI
$LiNO_3$-$NaNO_3$-KNO_3
Li_2SO_4-K_2SO_4
Li_2SO_4-Na_2SO_4-K_2SO_4
NaCl-Li_2SO_4

Surface tension

Na_2S
Na_2S_2
LiCl-$AlCl_3$
NaCl-$AlCl_3$
KCl-$AlCl_3$
NaCl-KCl-$AlCl_3$
LiCl-KCl-$CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiBr
LiF-LiCl-LiI
$LiNO_3$-$NaNO_3$-KNO_3
Li_2SO_4-K_2SO_4
Li_2SO_4-Na_2SO_4-K_2SO_4

Electrical conductivity

Na_2S
Na_2S_2
Na_2S_4
Na_2S_5
LiCl-KCl-$CaCl_2$
LiF-LiCl-LiBr
LiF-LiCl-LiI
Li_2SO_4-Na_2SO_4-K_2SO_4
NaCl-Li_2SO_4

Volume change on melting

Na_2S
Na_2S_2
KCl-$AlCl_3$
Na_2S_x
NaCl-KCl-$AlCl_3$
LiCl-KCl-$CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiBr
LiF-LiCl-LiI
$LiNO_3$-$NaNO_3$-KNO_3
Li_2SO_4-Na_2SO_4-K_2SO_4
NaCl-Li_2SO_4

(table continued)

Table I.9. --Continued

Diffusion

LiF
$MgCl_2$
$AlCl_3$
K_2CO_3
Li_2SO_4
Na_2SO_4
K_2SO_4
Na_2S
Na_2S_2
Na_2S_3
Na_2S_4
Na_2S_5
LiBr
LiI
$LiCl-AlCl_3$
$KCl-AlCl_3$
Na_2S_x
NaF-KF
LiF-LiCl
$NaCl-KCl-AlCl_3$
$LiCl-KCl-CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiBr
LiF-LiCl-LiI
$NaCl-Li_2SO_4$

Heat of fusion

Na_2S_2
Na_2S_3
Na_2S_4
NaCl-KCl
Na_2S_x
LiF-LiCl-LiBr
LiF-LiCl-LiI
$LiNO_3-NaNO_3-KNO_3$
$Li_2SO_4-K_2SO_4$
$Li_2SO_4-Na_2SO_4-K_2SO_4$

Thermal conductivity liquid

KF
$AlCl_3$
K_2CO_3
Li_2SO_4
Na_2SO_4
K_2SO_4
Na_2S_2
Na_2S_4
Na_2S_5
LiI
NaCl-KCl
$LiCl-AlCl_3$
$KCl-AlCl_3$
$NaCl-CaCl_2$
Na_2S_x
NaF-KF
LiF-LiCl
$NaCl-KCl-AlCl_3$
$LiCl-KCl-CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiBr
LiF-LiCl-LiI
$Li_2CO_3-Na_2CO_3-K_2CO_3$
$Li_2CO_3-K_2CO_3$
$Na_2CO_3-K_2CO_3$
$LiNO_3-NaNO_3-KNO_3$
$Li_2SO_4-K_2SO_4$
$Li_2SO_4-Na_2SO_4-K_2SO_4$
$NaCl-Li_2SO_4$

Cryoscopic constant

Na_2S_2
Na_2S_3
Na_2S_4
NaCl-KCl
Na_2S_x
LiF-LiCl-LiBr
LiF-LiCl-LiI
$NaNO_3-KNO_3$
$LiNO_3-NaNO_3-KNO_3$
$Li_2SO_4-K_2SO_4$
$Li_2SO_4-Na_2SO_4-K_2SO_4$

Heat capacity

Na_2S_2
Na_2S_3
Na_2S_4
Na_2S_5
NaCl-KCl
$LiCl-AlCl_3$
$NaCl-AlCl_3$
$KCl-AlCl_3$
$NaCl-CaCl_2$
Na_2S_x
NaF-KF
LiF-LiCl
$NaCl-KCl-AlCl_3$
$LiCl-KCl-CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiBr
LiF-LiCl-LiI
$Li_2CO_3-Na_2CO_2$
$LiNO_3-NaNO_3-KNO_3$
$Li_2SO_4-K_2SO_4$
$Li_2SO_4-Na_2SO_4-K_2SO_4$

Vapor pressure

Li_2SO_4
Na_2S
LiCl-KCl
$LiCl-AlCl_3$
NaF-KF
LiF-LiCl
$NaCl-KCl-AlCl_3$
$LiCl-KCl-CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiBr
LiF-LiCl-LiI
$NaNO_3-KNO_3$
$Li_2SO_4-K_2SO_4$
$Li_2SO_4-Na_2SO_4-K_2SO_4$
$NaCl-Li_2SO_4$

Thermal conductivity solid

KF
$CaCl_2$
$AlCl_3$
K_2CO_3
Li_2SO_4
Na_2SO_4
K_2SO_4
Na_2S
Na_2S_2
Na_2S_3
Na_2S_4
Na_2S_5
LiBr
LiI
NaCl-KCl
$LiCl-AlCl_3$
$NaCl-AlCl_3$
$KCl-AlCl_3$
$NaCl-CaCl_2$
Na_2S_x
NaF-KF
LiF-LiCl
$NaCl-KCl-AlCl_3$
$LiCl-KCl-CaCl_2$
LiCl-NaCl-KCl
LiF-LiCl-LiBr
LiF-LiCl-LiI
$Li_2CO_3-Na_2CO_3-K_2CO_3$
$Li_2CO_3-K_2CO_3$
$Na_2CO_3-K_2CO_3$
$NaNO_3-KNO_3$
$LiNO_3-NaNO_3-KNO_3$
$Li_2SO_4-K_2SO_4$
$Li_2SO_4-Na_2SO_4-K_2SO_4$
$NaCl-Li_2SO_4$

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I. Lithium Fluoride: LiF

1. *Melting Temperature (T_m)*

Melting point:
848° ± 2°C [1]

References [1-16].

2. *Density (ρ)*

Measurement method: Archimedean technique [17]

$$\rho = 2.3581 - 4.902 \times 10^{-4} T \quad (1.1)$$

precision: ± 0.11% uncertainty: ∿ ± 0.5%

Table 1.1. Densities from equation (1.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1140	(1.7993)	1230	1.7552
1150	1.7944	1240	1.7502
1160	1.7895	1250	1.7454
1170	1.7846	1260	1.7404
1180	1.7797	1270	1.7355
1190	1.7748	1280	1.7306
1200	1.7699	1290	1.7257
1210	1.7650	1300	1.7208
1220	1.7601	1310	1.7159

Value in parenthesis extrapolated beyond experimental temperature range.
References [17-20].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [21]

$$\gamma = 346.49 - 9.88 \times 10^{-2} T \quad (1.2)$$

precision: ± 0.3% uncertainty: ∿ ± 3%

For numerical values: see table 1.2

References [21-22].

4. *Viscosity (η)*

Measurement method: oscillating sphere [20]

$$\eta = 18.549 \times 10^{-2} \exp (5610/RT) \quad (1.3)$$

precision: ± 0.9% uncertainty: ∿ ± 20%

For numerical values: see table 1.3

References [20,23].

5. *Electrical Conductance (κ)*

Measurement method: ac; Kelvin bridge [24]

$$\kappa = -15.0389 + 3.53546 \times 10^{-2} T - 1.28145 \times 10^{-5} T^2 \quad (1.4)$$

precision: ± 0.3% uncertainty: ∿ ± 5%

For numerical values: see table 1.4

References [17, 24-27].

Table 1.2. Surface tension from equation (1.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1160	231.9	1350	213.1
1170	230.9	1360	212.1
1180	229.9	1370	211.1
1190	228.9	1380	210.1
1200	227.9	1390	209.2
1210	226.9	1400	208.2
1220	226.0	1410	207.2
1230	225.0	1420	206.2
1240	224.0	1430	205.2
1250	223.0	1440	204.2
1260	222.0	1450	203.2
1270	221.0	1460	202.2
1280	220.0	1470	201.3
1290	219.0	1480	200.3
1300	218.1	1490	199.3
1310	217.1	1500	198.3
1320	216.1	1510	197.3
1330	215.1	1520	196.3
1340	214.1	1530	195.3

Table 1.3. Viscosity from equation (1.3)

T (K)	η (cp)	T (K)	η (cp)
1140	2.21	1240	1.81
1160	2.11	1260	1.74
1180	2.03	1280	1.68
1200	1.95	1300	1.63
1220	1.88	1320	1.57
		1340	1.53

Table 1.4. Electrical conductance from equation (1.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1140	8.612	1230	9.060
1150	8.672	1240	9.097
1160	8.729	1250	9.132
1170	8.784	1260	9.164
1180	8.837	1270	9.193
1190	8.886	1280	9.220
1200	8.934	1290	9.244
1210	9.978	1300	9.266
1220	9.021	1310	9.285

6. Safety and Hazards

A. Hazard rating [28-30]

(i) Toxicity - severe

(ii) Vapor pressure: at m.pt. (848 °C), ∿ 8.8 x 10^{-3} mm; at 1080 °C, ∿ 1 mm

(iii) U.S. occupational standards: 3.4 mg m^{-3} air

B. Disaster hazards [31-33]

(i) Molten salt bath "explosion": i.e., explosive generating of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Fluorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

References [28-33].

7. Corrosion

Table 1.5. Corrosion studies from primary research literature

Studies	References
Cr	34
Ni-Cr-Fe alloys (INOR-8; Hastelloys N, B, W,...)	36-41
Al	42
Cb-Zr (99-1)	43-44
Ta-W-Zr-Cb (28-10.5-0.9-60.6) Ta-W-Cb (10-10-80)	44
Electrochemical behavior of oxide ions and related species in molten fluorides	45-47
Electro-analytical studies in molten fluorides	48
Annotated corrosion biblio.	49
Corrosion: molten fluorides (survey)	50

References [34-51].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [16,53]

Table 1.6. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
6.43	∿ ± 0.8%

References [16, 52-55].

10. Heat Capacity (Cp)

Measurement method: drop calorimetry [53]

$$C_p = 8.351 + 6.134 \times 10^{-3}T - 1.4694 \times 10^{4}T^{-2} \quad (1.5)$$

precision: ∿ ± 0.2% uncertainty: ∿ ± 1.5%

Table 1.7. Heat capacity from equation (1.5)

T (K)	C_p (cal $K^{-1}mol^{-1}$)	T (K)	C_p (cal $K^{-1}mol^{-1}$)
1120	15.21	1280	16.19
1130	15.27	1290	16.26
1140	15.33	1300	16.32
1150	15.39	1310	16.38
1160	15.46	1320	16.44
1170	15.52	1330	16.50
1180	15.58	1340	16.56
1190	15.64	1350	16.62
1200	15.70	1400	16.93
1210	15.76	1500	17.55
1220	15.82	1600	18.16
1230	15.89	1700	18.77
1240	15.95	1800	19.39
1250	16.01	1900	20.00
1260	16.07	2000	20.62
1270	16.13		

References [1,16,53,54,56].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary [57]

Table 1.8. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
29.4%	∿ ± 2%

References [57].

12. Vapor Pressure (p_{vap})

Measurement method: effusion [60,61]; boiling point [58,62]; estimated from data base [63]

$$\log p = A + B/T \quad (1.6)$$

Table 1.9. Coefficients of equation (1.6), precisions, and uncertainties

T range (K)	A	-B	Precision	Uncertainty
1121-1160	8.4768	11793	∿±0.6%	∿±5%
1170-1620	9.7633	13250	∿±3.1%	∿±10%
1630-1930	9.0006	11896	∿±0.8%	∿±5%

Table 1.10. Vapor pressure from equations in table 1.9

T (K)	p (mm)	T (K)	p (mm)
1120	0.0089	1630	50.4
1125	0.0099	1640	55.8
1130	0.0110	1650	61.8
1135	0.0122	1660	68.3
1140	0.0136	1670	75.4
1145	0.0150	1680	83.1
1150	0.0167	1690	91.5
1155	0.0185	1700	100.7
1160	0.0204	1710	110.6
1180	0.034	1720	121.4
1200	0.053	1730	133.1
1220	0.080	1740	145.8
1240	0.12	1750	159.5
1260	0.18	1760	174.4
1280	0.26	1770	190.4
1300	0.37	1780	207.7
1320	0.53	1790	226.4
1340	0.75	1800	246.4
1360	1.05	1810	268.1
1380	1.45	1820	291.3
1400	1.99	1830	316.3
1420	2.71	1840	343.1
1440	3.65	1850	371.8
1460	4.87	1860	402.6
1480	6.47	1870	435.6
1500	8.51	1880	470.9
1520	11.12	1890	508.7
1540	14.43	1900	549.0
1560	18.61	1910	592.0
1580	23.84	1920	637.9
1600	30.34	1930	686.9
1620	38.40		

References [58-63].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: quasi-steady state [64]

precision: not estimated uncertainty: $\sim \pm$ 25%

The results were reported in graphical form only.

Table 1.11. Thermal conductivity of melt

T (K)	$\lambda \times 10^4$ (cal $cm^{-1} sec^{-1} K^{-1}$)
1143	41.3

λ values at other temperatures in the range 1200-1450 K are reported in graphical form in [64].

References [51,64].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: absolute stationary [65]

precision: not estimated uncertainty: $\sim \pm$ 10%

The results were reported in graphical form only.

Table 1.12. Thermal conductivity of solid

T (K)	$\lambda \times 10^3$ (cal $cm^{-1} sec^{-1} K^{-1}$)
300	34.9
400	25.1
500	19.3
600	15.8
700	14.7
800	13.4
900	13.6
1000	14.3

Values interpolated from the graphical presentation in [65].

References [64-69].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [70]

Table 1.13. Cryoscopic constant

k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
10.4	$\sim \pm$ 0.8%

References [16,52-54,70-78].

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II. Sodium Fluoride: NaF

1. *Melting Temperature (T_m)*

Melting point:
995° ± 3°C [1,11].

References [1-15].

2. *Density (ρ)*

Measurement method: Archimedean technique [16]

$$\rho = 2.7550 - 6.36 \times 10^{-4} T \quad (2.1)$$

precision: ± 0.15% uncertainty: ∿ ± 0.5%

Table 2.1. Densities from equation (2.1)

T(K)	ρ(g cm^{-3})	T(K)	ρ(g cm^{-3})
1280	1.941	1330	1.909
1290	1.935	1340	1.903
1300	1.928	1350	1.896
1310	1.922	1360	1.890
1320	1.915	1370	1.884

References [12,16-29].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [30]

$$\gamma = 289.60 - 8.20 \times 10^{-2} T \quad (2.2)$$

precision: ∿ ± 0.5% uncertainty: ∿ ± 8%

Table 2.2. Surface tension from equation (2.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1270	185.5	1320	181.4
1280	184.6	1330	180.5
1290	183.8	1340	179.7
1300	183.0	1350	178.9
1310	182.2	1360	178.1

References [30-32].

4. *Viscosity (η)*

Measurement method: oscillating sphere [12]

$$\eta = 3.970 \times 10^{-2} \exp(9831/RT) \quad (2.3)$$

precision: ∿ ± 1.3% uncertainty: ∿ ± 15%

For numerical values: see table 2.3.

Table 2.3. Viscosity from equation (2.3)

T (K)	η (cp)	T (K)	η (cp)
1290	1.84	1390	1.40
1300	1.78	1400	1.36
1310	1.73	1410	1.33
1320	1.68	1420	1.29
1330	1.64	1430	1.26
1340	1.59	1440	1.23
1350	1.55	1450	1.20
1360	1.51	1460	1.18
1370	1.47	1470	1.15
1380	1.43		

References [12].

5. *Electrical Conductance (κ)*

Measurement method: ac; Kelvin bridge [33]

$$\kappa = 1.4633 + 2.7354 \times 10^{-3}T \quad (2.4)$$

precision: ± 0.2% uncertainty: ∿ ± 4%

Table 2.4. Electrical conductance from equation (2.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1270	4.937	1350	5.156
1280	4.965	1360	5.183
1290	4.992	1370	5.211
1300	5.019	1380	5.238
1310	5.047	1390	5.265
1320	5.074	1400	5.293
1330	5.101	1410	5.320
1340	5.129	1420	5.348

References [33-37].

6. *Safety and Hazards*

A. Hazard rating [38-40]

(i) Toxicity - severe

(ii) Vapor pressure: at m.pt. (995°C), ∿ 0.5 mm; at 1050°C, ∿ 1mm

(iii) U. S. occupational standards: 5.5 mg m^{-3} (air)

B. Disaster hazards [38,41-43]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Fluorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

References [38-43].

7. *Corrosion*

see table 2.5.

Table 2.5. Corrosion studies from primary research literature

Studies	References
Cr	44
Ni-Cr-Mo alloys (INOR-8; Hastelloys B, W, and N)	45,46
SSNi-12P	47
Quartz	48
Al	49
Various metals	50
Corrosion studies in molten salts with NaF as one component (e.g., Cl, CO_3,...)	51-67,74,75
Electro-chemical behavior of oxide ions and related species in molten fluorides	68-70
Electroanalytical studies in molten fluorides	71
Annotated corrosion biblio.	72
Corrosion: molten fluorides (survey)	73

References [44-75].

8. Diffusion

Measurement method: capillary [76-77]

List of diffusing species investigated in NaF as solvent

Na^+

Sodium, Na^+ (self-diffusion)

$$D_{Na^+} = 3.08 \times 10^{-3} \exp [-8700/RT] \quad (2.5)$$

precision: ± 3% uncertainty: ∿ ± 20%

Table 2.6. Self-diffusion coefficients from equation (2.5)

T (K)	$D_{Na^+} \times 10^5$ ($cm^2 sec^{-1}$)	T (K)	$D_{Na^+} \times 10^5$ ($cm^2 sec^{-1}$)
1290	10.34	1360	12.31
1300	10.61	1370	12.61
1310	10.89	1380	12.90
1320	11.17	1390	13.20
1330	11.45	1400	13.50
1340	11.74	1410	13.80
1350	12.02		

References [76-77].

9. Heat of Fusion (ΔH_f^o)

Measurement method: drop calorimetry [79]

Table 2.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
8.03	∿ ± 0.5%

References [15,78-81].

10. Heat Capacity (Cp)

Measurement method: drop calorimetry [79]

$$C_p = 10.91 + 4.654 \times 10^{-3}T - 9.3836 \times 10^{4}T^{-2} \quad (2.6)$$

precision: ∿ ± 0.2% uncertainty: ∿ ± 1%

Table 2.8. Heat capacity (liquid) from equation (2.6)

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
1270	16.76	1420	17.47
1280	16.81	1430	17.52
1290	16.86	1440	17.57
1300	16.90	1450	17.61
1310	16.95	1460	17.66
1320	17.00	1470	17.71
1330	17.05	1480	17.76
1340	17.09	1490	17.80
1350	17.14	1500	17.85
1360	17.19	1600	18.32
1370	17.24	1700	18.79
1380	17.28	1800	19.25
1390	17.33	1900	19.73
1400	17.38	2000	20.19
1410	17.42		

References [78-80, 82-84].

11. Volume Change on Melting (ΔV_f)

Measurement method: crystallization pycnometry [86]

Table 2.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
24.0%	∿ ± 2%

References [85-86].

12. Vapor Pressure ($p_{vap.}$)

Measurement method: boiling point [87,88]; transpiration [89]

$$\log p = 8.5954 - 11331/T \quad (2.7)$$

precision: ∿ ± 1.3% uncertainty: ∿ ± 5%

For numerical values: see table 2.10

Table 2.10. Vapor pressures from equation (2.7)

T (K)	p (mm)	T (K)	p (mm)
1280	0.55	1640	48.56
1300	0.76	1660	58.82
1320	1.03	1680	70.92
1340	1.38	1700	85.14
1360	1.84	1720	101.8
1380	2.42	1740	121.2
1400	3.18	1760	143.7
1420	4.13	1780	169.7
1440	5.33	1800	199.7
1460	6.83	1820	234.2
1480	8.70	1840	273.7
1500	11.00	1860	318.8
1520	13.83	1880	370.1
1540	17.28	1900	428.3
1560	21.48	1920	494.1
1580	26.54	1940	568.4
1600	32.62	1960	652.1
1620	39.90		

References [87-90].

13. *Thermal Conductivity (liquid)* (λ_ℓ)

Measurement method: coaxial cylinder [91]

$$\lambda = -14.85 \times 10^{-3} + 14.071 \times 10^{-6} T \quad (2.8)$$

precision: not estimated uncertainty: $\sim \pm 25\%$

Results were reported in graphical form only.

Table 2.11. Thermal conductivity of melt from equation (2.8)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
1270	30.2	1310	35.8
1280	31.6	1320	37.2
1290	33.0	1330	38.6
1300	34.4		

Eq. obtained by fitting the interpolated data from the graphical presentation in [91].

References [91].

14. *Thermal Conductivity (solid)* (λ_s)

Measurement method: absolute stationary state [92]

precision: not estimated uncertainty: $\sim \pm 10\%$

Results were reported in graphical form only.

For numerical values: see table 2.12.

Table 2.12. Thermal conductivity of solid

T (K)	$\lambda \times 10^3$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^3$ (cal $cm^{-1}sec^{-1}K^{-1}$)
300	36.1	700	14.1
400	25.8	800	12.6
500	20.1	900	11.5
600	16.2	1000	11.2

Sole investigation in this temperature range; values interpolated from the graphical presentation in [92].

References [92-93].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [94]

Table 2.13. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
16.7	~ ± 0.5%

References [78-81,94-105].

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III. Potassium Fluoride: KF

1. *Melting Temperature (T_m)*

Melting point:
856° ± 3°C [3,4]

References [1-8].

2. *Density (ρ)*

Measurement method: Archimedean technique [9]

$$\rho = 2.6464 - 6.515 \times 10^{-4} T \quad (3.1)$$

precision: ± 0.16% uncertainty: ∿ ± 0.6%

Table 3.1. Densities from equation (3.1)

T(K)	ρ(g cm^{-3})	T(K)	ρ(g cm^{-3})
1130	1.9102	1210	1.8581
1140	1.9037	1220	1.8516
1150	1.8972	1230	1.8451
1160	1.8907	1240	1.8385
1170	1.8841	1250	1.8320
1180	1.8776	1260	1.8255
1190	1.8711	1270	1.8190
1200	1.8646	1280	1.8125
		1290	1.8060

References [9-12].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [13]

$$\gamma = 176.666 + 7.392 \times 10^{-3} T - 3.330 \times 10^{-5} T^2 \quad (3.2)$$

precision: ± 0.2% uncertainty: ∿ ± 5%

Table 3.2. Surface tension from equation (3.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1200	137.6	1400	121.7
1210	136.9	1410	120.9
1220	136.1	1420	120.0
1230	135.4	1430	119.1
1240	134.6	1440	118.3
1250	133.9	1450	117.4
1260	133.1	1460	116.5
1270	132.3	1470	115.6
1280	131.6	1480	114.7
1290	130.8	1490	113.8
1300	130.0	1500	112.8
1310	129.2	1510	111.9
1320	128.4	1520	111.0
1330	127.6	1530	110.0
1340	126.8	1540	109.1
1350	126.0	1550	108.1
1360	125.1	1560	107.2
1370	124.3	1570	106.2
1380	123.5		
1390	122.6		

References [13].

4. *Viscosity (η)*

Measurement method: oscillating sphere [14]; uncertainty ± 20%

Table 3.3. Viscosity

T (K)	η (cp)
1246.2	1.59

References [14].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [15]

$$\kappa = 9.2728 \times 10^{-2} + 3.0628 \times 10^{-3} T \quad (3.3)$$

precision: ± 0.5% uncertainty: ∿ ± 5%

Table 3.4. Electrical conductance from equation (3.3)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1130	3.554	1220	3.829
1140	3.584	1230	3.860
1150	3.615	1240	3.891
1160	3.646	1250	3.921
1170	3.676	1260	3.952
1180	3.707	1270	3.982
1190	3.737	1280	4.013
1200	3.768	1290	4.044
1210	3.799		

References [11,15-21].

6. *Safety and Hazards*

A. Hazard rating [22-24]

(i) Toxicity - severe

(ii) Vapor pressure: at m.pt. (856°C), ∿ 0.5 mm; at 900°C, ∿ 1 mm

(iii) U. S. occupational standards: 7.6 mg m^{-3} (air)

B. Disaster hazards [22,25-27]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over and/or equipment failure; i.e., explosive expansion of "trapped" air

(ii) Fluorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes

References [22-27].

7. Corrosion

Table 3.5. Corrosion studies from primary research literature

Studies	References
Cr	28
Ni-Cr-Fe	29,30
INOR-8	30-33
Al	34,35
Ni-Mo-Cr-Fe (Hastelloy)	36
Inconel	33,37
Electro-chemical behavior of oxide ions and related species in molten fluorides	38-40
Electro-analytical studies in molten fluorides	41
Annotated corrosion biblio.	42
Corrosion: molten fluorides (survey)	43

References [28-43].

8. Diffusion

Measurement method: capillary [44]

List of diffusing species investigated in KF as solvent

K^+

Potassium, K^+ (self-diffusion)

$$D_{K^+} = 2.46 \times 10^{-3} \exp[-7500/RT] \quad (3.4)$$

precision: ± 2.5% uncertainty: ∿ ± 20%

Table 3.6. Self-diffusion coefficients from equation (3.4)

T (K)	$D_{K^+} \times 10^5$ ($cm^2 sec^{-1}$)	T (K)	$D_{K^+} \times 10^5$ ($cm^2 sec^{-1}$)
1140	8.97	1220	11.15
1150	9.24	1230	11.43
1160	9.50	1240	11.72
1170	9.77	1250	12.01
1180	10.04	1260	12.30
1190	10.31	1270	12.59
1200	10.59	1290	13.19
1210	10.87		

References [44].

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [45]

Table 3.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
7.05	∿ ±0.5%

References [45-49].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [45]

$$C_p = 11.845 + 2.762 \times 10^{-3}T - 9.11157 \times 10^{4}T^{-2} \quad (3.5)$$

precision: ∿ ± 0.2% uncertainty: ∿ ± 1%

Table 3.8. Heat capacity from equation (3.5)

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
1130	14.89	1370	15.58
1150	14.95	1390	15.64
1170	15.01	1400	15.66
1190	15.07	1410	15.69
1200	15.09	1430	15.75
1210	15.12	1450	15.81
1230	15.18	1470	15.86
1250	15.24	1490	15.92
1270	15.30	1500	15.95
1290	15.35	1600	16.23
1300	15.38	1700	16.51
1310	15.41	1800	16.79
1330	15.47	1900	17.07
1350	15.52	2000	17.35

References [45,50-53].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [54]

Table 3.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
17.2%	∿ ± 3%

References [54].

12. Vapor Pressure (p_{vap})

Measurement method: boiling point [55-56]

$$\log p = 8.4262 - 9820/T \quad (3.6)$$

precision: ∿ ± 0.01% uncertainty: ∿ ± 5%

For numerical values: see table 3.10.

KF

Table 3.10. Vapor pressure from equation (3.6)

T (K)	p (mm)	T (K)	p (mm)
1550	123.2	1670	351.5
1560	135.3	1680	381.0
1570	148.4	1690	412.6
1580	162.6	1700	446.4
1590	177.9	1710	482.5
1600	194.4	1720	521.1
1610	212.2	1730	562.2
1620	231.5	1740	606.1
1630	252.2	1750	652.8
1640	274.4	1760	702.5
1650	298.3	1770	755.4
1660	324.0		

References [55-57].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_f)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [58]

Table 3.11. Cryoscopic constant

k_f (K mol^{-1}kg^{-1})	Uncertainty
20.9	~ ± 0.5%

References [45,46,48,53,58-65].

16. References

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IV. Lithium Chloride: LiCl

1. *Melting Temperature (T_m)*

Melting point:
610° ± 2°C [2,6]

References [1-15].

2. *Density (ρ)*

Measurement method: Archimedean technique [3]

$$\rho = 1.8842 - 4.328 \times 10^{-4} T \quad (4.1)$$

precision: ± 0.34% uncertainty: ∿ ± 0.5%

Table 4.1. Densities from equation (4.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
910	1.4904	990	1.4557
920	1.4860	1000	1.4514
930	1.4817	1010	1.4471
940	1.4774	1020	1.4427
950	1.4730	1030	1.4384
960	1.4687	1040	1.4341
970	1.4644	1050	1.4298
980	1.4601		

References [1,3,9,11-14,16-28].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [29]

$$\gamma = 180.42 - 5.83 \times 10^{-2} T \quad (4.2)$$

precision: ± 0.3% uncertainty: ∿ ± 0.5%

Table 4.2. Surface tension from equation (4.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
890	128.5	1030	120.4
900	128.0	1040	119.8
910	127.4	1050	119.2
920	126.8	1060	118.6
930	126.2	1070	118.0
940	125.6	1080	117.5
950	125.0	1090	116.9
960	124.5	1100	116.3
970	123.9	1110	115.7
980	123.3	1120	115.1
990	122.7	1130	114.5
1000	122.1	1140	114.0
1010	121.5	1150	113.4
1020	121.0		

References [18,24,29-33].

4. Viscosity (η)

Measurement method: oscillating sphere [106]

$$\eta = 11.038 \times 10^{-2} \exp [4563.9/RT] \quad (4.3)$$

precision: ∿ ± 0.6% uncertainty: ∿ ± 10%

Table 4.3. Viscosity from equation (4.3)

T (K)	η (cp)	T (K)	η (cp)
900	1.417	1010	1.073
910	1.377	1020	1.049
920	1.340	1030	1.027
930	1.305	1040	1.005
940	1.271	1050	0.984
950	1.239	1060	0.964
960	1.208	1070	0.944
970	1.178	1080	0.926
980	1.150	1090	0.908
990	1.123	1100	0.891
1000	1.098	1110	0.874

References [13,34-40,106].

5. Electrical Conductance (κ)

Measurement method: ac technique [3,19]

$$\kappa = -2.0647 + 12.1271 \times 10^{-3}T - 3.7641 \times 10^{-6}T^2 \quad (4.4)$$

precision: ∿ ± 0.05% uncertainty: ∿ ± 2.5%

Table 4.4. Electrical conductance from equation (4.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
910	5.854	990	6.252
920	5.906	1000	6.298
930	5.958	1010	6.344
940	6.009	1020	6.389
950	6.059	1030	6.433
960	6.108	1040	6.476
970	6.157	1050	6.519
980	6.205		

References [3,12,15,17,19,20,24,25,27,35,37,41-51].

6. Safety and Hazards

A. Hazard rating [52-54]

(i) Toxicity - slight

(ii) Vapor pressure: at m.pt. (610°C), ∿ 25 x 10^{-2}mm; at 780°C, ∿ 1 mm

B. Disaster hazards [52,55-57]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides evolve highly toxic chloride fumes when heated to decomposition, or contacted with acids.

References [52-57].

7. Corrosion

Table 4.5. Corrosion studies from primary research literature

Studies	References
Mg, Ni, Zr, Ti	59
Ti, Zr, Hf, $ThCl_4$	60
Armco Fe	58,61
Solubility of metal oxides (Ni, Ca, Zn, Mg)	59,62
Thermodynamics of corrosion	59,63,64
Corrosion - annotated biblio.	65
Electrochemical aspects	66
Reviews: corrosion - molten salts	67-69

References [58-69].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in LiCl as solvent

Li^+, Cl^-, Na^+, Rb^+, Cs^+, Pb^{2+}, Ag^+, Zr^{2+}, Mo^{3+}, Cl_2

precision: in table 4.6.2 uncertainty: in table 4.6.1

Table 4.6.1. Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
capillary	∿±20%	Li^+, Cl^-, Na^+, Rb^+, Cs^+
chronopotentiometry	∿±10%	Pb^{2+}, Ag^+, Zr^{2+}, Mo^{3+}
Faradaic impedance	∿±50%	Cl_2

Equation:

$$D = A \exp[-E/RT] \quad (4.5)$$

For values of eq. parameters and precisions: see table 4.6.2.

Table 4.6.2. Parameters of diffusion equation (4.5), precisions, and recommended study

Species	A x 10^3 ($cm^2 sec^{-1}$)	E ($cal\ mol^{-1}$)	Temp. range (K)	Precision	Recommended study
Li^+	linear equation		883-1033		72
Cl^-	linear equation		883-1033		72
Na^+	2.10	5850	928-1085	∿±1.5%	75
Rb^+	2.06	6740	928-1091	∿±3.5%	75
Cs^+	0.93	6440	925-1089	∿±4%	75
Pb^{2+}	2.74	7479	903-1150	∿±3%	76
Ag^+	2.46	5516	911-1089	∿±2%	71
Zr^{2+}	2.95	7596	973-1105	∿±5%	70
Mo^{3+}	1.89	7194	935-1083	∿±6%	74, 78
Cl_2	1.09 x 10^{-7}	-32,211	935-1100	∿±26%	77

No entry in precision column indicates estimates not possible since results were reported as equations only

For Li^+, $D_{Li^+} = [10.6 + 0.0307\ (T-883)]x10^{-5}$; for Cl^-, $D_{Cl^-} = [5.8+0.0117(T-883)]x10^{-5}$

Table 4.6.3. Self-diffusion coefficients from equations in table 4.6.2

T (K)	D_{Li^+} x 10^5 ($cm^2 sec^{-1}$)	D_{Cl^-} x 10^5 ($cm^2 sec^{-1}$)
880	9.91	5.76
900	11.12	6.00
920	11.74	6.23
940	12.35	6.47
960	12.96	6.70
980	13.58	6.93
1000	14.19	7.17
1020	14.81	7.40
1040	15.42	7.64

For numerical values of other diffusing species: see table 4.6.4. (next page)

References: Li^+, 72; Cl^-, 72; Na^+, 75; Rb^+, 75; Cs^+, 75; Pb^{2+}, 76, 79; Ag^+, 71; Zr^{2+}, 70; Mo^{3+}, 74, 78; Cl_2, 77.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [80]

Table 4.7. Heat of Fusion

ΔH_f° ($kcal\ mol^{-1}$)	Uncertainty
4.76	∿ ± 1%

References [2,10,80-82].

Table 4.6.4. Diffusion coefficients, D x 10^5 (cm^2 sec^{-1}), from equations in table 4.6.2

T (K)	Na^+	Rb^+	Cs^+	Pb^{2+}	Ag^+	Zr^{2+}	Mo^{3+}	Cl_2
900				4.18				
910				4.38	11.64			
930	8.86	5.37	2.85	4.79	12.43		3.85	
950	9.47	5.80	3.07	5.21	13.24		4.18	280.5
970	10.09	6.24	3.29	5.66	14.06	5.73	4.52	197.3
990	10.73	6.70	3.52	6.12	14.90	6.21	4.88	140.8
1010	11.38	7.17	3.76	6.60	15.75	6.70	5.24	101.8
1030	12.05	7.65	4.00	7.09	16.61	7.21	5.62	74.5
1050	12.72	8.15	4.25	7.60	17.49	7.74	6.01	55.2
1070	13.40	8.65	4.50	8.13	18.37	8.28	6.41	41.4
1090	14.10	9.17	4.76	8.67	19.27	8.84	6.82	
1110				9.23		9.42		
1130				9.80				
1150				10.38				

10. Heat Capacity (C_p)

Measurement method: drop calorimetry + averaged [10,83,84]

$$C_p = 17.535 - 2.26 \times 10^{-3} T \quad (4.6)$$

precision: ± 0.1% uncertainty: ∿ ± 2%

Table 4.8. Heat capacity from equation (4.6)

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
900	15.501	1060	15.139
920	15.456	1080	15.094
940	15.411	1100	15.049
960	15.365	1120	15.004
980	15.320	1140	14.959
1000	15.275	1160	14.913
1020	15.230	1180	14.868
1040	15.185	1200	14.823

References [10,83-84].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [85]

Table 4.9. Volume change on melting

$(\Delta V_f / V_s)$	Uncertainty
26.2%	∿ ± 2%

References [85].

12. *Vapor Pressure (p_{vap})*

Measurement method: effusion [89]; Rodebush [92]

$\log p = 8.2848 - 8741/T$ (4.7)

precision: ∿ ± 1.20% uncertainty: ∿ ± 5%

Table 4.10. Vapor pressure from equation (4.7)

T (K)	p (mm)	T (K)	p (mm)
890	0.029	1140	4.14
900	0.037	1150	4.83
910	0.048	1160	5.62
920	0.061	1170	6.51
930	0.077	1180	7.54
940	0.097	1190	8.70
950	0.121	1200	10.01
960	0.151	1210	11.50
970	0.188	1220	13.18
980	0.232	1230	15.08
990	0.285	1240	17.20
1000	0.350	1250	19.59
1010	0.427	1260	22.26
1020	0.519	1270	25.24
1030	0.629	1280	28.57
1040	0.759	1290	32.27
1050	0.912	1300	36.39
1060	1.09	1310	40.95
1070	1.31	1320	46.01
1080	1.55	1330	51.60
1090	1.84	1340	57.77
1100	2.18	1350	64.56
1110	2.57	1360	72.04
1120	3.02	1370	80.26
1130	3.54		

References [86-93].

13. *Thermal Conductivity (liquid) (λ_ℓ)*

Measurement method: transient hot wire [94]

precision: not estimated uncertainty: ∿ ± 20%

Table 4.11. Thermal conductivity of melt

T (K)	$\lambda \times 10^4$ (cal $cm^{-1} sec^{-1} K^{-1}$)
943	10.88
1043	11.55

References [94-96].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: modified hot wire [96]

precision: not estimated uncertainty: ∿ ± 10%

Table 4.12. Thermal conductivity of solid

T (K)	$\lambda \times 10^4$ (cal cm^{-1} $sec^{-1}K^{-1}$)
823 to m. pt.	36.07

References [96].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [97]

Table 4.13. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
13.8	∿ ± 1%

References [7,80,97-105].

16. References

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V. Sodium Chloride: NaCl

1. *Melting Temperature (T_m)*

Melting point:
800° ± 2°C [4]

References [1-16].

2. *Density (ρ)*

Measurement method: Archimedean technique [14]

$$\rho = 2.1393 - 5.430 \times 10^{-4} T \quad (5.1)$$

precision: ± 0.1% uncertainty: ∿ ± 0.5%

Table 5.1. Densities from equation (5.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1080	1.553	1190	1.493
1090	1.547	1200	1.488
1100	1.542	1210	1.483
1110	1.537	1220	1.477
1120	1.531	1230	1.471
1130	1.526	1240	1.466
1140	1.520	1250	1.461
1150	1.515	1260	1.455
1160	1.509	1270	1.450
1170	1.504	1280	1.444
1180	1.499	1290	1.439

References [14,17-45].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [46]

$$\gamma = 191.4 - 7.19 \times 10^{-2} T \quad (5.2)$$

precision: ± 0.2% uncertainty: ∿ ± 1%

Table 5.2. Surface tension from equation (5.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1080	113.5	1170	107.0
1090	112.8	1180	106.3
1100	112.1	1190	105.6
1110	111.3	1200	104.9
1120	110.6	1210	104.1
1130	109.9	1220	103.4
1140	109.2	1230	102.7
1150	108.5	1240	102.0
1160	107.7	1250	101.3

References [10,37,46-57].

4. Viscosity (η)

Measurement method: oscillating cylinder [201]

$$\eta = 8.931 \times 10^{-2} \exp [5248.1/RT] \quad (5.3)$$

precision: ± 0.05% uncertainty: ∿ ± 3%

Table 5.3. Viscosity from equation (5.3)

T (K)	η (cp)	T (K)	η (cp)
1090	1.008	1150	0.888
1100	0.986	1160	0.871
1110	0.965	1170	0.854
1120	0.944	1180	0.838
1130	0.925	1190	0.822
1140	0.906	1200	0.807

The above viscosities are based on recent results from Trondheim (H. A. Øye, private communication to G. J. Janz (1978), see [201]) and receive additional support from work in progress at Bucharest (S. Zuca, private communication to G. J. Janz (1978)). These values supersede the data reference base [45]. Earlier values are as much as 40% too high at 1090K and this departure decreases uniformly to ∿ 10% at 1240K.

References [45,58-67,200,201].

5. Electrical Conductance (κ)

Measurement method: ac technique [1]

$$\kappa = -4.0896 + 1.1528 \times 10^{-2} T - 4.0534 \times 10^{-6} T^2 \quad (5.4)$$

precision: ∿ ± 0.27% uncertainty: ∿ ± 2%

Table 5.4. Electrical conductance from equation (5.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1100	3.687	1200	3.907
1110	3.712	1210	3.925
1120	3.737	1220	3.941
1130	3.761	1230	3.957
1140	3.785	1240	3.973
1150	3.807	1250	3.987
1160	3.820	1260	4.001
1170	3.849	1270	4.013
1180	3.869	1280	4.025
1190	3.889	1290	4.036

References [1,14,20,21,30,32,45,61,65,68-93].

6. Safety and Hazards

A. Hazard rating [94-96]

(i) Very low

(ii) Vapor pressure: at m.pt. (800°C), ∿ 0.34 mm;
at 860°C, ∿ 1 mm

B. Disaster hazards [94,97-99]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) When bulk NaCl is heated at high temperatures, vapor is evolved which is particularly irritating to the eyes; when heated to decomposition or contacted with acids, highly toxic chloride fumes are evolved.

References [94-99].

7. Corrosion

Table 5.5. Corrosion studies from primary research literature

Studies	References
Mo	100
Armco Fe	101-103
NiCr	104
Ti, Zr, Hf, $ThCl_4$	105
Cr	106
Cr, Fe-Cr	107
Ni alloys -	108
Ni-Cr-Al, Ni-Cr-W-Fe, Ni-Cr Mg, Ni, Zr, Ti	109
Au, Pt, MgO, Al_2O_3, Zirconia [NaCl with added Na_2O]	110
Electrochemical aspects of corrosion	111,112
Corrosion - annotated biblio.	113
Thermodynamic redox potentials (diagrammatic analysis)	109,114,115
Reviews: corrosion in molten salts	116-118

References [100-118].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in NaCl as solvent

Na^+, Cl^-, Li^+, K^+, Rb^+, Cs^+, Ca^{2+}, Pb^{2+}, Ag^+, Cd^{2+}, Zr^{2+}, Zr^{4+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Th^{4+}, U^{3+}, U^{4+}, Cl_2, *HCl*.

The italicized species indicate studies with insufficient data-sets for characterization of temperature dependence of diffusion coefficients. For these species, see: table 5.6.5.

precision: in table 5.6.2 uncertainty: in table 5.6.1

Table 5.6.1. Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
capillary	∿ ± 20%	Na^+, Cl^-, Li^+, K^+, Rb^+, Cs^+, Ca^{2+}
chronopotentiometry	∿ ± 10%	Pb^{2+}, Ag^+, Cd^{2+}, Zr^{2+}, Zr^{4+}, Th^{4+}, U^{3+}, U^{4+}, Co^{2+}, Ni^{2+}, Cl_2
rotating disc electrode	∿ ± 20%	Fe^{3+}, HCl, Cl_2

Equation:

$$D = A \exp[-E/RT] \quad (5.5)$$

For values of eq. parameters, and precisions: see table 5.6.2

For numerical values: see tables 5.6.3, 5.6.4, and 5.6.5

References: Na^+, 119-121, 122, 125, 135; Cl^-, 119, 120, 122, 125, 135; Li^+, 121; K^+, 121; Rb^+, 121, 125; Cs^+, 121, 125; Ca^{2+}, 136; Pb^{2+}, 126, 132; Ag^+, 133, 148; Cd^{2+}, 135, 137; Fe^{3+}, 123; Zr^{2+}, 129, 138; Zr^{4+}, 130, 138; Th^{4+}, 128; U^{3+}, 131, 140; U^{4+}, 131; Cl_2, 127, 141 - 143; Co^{2+}, 146; Ni^{2+}, 147; HCl, 124.

9. *Heat of Fusion (ΔH_f°)*

Measurement method: drop calorimetry [12,13]

Table 5.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
6.73	∿ ± 0.5%

References [5,12,13,149,150].

Table 5.6.2. Parameters of diffusion equation (5.5), precisions, and recommended study

Species	A x 10^3 ($cm^2 sec^{-1}$)	E ($cal\ mol^{-1}$)	Temp range (K)	Precision	Recommended study
Na^+	2.1	7140	1090-1295	∿±3%	122
Cl^-	1.9	7430	1100-1310	∿±3%	122
Li^+	1.38	5450	1090-1250	∿±2.5%	121
K^+	1.92	6780	1100-1240	∿±2.3%	121
Rb^+	2.04	7140	1105-1250	∿±3.6%	121
Cs^+	3.57	8620	1100-1250	∿±4%	121
Ca^{2+}	2.26	8270	1110-1220	∿±0.04%	136
Pb^{2+}	3.06	8492	1085-1190	∿±1.3%	126
Ag^+	4.66	8404	1095-1190	∿±1.4%	133
Cd^{2+}	2.97	8055	1100-1155	∿±3%	137
Fe^{3+}	22.9	13800	1120-1215	∿±0.08%	123
Zr^{2+}	4.46	8910	960-1215		129,138
Zr^{4+}	3.63	9335	1070-1220		130,138
Th^{4+}	7.27	10666	965-1210		128
U^{3+}	2.19	7733	1085-1205		140
U^{4+}	3.80	9335	920-1205		131
Cl_2	2.02 x 10^{-2}	-7554	1100-1225	∿±4.6%	141,143

No entry in precision column indicates estimates not possible, since results were reported as equations only.

Table 5.6.3. Self-diffusion coefficients from equations in table 5.6.2

T (K)	D_{Na^+} x 10^5 ($cm^2 sec^{-1}$)	D_{Cl^-} x 10^5 ($cm^2 sec^{-1}$)
1090	7.77	
1100	8.01	6.35
1110	8.25	6.54
1120	8.49	6.74
1140	8.99	7.15
1160	9.48	7.57
1180	9.99	7.99
1200	10.51	8.42
1220	11.04	8.86
1240	11.58	9.31
1260	12.12	9.77
1280	12.68	10.23
1300	13.24	10.70
1310		10.94

Table 5.6.4. Diffusion coefficients, D x 10^5 (cm^2sec^{-1}), from equations in table 5.6.2

T (K)	Li^+	K^+	Rb^+	Cs^+	Ca^{2+}	Pb^{2+}	Ag^+	Cd^{2+}	Fe^{3+}	Zr^{2+}	Zr^{4+}	Th^{4+}	U^{3+}	U^{4+}	Cl_2
920														2.30	
940														2.57	
960									4.18			2.71		2.85	
980									4.59			3.04		3.15	
1000									5.03			3.39		3.46	
1020									5.50			3.77		3.80	
1040									5.98			4.17		4.15	
1060									6.49			4.60		4.52	
1080						5.85			7.02	4.69		5.05	5.96	4.90	
1100	11.40	8.63	7.78	6.92		6.29	9.97	7.45	7.57	5.07		5.52	6.37	5.31	63.99
1120	11.92	9.12	8.25	7.42	5.50	6.74	10.67	7.96	8.14	5.47	4.64	6.03	6.78	5.73	60.16
1140	12.44	9.63	8.72	7.94	5.87	7.20	11.41	8.48	8.73	5.89	5.18	6.56	7.21	6.17	56.68
1160	12.97	10.13	9.21	8.48	6.25	7.69	12.16	9.02	9.34	6.32	5.75	7.11	7.65	6.62	53.51
1180	13.50	10.65	9.71	9.04	6.64	8.18	12.93		9.98	6.77	6.36	7.69	8.09	7.09	50.62
1200	14.04	11.18	10.21	9.61	7.04				10.63	7.24	7.02	8.30	8.55	7.58	47.97
1220	14.57	11.71	10.73	10.19	7.46				11.30	7.72	7.72				45.55
1240	15.11	12.25	11.25	10.80											
1250	15.38		11.51	11.10											

Table 5.6.5. Diffusion coefficients for species not included in tables 5.6.3 and 5.6.4

Species	T (K)	D x 10^5 (cm^2sec^{-1})	Recommended study
Co^{2+}	1079	2.12	146
Ni^{2+}	1078	2.81	147
HCl	1148	31.0	
	1173	25.0	124
	1223	17.0	

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [13]

$$C_p = 25.24 - 7.52 \times 10^{-3}T \quad (5.6)$$

precision: ∿ ± 0.1% uncertainty: ∿ ± 0.5%

Table 5.8. Heat capacity from equation (5.6)

T (K)	C_p (cal $K^{-1}mol^{-1}$)	T (K)	C_p (cal $K^{-1}mol^{-1}$)
1100	16.97	1200	16.22
1120	16.82	1220	16.07
1140	16.67	1240	15.92
1160	16.52	1260	15.76
1180	16.37	1280	15.61
		1300	15.46

References [13,151-153].

11. Volume Change on Melting (ΔV_f)

Measurement method: densities [26]

Table 5.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
26.06%	∿ ± 0.3%

References [23,26,154-160].

12. Vapor Pressure (p_{vap})

Measurement methods: boiling point [163]; Rodebush-Dixon [165].

$$\log p = 8.4459 - 9565/T \quad (5.7)$$

precision: ∿ ± 0.6% uncertainty: ∿ ± 5%

Table 5.10. Vapor pressure from equation (5.7)

T (K)	p (mm)	T (K)	p (mm)
1250	6.22	1400	41.1
1260	7.16	1410	45.9
1270	8.21	1420	51.3
1280	9.40	1430	57.2
1290	10.7	1440	63.6
1300	12.3	1450	70.7
1310	13.9	1460	78.4
1320	15.8	1470	86.9
1330	18.0	1480	96.2
1340	20.3	1490	106.3
1350	22.9	1500	117.3
1360	25.9	1510	129.3
1370	29.1	1520	142.3
1380	32.7	1530	156.4
1390	36.7		

References [161-170].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: coaxial cylinder steady state [173]

$$\lambda = 1.868 \times 10^{-3} + 4.73 \times 10^{-7} T \quad (5.8)$$

precision: not estimated uncertainty: ∿ ± 20%

Results were reported in graphical form only.

Table 5.11. Thermal conductivity of melt from equation (5.8)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
1100	23.88	1160	24.17
1110	23.93	1170	24.21
1120	23.98	1180	24.26
1130	24.02	1190	24.31
1140	24.07	1200	24.36
1150	24.12		

Eq. obtained by fitting the interpolated data from the graphical presentation

References [171-173].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: not cited [180]

precision: not estimated uncertainty: not estimated

Insufficient information for estimate of precision and uncertainty

Table 5.12. Thermal conductivity of solid

T (K)	$\lambda \times 10^3$ (cal $cm^{-1} sec^{-1} K^{-1}$)
80	84.0
100	62.4
120	47.5
140	38.0
160	32.4
180	28.5
200	25.6
220	23.2
240	21.1
260	19.1
280	17.4
300	15.8
320	14.5
340	13.6
360	12.9
380	12.2
400	11.6
420	11.0
440	10.5
460	9.6

References [174-184].

15. Cryoscopic Constant (k_f)

Measurement method: cryoscopy; and calc'd [185,186].

Table 5.13. Cryoscopic constant

k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
20.0	∿ ± 0.5%

References [185-199].

16. References

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VI. Potassium Chloride: KCl

1. *Melting Temperature (T_m)*

Melting point:
770° ± 1°C [4,9]

References [1-17].

2. *Density (ρ)*

Measurement method: Archimedean technique [2]

$$\rho = 2.1359 - 5.831 \times 10^{-4}T \quad (6.1)$$

precision: ± 0.5% uncertainty: ∿ ± 0.5%

Table 6.1. Densities from equation (6.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1060	1.5178	1130	1.4770
1070	1.5120	1140	1.4712
1080	1.5062	1150	1.4653
1090	1.5003	1160	1.4595
1100	1.4945	1170	1.4537
1110	1.4887	1180	1.4478
1120	1.4828	1190	1.4420
		1200	1.4362

References [2,3,6,8,10-12,14,16-49].

3. *Surface Tension (γ)*

Measurement method: derived from ref. 20, 50, 51, 52, 57, 59, 61, 62 [56]

$$\gamma = 179.1168 - 7.6026 \times 10^{-2}T \quad (6.2)$$

precision: ∿ ± 0.26% uncertainty: ∿ ± 0.5%

Table 6.2. Surface tension from equation (6.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1080	97.01	1190	88.65
1090	96.25	1200	87.89
1100	95.49	1210	87.13
1110	94.73	1220	86.37
1120	93.97	1230	85.61
1130	93.21	1240	84.84
1140	92.45	1250	84.08
1150	91.69	1260	83.32
1160	90.93	1270	82.56
1170	90.17	1280	81.80
1180	89.41		

References [29,35,50-64].

4. Viscosity (η)

Measurement method: oscillating sphere [226]

$$\eta = 7.32 \times 10^{-2} \exp [5601.7/RT] \quad (6.3)$$

precision: ∿ ± 0.6% uncertainty: ∿ ± 3%

Table 6.3. Viscosity from equation (6.3)

T (K)	η (cp)	T (K)	η (cp)
1070	1.020	1130	0.887
1080	0.996	1140	0.868
1090	0.972	1150	0.850
1100	0.950	1160	0.832
1110	0.928	1170	0.815
1120	0.907		

References [35,37,43,65-72,226].

5. Electrical Conductance (κ)

Measurement method: ac technique [2]

$$\kappa = -3.99005 + 9.0222 \times 10^{-3}T - 3.000 \times 10^{-6}T^2 \quad (6.4)$$

precision: ± 0.41% uncertainty: ∿ ± 1%

Table 6.4. Electrical conductance from equation (6.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1060	2.203	1140	2.396
1070	2.229	1150	2.418
1080	2.255	1160	2.439
1090	2.280	1170	2.459
1100	2.304	1180	2.479
1110	2.328	1190	2.498
1120	2.352	1200	2.517
1130	2.374		

References [2,3,6-8,10,14,15,20-22,32,34,47,71,73-112].

6 Safety and Hazards

A. Hazard rating [113,114]

(i) Very low

(ii) Vapor pressure: at m. pt. (770°C), ∿ 0.42 mm; at 820°C, ∿ 1 mm

B. Disaster hazards [116-118]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air

(ii) Chlorides evolve highly toxic fumes when heated to decomposition, or contacted with acids

References [113-118].

7. *Corrosion*

Table 6.5. Corrosion studies from primary research literature

Studies	References
Armco Fe; various steels	119,120,125,127
Cr	121
Cr, Fe-Cr	122
Mg, Ni, Zr, Ti	123
Ti, Zr, Hf, $ThCl_4$	124
Solubility of oxides (Ni, Ca, Zn, Mg)	123,128
Electrochemical aspects	129
Corrosion - annotated biblio.	130
Thermodynamic approach	123,131,132
Reviews: corrosion in molten salts	133-135

References [119-135].

8. *Diffusion*

Measurement method: cited in tabulations

List of diffusing species investigated in KCl as solvent

K^+, Cl^-, Na^+, Rb^+, Cs^+, Ca^{2+}, Pb^{2+}, *Cu^+*, Ag^+, *Au^+*, Cd^{2+}, Zr^{2+}, Zr^{4+}, Mo^{3+}, Fe^{3+}, *Co^{2+}*, *Ni^{2+}*, Th^{4+}, U^{3+}, U^{4+}, *Cl_2*, *HCl*

The italicized species indicate studies with insufficient data-sets for characterization of temperature dependence of diffusion coefficients. For these species, see table 6.6.5.

precision: in table 6.6.2 uncertainty: in table 6.6.1

Table 6.6.1. Diffusion techniques, uncertainties and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
capillary	∿ ± 20%	K^+, Cl^-, Na^+, Rb^+, Cs^+, Ca^{2+}
chronopotentiometry	∿ ± 10%	Pb^{2+}, Ag^+, Cd^{2+}, Zr^{2+}, Zr^{4+}, Mo^{3+}, Th^{4+}, U^{3+}, U^{4+}, Cl_2, Cu^+, Au^+, Co^{2+}, Ni^{2+}
rotating disc electrode	∿ ± 20%	Fe^{3+}, HCl

Equation:

$$D = A \exp[-E/RT] \qquad (6.5)$$

Table 6.6.2. Parameters of diffusion equation (6.5), precisions, and recommended study

Species	A x 10^3 ($cm^2 sec^{-1}$)	E ($cal\ mol^{-1}$)	Temp. range (K)	Precision	Recommended study
K^+	1.80	6880	1070 - 1260		149
Cl^-	1.80	7130	1065 - 1260		149
Na^+	3.03	7820	1070 - 1275		136
Rb^+	2.06	7070	1070 - 1275		136
Cs^+	1.09	5600	1070 - 1275		136
Ca^{2+}	1.29	7920	1055 - 1175	∿±0.2%	165
Pb^{2+}	2.46	8165	1065 - 1175	∿±1.9%	151
Ag^+	3.30	7709	1060 - 1190	∿±2.4%	147
Cd^{2+}	1.12	6209	1050 - 1135	∿±2.4%	156
Zr^{2+}	9.75	11500	965 - 1210		144
Zr^{4+}	7.94	11897	1070 - 1195		145
Mo^{3+}	6.64	10874	900 - 1100		157
Fe^{3+}	0.213	18830	1123 - 1213	∿±0.1%	139
Th^{4+}	7.46	11458	1000 - 1200		143
U^{3+}	2.45	8877	1050 - 1210		161
U^{4+}	3.09	10067	920 - 1205		146
Cl_2	data set does not fit either exponential or liner equations				

No entry in precision column indicates estimates not possible since results were reported as equations only.

Data set for Cl_2 in table 6.6.5

Table 6.6.3. Self-diffusion coefficients

T (K)	$D_{K^+} \times 10^5$ ($cm^2 sec^{-1}$)	$D_{Cl^-} \times 10^5$ ($cm^2 sec^{-1}$)
1060		6.10
1070	7.08	6.29
1080	7.29	6.49
1100	7.73	6.89
1120	8.18	7.31
1140	8.63	7.73
1160		8.16
1180	9.57	8.60
1200	10.05	9.05
1220	10.54	9.50
1240	11.03	9.97
1260	11.53	10.43

Table 6.6.4. Diffusion coefficients, D x 10^5 ($cm^2 sec^{-1}$), from equations in table 6.6.2

T (K)	Na^+	Rb^+	Cs^+	Ca^{2+}	Pb^{2+}	Ag^+	Cd^{2+}	Zr^{2+}	Zr^{4+}	Mo^{3+}	Fe^{3+}	Th^{4+}	U^{3+}	U^{4+}
900										1.52				
920										1.73				1.25
940										1.97				1.41
960								2.35		2.22				1.58
980								2.66		2.49				1.76
1000								2.99		2.79		2.34		1.95
1020								3.35		3.11		2.62		2.15
1040								3.73		3.44		2.92		2.37
1050				2.90			5.71	3.94		3.62		3.07	3.48	2.48
1060				3.00	5.10	8.49	5.87	4.15		3.80		3.24	3.62	2.60
1070	7.66	7.41	7.83	3.11	5.29	8.79	6.04	4.36	2.95	3.99		3.41	3.77	2.71
1080	7.92	7.64	8.02	3.22	5.48	9.09	6.20	4.59	3.11	4.18		3.58	3.91	2.84
1100	8.47	8.11	8.41	3.44	5.87	9.70	6.54	5.06	3.44	4.59		3.95	4.22	3.09
1120	9.02	8.59	8.80	3.67	6.27	10.33	6.88	5.56	3.79		4.51	4.33	4.54	3.35
1140	9.60	9.09	9.20	3.91	6.69	10.98	7.22	6.08	4.16		5.23	4.74	4.87	3.63
1160	10.19	9.59	9.60	4.15	7.12	11.64		6.64	4.55		6.03	5.17	5.21	3.92
1180	10.79	10.10	10.00	4.40	7.56	12.32		7.23	4.97		6.93	5.63	5.56	4.22
1190	11.10	10.36	10.21			12.66		7.53	5.18		7.41	5.87	5.74	4.38
1200	11.41	10.62	10.41					7.84	5.41		7.92	6.11	5.92	4.53
1210	11.72	10.88	10.61					8.16			8.45		6.11	4.69
1220	12.04	11.15	10.82											
1240	12.68	11.69	11.23											
1260	13.33	12.23	11.64											
1280	14.00	12.78	12.06											

Table 6.6.5. Diffusion coefficients for species not included in table 6.6.3 and 6.6.4

Species	T (K)	D x 10^5 ($cm^2 sec^{-1}$)	Recommended study
Cu^+	1088	2.14	141
Au^+	1088	2.20	141
Co^{2+}	1079	1.86	166
Ni^{2+}	1078	2.35	167
HCl	1123	31.0	140,163
	1153	35.0	
	1183	37.0	
Cl_2	1085	18.0	155
	1110	21.7	
	1117	23.2	
	1143	23.5	
	1173	24.0	

References K^+, 149; Cl^-, 149; Na^+, 136, 137, 162; Rb^+, 136; Cs^+, 136; Ca^{2+}, 165; Pb^{2+}, 151, 152; Ag^+, 141, 147, 148; Cd^{2+}, 156; Zr^{2+}, 144, 158; Zr^{4+}, 145, 158, 159; Mo^{3+}, 148, 150, 157; Fe^{3+}, 139; Th^{4+}, 143, 160; U^{3+}, 161; U^{4+}, 146; Cl_2, 138, 142, 154, 155, 164; Cu^+, 141; Au^+, 141; Co^{2+}, 166; Ni^{2+}, 167; HCl, 140, 163.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [169]

Table 6.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
6.34	∿ ± 1%

References [4,5,169-173].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [174]

Table 6.8. Heat capacity

C_p (cal $K^{-1} mol^{-1}$)	Temp. range (K)	Uncertainty
17.58	1050-1173	∿ ± 18%

References [172,174-176].

11. Volume Change on Melting (ΔV_f)

Measurement method: densities [24]

Table 6.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
22.27%	∿ ± 0.4%

References [24,177-184].

12. Vapor Pressure (p_{vap})

Measurement methods: transpiration [185]; boiling pt. [187]; Rodebush-Dixon [189]; Rodebush [196]

$$\log p = 8.2800 - 9032/T \quad (6.6)$$

precision: ∿ ± 0.7% uncertainty: ∿ ± 5%

Table 6.10. Vapor pressure from equation (6.6)

T (K)	p (mm)	T (K)	p (mm)
1180	4.22	1360	43.5
1190	4.90	1370	48.7
1200	5.67	1380	54.3
1210	6.54	1390	60.6
1220	7.53	1400	67.4
1230	8.65	1410	74.9
1240	9.91	1420	83.1
1250	11.3	1430	92.0
1260	12.9	1440	101.8
1270	14.7	1450	112.5
1280	16.7	1460	124.1
1290	19.0	1470	136.7
1300	21.5	1480	150.4
1310	24.3	1490	165.3
1320	27.4	1500	181.4
1330	30.8	1510	198.9
1340	34.7	1520	217.7
1350	38.9	1530	238.1

References [185-198].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: coaxial cylinder, modified hot wire [202,203].

$$\lambda = -23.43 \times 10^{-4} + 4.103 \times 10^{-6} T \quad (6.7)$$

precision: not estimated uncertainty: ∿ ± 20%

Results were reported in graphical or equation forms only.

Eq. obtained by fitting the mean values of [202] and [203]. For [202], values were interpolated from the graphical presentation.

For numerical values: see table 6.11.

Table 6.11. Thermal conductivity of melt from equation (6.7)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
1050	19.63	1130	22.93
1060	20.06	1140	23.34
1070	20.47	1150	23.75
1080	20.88	1160	24.16
1090	21.29	1170	24.58
1100	21.70	1180	24.99
1110	22.11	1190	25.40
1120	22.52	1200	25.81

References [199-205].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: not cited [208]

precision: not estimated uncertainty: not estimated

Insufficient information for estimate of precision and uncertainty

Table 6.12. Thermal conductivity of solid

T (K)	$\lambda \times 10^3$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^3$ (cal $cm^{-1}sec^{-1}K^{-1}$)
85	80.0	280	17.2
100	64.0	300	15.7
120	50.0	320	14.4
140	41.0	340	13.4
160	34.4	360	12.4
180	30.0	380	11.7
200	26.6	400	11.1
220	23.5	420	10.6
240	21.0	440	10.1
260	19.0	460	9.2

References [206-213].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [214]

Table 6.13. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
25.4	∿ ± 1%

References [169,214-225].

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VII. Magnesium Chloride: $MgCl_2$

1. *Melting Temperature (T_m)*

Melting point:
714° ± 2°C [3,12]

References [1-15].

2. *Density (ρ)*

Measurement method: Archimedean technique [16]

$$\rho = 1.976 - 3.02 \times 10^{-4}T \quad (7.1)$$

precision: ± 0.15% uncertainty: ∿ ± 0.2%

Table 7.1. Densities from equation (7.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1000	(1.675)	1120	1.638
1020	1.668	1140	1.632
1040	1.662	1160	1.626
1060	1.656	1180	(1.620)
1180	1.650	1200	(1.614)
1100	1.644	1220	(1.608)
		1240	(1.602)

Values in parentheses are extrapolated.

References [2,7-10,16-21].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [14]

$$\gamma = 76.73 - 1.0 \times 10^{-2}T \quad (7.2)$$

precision: ∿ ± 0.4% uncertainty: ∿ ± 0.8%

Table 7.2. Surface tension from equation (7.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
990	66.8	1110	65.6
1000	66.7	1120	65.5
1010	66.6	1130	65.4
1020	66.5	1140	65.3
1030	66.4	1150	65.2
1040	66.3	1160	65.1
1050	66.2	1170	65.0
1060	66.1	1180	64.9
1070	66.0	1190	64.8
1080	65.9	1200	64.7
1090	65.8	1210	64.6
1100	65.7		

References [1,14,22-25].

Viscosity (η)

Measurement method: oscillating sphere [26,27]

$$\eta = 14.903 - 2.039 \times 10^{-2}T + 7.625 \times 10^{-6}T^2 \quad (7.3)$$

precision: ± 2.29% uncertainty: ∿ ± 5%

Equation (7.3) averaged from [26-27]

Table 7.3. Viscosity from equation (7.3)

T (K)	η (cp)	T (K)	η (cp)
1000	2.14	1080	1.78
1010	2.09	1090	1.74
1020	2.04	1100	1.70
1030	1.99	1110	1.66
1040	1.94	1120	1.63
1050	1.90	1130	1.60
1060	1.86	1140	1.57
1070	1.82		

References [26,27].

Electrical Conductance (κ)

Measurement method: ac technique [11]

$$\kappa = -0.605419 + 1.34949 \times 10^{-3}T + 2.94264 \times 10^{-7}T^2 \quad (7.4)$$

precision: ± 0.24% uncertainty: ∿ ± 2%

Table 7.4. Electrical conductance from equation (7.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1000	1.038	1120	1.275
1020	1.077	1140	1.315
1040	1.116	1160	1.356
1060	1.156	1180	1.397
1080	1.195	1200	1.438
1100	1.235	1220	1.479
		1240	1.520

References [5,7,11,24,26,28-32].

Safety and Hazards

A. Hazard rating [33-35]

(i) Slight

(ii) Vapor pressure: at m.pt. (714°C) ∿ 0.11 mm; at 820°C, ∿ 1 mm

B. Disaster hazards [33,36-38]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides evolve highly toxic fumes when heated to decomposition, or contacted with acids.

References [33-38].

7. Corrosion

Table 7.5. Corrosion studies from primary research literature

Studies	References
Zr	39
Mg, Ni, Zr, Ti	40
Ti, Zr, Hf, $ThCl_4$	41
Thermodynamics of corrosion	41-43
Electrochemical approach	44,45
Corrosion in molten salts/ annotated biblio.	46

References [39-46].

8. Diffusion

No diffusion studies reported

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [6]

Table 7.6. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
10.30	∿ ± 0.5%

References [6,47,48].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [6,49]

Table 7.7. Heat capacity

C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
22.1	987-1500	∿ ± 0.5%

References [6,12,16,47,49].

11. Volume Change on Melting (ΔV_f)

Measurement method: densities [16]

Table 7.8. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
30.46%	∿ ± 2%

References [16,50].

12. Vapor Pressure (p_{vap})

Measurement method: boiling pt. [52]

$$\log p = -11735/T - 4.076 \log T + 23.15 \quad (7.5)$$

precision: ∿ ± 0.5% uncertainty: ∿ ± 5%

Table 7.9. Vapor pressure from equation (7.5)

T (K)	p (mm)	T (K)	p (mm)
1210	7.69	1320	34.70
1220	8.94	1330	39.25
1230	10.35	1340	44.31
1240	11.95	1350	49.91
1250	13.77	1360	56.11
1260	15.83	1370	62.95
1270	18.14	1380	70.51
1280	20.75	1390	78.82
1290	23.68	1400	87.95
1300	26.95	1410	97.97
1310	30.62		

References [51-53].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: constriction technique [54]

$$\lambda = -8.571 \times 10^{-3} + 11.231 \times 10^{-6} T \quad (7.6)$$

precision: not estimated uncertainty: ∿ ± 20%

Results were reported in graphical or equation forms only.

Table 7.10. Thermal conductivity of melt from equation (7.6)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
1020	28.85	1080	35.58
1030	29.97	1090	36.71
1040	31.09	1100	37.83
1050	32.22	1110	38.95
1060	33.34	1120	40.08
1070	34.46		

Reference [54].

Thermal Conductivity (solid) (λ_s)

Measurement method: constriction technique [54]

precision: not estimated uncertainty: ∿ ± 10%

Table 7.11. Thermal conductivity of solid

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
373	43.4	673	10.5
473	25.3	773	10.5
573	14.3	873	15.5
		923	20.0

Sole investigation; values interpolated from the graphical presentation.

Reference [54].

Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [55]

Table 7.12. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
17.90	∿ ± 0.5%

References [6,55-57].

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VIII. Calcium Chloride: $CaCl_2$

1. *Melting Temperature (T_m)*

Melting point:
782° ± 5°C [1,2,4,7]

References [1-17].

2. *Density (ρ)*

Measurement method: Archimedean technique [14]

$$\rho = 2.5261 - 4.225 \times 10^{-4}T \quad (8.1)$$

precision: ± 0.2% uncertainty: ∿ ± 0.9%

Table 8.1. Densities from equation (8.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1060	2.0783	1150	2.0402
1070	2.0740	1160	2.0360
1080	2.0698	1170	2.0318
1090	2.0656	1180	2.0276
1100	2.0614	1190	2.0233
1110	2.0571	1200	2.0191
1120	2.0529	1210	2.0149
1130	2.0487	1220	2.0107
1140	2.0445	1230	2.0064

References [14,18-20].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [13]

$$\gamma = 223.79 - 7.28 \times 10^{-2}T \quad (8.2)$$

precision: ± 0.3% uncertainty: ∿ ± 0.5%

Table 8.2. Surface tension from equation (8.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1040	148.1	1130	141.5
1050	147.4	1140	140.8
1060	146.6	1150	140.1
1070	145.9	1160	139.3
1080	145.2	1170	138.6
1090	144.4	1180	137.9
1100	143.7	1190	137.2
1110	143.0	1200	136.4
1120	142.3		

References [13,21,22].

4. *Viscosity:* (η)

Measurement method: oscillating (liquid filled) cylinder [23]

$$\eta = 619.541 - 1.54489\ T + 1.29259 \times 10^{-3} T^2 - 3.61856 \times 10^{-7} T^3 \quad (8.3)$$

precision: ± 3.5% uncertainty: ∿ ± 30%

Table 8.3. Viscosity from equation (8.3)

T (K)	η (cp)	T (K)	η (cp)
1060	3.34	1150	2.03
1070	3.11	1160	1.96
1080	2.90	1170	1.89
1090	2.72	1180	1.83
1100	2.57	1190	1.77
1110	2.43	1200	1.72
1120	2.31	1210	1.66
1130	2.20	1220	1.59
1140	2.11	1230	1.52
		1240	1.44

References [15,23,24].

. *Electrical Conductance* (κ)

Measurement method: ac technique [16]

$$\kappa = 19.628 \exp(-4749/RT) \quad (8.4)$$

precision: ± 0.25% uncertainty: ∿ ± 2.0%

Table 8.4. Electrical conductance from equation (8.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1060	2.059	1150	2.457
1070	2.103	1160	2.501
1080	2.147	1170	2.546
1090	2.191	1180	2.590
1100	2.235	1190	2.634
1110	2.279	1200	2.679
1120	2.324	1210	2.723
1130	2.368	1220	2.768
1140	2.412	1230	2.812

References [14,16,20,25-32].

Safety and Hazards

A. Hazard rating [33-35]

(i) Very low

(ii) Vapor pressure: at m.pt. (782°C), ∿ 2×10^{-4} mm; at 1230°C, ∿ 1 mm

B. Disaster hazards [33,36-38]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides evolve highly toxic fumes when heated to decomposition, or contacted with acids.

References [33-38].

7. Corrosion

Table 8.5. Corrosion studies from primary research literature

Studies	References
Zr	39
Ti, Zr, Hf, $ThCl_4$	40
Pb, Pb-Bi	41
Electrochemical aspects	42,43
Thermodynamic approach	44-46
Corrosion in molten salts/ annotated biblio.	47
Reviews: Corrosion in molten salts	48-50

References [39-50].

8. Diffusion

Measurement method: capillary [51]

List of diffusing species investigated in $CaCl_2$ as solvent

$$Ca^{2+},\ Cl^-$$

precision: not estimated uncertainty: ∿ ± 10%

Data reported in equation form only.

Equations:

$$D = A \exp [-E/RT] \quad (8.5)$$

Table 8.6.1. Parameters of diffusion equation (8.5)

Species	A x 10^3 ($cm^2 sec^{-1}$)	E ($cal\ mol^{-1}$)	Temp. range (K)
Ca^{2+}	0.38	6130	1060-1280
Cl^-	1.90	8860	1060-1290

For numerical values: see table 8.6.2.

References [51,52].

Table 8.6.2. Self-diffusion coefficients from equations in table 8.6.1

T (K)	$D_{Ca^{2+}} \times 10^5$ ($cm^2 sec^{-1}$)	$D_{Cl^-} \times 10^5$ ($cm^2 sec^{-1}$)
1060	2.07	2.83
1080	2.18	3.06
1100	2.30	3.30
1120	2.42	3.55
1140	2.54	3.80
1160	2.66	4.07
1180	2.78	4.34
1200	2.91	4.62
1220	3.03	4.91
1240	3.16	5.21
1260	3.28	5.52
1280	3.41	5.83
1290		5.99

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [1,3,4]

Table 8.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
6.78	∿ ± 0.5%

References [1,3,4].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [1]

$$C_p = 29.08 - 3.48 \times 10^{-3} T \quad (8.6)$$

precision: ± 0.2% uncertainty: ∿ ± 1%

Table 8.8. Heat capacity from equation (8.6)

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
1055	25.41	1260	24.70
1060	25.39	1280	24.63
1080	25.32	1300	24.56
1100	25.25	1320	24.49
1120	25.18	1340	24.42
1140	25.11	1360	24.35
1160	25.04	1380	24.28
1180	24.97	1400	24.21
1200	24.90	1500	23.86
1220	24.83	1600	23.51
1240	24.76	1700	23.16

References [1,4,7].

11. *Volume Change on Melting (ΔV_f)*

Measurement method: capillary technique [54]

Table 8.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
0.9%	∿ ± 15%

References [53-55].

12. *Vapor Pressure (p_{vap})*

Measurement methods: effusion [56]; boiling pt. [57]

$$\log p = 8.4073 - 12622/T \quad (8.7)$$

precision: ∿ ± 3% uncertainty: ∿ ± 10%

Table 8.10. Vapor pressure from equation (8.7)

T (K)	p (mm)	T (K)	p (mm)
1120	0.0014	1420	0.330
1140	0.0022	1440	0.439
1160	0.0034	1460	0.578
1180	0.0051	1480	0.757
1200	0.0077	1500	0.983
1220	0.0115	1520	1.269
1240	0.0169	1540	1.626
1260	0.0245	1560	2.071
1280	0.0352	1580	2.622
1300	0.0499	1600	3.300
1320	0.0700	1620	4.130
1340	0.0973	1640	5.140
1360	0.134	1660	6.363
1380	0.182	1680	7.838
1400	0.246	1700	9.607

References [56-58].

13. *Thermal Conductivity (liquid) (λ_ℓ)*

Measurement method: coaxial cylinder [60]

$$\lambda = -22.88 \times 10^{-2} + 31.18 \times 10^{-5}T - 8.68 \times 10^{-9}T^2 - 7.53 \times 10^{-11}T^3 \quad (8.8)$$

precision: ± 2% uncertainty: ∿ ± 20%

Table 8.11. Thermal conductivity of melt from equation (8.8)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
1070	26.80	1110	36.64
1080	30.03	1120	37.82
1090	32.74	1130	38.47
1100	34.95		

References [59,60].

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [4]

Table 8.12. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
35.5	~ ± 1%

References [1,4,61-63].

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IX. Aluminum Chloride: $AlCl_3$

1. Melting Temperature (T_m)

Melting point:
192° ± 1°C (at 2.3 atm)
sublimes at 180.1°C [4,5]

References [1-5,7-10].

2. Density (ρ)

Measurement method: Archimedean technique [1]

$$\rho = 2.18725 - 5.4045 \times 10^{-4}T - 1.13544 \times 10^{-5}T^2 + 3.04126 \times 10^{-8}T^3 \quad (9.1)$$

precision: ± 0.15% uncertainty: ∿ ± 2%

Table 9.1. Densities from equation (9.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
465	1.287	515	1.169
470	1.277	520	1.155
475	1.266	525	1.142
480	1.256	530	1.127
485	1.243	535	1.113
490	1.231	540	1.098
495	1.219	545	1.082
500	1.207	550	1.066
505	1.195	555	1.050
510	1.182	560	1.033

References [1-3,8,11,12].

3. Surface Tension (γ)

Measurement method: capillary rise [13]

$$\gamma = 42.43 - 7.04 \times 10^{-2}T \quad (9.2)$$

precision: ± 0.4% uncertainty: ∿ ± 1%

Table 9.2. Surface tension from equation (9.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
480	8.64	540	4.41
490	7.93	550	3.71
500	7.23	560	3.01
510	6.53	570	2.30
520	5.82	580	1.60
530	5.12	590	0.89

References [13].

4. Viscosity (η)

Measurement method: oscillating cylinder [6]

$$\eta = 3.2146 - 9.6606 \times 10^{-3}T + 7.4554 \times 10^{-6}T^2 \quad (9.3)$$

precision: ± 0.39% uncertainty: ∿ ± 5%

Table 9.3. Viscosity from equation (9.3)

T (K)	η (cp)	T (K)	η (cp)
470	0.321	520	0.207
480	0.295	530	0.189
490	0.271	540	0.172
500	0.248	550	0.157
510	0.227	560	0.143

References [1-3,6,8,13].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [1-3,8]

$$\kappa = 7.0270 \times 10^{-6} - 3.6646 \times 10^{-8} T + 4.8623 \times 10^{-11} T^2 \quad (9.4)$$

precision: ∿ ± 1.7% uncertainty: ∿ ± 3%

Table 9.4. Electrical conductance from equation (9.4)

T (K)	$\kappa \times 10^7$ ($ohm^{-1}cm^{-1}$)	T (K)	$\kappa \times 10^7$ ($ohm^{-1}cm^{-1}$)
475	5.91	500	8.60
480	6.40	505	9.21
485	6.91	510	9.84
490	7.45	515	10.50
495	8.01		

References [1-3,8,14,15].

6. *Safety and Hazards*

A. Hazard rating [16-18]

(i) Toxicity - severe

(ii) Vapor pressure: sublimes; at 100°C, ∿ 1 mm

B. Disaster hazards [16,19-21]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i/e., explosive expansion of "trapped" air.

(ii) Chlorides evolve highly toxic fumes when heated to decomposition, or contacted with acids. Reacts exothermically with moisture, to evolve HCl fumes.

References [16-21].

7. Corrosion

Table 9.5. Corrosion studies from primary research literature

Studies	References
metals	22
Ca	23
Al	24
Al, Ag, Au, Cu, Mo, Ni, Pd, Ti, Fe, Pt, stainless steel	25
Electrochemical approach	26,27
Thermodynamics of corrosion	28-30
Corrosion, annotated biblio.	31
Reviews	32-34

References [22-34].

8. Diffusion

No diffusion studies reported

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [7]

Table 9.6. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
8.5	∿ ± 3%

References [4,7,35,36].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [7]

Table 9.7. Heat capacity

C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
30	473-504	∿ ± 3%

References [4,7,36].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [37]

Table 9.8. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
83.0%	∿ ± 0.5%

References [37].

12. Vapor Pressure (p_{vap})

Measurement method: isoteniscope [43]

$$\log p = 7.42055 - 1948.55/T \quad (9.5)$$

precision: ∿ ± 0.1% uncertainty: ∿ ± 3%

Table 9.9. Vapor pressure from equation (9.5)

T (K)	p (mm)	T (K)	p (mm)
455	1374	495	3049
460	1530	500	3338
465	1699	505	3648
470	1882	510	3980
475	2081	515	4335
480	2297	520	4714
485	2529	525	5117
490	2779	530	5547

References [38-43].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [44]

Table 9.10. Cryoscopic constant

k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
6.7	∿ ± 3%

References [7,44].

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[18] Vapor pressure, calculated (see p. 99, this work).

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X. Lithium Carbonate: Li_2CO_3

1. *Melting Temperature (T_m)*

Melting point:
723° ± 3°C [1-3,8]

References [1-14].

2. *Density (ρ)*

Measurement method: Archimedean technique [1]

$$\rho = 2.2026 - 3.729 \times 10^{-4} T \quad (10.1)$$

precision: ± 0.1% uncertainty: ∿ ± 0.5%

Table 10.1. Densities from equation (10.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1010	1.8260	1070	1.8036
1020	1.8222	1080	1.7999
1030	1.8185	1090	1.7961
1040	1.8148	1100	1.7924
1050	1.8111	1110	1.7887
1060	1.8073	1120	1.7850

References [1,15].

3. *Surface Tension (γ)*

Measurement method: pin detachment [1]

$$\gamma = 284.59 - 4.06 \times 10^{-2} T \quad (10.2)$$

precision: ± 0.1% uncertainty: ∿ ± 0.3%

Table 10.2 Surface tension from equation (10.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1020	243.2	1080	240.7
1030	242.8	1090	240.3
1040	242.4	1100	239.9
1050	242.0	1110	239.5
1060	241.6	1120	239.1
1070	241.1	1130	238.7

References [1,16].

4. *Viscosity (η)*

Measurement method: oscillating (liquid-filled) cylinder [17]

$$\eta = -5259.12 + 14.8091\ T - 13.8581 \times 10^{-3} T^2 + 4.31294 \times 10^{-6} T^3 \quad (10.3)$$

precision: ∿ ± 3% uncertainty: ∿ ± 30%

Table 10.3. Viscosity from equation (10.3)

T (K)	η (cp)
1050	4.65
1060	4.35
1070	4.02
1080	3.68
1090	3.37
1100	3.11
1110	2.93
1120	2.84

References [17,18].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [1]

$$\kappa = 0.9877 - 1.3529 \times 10^{-3}T + 4.3873 \times 10^{-6}T^2 \quad (10.4)$$

precision: ± 0.007% uncertainty: ∿ ± 1.5%

Table 10.4. Electrical conductance from equation (10.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1010	4.097	1070	4.563
1020	4.172	1080	4.644
1030	4.249	1090	4.726
1040	4.326	1100	4.808
1050	4.404	1110	4.892
1060	4.483	1120	4.976

References [1,19-24].

6. *Safety and Hazards*

A. Hazard rating [25-27]

(i) Inhalation hazard: slight; toxic dose (human): 0.7 mg/kg (oral)

(ii) Vapor pressure: [CO_2 equilibrium dissociation pressure is ∿ 10 mm at approx. 730°C]

$$Li_2CO_3 \rightleftharpoons Li_2O + CO_2 \quad (10.5)$$

B. Disaster hazards [25,28-30]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e. explosive expansion of "trapped" air.

(ii) When heated with CO_2 pressures less than equilibrium dissociation pressures, decomposes to form alkali metal oxide; the toxicology and disaster hazards are the same as those of very caustic solutions, i.e. react with water or steam (exothermic) to form solutions that are markedly aggressive to all body tissues (chemical burns). Lithium carbonate itself is classified as a strong caustic.

References [25-30].

7. Corrosion

Table 10.5. Corrosion studies from primary research literature

Studies	References
Ti alloy	31
Au, Pt, Ag, Ni, Au-Pd	32
Pt, Au, Ag, MgO, BN	33,34
Ag, Co, Ni	35
Metals, alloys	36
Pt, Pd, Rh, Ir (O_2 environment)	37
Ag (O_2 + CO; H_2 + CO_2 environment)	38
Ag (O_2; Li_2CO_3-Li_2O)	14
Pt (N_2; Li_2CO_3-Li_2O)	39,40
Pt, Au (Ar; Li_2CO_3-Li_2O)	41
Ag, Pt, Ni; porcelain, quartz (Li_2CO_3-Li_2O; N_2 atmosphere)	10
Acid-base relationships in molten carbonates	42-46
Hydrolysis (H_2O) reactions	14,44,46,47
Corrosion in molten salts: annotated bibliography	48
Molten carbonates: fuel cells; thermal energy storage; coal gasification; power plant stack gases	49-54

References [10,14,31-54].

8. Diffusion

Measurement method: capillary [55,56]

List of diffusing species investigated in Li_2CO_3 as solvent

Na^+, CO_3^{2-}

precision: ∿ ± 3.5% uncertainty: ∿ ± 10%

Equation:

$$D = A \exp [-E/RT] \quad (10.6)$$

Li_2CO_3

Table 10.6.1. Parameters of diffusion equation (10.6)

Species	A x 10^3 ($cm^2 sec^{-1}$)	E (cal mol^{-1})	Temp. range (K)
Na^+	1.32	9630	1080-1180
CO_3^{2-}	1.35	9740	1120-1265

Table 10.6.2. Diffusion coefficients from equations in table 10.6.1

T (K)	D_{Na^+} x 10^5 ($cm^2 sec^{-1}$)	T (K)	$D_{CO_3^{2-}}$ x 10^5 ($cm^2 sec^{-1}$)
1080	1.48	1120	1.69
1090	1.55	1140	1.83
1100	1.61	1160	1.97
1120	1.74	1180	2.12
1140	1.88	1200	2.27
1160	2.02	1220	2.43
1170	2.10	1240	2.59
		1260	2.76

References [55,56].

9. *Heat of Fusion (ΔH_f°)*

Measurement method: drop calorimetry [11,57]

Table 10.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
9.8	∿ ± 10%

References [11,57,58].

10. *Heat Capacity (C_p)*

Measurement method: drop calorimetry [57]

$$C_p = 30.85 + 13.54 \times 10^{-3} T \quad (10.7)$$

precision: ∿ ± 0,3% uncertainty: ∿ ± 0,5%

Table 10.8. Heat capacity from equation (10.7)

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
1000	44.39	1080	45.47
1010	44.53	1090	45.61
1020	44.66	1100	45.74
1030	44.80	1110	45.88
1040	44.93	1120	46.01
1050	45.07	1130	46.15
1060	45.20	1140	46.29
1070	45.34	1150	46.42

References [57,58].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated; from densities [59]

Table 10.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
6.9%	∿ ± 8%

References [59].

12. Vapor Pressure (p_{vap})

Measurement method: cited with each data set [14,50,60].

No systematic studies of vaporization as "molecular carbonate" have been reported, viz:

$$Li_2CO_{3(\ell)} \rightleftharpoons Li_2CO_{3(g)} \quad (10.8)$$

Relative to the decomposition of molten carbonates, and other possible processes contributing to vaporization, the data for Li_2CO_3 are as follows.

Decomposition processes:

CO_2 dissociation and equilibrium pressures for molten Li_2CO_3

$$Li_2CO_{3(\ell)} \rightleftharpoons Li_2O_{(\ell)} + CO_{2(g)} \quad (10.9)$$

$$p_{CO_2} = K_d \left[a_{Li_2CO_{3(\ell)}} \Big/ a_{Li_2O_{(\ell)}} \right] \quad (10.10)$$

Here p is the equilibrium CO_2 dissociation pressure, and a the thermodynamically defined activity. For practical purposes, eq. (10.10) is generally expressed in the mol fraction scale [X] as:

$$p_{CO_2} = K_d \left[X_{Li_2CO_{3(\ell)}} \Big/ X_{Li_2O_{(\ell)}} \right] \quad (10.11)$$

The values of the equilibrium CO_2 pressures depend on both the oxide and carbonate content; the values will not be unique unless the composition is exactly defined, i.e. the oxide content. Further, the values will depend on the "quality" of the carbonate, and its previous history.

(i) Equilibrium dissociation constant, K_d

Measurement method: analytical technique [14]

$$\log K_d = -9970/T + 6.12 \quad (10.12)$$

precision: not estimated uncertainty: ∿ ± 1%

Table 10.10.1. CO_2 dissociation constant from equation (10.12)

T (K)	K_d (atm)	T (K)	K_d (atm)
(800)	(4.57×10^{-7})	1050	4.21×10^{-4}
(850)	(2.46×10^{-6})	1100	1.14×10^{-3}
(900)	(1.10×10^{-5})	1150	2.82×10^{-3}
(950)	(4.22×10^{-5})	1200	6.48×10^{-3}
1000	1.41×10^{-4}		

(ii) Equilibrium CO_2 dissociation pressures

Measurement method: dynamic TGA technique [60]

$$\log p(mm) = \frac{-17031.64}{T} + 17.96 \quad (10.13)$$

precision: $\sim \pm 0.5\%$ uncertainty: $\sim \pm 5\%$

Table 10.10.2. Equilibrium CO_2 dissociation pressures of $Li_2CO_{3(\ell)}$ from equation (10.13)

T (K)	p(mm) obsv'd	p(mm) calc'd	T (K)	p(mm) obsv'd	p(mm) calc'd
1000	8.5	46	1080	155	256
1020	18.3	73	1100	300	376
1040	38.3	113	1120	567	546
1060	78.1	171			

The p(obsv'd) were for Li_2CO_3 with oxide content $\sim 2.3 \times 10^{-3}$ mol/mol carbonate, eq. (10.13). The p(calc'd) follow from the data in table 10.10.1 and eq. (10.11).

It appears, from the preceding, that equilibrium was not attained by the dynamic technique except possibly at the upper temperatures.

The CO_2 dissociation pressure data reported by Lebeau (1905), Johnston (1908), and Howarth (1930) are understood if the (mol Li_2O/mol Li_2CO_3) ratios were, respectively: 3×10^{-2}, 8×10^{-2}, and 16×10^{-2}.

Vaporization of molten carbonates:

Measurement method: critical analysis [50]

Since O_2, H_2, and water vapor are present in fuel cell operations, the effects of these, [through contributing reactions leading to the formation of hydroxides, oxides, peroxides, and reduced alkali metals] should be considered. Such factors have been critically re-examined by Maru et al., (1976). Some of the possible contributing reactions, (relative to vaporization losses) are:

$$M_2CO_{3(\ell)} \rightleftharpoons M_2O_{(\ell)} + CO_{2(g)} \quad (10.14)$$

$$M_2CO_{3(\ell)} + \tfrac{1}{2}O_{2(g)} \rightleftharpoons M_2O_{2(\ell)} + CO_{2(g)} \quad (10.15)$$

$$M_2CO_{3(\ell)} + H_2O_{(g)} \rightleftharpoons 2MOH_{(\ell)} + CO_{2(g)} \quad (10.16)$$

$$M_2CO_{3(\ell)} + H_{2(g)} \rightleftharpoons 2M_{(\ell)} + H_2O_{(g)} + CO_{2(g)} \quad (10.17)$$

Calculations of the vaporization losses due to hydroxide requires consideration of the hydrolysis equilibrium (10.16) and the thermodynamic activity of the hydroxide in the molten carbonate. While the data are insufficient for quantitative calculations, it is apparent from such considerations that hydroxides are the major diluents (under fuel cell conditions), e.g. up to 6 mol % LiOH can be expected in molten Li_2CO_3. Using the vapor pressures of the molten hydroxides at fuel cell temperatures, as guidelines, viz:

Hydroxide:	LiOH	NaOH	KOH	$Li_2(OH)_2$
p(atm):	10^{-7}	10^{-7}	10^{-6}	10^{-7}

and assuming thermodynamic equilibrium between the feed gases and the molten carbonate, one predicts that the vaporization losses (due to hydroxide species) would be in the order:

$$K_2CO_3 > Li_2CO_3 \geq Na_2CO_3$$

The processes are undoubtedly more complex, for deviations from this order have been observed, e.g., $Li_2CO_3 > K_2CO_3$. Such observations may be understood thermodynamically if the local activity of Li_2CO_3 > that in the bulk electrolyte, or if the vapor saturation with LiOH > KOH. A more exact account is not possible without additional data.

References [14,50,60-67].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: steady state, radial heat flux [68]

$$\lambda = -3.2535 \times 10^{-3} + 7.961 \times 10^{-6}T \quad (10.18)$$

precision: not estimated uncertainty: $\sim \pm 20\%$

Results were reported in graphical and equation forms only.

Table 10.11. Thermal conductivity of melt from equation (10.18)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
1000	47.08	1160	59.81
1020	48.67	1180	61.40
1040	50.26	1200	63.00
1060	51.85	1220	64.59
1080	53.44	1240	66.18
1100	55.04	1260	67.77
1120	56.63	1280	69.37
1140	58.22	1300	70.96

References [68].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: absolute steady state radial heat flux [68]

$\lambda = 24.26 \times 10^{-3} - 49.04 \times 10^{-6}T + 28.19 \times 10^{-9}T^2$ (420-640 K) (10,19)

$\lambda = 18.17 \times 10^{-3} - 30.95 \times 10^{-6}T + 16.28 \times 10^{-9}T^2$ (700-1000 K) (10,20)

precision: not estimated uncertainty: $\sim \pm 10\%$

Results were reported in equation and graphical forms only.

Table 10.12. Thermal conductivity of solid from equations (10,19) and (10,20)

T (K)	$\lambda \times 10^3$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^3$ (cal $cm^{-1}sec^{-1}K^{-1}$)
420	8.64	740	4.18
440	8.14	760	4.05
460	7.67	780	3.93
480	7.22	800	3.83
500	6.79	820	3.74
520	6.38	840	3.66
540	6.00	860	3.59
560	5.64	880	3.54
580	5.30	900	3.50
600	4.98	920	3.47
620	4.69	940	3.46
640	4.42	960	3.46
700	4.48	980	3.47
720	4.32	1000	3.50

References [68].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [59]

Table 10.13. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
14.9	$\sim \pm 10\%$

References [11,59,69,70].

16. References

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XI. Sodium Carbonate: Na_2CO_3

1. *Melting Temperature (T_m)*

Melting point:
858° ± 1°C [1-5,11]

References [1-20].

2. *Density (ρ)*

Measurement method: Archimedean technique [1]

$$\rho = 2.4797 - 4.487 \times 10^{-4}T \quad (11.1)$$

precision: ± 0.7% uncertainty: ∿ ± 1%

Table 11.1. Densities from equation (11.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1140	1.9682	1210	1.9368
1150	1.9637	1220	1.9323
1160	1.9592	1230	1.9278
1170	1.9547	1240	1.9233
1180	1.9502	1250	1.9188
1190	1.9457	1260	1.9143
1200	1.9413	1270	1.9099
		1280	1.9054

References [1,21].

3. *Surface Tension (γ)*

Measurement method: pin detachment [1]

$$\gamma = 268.51 - 5.02 \times 10^{-2}T \quad (11.2)$$

precision: ± 0.1% uncertainty: ∿ ± 0.3%

Table 11.2. Surface tension from equation (11.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1140	211.3	1220	207.3
1150	210.8	1230	206.8
1160	210.3	1240	206.3
1170	209.8	1250	205.8
1180	209.3	1260	205.3
1190	208.8	1270	204.8
1200	208.3	1280	204.3
1210	207.8	1290	203.8

References [1].

4. *Viscosity (η)*

Measurement method: oscillating (liquid-filled) cylinder [22]

$$\eta = 3.832 \times 10^{-5} \exp (26260/RT) \quad (11.3)$$

precision: ∿ ± 0.5% uncertainty: ∿ ± 25%

For numerical values: see table 11.3

Table 11.3. Viscosity from equation (11.3)

T (K)	η (cp)
1160	3.40
1170	3.08
1180	2.80
1190	2.55
1200	2.32
1210	2.12
1220	1.94
1230	1.78
1240	1.63

References [22,23].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [1]

$$\kappa = 13.758 \exp(-3527/RT) \quad (11.4)$$

precision: ± 0.13% uncertainty: ∿ ± 1.5%

Table 11.4. Electrical conductance from equation (11.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1140	2.900	1200	3.134
1150	2.939	1210	3.173
1160	2.978	1220	3.211
1170	3.018	1230	3.249
1180	3.057	1240	3.288
1190	3.096		

References [1,9,12,24-27].

6. *Safety and Hazards*

A. Hazard rating [28-30]

(i) Moderate

(ii) Vapor pressure: [CO_2 equilibrium dissociation pressure is ∿ 1 mm at 950°C]

$$Na_2CO_3 \rightleftharpoons Na_2O + CO_2 \quad (11.5)$$

B. Disaster hazards [31-33]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e. explosive expansion of "trapped" air.

(ii) When heated with CO_2 pressures less than equilibrium dissociation pressures, decomposes to form alkali metal oxide; the toxicology and disaster hazards are the same as those of very caustic solutions, i.e. react with water or steam (exothermic) to form solutions that are markedly aggressive to all body tissues (chemical burns).

References [28-33].

7. Corrosion

Table 11.5. Corrosion studies from primary research literature

Studies	References
Silica	34
Pt	35
Metals	36
Cu-Zn	37
Pt, Au, Ag, MgO	38-41
Pt, Pd, Rh, Ir (O_2 environment)	42
Alumina (Monofrax-A)	59,61
Au, Ag, Al_2O_3 (O_2 environment, Na_2CO_3-Na_2O)	5
Al_2O_3, Pt (N_2 atmosphere, Na_2CO_3-Na_2O)	3,43,44
quartz, porcelain, Ag, Pt, Ni, (N_2 atmosphere; Na_2CO_3-Na_2O)	45
Boron nitride	41,58
Na-β-alumina	58
Fe [Na_2CO_3-NaX; X = F, Cl, Br, I]	59
Acid-base relationships in molten carbonates	46-49
Hydrolysis (H_2O) reactions	5,50,51
Corrosion in molten salts: annotated bibliography	52
Molten carbonates: fuel cells; thermal energy storage; coal gasification; power plant stack gases	53-57,59

References [3,5,34-61].

8. Diffusion

Measurement method: capillary [62]

List of diffusing species investigated in Na_2CO_3 as solvent

Na^+, CO_3^{2-}

precision: ∿ ± 1.5%, Na^+; ∿ ± 0.6%, CO_3^{2-} uncertainty: ∿ ± 10%

Equation

$$D = A \exp [-E/RT] \quad (11.6)$$

Table 11.6.1. Parameters of diffusion equation (11.6)

Species	A x 10^3 ($cm^2 sec^{-1}$)	E (cal mol^{-1})	Temp. range (K)
Na^+	10.0	12,170	1180-1320
CO_3^{2-}	2.86	10,620	1170-1335

Table 11.6.2. Self-diffusion coefficients from equations in table (11.6.1)

T (K)	D_{Na^+} x 10^5 ($cm^2 sec^{-1}$)	$D_{CO_3^{2-}}$ x 10^5 ($cm^2 sec^{-1}$)
1170		2.97
1180	5.57	3.09
1200	6.07	3.33
1220	6.60	3.58
1240	7.16	3.84
1260	7.74	4.11
1280	8.35	4.40
1300	8.99	4.69
1320	9.66	4.99
1340		5.30

References [62-64].

9. *Heat of Fusion (ΔH_f°)*

Measurement method: drop calorimetry [2,7,67]

Table 11.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
7.1	∿ ± 4%

References [2,5,7,65-67].

10. *Heat Capacity (C_p)*

Measurement method: drop calorimetry [7]

$$C_p = 33.99 + 10.70 \times 10^{-3} T \quad (11.7)$$

precision: ∿ ± 0.5% uncertainty: ∿ ± 5%

Table 11.8. Heat capacity from equation (11.7)

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
1130	46.08	1180	46.62
1140	46.19	1190	46.72
1150	46.30	1200	46.83
1160	46.40	1210	46.94
1170	46.51		

References [2,5,7,65,67].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated from densities [68]

Table 11.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
16.2%	∿ ± 8%

References [68].

12. Vapor Pressure (p_{vap})

Measurement method: cited with each data set [5,54,69]

No systematic studies of vaporization as "molecular carbonate" have been reported, viz:

$$Na_2CO_{3(\ell)} \rightleftharpoons Na_2CO_{3(g)} \quad (11.8)$$

Relative to the decomposition of molten carbonates and other possible processes contributing to vaporization, the data for Na_2CO_3 are as follows.

Decomposition processes:

CO_2 dissociation and equilibrium pressures for molten Na_2CO_3

$$Na_2CO_{3(\ell)} \rightleftharpoons Na_2O_{(\ell)} + CO_{2(g)} \quad (11.9)$$

$$p_{CO_2} = K_d \left[a_{Na_2CO_{3(\ell)}} \Big/ a_{Na_2O_{(\ell)}} \right] \quad (11.10)$$

Here p is the equilibrium CO_2 dissociation pressure, and a the thermodynamically defined activity. For practical purposes, eq. (11.10) is generally expressed in the mol fraction scale [X] as:

$$p_{CO_2} = K_d \left[X_{Na_2CO_{3(\ell)}} \Big/ X_{Na_2O_{(\ell)}} \right] \quad (11.11)$$

The values of p_{CO_2} thus depend on the quality of the "carbonate", i.e. the oxide content as well as carbonate. This will vary with the previous history. For example, conventional vacuum drying at elevated temperatures, where the sample is heated under dynamic vacuum, may lead to oxide formation if the pressures are less than the CO_2 equilibrium pressures. It is apparent that the p_{CO_2} equilibrium values will be unique only if the composition of the "carbonate" is exactly defined, i.e. the oxide content of carbonate.

(i) Equilibrium dissociation constant, K_d.

Measurement method: emf technique [5]

$$\log K_d = \frac{-15600}{T} + 6.99 \quad (11.12)$$

precision: not estimated uncertainty: ∿ ± 1%

Table 11.10.1. CO_2 dissociation constant from equation (11.12)

T (K)	K_d (atm)	T (K)	K_d (atm)
(800)	(3.09×10^{-13})	(1050)	(1.36×10^{-8})
(850)	(4.34×10^{-12})	(1100)	(6.43×10^{-8})
(900)	(4.54×10^{-11})	1150	2.66×10^{-7}
(950)	(3.71×10^{-10})	1200	9.77×10^{-7}
(1000)	(2.45×10^{-9})		

(ii) Equilibrium CO_2 dissociation pressures

Measurement method: dynamic TGA technique [69]

$$\log p \text{ (mm)} = \frac{-13242.51}{T} + 12.61 \quad (11.13)$$

precision: $\sim \pm 0.5\%$ uncertainty: $\sim \pm 5\%$

Table 11.10.2. Equilibrium CO_2 dissociation pressures from equation (11.13)

T (K)	p(mm) obsv'd	p(mm) calc'd	T (K)	p(mm) obsv'd	p(mm) calc'd
1130	7.8	7.8	1150	12.4	13.5
1140	9.9	10.2	1160	15.6	17.6

The p(mm) (calc'd) were calculated from the data in table 11,8,1 and eq. (11.11) and assuming Na_2O content, $\sim 1.5 \times 10^{-5}$ mol/mol Na_2CO_3, and eq. (11.13).

The thermal dissociation of anhydrous Na_2CO_3 to CO_2 (eq. 11.9) has been studied by Johnston (1908), Howarth and Turner (1930), Kroger and Stratmann (1961), and Spedding and Mills (1965). The CO_2 dissociation pressure data sets are understood from the preceding, if the mol Na_2O per mol Na_2CO_3, were, respectively: $\sim 2 \times 10^{-4}$, 3×10^{-2}, $\sim 8 \times 10^{-4}$, and $\sim 1.4 \times 10^{-4}$.

Vaporization of molten carbonates:

Measurement method: critical analysis [54]

The "vaporization" observations, based on electrolyte losses from high temperature molten carbonate fuel cells studies, and the thermodynamics of the associated reactions have been critically examined by Maru et al. (1976). For a summary of the results, refer: Li_2CO_3, present work.

References [5,54,62,69-76].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: steady state radial heat flux [77]

$$\lambda = 1.181 \times 10^{-3} + 2.816 \times 10^{-6} T \quad [11.14]$$

precision: not estimated uncertainty: $\sim \pm 20\%$

Results were reported in graphical and equation forms only.

Table 11.11. Thermal conductivity of melt from equation (11.14)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
1140	43.91	1210	45.88
1150	44.19	1220	46.17
1160	44.48	1230	46.45
1170	44.76	1240	46.73
1180	45.04	1250	47.01
1190	45.32	1260	47.29
1200	45.60		

References [77].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: absolute steady state radial heat flux [78].

$\lambda = 9.97 \times 10^{-5} + 8.57 \times 10^{-6}T - 9.87 \times 10^{-9}T^2$ (540-580 K) (11.15)

$\lambda = 2.04 \times 10^{-2} - 3.35 \times 10^{-5}T + 16.14 \times 10^{-9}T^2$ (700-1135 K) (11.16)

precision: not estimated uncertainty: $\sim \pm$ 10%

Results were reported in equation and graphical forms only.

Table 11.12. Thermal conductivity of solid from equations (11.15) and (11.16)

T (K)	$\lambda \times 10^3$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^3$ (cal $cm^{-1}sec^{-1}K^{-1}$)
540	1.85	880	3.40
550	1.83	900	3.31
560	1.80	920	3.23
570	1.78	940	3.16
580	1.75	960	3.10
700	4.85	980	3.05
720	4.64	1000	3.02
740	4.44	1020	3.00
760	4.25	1040	3.00
780	4.08	1060	3.00
800	3.92	1080	3.03
820	3.77	1100	3.06
840	3.64	1120	3.10
860	3.51		

References [78].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [68]

Table 11.13. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
37.9	$\sim \pm$ 3%

References [2,68,79].

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XII. Potassium Carbonate: K_2CO_3

1. *Melting Temperature (T_m)*

Melting point:
898° ± 3°C [1-3,9]

References [1-14].

2. *Density (ρ)*

Measurement method: Archimedean technique [6]

$$\rho = 2.4141 - 4.421 \times 10^{-4} T \quad (12.1)$$

precision: ∿ ± 0.7% uncertainty: ∿ ± 1%

Table 12.1. Densities from equation (12.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1180	1.8924	1230	1.8703
1190	1.8880	1240	1.8659
1200	1.8836	1250	1.8615
1210	1.8792	1260	1.8571
1220	1.8747	1270	1.8526
		1280	1.8482

References [6,15].

3. *Surface Tension (γ)*

Measurement method: pin detachment [6]

$$\gamma = 337.85 - 21.71 \times 10^{-2} T + 6.25 \times 10^{-5} T^2 \quad (12.2)$$

precision : ± 0.1% uncertainty: ∿ ± 0.3%

Table 12.2. Surface tension from equation (12.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1190	168.0	1240	164.7
1200	167.3	1250	164.1
1210	166.7	1260	163.5
1220	166.0	1270	162.9
1230	165.4	1280	162.4

References [6].

4. *Viscosity (η)*

Measurement method: oscillating (liquid-filled) cylinder [16]

$$\eta = 1.161 \times 10^{-5} \exp (29{,}487/RT) \quad (12.3)$$

precision: ∿ ± 1.23% uncertainty: ∿ ± 30%

For numerical values: see table 12.3

Table 12.3. Viscosity from equation (12.3)

T (K)	η (cp)
1190	3.02
1200	2.72
1210	2.46
1220	2.22
1230	2.01
1240	1.83
1250	1.66

References [16,17].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [6]

$$\kappa = 11.027 \exp(-3941/RT) \quad (12.4)$$

precision: ± 0.08% uncertainty: ∿ ± 1.5%

Table 12.4. Electrical conductance from equation (12.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1180	2.053	1240	2.227
1190	2.083	1250	2.256
1200	2.112	1260	2.285
1210	2.141	1270	2.313
1220	2.170	1280	2.342
1230	2.199		

References [6,10,18-22].

6. *Safety and Hazards*

A. Hazard rating [23-25]

(i) Severe

(ii) Vapor pressure: [CO_2 equilibrium dissociation pressure is ∿ 1 mm at approx. 1080°C]

$$K_2CO_3 \rightleftharpoons K_2O + CO_2 \quad (12.5)$$

B. Disaster hazards [26-28]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) When heated with CO_2 pressures less than equilibrium dissociation pressures, decomposes to form alkali metal oxide; the toxicology and disaster hazards are the same as those of very caustic solutions, i.e. react with water or steam (exothermic) to form solutions that are markedly aggressive to all body tissues (chemical burns). Potassium carbonate itself is classified as a strong caustic.

References [23-28].

7. *Corrosion*

Table 12.5. Corrosion studies from primary research literature

Studies	References
SS [(K, Mg/CO_3); (K_2CO_3, KCl, KF); (K/CO_3, F, Cl)]	29
Acid-base relationships in molten carbonates	30-33
Hydrolysis (H_2O) reactions	34-36
Corrosion in molten salts: annotated bibliography	37
Molten carbonates: fuel cells; thermal energy storage; coal gasification; power plant stack gases	29,38-42

References [29-42].

8. *Diffusion*

No diffusion studies reported.

9. *Heat of Fusion (ΔH_f°)*

Measurement method: drop calorimetry [2,3]

Table 12.6. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
6.6	∿ ± 1.0%

References [2,3,43].

10. *Heat Capacity (C_p)*

Measurement method: drop calorimetry [3]

$$C_p = 36.95 + 10.64 \times 10^{-3} T \quad (12.6)$$

precision: ∿ ± 0.5% uncertainty: ± 0.5%

For numerical values: see table 12.7

Table 12.7. Heat capacity from equation (12.6)

T (K)	C_p (cal $K^{-1}mol^{-1}$)	T (K)	C_p (cal $K^{-1}mol^{-1}$)
1170	49.40	1210	49.82
1180	49.51	1220	49.93
1190	49.61	1230	50.04
1200	49.72	1240	50.14
		1250	50.25

References [2,3,43].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated; from densities [44]

Table 12.8. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
16.4%	∿ ± 8%

References [44].

12. Vapor Pressure (p_{vap})

Measurement method: cited with each data set [36,38,45].

No systematic studies of vaporization as "molecular carbonate" have been reported, viz:

$$K_2CO_{3(\ell)} \rightleftarrows K_2CO_{3(g)} \quad (12.7)$$

Relative to the decomposition of molten carbonates and other possible processes contributing to vaporization, the data for K_2CO_3 are as follows.

Decomposition processes:

CO_2 dissociation and equilibrium pressures for molten K_2CO_3

$$K_2CO_{3(\ell)} \rightleftarrows K_2O_{(\ell)} + CO_{2(g)} \quad (12.8)$$

$$p_{CO_2} = K_d \left[a_{K_2CO_3(\ell)} / a_{K_2O(\ell)} \right] \quad (12.9)$$

Here p is the equilibrium dissociation pressure, and a the thermodynamically defined activity. For practical purposes, eq. (12.9) is expressed in the mol fraction scale [X] as:

$$p_{CO_2} = K_d \left[X_{K_2CO_3(\ell)} / X_{K_2O(\ell)} \right] \quad (12.10)$$

It is clear that the values of p_{CO_2}, thus, depend on the quality of the "carbonate", i.e. the oxide content as well as carbonate. The p_{CO_2} equilibrium values will be unique only if the composition of the "carbonate" is exactly defined, e.g., mols K_2O/mol K_2CO_3.

In the vacuum drying of carbonates, where the sample is heated under dynamic vacuum, the oxide content may be increased through this thermal dissociation if the pressures are less than the CO_2 equilibrium pressures.

(i) Equilibrium dissociation constant, K_d

Measurement method: emf technique [36]

$$\log K_d = \frac{-17850}{T} + 7.44 \quad (12.11)$$

precision: not estimated uncertainty: $\sim \pm 1\%$

Table 12.9.1. CO_2 dissociation constant from equation (12.11)

T (K)	K_d (atm)	T (K)	K_d (atm)
(800)	(1.34×10^{-15})	(1050)	(2.75×10^{-10})
(850)	(2.75×10^{-14})	(1100)	(1.63×10^{-9})
(900)	(4.04×10^{-13})	(1150)	(8.28×10^{-9})
(950)	(4.47×10^{-12})	1200	3.67×10^{-8}
(1000)	(3.89×10^{-11})		

(ii) Equilibrium CO_2 dissociation pressures

Measurement method: Knudsen effusion technique [45]

$$\log p(mm) = \frac{-10838.67}{T} + 8.63 \quad (12.12)$$

precision: $\sim \pm 0.2\%$ uncertainty: $\sim \pm 5\%$

Table 12.9.2. Equilibrium CO_2 dissociation pressures of $K_2CO_3(\ell)$ from equation (12.12)

T	p(mm)		T	p(mm)	
(K)	obsv'd	calc'd	(K)	obsv'd	calc'd
1170	0.23	0.17	1200	0.39	0.40
1180	0.28	0.22	1210	0.47	0.53
1190	0.33	0.30			

The p(mm) (calc'd) were calculated from the data in table 12.9.1 and eq. (12.10), and assuming K_2O content, $\sim 7 \times 10^{-5}$ mol/mol K_2CO_3, eq. (12.12).

Additional thermal dissociation data (anhydrous K_2CO_3 to CO_2) have been reported by Lebeau (1905), Howarth and Turner (1930), and Dubois and Millet (1968). The CO_2 pressures can be brought into accord if corrections for the oxide content is made. From the preceding, these are, respectively: $\sim 8 \times 10^{-6}$, $\sim 6 \times 10^{-3}$, and $\sim 2 \times 10^{-3}$.

Vaporization of molten carbonates:

Measurement method: critical analysis [38]

The various "vaporization" observations, based on electrolyte losses from high temperature molten carbonate fuel cells, and the thermodynamics of the associated reactions, have been critically examined by Maru et al. (1976). For a summary of the results, refer: Li_2CO_3, present work.

References [36,38,45-52].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [44]

Table 12.10. Cryoscopic constant

k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
57.1	∿ ± 1%

References [2,44,53].

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XIII. Lithium Nitrate: $LiNO_3$

1. *Melting Temperature (T_m)*

Melting point:
253° ± 2°C [5-7,12]

References [1-12].

2. *Density (ρ)*

Measurement method: Archimedean technique [13]

$$\rho = 2.070 - 5.49 \times 10^{-4} T \quad (13.1)$$

precision: ∿ ± 0.05% uncertainty: ∿ ± 1%

Table 13.1. Densities from equation (13.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
550	1.767	630	1.724
560	1.762	640	1.718
570	1.757	650	1.713
580	1.751	660	1.707
590	1.745	670	1.702
600	1.740	680	1.696
610	1.735	690	1.691
620	1.729		

References [13-16].

3. *Surface Tension (γ)*

Measurement method: plate detachment [17]

$$\gamma = 144.92 - 5.50 \times 10^{-2} T \quad (13.2)$$

precision: ± 0.5% uncertainty: ∿ ± 1%

Table 13.2. Surface tension from equation (13.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
570	113.6	680	107.5
580	113.0	690	107.0
590	112.5	700	106.4
600	111.9	710	105.9
610	111.4	720	105.3
620	100.8	730	104.8
630	110.3	740	104.2
640	109.7	750	103.7
650	109.2	760	103.1
660	108.6	770	102.6
670	108.1	780	102.0

References [17-19].

4. *Viscosity* (η)

Measurement method: capillary [9]

$$\eta = 70.567 - 20.188 \times 10^{-2}T + 14.976 \times 10^{-5}T^2 \quad (13.3)$$

precision: $\sim \pm 1.1\%$ uncertainty: $\sim \pm 2\%$

Table 13.3. Viscosity from equation (13.3)

T (K)	η (cp)	T (K)	η (cp)
540	5.222	600	3.352
550	4.835	610	3.146
560	4.479	620	2.969
570	4.152	630	2.822
580	3.856	640	2.705
590	3.589	650	2.619

References [9,11,20-22].

5. *Electrical Conductance* (κ)

Measurement method: dc technique [16]

$$\kappa = -1.5242 + 3.4674 \times 10^{-3}T + 1.8027 \times 10^{-6}T^2 \quad (13.4)$$

precision: $\pm$ 0.6% uncertainty: $\sim \pm 1.5\%$

Table 13.4. Electrical conductance from equation (13.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
550	0.928	600	1.205
560	0.983	610	1.262
570	1.038	620	1.318
580	1.093	630	1.376
590	1.149	640	1.433

References [13,15,16,23,24].

6. *Safety and Hazards*

A. Hazard rating [4,25,26]

(i) Inhalation: low; ingestion: moderate (toxicity)

(ii) Vapor pressure: $LiNO_3$ decomposes just above its m.pt. (253°C) to $LiNO_2$ and oxygen. If the container material is inert (glass is not), oxides of nitrogen are absent.

B. Disaster hazards [27-29]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) On decomposition, nitrates emit toxic fumes (oxides of nitrogen) viz:

$$MNO_3 \longrightarrow MNO_2 + \tfrac{1}{2}O_2 \qquad (13.5.1)$$

$$2MNO_2 \rightleftharpoons M_2O + NO + NO_2 \qquad (13.5.2)$$

The subsequent decomposition reactions are complex; if the gas phase is continuously removed, the nitrite decomposition (above) to NO and NO_2 is dominant. If the gas phase is not immediately removed, the NO may re-oxidize the nitrite to nitrate.

(iii) Nitrates are powerful oxidizing agents; violent (explosive) reactions possible in molten nitrates and carbonaceous materials (organic cpds oils; carbon;...); aluminum alloys and bath sludges (e.g. iron oxides); magnesium alloys. Dangerous.

References [4,25-29]

7. Corrosion

Table 13.5. Corrosion studies from primary research literature

Studies	References
Fe	30
Cu	31
Thermodynamic approach	32,33
Electrochemical approach	34,35
Annotated corrosion biblio.	36
Reviews/corrosion	37-39

References [30-39].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in $LiNO_3$ as solvent.

$$Li^+,\ NO_3^-,\ Na^+,\ K^+,\ Rb^+,\ Cs^+,\ Tl^+,\ Ag^+,\ Br^-.$$

precision: in table 13.6.2 uncertainty: in table 13.6.1

Table 13.6.1. Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
capillary	$\sim \pm 5\%$	Li^+, NO_3^-
chronopotentiometry	$\sim \pm 10\%$	Ag^+
electrophoresis	$\sim \pm 20\%$	Na^+, Cs^+
interferometry	$\sim \pm 20\%$	K^+, Rb^+, Tl^+, Br^-

Equation

$$D = A \exp[-E/RT] \qquad (13.6)$$

Table 13.6.2. Parameters of diffusion equation (13.6), precisions, and recommended study

Species	A x 10^3 (cm^2 sec^{-1}])	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
Li^+	2.47	5490	540-590	∿±1.7%	40
NO_3^-	1.95	6340	540-590	∿±3.3%	40
Na^+	0.43	3550	540-670		41
K^+	2.33	5776	540-615	∿±11%	45
Rb^+	0.87	4898	545-665	∿±3.6%	45
Cs^+	0.66	4540	540-675		41
Tl^+	3.95	6780	535-630	∿±7.8%	43
Ag^+	16.1	7900	530-590	∿±4.5%	46
Br^-	1.58	6290	530-625	∿±10%	47

No entry in precision column indicates estimates not possible since results were reported as equations only.

References Li^+, 40; NO_3^-, 40; Na^+, 41,45; K^+, 45; Rb^+, 45; Cs^+, 41,45; Tl^+, 43; Ag^+, 42,44,46; Br^-, 47.

Table 13.6.3. Self-diffusion coefficients

T (K)	D_{Li^+} x 10^5 (cm^2 sec^{-1})	$D_{NO_3^-}$ x 10^5 (cm^2 sec^{-1})
540	1.48	0.53
550	1.63	0.59
560	1.78	0.65
570	1.94	0.72
580	2.11	0.80
590	2.29	0.87

$LiNO_3$

Table 13.6.4. Diffusion coefficients,

$D \times 10^5$ ($cm^2 sec^{-1}$)

T (K)	Na^+	K^+	Rb^+	Cs^+	Tl^+	Ag^+	Br^-
530					0.63	0.89	0.40
540	1.57	1.07	0.91	0.96	0.71	1.02	0.45
560	1.77	1.30	1.07	1.12	0.89	1.33	0.55
580	1.98	1.55	1.24	1.28	1.10	1.70	0.67
590	2.08	1.69	1.33	1.37	1.22	1.91	0.74
600	2.19	1.83	1.43	1.47	1.34		0.81
610	2.30	1.99	1.53	1.56	1.47		0.88
620	2.41	2.14	1.63	1.66	1.61		0.96
630	2.52		1.74	1.76	1.76		1.04
650	2.75		1.96	1.96			
660	2.87		2.08	2.07			
670	2.99		2.20	2.18			
680				2.29			

9. Heat of Fusion (ΔH_f°)

Measurement method: reaction calorimetry [48]

Table 13.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
5.96	∿ ± 1.5%

References [5,8,48,49].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [50]

Table 13.8. Heat capacity

C_p (cal $K^{-1} mol^{-1}$)	Temp. range (K)	Uncertainty
26.6	∿ 540-670	∿ ± 2%

References [8,50].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [51]

Table 13.9. Volume change on melting

$(\Delta V_f / V_s)$	Uncertainty
21.4%	∿ ± 3%

References [51,52].

12. Vapor Pressure (p_{vap})

Measurement method: critical analysis (NSRDS study) [4]

$LiNO_3$ is unstable just above its m.pt. (250°C) viz:

$$LiNO_3 \longrightarrow LiNO_2 + \tfrac{1}{2}O_2 \quad (13.7)$$

Onset of this decomposition at approx. 290°C has been reported. Thermodynamically it is predicted that the decomposition to oxide and NO_2, viz:

$$2\ LiNO_3 \longrightarrow Li_2O + 2NO_2 + \tfrac{1}{2}O_2 \quad (13.8)$$

is negligible to approx. 327°C.

$LiNO_2$ is stable up to 300°C, and slow decomposition at ∿ 350°C has been noted, i.e.

$$2\ LiNO_2 \longrightarrow Li_2O + NO + NO_2 \quad (13.9)$$

The product gases, NO and NO_2, may re-oxidize the nitrite to $LiNO_3$ if not removed.

The "equilibrium pressures" thus reported for molten $LiNO_3$ by Centnerzwer and Blumenthal (1936) apply to "infinitely dilute" solutions of $LiNO_2$ in the melts.

References [4,53-55].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: concentric cylinder [60]

$$\lambda = 11.935 \times 10^{-4} + 5.00 \times 10^{-7} T \quad (13.10)$$

precision: not estimated uncertainty: ∿ ± 20%

Results were reported in equation form only.

Table 13.10. Thermal conductivity of melt from equation (13.10)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
530	14.59	640	15.14
540	14.64	650	15.19
550	14.69	660	15.24
560	14.74	670	15.29
570	14.79	680	15.34
580	14.84	690	15.39
590	14.89	700	15.44
600	14.94	710	15.49
610	14.99	720	15.54
620	15.04	730	15.59
630	15.09		

References [56-61].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: comparative, flat slab [62]

precision: not estimated uncertainty: ∿ ± 10%

Table 13.11. Thermal conductivity of solid

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
525	32.2
527	32.7

References [56,62].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [63]

Table 13.12. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
6.36	∿ ± 1.5%

References [8,63-68].

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XIV. Sodium Nitrate: $NaNO_3$

1. *Melting Temperature (T_m)*

Melting point:
307° ± 1°C [1,9]

References [1-12].

2. *Density (ρ)*

Measurement method: Archimedean technique [13]

$$\rho = 2.3339 - 7.665 \times 10^{-4} T \quad (14.1)$$

precision: ∿ 0.1% uncertainty: ∿ ± 1%

Table 14.1. Densities from equation (14.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
590	1.882	640	1.843
600	1.874	650	1.836
610	1.866	660	1.828
620	1.859	670	1.820
630	1.851	680	1.813
		690	1.805

References [13-27].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [28]

$$\gamma = 155.4 - 6.13 \times 10^{-2} T \quad (14.2)$$

precision: ± 0.3% uncertainty: ∿ ± 0.5%

Table 14.2. Surface tension from equation (14.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
590	119.4	740	110.2
600	118.8	750	109.6
610	118.1	760	109.0
620	117.5	770	108.3
630	116.9	780	107.7
640	116.3	790	107.1
650	115.7	800	106.5
660	115.1	810	105.9
670	114.5	820	105.3
680	113.9	830	104.7
690	113.2	840	104.0
700	112.6	850	103.4
710	112.0	860	102.8
720	111.4	870	102.2
730	110.8	880	101.6

References [28-33].

4. *Viscosity (η)*

Measurement method: capillary [37,40]

$$\eta = 25.0987 - 6.0544 \times 10^{-2}T + 3.8709 \times 10^{-5}T^2 \quad (14.3)$$

precision: $\sim \pm 0.6\%$ uncertainty: $\sim \pm 3\%$

Table 14.3. Viscosity from equation (14.3)

T (K)	η (cp)	T (K)	η (cp)
590	2.85	670	1.91
600	2.71	680	1.83
610	2.57	690	1.75
620	2.44	700	1.69
630	2.32	710	1.63
640	2.21	720	1.57
650	2.10	730	1.53
660	2.00		

References [34-40].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [26]

$$\kappa = -2.234486 + 6.533061 \times 10^{-3}T - 1.730567 \times 10^{-6}T^2 \quad (14.4)$$

precision: $\pm 0.05\%$ uncertainty: $\sim \pm 1\%$

Table 14.4. Electrical conductance from equation (14.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
590	1.018	650	1.281
600	1.062	660	1.323
610	1.107	670	1.366
620	1.151	680	1.408
630	1.195	690	1.449
640	1.238	700	1.491

References [14,25,26,41-47].

6. *Safety and Hazards*

A. Hazard rating [4,48,49]

(i) Inhalation: low; ingestion: permitted as a food additive

(ii) Vapor pressure: $NaNO_3$ (m.pt. 307°C) melts without decomposition; the melt is stable in air to approx. 500°C; at higher temperatures, decomposes to form $NaNO_2$ and oxygen, viz:

$$NaNO_3 \rightleftharpoons NaNO_2 + \tfrac{1}{2}O_2 \quad (14.5)$$

At 800°K, for example, the value of the equilibrium constant for this reaction has been reported as 1.34×10^{-2}.

B. Disaster hazards [4,48,50-52]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) On decomposition, nitrates emit toxic fumes (oxides of nitrogen) viz:

$$2MNO_3 \longrightarrow 2MNO_2 + O_2 \qquad (14.6.1)$$

$$2MNO_2 \longrightarrow M_2O + NO + NO_2 \qquad (14.6.2)$$

The subsequent decomposition reactions are complex; if the gas phase is continuously removed, the nitrite decomposition (above) to NO and NO_2 is dominant.

(iii) Nitrates are powerful oxidizing agents; violent (explosive) reactions possible in molten nitrates and carbonaceous materials (organic cpds., oils, carbon,....); aluminum alloys and bath sludges (e.g. iron oxides); magnesium alloys. Dangerous.

References [4,48-52].

7. Corrosion

Table 14.5. Corrosion studies from primary research literature

Studies	References
Fe	53,55,57
Fe, Co, Ni	54
Cu	56
Pt, S, steel	58
Oxide species	59
Electrochemical approach	60,61
Thermodynamic redox diagrams	62,63
Annotated corrosion biblio.	64
Reviews/molten salts	65-67

References [53-67].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in $NaNO_3$ as solvent

$$Na^+,\ NO_3^-,\ K^+,\ Rb^+,\ Cs^+,\ Sr^{2+},\ Ba^{2+},$$

$$Tl^+,\ Ag^+,\ F^-,\ Br^-,\ I^-,\ CO_3^{2-},\ SO_4^{2-}$$

The italicized species indicate studies with insufficient data-sets for characterization of temperature dependence of diffusion coefficients. For these species, see table 14.6.5.

precision: in table 14.6.2. uncertainty: in table 14.6.1.

Table 14.6.1. Diffusion techniques, uncertainties, and species

Diffusion techniques of recommended study	Uncertainty (in values of D)	Species
capillary	∿ ± 10%	Na^+, NO_3^-, K^+
	∿ ± 100%	Sr^{2+}, Ba^{2+}, Tl^+
chronopotentiometry	∿ ± 10%	Ag^+
interferometry	∿ ± 30%	Rb^+, F^-, Br^-, I^-, CO_3^{2-}, SO_4^{2-}
electrophoresis	∿ ± 25%	Cs^+, Tl^+

Equation:

$$D = A \exp[-E/RT] \quad (14.7)$$

For values of eq. parameters and precisions: see table 14.6.2.

For numerical values: see tables 14.6.3 - 14.6.5.

References: Na^+, 69-71, 75, 80, 81, 83-90, 100; NO_3^-, 69, 84; K^+, 90, 91; Rb^+, 79; Cs^+, 70, 75, 79, 83, 85, 88; Ag^+, 68, 77, 78, 82, 91-96, 99; F^-, 98; Br^-, 98; I^-, 98; CO_3^{2-}, 98; SO_4^{2-}, 98; Sr^{2+}, 73; Ba^{2+}, 73; Tl^+, 73, 87.

Table 14.6.2. Parameters of diffusion equation (14.7), precisions, and recommended study

Species	A x 10^3 ($cm^2 sec^{-1}$)	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
Na^+	1.29	4347	600-670	∿±2.3%	80
NO_3^-	0.90	5080	585-650	∿±1.4%	69,84
K^+	1.199	5144	590-670	∿±1.3%	90
Rb^+	0.694	4682	580-670	∿±4.5%	79
Cs^+	0.85	4740	580-720		75
Ag^+	1.07	4645	590-670	∿±2.6%	99
F^-	0.782	5730	620-650	∿±6.9%	98
Br^-	1.312	5671	590-670	∿±7.4%	98
I^-	1.712	5994	590-660	∿±6.6%	98
CO_3^{2-}	1.103	6432	590-650	∿±6.2%	98
SO_4^{2-}	0.762	5888	590-650	∿±4.2%	98

No entry in precision column indicates estimate not possible since results were reported as equations only.

Table 14.6.3. Self-diffusion coefficients

T (K)	$D_{Na^+} \times 10^5$ ($cm^2\ sec^{-1}$)	$D_{NO_3^-} \times 10^5$ ($cm^2\ sec^{-1}$)
580		1.10
590		1.18
600	3.37	1.27
610	3.57	1.36
620	3.79	1.46
630	4.00	1.56
640	4.23	1.66
650	4.46	1.76
660	4.69	
670	4.93	

Table 14.6.4. Diffusion coefficients, D x 10^5 ($cm^2 sec^{-1}$)

T (K)	K^+	Rb^+	Cs^+	Ag^+	F^-	Br^-	I^-	CO_3^{2-}	SO_4^{2-}
580		1.19	1.39						
590	1.49	1.28	1.49	2.04		1.04	1.03	0.457	0.502
600	1.60	1.37	1.60	2.17		1.13	1.12	0.501	0.546
610	1.72	1.46	1.70	2.32		1.22	1.22	0.547	0.592
620	1.84	1.55	1.81	2.47	0.746	1.31	1.32	0.596	0.641
630	1.97	1.65	1.93	2.62	0.804	1.41	1.43	0.647	0.691
640	2.10	1.75	2.05	2.77	0.863	1.52	1.54	0.701	0.744
650	2.23	1.85	2.17	2.93	0.925	1.63	1.65	0.758	0.799
660	2.37	1.95	2.29	3.10		1.74	1.77		
670	2.52	2.06	2.42	3.27		1.85			
680			2.55						
700			2.82						
720			3.09						

Table 14.6.5. Diffusion coefficients for species not included in tables 14.6.3 and 14.6.4

Species	T (K)	D x 10^5 ($cm^2\ sec^{-1}$)	Recommended study
Sr^{2+}	618	4.2	74
	633	4.4	
Ba^{2+}	633	3.7	74
Tl^+	589	1.83	87
	603	3.90	74
	633	4.30	

9. Heat of Fusion (ΔH_f°)

Measurement method: reaction calorimetry [12]

Table 14.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
3.70	∿ ± 1.0%

References [2,5,7-9,12,101-109].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry; DSC [5,110]

Table 14.8. Heat capacity

C_p (cal $K^{-1} mol^{-1}$)	Temp. range (K)	Uncertainty
37.0	600-700	∿ ± 5%

References [5,8,12,110].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [111]

Table 14.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
10.7%	∿ ± 5%

References [111-113].

12. Vapor Pressure (p_{vap})

Measurement method: critical evaluation; NSRDS study [4]

The stability of $NaNO_3$ (crystalline) relative to the hypothetical decomposition:

$$2NaNO_{3(c)} \rightleftharpoons Na_2O_{(s)} + 2NO_{2(g)} + \tfrac{1}{2}O_{2(g)} \qquad (14.8)$$

may be illustrated by the values of K_{equil}^m predicted thermodynamically.

Table 14.10.1. Equilibrium dissociation constants and pressures for equation (14.6)

T(K)	298.15	400	500	600	700	800
$K_{(equil^m)}$	2.29×10^{-81}	2.80×10^{-55}	3.58×10^{-40}	2.42×10^{-30}	6.24×10^{-24}	1.6×10^{-18}
$p_{(atm)}$	5.53×10^{-27}	4.56×10^{-18}	6.57×10^{-15}	1.61×10^{-9}	2.85×10^{-7}	2.1×10^{-5}

$NaNO_3$ (m.pt. 307°C) melts without decomposition; the molten salt is stable in air to ∿ 500°C. At higher temperature the decomposition to nitrite onsets:

$$NaNO_{3(\ell)} \rightleftharpoons NaNO_{2(\ell)} + \tfrac{1}{2}O_2 \qquad (14.9)$$

If the gas phase is not removed, a nitrate-nitrite interconversion equilibrium is established since $NaNO_3$ reacts with O_2. Values for the equilibrium constant, from an experimental study are as follows:

Table 14.10.2. Equilibrium dissociation constants and pressures for equation (14.7)

T(K)	800	850	900	950	1000
$K_{equil}{}^m[x10^2]$	1.34	3.62	8.80	19.5	398

Since $NaNO_2$ is soluble in $NaNO_3$ and the solution is virtually ideal,

$$K_{equil}{}^m = p_{O_2}^{\frac{1}{2}} \; [X_{NaNO_2}/X_{NaNO_3}] \qquad (14.10)$$

The enthalpy of reaction, $\Delta H^\circ_{298.1}$, from these data, is 26.13 kcal.

If the gas phase is continuously removed, the nitrite decomposition proceeds by decomposition to oxide and nitrogen oxides:

$$2NaNO_2 \rightleftharpoons Na_2O + NO + NO_2 \qquad (14.11)$$

If the nitrite decomposition is carried out in an inert atmosphere, the first decomposition product is N_2, and this is accompanied by increasing concentration of O_2 as the reaction proceeds. The evolution of N_2 has been attributed to the formation of a super-oxide (which subsequently decomposes to Na_2O and oxygen).

References [4,114-120].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: concentric cylinder [125]

$$\lambda = 9.696 \times 10^{-4} + 6.28 \times 10^{-7} T \qquad (14.12)$$

precision: not estimated uncertainty: ∿ ± 20%

Results were reported in equation form only.

Table 14.11. Thermal conductivity of melt from equation (14.12)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$
590	13.40	670	13.90
600	13.46	680	13.97
610	13.53	690	14.03
620	13.59	700	14.09
630	13.65	710	14.15
640	13.72	720	14.22
650	13.78	730	14.28
660	13.84	740	14.34

References [121-128].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: steady state concentric cylinder [128]

$$\lambda = 9.466 \times 10^{-4} + 8.02 \times 10^{-7} T \qquad (14.13)$$

precision: not estimated uncertainty: ∿ ± 10%

Results were reported in equation form only.

Table 14.12. Thermal conductivity of solid from equation (14.13)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
500	13.48	550	13.88
510	13.56	560	13.96
520	13.64	570	14.04
530	13.72	580	14.12
540	13.80		

References [128].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [101]

Table 14.13. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
15.4	~ ± 1%

References [12,101,107,108,129-132].

16. References

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XV. Potassium Nitrate: KNO_3

1. *Melting Temperature (T_m)*

Melting point:
337° ± 1°C [1,2,4,13]

References [1-15].

2. *Density (ρ)*

Measurement method: Archimedean technique [16]

$$\rho = 2.315 - 7.29 \times 10^{-4} T \quad (15.1)$$

precision: ± 0.1% uncertainty: ∿ ± 0.5%

Table 15.1. Densities from equation (15.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
620	1.863	750	1.768
630	1.856	760	1.761
640	1.848	770	1.754
650	1.841	780	1.746
660	1.834	790	1.739
670	1.827	800	1.732
680	1.819	810	1.725
690	1.812	820	1.717
700	1.805	830	1.710
710	1.797	840	1.703
720	1.790	850	1.695
730	1.783	860	1.688
740	1.776	870	1.681

References [7,16-24].

3. *Surface Tension (γ)*

Measurement method: pin detachment [25]

$$\gamma = 156.99 - 7.50 \times 10^{-2} T \quad (15.2)$$

precision: ± 0.1% uncertainty: ∿ ± 1.0%

Table 15.2. Surface tension from equation (15.2).

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
610	111.2	700	104.5
620	110.5	710	103.7
630	109.7	720	103.0
640	109.0	730	102.2
650	108.2	740	101.5
660	107.5	750	100.7
670	106.7	760	100.0
680	106.0	770	99.2
690	105.2		

References [12,25-29].

4. *Viscosity (η)*

Measurement method: capillary and oscillational techniques [40]

$$\eta = 28.404 - 67.52062 \times 10^{-3}T + 0.4220783 \times 10^{-4}T^2 \quad (15.3)$$

precision: ∿ ± 0.9% uncertainty: ∿ ± 2.0%

Table 15.3. Viscosity from equation (15.3)

T (K)	η (cp)	T (K)	η (cp)
620	2.77	700	1.82
630	2.62	710	1.74
640	2.48	720	1.67
650	2.35	730	1.61
660	2.23	740	1.55
670	2.11	750	1.51
680	2.01	760	1.47
690	1.91		

References [7,8,10,15,30-43].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [9]

$$\kappa = -2.11923 + 5.71490 \times 10^{-3}T - 3.01492 \times 10^{-6}T^2 \quad (15.4)$$

precision: ± 0.1% uncertainty: ∿ ± 1.0%

Table 15.4. Electrical conductance from equation (15.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
620	0.649	720	0.951
630	0.681	730	0.979
640	0.713	740	1.006
650	0.744	750	1.034
660	0.775	760	1.060
670	0.805	770	1.087
680	0.835	780	1.113
690	0.865	790	1.138
700	0.894	800	1.163
710	0.923	810	1.188

References [9,16,17,19,23,31,44-50].

6. *Safety and Hazards*

A. Hazard rating [4,51,52]

(i) Inhalation: low; ingestion: permitted as a food additive

(ii) Vapor pressure: KNO_3 (m.pt. 337°C) melts without decomposition to a liquid which is stable in air at least to 530°C; between 550° and 750°C, the quasi-equilibrium sets up:

$$KNO_3 \rightleftharpoons KNO_2 + \tfrac{1}{2}O_2 \quad (15.5)$$

i.e., the two salts interconvert in this temperature range (but: see below)

B. Disaster hazards [51,53-55]

(i) Molten salt bath "explosions": violent generation of steam due to bulk water "carry-over" and/or equipment failure; sudden explosive expansion of "trapped" air.

(ii) On decomposition, nitrates emit toxic fumes (oxides of nitrogen) viz:

$$MNO_3 \longrightarrow MNO_2 + \tfrac{1}{2}O_2 \qquad (15.6.1)$$

$$2MNO_2 \longrightarrow M_2O + NO + NO_2 \qquad (15.6.2)$$

The subsequent decomposition reactions are complex; if the gas phase is continuously removed, the nitrite decomposition (above) to NO and NO_2 is dominant.

In the temperature range 550-600°C, and under oxygen, the conversion of KNO_2 to KNO_3 goes to completion; between 650-750°C, the two salts interconvert (see above), KNO_3 becoming increasingly unstable; above 800°C, the nitrite decomposition: $2\ KNO_2 \longrightarrow K_2O + N_2 + {}^3/_2O_2$ goes to completion.

(iii) Nitrates are powerful oxidizing agents; violent (explosive) reactions possible in molten nitrates and carbonaceous materials (organic cpds., oils, carbon,...); aluminum alloys and bath sludges (e.g. iron oxides); magnesium alloys. Dangerous.

References [4,51-55].

7. Corrosion

Table 15.5. Corrosion studies from primary research literature

Studies	References
Fe	56
Pt, Rh, Ag	57
Oxide species	58
Electrochemical approach	59,60
Thermodynamic redox diagrams	61,62
Reviews/corrosion: molten salts	63-65
Annotated corrosion biblio.	66

References [56-66].

8. Diffusion

Measurement method: cited with each diffusing species

List of diffusing species investigated in KNO_3 as solvent

$$K^+,\ NO_3^-,\ \textit{Li}^+,\ Na^+,\ Rb^+,\ Cs^+,\ Sr^{2+},\ \textit{Ba}^{2+},$$
$$\textit{Tl}^+,\ Ag^+,\ \textit{Br}^-,\ \textit{I}^-$$

The italicized species indicate studies with insufficient data-sets for characterization of temperature dependence of diffusion coefficients. For these species, see table 15.6.5.

precision: in table 15.6.2 uncertainty: in table 15.6.1

Table 15.6.1. Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
capillary	∿ ± 20%	K^+, NO_3^-, Li^+
	∿ ± 100%	Tl^+, Br^-, I^-
chronopotentiometry	∿ ± 10%	Sr^{2+}, Ag^+
polarography	∿ ± 50%	Ba^{2+}, Tl^+, Br^-, I^-
interferometry	∿ ± 30%	Na^+, Rb^+, Cs^+

Equation:

$$D = A \exp[-E/RT] \quad (15.7)$$

For values of eq. parameters, and precisions: see table 15.6.2.

For numerical values: see tables 15.6.3 - 15.6.5.

References: K^+, 68, 71, 74, 77, 79, 87; NO_3^-, 68; Na^+, 70, 72, 73, 77, 80, 87; Rb^+, 73; Cs^+, 73; Sr^{2+}, 70, 81; Ag^+, 70, 75, 76, 83-86; Li^+, 72; Ba^{2+}, 67, 69; Tl^+, 67, 69; Br^-, 67, 69; I^-, 67, 69.

Table 15.6.2. Parameters of diffusion equation (15.7), precisions, and recommended study

Species	A x 10^3 (cm^2 sec^{-1})	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
K^+	1.48	5674	615-700	∿±3%	74,79
NO_3^-	1.42	5760	620-660	∿±2.7%	68
Na^+	2.925	6237	620-690	∿±4.2%	73
Rb^+	1.026	5321	610-725	∿±6.2%	73
Cs^+	0.593	4781	610-730	∿±6.8%	73
Sr^{2+}	6.63	8150	620-690	∿±4.5%	81
Ag^+	1.53	5280	620-720		76

No entry in precision column indicates estimates not possible since the results were reported as equations only.

KNO_3

Table 15.6.3. Self-diffusion coefficients

T (K)	$D_{K^+} \times 10^5$ ($cm^2\ sec^{-1}$)	$D_{NO_3^-} \times 10^5$ ($cm^2\ sec^{-1}$)
610	1.37	
620	1.48	1.32
630	1.59	1.43
640	1.71	1.53
650	1.83	1.64
660	1.96	1.76
670	2.09	
680	2.22	
690	2.36	
700	2.50	

Table 15.6.4. Diffusion coefficients

	D x 10^5 ($cm^2\ sec^{-1}$)				
T (K)	Na^+	Rb^+	Cs^+	Sr^{2+}	Ag^+
610		1.27	1.15		
620	1.85	1.37	1.22	0.888	2.11
630	2.01	1.46	1.30	0.986	2.25
640	2.17	1.56	1.38	1.09	2.41
650	2.34	1.67	1.46	1.21	2.57
660	2.52	1.77	1.55	1.33	2.73
670	2.70	1.89	1.63	1.46	2.90
680	2.89	2.00	1.72	1.59	3.07
690	3.09	2.12	1.81	1.74	3.25
710		2.36	2.00		3.63
720		2.49	2.10		3.82
730		2.62	2.19		

Table 15.6.5. Diffusion coefficients for species not included in tables 15.6.3 and 15.6.4

Species	T (K)	D x 10^5 ($cm^2\ sec^{-1}$)	Recommended study
Li^+	625	2.2	72
	645	2.6	
Ba^{2+}	643	2.1	70
Tl^+	618	3.2	70
	638	3.3	
	653	3.4	
Br^-	633	3.0	70
I^-	633	3.0	70

9. Heat of Fusion (ΔH_f°)

Measurement method: reaction calorimetry [88]

Table 15.7. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
2.41	∿ ± 1%

References [1,3,5,88-92].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [94]

Table 15.8. Heat capacity

C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
32.4	610-663	∿ ± 1.5%

References [90,93,94].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [95]

Table 15.9. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
3.3%	∿ ± 1.5%

References [95,96].

12. Vapor Pressure (p_{vap})

Measurement method: critical evaluation; NSRDS study [4]

KNO_3 (m.pt. 337°C) melts without decomposition. The melt is stable in air to at least 530°C. Decomposition reactions lead to the interconversion equilibrium:

$$KNO_{3(\ell)} \rightleftharpoons KNO_{2(\ell)} + \tfrac{1}{2}O_{2(g)} \qquad (15.8)$$

over a limited temperature range. Values of the equilibrium constant, from an experimental study, are in table 15.10.

Table 15.10. Equilibrium dissociation constants for equation (15.8)

T(K)	823.1	873.1	921.1	973.1	1023.1
$K_{equil}{}^m[x10^2]$	0.88	2.7	6.2	21.9	28.0

and the enthalpy for this reaction, from these data, is $\Delta H^\circ_{298.1} = 27.6 \pm 1.$ kcal mol^{-1}. In an oxygen atmosphere, in the temperature range 550°-600°C, the conversion of nitrite to nitrate goes to completion. From 650°-750°C, KNO_2 becomes increasingly more unstable. Experimentally it has been shown that the above reaction attains equilibrium in the range 650° to approx. 800°C. Above 800°C, the nitrite decomposition is dominant:

$$2\ KNO_2 \longrightarrow K_2O + N_2 + {}^3/_2O_2 \qquad (15.9)$$

If O_2 is removed, the nitrite decomposition leads to the formation of various oxides of nitrogen, e.g.

$$2KNO_2 \longrightarrow K_2O + NO_2 + NO \quad (15.10)$$

and the processes are more complicated.

References [4,13,97-102]

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: concentric cylinder [105]

$$\lambda = 5.665 \times 10^{-4} + 8.7 \times 10^{-7} T \quad (15.11)$$

precision: not estimated uncertainty: ∿ ± 20%

Results were reported in equation form only.

Table 15.11. Thermal conductivity of melt from equation (15.11)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
610	10.97	680	11.58
620	11.06	690	11.67
630	11.15	700	11.76
640	11.23	710	11.84
650	11.32	720	11.93
660	11.41	730	12.02
670	11.49		

References [103-113].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: comparative technique [114]

precision: not estimated uncertainty: ∿ ± 10%

Results were reported in graphical form only.

Table 15.12. Thermal conductivity of solid

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
353	22.9	408	19.1
363	23.2	413	19.4
373	23.4	423	19.6
383	23.7	433	20.1
393	24.1	443	20.6
403	20.3	453	21.0

Sole investigation in the temperature range 350-450 K; values interpolated from the graphical presentation in [114].

References [104,114].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [115]

Table 15.13. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
31.0	~ ± 1%

References [3,115-119].

16. References

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XVI. Lithium Sulfate: Li_2SO_4

1. *Melting Temperature (T_m)*

Melting point:
859° ± 3°C [1-3]

References [1-9].

2. *Density (ρ)*

Measurement method: Archimedean technique [10,11]

$$\rho = 2.4641 - 4.061 \times 10^{-4} T \quad (16.1)$$

precision: ± 0.02% uncertainty: ∿ ± 1%

Table 16.1. Densities from equation (16.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1140	2.001	1200	1.977
1150	1.997	1210	1.973
1160	1.993	1220	1.969
1170	1.989	1230	1.965
1180	1.985	1240	1.961
1190	1.981	1250	1.957

References [10,11].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [10]

$$\gamma = 300.96 - 6.72 \times 10^{-2} T \quad (16.2)$$

precision: ± 0.1% uncertainty: ∿ ± 1%

Table 16.2. Surface tension from equation (16.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1130	225.0	1260	216.3
1140	224.4	1270	215.6
1150	223.7	1280	214.9
1160	223.0	1290	214.3
1170	222.3	1300	213.6
1180	221.7	1310	212.9
1190	221.0	1320	212.3
1200	220.3	1330	211.6
1210	219.6	1340	210.9
1220	219.0	1350	210.2
1230	218.3	1360	209.6
1240	217.6	1370	208.9
1250	217.0		

References [10,12].

4. Viscosity (η)

No data.

5. Electrical Conductance (κ)

Measurement method: ac technique [13]

$$\kappa = -19.5390 + 35.410 \times 10^{-3}T - 12.7951 \times 10^{-6}T^2 \quad (16.3)$$

precision: ∿ ± 0.5% uncertainty: ∿ ± 5%

Table 16.3. Electrical conductance from equation (16.3)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1145	4.231	1175	4.403
1150	4.261	1180	4.429
1155	4.291	1185	4.455
1160	4.320	1190	4.480
1165	4.348	1195	4.504
1170	4.376	1200	4.528

References [13,39].

6. Safety and Hazards

A. Hazard rating [14-16]

(i) Unknown (the "toxic" qualities of sulfates, in general, are those of the cations with which the sulfate is combined)

(ii) Vapor pressure: Li_2SO_4 decomposes just above its m.pt. (859°C), evolving aggressive and toxic fumes (SO_3; SO_2), viz:

$$Li_2SO_4 \rightleftharpoons Li_2O + SO_3 \quad (16.4.1)$$

$$SO_3 \rightleftharpoons SO_2 + \tfrac{1}{2}O_2 \quad (16.4.2)$$

B. Disaster hazards [16-19]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air

(ii) When heated to decomposition, sulfates decompose, evolving SO_3, which in turn dissociates to SO_2 and O_2 (see above); toxic, corrosive fumes

References [14-19].

7. Corrosion

Table 16.4. Corrosion studies from primary research literature

Studies	References
Metals	20,21
Metals, Fe	22
Ag	23
Thermodynamic redox diagrams	20,23,24,25
Electrochemical approach	26
Reviews: molten salts corrosion	27-29
Corrosion: annotated biblio.	30

References [20-30].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [8,9]

Table 16.5. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
1.79	∿ ± 2%

References [4-9,31].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [8,9]

Table 16.6. Heat capacity

C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
48.3	1132-1179	∿ ± 0.5%

References [8,9].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated from densities [32]

Table 16.7. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
1.2%	∿ ± 8%

References [32].

12. *Vapor Pressure (p_{vap})*

Measurement method: critical evaluation; NSRDS study [1]

Li_2SO_4 (m. pt. 859°C) decomposes not far above its melting point, with the evolution of SO_3, SO_2, and oxygen:

$$Li_2SO_4 \rightleftharpoons Li_2O + SO_3 \quad (16.5)$$

$$SO_3 \rightleftharpoons SO_2 + \tfrac{1}{2}O_2 \quad (16.6)$$

The Li_2O is soluble in molten Li_2SO_4. Measurements of the decomposition pressure have not been reported. Thermal data appear insufficient for such pressures to be calculated thermodynamically.

References [1,33,34].

13. *Thermal Conductivity (liquid) (λ_ℓ)*

No thermal conductivity studies reported.

14. *Thermal Conductivity (solid) (λ_s)*

No thermal conductivity studies reported.

15. *Cryoscopic Constant (k_f)*

Measurement method: calculated from ΔH_f° [32]

Table 16.8. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
156	∿ ± 2%

References [8,9,31,32,35-38].

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XVII. Sodium Sulfate: Na_2SO_4

1. *Melting Temperature (T_m)*

Melting point:
884° ± 2°C [1,2]

References [1-9].

2. *Density (ρ)*

Measurement method: Archimedean technique [6]

$$\rho = 2.6523 - 5.034 \times 10^{-4} T \quad (17.1)$$

precision: ± 0.06% uncertainty: ∿ ± 0.5%

Table 17.1. Densities from equation (17.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1180	2.058	1230	2.033
1190	2.053	1240	2.028
1200	2.048	1250	2.023
1210	2.043	1300	1.998
1220	2.038	1350	1.973

References [6,10-13].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [6]

$$\gamma = 639.95 - 66.48 \times 10^{-2} T + 24.3 \times 10^{-5} T^2 \quad (17.2)$$

precision: ± 0.6% uncertainty: ∿ ± 8%

Table 17.2. Surface tension from equation (17.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1180	193.8	1270	187.6
1190	193.0	1280	187.1
1200	192.1	1290	186.7
1210	191.3	1300	186.4
1220	190.6	1310	186.1
1230	189.9	1320	185.8
1240	189.2	1330	185.6
1250	188.6	1340	185.4
1260	188.1	1350	185.3

References [6,14].

4. *Viscosity (η)*

Measurement method: oscillational viscometer [55]

$$\eta = 14.8 \times 10^{-2} \exp (9990/RT) \quad (17.3)$$

precision: not estimated uncertainty: ∿ ± 25%

Table 17.3. Viscosity from equation (17.3)

T (K)	η (cp)	T (K)	η (cp)	T (K)	η (cp)
1240	8.53	1320	6.68	1400	5.37
1260	8.00	1340	6.31	1420	5.10
1280	7.52	1360	5.97	1440	4.86
1300	7.08	1380	5.66	1460	4.63

References [55].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [4]

$$\kappa = -1.42689 + 3.18608 \times 10^{-3}T \quad (17.3)$$

precision: ∿ ± 0.1% uncertainty: ∿ ± 2%

Table 17.3. Electrical conductance from equation (17.3)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1180	2.333	1220	2.460
1190	2.365	1230	2.492
1200	2.396	1240	2.524
1210	2.428		

References [4,15].

6. *Safety and Hazards*

A. Hazard rating [16-18]

(i) Unknown (the "toxic" qualities of sulfates, in general, are those of the cations with which the sulfate is combined).

(ii) Vapor pressure: At the m.pt. of Na_2SO_4 (884°C), the vapor pressures due to volatilization and due to decomposition (to oxides of sulfur) are:

$$\sim < 10^{-5}\text{mm and} \sim < 10^{-10}\text{mm}$$

respectively; at 1500°C, the vapor pressure (volatilization) is ∿ 1 mm.

B. Disaster hazards [16,19-21]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Sulfates, when heated to decomposition, evolve SO_3, which in turn dissociates to SO_2 and O_2; toxic, aggressive fumes.

References [16-21].

7. Corrosion

Table 17.5. Corrosion studies from primary research literature

Studies	References
Ni, Co Co-W, Ni-W, Co-Mo, Cr-Ni, Co-Cr, Ni-Cr-Mo, Co-Cr-Mo, Co-Cr-Nb, Co-Cr-Ta, Ni-Cr-Al, Co-Cr-Mn, Co-Cr-Fe	22,29
Ni	23,24
Metals	25,26
Metals, Fe	27
Ag	28
"Hot corrosion" studies	30
Thermodynamic redox diagrams	25,27,31,32
Electrochemical aspects	33
Corrosion: molten salts (reviews)	34-36
Annotated corrosion biblio.	37

References [22-37].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [1,8]

Table 17.6. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
5.63	∿ ± 1%

References [1,7-9,38].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [1,8]

Table 17.7. Heat capacity

C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
47.3	1157-1850	∿ ± 1%

References [1,8,39].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated from densities [40]

Table 17.8. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
18.7%	∿ ± 8%

References [40].

12. Vapor Pressure (p_{vap})

Measurement method: merged from [41] (transpiration) and [46] (Knudsen mass spectrometer)

$$\log p = 8.9796 - 15980/T \quad (17.\ )$$

precision: ± 1.3% uncertainty: ∿ ± 15%

Table 17.9. Vapor pressure from equation (17.5)

T (K)	p x 10^4 (mm)	T (K)	p x 10^4 (mm)
1200	0.46	1340	11.3
1210	0.59	1350	13.9
1220	0.76	1360	17.0
1230	0.97	1370	20.7
1240	1.24	1380	25.1
1250	1.57	1390	30.4
1260	1.98	1400	36.8
1270	2.49	1410	44.3
1280	3.13	1420	53.8
1290	3.91	1430	63.8
1300	4.87	1440	76.3
1310	6.04	1450	91.0
1320	7.47	1460	108.0
1330	9.22	1470	128.0

Thermal Decomposition

All metal sulfates decompose on heating, eventually, with the evolution of SO_3, which in turn dissociates to SO_2 and O_2. Na_2SO_4 (m.pt. 884°C) melts to form a stable fluid; no weight loss was observed at ∿ 900°C. At 1000°C and 1200°C, after 2 hrs, losses of 0.04 wt. % and 1.05 wt. %, respectively, were noted. Analysis of the residue indicated both decomposition and volatilization had contributed. Decomposition pressure data for the melt have not been reported.

The equilibrium decomposition data for Na_2SO_4 (crystalline) near the m.pt., i.e. 827°C, calculated from thermal and thermodynamic values are:

$$Na_2SO_{4(c)} \rightleftharpoons Na_2O_{(c)} + SO_{3(g)}; \qquad K, 8.22 \times 10^{-20} \quad (17.6)$$

$$Na_2SO_{4(c)} \rightleftharpoons Na_2O_{(c)} + SO_{2(g)} + \tfrac{1}{2}O_{2(g)}; \quad K, 1.38 \times 10^{-19} \quad (17.7)$$

and the corresponding equilibrium pressures are in table 17.10.

Table 17.10. Equilibrium dissociation pressures

T(K)	p_{SO_2}(atm)	p_{SO_2}(atm)	p_{SO_3}(atm)	p_{total}(atm)
1100	3.37×10^{-13}	1.69×10^{-13}	8.22×10^{-20}	5.06×10^{-3}

References: [14,41-47].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [40]

Table 17.11. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
67.1	∿ ± 2%

References [9,40,48-54].

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XVIII. Potassium Sulfate: K_2SO_4

1. *Melting Temperature (T_m)*

Melting point:
1069° ± 3°C [1-3]

References [1-11].

2. *Density (ρ)*

Measurement method: Archimedean technique [12]

$$\rho = 2.47497 - 4.5108 \times 10^{-4} T \quad (18.1)$$

precision: ∿ ± 0.06% uncertainty: ∿ ± 1%

Table 18.1. Densities from equation (18.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
1350	1.866	1390	1.848
1360	1.861	1400	1.843
1370	1.857	1410	1.839
1380	1.853		

References [7,12,49-51].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [6]

$$\gamma = 245.20 - 7.65 \times 10^{-2} T \quad (18.2)$$

precision: ± 0.1% uncertainty: ∿ ± 0.5%

Table 18.2. Surface tension from equation (18.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
1350	141.9	1380	139.6
1360	141.2	1390	138.9
1370	140.4		

References [6,7,10,13-15].

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: ac technique [8]

$$\kappa = -0.806035 + 2.01030 \times 10^{-3} T \quad (18.3)$$

precision: ∿ ± 0.13% uncertainty: ∿ ± 3%

For numerical values: see table 18.3

Table 18.3. Electrical conductance from equation (18.3)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
1342	1.892	1352	1.912
1344	1.896	1354	1.916
1346	1.900	1356	1.920
1348	1.904	1358	1.924
1350	1.908	1360	1.928

References [5,8,16-19].

6. Safety and Hazards

A. Hazard rating [20-22]

(i) Inhalation: not reported; ingestion: severe (toxicity)

(ii) Vapor pressure: at m.pt. (1069°C), p $\sim$ 0.07 mm. K_2SO_4 melts to form a stable fluid; at 1270°C, p $\sim$ 1 mm; the decomposition pressures (due to dissociation to SO_3, SO_2, and oxygen) in this temperature range are $< 10^{-7}$ mm.

B. Disaster hazards [20,23-25]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Sulfates, when heated to decomposition, evolve SO_3, which, in turn, dissociates to SO_2 and O_2; toxic, aggressive fumes.

References [20-25].

7. Corrosion

Table 18.4. Corrosion studies from primary research literature

Studies	References
Metals	26
Metals, Fe	27
Ag	28
Electrochemical approach	29
Thermodynamic redox diagrams	26,27,30,31
Molten salts corrosion: reviews	32-34
Annotated corrosion biblio.	35

References [26-35].

8. Diffusion

No diffusion studies reported.

9. *Heat of Fusion (ΔH_f^o)*

Measurement method: averaged value; cryoscopy [2,9,36]

Table 18.5. Heat of fusion

ΔH^o_f (kcal mol^{-1})	Uncertainty
8.7	∿ ± 4%

References [2,9,36].

10. *Heat Capacity (C_p)*

Measurement method: drop calorimetry [37]

Table 18.6. Heat capacity

C_p (cal $K^{-1} mol^{-1}$)	Temp. range (K)	Uncertainty
47.8	1342-1400	∿ ± 3%

References [37].

11. *Volume Change on Melting (ΔV_f)*

Measurement method: estimated; from densities [38]

Table 18.7. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
26.9%	∿ ± 8%

References [38].

12. *Vapor Pressure (p_{vap})*

Measurement method: Knudsen effusion and transpiration [39]

$$\log p = 8.2510 - 12700/T \quad (18.4)$$

precision: not estimated uncertainty: ∿ ± 10%

Results reported in equation form.

Table 18.8. Vapor pressure from equation (18.4)

T (K)	p (mm)	T (K)	p (mm)
1350	0.070	1510	0.692
1360	0.082	1520	0.787
1370	0.096	1530	0.892
1380	0.112	1540	1.01
1390	0.130	1550	1.14
1400	0.151	1560	1.29
1410	0.175	1570	1.45
1420	0.203	1580	1.63
1430	0.234	1590	1.83
1440	0.270	1600	2.06
1450	0.311	1610	2.31
1460	0.357	1620	2.58
1470	0.409	1630	2.88
1480	0.468	1640	3.21
1490	0.534	1650	3.58
1500	0.609	1660	3.98

K_2SO_4

Thermal decomposition: critical analysis; NSRDS study [1]

All metal sulfates eventually decompose, evolving SO_3 which, in turn dissociates to SO_2 and O_2. K_2SO_4 (m.pt. 1069°C) melts without significant decomposition. The weight loss observed at 1000°C after 2 hrs was barely measurable, whereas at 1200°C, and comparable time, the weight loss was ∿ 3.6%. The interpretation of these data as due to two simultaneous processes, sublimation and decomposition is in conflict. High temperature thermal data are insufficient to resolve the discrepancies.

References [1,39-45].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [38]

Table 18.9. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
71.7	∿ ± 4%

References [2,9,36,38,46-48].

16. References

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[22] Vapor pressure, calculated (see p. 181, this work).

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XIX. Sulfur

1. *Melting Temperatures (T_m)*

Melting points [1-3,46]

Monoclinic: 115° ± 0.5°C
Rhombic: 110°C

Transition temperature:

Rhombic ⟶ monoclinic: 95°C

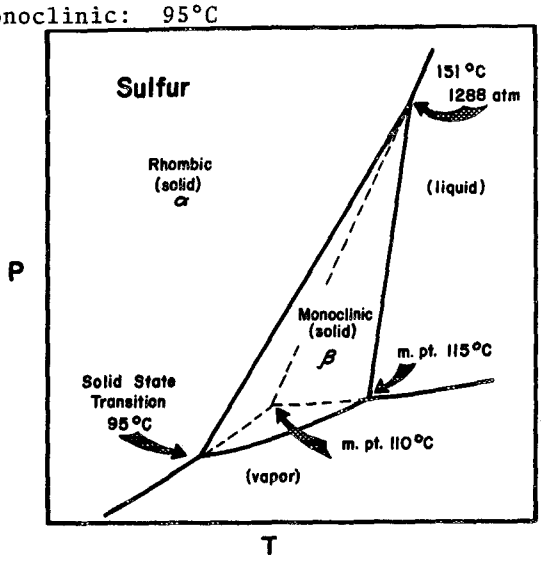

Figure 19.1. Sulfur phase diagram

References [1-7,46].

2. *Density (ρ)*

Measurement method: dilatometer [8-10]

$$\rho = a - bT \quad (19.1)$$

Table 19.1. Parameters of equation (19.1), precisions and uncertainties

Temp. range(K)	a	b x 10^3	Precision	Uncertainty
394-428	2.1365	0.84_6	±0.01%	~±0.5%
451-718	2.0445	0.610	±0.09%	~±0.5%

Table 19.2. Densities from equations in table 19.1

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
400	1.7982	560	1.7027
420	1.7813	580	1.6905
440	(1.771)	600	1.6783
460	1.7637	620	1.6661
480	1.7515	640	1.6538
500	1.7393	660	1.6416
520	1.7271	680	1.6294
540	1.7149	700	1.6172
550	1.7088	710	1.6111

Value in brackets interpolated.

References [8-13].

3. *Surface Tension (γ)*

Measurement method: capillary rise; maximum bubble pressure [14]

$$\gamma = 102.1 - 0.105\ T \quad (388\text{-}432\ K) \qquad (19.2)$$

$$\gamma = 81.2 - 0.0566\ T \quad (432\text{-}707\ K) \qquad (19.3)$$

precision: ∿ ± 0.5% uncertainty: ∿ ± 1%

Table 19.3. Surface tension from equations (19.2) and (19.3)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
380	(62.2)	510	52.3
385	(61.7)	520	51.8
390	61.1	530	51.2
395	60.6	540	50.6
400	60.1	550	50.0
405	59.6	560	49.5
410	59.0	570	48.9
415	58.5	580	48.4
420	58.0	590	47.8
425	57.5	600	47.2
430	56.9	610	46.7
440	56.3	620	46.1
450	55.7	630	45.5
460	55.2	640	45.0
470	54.6	650	44.4
480	54.0	660	43.8
490	53.5	670	43.3
500	52.9	680	42.7
		690	42.1
		700	41.6

References [8,12,14].

4. *Viscosity (η)*

Measurement method: capillary; rolling ball; and modified capillary [15, 6

$$\eta = a + bT + cT^2 \qquad (19.4)$$

precision: in table 19.4 uncertainty: ∿ ± 1.5%

Table 19.4. Parameters of equation (19.4) and precisions

a x 10^{-3}	-b x 10^{-2}	c x 10^{2}	T range(K)	Precision
31.886_5	1.1359_1	10.121_2	466-533	∿±3.5%
9.312_5	0.3148	2.665_4	544-589	∿±2.9%

Table 19.5. Viscosity from equations in table 19.4

T (K)	η (p)	T (K)	η (p)	T (K)	η (p)
322.1	0.759	427.6	0.065	511.0	250
333.2	0.491	430.4	0.067	522.1	160
344.3	0.342	432.1	0.12	533.2	110
355.4	0.253	436.0	120	544.3	74
366.5	0.193	438.8	210	555.4	52
377.6	0.149	444.3	460	566.5	34
388.8	0.119	455.4	890	577.6	22
394.3	0.110	461.0	930	588.7	18
399.9	0.100	466.5	910	590	(14)
405.4	0.089	472.1	820	600	(10)
411.0	0.080	477.6	730	610	(7)
416.5	0.074	488.7	570	620	(5)
422.1	0.067	499.9	390	630	(3.5)

Values in parenthesis, by extrapolation

References [15-17].

5. *Electrical Conductance (κ)*

Measurement method: dc technique [67,68].

$$\kappa = 2.60 \times 10^{-3} \exp[-22265/RT] \quad (490\text{-}690\ K) \quad (19.5)$$

precision: ∿ ± 5% uncertainty: ∿ ± 10%

Table 19.6.1. Electrical conductance[a]

T (K)	κ x 10^{14} ($ohm^{-1}cm^{-1}$)	T (K)	κ x 10^{14} ($ohm^{-1}cm^{-1}$)
398.15	0.9	428.15	1.8
403.15	1.2	433.15	1.5
408.15	1.4	438.15	1.8
413.15	1.7	443.15	2.3
418.15	2.05	448.15	2.7
423.15	2.4		

[a]Experimental values [67]; zone refined sulfur

Table 19.6.2. Electrical conductance from equation (19.5)[a]

T (K)	$\kappa \times 10^{12}$ ($ohm^{-1}cm^{-1}$)	T (K)	$\kappa \times 10^{12}$ ($ohm^{-1}cm^{-1}$)
490	0.305	600	20.16
500	0.481	610	27.38
510	0.747	620	36.82
520	1.14	630	49.05
530	1.71	640	64.77
540	2.53	650	84.79
550	3.69	660	110.1
560	5.31	670	141.9
570	7.54	680	181.4
580	10.59	690	230.3
590	14.69		

[a]Zone refined sulfur [68]

Table 19.6.3. Electrical conductivities of molten sulfur of various purities

Sulfur quality	$\kappa \times 10^{14}$ ($ohm^{-1}cm^{-1}$)			
	448.15 K	533.15 K	615 K	628 K
zone refined [67,68]	2.7	194	3178	4633
resublimed [66]			b	
refluxed with MgO [67,69][a]	16	130		
"hot spot" reflux [67,70][a]	22	320		
oxidation method [67,71][a]	2.0			
Zone refined sulfur				
doped with 0.02% benzil [67]	43			
doped with 0.015% bromine [67]	1100			
doped with 0.2% bromine [67]	22000			
Resublimed sulfur				
saturated with Na_2S_5 [66]				c

[a]Hydrocarbon content : 3.7×10^{-4}% [69,72]; 5.2×10^{-4}% [70,72]; 8.2×10^{-4}% [71,72]

[b]κ, $1 \times 10^{-8} ohm^{-1} cm^{-1}$

[c]κ, $1 \times 10^{-7} ohm^{-1}cm^{-1}$; for data at other temperatures in the range 576-690K, see [66]

References [18-23,66-72].

6. Safety and Hazards

A. Hazard rating [24-26]

(i) low

(ii) vapor pressure: at m.pt. of sulfur (115°C), ∿ 0.03 mm; increases rapidly to 1 mm at ∿ 185°C; the boiling point (atmospheric pressure) is ∿ 444.6°C

B. Disaster hazards [24,27-29]

(i) When heated to decomposition, sulfur burns with the formation of SO_2 and SO_3; toxic aggressive fumes.

References [24-29].

7. Corrosion

Table 19.7. Corrosion studies from primary research literature

Studies	References
Cast iron Mild steel SS-410, SS-430, SS-304 Hastelloy C Cu, Mn, Cu-Mn alloys Ni Monel, "K" Monel Inconel Ni-Resist	30
Ag-Zn; Ag-Al alloys	31
various metals (survey; 104 ref)	32
Fe	33

References [30-33].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in sulfur as solvent

P, S

The italicized species indicate studies with insufficient data-sets for characterization of temperature-dependence of diffusion coefficients. For these species: see table 19.8.4

Equation

$$D = A \exp[-E/RT] \quad (19.6)$$

precision: in table 19.8.2 uncertainty: in table 19.8.1

Table 19.8.1 Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
capillary	~ ± 20%	^{32}P
porous frit	~ ± 20%	^{35}S

Table 19.8.2. Diffusion equation parameters, precision, and recommended study

Species	A x 10^3 ($cm^2 sec^{-1}$)	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
^{35}S	281700	15167	395-420	± 5.5%	73
^{35}S	0.218	5348	540-590	± 2.5%	73

Table 19.8.3. Diffusion coefficients of sulfur[a]

T (K)	D x 10^6 ($cm^2 sec^{-1}$)	T (K)	D x 10^6 ($cm^2 sec^{-1}$)	T (K)	D x 10^6 ($cm^2 sec^{-1}$)
395.6	1.05	431.6	1.45	488.1	0.95
396.1	1.20	436.1	1.31	504.1	0.80
398.1	1.45	436.5	1.24	509.1	0.83
399.1	1.52	440.6	1.17	513.1	0.91
412.1	2.50	443.1	1.53	541.1	1.55
414.6	2.80	453.1	1.03	546.1	1.52
421.1	3.90	456.1	0.90	547.1	1.23
422.1	3.85	458.1	0.86	551.1	2.05
422.1	2.42	465.1	0.71	565.1	1.90
426.1	2.45	472.1	0.71	580.1	2.34
427.6	2.90	474.1	0.84	580.1	2.10
428.1	3.22	479.1	0.87	589.1	2.26

[a]Experimental values of diffusion coefficients.

Table 19.8.4. Diffusion coefficients for species not included in table 19.8.3.

Species	T (K)	D x 10^6 ($cm^2 sec^{-1}$)	Ref.
P	387	0.82	34

References: P, 34; S, 73.

9. *Heat of Fusion (ΔH_f°)*

Measurement method: adiabatic calorimetry [35]

Table 19.9. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
3.07[a]	∿ ± 0.5%

[a]calc'd as S_8

References [1,6,35-45].

10. *Heat Capacity (C_p)*

Measurement method: adiabatic calorimetry [36,42,43]

Table 19.10. Heat capacity[a]

T (K)	C_p (cal $K^{-1}mol^{-1}$)	T (K)	C_p (cal $K^{-1}mol^{-1}$)
393	7.40	498	8.53
398	7.42	503	8.52
403	7.44	508	8.51
408	7.46	513	8.51
413	7.49	518	8.50
418	7.54	523	8.50
423	7.61	528	8.50
428	7.83	533	8.50
432	8.33	538	8.51
435	12.48	543	8.51
438	11.59	548	8.52
443	10.70	553	8.53
448	10.13	558	8.55
453	9.73	563	8.56
458	9.46	568	8.56
463	9.22	573	8.57
468	8.98	578	8.60
473	8.83	583	8.62
478	8.73	588	8.65
483	8.66	593	8.68
488	8.57	598	8.70
493	8.55		

uncertainty: ∿ ± 1%

[a]The data cannot be expressed as a simple equation since there is an abrupt increase in C_p at ∿ 428 K (155°C) peaking at ∿ 432 K (159°C).

References [1,5,6,35,36,42,43,46,47].

11. *Volume Change on Melting (ΔV_f)*

Measurement method: estimated [48]

Table 19.11. Volume changes and uncertainties

Transition	Temp (°C)	$(\Delta V_f/V_s)$	Uncertainty
monoclinic → liquid	115	8.5%	∿±5%
liquid (ring) → liquid (polymer)	159	5.3%	∿±3%

References [48-51].

12. Vapor Pressure (p_{vap})

Measurement method: isoteniscope; modified dew point [55]

$$\log p = A + B/T \quad (19.7)$$

Table 19.12. Parameters of equation (19.7), temperature range, and precisions

Temp. range (K)	A	-B	Precision
413-453	9.3614	4263.7	±0.72%
463-613	8.1246	3682.3	±1.2%
613-653	7.5549	3347.6	±5.2%
663-693	7.4553	3282.5	±0.01%
693-723	7.4254	3261.7	±0.01%

Table 19.13. Vapor pressure from equations in table 19.12

T (K)	p (mm)	T (K)	p (mm)
420	0.16	580	59.7
430	0.28	590	76.5
440	0.47	600	97.1
450	0.77	610	122.5
460	1.32	620	143.1
470	1.95	630	174.3
480	2.84	640	211.0
490	4.07	650	254.0
500	5.75	660	303.6
510	8.02	670	359.8
520	11.0	680	424.7
530	15.0	690	499.0
540	20.2	700	583.2
550	26.9	710	678.4
560	35.4	720	785.7
570	46.2	730	906.4

References [52-57].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: horizontal plate [58]

precision: not estimated uncertainty: ∿ ± 20%

For numerical values: see table 19.14

Table 19.14. Thermal conductivity of melt

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
388	3.14	438	3.36
393	3.16	443	3.40
403	3.21	453	3.51
413	3.26	463	3.60
423	3.31	473	3.69
433	3.36	483	3.78

References [58-64].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: steady state linear heat flow [63]

precision: not estimated uncertainty: ∿ ± 10%

Table 19.15. Thermal conductivity of solid

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
Rhombic Sulfur	
285.03	6.58
292.61	6.56
306.38	6.42
316.76	6.33
322.26	6.28
332.26	6.22
337.27	6.17
347.23	6.08
354.80	6.00
Monoclinic Sulfur	
369.65	3.69
370.94	3.67
371.41	3.58
376.17	3.67
378.38	3.72
382.13	3.58
383.10	3.64
384.16	3.53
384.75	3.72
386.38	3.58
386.92	3.80
388.11	3.53
388.67	3.64

References [63-65].

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [48]

Table 19.16. Cryoscopic constant

k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
25.0	∿ ± 0.5%

References [48].

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XX. Sodium Sulfide: Na_2S

1. *Melting Temperature (T_m)*

Melting point:
1170° ± 10°C [1,4-8]

References [1-9].

2. *Density (ρ)*

No data.

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

No data.

6. *Safety and Hazards*

A. Hazard rating [10,11]

(i) Inhalation: variable

- as sulfides and polysulfides, the rating is similar to sodium hydroxide
- on reaction with moisture/water, H_2S is liberated; the inhalation hazard rating for H_2S is severe; i.e., highly toxic

(ii) vapor pressure: no data

B. Disaster hazards [10,12-14]

(i) Molten sulfides and polysulfides may react violently (explosively) with strong oxidants: H_2S evolved on contact with moisture/water can form explosive mixtures with air; H_2S, highly toxic.

(ii) Sulfides and polysulfides when heated to decomposition, or contacted with water, steam, acids, produce highly toxic fumes (oxides of sulfur, H_2S). Dangerous.

References [10-14].

7. *Corrosion*

For corrosion studies, see sodium polysulfides, Na_2S_x

8. *Diffusion*

No diffusion studies reported with molten Na_2S as solvent.

9. Heat of Fusion (ΔH_f°)

Measurement method: calc'd [19]

Table 20.1. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
5.0	∿ ± 20%

References [3,15-19].

10. Heat Capacity (C_p)

Measurement method: estimated [18,20]

$$C_p = 21.516 + 2.24 \times 10^{-4} T \quad (20.1)$$

precision: ∿ ± 0.2% uncertainty: ∿ ± 5-10%

Table 20.2. Heat capacity from equation (20.1)

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
1300	21.807	1480	21.848
1320	21.812	1500	21.852
1340	21.816	1600	21.874
1360	21.821	1700	21.897
1380	21.825	1800	21.919
1400	21.830	1900	21.942
1420	21.834	2000	21.964
1440	21.839		
1460	21.843		

References [18,20,21].

11. Volume Change on Melting (ΔV_f)

No data; but see NaF, NaCl, $NaNO_3$...

12. Vapor Pressure (p_{vap})

No vapor pressure data.

Caution: When heated to decomposition, or contacted with water vapor, H_2S is liberated (highly toxic).

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: comparative technique [22]

precision: not estimated uncertainty: ∿ ± 20%

For numerical values: see table 20.3.

Table 20.3. Thermal conductivity of melt

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	Sample type
573	4.06	a
623	4.06	
573	8.36	b
623	8.36	

[a] Na_2S-C-S composite with the graphite fibers randomly oriented.
[b] Na_2S-C-S composite with the graphite fibers oriented in the direction of heat flow.

References [22].

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [23]

Table 20.4. Cryoscopic constant

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
20.1	∿ ± 3%

Reference [23].

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XXI. Sodium Disulfide: Na_2S_2

1. *Melting Temperature (T_m)*

   Melting point:
   482° ± 2°C [1]

   References [1,2].

2. *Density (ρ)*

   No data; however, see sodium polysulfides, Na_2S_x.

3. *Surface Tension (γ)*

   No data; however, see sodium polysulfides, Na_2S_x.

4. *Viscosity (η)*

   No data; however, see sodium polysulfides, Na_2S_x.

5. *Electrical Conductance (κ)*

   No data; however, see sodium polysulfides, Na_2S_x.

6. *Safety and Hazards*

   No data; see Na_2S and Na_2S_x for observations on hazards.

   Vapor pressure: the sulfur pressure above molten Na_2S_2 at $\sim$ 1000°C is approx. 15 mm.

7. *Corrosion*

   For corrosion studies, see sodium polysulfides, Na_2S_x.

8. *Diffusion*

   No diffusion studies reported.

9. *Heat of Fusion (ΔH_f°)*

   No data; however, see sodium polysulfides, Na_2S_x.

10. *Heat Capacity (C_p)*

    No data; however, see sodium polysulfides, Na_2S_x.

11. *Volume Change on Melting (ΔV_f)*

    No data; however, see sodium polysulfides, Na_2S_x.

12. *Vapor Pressure (p_{vap})*

    See sodium polysulfides, Na_2S_x, for equilibrium vapor pressures of sulfur above molten polysulfides.

13. *Thermal Conductivity (liquid) (λ_ℓ)*

    No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

16. References

[1] Rosen, E., and Tegman, R., Acta Chem. Scand., 25, 3329 (1971).

[2] Rosen, E., and Tegman, R., Chimica Scripta, 2, 221 (1972).

XXII. Sodium Trisulfide: Na_2S_3

1. *Melting Temperature (T_m)*

Melting point:
230°C [4]

References [1-4].

2. *Density (ρ)*

See sodium polysulfides, Na_2S_x.

3. *Surface Tension (γ)*

See sodium polysulfides, Na_2S_x.

4. *Viscosity (η)*

See sodium polysulfides, Na_2S_x.

5. *Electrical Conductance (κ)*

See sodium polysulfides, Na_2S_x.

6. *Safety and Hazards*

No data; however, see Na_2S and Na_2S_x for observations on hazards.

Vapor pressure: the sulfur pressure above molten Na_2S_3 is approx. 10 mm at 750°C, and ∿300 mm at ∿1000°C.

References [5].

7. *Corrosion*

For corrosion studies; see sodium polysulfides, Na_2S_x.

8. *Diffusion*

No diffusion studies reported with molten Na_2S_3 as solvent.

9. *Heat of Fusion (ΔH_f°)*

No data; however, see sodium polysulfides, Na_2S_x.

10. *Heat Capacity (C_p)*

No data; however, see sodium polysulfides, Na_2S_x.

11. *Volume Change on Melting (ΔV_f)*

Measurement method: estimated [6]

Table 22.1. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
3.5%	∿ ± 5-10%

References [6].

12. Vapor Pressure (p_{vap})

See sodium polysulfides, Na_2S_x, for equilibrium vapor pressures of sulfur above molten polysulfides.

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: comparative technique [7]

precision: not estimated uncertainty: ∿ ± 20%

Table 22.2. Thermal conductivity of melt

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	Sample
573	6.45	a
623	6.45	
573	10.76	b
623	10.76	
573	5.23	c
623	5.23	
573	9.56	d
623	9.56	

[a] Na_2S_3-C-S composite with the graphite fibers randomly oriented.
[b] Na_2S_3-C-S composite with the graphite fibers oriented in the direction of heat flow.
[c] Na_2S_3-C-S composite with the graphite fibers randomly oriented, loading fraction of the cell one-half of that in (a) above
[d] Na_2S_3-C-S composite with the graphite fibers oriented in the direction of heat conduction and with a loading fraction of the cell corresponding to one-half of that in (b) above

References [7].

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

16. References

[1] Rosen, E., and Tegman, R., Acta Chem. Scand., 25, 3329 (1971).

[2] Rosen, E., and Tegman, R., Chimica Scripta, 2, 221 (1972).

[3] Oei, D. G., Inorg. Chem., 12, 435, 438 (1973).

[4] Janz, G. J., Downey, J. R., Jr., Coutts, J. C., Roduner, E., and Wasilczyk, G., Inorg. Chem., 15, 1751, 1755, 1759 (1976).

[5] Tiberg, A., and Tiberg, J., Acta Chemica Scand., 24, 991 (1970).

[6] Janz, G. J., et al., (MSDC-RPI) unpublished work (1977).

[7] Chatterji, D., General Electric Co., R. & D. Center, *"Development of Sodium-Sulfur Batteries for Utility Application"*, EPRI EM-266 (Dec., 1976).

XXIII. Sodium Tetrasulfide: Na_2S_4

1. *Melting Temperature (T_m)*

Melting point:
294° ± 2°C [1]

References [1-4].

2. *Density (ρ)*

Measurement method: pycnometric [3]

precision: not estimated uncertainty: ∿ ± 3%

Table 23.1. Densities

T (K)	ρ (g cm^{-3})
623	1.827
673	1.776
723	1.678

For densities of polysulfides with non-stoichiometric compositions, see: sodium polysulfides, Na_2S_x.

References [3].

3. *Surface Tension (γ)*

Measurement method: Wilhelmy slide plate method [3]

precision: not estimated uncertainty: ∿ ± 3%

Table 23.2. Surface tension

T (K)	γ (dyn cm^{-1})
623	136
673	134
713	130

For surface tension of polysulfides with non-stoichiometric compositions, see: sodium polysulfides, Na_2S_x.

References [3].

4. *Viscosity (η)*

No data; however, see sodium polysulfides, Na_2S_x.

5. *Electrical Conductance (κ)*

No data; however, see sodium polysulfides, Na_2S_x.

6. Safety and Hazards

No data, however, see Na_2S and Na_2S_x for observations on hazards.

Vapor pressure: the sulfur vapor pressure above molten Na_2S_4 is ∿ 18 mm at approx. 500°C, ∿ 200 mm at approx. 700°C, and ∿ 1 atm at approx. 850°C.

References [5,6].

7. Corrosion

For corrosion studies, see sodium polysulfides, Na_2S_x.

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

No data; however, see sodium polysulfides, Na_2S_x.

10. Heat Capacity (C_p)

No data; however, see sodium polysulfides, Na_2S_x.

11. Volume Change on Melting (ΔV_f)

Table 23.3. Volume change on melting

Measurement method: estimated [7]

$(\Delta V_f/V_s)$	Uncertainty
7.0%	∿ ± 10%

References [7].

12. Vapor Pressure (p_{vap})

See: sodium polysulfides, Na_2S_x, for equilibrium vapor pressures of sulfur above molten polysulfides.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

16. References

[1] Rosen, E., and Tegman, R., Acta Chem. Scand., 25, 3329 (1971).

[2] Rosen, E., and Tegman, R., Chimica Scripta, 2, 221 (1972).

[3] Øei, D. G., Inorg. Chem., 12, 435, 438 (1973).

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[5] Tiberg, A., and Tiberg, J., Acta Chemica Scand., 24, 991 (1970).

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[7] Janz, G. J., et al., (MSDC-RPI) unpublished work (1977).

XXIV. Sodium Pentasulfide: Na_2S_5

1. *Melting Temperature (T_m)*

Melting point:
264° ± 10°C [1-4].

References [1-4].

2. *Density (ρ)*

Measurement method: pycnometric [3]

precision: not estimated uncertainty: ∿ ± 3%

Table 24.1. Densities

T (K)	ρ (g cm^{-3})
623	1.754
673	1.728
723	1.669

For densities of polysulfides with non-stoichiometric compositions, see: sodium polysulfides, Na_2S_x.

References [3].

3. *Surface Tension (γ)*

Measurement method: plate, detachment [3]

precision: not estimated uncertainty: ∿ ± 3%

Table 24.2. Surface tension

T (K)	γ (dyn cm^{-1})
633	121
673	116
703	114

For surface tension of polysulfides with non-stoichiometric compositions, see: sodium polysulfides, Na_2S_x.

References [3].

4. *Viscosity (η)*

No data; however, see sodium polysulfides, Na_2S_x.

5. *Electrical Conductance (κ)*

No data; however, see sodium polysulfides, Na_2S_x.

6. *Safety and Hazards*

No data; however, see Na_2S and Na_2S_x for observations on hazards.

Vapor pressure: for equil. sulfur vapor pressures over some molten polysulfides see e.g., Na_2S_2, Na_2S_3 and Na_2S_4.

7. *Corrosion*

For corrosion studies, see sodium polysulfides, Na_2S_x.

8. *Diffusion*

No diffusion studies reported with molten Na_2S_5 as solvent.

9. *Heat of Fusion (ΔH_f°)*

No data; however, see sodium polysulfides, Na_2S_x.

10. *Heat Capacity (C_p)*

No data; however, see sodium polysulfides, Na_2S_x.

11. *Volume Change on Melting (ΔV_f)*

Measurement method: estimated [5]

Table 24.3. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
5.0%	$\sim \pm$ 10%

References [5].

12. *Vapor Pressure (p_{vap})*

See: sodium polysulfides, Na_2S_x, for equilibrium vapor pressures of sulfur above molten polysulfides.

13. *Thermal Conductivity (liquid) (λ_ℓ)*

No thermal conductivity studies reported.

14. *Thermal Conductivity (solid) (λ_s)*

No thermal conductivity studies reported.

15. *Cryoscopic Constant (k_f)*

No data.

16. *References*

[1] Rosen, E., and Tegman, R., Acta Chem. Scand., 25, 3329 (1971).

[2] Rosen, E., and Tegman, R., Chimica Scripta, 2, 221 (1972).

[3] Oei, D. G., Inorg. Chem., 12, 435,438 (1973).

[4] Janz, G. J., Downey, J. R., Jr., Coutts, J. C., Roduner, E., and Wasilczyk, G., Inorg. Chem., 15, 1751, 1755, 1759 (1976).

[5] Janz, G. J., et al., (MSDC-RPI), unpublished work (1977).

XXV. Lithium Bromide: LiBr

1. *Melting Temperature (T_m)*

Melting point:
552° ± 3°C [1,2,33]

References [1-9,33].

2. *Density (ρ)*

Measurement method: Archimedean technique [3]

$$\rho = 3.06546 - 6.5146 \times 10^{-4} T \quad (25.1)$$

precision: ∿ ± 0.02% uncertainty: ∿ ± 1.5%

Table 25.1. Densities from equation (25.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
830	2.5247	930	2.4596
840	2.5182	940	2.4531
850	2.5117	950	2.4466
860	2.5052	960	2.4401
870	2.4987	970	2.4335
880	2.4922	980	2.4270
890	2.4857	990	2.4205
900	2.4791	1000	2.4140
910	2.4726	1010	2.4075
920	2.4661	1020	2.4010

References [3-5,8,10,11].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [12]

$$\gamma = 185.2 - 6.91 \times 10^{-2} T \quad (25.2)$$

precision: not estimated uncertainty: ∿ ± 1%

Table 25.2. Surface tension from equation (25.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
860	125.8	990	116.8
870	125.1	1000	116.1
880	124.4	1010	115.4
890	123.7	1020	114.7
900	123.0	1030	114.0
910	122.3	1040	113.3
920	121.6	1050	112.6
930	120.9	1060	112.0
940	120.2	1070	111.3
950	119.5	1080	110.6
960	118.9	1090	109.9
970	118.2	1100	109.2
980	117.5	1110	108.5

References [12-14].

4. Viscosity (η)

Measurement method: oscillating sphere [7]

$$\eta = 13.8907 - 2.30413 \times 10^{-2}T + 1.0167 \times 10^{-5}T^2 \quad (25.3)$$

precision: ± 0.7% uncertainty: ∿ ± 25%

Table 25.3. Viscosity from equation (25.3)

T (K)	η (cp)	T (K)	η (cp)
870	1.536	960	1.141
880	1.488	970	1.107
890	1.437	980	1.075
900	1.389	990	1.044
910	1.342	1000	1.016
920	1.298	1010	0.993
930	1.256	1020	0.966
940	1.215	1030	0.944
950	1.177	1040	0.924

References [6,7].

5. Electrical Conductance (κ)

Measurement method: ac technique [3]

$$\kappa = -1.1362 + 8.6159 \times 10^{-3}T - 1.86212 \times 10^{-6}T^2 \quad (25.4)$$

precision: ± 0.47% uncertainty: ∿ ± 3.5%

Table 25.4. Electrical conductance from equation (25.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
830	4.7322	930	5.2660
840	4.7872	940	5.3174
850	4.8419	950	5.3683
860	4.8963	960	5.4189
870	4.9502	970	5.4692
880	5.0038	980	5.5190
890	5.0570	990	5.5685
900	5.1098	1000	5.6176
910	5.1622	1010	5.6663
920	5.2143	1020	5.7147

References [3,8,9,11,15-17].

6. Safety and Hazards

A. Hazard rating [18-20]

(i) Toxicity - moderate

(ii) Vapor pressure: at m.pt. (552°C), ∿ 9.2×10^{-3} mm; at 750°C, ∿ 1 mm

B. Disaster hazards [18,21-23]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air

(ii) Bromides when heated to decomposition, or contacted with acids, emit highly toxic fumes

References [18-23].

7. Corrosion

Table 25.5. Corrosion studies from primary research literature

Studies	References
Supremax glass	24-26
Molten salts corrosion : reviews	27-29
Annotated corrosion biblio.	30

References [24-30].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [2]

Table 25.6. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
4.22	∿ ± 1%

References [2,31].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [32]

Table 25.7. Heat capacity

C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
15.60	823-883	∿ ±2%

References [32,33].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [34]

Table 25.8. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
24.3%	∿ ± 3%

Reference [34].

12. *Vapor Pressure* (p_{vap})

Measurement method: boiling point [38]

$$\log p = 8.6340 - 8803/T \quad (25.5)$$

precision: ∿ ± 2.70% uncertainty: ∿ ± 10%

Table 25.9.1. Vapor pressure from equation (25.5)

T (K)	p (mm)	T (K)	p (mm)
1290	64.6	1420	272.1
1300	72.9	1430	300.7
1310	82.1	1440	331.7
1320	92.3	1450	365.6
1330	103.6	1460	402.3
1340	116.0	1470	442.2
1350	129.8	1480	485.3
1360	144.9	1490	532.0
1370	161.6	1500	582.6
1380	179.9	1510	637.1
1390	199.9	1520	695.9
1400	221.9	1530	759.3
1410	245.9		

Measurement method: effusion [37]

precison: not estimated uncertainty: ∿ ± 5%

Table 25.9.2. Additional vapor pressure data

T (K)	p (mm)
861	5.61×10^{-2}

References [35-38].

13. *Thermal Conductivity (liquid)* (λ_ℓ)

Measurement method: transient hot wire [39,40]

precision: not estimated uncertainty: ∿ ± 20%

Table 25.10. Thermal conductivity of melt

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
878	9.42
974	9.42

References [39,40].

14. *Thermal Conductivity (solid) (λ_s)*

No thermal conductivity studies reported.

15. *Cryoscopic Constant (k_f)*

Measurement method: calculated from ΔH_f° [41]

Table 25.11. Cryoscopic constant

k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
27.8	∿ ± 1%

References [2,41,42]

16. *References*

[1] Rossini, F. D., Wagman, D. D., Evans, W. H., Levine, S., and Jaffe, I., *"Selected Values of Chemical Thermodynamic Properties, NBS Circ. 500,"* U. S. Gov't Printing Office, Washington, D. C. (1952).

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[20] Vapor pressure, calculated (see p. 215, this work).

[21] *"Potential Hazards In Molten Salt Baths for Heat Treatment of Metals"*, National Board Fire Underwriters Research Report No. 2 (1954).

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XXVI. Lithium Iodide: LiI

1. *Melting Temperature (T_m)*

Melting point:
469° ± 3°C [1,2,27]

References [1-7,27].

2. *Density (ρ)*

Measurement method: Archimedean technique [5]

$$\rho = 3.79045 - 9.1780 \times 10^{-4} T \quad (26.1)$$

precision: ∿ ± 0.01% uncertainty: ∿ ± 2%

(partial decomposition of LiI reported at higher experimental temperatures)

Table 26.1. Densities from equation (26.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
760	3.0931	830	3.0289
770	3.0839	840	3.0197
780	3.0747	850	3.0105
790	3.0656	860	3.0013
800	3.0564	870	2.9922
810	3.0472	880	2.9830
820	3.0380		

References [5-7].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [8]

$$\gamma = 140.7 - 5.65 \times 10^{-2} T \quad (26.2)$$

precision: not estimated uncertainty: ∿ ± 1%

Table 26.2. Surface tension from equation (26.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
860	92.1	990	84.8
870	91.5	1000	84.2
880	91.0	1010	83.6
890	90.4	1020	83.1
900	89.9	1030	82.5
910	89.3	1040	81.9
920	88.7	1050	81.4
930	88.1	1060	80.8
940	87.6	1070	80.2
950	87.0	1080	79.7
960	86.5	1090	79.1
970	85.9	1100	78.5
980	85.3	1110	78.0

References [8,9].

Errata Sheet to accompany NSRDS-NBS 61, Part II
Physical Properties Data Compilations Relevant to Energy Storage.
II. Molten Salts: Data on Single and Multi-Component Salt Systems
G. J. Janz, C. B. Allen, N. P. Bansal, R. M. Murphy, and R. P. T. Tomkins

Page 175: The heading for the third column of table 17.10 should be p_{O_2} (atm).

Page 187: Replace table 19.4 with the following:

Table 19.4. Parameters of equation (19.4) and precisions[a]

a x 10^{-3}	-b x 10^{-2}	c x 10^{2}	T range (K)	Precision
-14.9135	-0.3452	-	440-460	~±11%
31.886_5	1.1359_1	10.121_2	466-533	~±3.5%
9.312_5	0.3148	2.665_4	544-589	~±2.9%

(a) for 330-420K, $\eta = 3.54642 \times 10^{-5} \exp(6305.9/RT)$, precision ~ ± 18%

Page 396: The missing tabular matter under the heading for table 45.1 is as follows:

a	b x 10^{7}	c x 10^{10}	Precision
2.06431	-4.76248	-5.60825	± 0.1%

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a	b x 10^{7}	c x 10^{10}	Precision
2.06431	-4.76248	-5.60825	± 0.1%

4. Viscosity (η)

Measurement method: oscillating sphere [4]

$$\eta = 17.1411 - 3.14517 \times 10^{-2}T + 1.54597 \times 10^{-5}T^2 \quad (26.3)$$

precision: ± 0.4% uncertainty: ∿ ± 25%

Table 26.3. Viscosity from equation (26.3)

T (K)	η (cp)	T (K)	η (cp)
		830	1.69
		840	1.63
750	2.25	850	1.58
760	2.17	860	1.53
770	2.09	870	1.48
780	2.01	880	1.44
790	1.94	890	1.39
800	1.87	900	1.36
810	1.81	910	1.32
820	1.75	920	1.29

References [4,10].

5. Electrical Conductance (κ)

Measurement method: ac technique [11]

$$\kappa = -3.64062 + 1.47826 \times 10^{-2}T - 6.28111 \times 10^{-6}T^2 \quad (26.4)$$

precision: ± 0.060% uncertainty: ∿ ± 2.5%

Table 26.4. Electrical conductance from equation (26.4)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
760	3.9662	820	4.2577
770	4.0179	830	4.3019
780	4.0684	840	4.3448
790	4.1176	850	4.3865
800	4.1655	860	4.4269
810	4.2122	870	4.4660
		880	4.5039

References [3,5-7,11].

6. Safety and Hazards

A. Hazard rating [12-14]

(i) Similar in toxicity to LiBr; moderate

(ii) Vapor pressure: at m.pt. (469°C), ∿ 2.8×10^{-3} mm; at 700°C, ∿ 1 mm

B. Disaster hazards [12,15-17]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air

(ii) Iodides when heated to decomposition can evolve highly toxic fumes of iodine and iodides; dangerous

References [12-17].

7. Corrosion

Table 26.5. Corrosion studies from primary research literature

Studies	References
Supremax glass	18-20
Molten salts corrosion: reviews	21-23
Annotated corrosion biblio.	24

References [18-24].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [25]

Table 26.6. Heat of fusion

ΔH_f° (kcal mol^{-1})	Uncertainty
3.50	∿ ± 1.5%

References [25].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [26]

Table 26.7. Heat capacity

C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
15.10	742-802	∿ ± 2%

References [26,27].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated; from densities [28]

Table 26.8. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
24.7%	∿ ± 8%

References [28].

12. Vapor Pressure (p_{vap})

Measurement method: boiling point [29]

$$\log p = 8.5901 - 8270/T \quad (26.5)$$

precision: ∿ ± 1.5% uncertainty: ∿ ± 10%.

Table 26.9. Vapor pressure from equation (26.5)

T (K)	p (mm)	T (K)	p (mm)
1230	73.5	1330	235.5
1240	83.3	1340	262.1
1250	94.2	1350	291.2
1260	106.3	1360	323.0
1270	119.8	1370	357.8
1280	134.6	1380	395.7
1290	151.1	1390	437.0
1300	169.3	1400	481.9
1310	189.3	1410	530.7
1320	211.3		

References [29,30].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calculated from ΔH_f° [28]

Table 26.10. Cryoscopic constant

k_f (K mol^{-1}kg^{-1})	Uncertainty
41.8	∿ ± 1.5%

References [25,28].

16. References

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XXVII. Lithium Chloride-Potassium Chloride: LiCl-KCl

1. Melting Temperatures (T_m)

Pure substance melting points:

LiCl : 610°C

KCl : 770°C

Eutectic melting point:

355°C, composition: 58.5 mol % LiCl

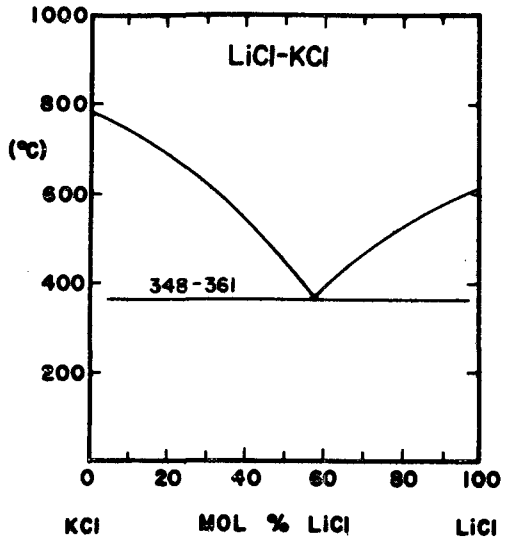

Figure 27.1. LiCl-KCl phase diagram

References [1-3].

2. Density (ρ)

Measurement method: Archimedean technique [4]

Two-independent-variable equation

$$\rho = a + bT + cC + dT^3 + eC^3 + fTC^2 \quad (C = \text{mol \% LiCl}) \quad (27.1)$$

precision: ± 0.15% uncertainty: ∿ ± 0.5%

Table 27.1. Coefficients for two-independent-variable equation (27.1)

a	b x 10^4	c x 10^3	d x 10^{11}	e x 10^7	f x 10^8
1.98715	-5.89069	2.02443	5.31098	1.21294	-2.16826

Table 27.2. Densities (g cm^{-3}) from two-independent-variable equation (27.1)

T (K)	Mol % LiCl											
	100	90	80	70	60	50	40	30	20	10	0	59.5
720					1.646							
740				1.622	1.636							1.636
760			1.598	1.612	1.625							1.626
780			1.588	1.602	1.615	1.627						1.615
800			1.578	1.591	1.604	1.616						1.605
820		1.552	1.568	1.581	1.594	1.605						1.594
840		1.542	1.558	1.571	1.583	1.595						1.584
860		1.533	1.548	1.562	1.573	1.584	1.595					1.574
880		1.523	1.539			1.574	1.584					1.564
900	1.496	1.514				1.563	1.573	1.583				
920	1.487	1.505				1.553	1.562	1.572				
940	1.478	1.496				1.543	1.552	1.561				
960	1.469						1.541	1.550				
980	1.460						1.531	1.539	1.548			
1000	1.451						1.521	1.528	1.536			
1020	1.443							1.518	1.525	1.534		
1040	1.434							1.507	1.514	1.522		
1060								1.497	1.503	1.510	1.520	
1080									1.492	1.499	1.507	
1100									1.481	1.487	1.495	
1120									1.471	1.476	1.483	
1140										1.465	1.471	
1160										1.454	1.459	
1180											1.447	
1200											1.436	

References [4-24].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [10,11]

Single variable equation

$$\gamma = a - bT \quad (27.2)$$

precision: in table 27.3 uncertainty: $\sim \pm 0.5\%$

Table 27.3. Coefficients of equation (27.2), and precisions

Mol % LiCl	a	b x 10^2	Precision
10	187.4541	8.30993	± 0.13%
15	189.5651	8.49146	± 0.08%
22	196.2269	9.16605	± 0.20%
30	190.9364	8.69217	± 0.24%
40	189.4704	8.45251	± 0.25%
50	187.3435	8.08096	± 0.21%
58	189.5657	8.23478	± 0.70%
69	188.3650	7.82852	± 0.22%
79	183.5300	7.10111	± 0.38%
90	183.3852	6.75324	± 0.20%

Two-independent-variable equation

$$\gamma = a + bT + cC + dT^2 + eC^2 + fTC + gTC^2 \quad (C = \text{mol \% KCl}) \quad (27.3)$$

precision: ∿ ± 0.4% uncertainty: ∿ ± 1%

Table 27.4. Coefficients for two-independent-variable equation (27.3)

a	b x 10^2	c x 10^2	d x 10^6	e x 10^3	f x 10^4	g x 10^6
177.43373	-5.43167	34.0743	-3.73703	-3.19922	-7.20291	5.57068

Table 27.5. Surface tension (dyn cm^{-1}) from equations in table 27.3

	Mol % LiCl									
T(K)	90	79	69	58	50	40	30	22	15	10
660				135.22						
680				133.57						
700				131.92						
720				130.28						
740				128.63						
760				126.98						
780			127.30	125.33	124.31					
800			125.74	123.69	122.70					
820			124.17	122.04	121.08					
840		123.88	122.61	120.39	119.46					
860		122.46	121.04	118.75	117.85					
880	123.96	121.04	119.47	117.10	116.23	115.09				
900	122.61	119.62		115.45	114.61	113.40				
920	121.26	118.20		113.81	113.00	111.71	110.97			
940	119.90	116.78			111.38	110.02	109.23			
960	118.56	115.36			109.77	108.33	107.49			
980	117.20	113.94			108.15	106.64	105.75	106.40		
1000	115.85	112.52			106.53	104.95	104.01	104.57		
1020	114.50	111.10			104.92	103.25	102.28	102.73	102.95	
1040	113.15						100.54	100.90	101.25	101.03
1060	111.80						98.80	99.07	99.56	99.37
1080									97.86	97.71
1100									96.16	96.04

References [4-11,25].

4. *Viscosity (η)*

Measurement method: oscillating sphere [13]

$$\eta = a + bT + cT^2 + dT^3 \quad (27.4)$$

precision: in table 27.6 uncertainty: ∿ ± 15%

Table 27.6. Coefficients of equation (27.4), and precisions

LiCl (mol %)	a	-b x 10^2	c x 10^6	d x 10^9	Precision
0	13.5546	2.0050	7.8613	0	±0.76%
60	8.5113	0.7401	-4.8633	4.8121	±0.59%
100	10.0147	0.5158	-13.0241	9.2997	±1.36%

$$\eta = A \exp (E/RT) \quad (27.5)$$

precision: in table 27.7 uncertainty: ∿ ± 5%

Table 27.7. Coefficients of equation (27.5), and precisions

LiCl (mol %)	A x 10^2	E (cal mol^{-1})	Precision
20	7.037	5707	±0.69%
30	9.019	5097	±1.69%
40	7.793	5337	±1.01%
50	7.860	5249	±1.09%
80	8.893	4980	±0.98%

Table 27.8. Viscosity (cp) from equations in tables 27.6, and 27.7.

T (K)	Mol % LiCl							
	100	80	60	50	40	30	20	0
890			1.46					
900	1.60		1.42					
910	1.54	1.40	1.38					
920	1.49	1.36	1.33		1.45	1.47		
930	1.43	1.32	1.29	1.35	1.40	1.42		
940	1.38	1.28	1.25	1.31	1.36	1.38		
950	1.33	1.24	1.22	1.27	1.32	1.34		
960	1.29	1.21	1.18	1.23	1.28	1.31		
970	1.24	1.18	1.15	1.20	1.24	1.27	1.36	
980	1.20	1.15	1.12	1.17	1.21	1.24	1.32	
990	1.17	1.12	1.09	1.13	1.18	1.20	1.28	
1000	1.13	1.09	1.06	1.10	1.14	1.17	1.24	
1010	1.10	1.06	1.03	1.08	1.11	1.14	1.21	
1020	1.07	1.04	1.01	1.05	1.09	1.12	1.18	
1030	1.05	1.01	0.99	1.02	1.06	1.09	1.14	
1040	1.02	0.99	0.97	1.00	1.03	1.06	1.11	
1050	1.01	0.97	0.95	0.97	1.01	1.04	1.09	
1060	0.99	0.95	0.93	0.95	0.98	1.01	1.06	
1070	0.98	0.93	0.92	0.93	0.96	0.99	1.03	
1080						0.97	1.01	
1090								1.04
1100								1.01
1110								0.99
1120								0.96
1130								0.94
1140								0.92
1150								0.89

References [4-14,26-29].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [4]

$$\kappa = a + bT + cT^2 \quad (27.6)$$

precision: in table 27.9
uncertainty: ∿ ± 0.5% at T < 1050 , and increasing to
∿ ± 4% for T > 1050

Table 27.9. Coefficients of equation (27.6), and precisions

Mol % LiCl	-a	b x 10^2	-c x 10^6	Precision
0	5.5231	1.1714	4.1800	±0.19%
19.96	5.9678	1.2866	4.7560	±0.17%
40.45	8.5932	1.8845	7.8109	±0.24%
58.80	5.6492	1.3732	5.1788	±0.18%
70.36	11.0108	2.7461	13.2471	±0.49%
81.77	6.7217	1.8182	7.4002	±0.09%
100	7.3766	2.2747	9.0623	±0.35%

For numerical values: see table 27.10.

Table 27.10. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 27.9

T (K)	Mol % LiCl						
	100	81.77	70.36	58.80	40.45	19.96	0
670				1.227			
690				1.360			
710				1.490			
730			1.976	1.615			
750			2.133	1.737			
770			2.280	1.854			
790			2.416	1.967			
810		3.150	2.541	2.076			
830		3.271	2.656	2.181			
850		3.386	2.760	2.281			
870		3.495	2.854		1.890		
890		3.599			1.992		
910	5.819				2.087		
930	5.940				2.177		
950	6.054				2.260		
970	6.161				2.337		
990	6.261				2.408	2.108	
1010	6.353				2.472	2.175	
1030	6.439					2.239	
1050	6.517					2.298	
1070						2.354	2.225
1090						2.406	2.279
1110						2.454	2.329
1130							2.376
1150							2.420
1170							2.460
1190							2.497

References [4-11,28,30-37].

6. Safety and Hazards

A. Hazard rating [38-40]

(i) Toxicity: LiCl, slight; KCl, slight.

(ii) Vapor pressure: eutectic (m.pt. 355°C): ~ 1 mm at 800°C (estimated).

B. Disaster hazards [38,41-43]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides evolve highly toxic chloride fumes when heated to decomposition, or contacted with acids.

References [38-43].

7. Corrosion

Table 27.11. Corrosion studies from primary research literature

Studies	References
Cu	44
Fe	45, 46
U-Bi	47
Cr, Pt	48
Cu, CuO; Pt, PtO; Bi, Bi_2O_3; Ni, NiO	49
Zn-rare earth metal alloys	50
Ni	51
Ag, Cu, Ni, Co, Au	52
Ti-Al-Mo-V	53
Pt	54
Mild steel, Armco iron	55, 56
Various steels	57
Mo, Ni, Nb, various steels, various Inconels (LiCl-KCl, with FeS and FeS_2 as additives)	58
H_2O (trace amts)	59
Emf. series	48
Electrochemical approach	60
Thermodynamic principles (redox diagrams)	61-63
Annotated corrosion biblio.	64
Reviews: corrosion in molten salts	65-67

References [44-67].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in LiCl-KCl as solvent

Na^+, Tl^+, *Ge^{2+}*, Pb^{2+}, *Sb^{3+}*, Bi^{3+}, Cu^+, Ag^+, Au^+, *Zn^{2+}*, Cd^{2+}, *Hg^{2+}*, *Y^{3+}*, La^{3+}, *V^{5+}*, *VO^{2+}*, *Nb^{2+}*, Nb^{3+}, *Nb_3Cl_8*, *$[TaCl_6]^{2-}$*, Cr^{3+}, Mo^{3+}, *$[MoCl_6]^{3-}$*, *W^{3+}*, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, *Pd^{2+}*, *Pt^{2+}*, Ce^{3+}, *Pr^{3+}*, *Nd^{3+}*, *Sm^{3+}*, *Eu^{3+}*, *Gd^{3+}*, *Tb^{3+}*, *Dy^{3+}*, *Ho^{3+}*, *Er^{3+}*, *Tm^{3+}*, *Yb^{3+}*, *Lu^{3+}*, U^{3+}, U^{4+}, UO_2^{2+}, Np^{3+}, Np^{4+}, *NpO_2^+*, *NpO_2^{2+}*, Pu^{3+}, Pu^{4+}, Am^{3+}, Cm^{3+}, *O^{2-}*, *VO_3^-*, *CrO_4^{2-}*, *MoO_4^{2-}*, *MoO_2Cl_2*, *PO_4^{3-}*, *S_x^{2-}*, *Cl_2*, *HCl*, *H_2O*.

The italicized species indicate studies with insufficient data-sets for characterization of temperature-dependence of diffusion coefficients. For these species: see table 27.12.4.

Equation $D = A \exp [-E/RT]$ (27.7)

precision: in table 27.12.2 uncertainty: in table 27.12.1

Table 27.12.1. Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
capillary	∿ ± 10%	Na^+, Cu^+, U^{4+}, UO_2^{2+}
chronopotentiometry	∿ ± 10%	Cu^+, Ag^+, Au^+, La^{3+}, Nb^{3+}, Mo^{3+}, Fe^{2+}, Ni^{2+}, Ce^{3+}, U^{3+}, U^{4+}, Np^{3+}, Np^{4+}, Pu^{3+}, Pu^{4+}, Am^{3+}, Cm^{3+}, Ge^{2+}, Zn^{2+}, Hg^{2+}, V^{5+}, VO^{2+}, Nb_3Cl_8, $TaCl_6^{2-}$, $MoCl_6^{3-}$, W^{3+}, Pd^{2+}, NpO_2^+, NpO_2^{2+}, O^{2-}, VO_3^-, CrO_4^{2-}, MoO_4^{2-}, MoO_2Cl_2, PO_4^{3-}, S_x^{2-}, Cl_2, HCl, H_2O
voltammetry	∿ ± 20%	Bi^{3+}, Tl^+, Cd^{2+}, Cr^{3+}, Mn^{2+}, Co^{2+}
polarography	∿ ± 20%	Sb^{3+}, Pd^{2+}, Pt^{2+}
rotating disc electrode	∿ ± 20%	Y^{3+}, Pr^{3+}, Nd^{3+}, Sm^{3+}, Eu^{3+}, Gd^{3+}, Tb^{3+}, Dy^{3+}, Ho^{3+}, Er^{3+}, Tm^{3+}, Yb^{3+}, Lu^{3+}

For diffusion equation parameters, and precisions: see table 27.12.2

Table 27.12.2 Diffusion equation parameters, precisions, and recommended study

Species	A x 10^3 ($cm^2 sec^{-1}$)	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
Tl^{+}	3.08	6498	650-810		93
Pb^{2+}	2.84	7313	650-810		93
Bi^{3+}	6.03	10067	630-800		93
Cu^{+}	0.601	4550	670-750		116
Ag^{+}	1.32	5800	670-870		83
Au^{+}	1.14	6300	670-870		83
Cd^{2+}	5.94	8502	640-800		98
La^{3+}	2.69	7688	710-940		79
Nb^{3+}	2.18	7000	670-870		86
Cr^{3+}	6.35	10424	690-810		93
Mo^{3+}	3.89	9212	810-1190		77,104
Mn^{2+}	10.9	9706	640-810		93
Fe^{2+}	1.53	7200	670-870		83
Co^{2+}	2.45	8054	670-820		93
Ni^{2+}	1.56	7100	670-870		83
Ce^{3+}	1.78	7670	670-920		109
U^{3+}	1.739	8502	650-810	±4.1%	91
U^{4+}	1.13	6300	640-880	± 3%	90
U^{4+}[a]	*5.788*	*8757*	*690-820*	*±3.6%*	*91*
UO_2^{2+}	1.76	7500	665-800	±0.14%	90
Np^{3+}	3.05	8699	670-920	± 3%	85
Np^{4+}	3.447	8787	670-820	±4.6%	110
Pu^{3+}	3.314	8792	670-920	± 2%	122
Pu^{4+}	5.918	9665	670-920	±2.1%	84
Am^{3+}	5.657	9770	670-920	±8.3%	92
Cm^{3+}	8.799	10397	670-820	± 14%	125

No entry in precision column indicates estimates not possible since results were reported as equations only.

[a]The italicized U^{4+} is for a study in presence of added F^- ions, diffusing species is uncertain.

Table 27.12.3 (Part 1). Diffusion coefficients, D x 10^5(cm^2sec^{-1}), from equations in table 27.12.2

T (K)	Tl^+	Pb^{2+}	Bi^{3+}	Cu^+	Ag^+	Au^+	Cd^{2+}	La^{3+}	Nb^{3+}	Cr^{3+}	Mo^{3+}	Mn^{2+}	Fe^{2+}	Co^{2+}
630			0.194											
640			0.220				0.742					0.528		
650	2.01	0.99	0.248				0.822					0.594		
670	2.34	1.17	0.314	1.97	1.69	1.00	1.00		1.14			0.743	0.685	0.578
690	2.69	1.37	0.390	2.18	1.92	1.15	1.20		1.32	0.317		0.918	0.802	0.689
710	3.08	1.59	0.480	2.39	2.16	1.31	1.43	1.16	1.53	0.393		1.12	0.93	0.813
730	3.49	1.84	0.584	2.61	2.42	1.48	1.69	1.34	1.75	0.481		1.35	1.07	0.950
750	3.93	2.10	0.702	2.84	2.69	1.66	1.98	1.55	1.99	0.582		1.62	1.22	1.10
770	4.41	2.39	0.837		2.98	1.86	2.29	1.77	2.25	0.698		1.92	1.38	1.27
790	4.91	2.69	0.989		3.28	2.06	2.64	2.01	2.52	0.829		2.25	1.56	1.45
800	5.17	2.85	1.07		3.44	2.17	2.83	2.14	2.67	0.901		2.43	1.65	1.54
810	5.43	3.02			3.59	2.28		2.27	2.82	0.977	1.27	2.62	1.75	1.64
830					3.92	2.50		2.54	3.13		1.46		1.94	
850					4.26	2.74		2.84	3.46		1.66		2.15	
870					4.61	2.98		3.15	3.80		1.89		2.38	
890								3.48			2.13			
930								4.20			2.66			
950											2.96			
970											3.27			
990											3.60			
1010											3.95			
1030											4.32			
1050											4.70			
1070											5.11			
1090											5.53			
1110											5.97			
1130											6.43			
1150											6.90			
1170											7.40			
1190											7.91			

Table 27.12.3 (Part 2) Diffusion coefficients, D x 10^5(cm^2sec^{-1}), from equations in table 27.12.2

T (K)	Ni^{2+}	Ce^{3+}	U^{3+}	U^{4+}	U^{4+}[a]	UO_2^{2+}	Np^{3+}	Np^{4+}	Pu^{3+}	Pu^{4+}	Am^{3+}	Cm^{3+}
630												
640				0.797								
650			0.241	0.860								
670	0.753	0.560	0.293	0.995		0.629	0.443	0.469	0.449	0.416	0.368	0.357
690	0.879	0.662	0.353	1.14	0.974	0.741	0.536	0.568	0.544	0.514	0.455	0.448
710	1.02	0.775	0.420	1.30	1.17	0.864	0.640	0.680	0.651	0.626	0.556	0.554
730	1.17	0.899	0.495	1.47	1.38	1.00	0.758	0.806	0.773	0.756	0.672	0.678
750	1.33	1.04	0.579	1.65	1.62	1.15	0.890	0.948	0.908	0.903	0.804	0.821
770	1.51	1.18	0.671	1.84	1.89	1.31	1.04	1.11	1.06	1.07	0.954	0.985
790	1.69	1.34	0.773	2.04	2.19	1.48	1.20	1.28	1.22	1.25	1.12	1.17
800	1.79	1.43	0.827	2.15	2.34	1.57	1.28	1.37	1.31	1.35	1.21	1.27
810	1.89	1.52	0.883	2.26	2.51		1.37	1.47	1.41	1.46	1.31	1.38
830	2.11	1.70		2.48			1.56		1.60	1.69	1.51	
850	2.33	1.90		2.71			1.77		1.82	1.94	1.74	
870	2.57	2.11		2.95			1.99		2.05	2.21	1.99	
890		2.33					2.23		2.30	2.50	2.26	
910		2.56					2.48		2.56	2.82	2.55	

[a]The *U^{4+}* in italics is for a diffusion study in the presence of added F^- ions.

Table 27.12.4. Diffusion coefficients for species not included in table 27.12.3

Species	T (K)	D x 10^5 ($cm^2 sec^{-1}$)	Recommended study
Na^+	677	1.97	116
	755	2.65	
Ge^{2+}	723	2.2	129
Sb^{3+}	723	1.2	108
Zn^{2+}	723	1.15	74, 96, 99
Hg^{2+}	723	1.67	132
Y^{3+}	673	0.057	126
V^{5+}	723	0.8	112
VO^{2+}	723	2.68	88
Nb^{2+}	723	3.5	94
Nb_3Cl_8	773	3.2	135
	948	9.3	
$[TaCl_6]^{2-}$[a]	773	9.0	105
	873	25.0	
	948	46.0	
$[MoCl_6]^{3-}$	873	1.43	127
	973	2.89	
	1023	3.8	
W^{3+}	723	0.71	137
Pd^{2+}	723	1.39	108
	758	1.68	107
Pt^{2+}	723	1.49	108
Pr^{3+}	673	0.037	124
Nd^{3+}	673	0.064	124
Sm^{3+}	673	0.153	124
Eu^{3+}	673	0.111	124
Gd^{3+}	673	0.054	124
Tb^{3+}	673	0.046	124
Dy^{3+}	673	0.043	124
Ho^{3+}	673	0.045	124
Er^{3+}	673	0.046	124
Tm^{3+}	673	0.056	124
Yb^{3+}	673	0.080	124
Lu^{3+}	673	0.060	124
NpO_2^+	673	0.48	123
NpO_2^{2+}	673	0.20	123
O^{2-}	673	1.6	76
	713	2.6	
	753	4.8	
	783	7.2	
VO_3^-	723	0.76	131
CrO_4^{2-}	723	0.96	118, 137
MoO_4^{2-}	723	1.64	130
MoO_2Cl_2	723	1.08	130
PO_4^{3-}	723	0.80	119
S_x^{2-}	693	0.312	121
Cl_2	673	6.0	114, 115
	723	16	
	773	17	
	843	23	
HCl	677	18	133, 134
	735	25	
	793	21	
H_2O	723	1.77	117

[a] $[TaCl_6]^{2-}$; values of diffusion coefficients appear improbable: possibly a factor of 10 too high

References:

Na^+, 116; Tl^+, 68, 72, 73, 93, 96, 98; Ge^{2+}, 129; Pb^{2+}, 68, 70, 72-74, 93, 96, 100, 101, 136; Sb^{3+}, 108; Bi^{3+}, 69, 70, 74, 93, 96, 108, 136; Cu^+, 69, 83, 93, 95, 96, 116, 136; Ag^+, 69-73, 83, 93, 96, 97, 120, 136; Au^+, 83; Zn^{2+}, 74, 96, 99; Cd^{2+}, 68-70, 74, 91, 93, 95, 96, 98-101, 128; Hg^{2+}, 132; Y^{3+}, 126; La^{3+}, 79, 124; V^{5+}, 112; VO^{2+}, 88; Nb^{2+}, 94; Nb^{3+}, 86, 94; Nb_3Cl_8, 135; $TaCl_6^{2-}$, 105; Cr^{3+}, 81, 89, 93, 98, 102, 103; Mo^{3+}, 77, 104; $MoCl_6^{3-}$, 127; W^{3+}, 137; Mn^{2+}, 93, 99, 106; Fe^{2+}, 83, 46; Co^{2+}, 68, 82, 93, 98, 101; Ni^{2+}, 75, 80, 83, 95, 96, 98, 101, 106; Pd^{2+}, 107, 108; Pt^{2+}, 108; Ce^{3+}, 109, 124; Pr^{3+}, 124; Nd^{3+}, 124; Sm^{3+}, 124; Eu^{3+}, 124; Gd^{3+}, 124; Tb^{3+}; 124; Dy^{3+}, 124; Ho^{3+}, 124; Er^{3+}, 124; Tm^{3+}, 124; Yb^{3+}, 124; Lu^{3+}, 124; U^{3+}, 78, 91, 113; U^{4+}, 70, 78, 84, 85, 90, 91, 110, 113; UO_2^{2+}, 90, 113; Np^{3+}, 85, 92; Np^{4+}, 84, 110, 113; NpO_2^+, 123; NpO_2^{2+}, 123; Pu^{3+}, 91, 92, 111, 122; Pu^{4+}, 84; Am^{3+}, 92; Cm^{3+}, 125; O^{2-}, 76; VO_3^-, 131; CrO_4^{2-}, 87, 118; MoO_4^{2-}, 130; MoO_2Cl_2, 130; PO_4^{3-}, 119; S_x^{2-}, 121; Cl_2, 114, 115; HCl, 133, 134; H_2O, 117.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [138,139]

Table 27.13. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
3.13	∿ ± 1%

References [138-140].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [138]

Table 27.14. Heat capacity of eutectic

C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
17.3	625-852	∿ ± 3.5%

References [138,140].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated from densities [141]

Table 27.15. Volume change on melting of eutectic

Binary mixture (mol % LiCl)	$(\Delta V_f/V_s)$	Uncertainty
58.5	15.8%	∿ ± 5%

References [141].

12. Vapor Pressure (p_{vap})

No vapor pressure studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: transient hot wire [142]

Precision: not estimated, uncertainty: ∿ ± 20%

Table 27.16. Thermal conductivity of eutectic melt

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
626.5	16.5

References [142].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: transient hot wire [142]]

Precision: not estimated, uncertainty: ∿ ± 10%

Table 27.17. Thermal conductivity of solid

T (K)	$\lambda \times 10^4$ (cal cm^{-1} $sec^{-1}K^{-1}$)
528	35.4
586	27.0
624	24.1

Sole investigation.

References [142].

15. Cryoscopic Constant (k_f)

Measurement method: calc'd from ΔH_f° [141]

Table 27.18. Cryoscopic constant of eutectic

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
14.0	∿ ± 1%

References [139,141,143,144].

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XXVIII. Sodium Chloride - Potassium Chloride: NaCl-KCl

1. *Melting Temperatures (T_m)*

Pure substance melting points:
NaCl: 800°C
KCl: 770°C

Solid solution, minimum melting point:
685°C, composition: 50 mol % NaCl.

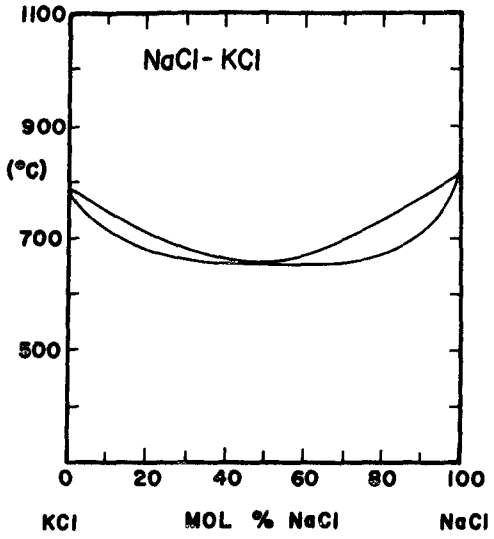

Figure 28.1. NaCl-KCl phase diagram

References [1-3].

2. *Density (ρ)*

Measurement method: Archimedean technique [4]

Single variable equation

$$\rho = a + bT \quad (28.1)$$

precision: in table 28.1 uncertainty: ∿ ± 0.5%

Table 28.1. Coefficients for single variable equation (28.1), and precisions

Mol % NaCl	a	$-b \times 10^4$	Precision
0	2.1376	5.8445	±0.03%
20.75	2.1377	5.8127	±0.01%
41.00	2.1342	5.7477	±0.02%
51.23	2.1314	5.6793	±0.01%
65.15	2.1338	5.5749	±0.01%
72.94	2.1374	5.5900	±0.02%
84.77	2.1400	5.5381	±0.02%
100	2.1365	5.4052	±0.05%

Two-independent-variable equation

$$\rho = a + bT + cC^3 + dTC + eCT^2 \quad (C=\text{mol \% KCl}) \quad (28.2)$$

precision: ± 0.11% uncertainty: ∿ + 0.5%

Table 28.2. Coefficients for two-independent-variable equation (28.2)

a	b x 10^4	c x 10^8	d x 10^7	e x 10^{10}
2.14250	-5.45436	2.79726	-9.89901	2.78444

Table 28.3. Densities (g cm^{-3}) from equations (28.1) and (28.2)

T (K)	Mol % NaCl								
	100	84.77	72.94	65.15	51.23	50.00	41.00	20.75	0
945									
960					1.586	1.588	1.582		
975					1.578		1.574		
990			1.584	1.582	1.569	1.571	1.565		
1005			1.576	1.574	1.561		1.557	1.554	
1020			1.567	1.565	1.552	1.554	1.548	1.545	
1035			1.559	1.557	1.544		1.539	1.536	
1050			1.550	1.548	1.535	1.537	1.531	1.527	
1065		1.550	1.542	1.540	1.527		1.522	1.519	1.515
1080	1.553	1.542	1.534	1.532	1.518	1.520	1.513	1.510	1.506
1095	1.545	1.534	1.525	1.523	1.510		1.505	1.501	1.498
1110	1.537	1.525	1.517	1.515	1.501	1.508	1.496	1.493	1.489
1125	1.528	1.517	1.509	1.507	1.493		1.488	1.484	1.480
1140	1.520	1.509	1.500	1.498	1.484	1.486	1.479	1.475	1.471
1155	1.512	1.500	1.492	1.490	1.475		1.470	1.466	1.463
1170	1.504	1.492	1.483	1.482	1.467		1.462	1.458	1.454
1185	1.496	1.484	1.475	1.473				1.449	1.445
1200	1.488							1.440	1.436
1215	1.480								
1230	1.472								
1245	1.464								
1260	1.455								
1275	1.447								
1290	1.439								

References [4-19].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [11]

Single variable equation

$$\gamma = a + bT \quad (28.3)$$

precision: ± 0.2% uncertainty: ∿ ± 2%

Table 28.4. Coefficients for single variable equation (28.3)

Mol % NaCl	a	$-b \times 10^2$
0	176.8	7.5
10	178.1	7.5
25	178.0	7.4
40	177.3	7.2
50	179.3	7.2
60	180.4	7.2
75	181.2	7.0
90	183.5	6.8
100	187.0	6.8

Two-independent-variable equation

$$\gamma = a + bT + cC + dC^2 + eC^3 + fTC^2 + gCT^2 \quad (C = \text{mol \% KCl}) \quad (28.4)$$

precision: ± 0.20% uncertainty: ∿ ± 2%

Table 28.5. Coefficients for two-independent-variable equation (28.4).

a	$b \times 10^2$	$c \times 10^2$	$d \times 10^3$	$e \times 10^5$	$f \times 10^8$	$g \times 10^8$
186.76500	-6.77993	-3.41591	3.42500	-1.28519	-3.15694	-3.79717

Table 28.6. Surface tension (dyn cm^{-1}) from equations in table 28.4

	Mol % NaCl								
T(K)	100	90	75	60	50	40	25	10	0
980		116.9	112.6	109.8	108.7	106.7	105.5	104.6	
990		116.2	111.9	109.1	108.0	106.0	104.7	103.9	
1000	119.3	115.5	111.2	108.4	107.3	105.3	104.0	103.1	
1010	118.3	114.8	110.5	107.7	106.6	104.6	103.3	102.4	
1020	117.6	114.1	109.8	107.0	105.9	103.9	102.5	101.6	
1030	117.0	113.5	109.1	106.2	105.1	103.1	101.8	100.9	
1040	116.3	112.8	108.4	105.5	104.4	102.4	101.0	100.1	
1050	115.6	112.1	107.7	104.8	103.7	101.7	100.3	99.4	
1060	114.9	111.4	107.0	104.1	103.0	101.0	99.6	98.6	
1070	114.2	110.7	106.3	103.4	102.3	100.3	98.8	97.9	
1080	113.6	110.1	105.6	102.6	101.5	99.5	98.1	97.1	95.8
1090	112.9	109.4	104.9	101.9	100.8	98.8	97.3	96.4	95.1
1100	112.2	108.7	104.2	101.2	100.1	98.1	96.6	95.6	94.3
1110	111.5	108.0	103.5	100.5	99.4	97.4	95.9	94.9	93.6
1120	110.8	107.3	102.8	99.8	98.7	96.7	95.1	94.1	92.8
1130	110.2	106.7	102.1	99.0	97.9	95.9	94.4	93.4	92.1
1140	109.5	106.0	101.4	98.3	97.2	95.2	93.6	92.6	91.3
1150	108.8	105.3	100.7	97.6	96.5	94.5	92.9	91.9	90.6
1160	108.1	104.6	100.0	96.9	95.8	93.8	92.2	91.1	89.8
1170	107.4	103.9	99.3	96.2	95.1	93.1	91.4	90.4	89.1
1180	106.8								88.3
1190	106.1								87.6
1200	105.4								86.8
1210	104.7								86.1
1220	104.0								85.3

References [4-12,19-23].

4. Viscosity (η)

Measurement method: oscillating sphere [7]

$$\eta = a + bT + cT^2 + dT^3 \quad (28.5)$$

precision: in table 28.7 uncertainty: ∿ ± 25%

Table 28.7. Coefficients of equation (28.5), and precisions

NaCl (mol %)	a	$-b \times 10^2$	$c \times 10^6$	$d \times 10^9$	Precision
0	1.7091	-1.5846	-27.7213	11.5836	±0.57%
20.75	14.1361	1.9076	5.0784	1.2900	±0.29%
41.00	11.6454	1.1612	-1.9476	3.4160	±0.55%
51.23	18.3576	2.5649	7.1721	1.6990	±0.61%
65.15	16.2796	2.0228	3.0276	2.5895	±0.38%
84.77	15.2401	1.4962	-3.3789	4.9174	±0.25%

$$\eta = A \exp (E/RT) \quad (28.6)$$

precision: in table 28.8, uncertainty: ∿ ± 5%

Table 28.8. Coefficients of equation (28.6), and precisions

LiCl (mol %)	$A \times 10^2$	E (cal mol^{-1})	Precision
72.90	2.231	8699	± 0.60%
100	1.821	9341	± 0.47%

Table 28.9. Viscosity (cp) from equations in tables 28.7 and 28.8

T (K)	Mol % NaCl							
	100	84.77	72.90	65.15	51.23	41.00	20.75	0
1000			1.777	1.668	1.580	1.502		
1010			1.702	1.605	1.519	1.450		
1020			1.631	1.545	1.460	1.400	1.331	
1030			1.565	1.486	1.404	1.351	1.285	
1040		1.557	1.502	1.430	1.351	1.305	1.241	
1050		1.498	1.443	1.376	1.300	1.260	1.199	
1060		1.441	1.387	1.324	1.252	1.217	1.158	1.154
1070		1.387	1.335	1.274	1.206	1.175	1.119	1.116
1080		1.335	1.285	1.226	1.162	1.136	1.082	1.080
1090		1.285	1.238	1.181	1.121	1.098	1.047	1.046
1100	1.307	1.239	1.194	1.139	1.083	1.062	1.014	1.014
1110	1.258	1.195	1.152	1.098	1.047	1.028	0.983	0.984
1120	1.211	1.153	1.112	1.060	1.014	0.996	0.954	0.957
1130	1.167	1.114	1.074	1.024	0.984	0.966	0.926	0.931
1140	1.125	1.078	1.038	0.990	0.956	0.937	0.900	0.908
1150	1.086	1.044	1.004	0.959	0.930	0.911	0.877	0.887
1160	1.048	1.013	0.972	0.931	0.907	0.887	0.855	0.869
1170	1.012	0.985	0.941	0.904	0.887	0.864	0.835	0.853

References [4-12,16,19,23-27].

5. Electrical Conductance (κ)

Measurement method: ac technique [4]

$$\kappa = a + bT + cT^2 \quad (28.7)$$

precision: in table 28.10 uncertainty: ∿ ± 4% at T > 1050 K

Table 28.10. Coefficients of equation (28.7), and precisions

Mol % NaCl	-a	b x 10^2	-c x 10^5	Precision
0.00	5.5231	1.1714	0.4180	±0.19%
20.40	2.9567	0.7368	0.2270	±0.29%
41.00	6.3093	1.3765	0.5147	±0.22%
51.23	3.3119	0.8380	0.2641	±0.40%
65.15	3.1690	0.8265	0.2477	±0.19%
72.94	4.0668	1.0120	0.3317	±0.30%
84.77	1.3797	0.5656	0.1274	±0.24%
100.00	2.3356	0.7783	0.2118	±0.22%

Table 28.11. Specific conductance (ohm^{-1}cm^{-1}) from equations in table 28.10

T (K)	Mol % NaCl							
	100.00	84.77	72.94	65.15	51.23	41.00	20.40	0.00
940								
950								
960					2.299	2.162		
970				2.517	2.332	2.200		
980				2.552	2.364	2.237		
990				2.586	2.396	2.273		
1000			2.736	2.619	2.427	2.309		
1010			2.771	2.652	2.458	2.343	2.169	
1020			2.805	2.684	2.488	2.376	2.197	
1030			2.838	2.716	2.518	2.408	2.224	
1040		3.125	2.870	2.748	2.547	2.439	2.251	
1050		3.154	2.902	2.778	2.575	2.469	2.277	
1060		3.184	2.933	2.809	2.603	2.498	2.303	2.197
1070		3.214	2.964	2.839	2.631	2.526	2.328	2.225
1080	3.600	3.243	2.993	2.868	2.658	2.553	2.353	2.252
1090	3.632	3.272	3.023	2.897	2.685	2.579	2.377	2.279
1100	3.663	3.300	3.052	2.925	2.710	2.604	2.401	2.304
1110	3.694	3.329	3.079	2.953	2.736	2.628	2.425	2.329
1120	3.724	3.357	3.107	2.981	2.761	2.651	2.448	2.353
1130	3.755	3.385	3.133	3.008	2.785	2.673	2.471	2.376
1140	3.784	3.412	3.159	3.034	2.809	2.694	2.493	2.399
1150	3.814	3.440	3.184	3.060	2.832	2.714	2.514	2.420
1160	3.843	3.467	3.209	3.085	2.855	2.732	2.536	2.440
1170	3.871	3.494	3.233	3.110	2.877	2.750	2.556	2.460
1180	3.899	3.520	3.256	3.135	2.899	2.767	2.577	2.479
1190	3.927	3.547	3.279	3.159			2.597	2.497
1200	3.954	3.573	3.301	3.182			2.616	
1210	3.981			3.205				
1220	4.007							
1230	4.033							
1240	4.059							
1250	4.084							
1260	4.108							
1270	4.133							
1280	4.156							
1290	4.180							

References [4-13,19,28-39].

6. Safety and Hazards

A. Hazard rating [40-42]

(i) Toxicity: NaCl, very low; KCl, slight

(ii) Vapor pressure: no data for mixture; but see: NaCl, KCl.

B. Disaster hazards [40,43-45]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides evolve highly toxic fumes when heated to decomposition or contacted with acids.

References [40-45].

7. Corrosion

Table 28.12. Corrosion studies from primary research literature

Studies	References
Ni, Fe	46
Zr, Be, Ti, Hf, U	47
Ni-Cr-Fe	48
Ti	49,50
Cr_2O_3 + C electrode	51
Fe	52
Ni-Cr	53
Fe, Ni	54
Steel 3	55
Ni-Fe	46,56
Au, Pt, W	57
Several metals	58
Fe	59
Ni	60
Zr	47
Rh	61
Al	62
Cr, Fe-Cr	63
W	64
Emf. series	58
Thermodynamic redox diagrams	46,65
Electrochemical approach	66,67
Reviews (molten salts corrosion)	68-70
Annotated corrosion biblio.	71

References [46-71].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in NaCl-KCl as solvent

Be^{2+}, Mg^{2+}, Al^{3+}, Tl^{+}, Pb^{2+}, *Cu^{+}*, Ag^{+}, *Zn^{2+}*, Cd^{2+}, Y^{3+}, Zr^{2+}, Zr^{4+}, ZrF_6^{2-}, Hf^{2+}, Hf^{4+}, HfF_6^{2-}, Nb^{2+}, Nb^{3+}, *Nb_3Cl_8*, *K_2NbF_7*, Cr^{3+}, *Mo^{3+}*, W^{4+}, W^{5+}, Fe^{2+}, *Co^{2+}*, *Ni^{+}*, *Ni^{2+}*, Th^{4+}, U^{3+}, U^{4+}, UO_2^{2+}, *PO_4^{3-}*, Cl_2, *HCl*, *SO_3*, *CO_2*.

The italicized species indicate studies with insufficient data-sets for characterization of temperature dependence of diffusion coefficients. For these species see table 28.13.4.

Equation: $D = A \exp [-E/RT]$ (28.8)

precision: in table 28.13.2 uncertainty: in table 28.13.1

Table 28.13.1. Diffusion techniques, uncertainties, and species

Diffusion techniques of recommended study	Uncertainty (in values of D)	Species
chronopotentiometry	∿± 10%	Be^{2+}, Mg^{2+}, Al^{3+}, Tl^{+}, Pb^{2+}, Ag^{+}, Cd^{2+}, Y^{3+}, Zr^{2+}, Zr^{4+}, ZrF_6^{2-}, Hf^{2+}, Hf^{4+}, HfF_6^{2-}, Nb^{2+}, Nb^{3+}, K_2NbF_7, W^{4+} W^{5+}, Fe^{2+}, Th^{4+}, U^{3+}, U^{4+}, UO_2^{2+}, Cl_2, Zn^{2+}, Nb_3Cl_8, CO^{2+}, Ni^{+}, Ni^{2+}, PO_4^{3-}, SO_3, CO_2
galvanostatic	∿± 20%	Cr^{3+}
voltammetry	∿± 20%	Cu^{+}
rotating disc electrode	∿± 20%	HCl

Table 28.13.2. Diffusion equation parameters, precisions, and recommended study

Species	A x 10^3 ($cm^2 sec^{-1}$)	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
Be^{2+}	5.27	10700	950-1070		83
Mg^{2+}	3.80	8328	1020-1120		103
Al^{3+}	1.096	6543	950-1090		89
Tl^{+}	5.16	8526	945-1040	±2.6%	94
Pb^{2+}	1.582	7678	970-1200	±3.4%	90
Ag^{+}	1.91	6411	980-1150	±2.8%	87
Cd^{2+}	1.63	7030	950-1070		96
Y^{3+}	1.49	8359	950-1090		76
Zr^{2+}	5.40	11100	970-1170	±0.4%	86
Zr^{4+}	6.20	9800	970-1170		86
ZrF_6^{2-}	3.60	14963	970-1070		72
Hf^{2+}	2.73	7950	970-1170		84
Hf^{4+}	4.40	9200	970-1170		120
HfF_6^{2-}	9.55	12767	950-1130		100
Nb^{2+}	9.12	9152	970-1110		85
Nb^{3+}	4.36	10500	970-1110		85
Cr^{3+}	5.75	11472	1020-1120		82
W^{4+}	11.38	12643	970-1130		81
W^{5+}	15.21	13480	970-1130		81
Fe^{2+}	6.53	9839	960-1180		79
Th^{4+}	17.46	12776	950-1100		78
Th^{4+} [b]	60.26	15897	950-1100		78
U^{3+}	2.83	8800	950-1170		110
U^{4+}	9.55	11797	950-1160		110
UO_2^{2+}	2.94	10726	950-1120		110
Cl_2	linear equation[a]		1010-1110		111

No entry in precision column indicates estimate not possible since results were reported as equations only.

[a] Cl_2: $D_{Cl_2} = 0.95 \times 10^{-3} - 0.9 \times 10^{-6}(T-931)$

[b] *Th^{4+}*: The italics indicate that in this study, the diffusion of Th^{4+} was investigated in the presence of added F^- ions; diffusing species uncertain.

Table 28.13.3 (Part 1). Diffusion coefficients D x 10^5(cm^2sec^{-1}), from equations in table 28.13.2

T (K)	Be^{2+}	Mg^{2+}	Al^{3+}	Tl^{+}	Pb^{2+}	Ag^{+}	Cd^{2+}	Y^{3+}	Zr^{2+}	Zr^{4+}	ZrF_6^{2-}	Hf^{2+}	Hf^{4+}	HfF_6^{2-}
950	1.82		3.42	5.64			3.93	1.78						1.10
970	2.05		3.68	6.19	2.95		4.25	1.95	1.70	3.84	1.53	4.41	3.72	1.27
980	2.17		3.81	6.47	3.07	7.10	4.41	2.04	1.81	4.04	1.66	4.60	3.91	1.36
1000	2.42		4.07	7.07	3.32	7.53	4.74	2.22	2.02	4.47	1.93	5.00	4.29	1.55
1020	2.69	6.24	4.34	7.69	3.58	8.08	5.08	2.41	2.26	4.93	2.24	5.40	4.70	1.76
1040	2.97	6.75	4.62	8.33	3.85	8.58	5.43	2.61	2.51	5.41	2.58	5.83	5.13	1.98
1060	3.28	7.29	4.91		4.13	9.10	5.79	2.82	2.78	5.91	2.96	6.27	5.58	2.23
1070	3.44	7.56	5.05		4.27	9.36	5.97	2.92	2.92	6.17	3.16	6.49	5.81	2.36
1090		8.13	5.34		4.57	9.90		3.14	3.21	6.72		6.95	6.29	2.63
1100		8.41			4.72	10.17			3.36	7.00		7.19	6.54	2.78
1120		9.01			5.02	10.71			3.68	7.58		7.67	7.05	3.08
1130					5.18	10.99			3.85	7.87		7.92	7.31	3.24
1150					5.50	11.55			4.20	8.51		8.42	7.85	
1170					5.82				4.56	9.16		8.93	8.41	
1190					6.15									
1200					6.32									

[Al^{3+}; for Al^{3+} conc'ns < 0.18 wt%]

Table 28.13.3 (Part 2). Diffusion coefficients, D x 10^5(cm^2sec^{-1}), from equations in table 28.13.2

T (K)	Nb^{2+}	Nb^{3+}	Cr^{3+}	W^{4+}	W^{5+}	Fe^{2+}	Th^{4+}	*Th^{4+}*	U^{3+}	U^{4+}	UO_2^{2+}	Cl_2
950							2.01	1.33	2.67	1.84	1.00	
960						3.76	2.15	1.45	2.81	1.97	1.06	
970	7.90	1.88		1.61	1.40	3.96	2.31	1.58	2.94	2.10	1.13	
980	8.30	1.99		1.72	1.50	4.17	2.47	1.72	3.08	2.23	1.19	
990	8.70	2.10		1.84	1.61	4.39	2.64	1.86	3.23	2.37	1.26	
1000	9.11	2.21		1.96	1.72	4.62	2.82	2.02	3.38	2.52	1.33	
1010	9.54	2.33		2.09	1.84	4.85	3.00	2.19	3.53	2.67	1.40	87.9
1020	9.97	2.45	2.00	2.22	1.97	5.09	3.19	2.36	3.68	2.83	1.48	87.0
1040	10.88	2.71	2.23	2.51	2.23	5.59	3.61	2.75	4.00	3.17	1.64	85.2
1060	11.83	2.98	2.48	2.81	2.53	6.11	4.05	3.18	4.34	3.53	1.81	83.4
1070	12.32	3.12	2.61	2.98	2.68	6.38	4.29	3.41	4.51	3.72	1.89	82.5
1090	13.33	3.42	2.88	3.32	3.01	6.95	4.79	3.91	4.87	4.12	2.08	80.7
1100	13.85	3.57	3.02	3.50	3.19	7.24	5.05	4.18	5.05	4.33	2.17	79.8
1110	14.38	3.73	3.17	3.69	3.37	7.54			5.24	4.54	2.27	78.9
1120			3.32	3.88	3.56	7.85			5.43	4.76	2.37	
1130				4.08	3.76	8.16			5.62	4.99		
1150						8.81			6.02	5.47		
1170						9.48			6.43			
1180						9.83						

[*Th^{4+}*; italicized indicates study with added F^- ions; diffusing species uncertain]

Table 28.13.4. Diffusion coefficients for species not included in table 28.13.3

Species	T (K)	D x 10^5 ($cm^2 sec^{-1}$)	Recommended study
Cu^+	773	6.7	116
	1123	23.0	114,115
Zn^{2+}	973	4.6	91,93
Nb_3Cl_8	948	8.6	124
K_2NbF_7	1023	4.9	121
Mo^{3+}	1000	2.9	101
Co^{2+}	973	2.04	102
	1079	2.59	
Ni^+	1003	70	106
Ni^{2+}	978	2.36	91,104,105,106
	1080	2.87	
PO_4^{3-}	1053	0.82	122
HCl	988	10	75,112
	1068	25	
	1093	27	
	1180	30	
SO_3	1023	20	117
CO_2	973	17	125

Temperature dependence of D reported in graphical form.

References

Be^{2+}, 83; Mg^{2+}, 103; Al^{3+}, 89; Tl^+, 94, 119; Pb^{2+}, 73,88,90,91, 93,95,107,108; Cu^+, 114-116; Ag^+, 72,87,88,91,95; Zn^{2+}, 91,93; Cd^{2+}, 80,88,91,93,95-98; Y^{3+}, 76; Zr^{2+}, 72,86,99; Zr^{4+}, 72,86; ZrF_6^{2-}, 72; Hf^{2+}, 84; Hf^{4+}, 100,120; HfF_6^{2-}, 100; Nb^{2+}, 85; Nb^{3+}, 85; Nb_3Cl_8, 124; K_2NbF_7, 121; Cr^{3+}, 82,118; Mo^{3+}, 101; W^{4+}, 81; W^{5+}, 81; Fe^{2+}, 79; Co^{2+}, 102; Ni^+, 106; Ni^{2+}, 91,104-106; Th^{4+}, 78; U^{3+}, 109,110,123; U^{4+}, 109,110,123; UO_2^{2+}, 92,109,110, 123; PO_4^{3-}, 122; Cl_2, 74,77,111,113; HCl, 75,112; SO_3, 117; CO_2, 125

9. Heat of Fusion (ΔH_f°)

No data.

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [126]

Table 28.14. Volume change on melting of minimum melting solid solution

$(\Delta V_f/V_s)$	Uncertainty
14.8%	∿ ± 4%

References [126].

12. Vapor Pressure ($\tilde{p}_{vap}$)

Measurement method: transpiration [127]

precision: not estimated uncertainty: ∿ ± 10%

Table 28.15. Vapor pressure(mm)

Mol % KCl	T (K)		
	1133	1223	1263
25.2	2.9		
49.8	3.1		
74.7	4.0		
25.8		9.6	
49.6		9.7	
74.4		10.8	
24.3			16.5
49.5			16.5
75.9			17.9

References [127,128].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_ℓ)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

16. References

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XXIX. Lithium Chloride-Aluminum Chloride: $LiCl-AlCl_3$

1. *Melting Temperature (T_m)*

Pure substance melting points:

$LiCl$: 610°C
$AlCl_3$: 192°C

Eutectic melting point:

114°C, composition: 40 mol % $LiCl$

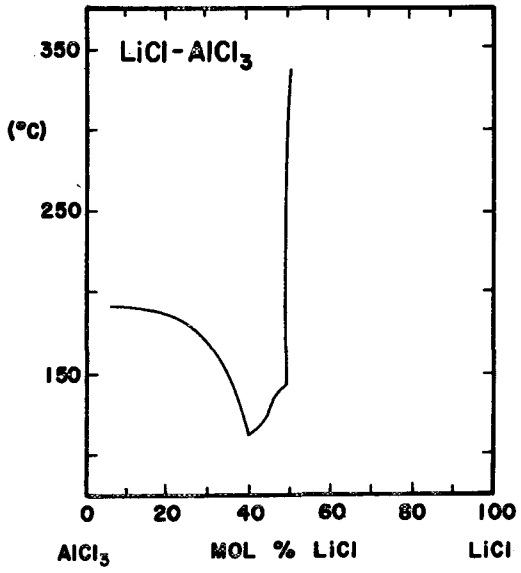

Figure 29.1. $LiCl-AlCl_3$ phase diagram

References [1-3].

2. *Density (ρ)*

Measurement method: dilatometric technique [3]

Two-independent-variable equation

$$\rho = a + bC + cT + dC^2 + eCT + fC^2T \quad (C=\text{Mol \% } AlCl_3) \quad (29.1)$$

precision: ± 0.11% uncertainty: ∿ ± 1%

Table 29.1. Coefficients for two-independent-variable equation (29.1)

a	b x 10^2	c x 10^3	d x 10^4	e x 10^5	f x 10^7
2.47542	-2.02834	-2.15321	1.97633	5.76140	-5.91700

Table 29.2. Densities (g cm^{-3}) from equation (29.1)

T (K)	Mol % $AlCl_3$ 50.00	55.00	60.00	65.00	70.00	75.00
420	1.6396					
430	1.6321					
440	1.6246					
450	1.6170					
460	1.6095					
470	1.6020	1.5937	1.5814	1.5651	1.5448	1.5204
480	1.5945	1.5860	1.5732	1.5560	1.5346	1.5088
490	1.5870	1.5782	1.5649	1.5470	1.5244	1.4972
500	1.5795	1.5705	1.5566	1.5379		1.4856
510	1.5719	1.5628	1.5484	1.5288		1.4740
520	1.5644	1.5550	1.5401			1.4624
530	1.5569		1.5319			
540			1.5236			

References [3-5].

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: ac technique [7]

Single variable equation

$$\kappa = A \exp(-E/RT) \quad (29.2)$$

precision: in table 29.3 uncertainty: $\sim \pm 5\%$

Table 29.3. Coefficients of equation (29.2), and precisions

Mol % $AlCl_3$	A	E (cal mol^{-1})	Precision
49.25	4.09405	2168	± 4.40
55.00	4.49855	2536	± 1.50
59.98	3.98840	2650	± 1.00
64.92	3.11955	2614	± 0.69
69.99	2.99865	2800	± 0.16
75.10	1.68110	2579	± 0.83

Two-independent-variable-equation

$$\kappa = a + bC + cT + eCT + fC^2T \quad (29.3)$$

precision: ± 5.1% uncertainty $\sim \pm 5\%$

Table 29.4. Coefficients for two-independent-variable equation (29.3)

a	b x 10^2	c x 10^3	d x 10^4	e x 10^4	f x 10^7
-1.86688	2.69890	7.40140	-0.50263	-1.30430	5.1200

Table 29.5. Specific conductance (ohm^{-1} cm^{-1}) from equations in table 29.3

	Mol % $AlCl_3$					
T(K)	49.25	55.00	59.98	64.92	69.99	75.10
420						
430		0.23128	0.17944			
440	0.34301	0.24742	0.19255	0.15693		
450	0.36244	0.26389	0.20596	0.16771		
460	0.38205	0.28067	0.21967	0.17872		
470	0.40182	0.29774	0.23364	0.18993		0.10626
480	0.42173	0.31507	0.24787	0.20133	0.15924	0.11255
490	0.44176	0.33264	0.26233	0.21291		0.11894
500	0.46187	0.35042	0.27701	0.22466		0.12541
510	0.48206	0.36841	0.29188	0.23655		0.13195
520	0.50231	0.38657	0.30693	0.24858		0.13857
530	0.52259	0.40489	0.32215	0.26073		
540	0.54290	0.42335	0.33751	0.27299		
550	0.56321	0.44194	0.35301			
560	0.58352	0.46063	0.36863			
570	0.60381	0.47942	0.38436			
580	0.62407	0.49829				
590	0.64428	0.51723				
600	0.66445					
610	0.68455					
620	0.70459					

References [4-7].

6. Safety and Hazards

A. Hazard rating [8,9]

(i) Toxicity: LiCl, slight; $AlCl_3$, severe.

(ii) Vapor pressure: appreciable; see [23,24]

B. Disaster hazards [8,10-12]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides when heated to decomposition, or contacted with acids, emit highly toxic fumes; $AlCl_3$ reacts exothermically with moisture/water evolving HCl fumes.

References [8-12].

7. Corrosion

Table 29.6. Corrosion studies from primary research literature

Studies	References
Pyrex glass, Pt, quartz, silica	4-6
Electrochem. approach	13,14
Thermodynamic redox diagrams	15-17
Reviews: corrosion	18-20
Annotated biblio.	21

References [4-6,13-21].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: estimated [22]

Table 29.7. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
5.8	∿ ± 5%

References [22].

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated from densities [22]

Table 29.8. Volume change on melting

Binary eutectic (mol % LiCl)	$(\Delta V_f/V_s)$	Uncertainty
40	36.4%	∿ ± 5%

References [22].

12. Vapor Pressure (p_{vap})

Measurements in progress [23,24]

References [23,24].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: estimated [22]

Table 29.9. Cryoscopic constant

Binary mixture (mol % LiCl)	k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
60	4.07	∿ ± 5%

References [22].

16. References

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XXX. Sodium Chloride-Aluminum Chloride: $NaCl-AlCl_3$

1. *Melting Temperatures (T_m)*

Pure substance melting points:
NaCl: 800°C
$AlCl_3$: 192°C

Eutectic melting point:
105-108°C, composition: 36.8 mol % NaCl

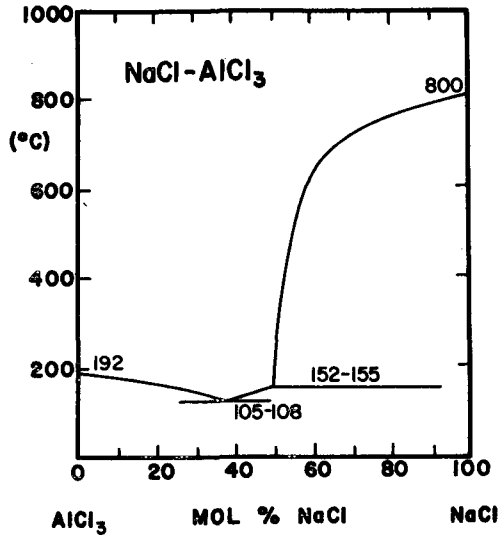

Figure 30.1. $NaCl-AlCl_3$ phase diagram

References [1-5].

2. *Density (ρ)*

Measurement method: flotation technique [6]

$$\rho = a + bT \quad (30.1)$$

precision: in table 30.1 uncertainty: ∿ ± 5%

Table 30.1. Coefficients of equation (30.1), and precisions

Mol % NaCl	a	$-b \times 10^3$	Precision
0.0	2.371	2.330	±0.14%
27.0	2.011	0.920	±0.07%
38.2	2.034	0.866	±0.04%
48.0	2.068	0.838	±0.05%

Table 30.2. Densities (g cm^{-3}) from equations in table (30.1)

T (K)	Mol % NaCl			
	48.0	38.2	27.0	0.0
400	1.733			
410	1.724			
420	1.716			
430	1.708			
440	1.699	1.653		
450	1.691	1.644		
460	1.682	1.635	1.588	
470	1.674	1.627	1.579	
480	1.666	1.618	1.570	1.252
490	1.657	1.609	1.561	1.229
500	1.649	1.601	1.551	
510	1.641	1.592	1.542	
520	1.632	1.583	1.533	
530	1.624	1.575	1.524	
540	1.615	1.566	1.515	
550	1.607		1.505	
560	1.598		1.496	
570			1.487	
580			1.478	
590			1.469	
600			1.459	
610			1.450	

References [6-18].

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

Measurement method: oscillation cylinder [19]

$$\eta = A \exp(E/RT) \quad (30.2)$$

precision: in table 30.3 uncertainty: $\sim \pm 5\%$

Table 30.3. Parameters of equation (30.2), temperature range, and precisions

Mol % $AlCl_3$	Temp. range (K)	A x 10^3	E (cal mol^{-1})	Precision
50.00	453-577	7.2702	3285.3	±1.11%
55.00	455-574	6.8398	3413.5	±0.99%
59.99	448-578	5.7828	3661.1	±1.48%
64.96	443-577	4.9477	3850.2	±1.29%
69.92	453-573	4.2341	3966.7	±0.75%
74.80	468-579	3.6622	3977.5	±0.52%
79.72	472-575	2.8309	3985.8	±1.25%

Table 30.4. Viscosity (cp) from equations in table 30.3

T (K)	Mol % $AlCl_3$						
	50.00	55.00	59.99	64.96	69.92	74.80	79.72
440							
450			3.469	3.667			
460	2.645	2.863	3.174	3.339	3.246		
470	2.450	2.644	2.914	3.053	2.960	2.590	
480	2.277	2.450	2.686	2.802	2.709	2.370	1.848
490	2.123	2.278	2.483	2.580	2.489	2.177	1.697
500	1.984	2.124	2.304	2.384	2.294	2.006	1.564
510	1.859	1.985	2.143	2.210	2.121	1.854	1.445
520	1.747	1.861	1.999	2.054	1.967	1.720	1.340
530	1.645	1.748	1.870	1.915	1.830	1.599	1.246
540	1.553	1.646	1.753	1.789	1.707	1.491	1.162
550	1.469	1.554	1.648	1.676	1.596	1.394	1.086
560	1.392	1.470	1.552	1.574	1.496	1.306	1.017
570	1.322	1.393	1.465	1.481	1.405	1.227	0.955

References [6-16,19].

5. *Electrical Conductance* (κ)

Measurement method: ac technique [14]

$$\kappa = a + bT + cT^2 \quad (30.3)$$

precision: in table 30.5, uncertainty: $\sim \pm 4\%$

Table 30.5. Coefficients of equation (30.3), and precisions

Mol % NaCl	-a	b x 10^3	c x 10^6	Precision
18.9	0.2067	0.6780	0	±0.63%
19.4	0.1839	0.6342	0	±0.87%
30.9	0.4258	1.3836	0	±0.69%
31.0	-0.6993	-3.3027	4.8037	±2.07%
42.2	0.5852	1.9443	0	±0.95%
49.2	0.6548	2.4082	0	±1.32%
50.0	0.7966	2.7366	0	±0.52%

Table 30.6. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 30.5

T (K)	Mol % NaCl						
	50.0	49.2	42.2	31.0	30.9	19.4	18.9
420				0.160			
430				0.167			
440				0.176			
450				0.186	0.197		
460	0.462	0.453	0.309	0.197	0.211		
470	0.490	0.477	0.329	0.208	0.224		
480	0.517	0.501	0.348	0.221	0.238	0.121	0.119
490	0.544	0.525	0.368	0.234	0.252	0.127	0.126
500	0.572	0.549	0.387	0.249		0.133	0.132
510	0.599	0.573	0.406	0.264		0.140	0.139
520	0.626	0.598	0.426				
530	0.654	0.622	0.445				
540	0.681	0.646	0.465				

References [6-16,20].

3. *Safety and Hazards*

A. Hazard rating [21-23]

(i) Toxicity: NaCl, very low; $AlCl_3$, severe

(ii) Vapor pressure: appreciable; see Table 30.11.2 (p.273) and [56]

B. Disaster hazards [24-26]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes; $AlCl_3$ reacts exothermically with moisture/water, to evolve HCl fumes.

References [21-26,56]

7. Corrosion

Table 30.7. Corrosion studies from primary research literature

Studies	References
Al, Ag, Cu, Mo, Ni, Pd, Ti, Fe, Pt, stainless steels	27
quartz, pyrex glass, Pt, Ni, vycor	6,14,20,28
Thermodynamic and electrochemical approach	29-31
Reviews (molten salts corrosion)	32-34
Annotated corrosion biblio.	35

References [6,14,20,27-35].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in $NaCl-AlCl_3$ as solvent

Na^+, Sn^{2+}, Pb^{2+}, Cu^+, Ag^+, Cd^{2+}, Ti^{2+}, Zr^{4+}, Nb^{5+}, Fe^{3+}, U^{4+}, I^-

The italicized species indicate studies with insufficient data-sets for characterization of temperature dependence of diffusion coefficients. For these species, see table 30.8.4.

precision: in table 30.8.2 uncertainty: in table 30.8

Table 30.8.1. Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
chronopotentiometry	∿±10%	U^{4+}, Na^+, Sn^{2+}, Pb^{2+}, Ti^{2+}, I^-
cyclic voltammetry	∿±20%	Zr^{4+}, I^-
linear sweep voltammetry	∿±20%	Sn^{2+}, Pb^{2+}, Cu^+, Cd^{2+}, Ti^{2+}, Nb^{5+}
pulse polarography	∿±20%	I^-, Ag^+, Fe^{3+}
chronoamperometry	∿±20%	Ti^{2+}, Fe^{3+}
rotating disc electrode	∿±20%	Fe^{3+}

Equation $D = A \exp[-E/RT]$ (30.4)

Table 30.8.2. Diffusion equation parameters, precisions, and recommended study

Species	A x 10^3 (cm^2 sec^{-1})	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
	(a) $NaCl-AlCl_3$ (eutectic)				
U^{4+}	3.82	4150	520-670	~8.5%	37
	(b) $NaCl-AlCl_3$ (50 mol % NaCl)				
Nb^{5+}	1.99	5033	430-570	~9.2%	38
U^{4+}	8.36	5324	520-670	~2.8%	37
	(c) $NaCl-AlCl_3$ (48 mol % NaCl)				
Zr^{4+}	15.17	6859	450-490	~12%	41

Table 30.8.3. Diffusion coefficients, D x 10^5 (cm^2 sec^{-1}), from equations in table 30.8.2

T (K)	Eutectic melt	50 mol % NaCl		48 mol % NaCl
	U^{4+}	Nb^{5+}	U^{4+}	Zr^{4+}
430		0.550		
450		0.715		0.707
460		0.808		0.836
470		0.909		0.980
480		1.02		1.14
490		1.13		1.32
500		1.26		
520	6.88	1.53	4.84	
540	7.98	1.83	5.85	
560	9.16	2.16	6.99	
570	9.78	2.34	7.60	
590	11.08		8.91	
610	12.44		10.34	
630	13.87		11.89	
650	15.36		13.55	
670	16.91		15.33	

Table 30.8.4. Diffusion coefficients for species not included in table 30.8.3

Species	Melt composition (mol % NaCl)	T (K)	D x 10^5 (cm^2 sec^{-1})	Recommended study
Na^+	37	413	0.10	43
Sn^{2+}	33.3	433	0.12	45
	48	433	0.19	44[a]
Pb^{2+}	33.3	433	0.27	45
	48	433	0.24	44[a]
Cu^+	48	433	0.53	44[a]
Ag^+	50	448	0.30	42
Cd^{2+}	48	433	0.18	44[a]
Ti^{2+}	35	458	0.295 0.275 0.424	39
	35	533	0.60	39
Fe^{3+}	50	448	0.91	42
		523	2.20	36
I^-	37	448	0.202 0.107 0.241	40
	50	448	0.268 0.211 0.243	40

[a]Ref. [44] reported data in graphical form in the temperature range 430-500 K.

References: Na^+, 43; Sn^{2+}, 45; Pb^{2+}, 44, 45; Cu^+, 44; Ag^+, 42; Cd^{2+}, 44; Ti^{2+}, 39; Zr^{4+}, 41; Nb^{5+}, 38; Fe^{3+}, 36, 42; U^{4+}, 37; I^-, 40

9. *Heat of Fusion (ΔH_f°)*

Measurement method: estimated [46]

Table 30.9. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
7.2	~ ± 5%

References [46].

10. *Heat Capacity (C_p)*

No data.

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated from densities [46]

Table 30.10. Volume change on melting

Binary eutectic (mol % NaCl)	$(\Delta V_f/V_s)$	Uncertainty
36.8	35.9%	∿ ± 5%

References [46].

12. Vapor Pressure (p_{vap})

Measurement method: isoteniscope [47]

$$\log p = A + B/T \quad (30.5)$$

precision: in table 30.11.1 uncertainty: ∿ ± 5%

Table 30.11.1. Parameters of equation (30.5), and precisions

Mol % $AlCl_3$	A	-B	Precision	Temp. range (K)
53.790	4.71496	1771.0	±3.53%	431-491
54.250	5.94281	2304.5	±4.96%	418-524
55.513	5.77583	2177.5	±5.43%	415-476
58.062	6.72729	2416.6	±1.93%	379-521
60.977	7.34912	2542.8	±1.32%	408-524
62.677	7.27205	2427.5	±1.02%	410-524
63.046	7.09260	2304.9	±1.11%	407-530
65.904	6.66296	1952.0	±0.43%	429-524
66.036	7.20848	2208.4	±0.80%	427-524
69.277	6.96901	1951.6	±0.35%	439-523
70.255	7.04376	1956.6	±0.07%	448-483
73.929	7.14703	1894.8	±0.16%	455-524

Table 30.11.2. Vapor pressure (mm) from equations in table 30.11.1

T	Mol % $AlCl_3$											
(K)	53.790	54.250	55.513	58.062	60.977	62.677	63.046	65.904	66.036	69.277	70.255	73.929
380				2.33								
390				3.40								
400				4.85								
410				6.81	14.03	22.46	29.57					
420		2.86	3.90	9.41	19.72	31.07	40.25					
430		3.83	5.15	12.80	27.27	42.34	54.00	132.87	118.21			
440	4.90	5.07	6.71	17.18	37.16	56.89	71.48	168.50	154.57	341.63		
450	6.02	6.63	8.65	22.75	49.94	75.44	93.46	211.44	199.95	428.67	496.32	
460	7.33	8.57	11.02	29.77	66.27	98.83	120.77	262.72	255.63	532.61	617.00	1066.37
470	8.85	10.96	13.89	38.51	86.88	127.99	154.37	323.43	323.42	655.66	759.95	1304.81
480	10.60	13.86		49.28	112.62	163.97	195.31	394.73	405.18	800.17	927.93	1583.20
490	12.61	17.37		62.44	144.46	207.96	244.75	477.85	502.98	968.63		1905.89
500		21.57		78.36	183.45	261.25	303.95	574.07	618.99	1163.64		2277.39
510		26.56		97.47	230.80	325.28	374.28	684.72	755.60	1387.87		2702.36
520		32.44		120.22	287.82	401.59	457.20	811.19	915.30	1644.14		3185.60

For vapor pressure of mixtures with 0-50 mol% $AlCl_3$, see [56]

References [47-54,56].

13. *Thermal Conductivity (liquid) (λ_ℓ)*

Measurement method: steady state concentric cylinder [55]

precision: not estimated uncertainty: ∿ ± 20%

Table 30.12. Thermal conductivity of eutectic melt

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
467	5.3

References [55].

14. *Thermal Conductivity (solid) (λ_s)*

No thermal conductivity studies reported.

15. *Cryoscopic Constant (k_f)*

Measurement method: estimated [46]

Table 30.13. Cryoscopic constant of eutectic

Binary eutectic (mol % NaCl)	k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
36.8	4.2	∿ ± 5%

References [46].

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XXXI. Potassium Chloride-Aluminum Chloride: $KCl-AlCl_3$

1. *Melting Temperatures (T_m)*

Pure substance melting points:

KCl: 770°C
$AlCl_3$: 192°C

Eutectic melting point:

128°C, composition: 33 mol % KCl

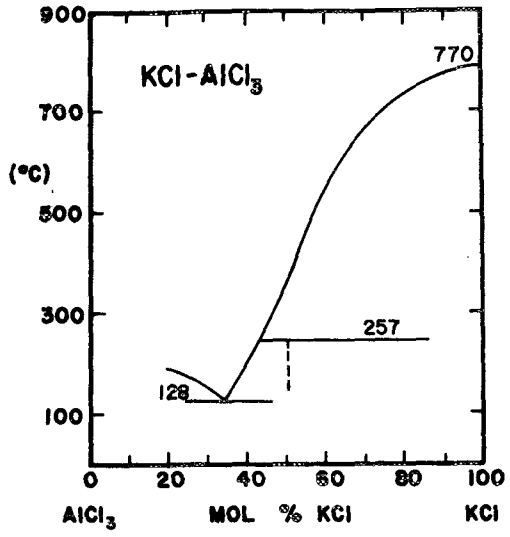

Figure 31.1. $KCl-AlCl_3$ phase diagram

References [1-3].

2. *Density (ρ)*

Measurement method: float technique [4]

$$\rho = a + bT \quad (31.1)$$

precision: in table 31.1 uncertainty: $\sim \pm 0.5\%$

Table 31.1. Coefficients of equation (31.1), and precisions

Mol. % KCl	a	$-b \times 10^3$	Precision
20.00	2.0252	1.0038	±0.11%
33.33	1.9889	0.7901	±0.14%
50.03	1.9556	0.6622	±0.05%
66.66	1.9734	0.6101	±0.02%

For numerical values: see table 31.2

Table 31.2. Densities (g cm^{-3}) from equations in table 31.1

	Mol % KCl			
T (K)	66.66	50.03	33.33	20.00
480				1.543
500			1.594	1.523
520			1.578	1.503
540			1.562	1.483
560			1.547	
580			1.531	
600			1.515	
620			1.499	
640			1.483	
660			1.468	
680			1.452	
700			1.436	
720			1.420	
740		1.466	1.404	
760		1.452	1.389	
780		1.439	1.373	
800		1.426		
820		1.413		
840		1.399		
860		1.386		
880		1.373		
900		1.360		
920		1.346		
940		1.333		
960	1.388	1.320		
980	1.376	1.307		
1000	1.363	1.293		
1020	1.351	1.280		
1040	1.339	1.267		

References [4-12].

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: ac technique [5,9]

$$\kappa = a + bT + cT^2 \quad (31.2)$$

precision: in table 31.3 uncertainty: ∿ ± 3%

Table 31.3.1. Coefficients of equation (31.2), and precisions

Mol % KCl	-a	b x 10^3	c x 10^6	Precision
19.4	0.0842	0.1364	0.5637	±0.50%
19.75	0.2107	0.6730	0	±0.74%
28.80	0.4986	1.6155	-0.4808	±0.21%
30.75	0.2948	0.7560	0.4625	±0.52%
39.45	0.5271	1.5402	0	±1.18%
49.35	0.7979	2.1891	0	±0.74%

Table 31.3.2. Coefficients of equation (31.2) and precisions for additional mixtures

Mol % KCl	-a	b x 10^3	-c x 10^6	Precision
40	1.60616	4.5104	2.0094	±0.01%
50	1.06946	3.3785	1.2854	±0.36%
60	0.24510	0.6700	0.0	±2.03%
70	0.11300	0.8500	0.0	±1.99%
80	0.17700	1.0000	0.0	±0.00%
90	0.29910	1.2000	0.0	±0.68%
100	-0.19590	2.2500	0.0	±1.30%

uncertainty: ∿ ± 4%

Table 31.4.1. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 31.3.1.

	Mol % KCl					
T (K)	49.35	39.45	30.75	28.80	19.75	19.4
470				0.1544	0.1056	0.1044
480		0.2122	0.1746	0.1660	0.1123	0.1111
490		0.2276	0.1867	0.1775	0.1191	0.1180
500		0.2430	0.1988	0.1889	0.1258	0.1249
510		0.2584	0.2111	0.2002	0.1325	0.1320
520		0.2738	0.2234	0.2114	0.1393	0.1392
530	0.3623	0.2892	0.2358	0.2225	0.1460	0.1464
540	0.3842	0.3046	0.2483	0.2335	0.1527	0.1538
550	0.4061	0.3200	0.2609		0.1595	0.1613
560	0.4280	0.3354	0.2736		0.1662	
570	0.5599		0.2864			

Table 31.4.2. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 31.3.2.

T (K)	Mol % KCl						
	40	50	60	70	80	90	100
880	0.807	0.908					
900	0.826	0.930					
920	0.843	0.951					
940	0.858	0.971					
960	0.872	0.989					
980	0.884	1.007	0.902	0.946			
1000	0.895	1.024	0.915	0.963			
1020	0.904	1.039	0.929	0.980			
1040	0.911	1.054	0.942	0.997			
1060	0.917	1.067	1.955	1.014			
1080		1.080	0.969	1.031	1.257	1.595	2.234
1100		1.092	0.982	1.048	1.277	1.619	2.279
1120		1.102	0.996	1.065	1.297	1.643	2.324
1140		1.112	1.009	1.082	1.317	1.667	2.369
1160		1.120	1.022	1.099	1.337	1.691	2.414
1180		1.127	1.036	1.116	1.357	1.715	2.459
1200		1.134	1.049	1.133	1.377	1.739	2.504
1220		1.139	1.063	1.150	1.397	1.763	2.549
1240		1.143	1.076	1.167	1.417	1.787	2.594
1260		1.147	1.089	1.184	1.437	1.811	2.639

References [4-6,8,9,11-16].

6. *Safety and Hazards*

A. Hazard rating [17-19]

(i) Toxicity: KCl, slight; $AlCl_3$, severe

(ii) Vapor pressure: appreciable; see [32-34] and Table 31.9 (p.282)

B. Disaster hazards [17,20-22]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides, when heated to decomposition, or contacted with acids emit highly toxic fumes; $AlCl_3$ reacts exothermically with moisture/water to evolve HCl fumes.

References [17-22].

7. Corrosion

Table 31.5. Corrosion studies from primary research literature

Studies	References
Quartz, vycor, Ni, Pt	4,5,9,23
Electrochemical approach	24,25
Thermodynamic redox diagrams	26
Annotated corrosion biblio.	27
Reviews: molten salts corrosion	28-30

References [4,5,9,23-30].

8. Diffusion

No diffusion studies reported with molten $KCl\text{-}AlCl_3$ as solvent.

9. Heat of Fusion (ΔH_f°)

Measurement method: estimated [31]

Table 31.6. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
6.9	∿ ± 5%

References [31].

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated from densities [31]

Table 31.7. Volume change on melting

Binary eutectic (mol % KCl)	$(\Delta V_f/V_s)$	Uncertainty
33	35.5%	∿ ± 5%

References [31].

12. Vapor Pressure (p_{vap})

Measurement method: static technique [32]

$$\log p = A + B/T \quad (31.3)$$

precision: in table 31.8 uncertainty: ∿ ± 10%

Table 31.8. Parameters of equation (31.3), and precisions

Mol % $AlCl_3$	A	-B	Temp. range (K)	Precision
50.1	7.3950	5860	861-1073	± 1.87%
48.5	9.2386	7846	905-1073	± 3.50%
42.4	8.9430	7634	917-1029	± 1.10%
36.2	8.4231	7212	943-1037	± 0.90%

For vapor pressure of mixtures with 0-50 mol% $AlCl_3$, see [34]

Table 31.9. Vapor pressure (mm) from equations in table 31.8

T (K)	Mol % $AlCl_3$			
	36.2	42.4	48.5	50.1
870				4.6
880				5.4
890				6.5
900				7.7
910			4.1	9.0
920		4.4	5.1	10.6
930		5.4	6.3	12.4
940		6.6	7.8	14.5
950	6.8	8.1	9.5	16.8
960	8.1	9.8	11.6	19.5
970	9.7	11.8	14.1	22.6
980	11.6	14.2	17.1	26.0
990	13.7	17.1	20.6	29.9
1000	16.3	20.4	24.7	34.3
1010	19.2	24.2	29.5	39.2
1020	22.5	28.8	35.2	44.7
1030	26.4	34.0	41.8	50.8
1040			49.5	57.6
1050			58.4	65.2
1060			68.7	73.6
1070			80.5	82.9

References [32-34].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: estimated [31]

Table 31.10. Cryoscopic constant of eutectic

k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
5.3	∿ ± 5%

References [31].

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[19] Vapor pressure, calculated (see p.282, this work).

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XXXII. Sodium Chloride-Calcium Chloride: $NaCl-CaCl_2$

1. Melting Temperatures (T_m)

Pure substance melting points:
$NaCl$: 800°C
$CaCl_2$: 782°C

Eutectic melting point:
500°C, composition: 48 mol % NaCl

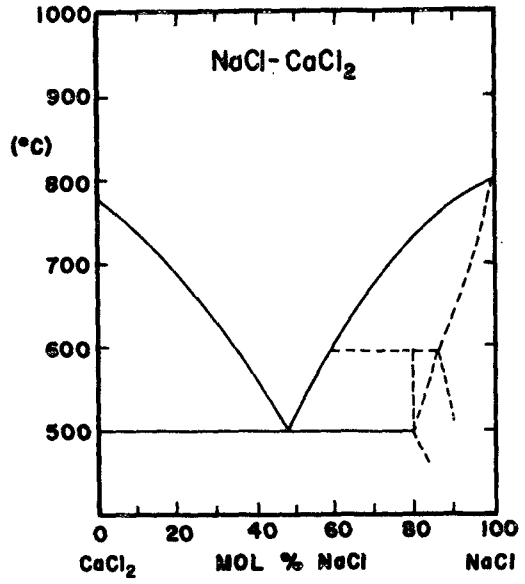

Figure 32.1. $NaCl-CaCl_2$ phase diagram

References [1-3].

2. Density (ρ)

Measurement method: Archimedean technique [4]

Single variable equation

$$\rho = a + bT \quad (32.1)$$

precision: in table 32.1 uncertainty: ∿ + 1%

Table 32.1. Coefficients of single variable equation (32.1), and precisions

Mol. % NaCl	a	$-b \times 10^4$	Precision
0	2.4986	3.976	±0.05%
19.8	2.4651	4.444	±0.03%
22.5	2.4637	4.554	±0.02%
35.9	2.4925	5.367	±0.18%
49.1	2.3800	4.955	±0.02%
67.5	2.1791	4.006	±0.01%
85.0	2.1305	4.546	±0.01%
100.0	2.1319	5.297	±0.04%

$NaCl-CaCl_2$

Two-independent-variable equation

$$\rho = a + bT + cC + dC^2 \quad (C = \text{mol \% } CaCl_2) \quad (32.2)$$

precision: ± 0.18% uncertainty: ∿ ± 1%

Table 32.2. Coefficients of two-independent-variables equation (32,2)

a	b x 10^4	c x 10^3	d x 10^5
2.06606	-4.72915	6.20063	-1.04771

Table 32.3. Densities (g cm^{-3}) from equations in table 32.1

T (K)	Mol % NaCl							
	100	85.0	67.5	49.1	35.9	22.5	19.8	0
1040							2.003	
1050							1.998	
1060				1.855			1.994	
1070				1.850			1.990	2.073
1080				1.845	1.913	1.972	1.985	2.069
1090	1.555	1.635	1.742	1.840	1.908	1.967	1.981	2.065
1100	1.549	1.630	1.738	1.835	1.903	1.963	1.976	2.061
1110	1.544	1.626	1.734	1.830	1.897	1.958	1.972	2.057
1120	1.539	1.621	1.730	1.825	1.892	1.954	1.967	2.053
1130	1.533	1.617	1.726	1.820	1.887	1.949		2.049
1140	1.528	1.612	1.722	1.815	1.881	1.945		2.045
1150	1.523	1.608	1.718	1.810	1.876	1.940		
1160	1.517	1.603		1.805	1.871	1.935		
1170	1.512	1.599			1.865	1.931		

References [4-23].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [16]

$$\gamma = a + bT \quad (32.3)$$

precision: ∿ ± 0.8% uncertainty: ∿ ± 0.5%

Table 32.4. Parameters of equation (32.3)

Mol % NaCl	a	$-b \times 10^2$
0	205.83	5.61
20	224.81	8.37
23.72	211.92	7.40
30	204.57	7.00
35	199.68	6.66
40	204.49	7.36
50	194.15	6.62
60	201.34	7.55
70	206.22	8.24
80	206.36	8.42
90	199.67	7.90
100	198.14	7.80

Table 32.5. Surface tension (dyn cm^{-1}) from equations in table 32.4

	Mol % NaCl											
T(K)	100	90	80	70	60	50	40	35	30	23.72	20	0
830						139.20	143.40					
840						138.54	142.67					
850						137.88	141.93					
860						137.22	141.19					
870						136.56	140.46					
880					134.90	135.89	139.72	141.07				
890					134.15	135.23	138.99	140.41				
900					133.39	134.57	138.25	139.74				
910					132.64	133.91	137.51	139.07				
920					131.88	133.25	136.78	138.41				
930					131.13	132.58	136.04	137.74	139.47			
940					130.37	131.92	135.31	137.08	138.77			
950				127.94	129.62	131.26	134.57	136.41	138.07			
960				127.12	128.86	130.60	133.83	135.74	137.37			
970				126.29	128.11	129.94	133.10	135.08	136.67	140.14		
980				125.47	127.35	129.27	132.36	134.41	135.97	139.40	142.78	
990				124.64	126.60	128.61	131.63	133.75	135.27	138.66	141.95	
1000				123.82	125.84	127.95	130.89	133.08	134.57	137.92	141.11	
1010				123.00	125.09	127.29	130.15	132.41	133.87	137.18	140.27	149.17
1020			120.48	122.17	124.33	126.63	129.42	131.75	133.17	136.44	139.44	148.61
1030			119.63	121.35	123.58	125.96	128.68	131.08	132.47	135.70	138.60	148.05
1040			118.79	120.52	122.82	125.30	127.95	130.42	131.77	134.96	137.76	147.49
1050			117.95	119.70	122.07	124.64	127.21	129.75	131.07	134.22	136.93	146.93
1060			117.11	118.88	121.31	123.98	126.47	129.08	130.37	133.48	136.09	146.36
1070		115.14	116.27	118.05	120.56	123.32	125.74	128.42	129.67	132.74	135.25	145.80
1080	113.90	114.35	115.42	117.23	119.80				128.97	132.00	134.41	145.24
1090	113.12	113.56	114.58	116.40						131.26	133.58	144.68
1100	112.34	112.77	113.74	115.58						130.52		144.12
1110	111.56	111.98	112.90	114.76								143.56
1120	110.78	111.19	112.06									143.00
1130	110.00	110.40										142.44
1140												141.88

References [4-18,24,25].

4. *Viscosity (η)*

Measurement method: oscillating sphere [10]

$$\eta = a + bT + cT^2 + dT^3 \quad (32.4)$$

precision: in table 32.6 uncertainty: ∿ ± 25%

Table 32.6. Parameters of equation (32.4), and precisions

NaCl (mol %)	a	b x 10^2	c x 10^5	d x 10^9	Precision
0	69.3492	-10.3644	3.5858	3.8776	0.73%
10	20.1917	2.8465	-8.3002	39.9729	0.34%
20	30.0118	-0.1588	-5.5677	32.2866	0.41%
40	12.1701	0.9805	-3.4259	16.2560	0.67%
50	44.5576	-8.7561	6.2253	-15.5917	0.65%
60	10.4758	1.2168	-3.6226	16.8297	0.68%
70	19.1369	-1.1116	-1.3786	8.9463	0.58%
80	33.3003	-3.3357	-0.9395	12.5058	0.69%
90	30.9838	-2.2958	-2.2975	17.8387	0.64%
100	[-22.9126]	[4.8514]	[-2.4000]	0	

Table 32.7. Viscosity (cp) from equations in table 32.6

T (K)	Mol % NaCl									
	100	90	80	70	60	50	40	20	10	0
930					4.00	4.43	4.73			
940					3.88	4.31	4.62			
950					3.77	4.19	4.50			
960					3.66	4.08	4.39			
970					3.55	3.97	4.28			
980				3.42	3.45	3.86	4.18	5.37		
990				3.30	3.35	3.76	4.07	5.20		
1000			3.05	3.18	3.25	3.66	3.97	5.03		
1010			2.91	3.06	3.15	3.56	3.87	4.88		
1020			2.77	2.95	3.06	3.47	3.78	4.73		
1030			2.64	2.84	2.97	3.38	3.69	4.59	5.13	4.88
1040			2.51	2.73	2.88	3.29	3.60	4.46	4.98	4.71
1050		2.20	2.39	2.62	2.80	3.20	3.51	4.34	4.84	4.55
1060		2.08	2.28	2.52	2.72	3.12	3.43	4.22	4.71	4.40
1070		1.97	2.17	2.42	2.64	3.04	3.35	4.12	4.59	4.25
1080		1.86	2.07	2.32	2.56	2.96	3.28	4.03	4.47	4.12
1090		1.76	1.97	2.23	2.49	2.89	3.21	3.94	4.37	4.00
1100	[1.41]	1.67	1.88	2.14	2.43	2.82	3.14	3.87	4.27	3.89
1110	[1.37]	1.59	1.80	2.05	2.37	2.74	3.08	3.81	4.19	3.79
1120	[1.32]	1.51	1.72	1.96	2.31	2.68	3.02	3.75	4.11	3.70
1130	[1.26]	1.44	1.65	1.88	2.25	2.61	2.96	3.71	4.05	3.61
1140	[1.20]	1.38	1.59	1.80	2.20	2.54	2.91	3.68	3.99	3.54

Values in brackets are based on minimal data base.

References [4-18].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [14]

$$\kappa = a + bT + cT^2 \quad (32.5)$$

precision: in table 32.8 uncertainty: ∿ ± 1.5%

Table 32.8. Parameters of equation (32.5), and precisions

Mol % NaCl	-a	b x 10^3	-c x 10^7	Precision[a]
33.3	[3.4536]	[6.1849]	[9.4099]	
51.8	3.9865	7.7171	17.9443	±0.07%
73.6	[3.9759]	[8.6268]	[23.5295]	
88.5	-[0.2981]	[2.5926]	—	

[a]No entry indicates insufficient data for precision estimates

Table 32.9.1 Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 32.8

T (K)	Mol % NaCl		
	88.5	73.6	33.3
970			[1.660]
980		[2.219]	[1.704]
990		[2.259]	[1.747]
1000		[2.298]	[1.790]
1010		[2.337]	[1.833]
1020		[2.375]	[1.876]
1030		[2.414]	[1.919]
1040		[2.451]	[1.961]
1050		[2.488]	[2.003]
1060	[3.046]	[2.525]	[2.045]
1070	[3.072]	[2.561]	[2.087]
1080	[3.098]	[2.597]	

Values in brackets are based on minimal data base.

Table 32.9.2. Specific conductance for additional mixture (51.8 mol % NaCl)

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
830	1.183	960	1.768
840	1.230	970	1.811
850	1.277	980	1.853
860	1.323	990	1.895
870	1.369	1000	1.936
880	1.415	1010	1.977
890	1.460	1020	2.018
900	1.505	1030	2.058
910	1.550	1040	2.098
920	1.594	1050	2.138
930	1.638	1060	2.177
940	1.682	1070	2.216
950	1.725	1080	2.255

References [4-19,21,26-28].

6. Safety and Hazards

A. Hazard rating [29-31]

(i) Toxicity: NaCl, very low; $CaCl_2$, very low.

(ii) Vapor pressure: no data for mixture; but see, NaCl; $CaCl_2$.

B. Disaster hazards [29,32-34]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

References [29-34].

7. Corrosion

Table 32.10. Corrosion studies from primary research literature

Studies	References
Armco Fe, steels	35
Ti, Zr, Hf, $ThCl_4$	36
Quartz, Pt, Mo, Ni, Al_2O_3	11,14,15,21
Thermodynamic redox diagrams	37
Electrochem. approach	38,39
Reviews: molten salts corrosion	40-42
Annotated corrosion biblio.	43

References [11,14,15,21,35-43].

8. Diffusion

Measurement method: chronopotentiometry [44]

Diffusing species investigated in $NaCl-CaCl_2$ as solvent:

Fe^{2+}

precision: insufficient data for estimate

Table 32.11. Diffusion coefficients and uncertainties

Species	T (K)	$D \times 10^5$ ($cm^2\ sec^{-1}$)	Uncertainty
Fe^{2+}	873	2.36	$\sim \pm 10\%$

References [44].

9. Heat of Fusion (ΔH_f°)

Measurement method: estimated [45]

Table 32.12. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
5.7	∿ ± 5%

References [45].

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated from densities [46].

Table 32.13. Volume change on melting

Binary eutectic (mol % NaCl)	$(\Delta V_f/V_s)$	Uncertainty
48	14.5%	∿ ± 8%

References [46].

12. Vapor Pressure (p_{vap})

Measurement method: Rodebush-Dixon [47]

Table 32.14. Vapor pressures (mm)

Mol % NaCl	1373 K	1423 K	Mol % NaCl	1373 K	1423 K
13	1.46	2.90	84	24.48	41.10
29	3.77	7.32	86	25.71	43.18
42	7.37	13.79	88	27.19	46.08
53	11.35	18.37	90	28.43	47.70
61	14.30	24.79	91	28.87	48.91
69	17.47	30.08	100	32.07	56.34
78	20.92	36.05			

Values at 100% NaCl are 8-10% higher than the recommended vapor pressure for NaCl at 1373 and 1423 K.

References [47].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_ℓ)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: estimated [45]

Table 32.15. Cryoscopic constant

Binary eutectic (mol % NaCl)	k_f ($K\ mol^{-1}kg^{-1}$)	Uncertainty
48	17.7	∿ ± 5%

References [45].

16. References

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XXXIII. Sodium Polysulfides: Na_2S_x (2,·····, 5.2)

1. *Melting Temperatures (T_m)*

Pure substance melting points:

Na_2S : 1170°C

Sulfur: 115°C

Compound melting points:

Na_2S_2: 482°C

Na_2S_3: 230°C

Na_2S_4: 294°C

Na_2S_5: 255°C

Eutectic melting points:

Eutectic 1: 235°C, composition: Na_2S_2-Na_2S_4 (50 mol % Na_2S_2)

Eutectic 2: 237°C, composition: Na_2S_4-Na_2S_5 (33.3 mol % Na_2S_4)

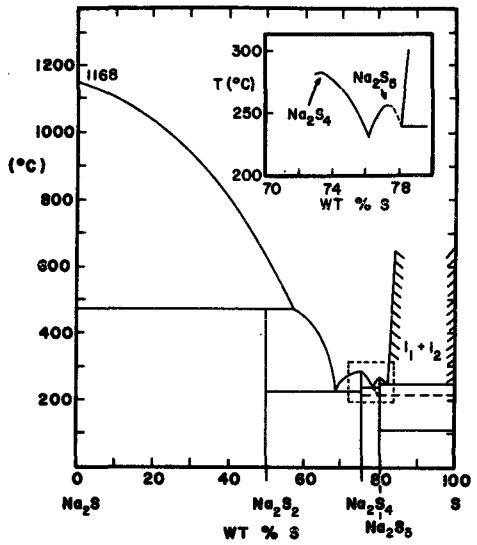

Figure 33.1. Na_2S_x phase diagram

References [1-11].

2. *Density (ρ)*

Measurement method: modified dilatometric [12]

$$\rho = a + bT \quad (33.1)$$

precision: in table 33.1 uncertainty: ∿ ± 2%

Table 33.1. Parameters of equation (33.1), and precisions

Melt	Wt % S	Temp. range (K)	a	$-b \times 10^3$	Precision
$Na_2S_{3.0}$	67.6	590 - 683	2.2270	0.5658	±0.18%
$Na_2S_{3.3}$	69.7	576 - 689	2.3802	0.7989	±0.40%
$Na_2S_{3.7}$	72.0	563 - 669	2.2538	0.5459	±0.13%
$Na_2S_{4.4}$	75.4	571 - 680	2.2687	0.6664	±0.26%
$Na_2S_{4.8}$	77.0	573 - 683	2.3056	0.7156	±0.27%

Table 33.2. Densities (g cm^{-3}) from equations in table 33.1

T (K)	$Na_2S_{3.0}$	$Na_2S_{3.3}$	$Na_2S_{3.7}$	$Na_2S_{4.4}$	$Na_2S_{4.8}$
560					
570			1.9426		
580		1.9169	1.9372	1.8822	1.8905
590		1.9089	1.9317	1.8756	1.8834
600	1.8875	1.9009	1.9263	1.8689	1.8762
610	1.8818	1.8929	1.9208	1.8622	1.8691
620	1.8762	1.8850	1.9153	1.8556	1.8619
630	1.8705	1.8770	1.9099	1.8489	1.8547
640	1.8648	1.8690	1.9044	1.8422	1.8476
650	1.8592	1.8610	1.8990	1.8356	1.8404
660	1.8535	1.8530	1.8935	1.8289	1.8333
670	1.8479	1.8450		1.8223	1.8261
680	1.8422	1.8370		1.8156	1.8190

References [12,13].

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [12]

$$\gamma = a + bT \quad (33.2)$$

precision: in table 33.3 uncertainty: $\approx \pm 1.5\%$

Table 33.3. Parameters of equation (33.2), and precisions

Melt	Wt % S	Temp. range (K)	a	-b x 10^2	Precision
$Na_2S_{3.0}$	67.7	583-691	210.22	6.070	± 0.4%
$Na_2S_{3.1}$	68.5	588-673	237.21	11.98	± 0.4%
$Na_2S_{3.3}$	69.7	586-671	191.61	6.496	± 0.3%
$Na_2S_{3.6}$	71.5	589-677	162.00	3.395	± 0.2%
$Na_2S_{3.9}$	72.4	539-676	153.62	3.592	± 0.2%
$Na_2S_{4.1}$	74.0	556-641	163.08	5.809	± 0.4%
$Na_2S_{4.3}$	75.1	602-676	168.25	6.729	± 1.0%
$Na_2S_{4.7}$	76.3	562-671	169.80	7.100	± 0.5%
$Na_2S_{4.8}$	76.8	625-688	182.95	9.153	± 1.2%
$Na_2S_{5.2}$	78.4	616-661	138.74	3.901	± 0.4%

Table 33.4. Surface tension (dyn cm^{-1}) from equations in table 33.3

T (K)	$Na_2S_{3.0}$	$Na_2S_{3.1}$	$Na_2S_{3.3}$	$Na_2S_{3.6}$	$Na_2S_{3.9}$	$Na_2S_{4.1}$	$Na_2S_{4.3}$	$Na_2S_{4.7}$	$Na_2S_{4.8}$	$Na_2S_{5.2}$
530										
540					134.22					
550					133.86					
560					133.51	130.54				
570					133.13	129.96		129.33		
580					132.79	129.38		128.64		
590	174.41	166.52	153.28	141.97	132.43	128.80		127.93		
600	173.80	165.32	152.63	141.63	132.07	128.22		127.22		
610	173.19	164.12	151.98	141.29	131.71	127.64	127.20	126.52		
620	172.59	162.93	151.33	140.95	131.35	127.06	126.53	125.81		114.56
630	171.98	161.73	150.68	140.61	130.99	126.48	125.85	125.10	125.29	114.17
640	171.37	160.53	150.03	140.27	130.63	125.90	125.18	124.39	124.37	113.78
650	170.77	159.33	149.38	139.94	130.27		124.51	123.68	123.46	113.39
660	170.16	158.13	148.73	139.60	129.91		123.83	122.94	122.54	113.00
670	169.55	156.94	148.09	139.26	129.55		123.16	122.23	121.63	
680	168.94								120.71	
690	168.34									

References [12].

4. Viscosity (η)

Measurement method: modified capillary [12]

$$\eta = A \exp[E_\eta/R(T-T_o)] \quad (33.3)$$

precision: in table 33.5 uncertainty: ∿ ± 5%

Table 33.5. Parameters of equation (33.3), and precisions

Melt	Wt. % S	Temp. range (K)	A (cp)	E_η (cal mol^{-1})	T_o (K)	Precision
$Na_2S_{3.1}$	68.4	577-653	0.5624	2018	332	± 0.5%
$Na_2S_{3.3}$	70.0	589-647	0.3370	2683	288	± 0.1%
$Na_2S_{3.6}$	71.7	558-646	0.6193	1906	342	± 0.2%
$Na_2S_{3.9}$	73.1	533-652	0.4046	2221	326	± 0.8%
$Na_2S_{4.1}$	74.0	587-641	0.4070	2234	328	± 0.2%
$Na_2S_{4.3}$	75.1	572-675	0.8071	1438	390	± 0.4%
$Na_2S_{4.7}$	76.8	557-654	0.4684	1963	356	± 0.6%
$Na_2S_{5.2}$	78.5	620-648	1.7411	742.1	465	± 0.3%

For $Na_2S_{3.9}$, viscosity values at temperatures less than 553 K are for the supercooled melt.

Table 33.6. Viscosity (cp) from equations in table 33.5

T (K)	$Na_2S_{3.1}$	$Na_2S_{3.3}$	$Na_2S_{3.6}$	$Na_2S_{3.9}$	$Na_2S_{4.1}$	$Na_2S_{4.3}$	$Na_2S_{4.7}$	$Na_2S_{5.2}$
540				75.03				
550				59.43				
560			50.43	48.02			59.38	
570			41.58	39.48			47.35	
580	33.76		34.84	32.96		36.39	38.53	
590	28.81	29.46	29.62	27.90	29.72	30.08	31.92	
600	24.87	25.53	25.50	23.91	25.39	25.32	26.85	
610	21.70	22.32	22.19	20.71	21.93	24.65	22.89	
620	19.12	19.67	19.51	18.12	19.13	18.76	19.75	19.37
630	16.98	17.46	17.31	15.99	16.84	16.46	17.23	16.74
640	15.20	15.61	15.48	14.22	14.94	14.59	15.18	14.71
650	13.71			12.74		13.05	13.48	
660						11.77		
670						10.70		

References [12].

5. Electrical Conductance (κ)

Measurement method: Wayne-Kerr ac technique [14]

$$\kappa = A \exp[-E_\kappa/R(T-T_o)] \quad (33.4)$$

precision: in table 33.7 uncertainty: ∿ ± 2.5%

Table 33.7. Parameters of equation (33.4), and precisions

Melt	Wt % S	Temp. range (K)	A ($ohm^{-1}cm^{-1}$)	E cal mol^{-1}	T_o (K)	Precision
$Na_2S_{2.1}$	60.0	728-840	5.4770	736.1	499	±1.3%
$Na_2S_{2.9}$	66.1	642-698	3.8590	595.4	458	±0.9%
$Na_2S_{3.0}$	67.5	582-693	7.0407	1362	329	±0.5%
$Na_2S_{3.2}$	70.1	458-694	7.0650	1402	330	±1.0%
$Na_2S_{3.8}$	72.3	428-694	7.0860	1541	325	±0.7%
$Na_2S_{4.2}$	74.8	456-671	6.2783	1475	341	±1.4%
$Na_2S_{5.1}$	77.8	477-681	5.7935	1513	344	±1.0%

For the following polysulfides, conductivity measurements have been extended into the supercooled liquid state region [refer phase diagram]: $Na_2S_{2.1}$ ($T < 748K$); $Na_2S_{3.2}$ ($T < 538K$); $Na_2S_{3.8}$ ($T < 553K$); $Na_2S_{4.2}$ ($T < 543K$); Na_2S_5 ($T < 533K$).

Table 33.8.1. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 33.7

T (K)	$Na_2S_{2.9}$	$Na_2S_{3.0}$	$Na_2S_{3.2}$	$Na_2S_{3.8}$	$Na_2S_{4.2}$	$Na_2S_{5.1}$
430				0.0044		
440				0.0084		
450				0.0143		
460			0.0311	0.0227	0.0123	
470			0.0458	0.0337	0.0199	
480			0.0640	0.0476	0.0301	0.0215
490			0.0859	0.0645	0.0431	0.0315
500			0.1114	0.0843	0.0589	0.0440
510			0.1402	0.1071	0.0777	0.0591
520			0.1724	0.1328	0.0993	0.0767
530			0.2075	0.1613	0.1237	0.0967
540			0.2455	0.1923	0.1506	0.1192
550			0.2860	0.2257	0.1801	0.1439
560			0.3288	0.2614	0.2118	0.1708
570			0.3736	0.2991	0.2456	0.1996
580			0.4202	0.3386	0.2812	0.2302
590		0.5095	0.4684	0.3798	0.3186	0.2625
600		0.5613	0.5179	0.4224	0.3574	0.2963
610		0.6142	0.5686	0.4663	0.3976	0.3313
620		0.6679	0.6202	0.5114	0.4390	0.3675
630		0.7223	0.6726	0.5574	0.4813	0.4047
640		0.7771	0.7256	0.6043	0.5245	0.4428
650	0.8105	0.8324	0.7791	0.6518	0.5683	0.4816
660	0.8756	0.8878	0.8329	0.7000	0.6128	0.5211
670	0.9390	0.9434	0.8870	0.7485	0.6577	0.5611
680	1.001	0.9990	0.9412	0.7975		0.6014
690	1.060	1.055	0.9954	0.8467		
700						

Table 33.8.2. Specific conductance for additional mixture, $Na_2S_{2.1}$

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
730	1.102	790	1.534
740	1.178	800	1.600
750	1.252	810	1.664
760	1.325	820	1.727
770	1.396	830	1.789
780	1.466	840	1.848

References [14].

6. Safety and Hazards

A. Hazard rating [15-17]

(i) Inhalation: variable

- as sulfides and polysulfides, the rating is similar to sodium hydroxide
- on reaction with moisture/water, H_2S is liberated; the inhalation hazard rating for H_2S is severe; i.e., highly toxic

(ii) Vapor pressure: the sulfur pressure above some molten polysulfide compositions has been reported, e.g., at ∿ 1000°C, the sulfur pressures above Na_2S_2, Na_2S_3, and Na_2S_4 are respectively, ∿ 15 mm, ∿ 300 mm, and ∿ 2000 mm.

B. Disaster hazards [15,18-20]

(i) Molten sulfides and polysulfides may react violently (explosively) with strong oxidizers; H_2S evolved on contact with moisture/water can form explosive mixtures with air; H_2S, highly toxic.

(ii) Polysulfides, when heated to decomposition, or contacted with water, steam, acids, produce highly toxic fumes (oxides of sulfur; H_2S). Dangerous.

References [15-20].

7. Corrosion

Table 33.9.1. Corrosion screening studies [21-23]

Extensively corroded materials

TaB_2, ZrC, VN, VC, NbB_2, $ZrSi_2$, $TiSi_2$, CrB_2, ZrN, CrC, $CaTiO_3$ (+ 0.3% Fe_2O_3), anodized Ti, Ti

Corrosion protection from sulfide or oxide film formation

Zr, $CrSi_2$, TiC, ZrB_2, TiN, Si, TaC, TaN, AISI 446 stainless steel, Inconel600 and 601, Mo

Table 33.9.1. - - Continued

Intrinsically Corrosion Resistant Materials
Cr_2O_3, MoS_2, ZrO_2, $La_{0.84}Sr_{0.16}CrO_3$, TiO_2 (single crystal and polycrystalline doped with Ta). $SrTiO_3$, $CaTiO_3$ (+ 3.0% Fe_2O_3) Polyphenylene (PpH), Polyphenylene-graphite composites, oxidized stainless steels, NiO

Table 33.9.2. Corrosion studies: static techniques [21-23]

(i) All metals and alloys are attacked to some extent. Sulfides of metals appear to be thermodynamically more stable than the unreacted metals.

(ii) Certain metals - Fe, Cu, Ni, Au, and Ti - are rapidly corroded, i.e., rapid dissolution of the sulfide product in the polysulfides

(iii) With the metals Cr, Hf, Zr and Mo the attack is less severe, i.e., apparently a slow dissolution of the sulfide product in the polysulfides

(iv) Alloys containing an appreciable concentration of Cr ($\sim$ 20%) are slowly attacked at a rate similar to that for Cr metal itself. Both ferritic and austenitic stainless steels and several grades of Inconel exhibit this characteristic; i.e., apparently an accumulation of Cr sulfide in the corrosion inhibiting layer.

(v) The oxides of the reactive metallic elements studied thus far are instrinsically stable in molten polysulfide; i.e., correlates with the relative thermodynamic stabilities of oxides and sulfides of these elements

(vi) In general, metallic borides, carbides, nitrides, and silicides are rapidly attacked.

(vii) Certain forms of carbon are stable. Graphite, vitreous carbon, and a thermosetting polyphenylene resin have been found to be intrinsically stable.

Table 33.9.3. Corrosion studies from primary research literature: dynamic studies (electrochemical) [21,24,25,27]

Studies	Conditions
Fe (99.98%)	Steady-state current-potential measurements
18-8 SS	anodic and cathodic corrosion properties
E-Brite - SS	pre-oxidized (750°C, 1 hr); anodic and cathodic
AISI-446-SS	pre-oxidized (750°C, 20 hr); anodic and cathodic
Fe-Co-Ni	-

Table 33.9.4. Corrosion studies from primary research literature: various additional studies [21-23,26]

Studies	Conditions
AISI-446-SS E-Brite-SS	preoxidized; static corrosion studies at 300°, 350°C, 400°C
AISI-446-SS	pre-oxidized; statis corrosion studies; various polysulfide compositions (Na_2S_3, Na_2S_4, Na_2S_5)
Fe, Zr, Hf	static corrosion studies in Na_2S_3
AISI-446-SS	static corrosion studies in Na_2S
Corrosion in molten salts	annotated bibliography
Metal sulfides	saturation solubilities

t (°C)	solute	solvent (polysulfide)	solubility (mg/g)
375	CrS	Na_2S_5	71.4 × 10^{-3}
		Na_2S_4	46.2 × 10^{-3}
		$Na_2S_{3.2}$	40.6 × 10^{-3}
		$Na_2S_{2.74}$	6.0 × 10^{-3}
375	MnS	Na_2S_5	3.42
		Na_2S_4	2.12
		$Na_2S_{3.2}$	1.18
		$Na_2S_{2.74}$	0.50
375	FeS	Na_2S_5	0.17
		Na_2S_4	1.28
		$Na_2S_{3.2}$	2.72
		$Na_2S_{2.74}$	3.99
375	NiS	Na_2S_5	0.15
		Na_2S_4	0.47
		$Na_2S_{3.2}$	1.18
		$Na_2S_{2.74}$	4.64
325	CrS	Na_2S_4	30
	FeS		0.6
300	FeS	Na_2S_5	0.1
	NiS		0.1
300	FeS	$Na_2S_{2.9}$	2
	NiS		0.8

References [21-27].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

No data.

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

No data.

12. Vapor Pressure (p_{vap})

Measurement method: transpiration; emf. [28-30]

Polysulfides exhibit equilibrium sulfur vapor pressures. The equilibrium sulfur pressures for a series of polysulfides covering the composition range from $Na_2S_{1.7}$ to $Na_2S_{5.5}$ reported herewith have been calculated from the Tegman data-base [28-30].

Vaporization studies of molten polysulfides as molecular polysulfide species have not been reported. In the Tegman studies of sulfur equilibrium pressures, the observation is reported that a faint condensate due to polysulfide molecular species was evident in the temperature range of 1173-1273 K. From this it is apparent that the vapor pressures as molecular polysulfides are much smaller than the equilibrium sulfur pressures, i.e. possibly more comparable to the alkali metal halides.

Equilibrium sulfur pressures for Na_2S_x

$$\log p = A + B/T \quad (33.5)$$

precision: in table 33.10.1 uncertainty: $\sim \pm 10\%$

Table 33.10.1. Parameters of equation (33.5) precisions, and temp. range

Na_2S_x	A	-B	Precision	Temp. range (K)	Na_2S_x	A	-B	Precision	Temp. range (K)
$Na_2S_{1.70}$	8.132	8656	0.0%	1073-1173	$Na_2S_{3.70}$	9.710	6804	± 10%	523-873
$Na_2S_{1.80}$	7.814	8139	0.0%	1073-1173	$Na_2S_{3.80}$	9.720	6734	± 10%	523-873
$Na_2S_{1.90}$	6.456	6424	± 30%	973-1173	$Na_2S_{3.90}$	9.726	6669	± 10%	523-873
$Na_2S_{2.00}$	6.547	6285	0.0%	973-1073	$Na_2S_{4.00}$	9.737	6611	± 10%	523-873
$Na_2S_{2.10}$	6.327	5912	± 5%	873-1073	$Na_2S_{4.10}$	9.752	6566	± 5%	523-873
$Na_2S_{2.20}$	5.636	5182	± 10%	873-1073	$Na_2S_{4.20}$	9.768	6516	± 10%	523-873
$Na_2S_{2.30}$	5.736	5164	0.0%	873-973	$Na_2S_{4.30}$	9.783	6469	± 8%	523-873
$Na_2S_{2.40}$	7.497	6707	± 30%	773-973	$Na_2S_{4.40}$	9.797	6418	± 7%	523-873
$Na_2S_{2.50}$	7.159	6275	± 30%	773-973	$Na_2S_{4.50}$	9.808	6375	± 5%	523-873
$Na_2S_{2.60}$	8.082	6948	± 15%	623-973	$Na_2S_{4.60}$	9.814	6331	± 10%	523-873
$Na_2S_{2.70}$	8.254	6928	± 15%	623-973	$Na_2S_{4.70}$	9.813	6286	± 5%	523-873
$Na_2S_{2.80}$	9.077	7356	± 3%	623-873	$Na_2S_{4.80}$	9.805	6238	± 5%	523-873
$Na_2S_{2.90}$	9.209	7319	± 3%	623-873	$Na_2S_{4.90}$	9.787	6186	± 5%	573-873
$Na_2S_{3.00}$	9.396	7330	± 2%	573-873	$Na_2S_{5.00}$	9.757	6130	± 5%	573-873
$Na_2S_{3.10}$	9.316	7146	± 2%	523-873	$Na_2S_{5.10}$	9.775	6112	± 5%	573-873
$Na_2S_{3.20}$	9.367	7065	± 3%	523-873	$Na_2S_{5.20}$	9.715	6041	± 4%	623-873
$Na_2S_{3.30}$	9.399	6979	± 4%	523-873	$Na_2S_{5.30}$	9.629	5955	± 8%	623-873
$Na_2S_{3.40}$	9.421	6894	± 6%	523-873	$Na_2S_{5.40}$	9.316	5692	± 8%	673-873
$Na_2S_{3.50}$	9.568	6888	± 6%	523-873	$Na_2S_{5.50}$	7.330	4033	0.0%	773-873
$Na_2S_{3.60}$	9.566	6802	± 6%	523-873	$Na_2S_{5.60}$	7.870	4486	0.0%	773-873

Note: For the composition ranges $Na_2S_{1.7}$-$Na_2S_{2.5}$ and $Na_2S_{5.4}$-$Na_2S_{5.6}$, the data-sets were very limited (i.e. 3 values).

Table 33.10.2. Equilibrium sulfur pressures for some polysulfides from equations in table 33.10.1

T (K)	p (mm)							
	Na_2S_2	$Na_2S_{2.5}$	Na_2S_3	$Na_2S_{3.5}$	Na_2S_4	$Na_2S_{4.5}$	Na_2S_5	$Na_2S_{5.5}$
540				0.0008	0.0031	0.0101	0.0254	
560				0.0023	0.0085	0.0266	0.0647	
580			0.0006	0.0061	0.0218	0.0656	0.1542	
600			0.0015	0.0151	0.0523	0.1524	0.3470	
620			0.0037	0.0353	0.1186	0.3355	0.7411	
640			0.0088	0.0786	0.2555	0.7032	1.5096	
660			0.0195	0.1666	0.5252	1.4090	2.9453	
680			0.0414	0.3377	1.0350	2.7102	5.5245	
700			0.0841	0.6577	1.9621	5.0218	9.9968	
720			0.1642	1.2341	3.5897	8.9916	17.5031	
740			0.3095	2.2382	6.3565	15.6005	29.7317	
760			0.5640	3.9341	10.9224	26.2933	49.1150	
780		0.1301	0.9967	6.7179	18.2542	43.1446	79.0733	144.3749
800		0.2067	1.7120	11.1687	29.7340	69.0643	124.3096	194.4262
820		0.321	2.8640	18.1135	47.2943	108.0473	191.1592	258.0551
840		0.488	4.6753	28.7080	73.5810	165.4699	287.9958	337.9208
860		0.7286	7.4601	44.5350	112.1489	248.4358	425.6952	436.9892
880		1.0674						
900		1.5374						
920		2.1795						
940		3.0442						
960		4.1932						
980	1.3606							
1000	1.8281							
1020	2.4279							
1040	3.1896							
1060	4.1472							

References [6,28-33].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

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[32] vide infra ref. [17].

[33] *vide infra* ref. [9].

XXXIV. Sodium Fluoride-Potassium Fluoride: NaF-KF

1. *Melting Temperatures (T_m)*

Pure substance melting points:
NaF: 995°C
KF: 856°C

Eutectic melting point:
710°C, composition: 40 mol % NaF

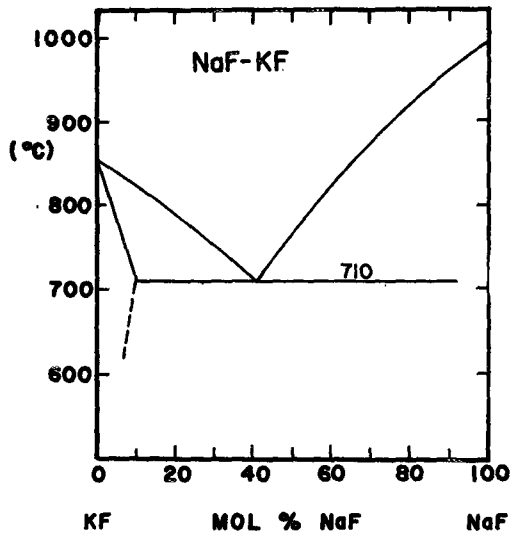

Figure 34.1. NaF-KF phase diagram

References [1-8].

2. *Density (ρ)*

Measurement method: Archimedean technique [9]

$$\rho = a + bT \quad (34.1)$$

precision: in table 34.1 uncertainty: ∿ ± 2%

Table 34.1. Parameters of equation (34.1), and precisions

Mol % NaF	a	$-b \times 10^4$	Precision
0.0	2.555	6.241	±0.15%
12.0	1.867	1.011	±1.08%
25.0	2.114	2.853	±0.80%
40.0	2.568	6.000	±0.67%
60.0	2.530	5.641	±0.15%
80.0	2.601	5.878	±0.12%
100.0	2.682	6.151	±0.13%

Table 34.2. Densities (g cm^{-3}) from equations in table 34.1

	Mol % NaF						
T (K)	100.0	80.0	60.0	40.0	25.0	12.0	0.0
1050				1.938			
1065				1.929	1.810		
1080				1.920	1.806		
1095				1.911	1.802	1.756	
1110				1.902	1.797	1.755	
1125			1.895	1.893	1.793	1.753	
1140			1.887	1.884	1.789	1.752	1.844
1155			1.878	1.875	1.784	1.750	1.834
1170			1.870	1.866	1.780	1.749	1.825
1185			1.862	1.857	1.776	1.747	1.815
1200		1.896	1.853	1.848	1.772	1.746	1.806
1215		1.887	1.845	1.839	1.767	1.744	1.797
1230		1.878	1.836	1.830	1.763	1.743	1.787
1245		1.869	1.828	1.821	1.759	1.741	1.778
1260		1.860	1.819	1.812	1.755	1.740	1.769
1275	1.898	1.852	1.811	1.803	1.750	1.738	1.759
1290	1.889	1.843	1.802	1.794	1.746	1.737	1.750
1305	1.879	1.834	1.794	1.785	1.742	1.735	1.741
1320	1.870	1.825	1.785	1.776	1.737	1.734	1.731
1335	1.861	1.816	1.777	1.767	1.733	1.732	1.722
1350	1.852	1.807	1.768	1.758	1.729	1.731	1.712

References [9-13].

3. Surface Tension (γ)

Measurement method: maximum bubble pressure [12]

$$\gamma = 243.73 - 7.92 \times 10^{-2} T \quad (34.2)$$

precision: $\sim \pm 0.3\%$ uncertainty: $\sim \pm 1.0\%$

For numerical values see table 34.3

Table 34.3. Surface tension for the eutectic from equation (34.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
910	171.7 *	1030	162.2
920	170.9 *	1040	161.4
930	170.1 *	1050	160.6
940	169.3 *	1060	159.8
950	168.5 *	1070	159.0
960	167.7 *	1080	158.2
970	166.9 *	1090	157.4
980	166.1 *	1100	156.6
990	165.3	1110	155.8
1000	164.5	1120	155.0
1010	163.7	1130	154.2
1020	162.9		

References [9-12]. * Values are for supercooled liquid.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: ac technique [10]

$$\kappa = a + bT \quad (34.3)$$

precision: in table 34.4 uncertainty: $\sim \pm 4\%$

Table 34.4. Parameters of equation (34.3), and precisions

Mol % NaF	a x 10^2	b x 10^3	Precision
0.0	38.84	2.940	±0.47%
12.0	-39.59	3.525	±0.65%
25.0	-86.67	3.958	±0.26%
40.0	-54.67	3.580	±1.09%
60.0	-12.82	3.500	±0.55%
80.0	17.97	3.420	±0.60%
100.0	-206.0	5.640	±1.21%

Table 34.5. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 34.4.

	Mol % NaF						
T(K)	100.0	80.0	60.0	40.0	25.0	12.0	0.0
1050				3.21			
1060				3.25			
1070				3.28			
1080				3.32	3.41		
1090				3.36	3.45	3.45	
1100				3.39	3.49	3.48	
1110			3.76	3.43	3.53	3.52	
1120			3.79	3.46	3.57	3.55	
1130			3.83	3.50	3.61	3.59	
1140			3.86	3.54	3.65	3.62	3.74
1150			3.90	3.57	3.69	3.66	3.77
1160			3.93	3.61	3.73	3.69	3.80
1170			3.97	3.64	3.76	3.73	3.83
1180			4.00	3.68	3.80	3.76	3.86
1190			4.04	3.71	3.84	3.80	3.89
1200			4.07	3.75	3.88	3.83	3.92
1210			4.11	3.79	3.92	3.87	3.95
1220			4.14	3.82	3.96	3.91	3.98
1230		4.39	4.18	3.86	4.00	3.94	4.01
1240		4.42	4.21	3.89	4.04	3.98	4.03
1250		4.46	4.25	3.93	4.08	4.01	4.06
1260		4.49	4.28	3.96	4.12	4.05	4.09
1270		4.52	4.32	4.00	4.16	4.08	4.12
1280		4.56	4.35	4.04	4.20	4.12	4.15
1290		4.59	4.39	4.07	4.24	4.15	4.18
1300		4.63	4.42	4.11	4.28	4.19	4.21
1310	5.33	4.66	4.46	4.14	4.32	4.22	4.24
1320	5.39	4.69	4.49	4.18	4.36	4.26	4.27
1330	5.44	4.73	4.53	4.22	4.40	4.29	4.30
1340	5.50	4.76	4.56	4.25	4.44	4.33	4.33

References [9-13].

6. Safety and Hazards

A. Hazard rating [14-16]

(i) Toxicity: NaF, severe; KF, severe.

(ii) Vapor pressure: no data for mixture; but see: NaF, KF.

(iii) U. S. occupational standards: NaF, 5.5 mg/m^3 (air); KF, 7.6 mg/m^3 (air).

B. Disaster hazards [14,17-19]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Fluorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

References [14-19].

7. Corrosion

Table 34.6. Corrosion studies from primary research literature

Studies	References
Cr	20
Ni-Cr-Fe	21-25
Quartz	26
Al	27
Inconel 600; Hastelloy B (Ni base, 28% Mo, 5% Fe); Hastelloy W (Ni base, 25% Mo, 5% Cr, 5.5% Fe); Hastelloy N (i.e. INOR-8, Ni base, 15% Mo, 6% Cr, 5% Fe)	28-29
Electrochemical behavior of oxide ions and related species in molten fluorides	30-32
Electroanalytical studies in molten fluorides	33
Annotated corrosion biblio.	34
Corrosion in molten fluorides (survey)	35

References [20-35].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: calc'd, from cryoscopy [36]

Table 34.7. Heat of fusion

Binary eutectic (mol % NaF)	ΔH_f° (kcal mol^{-1})	Uncertainty
40	4.97	∿ ± 2%

References [36,37].

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated; from densities [36]

Table 34.8. Volume change on melting

Binary eutectic (mol % NaF)	$(\Delta V_f/V_s)$	Uncertainty
40	17.9%	∿ ± 8%

References [36].

12. Vapor Pressure (p_{vap})

No vaporization studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_ℓ)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: cryoscopy [38]

Table 34.9. Cryoscopic constant

Binary eutectic (mol % NaF)	k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
40	20	∿ ± 2%

References [38].

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XXXV. Lithium Fluoride-Lithium Chloride: LiF-LiCl

1. *Melting Temperatures (T_m)*

Pure substance melting points:

LiF: 848°C
LiCl: 610°C

Eutectic melting point:

484°C, composition: 69.5 mol % LiCl

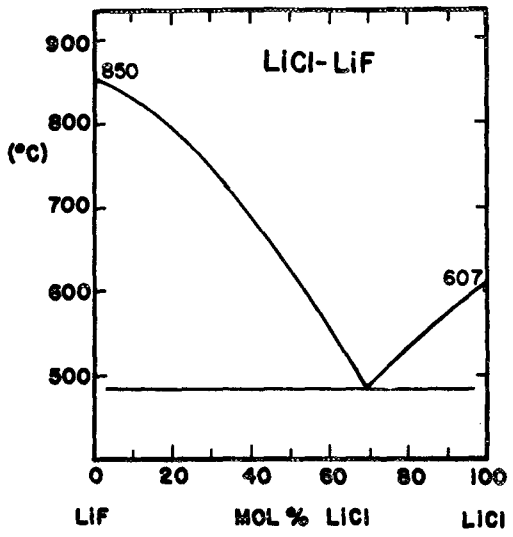

Figure 35.1. LiF-LiCl phase diagram

References [1-3].

2. *Density (ρ)*

Measurement method: Archimedean technique [4]

Single variable equation

$$\rho = a + bT \quad (35.1)$$

precision: in table 35.1 uncertainty: ∿ ± 2%

Table 35.1. Parameters of single variable equation (35.1), and precisions

Mol % LiCl	a	$-b \times 10^3$	Precision
0	2.266	0.414	±0.11%
12	2.160	0.417	±0.17%
25	2.116	0.443	±0.18%
37	2.050	0.436	±0.18%
50	2.000	0.438	±0.13%
63	1.962	0.440	±0.26%
75	1.928	0.437	±0.26%
88	1.905	0.438	±0.27%
100	1.896	0.446	±0.34%

Two-independent variable equation

$$\rho = a + bC + cT + dC^2 + eC^3 + fTC^2 + gCT^2 \quad (C = \text{mol \% LiCl}) \quad (35.2)$$

precision: ± 0,004%, uncertainty: ∿ ± 2%

Table 35,2. Parameters of two-independent-variable equation (35,2)

a	$b \times 10^3$	$c \times 10^4$	$d \times 10^5$	$e \times 10^7$	$f \times 10^9$	$g \times 10^{10}$
2.25621	-8.20475	-4.09235	6.37250	-2.52846	8.73570	-5.11184

Table 35,3. Densities (g cm^{-3}) from equations in table 35,1

	Mol % LiCl								
T (K)	100	88	75	63	50	37	25	12	0
940	1.477	1.493	1.517	1.548	1.588	1.640	1.699	1.768	1.877
960	1.468	1.485	1.508	1.540	1.579	1.631	1.691	1.760	1.869
980	1.459	1.476	1.500	1.531	1.571	1.623	1.682	1.751	1.860
1000	1.450	1.467	1.491	1.522	1.562	1.614	1.673	1.743	1.852
1020	1.441	1.458	1.482	1.513	1.553	1.605	1.664	1.735	1.844
1040	1.432	1.449	1.473	1.504	1.544	1.597	1.655	1.726	1.835
1060	1.423	1.441	1.465	1.496	1.536	1.588	1.646	1.718	1.827
1080	1.414	1.432	1.456	1.487	1.527	1.579	1.637	1.710	1.819
1100	1.405	1.423	1.447	1.478	1.518	1.570	1.629	1.701	1.811
1120	1.396	1.414	1.439	1.469	1.509	1.562	1.620	1.693	1.802
1140	1.387	1.406	1.430	1.460	1.501	1.553	1.611	1.685	1.794
1160	1.379	1.397	1.421	1.452	1.492	1.544	1.602	1.676	1.786
1180	1.370	1.388	1.412	1.443	1.483	1.535	1.593	1.668	1.777
1200	1.361	1.379	1.404	1.434	1.474	1.527	1.584	1.660	1.769
1220	1.352	1.371	1.395	1.425	1.466	1.518	1.575	1.651	1.761
1240	1.343	1.362	1.386	1.416	1.457	1.509	1.567	1.643	1.753
1260	1.334	1.353	1.377	1.408	1.448	1.501	1.558	1.635	1.744

References [4-7].

3. Surface Tension (γ)

Measurement method: maximum bubble pressure [8]

Single variable equation $\gamma = a + bT$ (35.3)

precision: $\sim \pm$ 0.5% uncertainty: $\sim \pm$ 1%

Table 35.4. Parameters of single variable equation (35.3)

Mol % LiCl	a	$-b \times 10^2$
0	350.2	9.86
12	323.8	9.49
25	303.3	9.58
37	281.7	9.22
50	264.4	9.13
63	250.0	9.06
75	234.1	8.53
88	223.2	8.42

Two-independent-variable equation

$$\gamma = a + bTC + cC^2 + dCT^2 + eTC^2 + fT^3 \quad (C = \text{mol \% LiCl}) \quad (35.4)$$

precision: $\sim \pm$ 0.2%, uncertainty: $\sim \pm$ 1%

Table 35.5. Parameters of two-independent-variable equation (35.4)

a	$b \times 10^3$	$c \times 10^4$	$d \times 10^6$	$e \times 10^6$	$f \times 10^8$
271.25732	-2.89297	-4.13850	1.04392	7.27278	-2.26107

Table 35.6. Surface tension (dyn cm^{-1}) from equations in table 35.4

T	Mol % LiCl							
(K)	88	75	63	50	37	25	12	0
930	144.9							
960	142.4	152.2						
980	140.7	150.5	161.2					
1000	139.0	148.8	159.4					
1020	137.3	147.1	157.6	171.3				
1040	135.6	145.4	155.8	169.4				
1060	133.9	143.7	154.0	167.6	184.0			
1080	132.3	142.0	152.1	165.8	182.1	199.8		
1100	130.6	140.3	150.3	164.0	180.3	197.9	219.4	241.7
1120		138.6	148.5	162.1	178.4	196.0	217.5	239.8
1140		136.9	146.7	160.3	176.6	194.1	215.6	237.8
1160				158.5	174.7	192.2	213.7	235.8
1180					172.9	190.3	211.8	233.9
1200						188.3	209.9	231.9
1220							208.0	229.9
1240								227.9

References [6,8].

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: ac technique [4]

$$\kappa = a + bT + cT^2 + dT^3 \quad (35.5)$$

precision: in table 35.7 uncertainty: $\sim \pm 3\%$

Table 35.7. Parameters of equation (35.5), and precisions

Mol % LiCl	-a	b x 10^2	-c x 10^6	-d x 10^{10}	Precision
100	2.38328	1.30626	4.38178		± 0.02%
88	3.79487	1.53803	6.54756	7.08847	± 0.03%
75	4.53422	1.39024	4.16275		± 0.03%
63	5.09117	1.40770	3.99430		± 0.03%
50	4.45470	1.14329	0.81203	10.05267	± 0.02%
37	6.50401	1.59769	4.07234		± 0.03%
25	6.35426	1.67159	4.48874		± 0.02%
12	6.13153	1.72097	4.67529		± 0.04%
0	6.62282	1.90497	5.17567		± 0.03%

Table 35.8. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 35.7

	Mol % LiCl								
T(K)	100	88	75	63	50	37	25	12	0
940	6.023	5.463	4.856	4.610	4.741	4.915	5.391	5.912	6.708
960	6.118	5.566	4.973	4.743	4.880	5.081	5.556	6.081	6.895
980	6.211	5.656	5.095	4.867	5.025	5.244	5.717	6.245	7.077
1000	6.299	5.749	5.205	4.994	5.161	5.402	5.875	6.403	7.254
1020	6.379	5.833	5.317	5.110	5.295	5.552	5.026	6.561	7.421
1040	6.464	5.915	5.419	5.229	5.427	5.709	6.175	6.706	7.590
1060	6.541	5.996	5.527	5.345	5.556	5.856	6.321	6.860	7.755
1080	6.613	6.072	5.626	5.452	5.679	6.000	6.461	7.005	7.917
1100	6.684	6.143	5.720	5.562	5.801	6.143	6.603	7.139	8.071
1120	6.749	6.213	5.816	5.665	5.917	6.282	6.738	7.283	8.218
1140	6.811	6.282	5.903	5.763	6.035	6.421	6.867	7.410	8.368
1160	6.875	6.342	5.992	5.864	6.147	6.547	6.999	7.539	8.510
1180	6.931	6.401	6.072	5.959	6.253	6.677	7.118	7.664	8.645
1200	6.981	6.455	6.155	6.048	6.357	6.805	7.241	7.788	8.784
1220	7.031	6.512	6.232	6.136	6.460	6.926	7.357	7.900	8.914
1240	7.076	6.561	6.304	6.222	6.557	7.045	7.471	8.021	9.042
1260	7.120	6.608	6.374	6.307	6.651	7.163	7.583	8.134	9.164

References [4,7].

6. Safety and Hazards

A. Hazard rating [9-11]

(i) Toxicity: LiF, severe; LiCl, slight.

(ii) Vapor pressure: no data for mixture; but see, LiF, LiCl.

(iii) U. S. occupational standards: LiF, 3.5 mg/m^3 (air)

B. Disaster hazards [12-14]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Fluorides and chlorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

References [9-14].

7. Corrosion

No data; see LiCl and LiF, respectively, for possible guidelines.

8. Diffusion

No diffusion studies reported.

9. *Heat of Fusion (ΔH_f°)*

Measurement method: cryoscopic [15]

Table 35.9. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
4.8	∿ ± 6%

References [15].

10. *Heat Capacity (C_p)*

No Data.

11. *Volume Change on Melting (ΔV_f)*

Measurement method: estimated; from densities [16]

Table 35.10. Volume change on melting

Binary etuectic (mol % LiF)	$(\Delta V_f/V_s)$	Uncertainty
69.5	32.3%	∿ ± 8%

References [16].

12. *Vapor Pressure (p_{vap})*

No vaporization studies reported.

13. *Thermal Conductivity (liquid) (λ_ℓ)*

No thermal conductivity studies reported.

14. *Thermal Conductivity (solid) (λ_s)*

No thermal conductivity studies reported.

15. *Cryoscopic Constant (k_f)*

Measurement method: cryoscopic [15]

Table 35.11. Cryoscopic Constant

Binary eutectic (mol % LiCl)	k_f (K mol^{-1} kg^{-1})	Uncertainty
69.5	9.3	∿ ± 6%

References [15].

16. *References*

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[11] Vapor pressure; estimated (MSDC-RPI) unpublished work (1978).

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XXXVI. Sodium Chloride-Potassium Chloride-Aluminum Chloride: $NaCl-KCl-AlCl_3$

1. Melting Temperatures (T_m)

Pure substance melting points:
NaCl: 800°C
KCl: 770°C
$AlCl_3$: 192°C

Eutectic melting point:
88.9°C, composition: 20 mol % NaCl, 16.5 mol % KCl, 63.5 mol % $AlCl_3$

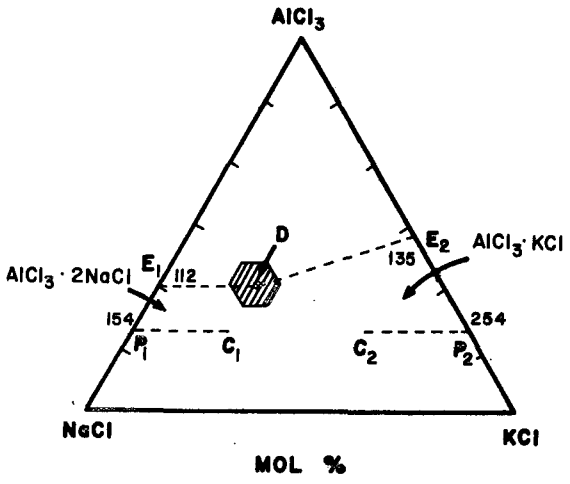

Figure 36.1. $NaCl-KCl-AlCl_3$ phase diagram. E_1D, E_2D: lines from binary eutectics; D: ternary eutectic; P_1C_1, P_2C_2: approx. boundaries between fields in ternary system

References [1-10].

2. Density (ρ)

Measurement method: Archimedean technique [11]

Table 36.1. Compositions of mixtures investigated

Mixture	$AlCl_3$	NaCl	KCl
	Mol %		
A	50	40	10
B	55	25	20
C	60	30	10
D	60	20	20
E	60	10	30
F	65	25	10
G	65	10	25

$$\rho = a + bT \quad (36.1)$$

precision: not estimated , uncertainty: not estimated; insufficient data

Results were reported in equation form.

Table 36.2. Parameters of equation (36.1)

Mixture	a	$-b \times 10^4$
A	2.136	9.23
B	2.105	9.03
C	2.096	8.82
D	2.117	9.70
E	2.059	8.22
F	2.059	8.77
G	2.115	10.2

Table 36.3. Densities (g cm^{-3}) from equations in table 36.2

	Mixtures						
T(K)	A	B	C	D	E	F	G
430			1.7167	1.6999		1.6819	1.6764
440		1.7077	1.7079	1.6902		1.6731	1.6662
450		1.6987	1.6991	1.6905		1.6644	1.6560
460		1.6896	1.6903	1.6708		1.6556	1.6458
470		1.6806	1.6815	1.6611	1.6727	1.6468	1.6356
480		1.6716	1.6726	1.6514	1.6644	1.6380	1.6254
490					1.6562		
500	1.6745				1.6480		
510	1.6653				1.6398		
520	1.6560				1.6316		
530	1.6468						
540	1.6376						

References [11,12].

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: ac technique [13]

Table 36.4. Compositions of mixtures investigated

Mixtures	NaCl	KCl	$AlCl_3$
	Mol %		
A	35.3	6.9	57.8
B	21.3	12.0	66.7
C	22.0	15.0	63.0
D	32.0	16.8	51.2
E	40.4	7.9	51.7
F	31.0	16.2	52.8

$$\kappa = a + bT \quad (36.2)$$

precision: $\sim \pm 1\%$ uncertainty: $\sim \pm 5\%$

Table 36.5. Parameters of equation (36.2)

Mixture	-a	b x 10^3	Temp. range (K)
A	0.616	1.95	405 - 458
B	0.476	1.47	404 - 463
C	0.585	1.80	403 - 464
D	0.733	2.30	411 - 473
E	0.911	2.78	427 - 466
F	0.785	2.39	415 - 463

For numerical values: see table 36.6

Table 36.6. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 36.5

	Mixtures					
T(K)	A	B	C	D	E	F
405	0.174	0.119	0.144			
410	0.183	0.127	0.153			
415	0.193	0.134	0.162	0.221		0.207
420	0.203	0.141	0.171	0.233		0.219
425	0.213	0.149	0.180	0.245		0.231
430	0.223	0.156	0.189	0.256	0.284	0.243
435	0.232	0.163	0.198	0.267	0.298	0.255
440	0.242	0.171	0.207	0.279	0.312	0.267
445	0.252	0.178	0.216	0.291	0.326	0.279
450	0.261	0.185	0.225	0.302	0.340	0.291
455	0.271	0.193	0.234	0.313	0.354	0.302
460		0.200	0.243	0.325	0.368	0.314
465				0.337	0.382	
470				0.348		

References [12,13].

6. Safety and Hazards

A. Hazard rating [14-16]

(i) Toxicity: NaCl, very low; KCl, very low; $AlCl_3$, severe.

(ii) Vapor pressure: no data for mixture; but see, NaCl; KCl; $AlCl_3$.

B. Disaster hazards [14,17-19]

(i) Molten salt bath "explosions"; i.e, explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e. explosive expansion of "trapped" air.

(ii) Chlorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes; $AlCl_3$ reacts exothermically with moisture/water to evolve HCl fumes.

References [14-19].

7. Corrosion

Table 36.7. Corrosion studies from primary research literature

Studies	References
Al	20
Electrochem. approach	21,22
Thermodynamic redox diagrams	23
Annotated corrosion biblio.	24
Reviews: molten salts corrosion	25-27

References [20-27].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: estimated [28]

Table 36.8. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
6.9	~ ± 5%

References [28].

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

No data; but see NaCl, KCl, $AlCl_3$.

12. Vapor Pressure (p_{vap})

No vaporization studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: estimated [28]

Table 36.9. Cryoscopic constant

Mixture	k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
ternary eutectic	4.1	∿ ± 5%

References [28].

16. References

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XXXVII. Lithium Chloride-Potassium Chloride-Calcium Chloride: $LiCl-KCl-CaCl_2$

1. *Melting Temperatures (T_m)*

Pure substance melting points:

LiCl: 610°C
KCl: 770°C
$CaCl_2$: 782°C

Eutectic melting points:

Eutectic 1: 412°C, composition: 52.4 mol % LiCl, 11.5 mol % KCl, 36.1 mol % $CaCl_2$

Eutectic 2: 332°C, composition: 50.5 mol % LiCl, 44.2 mol % KCl, 5.3 mol % $CaCl_2$

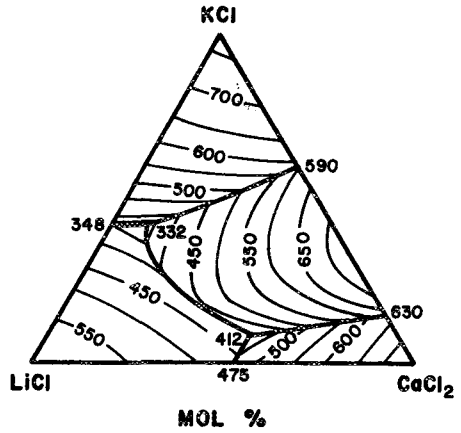

Figure 37.1. $LiCl-KCl-CaCl_2$ phase diagram

References [1-4].

2. *Density (ρ)*

No data.

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

No data.

6. Safety and Hazards

A. Hazard rating [5-7]

(i) Toxicity: LiCl, slight; KCl, very low; $CaCl_2$, very low.

(ii) Vapor pressure: no data for mixture; but see, LiCl; KCl; $CaCl_2$.

B. Disaster hazards [5,8-10]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

7. Corrosion

No corrosion studies reported; for guidelines, see LiCl-KCl, and $CaCl_2$.

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f^o)

Measurement method: estimated [11]

Table 37.1. Heats of fusion and uncertainty

Mixture	ΔH_f° (kcal mol^{-1})	Uncertainty
Eutectic 1	4.7	∿±5%
Eutectic 2	4.3	∿±5%

References [11].

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

No data; but see LiCl, KCl, $CaCl_2$ for guidelines.

12. Vapor Pressure (p_{vap})

No vaporization studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: estimated [11]

Table 37.2. Cryoscopic constants and uncertainty

Mixture	k_f (K mol $^{-1}$kg^{-i})	Uncertainty
Eutectic 1	9.6	∿±5%
Eutectic 2	15.4	∿±5%

References [11].

16. References

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[11] Janz, G. J., et al., (MSDC-RPI) unpublished work (1977).

XXXVIII. Lithium Chloride-Sodium Chloride-Potassium Chloride: LiCl-NaCl-KCl

1. *Melting Temperatures (T_m)*

Pure substance melting points:

LiCl: 610°C
NaCl: 800°C
KCl: 770°C

Eutectic melting point:

348°C, composition: 53.5 mol % LiCl, 8.5 mol % NaCl, 38 mol % KCl

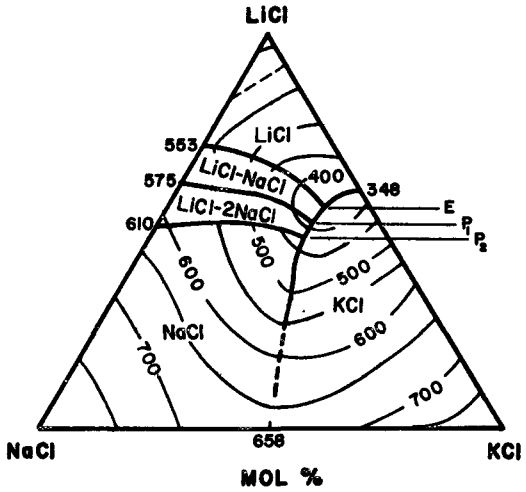

Figure 38.1. LiCl-NaCl-KCl phase diagram; E, eutectic; P_1, P_2, peritectics

References [1-4].

2. *Density (ρ)*

No data.

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: ac technique [5]

Table 38.1. Compositions of mixtures investigated

Mixture	KCl	LiCl	NaCl
	Mol %		
A	41.95	57.93	0.12
B	41.89	57.85	0.26
C	41.80	57.72	0.48
D	41.49	57.30	1.21
E	40.39	55.77	3.84

$$\kappa = A \exp(-E/RT) \quad (38.1)$$

precision: in table 38.2 uncertainty: ∿ ± 3%

Table 38.2. Coefficients of equation (38.1), and precisions

Mixture	$A(ohm^{-1}cm^{-1})$	$E(cal\ mol^{-1})$	Precision
A	43.70816	4687.94	±0.15%
B	47.63575	4791.01	±0.10%
C	53.75324	4961.16	±0.07%
D	56.27187	5023.06	±0.04%

$$\kappa = a + bT \quad (38.2)$$

precision: in table 38.3 uncertainty: ∿ ± 3%

Table 38.3. Parameters of equation (38.2), and precision

Mixture	-a	$b \times 10^3$	Precision
E	3.80334	7.59545	±0.11%

Table 38.4. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in tables 38.2 and 38.3

T(K)	Mixtures				
	A	B	C	D	E
635	1.064	1.069	1.054	1.051	1.020
640	1.096	1.101	1.087	1.084	1.058
645	1.127	1.134	1.120	1.118	1.096
650	1.160	1.167	1.154	1.152	1.134
655	1.192	1.201	1.189	1.187	1.172
660	1.225	1.234	1.223	1.222	1.210
665	1.259	1.269	1.259	1.257	1.248
670	1.292	1.304	1.295	1.294	1.286

References [5].

6. Safety and Hazards

A. Hazard rating [6-8]

(i) Toxicity: LiCl, slight; KCl, very low; NaCl, very low

(ii) Vapor pressure: no data for mixture; but see, LiCl; NaCl; KCl.

B. Disaster hazards [6,9-11]

(i) Molten salt bath "explosions", i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Chlorides, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

7. Corrosion

Table 38.5. Corrosion studies from primary research literature

Studies	References
Cu, Al, Al-Cu	12
Electrochem. approach	13,14
Thermodynamic redox diagrams	15
Annotated corrosion biblio.	16
Reviews: molten salts corrosion	17-19

References [12-19].

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: estimated [20]

Table 38.6. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
4.8	~ ± 5%

References [20].

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

No data; but see LiCl, NaCl, KCl for guidelines

12. Vapor Pressure (p_{vap})

No vaporization studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: estimated [20]

Table 38.7. Cryoscopic constant

Mixture	k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
Ternary eutectic	9.0	5%

References [20].

16. References

[1] Akopov, E. K., Zhur. Neorg. Khim., 1, 1024 (1956).

[2] Akopov, E. K., and Bergman, A. G., ibid., 2, 383 (1957); 11, 1751 (1966).

[3] Janz, G. J., Downey, J. R., Jr., Allen, C. B., and Tomkins, R. P. T., *"Eutectic Data"* - 2 vols.; ERDA-TID-27163-P1 & P2; NTIS, Washington, D. C. (1977).

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[18] Inman, D., and Wrench, N. S., Brit. Corr. J., 1, 246 (1966).

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XXXIX. Lithium Fluoride-Lithium Chloride-Lithium Bromide: LiF-LiCl-LiBr

1. *Melting Temperatures (T_m)*

Pure substance melting points:

LiF: 848°C
LiCl: 610°C
LiBr: 552°C

Eutectic melting point:

445°C, composition: 22 mol % LiF, 31 mol % LiCl, 47 mol % LiBr

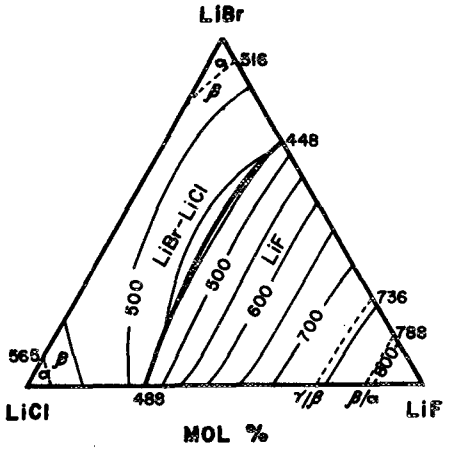

Figure 39.1. LiF-LiCl-LiBr phase diagram

References [1-4].

2. *Density (ρ)*

Measurement method: no information [4]

Table 39.1. Density

Composition	T (K)	ρ (g cm^{-3})
ternary eutectic	773	2.19

Reference [4]

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

No data.

6. *Safety and Hazards*

A. Hazard rating [5-7]

(i) Toxicity: LiF, severe; LiBr, moderate; LiCl, slight.

(ii) Vapor pressure: no data for mixture; but see, LiCl; LiBr; LiF.

B. Disaster hazards [5,8-10]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Halide salts, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

References [5-10].

7. Corrosion

No corrosion studies reported; for guidelines, see LiF, LiCl, and LiBr and mixtures.

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

No data.

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

No data; but see LiF, LiCl, LiBr for guidelines.

12. Vapor Pressure (p_{vap})

No vaporization studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

16. References

[1] Bergman, A. G., and Arabadzhan, A. S., Zh. Neorgan. Khim., 8[5], 1228 (1963); Russ. J. Inorg. Chem., 8, 637 (1963).

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[4] Ackerman, J. P., and Sim, J. W., "Electrolyte Studies", cited in Argonne National Laboratory Rpt. ANL-76-35, NTIS, U. S. Dept. Commerce, Springfield, Va. (1976).

[5] *"Dangerous Properties of Materials"*, Sax, N. I., Van Nostrand Reinhold Co., N. Y. (1969).

[6] *"Registry of Toxic Effects of Chemical Substances"*, Christensen, H. E., and Lubinbyhl, T. T., eds., U. S. Dept. H. E. W., U. S. Gov't Printing Office, Washington, D. C. (1975).

[7] Vapor pressure; estimated (MSDC-RPI) unpublished work (1978).

[8] *"Potential Hazards In Molten Salt Baths for Heat Treatment of Metals"*, National Board Fire Underwriters Research Report No. 2 (1954).

[9] *"Handbook of Reactive Chemical Hazards"*, Bretherwick, L., Butterworths Co., London (1975).

[10] Janz, G. J., Tomkins, R. P. T., Downey, J. R., Jr., and Allen, C. B., *"Safety and Hazards"*, Chapter in *"Eutectic Data"*, ERDA TID-27163-P1; NTIS, U. S. Dept. Commerce, Springfield, Va. (1977).

XL. Lithium Fluoride-Lithium Chloride-Lithium Iodide: LiF-LiCl-LiI

1. *Melting Temperatures (T_m)*

Pure substance melting points:

LiF: 848°C
LiCl: 610°C
LiI: 469°C

Eutectic melting point:

340.9°C, composition: 11.7 mol % LiF, 29.1 mol % LiCl, 59.2 mol % LiI

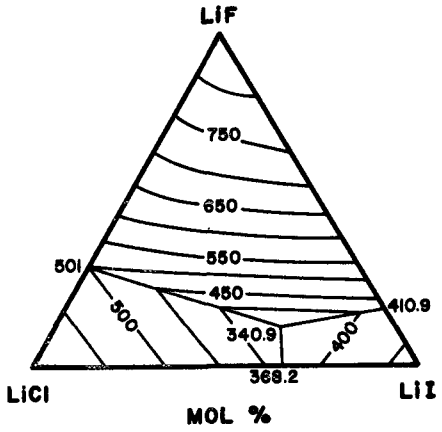

Figure 40.1. LiF-LiCl-LiI phase diagram

References [1-4].

2. *Density (ρ)*

No data.

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

No data.

6. *Safety and Hazards*

A. Hazard rating [5-7]

(i) Toxicity: LiF, severe; LiI, moderate; LiCl, slight.

(ii) Vapor pressure: no data for mixture; but see LiF; LiCl; LiI

(iii) U. S. occupational standards: LiF, $\sim$ 3.4 mg/m^3 (air)

B. Disaster rating [5,8-10]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Halide salts, when heated to decomposition, or contacted with acids, emit highly toxic fumes.

References [5-10].

7. *Corrosion*

No corrosion studies reported; for guidelines, see LiF, LiCl, LiI and mixtures.

8. *Diffusion*

No diffusion studies reported.

9. *Heat of Fusion* (ΔH_f°)

No data.

10. *Heat Capacity* (C_p)

No data.

11. *Volume Change on Melting* (ΔV_f)

No data; but see LiF, LiCl, LiI for guidelines.

12. *Vapor Pressure* (p_{vap})

No vaporization studies reported.

13. *Thermal Conductivity (liquid)* (λ_ℓ)

No thermal conductivity studies reported.

14. *Thermal Conductivity (solid)* (λ_s)

No thermal conductivity studies reported.

15. *Cryoscopic Constant* (k_f)

No data.

16. *References*

[1] Johnson, C. E., and Hathaway, E. J., J. Electrochem. Soc., 118, 631 (1971).

[2] Cairns, E. J., et al., Argonne National Lab. Report ANL-7316, p. 219 (1967).

[3] Janz, G. J., Downey, J. R., Jr., Allen, C. B., and Tomkins, R. P. T., *"Eutectic Data"* - 2 vols.; ERDA-TID-27163-P1 & P2; NTIS, Washington, D. C. (1977).

[4] Janz, G. J., Downey, J. R., Jr., Allen, C. B., and Tomkins, R. P. T., *"Physical Properties Data Compilations Relevant to Energy Storage. I Molten Salts: Eutectic Data"*, NSRDS-NBS-61, U. S. Gov't Printing Office, Washington, D. C. (1978).

[5] *"Dangerous Properties of Materials"*, Sax, N. I., Van Nostrand Reinhold Co., N. Y. (1969).

[6] *"Registry of Toxic Effects of Chemical Substances"*, Christensen, H. E., and Lubinbyhl, T. T., eds., U. S. Dept. H. E. W., U. S. Gov't Printing Office, Washington, D. C. (1975).

[7] Janz, G. J. et al. (MSDC-RPI), unpublished work (1978).

[8] *"Potential Hazards In Molten Salt Baths for Heat Treatment of Metals"*, National Board Fire Underwriters Research Report No. 2 (1954).

[9] *"Handbook of Reactive Chemical Hazards"*, Bretherwick, L., Butterworths Co., London (1975).

[10] Janz, G. J., Tomkins, R. P. T., Downey, J. R., Jr., and Allen, C. B., *"Safety and Hazards"*, Chapter in *"Eutectic Data"*, ERDA TID-27163-P1; NTIS, U. S. Dept. Commerce, Springfield, Va. (1977).

XLI. Lithium Carbonate-Sodium Carbonate-Potassium Carbonate: Li_2CO_3-Na_2CO_3-K_2CO_3

1. *Melting Temperatures (T_m)*

Pure substance melting points:
Li_2CO_3: 723°C
Na_2CO_3: 858°C
K_2CO_3: 898°C

Eutectic melting point:
397°C, composition: 43.5 mol % Li_2CO_3, 31.5 mol % Na_2CO_3, 25.0 mol % K_2CO_3

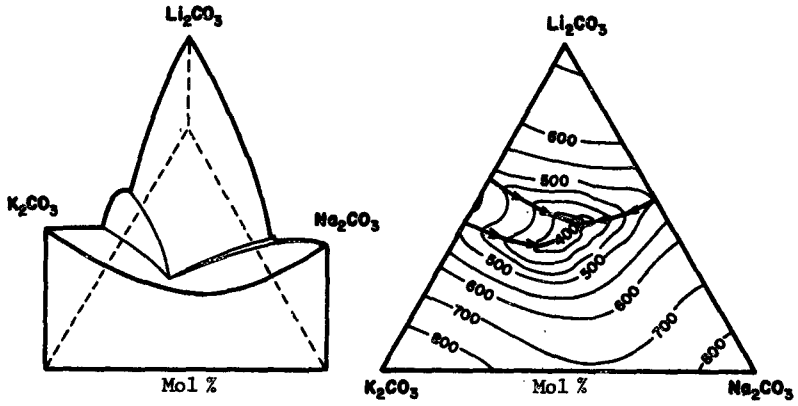

Figure 41.1. Li_2CO_3-Na_2CO_3-K_2CO_3 phase diagram

References [1-5].

2. *Density (ρ)*

Measurement method: Archimedean technique [6]

$$\rho = 2.5128 - 5.4405 \times 10^{-4} T \quad (41.1)$$

precision: ± 0.8% uncertainty: ∿ ± 1%

Table 41.1. Densities (g cm^{-3}) from equation (41.1)

T (K)	ρ (g cm^{-3})	T (K)	ρ (g cm^{-3})
680	2.1429	880	2.0340
700	2.1320	900	2.0232
720	2.1211	920	2.0123
740	2.1102	940	2.0014
760	2.0993	960	1.9905
780	2.0885	980	1.9796
800	2.0776	1000	1.9688
820	2.0667	1020	1.9579
840	2.0558	1040	1.9470
860	2.0449	1060	1.9361

References [6].

Li_2CO_3-Na_2CO_3-K_2CO_3

3. *Surface Tension (γ)*

Measurement method: pin detachment [6]

$$\gamma = 287.07 - 6.944 \times 10^{-2} T \quad (41.2)$$

precision: $\sim \pm 0.4\%$ uncertainty: $\sim \pm 0.5\%$

Table 41.2. Surface tension from equation (41.2)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
740	235.7	840	228.7	940	221.8
750	235.0	850	228.0	950	221.1
760	234.3	860	227.4	960	220.4
770	233.6	870	226.7	970	219.7
780	232.9	880	226.0	980	219.0
790	232.2	890	225.3	990	218.3
800	231.5	900	224.6	1000	217.6
810	230.8	910	223.9	1010	216.9
820	230.1	920	223.2	1020	216.2
830	229.4	930	222.5	1030	215.5
				1040	214.9
				1050	214.2

References [6].

4. *Viscosity (η)*

Measurement method: oscillating (liquid filled) cylinder [7]

$$\eta = 4.64 \times 10^{-3} \exp (10{,}661/RT) \quad (41.3)$$

precision: $\sim \pm 0.05\%$ uncertainty: $\sim \pm 25\%$

Table 41.3. Viscosity from equation (41.3)

T (K)	η (cp)	T (K)	η (cp)
760	5.402	820	3.223
770	4.929	830	2.978
780	4.507	840	2.758
790	4.132	850	2.558
800	3.795	860	2.377
810	3.494	870	2.213

References [7].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [6,8]

Li_2CO_3-Na_2CO_3-K_2CO_3

Table 41.4. Compositions of mixtures investigated

Mixture	Li_2CO_3	Na_2CO_3	K_2CO_3	Ref.
	Mol %			
Eutectic	43.5	31.5	25.1	6
A	50	33.3	16.67	8
B	40	30	30	
C	33.3	33.3	33.3	

$$\kappa = A \exp(-E/RT) \quad (41.4)$$

precision: in table 41.5 uncertainty: eutectic, ∿ ± 2%; other mixtures, ∿ ± 4%

Table 41.5. Parameters of equation (41.4), and precisions

Mixture	A ($ohm^{-1}cm^{-1}$)	E ($cal\ mol^{-1}$)	Precision
Eutectic	83.8192	7385	±0.5%
A	38.2364	5910	±1.7%
B	32.777	5904	±2.0%
C	27.208	5619	±1.3%

For numerical values: see table 41.6.

Table 41.6. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 41.5

T(K)	Mixtures			
	Eutectic	A	B	C
670	0.3269			
700	0.4146			
730	0.5157			
760	0.6305			
790	0.7591			
820	0.9017			
850	1.0581	1.16	0.95	0.94
880	1.2282	1.30	1.08	1.09
910	1.4117	1.46	1.25	1.22
940	1.6082	1.62	1.39	1.34
970	1.8174	1.78	1.53	1.47
1000	2.0387	1.95	1.68	1.61
1030		2.13	1.83	1.75
1060		2.31	1.99	1.89
1090		2.50	2.15	2.03
1120		2.69	2.31	2.18

References [6,8].

6. Safety and Hazards

A. Hazard rating [9-11]

(i) Toxicity: Li_2CO_3, toxic dose (oral; human), 0.7 mg/kg; K_2CO_3, severe; Na_2CO_3, moderate.

(ii) Vapor pressure: Carbonates dissociate on heating

$$M_2CO_{3(\ell)} \longrightarrow M_2O_{(\ell)} + CO_{2(g)} \qquad (41.5)$$

For the ternary eutectic (m.pt. 397°C) the CO_2 equilibrium dissociation pressure is ∿ 31 mm at approx. 827°C

B. Disaster hazards [9,12-14]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) When heated at CO_2 pressures less than equilibrium, carbonates decompose to alkali metal oxides; the toxicology and disaster hazards of such oxides are the same as very strong caustics; i.e. react with water or steam exothermically to form hydroxides that are very aggressive to body tissues (chemical burns); Li_2CO_3 by itself is classed as a strong caustic.

References [9-14].

Li_2CO_3-Na_2CO_3-K_2CO_3

7. Corrosion

Table 41.7. Corrosion studies from primary research literature

Studies	References
Ti	15
Ti alloys	16
Fe, Ni, Cu	17,29,30
Au-Pd, Ni, 347-SS	18,42
Cu-Zn	19
Metals (anodic behavior)	20
Pt, Ag	18,21,22,23
Alumina (Monofrax A)	45
SS-347; SS-321; SS-304; Incoloy 800; Carpenter 7 Mo; Hastelloy G; Inconel 600; Haynes G; Hastelloy X; Aluminized SS-347; Alumina (Monofrax A; Monofrax H; Coors AD-998); graphite (various environments; dry air; wet air; argon; $SO_3^=$; $S^=$; $SO_4^=$; C; NaOH)	24,25
Pythagoras porcelain, aluminates	26-28
Au(O_2 environment; ternary eutectic + Na_2O)	31
Boron nitride Na-β-alumina	44
Thermodynamics of corrosion (E-pCO_2 diagrams); acid-base properties	26,32,35,36
emf series of metals	32-34
Hydrolysis (H_2O) reactions	37,38
Corrosion in molten salts: annotated bibliography	39
Molten carbonates: fuel cells; thermal energy storage; coal gasification; power plant stack gases	40-43

References [15-45].

Li_2CO_3-Na_2CO_3-K_2CO_3

8. Diffusion

Measurement method: capillary [46]

List of diffusing species investigated in Li_2CO_3-Na_2CO_3-K_2CO_3 as solvent

Na^+, K^+, CO_3^{2-}

precision in table 41.8.1 uncertainty: ∿ ± 20%

Equations:

$$D = A \exp [-E/RT] \quad (41.6)$$

Table 41.8.1. Parameters of diffusion equation (41.6), and precisions

Species	A x 10^3 (cm^2 sec^{-1})	E (cal mol^{-1})	Temp. range (K)	Precision
Na^+	8.06	11,035	830-1040	∿±3.6%
K^+	9.73	11,880	885-1115	∿±1%
CO_3^{2-}	1.58	10,070	690-1130	∿±6%

For numerical values: see table 41.8.2.

Table 41.8.2. Self-diffusion coefficients, D x 10^5($cm^2 sec^{-1}$), from equations in table 41.8.1.

T (K)	Na^+	K^+	CO_3^{2-}
690			0.102
710			0.126
730			0.153
750			0.184
770			0.219
790			0.259
810			0.303
830	1.00		0.352
850	1.17		0.407
870	1.36		0.466
890	1.57	1.18	0.532
910	1.80	1.36	0.603
930	2.06	1.57	0.679
950	2.33	1.80	0.762
970	2.63	2.05	0.850
990	2.95	2.32	0.945
1010	3.30	2.61	1.046
1030	3.67	2.93	1.153
1040	3.87	3.10	1.209
1060		3.46	1.325
1080		3.84	1.448
1100		4.24	1.577
1120		4.67	1.712
1130			1.782

References [46].

9. *Heat of Fusion* (ΔH_f°)

Measurement method: drop calorimetry [3,47]

Table 41.9. Heat of fusion

Composition	ΔH_f° (kcal mol^{-1})	Uncertainty
ternary eutectic	6.55	~ ± 1%

References [3,47].

Li_2CO_3-Na_2CO_3-K_2CO_3

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [47]

$$C_p = 28.41 + 16.56 \times 10^{-3} T \quad (41.7)$$

precision: ∿ ± 0.5% uncertainty: ∿ ± 1%

Table 41.10. Heat capacity from equation (41.7)

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
680	39.67	900	43.31
700	40.00	920	43.65
720	40.33	940	44.98
740	40.66	960	44.31
760	41.00	980	44.64
780	41.33	1000	44.97
800	41.66	1020	45.30
820	41.99	1040	45.63
840	42.32	1060	45.96
860	42.65	1080	46.29
880	42.98	1100	46.63

References [47].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated; from densities [48]

Table 41.11. Volume change on melting

Composition	$(\Delta V_f / V_s)$	Uncertainty
ternary eutectic	3.6%	∿ ± 8%

References [48].

12. Vapor Pressure (p_{vap})

Measurement method: cited with each data set [31,41,46]

No systematic studies of vaporization as molecular carbonates have been reported, viz:

$$M_2CO_{3(\ell)} \rightleftharpoons M_2CO_{3(g)} \quad (41.8)$$

Relative to the CO_2 decomposition of molten carbonates and other possible processes contributing to vaporization, the data for the ternary carbonate eutectic are as follows:

Decomposition processes:

CO_2 dissociation and equilibrium pressures for the molten ternary carbonate eutectic ($Li_2CO_3/Na_2CO_3/K_2CO_3$: 43.5/31.5/25.0 mol %; m.pt. 397°C).

$$M_2CO_{3(\ell)} \rightleftharpoons M_2O_{(\ell)} + CO_{2(g)} \quad (41.9)$$

$$p_{CO_2}(atm) = K_d \left[a_{M_2CO_{3(\ell)}} / a_{M_2O_{(\ell)}} \right] \quad (41.10)$$

where M is the Li, Na, K cationic mixture of the ternary eutectic, p is the equilibrium CO_2 dissociation pressure, and a the thermodynamically defined activity. For practical purposes, eq. (41.10) is generally expressed in the mol fraction scale [X].

$$p_{CO_2}\ (atm) = K_d[X_{M_2CO_3(\ell)}/X_{M_2O(\ell)}] \qquad (41.11)$$

As noted for the single salts, the values for p_{CO_2} cannot be uniquely defined unless the oxide content of the carbonate is specified, i.e. the pressures depend on the quality of the "carbonate", and its previous history, e.g. drying techniques; vacuum pumping;... or related conditions which may promote CO_2 decomposition of the carbonates.

(i) Equilibrium dissociation constant, K_d

Measurement method: emf technique [31]

$$\log K_d = -13530/T + 6.75 \qquad (41.12)$$

precision: not estimated uncertainty: ∿ ± 1%

Table 41.12.1. CO_2 dissociation constant from equation (41.12)

T (K)	K_d (atm)	T (K)	K_d (atm)
800	6.88×10^{-11}	1050	7.32×10^{-7}
850	6.80×10^{-10}	1100	2.82×10^{-6}
900	5.21×10^{-9}	1150	9.66×10^{-6}
950	3.22×10^{-8}	1200	2.98×10^{-5}
1000	1.66×10^{-7}		

(ii) Equilibrium CO_2 dissociation pressures

Measurement method: static technique [46]

$$\log p(mm) = \frac{-6300.57}{T} + 7.22 \qquad (41.13)$$

precision: ∿ ± 3% uncertainty: ∿ ± 5%

Table 41.12.2. Equilibrium CO_2 dissociation pressures for the ternary carbonate eutectic(ℓ) from equation (41.13)

T (K)	CO_2 pressure (mm) (obsv'd) eq. (41.13)	calc'd from eq. (41.10), (41.11) $X_{M_2O} = 3 \times 10^{-5}$	1×10^{-4}	3×10^{-4}
1020	11	7.7	2.3	0.8
1060	19	24		
1100	31	71	21	
1140	50		58	19
1180	77		146	49
1220	115			115

Remarks: In the first approximation, it is seen that the observed CO_2 pressures are in accord with increasing oxide content with increasing temperatures.

The CO_2 dissociation pressures of Lorenz and Janz (1970; emf technique) are in accord with the preceding if a correction for oxide content (mol M_2O/mol eutectic) of $\sim 5 \times 10^{-2}$ is applied from the preceding viewpoints.

Vaporization of molten carbonates:

Measurement method: critical analyses [41]

The various "vaporization" data, based on electrolyte losses from high temperature molten carbonate fuel cells, and the thermodynamics of the associated reactions, have been critically examined by Maru et al. (1976). For a summary of the data status, refer: Li_2CO_3, present work.

References [31,41,46,49-53].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calc'd; from ΔH_f° [48]

Table 41.13. Cryoscopic constant

Composition	k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
ternary eutectic	13.5	$\sim \pm 1\%$

References [1,3,47,48].

16 References

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XLII. Lithium Carbonate-Sodium Carbonate: Li_2CO_3-Na_2CO_3

1. *Melting Temperatures (T_m)*

Pure substance melting points:
Li_2CO_3: 723°C
Na_2CO_3: 858°C

Eutectic melting point:
495.8°C, composition: 53.3 mol % Li_2CO_3

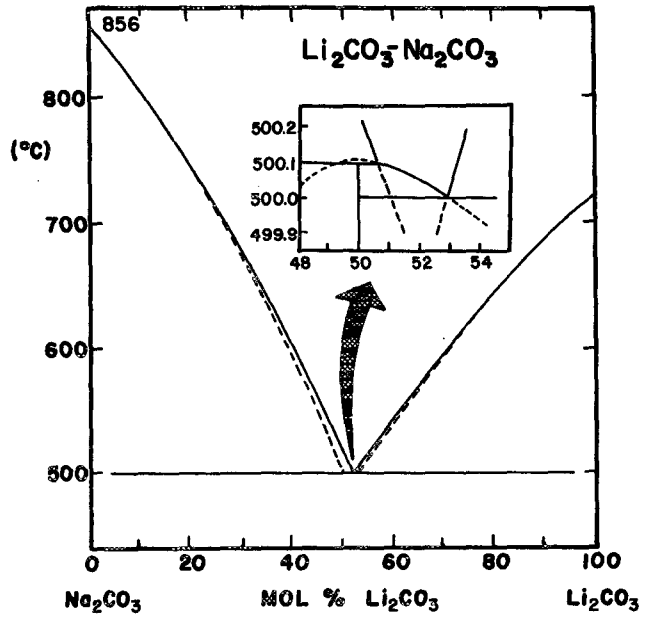

Figure 42.1. Li_2CO_3-Na_2CO_3 phase diagram

References [1-6].

2. *Density (ρ)*

Measurement method: Archimedean technique [7]

Single variable equation

$$\rho = a + bT \quad (42.1)$$

precision: ∿ ± 0.2% uncertainty: ∿ ± 0.5%

Li_2CO_3-Na_2CO_3

Table 42.1. Parameters of equation (42.1)

Mol % Na_2CO_3	a	-b x 10^3	Temp. range (K)
0	2.2365	0.4041	1020 - 1120
10	2.2435	0.3991	980 - 1200
20	2.2885	0.4120	960 - 1220
30	2.3474	0.4378	940 - 1200
40	2.3557	0.4337	920 - 1180
46.7	2.3581	0.4325	820 - 1180
50	2.3532	0.4249	900 - 1180
60	2.3653	0.4262	880 - 1180
70	2.3890	0.4230	960 - 1180
80	2.4461	0.4437	1060 - 1220
90	2.4443	0.4301	1120 - 1220
100	2.4532	0.4267	1140 - 1240

Two-independent-variable equation

$$\rho = a + bT + cC + dC^2 + eC^3 + fTC + gTC^2 \quad (C = \text{mol \% } Na_2CO_3) \qquad (42.2)$$

precision: ± 0.4% uncertainty: ∿ ± 0.5%

Table 42.2. Parameters of two-independent-variable equation (42.2)

a	b x 10^4	c x 10^4	d x 10^6	e x 10^7	f x 10^6	g x 10^8
2.3278	-4.94895	-1.07485	-2.75396	1.90622	2.95891	-2.43405

Table 42.3. Densities (g cm^{-3}) from equations in table 42.1

	Mol % Na_2CO_3											
T(K)	100	90	80	70	60	50	46.7	40	30	20	10	0
820							2.003					
840							1.995					
860							1.986					
880					1.990		1.978					
900					1.982	1.971	1.969					
920					1.973	1.962	1.960	1.957				
940					1.965	1.954	1.952	1.948	1.936			
960				1.983	1.956	1.945	1.943	1.939	1.927			
980				1.974	1.948	1.937	1.934	1.931	1.918	1.885		
1000				1.966	1.939	1.928	1.926	1.922	1.910	1.877	1.844	
1020				1.958	1.931	1.920	1.917	1.913	1.901	1.868	1.836	1.824
1040				1.949	1.922	1.911	1.908	1.905	1.892	1.860	1.828	1.816
1060			1.976	1.941	1.914	1.903	1.900	1.896	1.883	1.852	1.820	1.808
1080			1.967	1.932	1.905	1.894	1.891	1.887	1.875	1.844	1.812	1.800
1100			1.958	1.924	1.896	1.886	1.882	1.879	1.866	1.835	1.804	1.792
1120		1.963	1.949	1.915	1.888	1.877	1.874	1.870	1.857	1.827	1.797	1.784
1140	1.967	1.954	1.940	1.907	1.879	1.869	1.865	1.861	1.848	1.819	1.789	
1160	1.958	1.945	1.931	1.898	1.871	1.860	1.856	1.853	1.840	1.811	1.781	
1180	1.950	1.937	1.923	1.890	1.862	1.852	1.848	1.844	1.831	1.802	1.774	
1200	1.941	1.928	1.914						1.822	1.794	1.765	
1220	1.933	1.920	1.905							1.786		
1240	1.924											

References [7-9].

Li_2CO_3-Na_2CO_3

3. Surface Tension (γ)

Measurement method: pin detachment [8]; maximum bubble pressure [10]

$$\gamma = 313.5 - 7.66 \times 10^{-2}T \quad (42.3)$$

precision: ± 0.7% uncertainty: ∿ ± 1.5%

Table 42.4. Surface tension of eutectic from equation (42.3)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
830	249.9	930	242.3
840	249.2	940	241.5
850	248.4	950	240.7
860	247.6	960	240.0
870	246.9	970	239.2
880	246.1	980	238.4
890	245.3	990	237.7
900	244.6	1000	236.9
910	243.8	1010	236.1
920	243.0	1020	235.4

Single variable equation

$$\gamma = a + bT \quad (42.4)$$

precision: in table 42.4 uncertainty: ∿ ± 1.5%

Table 42.5. Coefficients of single variable equation (42.4), and precisions

Li_2CO_3 (mol %)	a	$-b \times 10^3$	Temp. range (K)	Precision
0	292.2	72.0	1159-1263	±0.3%
10	279.3	56.3	1092-1181	±0.5%
30	307.8	77.9	962-1170	±0.8%
50	308.0	74.6	822-1195	±0.6%
70	298.1	60.4	903-1174	±0.4%
90	289.0	48.2	973-1172	±0.1%
100	281.5	36.6	1023-1173	±0.4%

Two-independent-variable equation

$$\gamma = a + bT + cC + dC^2 + eT^3 + fC^3 + gTC^2 + hCT^2 \quad (C = \text{mol \% } Na_2CO_3) \quad (42.5)$$

precision: ∿ ± 0.3% uncertainty: ∿ ± 1.5%

Table 42.6. Coefficients of two-independent-variable equation (42.5)

a	$b \times 10^2$	$c \times 10^2$	$d \times 10^2$	$e \times 10^9$	$f \times 10^5$	$g \times 10^6$	$h \times 10^7$
300.11719	-8.10195	58.4934	-1.20938	2.24208	2.59350	7.81488	-1.86765

Table 42.7. Surface tension (dyn cm^{-1}) from equations in table 42.5

T (K)	Mol % Na_2CO_3						
	100	90	70	50	30	10	0
830				246.3			
850				244.8			
870				243.3			
890				241.8			
910				240.3	243.0		
930				238.8	241.8		
950				237.3	240.6		
970			232.2	235.8	239.4		
990			230.7	234.3	238.2	241.3	
1010			229.1	232.9	237.0	240.3	
1030			227.6	231.4	235.8	239.4	243.8
1050			226.0	229.8	234.6	238.4	243.1
1070			224.0	228.4	233.4	237.4	242.3
1090		217.9	222.9	226.9	232.2	236.5	241.6
1110		216.8	221.3	225.4	230.9	235.5	240.9
1130		215.7	219.8	223.9	229.7	234.5	240.1
1150		214.6	218.2	222.4	228.5	233.6	239.4
1170	208.7	213.4	216.7	220.9	227.3	232.6	238.7

References [8,10].

4. *Viscosity* (η)

Measurement method: oscillating sphere [11]

precision: not estimated uncertainty: $\sim \pm 25\%$

Values interpolated from graphical data.

For numerical values: see table 42.8.

Li_2CO_3-Na_2CO_3

Table 42.8. Viscosity (cp)

Li_2CO_3 (mol %)	T (K)				
	973	1023	1073	1123	1173
0				4.03	3.57
10			4.44	3.87	3.41
20		5.16	4.37	3.76	3.29
30		5.16	4.37	3.73	3.26
40	6.35	5.28	4.44	3.80	3.31
50	6.51	5.41	4.55	3.86	3.36
60	6.66	5.52	4.61	3.91	3.41
70	6.77	5.58	4.68	3.98	3.46
80	6.89	5.69	4.76	4.06	3.54
90	7.09	5.96	5.04	4.29	3.72
100		6.43	5.47	4.70	4.07

References [11].

5. *Electrical Conductance* (κ)

Measurement method: ac technique [13]

$$\kappa = A \exp(-E/RT) \quad (42.6)$$

precision: not estimated uncertainty: $\sim \pm 2.5\%$

Results reported in equation form only.

Table 42.9. Parameters of equation (42.6)

Na_2CO_3 (mol %)	A ($ohm^{-1}cm^{-1}$)	E (cal mol^{-1})	Temp. range (K)
0	29.22	3940	1013-1153
10	28.00	3980	1007-1201
20	25.05	3930	973-1196
30	23.21	4000	973-1196
40	21.74	4050	953-1253
46.7	20.84	4050	913-1220
50	20.36	4030	933-1212
60	18.85	3940	983-1239
70	17.29	3820	983-1234
80	15.88	3710	1013-1224
90	14.71	3620	1077-1232
100	14.12	3590	1145-1238

Table 42.10. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 42.9

	Mol % Na_2CO_3											
T(K)	100	90	80	70	60	50	46.7	40	30	20	10	0
920							2.274					
940						2.354	2.384		2.727			
960						2.462	2.494	2.602	2.851			
980						2.571	2.604	2.717	2.976	3.330		
1000				2.529	2.596	2.679	2.715	2.832	3.101	3.467		
1020			2.546	2.625	2.698	2.788	2.826	2.948	3.226	3.604	3.930	4.183
1040			2.638	2.723	2.801	2.897	2.936	3.063	3.350	3.741	4.081	4.342
1060			2.729	2.820	2.904	3.005	3.047	3.179	3.475	3.877	4.232	4.501
1080		2.723	2.819	2.916	3.006	3.114	3.157	3.294	3.599	4.014	4.383	4.660
1100		2.808	2.909	3.012	3.108	3.222	3.268	3.409	3.723	4.149	4.533	4.818
1120		2.892	2.999	3.107	3.210	3.330	3.378	3.523	3.847	4.285	4.683	4.976
1140		2.976	3.087	3.202	3.311	3.437	3.487	3.638	3.970	4.420	4.832	5.133
1160	2.975	3.059	3.176	3.297	3.412	3.544	3.596	3.752	4.093	4.554	4.981	
1180	3.054	3.142	3.264	3.391	3.512	3.651	3.705	3.865	4.215	4.687	5.129	
1200	3.133	3.223	3.351	3.484	3.612	3.757	3.813	3.978	4.337	4.819	5.276	
1220	3.212	3.305	3.438	3.577	3.711		3.921					
1240					3.810							

References [8,9,12,13].

6. Safety and Hazards

A. Hazard rating [14-16]

(i) Toxicity: Li_2CO_3, toxic dose (oral, human), 0.7 mg/kg; Na_2CO_3, moderate

(ii) Vapor pressure: carbonates dissociate on heating:

$$M_2CO_{3(\ell)} \rightleftharpoons M_2O_{(\ell)} + CO_{2(g)} \qquad (42.7)$$

For the binary eutectic (m.pt. 495.8°C), the CO_2 equilibrium dissociation pressure is $\sim 4.8 \times 10^{-2}$ mm at approx. 530°C.

B. Disaster hazards [14,17-19]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e. explosive expansion of "trapped" air

(ii) When heated at CO_2 pressures less than equilibrium, carbonates decompose to alkali metal oxides; the toxicology and disaster hazards of such oxides are the same as very strong caustics, i.e. react with water or steam exothermically to form hydroxides that are very aggressive to body tissues (chemical burns); Li_2CO_3 is itself classed as a strong caustic.

References [14-19].

7. Corrosion

Table 42.11. Corrosion studies from primary research literature

Studies	References
Ti alloys; Cr-Ni alloys	20,41
Au, Pt, Ag, Ni, Au-Pd	21
Pt, Au, Ag, MgO	22
Ag, Co, Ni	23
310-SS; 321-SS; 347-SS; Kanthal A; Kanthal A-1; [various gas environments]	24
Thermodynamics of corrosion (E-pCO_2 diagrams); acid-base concepts	25,26,30,31
Ag(fuel cell environment)	27,28
Ag; Al_2O_3 (O_2 environment; eutectic + Li_2O)	29
Hydrolysis (H_2O) reactions	29,32,33
Corrosion in molten salts: annotated bibliography	34
Molten carbonates: fuel cells; thermal energy storage; coal gasification; power plant stack gases	35-40

References [20-41].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in Li_2CO_3-Na_2CO_3 as solvent

Na^+, CO_3^{2-}, H_2

precision: in table 42.12.2 uncertainty: in table 42.12.1

Table 42.12.1. Diffusion techniques, uncertainties, and species

Diffusion techniques of recommended study	Uncertainty (in values of D)	Species
capillary	∿±20%	Na^+, CO_3^{2-}
chronopotentiometry	∿±10%	H_2
voltammetry (linear sweep)	∿±20%	H_2

Li_2CO_3-Na_2CO_3

Equation:

$$D = A \exp [-E/RT] \quad (42.8)$$

Table 42.12.2. Parameters of diffusion equation (42.8), precision and recommended study

Species	A x 10^3 (cm^2 sec^{-1})	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
	(a) Li_2CO_3-Na_2CO_3 eutectic				
Na^+	9.81	10,990	850-1130	~±1.3%	42
CO_3^{2-}	7.36	11,560	840-1115	~±4.8%	42
H_2	6.45	4,346	780-970	~±3%	44
	(b) Li_2CO_3-Na_2CO_3 (25 mol % Na_2CO_3)				
Na^+	4.42	10,060	1030-1210		43
CO_3^{2-}	3.57	10,920	1030-1210		43
	(c) Li_2CO_3-Na_2CO_3 (75 mol % Na_2CO_3)				
Na^+	9.40	11,910	1050-1205		43
CO_3^{2-}	4.26	11,130	1050-1205		43

No entry in precision column indicates estimates not possible since results were reported as equations only.

Li_2CO_3-Na_2CO_3

Table 42.12.3. Self-diffusion coefficients, D x 10^5(cm^2 sec^{-1})

T (K)	Eutectic melt		25 mol % Na_2CO_3		75 mol % Na_2CO_3	
	Na^+	CO_3^{2-}	Na^+	CO_3^{2-}	Na^+	CO_3^{2-}
840		0.723				
850	1.47	0.784				
870	1.70	0.918				
890	1.96	1.066				
910	2.25	1.231				
930	2.56	1.413				
950	2.91	1.612				
970	3.28	1.828				
990	3.68	2.064				
1010	4.11	2.319				
1030	4.57	2.593	3.24	1.72		
1050	5.06	2.888	3.56	1.90	3.12	2.05
1070	5.58	3.203	3.90	2.10	3.47	2.27
1090	6.14	3.539	4.25	2.31	3.85	2.50
1110	6.72	3.896	4.62	2.53	4.25	2.74
1130	7.34		5.01	2.76	4.67	3.00
1150			5.41	3.00	5.12	3.27
1170			5.84	3.26	5.60	3.55
1190			6.28	3.52	6.10	3.85
1210			6.73	3.80	6.63	4.16

Table 42.12.4. Diffusion coefficients in the eutectic melt

T (K)	D_{H_2} x 10^5 (cm^2 sec^{-1})	T (K)	D_{H_2} x 10^5 (cm^2 sec^{-1})
780	39.1	880	53.7
790	40.5	890	55.2
800	41.9	900	56.8
810	43.3	910	58.3
820	44.8	920	59.8
830	46.2	930	61.4
840	47.7	940	63.0
850	49.2	950	64.5
860	50.7	960	66.1
870	52.2	970	67.6

References: Na^+, 42,43; CO_3^{2-}, 42,43; H_2, 44.

9. Heat of Fusion (ΔH_f°)

Measurement method: estimated [45]

Table 42.13. Heat of fusion of eutectic

ΔH_f° (kcal mol^{-1})	Uncertainty
7.9	∿ ± 5%

References [45].

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated [46]

Table 42.14. Volume change on melting

Mol % Li_2CO_3	$(\Delta V_f/V_s)$	Uncertainty
52.7	13.5%	∿ ± 8%

References [46].

12. Vapor Pressure (p_{vap})

Measurement method: cited with each data set [29,36,45]

No systematic studies of vaporization as molecular carbonates have been reported, i.e:

$$M_2CO_{3(\ell)} \rightleftharpoons M_2CO_{3(g)} \quad (42.9)$$

Concerning the CO_2 decomposition of molten carbonates and other possible processes contributing to vaporization, the data for the binary carbonate eutectic are as follows:

Decomposition processes

CO_2 dissociation and equilibrium pressures for the molten eutectic (Li_2CO_3/Na_2CO_3: 53.3/46.7 mol %; m.pt. 495.8°C).

$$M_2CO_{3(\ell)} \rightleftharpoons M_2O_{(\ell)} + CO_{2(g)} \quad (42.10)$$

$$p_{CO_2}(atm) = K_d[a_{M_2CO_{3(\ell)}}/a_{M_2O_{(\ell)}}] \quad (42.11)$$

Here M is the Li, Na cationic mixture of the binary eutectic, p is the equilibrium dissociation pressure, and a is the thermodynamically defined activity. For practical purposes, eq. (42.11) is approximated, in the first instance, in the mol fraction scale [X], as:

$$p_{CO_2}(atm) = K_d[X_{M_2CO_{3(\ell)}}/X_{M_2O_{(\ell)}}] \quad (42.12)$$

The values of $p(CO_2)$ are not uniquely defined unless the oxide content of the carbonate is known exactly; the "equilibrium pressures" will thus depend on the quality of the "carbonate", and its previous history, e.g. to conditions which may promote oxide formation, such as high temperatures at partial pressures < equilibrium dissociation pressure for minimal oxide content.

(i) Equilibrium dissociation constant, K_d

Measurement method: emf technique [29]

$$\log K_d = -12500/T + 6.60 \quad (42.13)$$

precision: not estimated uncertainty: $\sim \pm 1\%$

Table 42.15.1. CO_2 dissociation constant for the binary eutectic from equation (42.13)

T (K)	K_d (atm)	T (K)	K_d (atm)
800	9.44×10^{-10}	1050	4.96×10^{-6}
850	7.84×10^{-9}	1100	1.72×10^{-5}
900	5.14×10^{-8}	1150	5.38×10^{-5}
950	2.77×10^{-7}	1200	1.53×10^{-4}
1000	1.26×10^{-6}		

(ii) Equilibrium CO_2 dissociation pressures

Measurement method: thermodynamic; calc'd [45]

No direct measurements of the equilibrium CO_2 dissociation pressures have been reported. Based on Andersen's (1975) values for K_d, and the preceding expressions for p_{CO_2} the equation for the CO_2 pressure as a function of temperature and oxide content of this molten carbonate eutectic is, (if n is very small, n <<< 1)

$$\log p_{CO_2}(mm) = -12500/T + 9.4808 - \log n \quad (42.14)$$

where n is the oxide content of the molten carbonate in moles oxide per mole carbonate. The values in table 42.15.2 illustrate the thermodynamically predicted equilibrium CO_2 pressures for a range of n (comparable to those observed in related systems, i.e. Li_2CO_3; ternary eutectic).

Table 42.15.2. Equilibrium CO_2 dissociation pressures (mm) for the binary eutectic from equation (42.14)

T (K)	n (mol oxide per mol carbonate)			
	1.5×10^{-5}	3×10^{-5}	1.5×10^{-4}	3×10^{-4}
	CO_2 pressure (mm)			
800	4.8×10^{-2}	2.4×10^{-2}	4.8×10^{-3}	2.4×10^{-3}
900	2.6	1.3	0.26	0.13
1000	64	32	6.4	3.2
1100	870	440	87	44
1200	7700	3800	77	38

Remarks: It is seen that since the molten carbonate is a solution, and the values of the equilibrium pressures depend on the solution composition, the dissociation pressure does not have a unique value unless the value of n is specified.

Vaporization of molten carbonates

Measurement method: critical analysis [36]

The various "vaporization" data, based on electrolyte losses from high temperature molten carbonate fuel cells, and the thermodynamics of the associated reactions, have been critically examined by Maru et al., (1976). For a summary of the data status, refer: Li_2CO_3, present work.

References [27,29,36,45,47-49].

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: steady state radial heat flow [50]

$$\lambda = 2.271 \times 10^{-3} + 5.58 \times 10^{-7}\ T \quad (42.15)$$

precision: not estimated uncertainty: $\sim \pm 20\%$

Results were reported in graphical form only.

Table 42.16. Thermal conductivity from equation (42.15)

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)	T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
800	27.17	980	28.18
820	27.29	1000	28.29
840	27.40	1020	28.40
860	27.51	1040	28.51
880	27.62	1060	28.62
900	27.73	1080	28.74
920	27.84	1100	28.85
940	27.96		
960	28.07		

Sole investigation; equation obtained by fitting the interpolated values from graphical presentation in [50].

References [50].

14. Thermal Conductivity (solid) (λ_s)

Measurement method: steady state radial heat flow [50]

precision: not estimated uncertainty: $\sim \pm 10\%$

For numerical values: see table 42.17.

Li_2CO_3-Na_2CO_3

Table 42.17. Thermal conductivity

T (K)	$\lambda \times 10^4$ (cal $cm^{-1}sec^{-1}K^{-1}$)
400	50.6
450	40.6
500	30.6
550	21.5
600	19.1
650	17.0
700	16.7
750	16.7

References [50].

15. Cryoscopic Constant (k_f)

Measurement method: estimated [45]

Table 42.18. Cryoscopic constant

Mol % Li_2CO_3	k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
53.3	13.4	~ ± 5%

References [45].

16. References

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XLIII. Lithium Carbonate-Potassium Carbonate: Li_2CO_3-K_2CO_3

1. *Melting Temperatures (T_m)*

Pure substance melting points:
Li_2CO_3: 723°C
K_2CO_3: 898°C

Eutectic melting points:
Eutectic 1: 498°C, composition: 42.7 mol % Li_2CO_3
Eutectic 2: 488°C, composition: 62 mol % Li_2CO_3

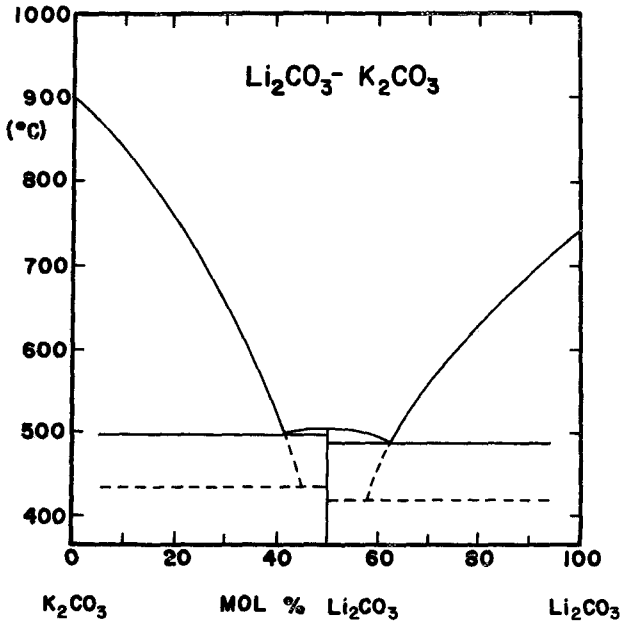

Figure 43.1. Li_2CO_3-K_2CO_3 phase diagram

References [1-4].

2. *Density (ρ)*

Measurement method: Archimedean technique [5]

Single variable equation

$$\rho = a + bT \quad (43.1)$$

precision: ∿ ± 0.2% uncertainty: ∿ ± 0.5%

Li_2CO_3-K_2CO_3

Table 43.1. Coefficients of single variable equation (43.1)

Mol % Li_2CO_3	a	$-b \times 10^3$	Temp. range (K)
0	2.4295	0.4543	1190 - 1250
10	2.4094	0.4422	1130 - 1250
20	2.3942	0.4385	1050 - 1250
30	2.4184	0.4761	950 - 1170
40	2.3795	0.4527	890 - 1150
42.7	2.3711	0.4623	890 - 1190
50	2.3599	0.4548	870 - 1150
60	2.3593	0.4569	890 - 1150
62	2.3526	0.4532	850 - 1210
70	2.3251	0.4390	970 - 1150
80	2.2966	0.4264	990 - 1170
90	2.2687	0.4180	1010 - 1170
100	2.2365	0.4041	1030 - 1130

Two-independent-variable equation:

$$\rho = a + bT + cC + dC^2 + eC^3 \quad (C = \text{mol \% } Li_2CO_3) \quad (43.2)$$

precision: $\sim \pm 0.3\%$ uncertainty: $\sim \pm 0.5\%$

Table 43.2. Coefficients of two-independent-variable equation

a	$b \times 10^4$	$c \times 10^3$	$d \times 10^5$	$e \times 10^8$
2.42818	-4.45548	-1.82681	1.20594	-8.42184

Table 43.3. Densities (g cm^{-3}) from equations in table 43.1

	Mol % Li_2CO_3												
T(K)	100	90	80	70	62	60	50	42.7	40	30	20	10	0
850					1.967								
870					1.958		1.964						
890					1.949	1.953	1.955	1.960	1.977				
910					1.940	1.944	1.946	1.950	1.968				
930					1.931	1.934	1.937	1.941	1.958				
950					1.922	1.925	1.928	1.932	1.949	1.966			
970				1.899	1.913	1.916	1.919	1.923	1.940	1.957			
990			1.874	1.890	1.904	1.907	1.910	1.913	1.931	1.947			
1010		1.847	1.866	1.882	1.895	1.898	1.901	1.904	1.922	1.938			
1030	1.820	1.838	1.857	1.873	1.886	1.889	1.891	1.895	1.913	1.928			
1050	1.812	1.830	1.849	1.864	1.877	1.880	1.882	1.886	1.904	1.918	1.934		
1070	1.804	1.821	1.840	1.855	1.868	1.870	1.873	1.876	1.895	1.909	1.925		
1090	1.796	1.813	1.832	1.847	1.859	1.861	1.864	1.867	1.886	1.899	1.916		
1110	1.788	1.805	1.823	1.838	1.850	1.852	1.855	1.858	1.877	1.890	1.907		
1130	1.780	1.796	1.815	1.829	1.840	1.843	1.846	1.849	1.868	1.880	1.899	1.910	
1150		1.788	1.806	1.820	1.831	1.834		1.839	1.859	1.871	1.890	1.901	
1170		1.780	1.798		1.822			1.830		1.861	1.881	1.892	
1190					1.813			1.821			1.872	1.883	1.889
1210					1.804						1.864	1.874	1.880
1230											1.855	1.865	1.871
1250											1.846	1.857	1.862

References [5-7].

3. Surface Tension (γ)

Measurement method: pin detachment; maximum bubble [6,8]

$$\gamma = 324.09 - 124.8 \times 10^{-3}T \quad (43.3)$$

precision: ± 0.8% uncertainty: ∿ ± 1.5%

Table 43.4. Surface tension of eutectic 1 from equation (43.3)

T (K)	γ (dyn cm^{-1})	T (K)	γ (dyn cm^{-1})
840	219.3	960	204.3
860	216.8	980	201.8
880	214.3	1000	199.3
900	211.8	1020	196.8
920	208.0	1040	194.3
940	206.8	1060	191.8
		1080	189.3

$$\gamma = a - bT \quad (43.4)$$

precision: in table 43.5 uncertainty: ∿ ± 3%

Table 43.5. Coefficients of equation (43.4), and precisions

Mol % Li_2CO_3	a	b x 10^3	Temp. range (K)	Precision
0	241.07	61.4	1173-1308	±0.41%
10	262.92	79.9	1114-1173	±0.12%
30	241.94	58.0	931-1173	±0.83%
50	229.59	39.5	800-1172	±0.68%
70	231.18	29.2	842-1173	±0.25%
90	253.42	33.4	965-1172	±0.62%
100	281.50	36.6	1023-1173	±0.46%

Table 43.6. Surface tension (dyn cm^{-1}) from equations in table 43.5

	Mol % Li_2CO_3				
T(K)	90	70	50	30	10
800			198.0		
820			197.2		
840		206.7	196.4		
860		206.1	195.6		
880		205.5	194.8		
900		204.9	194.0		
920		204.3	193.3		
940		203.7	192.5	187.4	
960		203.1	191.7	186.3	
980	220.7	202.6	190.9	185.1	
1000	220.0	202.0	190.1	183.9	
1020	219.4	201.4	189.3	182.8	
1040	218.7	200.8	188.5	181.6	
1060	218.0	200.2	187.7	180.5	
1080	217.3	199.6	186.9	179.3	
1100	216.7	199.1	186.1	178.1	
1120	216.0	198.5	185.4	177.0	173.4
1140	215.3	197.9	184.6	175.8	171.8
1160	214.7	197.3	183.8	174.7	170.2
1180					168.6

References [6,8].

4. *Viscosity* (η)

Measurement method: oscillating sphere [9]

$$\eta = a + bT + cT^2 \quad (43.5)$$

precision: in table 43.7 uncertainty: $\sim \pm 25\%$

Table 43.7. Parameters of equation (43.5), and precisions

Li_2CO_3 (mol %)	a	-b x 10^2	c x 10^5	Temp. range (K)	Precision
10	10.776	0.6800		1123-1173	
20	50.590	7.576	2.980	1023-1173	±0.4%
30	53.599	8.100	3.202	973-1173	±0.4%
40	56.671	8.601	3.405	973-1173	±0.6%
50	56.353	8.467	3.317	973-1173	±0.7%
60	64.086	9.816	3.917	973-1173	±0.5%
70	69.752	10.785	4.347	973-1173	±0.5%
75	72.031	11.138	4.490	973.1173	±0.6%
80	75.469	11.719	4.747	973-1173	±1.0%
85	70.975	10.785	4.289	973-1173	±0.5%
90	79.076	12.136	4.866	1023-1173	±0.5%
95	16.121	0.5749	-0.3958	1023-1173	±4.5%
100	9.621	-0.6993	-0.9960	1023-1173	±4.1%

Table 43.8. Viscosity (cp) from equations in table 43.7

T (K)	Mol % Li_2CO_3												
	10	20	30	40	50	60	70	75	80	85	90	95	100
980			4.97	5.08	5.23	5.51	5.81	6.00	6.21	6.47			
990			4.79	4.89	5.04	5.30	5.59	5.77	5.98	6.24			
1000			4.62	4.71	4.85	5.10	5.37	5.55	5.75	6.01			
1010			4.45	4.54	4.67	4.90	5.17	5.34	5.53	5.80			
1020			4.29	4.37	4.50	4.72	4.97	5.14	5.32	5.59			
1030		4.17	4.14	4.20	4.33	4.54	4.78	4.94	5.12	5.39	5.70	6.00	6.26
1040		4.03	3.99	4.05	4.17	4.37	4.61	4.76	4.93	5.20	5.49	5.86	6.12
1050		3.90	3.85	3.90	4.02	4.20	4.44	4.58	4.76	5.02	5.30	5.72	5.98
1060		3.77	3.72	3.76	3.87	4.05	4.27	4.42	4.58	4.85	5.11	5.58	5.84
1070		3.64	3.59	3.62	3.73	3.90	4.12	4.26	4.42	4.68	4.93	5.44	5.70
1080		3.53	3.47	3.50	3.60	3.76	3.98	4.11	4.27	4.52	4.76	5.30	5.56
1090		3.42	3.35	3.37	3.47	3.63	3.84	3.97	4.13	4.38	4.61	5.15	5.41
1100		3.31	3.24	3.26	3.35	3.51	3.72	3.84	4.00	4.24	4.46	5.01	5.26
1110		3.21	3.14	3.15	3.24	3.39	3.60	3.72	3.88	4.11	4.32	4.86	5.11
1120		3.12	3.04	3.05	3.13	3.28	3.49	3.61	3.76	3.98	4.19	4.72	4.96
1130	3.09	3.03	2.96	2.96	3.03	3.18	3.39	3.50	3.66	3.87	4.07	4.57	4.81
1140	3.02	2.95	2.87	2.87	2.94	3.09	3.30	3.41	3.56	3.77	3.96	4.42	4.65
1150	2.96	2.88	2.80	2.79	2.85	3.00	3.21	3.32	3.48	3.67	3.86	4.28	4.49
1160	2.89	2.81	2.73	2.72	2.77	2.93	3.14	3.25	3.40	3.58	3.78	4.13	4.33
1170	2.82	2.74	2.66	2.65	2.70	2.86	3.07	3.18	3.34	3.50	3.70	3.98	4.17

References [9].

5. *Electrical Conductance (κ)*

Measurement method: classical ac [10]

$$\kappa = A \exp(-E/RT) \quad (43.6)$$

precision: estimate not possible uncertainty: ∿ ± 2.5%

Data reported in equation form.

Table 43.9. Parameters of equation (43.6)

K_2CO_3 (mol %)	A	E (cal mol^{-1})	Temp. range (K)
100	10.52	3830	1178-1281
90	10.85	3840	996-1136
80	11.41	3890	972-1165
70	13.32	4180	973-1193
60	14.49	4320	1003-1197
57.3	14.56	4320	1013-1223
50	14.96	4330	1013-1222
40	16.63	4240	993-1227
30	20.27	4180	1001-1239
20	23.37	4110	1034-1246
10	26.46	4030	1133-1260
0	29.22	3940	1013-1153

Table 43.10. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 43.9

T(K)	Mol % Li_2CO_3											
	100	90	80	70	60	50	42.7	40	30	20	10	0
980									1.557	1.548		
1000				2.473	1.969			1.648	1.625	1.611	1.571	
1020	4.183			2.577	2.053	1.766	1.728	1.719	1.694	1.674	1.631	
1040	4.342		3.198	2.682	2.137	1.840	1.800	1.791	1.762	1.737	1.692	
1060	4.501		3.320	2.786	2.221	1.915	1.872	1.863	1.831	1.800	1.752	
1080	4.660		3.443	2.890	2.306	1.989	1.945	1.936	1.899	1.862	1.813	
1100	4.818		3.565	2.994	2.390	2.063	2.017	2.008	1.968	1.925	1.873	
1120	4.976		3.686	3.098	2.474	2.138	2.090	2.080	2.036	1.987	1.932	
1140	5.133	4.466	3.808	3.202	2.558	2.212	2.162	2.152	2.104	2.049		
1160		4.605	3.929	3.306	2.642	2.286	2.235	2.224	2.172	2.110		
1180		4.744	4.049	3.409	2.726	2.360	2.307	2.296	2.240			2.054
1200		4.882	4.169	3.512	2.809	2.434	2.379					2.117
1220		5.019	4.289	3.614	2.893	2.507	2.450					2.167
1240		5.155	4.408	3.716								2.223
1260		5.291										2.278
1280												2.334

References [6,7,10,11].

6. Safety and Hazards

A. Hazard rating [12-14]

(i) Toxicity: Li_2CO_3, toxic dose (oral, human), 0.7 mg/kg; K_2CO_3, severe

(ii) Vapor pressure: Carbonates dissociate on heating:

$$M_2CO_{3(\ell)} \rightleftharpoons M_2O_{(\ell)} + CO_{2(g)} \qquad (43.7)$$

For the equimolar mixture the CO_2 equilibrium dissociation pressure is $\sim 1.6 \times 10^{-3}$ mm at approx. 530°C.

B. Disaster hazards [12,15-17]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e. explosive expansion of "trapped air.

(ii) When heated at CO_2 pressures less than equilibrium, carbonates decompose to alkali metal oxides; the toxicology and disaster hazards of such oxides are the same as very strong caustics, i.e. react with water or steam exothermically to form hydroxides that are very aggressive to body tissues (chemical burns); Li_2CO_3 by itself is classed as a strong caustic.

References [12-17].

7. Corrosion

Table 43.11. Corrosion studies from primary research literature

Studies	References
Ti alloy	18
oxides (polarographic studies)	19
SS-304; Al	20,21
Acid-base relationships in molten carbonates	22-25
Hydrolysis (H_2O) reactions	26-28
Corrosion in molten salts: annotated bibliography	29
Molten carbonates: fuel cells; thermal energy storage; coal gasification; power plant stack gases	30-35

References [18-35].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in Li_2CO_3-K_2CO_3 as solvent

K^+, CO_3^{2-}, *Pb^{2+}*, *Cu^+*, *Cd^{2+}*, *Ni^{2+}*, *$Cr_2O_7^{2-}$*, *Cl^-*, *Br^-*, *I^-*.

The italicized species indicate studies with insufficient data-sets for temperature-dependence characterization of diffusion coefficients. For these species: see table 43.12.4.

precision: in table 43.12.2 uncertainty: in table 32.12.1

Table 43.12.1. Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty (in values of D)	Species
capillary	∿±20%	K^+, CO_3^{2-}
chronopotentiometry	∿±10%	Pb^{2+}, Cu^+, Cd^{2+}, Ni^{2+}, $Cr_2O_7^{2-}$, Cl^-, Br^-, I^-

Li_2CO_3-K_2CO_3

Equations:

$$D = A \exp[-E/RT] \quad (43.8)$$

Table 43.12.2. Parameters of diffusion equation (43.8), precisions, and recommended study

Species	A x 10^3 (cm^2 sec^{-1})	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
K^+	7.26	11,490	890-1130	∿±3.5%	36
CO_3^{2-}	7.94	11,860	850-1135	∿±3.5%	36

Table 43.12.3. Self-diffusion coefficients from equations in table 43.12.2

T (K)	D_{K^+} x 10^5 (cm^2 sec^{-1})	$D_{CO_3^{2-}}$ x 10^5 (cm^2 sec^{-1})
850		0.71
870		0.83
890	1.09	0.97
920	1.35	1.21
950	1.65	1.48
980	1.99	1.80
1010	2.37	2.15
1040	2.79	2.55
1070	3.27	3.00
1100	3.78	3.49
1130	4.35	4.03

Table 43.12.4. Diffusion coefficients for species not included in table 43.12.3

Species	D x 10^5 (cm^2 sec^{-1})	Species	D x 10^5 (cm^2 sec^{-1})
Pb^{2+}	2.74	$Cr_2O_7^{2-}$	4.12
Cu^+	4.89	Cl^-	0.089
Cd^{2+}	2.71	Br^-	0.081
Ni^{2+}	3.78	I^-	0.071

References: K^+, 36; CO_3^{2-}, 36; Pb^{2+}, 37; Cu^+, 37; Cd^{2+}, 37; Ni^{2+}, 37; $Cr_2O_7^{2-}$, 37; Cl^-, 37; Br^-, 37; I^-, 37.

9. *Heat of Fusion (ΔH_f°)*

Measurement method: drop calorimetry [38]

Table 43.13. Heat of fusion

Mol % Li_2CO_3	ΔH_f° (kcal mol^{-1})	Uncertainty
50	8.7	∿ ± 1.5%

References [38].

10. *Heat of Capacity (C_p)*

Measurement method: drop calorimetry [38]

Table 43.14. Heat capacity

Mol % Li_2CO_3	C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
50	44.65 ± 0.1	778-1200	∿ ± 0.5%

References [38].

11. *Volume Change on Melting (ΔV_f)*

Measurement method: estimated [39]

Table 43.15. Volume changes on melting

Mol % Li_2CO_3	T_m(°C)	$(\Delta V_f/V_s)$	Uncertainty
42.2	498	9.3%	∿±8%
50	505	9.6%	
63	488	8.5%	

References [39].

12. *Vapor Pressure (p_{vap})*

Measurement method: cited with each data set

No systematic studies of vaporization as molecular carbonates have been reported, i.e.,

$$M_2CO_{3(\ell)} \rightleftharpoons M_2CO_{3(g)} \quad (43.9)$$

For the CO_2 decomposition of molten carbonates and other possible processes contributing to vaporization, the data for the equimolar binary carbonate system are as follows.

Decomposition processes

CO_2 dissociation and equilibrium processes for the molten equimolar binary Li,K/CO_3 system (m.pt. 505°C)

$$M_2CO_{3(\ell)} \rightleftharpoons M_2O_{(\ell)} + CO_{2(g)} \quad (43.10)$$

Li_2CO_3-K_2CO_3

$$p_{CO_2}\ (atm) = K_d\ [a_{M_2CO_3\ (\ell)} / a_{M_2O\ (\ell)}] \quad (43.11)$$

where M is the Li, K cationic mixture of the equi-molar binary mixture, p is the equilibrium CO_2 dissociation pressure, and a the thermodynamically defined activity. For practical purposes, eq. (43.11) is generally expressed in the mol fraction scale [X], as:

$$p_{CO_2}\ (atm) = K_d\ [X_{M_2CO_3\ (\ell)} / X_{M_2O\ (\ell)}] \quad (43.12)$$

The "equilibrium pressures" thus depend on the quality of the "carbonate" and its previous history, i.e. the oxide content, since the molten system is a solution.

(i) Equilibrium dissociation constant, K_d

Measurement method: emf technique [28]

$$\log K_d = -13810/T + 6.77 \quad (43.13)$$

precision: not estimated uncertainty: $\sim \pm 1\%$

Table 43.16.1. CO_2 dissociation constant for the equimolar mixture from equation (43.13)

T (K)	K_d (atm)	T (K)	K_d (atm)
800	3.22×10^{-11}	1050	4.15×10^{-7}
850	3.33×10^{-10}	1100	1.64×10^{-6}
900	2.66×10^{-9}	1150	5.77×10^{-6}
950	1.71×10^{-8}	1200	1.83×10^{-5}
1000	9.12×10^{-8}		

(ii) *Equilibrium CO_2 dissociation pressures*

Measurement method: thermodynamic; calc'd [40]

No direct measurements of the equilibrium CO_2 dissociation pressures have been reported. Based on Andersen's (1975) values for K_d, and the preceding expressions for p_{CO_2}, the equation for p_{CO_2} as a function of T and oxide content for the molten binary system is:

$$\log p_{CO_2}(mm) = -13810/T + 9.6508 - \log n \quad (43.14)$$

Here n is the oxide content in mols oxide/mol carbonate, and $n \ll$ unity. The values in table 43.16.2 illustrate the thermodynamically predicted equilibrium CO_2 pressures for a range of n (comparable to the oxide contents observed in related systems, e.g. Li_2CO_3; K_2CO_3; ternary eutectic).

Table 43.16.2. Equilibrium CO_2 dissociation pressures (mm) for the equimolar mixture from equation (43.14)

T	n (mol oxide per mole carbonate)			
(K)	1.5×10^{-5}	3×10^{-5}	1.5×10^{-4}	3×10^{-4}
	CO_2 pressure (mm)			
800	1.6×10^{-3}	8.1×10^{-4}	1.6×10^{-4}	8.1×10^{-5}
900	0.13	6.7×10^{-2}	1.3×10^{-2}	6.7×10^{-3}
1000	4.6	2.3	0.46	0.23
1100	83	42	8.3	4.2
1200	930	465	93	46

Remarks: Since the molten carbonate/oxide system is a solution, and the values of the equilibrium pressures depend on the solution composition, the dissociation pressures do not have a unique value unless the value of n is specified.

Vaporization of molten carbonates

Measurement method: critical analysis [31]

The various "vaporization" data, based on electrolyte losses from high temperature molten carbonate fuel cells, and the thermodynamics of the associated reactions, have been critically examined by Maru et al. (1976). For a summary of the data status, refer: Li_2CO_3, present work.

References [28,31,40-44].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calc'd from ΔH_f° [40]

Table 43.17. Cryoscopic constant

Mol % Li_2CO_3	k_f (K $mol^{-1}kg^{-1}$)	Uncertainty
50	14.6	$\sim \pm 1.5\%$

References [38,40].

16. References

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XLIV. Sodium Carbonate-Potassium Carbonate: Na_2CO_3-K_2CO_3

1. Melting Temperatures (T_m)

Pure substance melting points:
Na_2CO_3: 858°C
K_2CO_3: 898°C

Minimum melting solid solution melting point:
710°C, composition: 58 mol % Na_2CO_3

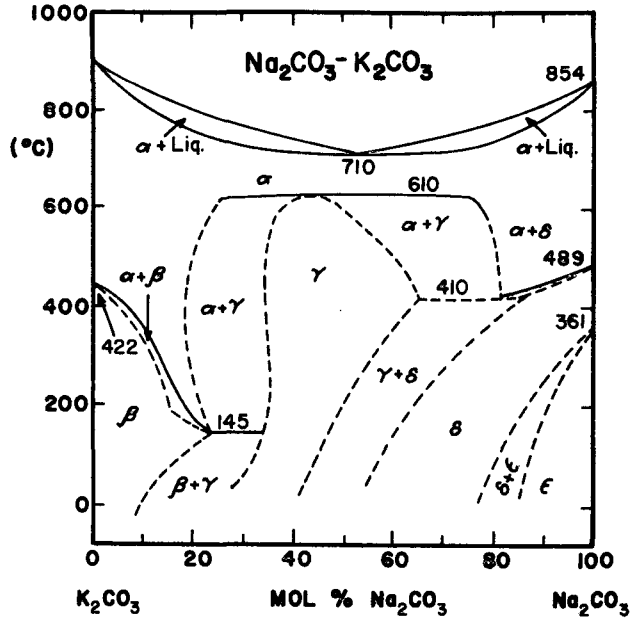

Figure 44.1. Na_2CO_3-K_2CO_3 phase diagram

References [1-5].

2. Density (ρ)

Measurement method: Archimedean technique [6]

Single variable equation

$$\rho = a + bT \quad (44.1)$$

precision: ∿ ± 0.2% uncertainty: ∿ ± 0.5%

Table 44.1. Parameters of single variable equation (44.1)

Mol % Na_2CO_3	a	-b x 10^3	Temp. range (K)
0	2.4295	0.4543	1190 - 1260
10	2.4179	0.4419	1180 - 1260
20	2.4130	0.4329	1140 - 1260
25	2.4243	0.4405	1070 - 1270
30	2.4240	0.4375	1070 - 1260
40	2.4278	0.4366	1020 - 1240
50	2.4359	0.4393	1000 - 1230
58	2.4413	0.4406	1050 - 1240
60	2.4506	0.4467	1040 - 1230
70	2.4509	0.4419	1070 - 1240
75	2.4614	0.4465	1090 - 1240
80	2.4723	0.4520	1070 - 1230
90	2.4862	0.4581	1120 - 1240
100	2.4532	0.4267	1140 - 1240

Two-independent-variable equation

$$\rho = a + bC + cT^2 + dC^2 + eT^3 \quad (C = \text{mol \% } Na_2CO_3) \qquad (44.2)$$

precision: ± 0.6% uncertainty: ∿ ± 0.5%

Table 44.2. Coefficients of two-independent-variable equation (44.2)

a	b x 10^4	c x 10^7	d x 10^6	e x 10^{11}
2.22615	4.05178	-3.40228	1.84011	8.55883

Table 44.3. Densities(g cm^{-3}) from equations in table 44.1

	Mol % Na_2CO_3													
T(K)	100	90	80	75	70	60	58	50	40	30	25	20	10	0
1000								1.997						
1010								1.992						
1020								1.988	1.982					
1030								1.983	1.978					
1040						1.986		1.979	1.974					
1050						1.982	1.979	1.975	1.969					
1060						1.977	1.974	1.970	1.965					
1070			1.989		1.978	1.973	1.970	1.966	1.961					
1080			1.984		1.974	1.968	1.965	1.961	1.956	1.952	1.949			
1090			1.980	1.975	1.969	1.964	1.961	1.957	1.952	1.947	1.944			
1100			1.975	1.970	1.965	1.959	1.957	1.953	1.948	1.943	1.940			
1120		1.973	1.966	1.961	1.956	1.950	1.948	1.948	1.943	1.938	1.935			
1130		1.969	1.962	1.957	1.952	1.946	1.943	1.944	1.939	1.934	1.931			
1140	1.967	1.964	1.957	1.952	1.947	1.941	1.939	1.939	1.934	1.930	1.927	1.924		
1150	1.962	1.959	1.953	1.948	1.943	1.937	1.935	1.935	1.930	1.925	1.922	1.919		
1160	1.958	1.955	1.948	1.943	1.938	1.932	1.930	1.931	1.926	1.921	1.918	1.915		
1170	1.954	1.950	1.943	1.939	1.934	1.928	1.926	1.926	1.921	1.917	1.913	1.911		
1180	1.950	1.946	1.939	1.935	1.929	1.923	1.921	1.922	1.917	1.912	1.909	1.907	1.901	
1190	1.945	1.941	1.934	1.930	1.925	1.919	1.917	1.918	1.913	1.908	1.905	1.902	1.896	1.893
1200	1.941	1.936	1.930	1.926	1.921	1.915	1.913	1.913	1.908	1.903	1.900	1.898	1.892	1.889
1210	1.927	1.932	1.925	1.921	1.916	1.910	1.908	1.909	1.904	1.899	1.896	1.894	1.888	1.884
1220	1.933	1.927	1.921	1.917	1.912	1.906	1.904	1.904	1.900	1.895	1.891	1.889	1.883	1.880
1230	1.928	1.923	1.916	1.912	1.907	1.901	1.899	1.900	1.895	1.890	1.887	1.885	1.879	1.875
1240	1.924	1.918		1.908	1.903		1.895		1.891	1.886		1.881	1.874	1.871
1250										1.882		1.876	1.870	1.866
1260										1.877		1.872	1.866	1.862

References [6-9].

3. *Surface Tension (γ)*

Measurement method: pin detachment, maximum bubble pressure [7,10,11]

$$\gamma = a + bT + cT^2 \quad (44.3)$$

precision: in table 44.4 uncertainty: $\sim \pm$ 0.5%

Table 44.4. Parameters of equation (44.3), and precisions

Mol % Na_2CO_3	a	-b x 10^2	c x 10^5	Precision
0	243.908	6.37144		±0.15%
25	866.024	115.2236	47.8798	±1.31%
50	272.280	9.72033	1.61667	±0.04%
58	202.781	8.35561	-7.45722	±0.18%
75	259.582	5.83335		±0.09%
100	304.552	10.97145	2.44999	±0.06%

Table 44.5. Surface tension (dyn cm^{-1}) from equations in table 44.4

T (K)	Mol % Na_2CO_3					
	100	75	58	50	25	0
1000			211.8	191.2		
1020			210.4	190.0		
1040			209.0	188.7		
1060		197.8	207.6	187.4		
1080		196.6	206.0	186.2	180.1	
1100		195.4	204.5	184.9	177.9	
1120		194.3	202.8	183.7	176.1	
1140	211.3	193.1	201.1	182.5	174.7	
1160	210.3	191.9		181.3	173.7	
1180	209.2	190.8			173.1	168.7
1200	208.2	189.6			172.8	167.5
1220	207.2					166.2
1240	206.2					164.9
1260	205.2					163.6
1280	204.3					162.4

References [6,9-11].

4. *Viscosity (η)*

Measurement method: oscillating sphere [12]

precision: not estimated uncertainty: ∿ ± 25%

Values interpolated from the graphical data.

Table 44.6. Viscosity(cp)

Mol % Na_2CO_3	T (K)			
	1023	1073	1123	1173
0				2.83
10			3.41	3.05
20			3.47	3.10
30	4.75	4.06	3.56	3.18
40	4.82	4.20	3.64	3.24
50	4.96	4.30	3.73	3.29
60	5.12	4.41	3.81	3.37
70	5.21	4.48	3.84	3.39
80	5.25	4.50	3.88	3.38
90			3.94	3.45
100			4.04	

References [12].

Na_2CO_3-K_2CO_3

5. Electrical Conductance (κ)

Measurement method: ac technique [14]

$$\kappa = A \exp(-E/RT) \quad (44.4)$$

precision: estimate not possible uncertainty: ≈ ± 2.5%

Data reported in equation form.

Table 44.7. Parameters of equation (44.4)

Mol % Na_2CO_3	A (ohm^{-1} cm^{-1})	E (cal mol^{-1})	Temp. range (K)
0	10.52	3830	1178-1281
10	10.85	3850	1157-1250
20	11.32	3880	1148-1258
30	11.49	3870	1076-1237
40	11.79	3860	1047-1246
50	12.20	3900	1044-1230
58	12.38	3910	1043-1226
60	12.98	3990	1073-1230
70	13.20	3910	1071-1222
80	13.65	3800	1086-1236
90	13.95	3700	1143-1254
100	14.12	3590	1145-1238

Table 44.8. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 44.7

	Mol % Na_2CO_3											
T(K)	100	90	80	70	60	58	50	40	30	20	10	0
1040						1.866	1.848					
1060						1.934	1.915	1.886	1.830			
1080				2.134	2.022	2.002	1.982	1.951	1.893			
1100			2.399	2.206	2.092	2.069	2.049	2.016	1.956			
1120			2.475	2.278	2.161	2.136	2.114	2.081	2.019			
1140		2.724	2.550	2.349	2.230	2.203	2.181	2.145	2.081			
1160	2.974	2.802	2.625	2.420	2.299	2.270	2.247	2.209	2.144	2.072	2.042	
1180	3.054	2.879	2.699	2.491	2.367	2.336	2.312	2.273	2.205	2.133	2.100	2.054
1200	3.133	2.956	2.773	2.561	2.435	2.402	2.377	2.336	2.267	2.224	2.159	2.111
1220	3.211	3.032	2.847	2.631	2.503	2.467	2.442	2.399	2.328	2.284	2.217	2.167
1240	3.289	3.107						2.461	2.389	2.344	2.274	2.223
1260										2.403		2.278
1280												2.334

References [7,13,14].

6. Safety and Hazards

A. Hazard rating [15-17]

(i) Toxicity: K_2CO_3, severe; Na_2CO_3, slight.

(ii) Vapor pressure: Carbonates dissociate on heating:

$$M_2CO_{3(\ell)} \rightleftharpoons M_2O_{(\ell)} + CO_{2(g)} \quad (44.5)$$

For the min. melting mixture (m.pt. 710°C), the CO_2 equilibrium dissociation pressure is $\sim 1.1 \times 10^{-6}$ mm at approx. 530°C

B. Disaster hazards [15,18-20]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e. explosive expansion of "trapped" air.

(ii) When heated at CO_2 pressures less than equilibrium, carbonates decompose to alkali metal oxides; the toxicology and disaster hazards of such oxides are the same as very strong caustics, i.e. react with water or steam exothermically to form hydroxides that are very aggressive to body tissues (chemical burns).

References [15-20].

7. Corrosion

Table 44.9. Corrosion studies from primary research literature

Studies	References
Corundum, mullite, fosterite	21
Ag; Al_2O_3 (O_2 atmosphere; Na_2CO_3-K_2CO_3-Na_2O)	22
Acid-base relationships in molten carbonates	23-26
Hydrolysis (H_2O) reactions	22,27,28
Corrosion in molten salts: annotated bibliography	29
Molten carbonates: fuel cells; thermal energy storage; coal gasification, power plant stack gases	30-35

References [21-36].

8. Diffusion

Measurement method: capillary [37]

List of diffusing species investigated in Na_2CO_3-K_2CO_3 as solvent

$$Na^+,\ K^+,\ CO_3^{2-}$$

Equation

$$D = A \exp[-E/RT] \quad (44.6)$$

precision: in table 44.10.1 uncertainty: $\sim \pm$ 20%

Table 44.10.1. Parameters of diffusion equation (44.6), and precisions

Species	A x 10^3 (cm^2 sec^{-1})	E (cal mol^{-1})	Temp. range (K)	Precision
K^+	7.61	11,840	1065-1240	±1.5%
Na^+	8.18	11,820	1080-1240	±3.1%
CO_3^{2-}	2.71	11,030	1030-1190	±2.4%

Table 44.10.2. Self-diffusion coefficients, D x 10^5(cm^2sec^{-1}), from equations in table 44.10.1

T (K)	Na^+	K^+	CO_3^{2-}
1030			1.24
1040			1.30
1060		2.75	1.44
1080	3.32	3.06	1.59
1100	3.67	3.38	1.74
1120	4.04	3.72	1.91
1140	4.43	4.09	2.08
1160	4.85	4.47	2.26
1180	5.29	4.88	2.45
1190	5.52	5.09	2.55
1200	5.75	5.31	
1220	6.24	5.76	
1240	6.75	6.23	

References [37].

9. *Heat of Fusion* (ΔH_f°)

Measurement method: drop calorimetry [38]

Table 44.11. Heat of fusion

Mol % Na_2CO_3	ΔH_f° (kcal mol^{-1})	Uncertainty
56	4.7	∿ ± 2%

References [38].

Na_2CO_3-K_2CO_3

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [38]

Table 44.12. Heat capacity

Mol % Na_2CO_3	C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
56	44.3 ± 0.1	983-1197	∿ ± 0.5%

References [38].

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated; from densities [39]

Table 44.13. Volume change on melting

Mol % Na_2CO_3	$(\Delta V_f/V_s)$	Uncertainty
56	14.4%	∿ ± 8%

References [39].

12. Vapor Pressure (p_{vap})

Measurement method: cited with each data set [22,31,39]

No systematic studies of vaporization as molecular carbonates have been reported, i.e.,

$$M_2CO_{3(\ell)} \rightleftharpoons M_2CO_{3(g)} \quad (44.7)$$

For the CO_2 decomposition of molten carbonates and other possible processes contributing to vaporization, the data for the molten minimum melting Na,K/CO_3 system are as follows.

Decomposition Processes

CO_2 dissociation and equilibrium pressure for the molten minimum melting Na,K/CO_3 mixture (56:44; m.pt. 710°C)

$$M_2CO_{3(\ell)} \rightleftharpoons M_2O_{(\ell)} + CO_{2(g)} \quad (44.8)$$

$$p_{CO_2}\ (atm) = K_d[a_{M_2CO_{3(\ell)}}/a_{M_2O_{(\ell)}}] \quad (44.9)$$

Here M is the Na,K cationic mixture in this molten binary system, p is the equilibrium CO_2 dissociation pressure, and a the thermodynamically defined activity. For practical purposes, eq. (44.9) is generally expressed in the mol fraction scale [X], as:

$$p_{CO_2}\ (atm) = K_d[X_{M_2CO_{3(\ell)}}/X_{M_2O_{(\ell)}}] \quad (44.10)$$

Thus the "equilibrium pressures" depend on the oxide content, i.e. the quality of the "carbonate", and its previous history.

(i) Equilibrium dissociation constant, K_d

Measurement method: emf technique [22]

$$\log K_d = -16780/T + 7.32 \quad (44.11)$$

Precision: not estimated, uncertainty: $\sim \pm 1\%$

Table 44.14.1. CO_2 dissociation constants from equation (44.11) for minimum melting mixture

T (K)	K_d (atm)	T (K)	K_d (atm)
800	2.21×10^{-14}	1050	2.18×10^{-9}
850	3.79×10^{-13}	1100	1.16×10^{-8}
900	4.72×10^{-12}	1150	5.35×10^{-8}
950	4.54×10^{-11}	1200	2.17×10^{-7}
1000	3.47×10^{-10}		

(ii) Equilibrium CO_2 dissociation pressures

Measurement method: thermodynamic; calc'd [39]

No direct measurements of the equilibrium CO_2 dissociation pressures have been reported. Based on Andersen's (1975) values for K_d, and the preceding expressions for p_{CO_2}, the equation for p_{CO_2} as a function of T and oxide content for this molten binary system is:

$$\log p_{CO_2}(\text{mm}) = \frac{-16780}{T} + 10.2008 - \log n \quad (44.12)$$

where n is the oxide content (i.e. mols oxide/mol carbonate) if $n \ll$ unity. The values in table 44.14.2 summarize the thermodynamically predicted p_{CO_2} pressures for a range of n (comparable to the oxide content in related systems, e.g. Na_2CO_3; K_2CO_3; ternary eutectic).

Table 44.14.2. Equilibrium CO_2 dissociation pressures (mm) from equation (44.12) for minimum melting mixture

T	n(mol oxide per mol carbonate)			
(K)	1.5×10^{-5}	3×10^{-5}	1.5×10^{-4}	3×10^{-4}
	CO_2 pressure (mm)			
800	1.1×10^{-6}	5.6×10^{-7}	1.1×10^{-7}	5.6×10^{-8}
900	2.4×10^{-4}	1.2×10^{-4}	2.4×10^{-5}	1.2×10^{-5}
1000	1.7×10^{-2}	8.8×10^{-3}	1.7×10^{-3}	8.8×10^{-4}
1100	0.6	0.3	6×10^{-2}	3×10^{-2}
1200	11	5.5	1.1	0.55

Remarks: The oxide is dissolved in the molten carbonate, and since the values of the equilibrium pressures depend on the composition of the solution, the dissociation pressures do not have unique values unless the values of n are specified.

Vaporization of molten carbonates

Measurement method: critical analyses [31]

The various "vaporization" data, based on electrolyte losses from high temperature molten carbonate fuel cells, and the thermodynamics of associated reactions, have been critically examined by Maru et al., (1976). For a summary of the data status, refer: Li_2CO_3, present work.

References [22,31,39-43].

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calc'd; from ΔH_f° [39]

Table 44.15. Cryoscopic constant

Mol % Na_2CO_3	k_f (K mol^{-1} kg^{-1})	Uncertainty
56	49.1	~ ± 2%

References [38,39].

16. References

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XLV. Sodium Nitrate-Potassium Nitrate: $NaNO_3$-KNO_3

1. *Melting Temperatures (T_m)*

Pure substance melting points:

$NaNO_3$: 307°C

KNO_3: 337°C

Minimum melting mixture:

222°C, composition: 54 mol % KNO_3

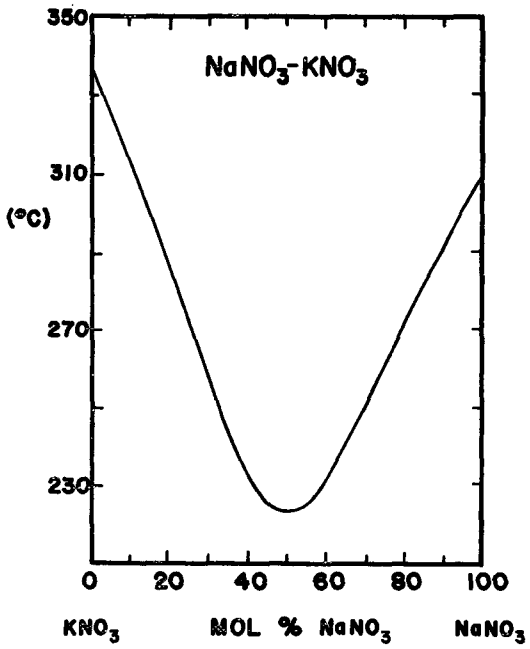

Figure 45.1. $NaNO_3$-KNO_3 phase diagram

References [1-4].

2. *Density (ρ)*

Measurement method: Archimedean technique [5]

Two-independent-variable equation

$$\rho = a + bT^2 + cCT^2 \quad (C = \text{mol \% } KNO_3) \quad (45.1)$$

precision: in table 45.1 uncertainty: ∿ ± 0.5%

Table 45.1. Coefficients of two-independent-variable equation (45.1)

Table 45.2. Densities (g cm^{-3}) from two-independent-variable equation (45.1)

	Mol % $NaNO_3$											
T(K)	100	90	80	70	60	50	40	30	20	10	0	46
625	1.878	1.876	1.874	1.872	1.870	1.867	1.865	1.863	1.861	1.859	1.856	1.866
630	1.875	1.873	1.871	1.869	1.866	1.864	1.862	1.860	1.857	1.855	1.853	1.863
635	1.872	1.870	1.868	1.865	1.863	1.861	1.859	1.856	1.854	1.852	1.850	1.860
640	1.869	1.867	1.865	1.862	1.860	1.858	1.855	1.853	1.851	1.849	1.846	1.857
645	1.866	1.864	1.862	1.859	1.857	1.855	1.852	1.850	1.548	1.845	1.843	1.854
650	1.863	1.861	1.858	1.856	1.854	1.851	1.849	1.847	1.844	1.842	1.839	1.850
655	1.860	1.858	1.855	1.853	1.850	1.848	1.846	1.843	1.841	1.838	1.836	1.847
660	1.857	1.854	1.852	1.850	1.847	1.845	1.842	1.840	1.837	1.835	1.832	1.844
665	1.854	1.851	1.849	1.846	1.844	1.841	1.839	1.836	1.834	1.831	1.829	1.840
670	1.851	1.848	1.845	1.843	1.840	1.838	1.835	1.833	1.830	1.828	1.825	1.837
675	1.847	1.845	1.842	1.840	1.837	1.835	1.832	1.829	1.827	1.824	1.822	1.834
680	1.844	1.842	1.839	1.836	1.834	1.831	1.829	1.826	1.823	1.821	1.818	1.830
685	1.841	1.838	1.836	1.833	1.830	1.828	1.825	1.822	1.820	1.817	1.815	1.827
690	1.838	1.835	1.832	1.830	1.827	1.824	1.822	1.819	1.816	1.814	1.811	1.823
695	1.834	1.832	1.829	1.826	1.823	1.821	1.818	1.815	1.813	1.810	1.807	1.820
700	1.831	1.828	1.825	1.823	1.820	1.817	1.814	1.812	1.809	1.806	1.803	1.816
705	1.828	1.825	1.822	1.819	1.816	1.814	1.811	1.808	1.805	1.803	1.800	1.813
710	1.824	1.821	1.819	1.816	1.813	1.810	1.807	1.804	1.802	1.799	1.796	1.809
715	1.821	1.818	1.815	1.812	1.809	1.807	1.804	1.801	1.798	1.795	1.792	1.805
720	1.817	1.815	1.812	1.809	1.806	1.803	1.800	1.797	1.794	1.791	1.788	1.802

References [5-17].

3. *Surface Tension (γ)*

Measurement method: plate detachment [18]

Two-independent-variable equation

$$\gamma = a + bT + cCT^2 + dTC^2 \quad (C = \text{mol \% } KNO_3) \quad (45.2)$$

precision: in table 45.3 uncertainty: ∿ ±1%

Table 45.3. Coefficients of two-independent-variable equation (45.2)

a	b x 10^2	c x 10^7	d x 10^7	Precision
155.67822	-6.27403	-2.31449	5.98777	± 0.1%

Table 45.4. Surface tension (dyn cm^{-1}) from two-independent-variable equation (45.2)

	Mol % $NaNO_3$											
T(K)	100	90	80	70	60	50	40	30	20	10	0	46
500						122.2						122.1
510					121.8	121.4	121.2					121.3
520					121.0	120.7	120.4					120.6
530					120.3	120.0	119.7	119.4				119.8
540				120.1	119.6	119.2	118.9	118.7				119.1
550				119.4	118.9	118.5	118.2	117.9	117.7			118.4
560			119.2	118.7	118.2	117.8	117.4	117.1	116.9			117.6
570			118.5	118.0	117.5	117.0	116.6	116.3	116.1	115.9		116.9
580			117.9	117.3	116.7	116.3	115.9	115.5	115.3	115.1		116.1
590		117.9	117.2	116.6	116.0	115.5	115.1	114.8	114.5	114.3	114.1	115.3
600		117.2	116.5	115.9	115.3	114.8	114.3	114.0	113.7	113.4	113.3	114.6
610		116.6	115.8	115.2	114.5	114.0	113.6	113.2	112.9	112.6	112.4	113.8
620	116.8	115.9	115.1	114.4	113.8	113.3	112.8	112.4	112.0	111.8	111.6	113.1
630	116.2	115.3	114.5	113.7	113.1	112.5	112.0	111.6	111.2	110.9	110.7	112.3
640	115.5	114.6	113.8	113.0	112.3	111.7	111.2	110.8	110.4	110.1	109.9	111.5
650	114.9	114.0	113.1	112.3	111.6	111.0	110.4	110.0	109.6	109.2	109.0	110.8
660	114.3	113.3	112.4	111.6	110.9	110.2	109.6	109.1	108.7	108.4	108.1	110.0
670	113.6	112.6	111.7	110.9	110.1	109.5	108.9	108.3	107.9	107.5	107.3	109.2

References [2,18-22].

4. Viscosity (η)

Measurement method: oscillating sphere [12]

$$\eta = a + bT + cT^2 + dT^3 \quad (45.3)$$

precision: in table 45.5 uncertainty: $\sim \pm$ 10%

Table 45.5. Coefficients of equation (45.3), and precisions

Mol % $NaNO_3$	a	-b x 10^2	c x 10^5	d x 10^8	Precision
50	90.8112	35.1716	46.64877	-20.8610	± 2.2%
75	25.6156	6.2877	4.08206	0	± 0.47%
100	14.2464	1.1549	-3.46657	3.6440	± 0.33%

$$\eta = A \exp(E/RT) \quad (45.4)$$

precision: in table 45.6 uncertainty: $\sim \pm$ 3%

Table 45.6. Coefficients of equation (45.4), and precisions

Mol % $NaNO_3$	A x 10^2	E (cal mol^{-1})	Precision
0	7.127	4506	±0.35%
25	8.710	4141	±0.51%

Table 45.7. Viscosity (cp) from equations in tables 45.5 and 45.6

T (K)	Mol % $NaNO_3$				
	100	75	50	25	0
520			4.725		
530			4.381		
540			4.064		
550			3.772		
560			3.506		
570		3.038	3.262	3.372	
580		2.879	3.040	3.165	
590		2.728	3.839	2.978	
600	2.708	2.585	2.657	2.808	
610	2.574	2.450	2.494	2.653	
620	2.445	2.323	2.348	2.511	2.763
630	2.323	2.205	2.217	2.380	2.608
640	2.208	2.094	2.100	2.260	2.465
650	2.101	1.992	1.997	2.150	2.334
660	2.000	1.899	1.906	2.048	2.214
670	1.907	1.812	1.826	1.954	2.102
680	1.822	1.735	1.755	1.867	2.001
690	1.744	1.665	1.692	1.786	1.906
700	1.675	1.604	1.636	1.710	1.819
710	1.614	1.551	1.585	1.640	1.738
720	1.562	1.506	1.540	1.574	1.662

References [2,6,12,16,23-29].

5. *Electrical Conductance (κ)*

Measurement method: ac technique [30]

$$\kappa = a + bT + cT^2 \quad (45.5)$$

precision: in table 45.8 uncertainty: ∿ ± 0.5%

Table 45.8. Parameters of equation (45.5), and precisions

Mol % $NaNO_3$	-a	b x 10^2	-c x 10^5	Precision
0	2.4566	0.67289	0.27583	±0.1%
24.85	2.0386	0.56214	0.18254	±0.08%
50.31	2.4156	0.68424	0.25391	±0.23%
75.09	3.0522	0.89412	0.39159	±0.20%
100	2.9565	0.88732	0.35949	±0.15%

Table 45.9. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 45.8

	Mol % $NaNO_3$				
T(K)	100	75.09	50.31	24.85	0
560			0.620	0.537	
570			0.660	0.573	
580		0.816	0.699	0.608	
590		0.860	0.738	0.643	
600		0.903	0.776	0.677	
610	1.118	0.945	0.813	0.711	
620	1.163	0.986	0.851	0.745	
630	1.207	1.027	0.887	0.778	0.688
640	1.250	1.066	0.924	0.811	0.720
650	1.292	1.105	0.959	0.844	0.752
660	1.334	1.143	0.994	0.876	0.783
670	1.375	1.181	1.029	0.908	0.814
680	1.415		1.063	0.940	0.844
690	1.454		1.097	0.971	0.873
700	1.493				
710	1.531				
720	1.569				

References [2,5,7,8,10,16,30-42].

6. Safety and Hazards

A. Hazard rating [43-45]

(i) Toxicity: $NaNO_3$, low; KNO_3, low; (permitted as food additive)

(ii) Vapor pressure: eutectic (m.pt. 222°C) melts without decomposition; the melt is stable in air to approx. 500°C; at higher temperatures, nitrates dissociate:

$$MNO_3 \rightleftarrows MNO_2 + \tfrac{1}{2}O_2 \qquad (45.6)$$

The nitrite and nitrate undoubtedly co-exist in quasi-equilibrium in a temperature range comparable to the single components (i.e., to ∿ 800°C), but the binary mixture (above) has not been investigated.

B. Disaster hazards [43,46-48]

(i) Molten salt bath "explosions": violent generation of steam due to bulk water "carry-over" and/or equipment failure; sudden explosive expansion of "trapped" air.

(ii) On decomposition, nitrates emit toxic fumes (oxides of nitrogen) viz:

$$MNO_3 \longrightarrow MNO_2 + \tfrac{1}{2}O_2 \quad (45.7.1)$$

$$2MNO_2 \longrightarrow M_2O + NO + NO_2 \quad (45.7.2)$$

The subsequent decomposition reactions are complex; if the gas phase is continuously removed, the nitrite decomposition (above) to NO and NO_2 is dominant. If the gas phase is not immediately removed, the NO may re-oxidize the nitrite to nitrate.

(iii) Nitrates are powerful oxidizing agents; violent (explosive) reactions possible in molten nitrates and carbonaceous materials (organic compds; oils; carbon;...); aluminum alloys and bath sludges (e.g., iron oxides); magnesium alloys. Dangerous.

References [43-48].

7. Corrosion

Table 45.10. Corrosion studies from primary research literature

Studies	References
Cu, Cd, Pb, Ni, Zn	49
Cr-Mo alloys, cast iron	50
Pt, Au, Ag, Ni, Cu, Hg, W	51
Metals	52
Fe, low carbon steels	53
Various steels and Ti alloys	54
Hydrogen, H_2O behavior	55
Electrochem. approach	56,57
Thermodynamic redox diagrams	58,59
Reviews: corrosion, molten salts	60-62
Annotated corrosion biblio.	63

References [49-63].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in $NaNO_3$-KNO_3 as solvent

Na^+, K^+, Li^+, Tl^+, Pb^{2+}, Ag^+, Cd^{2+}, Hg_2^{2+}, Hg^{2+}, Ce^{3+}, Pr^{3+}, Nd^{3+}, O_2^-, O_2^{2-}, O^{2-}, OH^-, CO_3^{2-}, $C_2O_4^{2-}$, NO_2^-, Cl^-, Br^-, I^-, H_2, O_2, CO_2, H_2O

The italicized species indicate studies with insufficient data-sets for temperature dependence characterization of diffusion coefficients. For numerical values: see table 45.11.5.

precision: in table 45.11.2 uncertainty: in table 45.11.1

For diffusion techniques, uncertainties, and species: see table 45.11.1

Equation $D = A \exp[-E/RT]$ (45.8)

Table 45.11.1. Diffusion techniques, uncertainties, and species

Diffusion techniques of recommended study	Uncertainty (in values of D)	Species
capillary	∿±15%	Li^+, Na^+, K^+
chronopotentiometry	∿±10%	Ag^+, Cd^{2+}, O^{2-}, $C_2O_4^{2-}$
linear sweep voltammetry	∿±20%	Tl^+, Pb^{2+}, Ag^+, Cd^{2+}, Cl^-, Br^-, OH^-
voltammetry (cyclic)	∿±20%	Hg^{2+}
pulse polarography	∿±20%	Cl^-, Br^-, I^-
rotating disc electrode	∿±20%	I^-, CO_3^{2-}, CO_2, O_2^-, O_2^{2-}, H_2, O_2, H_2O, Hg_2^{2+}
paper electrophoresis	∿±15%	Na^+, K^+

For numerical values: see tables 45.11.2 - 45.11.5

Table 45.11.2. Parameters of diffusion equation (45.8), precisions, recommended study

Species	A x 10^3 (cm^2 sec^{-1})	E (cal mol^{-1})	Temp. range (K)	Precision	Recommended study
	(a) $NaNO_3$-KNO_3 eutectic				
Na^+	0.533	4013	550-720	±3.7%	73
K^+	1.352	5380	550-720	±4.8%	73
OH^-	12.935	8581	510-620	±0.8%	77,79
	(b) $NaNO_3$-KNO_3 (30.3 mol % $NaNO_3$)				
Na^+	1.323	5220	590-670	±0.2%	75
K^+	1.357	5468	590-670	±0.1%	75
	(c) $NaNO_3$-KNO_3 (51.7 mol % $NaNO_3$)				
Na^+	1.404	5228	590-670	±0.13%	75
K^+	1.438	5462	590-670	±0.35%	75
	(d) $NaNO_3$-KNO_3 (79.7 mol % $NaNO_3$)				
Na^+	1.180	4958	590-670	±0.65%	75
K^+	1.425	5401	590-670	±0.25%	75

Table 45.11.3. Self-diffusion coefficients, D x 10^5 (cm^2sec^{-1})

T (K)	Eutectic Melt		30.3 mol % $NaNO_3$		56.7 mol % $NaNO_3$		79.7 mol % $NaNO_3$	
	Na^+	K^+	Na^+	K^+	Na^+	K^+	Na^+	K^+
550	1.36	0.984						
570	1.54	1.17						
590	1.74	1.37	1.54	1.28	1.62	1.36	1.72	1.42
610	1.95	1.60	1.78	1.49	1.88	1.59	1.97	1.65
630	2.16	1.84	2.04	1.72	2.16	1.83	2.25	1.91
650	2.38	2.10	2.32	1.97	2.45	2.10	2.54	2.18
670	2.62	2.38	2.62	2.23	2.77	2.38	2.85	2.47
690	2.86	2.67						
710	3.10	2.98						
720	3.23	3.15						

Table 45.11.4. Diffusion coefficients in the eutectic melt

T (K)	$D_{OH^-} \times 10^5$ ($cm^2\ sec^{-1}$)	T (K)	$D_{OH^-} \times 10^5$ ($cm^2\ sec^{-1}$)
510	0.272	570	0.663
520	0.320	580	0.755
530	0.374	590	0.857
540	0.435	600	0.968
550	0.503	610	1.09
560	0.579	620	1.22

Table 45.11.5. Diffusion coefficients for species not included in tables 45.11.2 to 45.11.4

Species	Melt composition (mol % $NaNO_3$)	T (K)	$D \times 10^5$ ($cm^2\ sec^{-1}$)	Recommended study
Li^+	51.7	522 619 675	1.1 2.2 3.2	67
$\underline{Tl^+}$	eutectic	525	1.07	90
$\underline{Pb^{2+}}$	eutectic	518	0.40	66,83,90
Ag^+	eutectic	523 536 553 570 590	0.40 0.73 1.10 1.30 1.59	64,66,70,72 82,83
Ag^+	20	588 613 633	1.65 1.94 2.14	74
Ag^+	40	588 613 633	1.76 2.11 2.26	74
Ag^+	45	573	1.68	80
Ag^+	60	588 613 633	1.83 2.14 2.32	74
Ag^+	80	588 613 633	1.94 2.25 2.47	74
$\underline{Cd^{2+}}$	eutectic	523	0.47	66,71,83,90
Cd^{2+}	40	523	2.34[a]	76
Cd^{2+}	45	529 598	0.30 0.80	80
Hg_2^{2+}	eutectic	523	0.14	69

Table 45.11.5. Diffusion coefficients for species not included in tables 45.11.2 to 45.11.4--Continued

Species	Melt composition (mol % $NaNO_3$)	T (K)	D x 10^5 (cm^2 sec^{-1})	Recommended study
Hg^{2+}	eutectic	523	0.13	69
Ce^{3+}	40	523	19.5[a]	76,81
Pr^{3+}	40	523	0.5	76
Nd^{3+}	40	523	14.0[a]	81
$\underline{Cl^-}$	eutectic	518	0.69	84,90,91
$\underline{Br^-}$	eutectic	518	0.70	84,90,91
$\underline{I^-}$	eutectic	518	0.68	78,84
O_2^-	eutectic	502	0.48	86
O_2^{2-}	eutectic	502	0.31	86
O^{2-}	eutectic	523	2.24	88
$\underline{CO_3^{2-}}$	eutectic	510	0.31	87
$C_2O_4^{2-}$	eutectic	523	1.03	88
NO_2^-	eutectic	523	2.75	88
H_2	eutectic	571 513	5.20 7.80	89 92
O_2	eutectic	550	31.0	68
$\underline{CO_2}$	eutectic	510	1.9	87
H_2O	eutectic	503	1.9	85

[a] Values are improbable, possibly by a factor of 20.
For the underlined species the temperature dependence of D reported in graphical form; see [90, 91, 78, 87].

References:

Na^+, 73, 75; K^+, 73, 75; Li^+, 67; Tl^+, 90; Pb^{2+}, 66, 83, 90; Ag^+, 64, 66, 70, 72, 82, 83; Cd^{2+}, 66, 71, 76, 80, 83, 90; Hg_2^{2+}, 69; Hg^{2+}, 69; Ce^{3+}, 76, 81; Pr^{3+}, 76, 83; Nd^{3+}, 81; O_2^-, 86; O_2^{2-}, 86; O^{2-}, 88; OH^-, 77, 79, 82; CO_3^{2-}, 87; $C_2O_4^{2-}$, 88; NO_2^-, 88; Cl^-, 84, 90, 91; Br^-, 84, 90, 91; I^-, 78, 84, 90, 91; H_2, 89; O_2, 92; CO_2, 87; H_2O, 85.

9. Heat of Fusion (ΔH_f°)

Measurement method: differential calorimetry [93]

precision: not estimated uncertainty: ∿ ± 2%

Table 45.12. Heats of fusion

Composition (mol % KNO_3)	ΔH_f° (kcal mol^{-1})	T_m (°C)
0	3.600	310
25	3.382	275
40	3.290	243
50	3.195	227
60	3.100	230
75	2.802	260
87	2.685	300
100	2.300	337

T_m is defined as the temperature at which disappearance of last traces of solid would be noted during fusion; interpolated from phase diagram.

The value for KNO_3 (100%) appears low relative to the recommended value (see KNO_3). The value for $NaNO_3$ (100%) is in close accord with recommended value (see $NaNO_3$).

References [93].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [94]

$$C_p = 53.44 - 2.638 \times 10^{-2} T \quad (45.9)$$

precision: ∿ ± 0.5% uncertainty ∿ ± 3%

Table 45.13. Heat capacity from equation (45.9) for minimum melting mixture

T (K)	C_p (cal $K^{-1} mol^{-1}$)	T (K)	C_p (cal $K^{-1} mol^{-1}$)
510	39.99	650	36.29
520	39.72	660	36.03
530	39.46	670	35.77
540	39.19	680	35.50
550	38.93	690	35.24
560	38.67	700	34.97
570	38.40	710	34.71
580	38.14	720	34.45
590	37.88	730	34.18
600	37.61	740	33.92
610	37.35	750	33.66
620	37.08	760	33.39
630	36.82	770	33.13
640	36.56		

References [94].

11. Volume Change on Melting (ΔV_f)

Measurement method: capillary technique [95]

Table 45.14. Volume change on melting

$(\Delta V_f/V_s)$	Uncertainty
4.6%	∿ ± 12%

References [95,96].

12. Vapor Pressure (p_{vap})

No vaporization studies. For observations on thermal decomposition processes in molten nitrates (to nitrites, oxides, with formation of gaseous oxides of nitrogen, oxygen): see $NaNO_3$ and KNO_3.

13. Thermal Conductivity (liquid) (λ_ℓ)

Measurement method: concentric cylinder [99]

$$\lambda = a + bT \quad (45.10)$$

precision: not estimated uncertainty: ∿ ± 20%

Results were reported as equations only.

Table 45.15. Parameters of equation (45.10), and temp. range

Mol % KNO_3	a x 10^4	b x 10^7	Temp. range (K)
25	10.490	3.70	604 - 730
50	9.318	4.60	612 - 727
75	7.0298	7.40	624 - 727

Table 45.16. Thermal conductivity from equations in table 45.15

T (K)	25 mol % KNO_3	50 mol % KNO_3	75 mol % KNO_3
610	12.75	12.12	
620	12.78	12.17	
630	12.82	12.22	11.69
640	12.86	12.26	11.77
650	12.90	12.31	11.84
660	12.93	12.35	11.91
670	12.97	12.40	11.99
680	13.01	12.45	12.06
690	13.04	12.49	12.14
700	13.08	12.54	12.21
710	13.12	12.58	12.28
720	13.15	12.63	12.36
730	13.19	12.68	12.43

References [97-100].

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

16. References

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XLVI. Lithium Nitrate-Sodium Nitrate-Potassium Nitrate: $LiNO_3$-$NaNO_3$-KNO_3

1. *Melting Temperatures (T_m)*

Pure substance melting points:

$LiNO_3$: 253°C

$NaNO_3$: 307°C

KNO_3: 337°C

Eutectic melting point:

120°C, composition: 37.5 mol % $LiNO_3$, 18 mol % $NaNO_3$, 44.5 mol % KNO_3

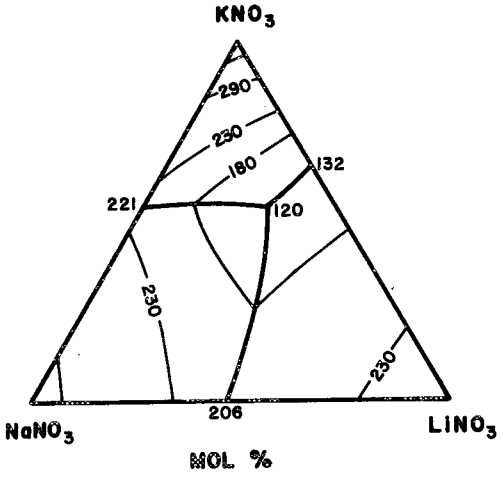

Figure 46.1. $LiNO_3$-$NaNO_3$-KNO_3 phase diagram

References [1-4].

2. *Density (ρ)*

No data.

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: dc technique [5]

$$\kappa = 1.40865 - 1.19760 \times 10^{-2}T + 2.84423 \times 10^{-5}T^2 - 1.69292 \times 10^{-8}T^3 \quad (46.1)$$

precision: $\sim \pm 0.35\%$ uncertainty: $\sim \pm 2\%$

Table 46.1. Specific conductance from equation (46.1) for eutectic composition

T (K)	κ ($ohm^{-1}cm^{-1}$)	T (K)	κ ($ohm^{-1}cm^{-1}$)
410	0.1129	540	0.5696
420	0.1417	550	0.6090
430	0.1720	560	0.6485
440	0.2035	570	0.6881
450	0.2363	580	0.7275
460	0.2703	590	0.7667
470	0.3052	600	0.8056
480	0.3410	610	0.8441
490	0.3777	620	0.8820
500	0.4151	630	0.9194
510	0.4531	640	0.9561
520	0.4915	650	0.9919
530	0.5304		

References [5].

6. Safety and Hazards

A. Hazard rating [6-8]

(i) Toxicity: $LiNO_3$, moderate; $NaNO_3$, low; KNO_3, low

(ii) Vapor pressure: eutectic (m.pt. 120°C): no data on thermal stability; the nitrates decompose thermally to form the corresponding nitrites and oxygen:

$$MNO_3 \rightleftarrows MNO_2 + \tfrac{1}{2}O_2 \qquad (46.2)$$

$LiNO_3$ is the least stable, and decomposes just above its m.pt. (253°C) to $LiNO_2$. If the container material is not inert; oxides of nitrogen are evolved.

B. Disaster hazards [6-9]

(i) Molten salt bath "explosions": i.e. explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) On decomposition, nitrates emit toxic fumes (oxides of nitrogen) viz:

$$MNO_3 \longrightarrow MNO_2 + \tfrac{1}{2}O_2 \qquad (46.3.1)$$
$$2MNO_2 \longrightarrow M_2O + NO + NO_2 \qquad (46.3.2)$$

The subsequent decomposition reactions are complex; if the gas phase is continuously removed, the nitrite decomposition (above) to NO and NO_2 is dominant. If the gas phase is not immediately removed, the NO may re-oxidize the nitrite to nitrate.

(iii) Nitrates are powerful oxidizing agents; violent (explosive) reactions possible in molten nitrates and carbonaceous materials (organic compds.; oils; carbon;...) aluminum alloys and bath sludges (e.g., iron oxides); magnesium alloys. Dangerous.

References [6-11].

7. Corrosion

No corrosion studies reported; for guidelines, see each component as single-salt melts and binary combinations.

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in $LiNO_3$-$NaNO_3$-KNO_3 as solvent

Tl^+, Pb^{2+}, Zn^{2+}, Cd^{2+}, Co^{2+}, Ni^{2+}, Eu^{3+}, Cl_2, Br_2, I_2, NO_2

The italicized species indicate studies with data-sets inadequate for temperature-dependence characterization of diffusion coefficients.

precision: not estimated uncertainty: in table 46.2.1

Table 46.2.1. Diffusion techniques, uncertainties and species

Diffusion techniques of recommended study	Uncertainty (in values of D)	Species
polarography	∿± 20%	Pb^{2+}, Zn^{2+}, Cd^{2+}, Co^{2+}, Ni^{2+}
oscillographic polarography	∿± 20%	Tl^+, Pb^{2+}, Zn^{2+}, Cd^{2+}, Ni^{2+}, Eu^{3+}
rotating disc electrode	∿± 20%	Tl^+, Cl_2, Br_2, I_2, NO_2

For numerical values: see table 46.2.2

Table 46.2.2. Diffusion coefficients

Species	T (K)	D x 10^5 (cm^2 sec^{-1})	Recommended study
$\underline{Tl^+}$	423	8.4[a]	15,16
$\underline{Pb^{2+}}$	423	0.087	16,18
$\underline{Zn^{2+}}$	433	0.15	13,16
$\underline{Cd^{2+}}$	422	0.10	14,16
Co^{2+}	421	0.08	14
$\underline{Ni^{2+}}$	416	0.035	14,16
$\underline{Eu^{3+}}$	433	0.044	19
Cl_2	423	5.8	17
Br_2	423	5.1	17
I_2	423	4.2	15,17
NO_2	423	7.0	15

[a]Value appears improbably high.

For the underlined species, the temperature dependence of D reported in graphical form; see [16,19].

References

Tl^+, 15, 16, 20; Pb^{2+}, 13, 14, 16, 18, 20; Zn^{2+}, 13, 16, 20; Cd^{2+}, 13, 14, 16, 20; Co^{2+}, 14; Ni^{2+}, 13, 14, 16, 20; Eu^{3+}, 19, 20; Cl_2, 17; Br_2, 17; I_2, 15, 17; NO_2, 15

9. *Heat of Fusion (ΔH_f°)*

No data.

10. *Heat Capacity (C_p)*

No data.

11. *Volume Change on Melting (ΔV_f)*

No data; but see $LiNO_3$, $NaNO_3$, KNO_3, and $NaNO_3$-KNO_3 for guidelines

12. *Vapor Pressure (p_{vap})*

No vaporization studies reported. For thermal decomposition processes in molten nitrates (to nitrites, oxides, with formation of gaseous oxides and oxides of nitrogen) see $LiNO_3$, $NaNO_3$, and KNO_3.

13. *Thermal Conductivity (liquid) (λ_ℓ)*

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

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XLVII. Lithium Sulfate-Potassium Sulfate: Li_2SO_4-K_2SO_4

1. Melting Temperatures (T_m)

Pure substance melting points:

Li_2SO_4: 859°C

K_2SO_4: 1069°C

Eutectic melting points:

Eutectic 1: 535°C, composition: 80 mol % Li_2SO_4

Eutectic 2: 700-712°C, composition: 39.5 mol % Li_2SO_4

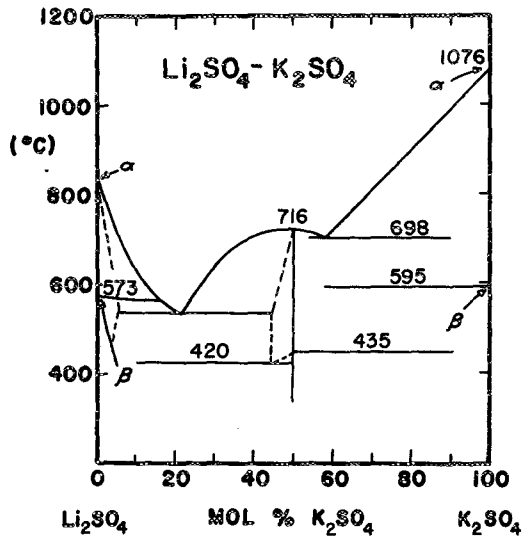

Figure 47.1. Li_2SO_4-K_2SO_4 phase diagram

References [1-3].

2. Density (ρ)

Measurement method: Archimedean technique [4,5]

$$\rho = a - bT \quad (47.1)$$

precision: ∿ ± 0.1% uncertainty: ∿ ± 1%

Table 47.1. Coefficients of equation (47.1)

Mixture	Mol % Li_2SO_4	a	b x 10^4
A	80	2.455	4.07
B	50	2.469	4.337

Table 47.2.1. Densities for mixture A from equation in table 47.1

T(K)	ρ(g cm^{-3})	T(K)	ρ(g cm^{-3})
860	2.1050	950	2.0683
870	2.1009	960	2.0643
880	2.0968	970	2.0602
890	2.0928	980	2.0561
900	2.0887	990	2.0521
910	2.0846	1000	2.0480
920	2.0806	1010	2.0439
930	2.0765	1020	2.0399
940	2.0724		

Table 47.2.2. Densities for mixture B from equations in table 47.1

T(K)	ρ(g cm^{-3})	T(K)	ρ(g cm^{-3})
1070	2.004	1170	1.962
1080	2.001	1180	1.957
1090	1.996	1190	1.953
1100	1.992	1200	1.949
1110	1.988	1210	1.944
1120	1.983	1220	1.940
1130	1.979	1230	1.936
1140	1.975	1240	1.931
1150	1.970	1250	1.927
1160	1.966	1260	1.923

References [4,5].

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

Measurement method: ac technique [6]

$$\kappa = a + bT + cT^2 + dT^3 \quad (47.2)$$

precision: in table 47.3 uncertainty: $\sim \pm 2.5\%$

Table 47.3. Parameters of equation (47.2), and precisions

Mol % K_2SO_4	-a	b x 10^3	c x 10^6	-d x 10^9	Precision
3.00	1.79337	-0.57431	9.45601	4.01944	±0.008%
4.89	3.25757	3.49123	5.45248	2.76495	±0.06%
20.00	3.36276	3.96153	2.76059	1.56802	±0.20%
25.00	14.44603	35.91980	-28.07680	-8.24127	±0.50%
40.00	3.51175	5.55568	-0.81426		±0.15%
60.00	2.99969	4.69725	-0.70820		±0.13%
80.00	1.39083	2.43733			±0.03%
100.00	0.81133	2.01416			±0.10%

Table 47.4. Specific conductance ($ohm^{-1}cm^{-1}$) from equations in table 47.3

	Mol % K_2SO_4							
T(K)	3.00	4.89	20.00	25.00	40.00	60.00	80.00	100
840				0.800				
850				0.861				
860				0.921				
870			1.141	0.980				
880			1.193	1.037				
890			1.244	1.093				
900			1.296	1.147				
910			1.347	1.201				
920			1.397	1.253				
930			1.448	1.305				
940			1.498	1.355				
950			1.548	1.404				
960			1.597	1.453				
970			1.646	1.500				
980			1.695	1.547				
990			1.743	1.593	1.190	0.956		
1000			1.791	1.638	1.230	0.989		
1010			1.839	1.683	1.269	1.022		
1020			1.886	1.727	1.308	1.055		
1030			1.933	1.770	1.347	1.087		
1040			1.979	1.813	1.385	1.119		
1050		3.219	2.025	1.855	1.424	1.152		
1060		3.277	2.071	1.897	1.462	1.184		
1070		3.333	2.116	1.939	1.501	1.215		
1080	3.553	3.390	2.160	1.980	1.539	1.247		
1090	3.610	3.445	2.205	2.021	1.577	1.279		
1100	3.667	3.500	2.248	2.062	1.614	1.310		
1110	3.723	3.554	2.291	2.103	1.652	1.342		
1120	3.778	3.608	2.334	2.143	1.689	1.373		
1130	3.832	3.660	2.376	2.183	1.726	1.404		
1140	3.886	3.712	2.418	2.224	1.763	1.435		
1150	3.939	3.763	2.459	2.264	1.800	1.466		
1160	3.991	3.813	2.500	2.305	1.837	1.496		
1170	4.041	3.863	2.540	2.345	1.874	1.527		
1180		3.911		2.386				
1190				2.427				
1200				2.468				
1210				2.510				
1220							1.583	
1230							1.607	
1240								1.888
1250								1.908
1260								1.928

References [6].

6. Safety and Hazards

A. Hazard rating [7-9]

(i) Toxicity: Li_2SO_4, unknown; "toxic" qualities of Li salts; K_2SO_4, severe

(ii) Vapor pressure: eutectics melt to form stable liquids. Note: Li_2SO_4 decomposes at ∿ 860°C, evolving aggressive and toxic fumes (oxides of sulfur).

B. Disaster hazards [7,10-12]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure, i.e., explosive expansion of "trapped" air.

(ii) When heated to decomposition, sulfates decompose, evolving SO_3, which in turn dissociates to SO_2 and O_2 (see above); toxic, corrosive fumes.

References [7-12].

7. Corrosion

Table 47.5. Corrosion studies from primary research literature

Studies	References
Fe, Ni	13
Ferrite steels	
Fe-Mo,	
Fe-Cr-Mo,	14
Fe-Cr	
Fe	15
Cu,Pd,Rh,Ag	16
Emf. series	16,17
Thermodynamic redox diagrams	13-15
Electrochem. approach	18,19
Reviews: molten salts corrosion	17,20,21
Annotated corrosion biblio.	22

References [13-22].

8. Diffusion

Measurement method: cited in tabulations

List of diffusing species investigated in Li_2SO_4-K_2SO_4 as solvent.

In^{3+}, Pb^{2+}, Bi^{3+}, Cu^{+}, Cu^{2+}, Ag^{+}, Zn^{2+}, Cd^{2+}, Fe^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}

precision: not estimated uncertainty: in table 47.6.1

Table 47.6.1. Diffusion techniques, uncertainties, and species

Diffusion technique of recommended study	Uncertainty	Species
chronopotentiometry	∿ ± 10%	In^{3+}, Pb^{2+}, Bi^{3+}, Cu^{+}, Cu^{2+}, Ag^{+}, Zn^{2+}, Cd^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}

Equations: insufficient data-sets for characterization of temperature dependence of diffusion coefficients.

Table 47.6.2. Diffusion coefficients

Species	Melt composition (mol % Li_2SO_4)	T (K)	D x 10^5 ($cm^2 sec^{-1}$)	Recommended study
In^{3+}	86.38	873	0.05	23
Pb^{2+}	86.38	873	0.79	23
Bi^{3+}	86.38	873	0.16	23
Cu^{+}	86.38	873	1.58	23
	80	898	2.00	24
Cu^{2+}	86.38	873	0.28	23
Ag^{+}	86.38	873	2.07	23
Zn^{2+}	86.38	873	0.42	23
Cd^{2+}	86.38	873	0.46	23
Fe^{2+}	86.38	873	0.39	25
Fe^{3+}	86.38	873	0.145	25
Co^{2+}	86.38	873	0.25	23
Ni^{2+}	86.38	873	0.33	23

References: In^{3+}, 23; Pb^{2+}, 23; Bi^{3+}, 23; Cu^{+}, 23, 24; Cu^{2+}, 23; Ag^{+}, 23, 13; Zn^{2+}, 23; Cd^{2+}, 23; Fe^{2+}, 25; Fe^{3+}, 25; Co^{2+}, 23; Ni^{2+}, 23.

9. Heat of Fusion (ΔH_f^o)

No data.

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

Measurement method: estimated; from densities [26]

Table 47.7. Volume change on melting, and uncertainty

Binary mixtures (mol % Li_2SO_4)	T_m (°C)	$(\Delta V_f/V_s)$	Uncertainty
80	535	∿ - 1.0%	∿±10%
39.5	710	∿ 11.2%	∿±10%

References [26].

12. Vapor Pressure (p_{vap})

No vaporization studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

16. References

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XLVIII. Lithium Sulfate-Sodium Sulfate-Potassium Sulfate: Li_2SO_4-Na_2SO_4-K_2SO_4

1. *Melting Temperatures (T_m)*

Pure substance melting points:

Li_2SO_4: 859°C
Na_2SO_4: 884°C
K_2SO_4: 1069°C

Eutectic melting point:

512°C, composition: 78 mol % Li_2SO_4, 8.5 mol % Na_2SO_4, 13.5 mol % K_2SO_4

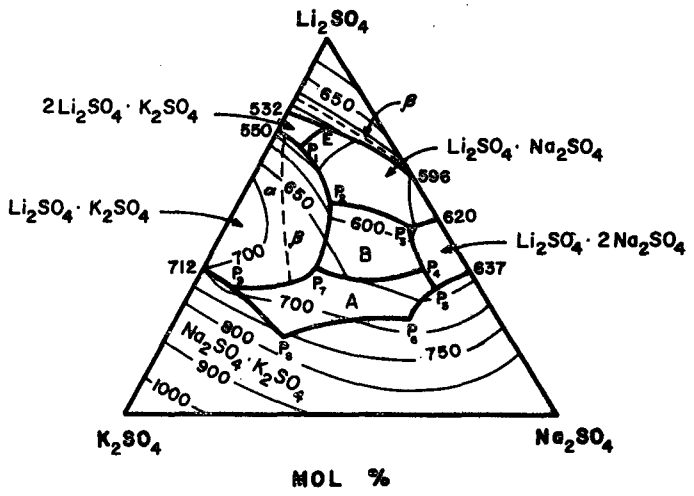

Figure 48.1. Li_2SO_4-Na_2SO_4-K_2SO_4 phase diagram; E, eutectic; P's, peritectics

References [1-3].

2. *Density (ρ)*

No data.

3. *Surface Tension (γ)*

No data.

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

No data.

6. Safety and Hazards

A. Hazard rating [4-6]

(i) Toxicity: Li_2SO_4, unknown: "toxic" qualities of Li cations; Na_2SO_4, unknown: "toxic" qualities of Na cations; K_2SO_4, severe

(ii) Vapor pressure: eutectic (m.pt. 512°C) melts to form a stable liquid.

Note: Li_2SO_4 decomposes at ∿ 860°C, evolving aggressive and toxic fumes (oxides of sulfur).

B. Disaster hazards [4,7-9]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) Sulfates, when heated to decomposition, evolve SO_3, which, in turn, dissociates to SO_2 and O_2; toxic, aggressive fumes

References [4-9].

7. Corrosion

Table 48.1. Corrosion studies from primary research literature

Studies	References
SS(18-8)	10
Nimonic-105 alloy (19 Co, 16 Cr, 4 Al, 4 Ti, 1.5 Mo, balance Ni)	
Emf series	11,12
Thermodynamic redox diagrams	13
Electrochem. approach	14,15
Reviews: molten salts corrosion	12,16,17
Annotated corrosion biblio.	18

References [

8. Diffusion

Measurement method: chronopotentiometry [10]

List of diffusing species investigated in Li_2SO_4-Na_2SO_4-K_2SO_4 as solvent

SO_3

Table 48.2. Diffusion coefficients and uncertainties

Species	D x 10^5 (cm^2 sec^{-1})	Temp. (K)	Uncertainty
SO_3	0.6	873	∿ ± 5%

References [10].

9. Heat of Fusion (ΔH_f°)

No data.

10. Heat Capacity (C_p)

No data.

11. Volume Change on Melting (ΔV_f)

No data; but see LiCl, NaCl, KCl, NaCl-KCl, and nitrates for guidelines.

12. Vapor pressure (p_{vap})

No vaporization studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

No data.

16. References

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XLIX. Sodium Chloride-Lithium Sulfate: NaCl-Li_2SO_4

1. *Melting Temperatures (T_m)*

Pure substance melting points:

NaCl: 800°C
Li_2SO_4: 859°C

Eutectic melting point:

499°C, composition: 26.0 mol % NaCl

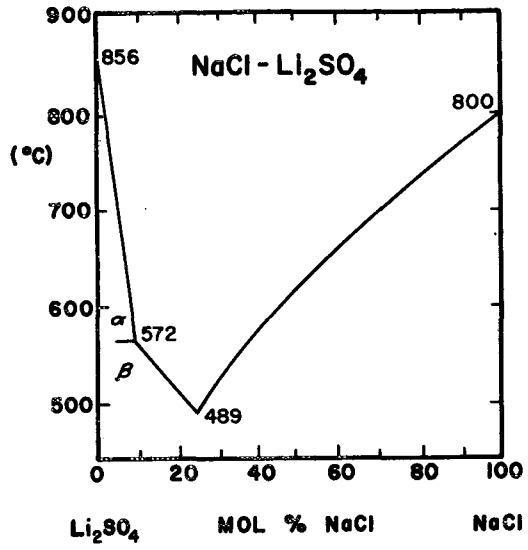

Figure 49.1. NaCl-Li_2SO_4 phase diagram

References [1-3].

2. *Density (ρ)*

No data.

3. *Surface Tension (γ)*

Measurement method: maximum bubble pressure [4]

$$\gamma = a + bT + cT^2 \quad (49.1)$$

precision: in table 49.1 uncertainty: ∿ ± 3%

Table 49.1. Parameters of equation (49.1), and precisions

NaCl (Mol %)	a	b x 10^2	-c x 10^6	Precision
0	-67.289	51.487	227.30	±0.12%
1.0	299.27	-7.20		±0.66%
1.5	289.63	-6.60		±0.13%
2.0	294.32	-7.00		±0.13%
2.5	154.3	14.784	85.55	±0.07%
10.0	85.37	23.002	113.90	±0.50%
30.0	236.64	-5.800		±0.50%
50.0	-41.197	36.204	170.50	±0.32%
75.0	-11.475	28.824	142.30	±0.16%
100.0	-38.168	29.224	142.30	±0.53%

Table 49.2. Surface tension (dyn cm^{-1}) from equations in table 49.1

	Mol % NaCl									
T(K)	0	1.0	1.5	2.0	2.5	10	30	50	75	100
1180	223.8	214.3	211.8	211.7	209.6	198.2	168.2	148.6	130.5	108.5
1190	223.5	213.6	211.1	211.0	209.1	197.8	167.6	148.2	130.0	108.1
1200	223.2	212.9	210.4	210.3	208.5	197.4	167.0	147.7	129.5	107.6
1210	222.9	212.2	209.8	209.6	207.9	196.9	166.5	147.2	129.0	107.1
1220	222.5	211.4	209.1	208.9	207.3	196.5	165.9	146.7	128.4	106.6
1230	222.1	210.7	208.5	208.2	206.7	196.0	165.3	146.2	127.8	106.0
1240	221.7	210.0	207.8	207.5	206.1	195.5	164.7	145.6	127.1	105.4
1250	221.1	209.3	207.1	206.8	205.4	194.9	164.1	144.9	126.5	104.8
1260	220.6	208.6	206.5	206.1	204.8	194.4	163.6	144.3	125.8	104.1
1270	220.0	207.8	205.8	205.4	204.1	193.8	163.0	143.6	125.1	103.5
1280	219.3	207.1	205.2	204.7	203.4	193.2	162.4	142.9	124.3	102.8
1290	218.6	206.4	204.5	204.0	202.6	192.6	161.8	142.1	123.6	102.0
1300	217.9	205.7	203.8	203.3	201.9	191.9	161.2	141.3	122.8	101.3
1310	217.1	205.0	203.2	202.6	201.2	191.2	160.7	140.5	121.9	100.5
1320	216.3	204.2	202.5	201.9	200.4	190.5	160.1	139.6	121.1	99.6
1330	215.4	203.5	201.9	201.2	199.6	189.8	159.5	138.7	120.2	98.8
1340	214.5	202.8	201.2	200.5	198.8	189.1	158.9	137.8	119.3	97.9
1350	213.5	202.1	200.5	199.8	198.0	188.3	158.3	136.8	118.3	97.0
1360	212.5	201.4	199.9	199.1	197.1	187.5	157.8	135.8	117.3	96.1
1370	211.5	200.6	199.2	198.4	196.3	186.7	157.2	134.8	116.3	95.1
1380	210.4	199.9	198.6	197.7	195.4	185.9	156.6	133.7	115.3	94.1

References [4].

4. *Viscosity (η)*

No data.

5. *Electrical Conductance (κ)*

No data.

6. Safety and Hazards

A. Hazard rating [5-7]

(i) Toxicity: Li_2SO_4, unknown: "toxic" qualities of Li cations; NaCl, very low.

(ii) Vapor pressure: eutectic (m.pt. 499°C) melts to form a stable liquid; Note: Li_2SO_4 decomposes at ∿ 860°C, evolving oxides of sulfur (toxic, aggressive fumes).

B. Disaster hazards [5,8-10]

(i) Molten salt bath "explosions": i.e., explosive generation of steam due to bulk water "carry-over" and/or equipment failure; i.e., explosive expansion of "trapped" air.

(ii) When bulk NaCl is heated at high temperatures, vapor is evolved which is particularly irritating to the eyes; when heated to decomposition or contacted with acids, highly toxic chloride fumes are evolved.

(iii) Sulfates, when heated to decomposition, evolve SO_3, which in turn dissociates to SO_2 and O_2; toxic, aggressive fumes.

References [5-10].

7. Corrosion

No corrosion studies; see NaCl and Li_2SO_4 for guidelines.

8. Diffusion

No diffusion studies reported.

9. Heat of Fusion (ΔH_f°)

Measurement method: drop calorimetry [11]

Table 49.3. Heat of fusion

Binary eutectic (mol % Li_2SO_4)	ΔH_f° (kcal mol^{-1})	Uncertainty
58.1	7.48	∿ ± 2%

Reference [11].

10. Heat Capacity (C_p)

Measurement method: drop calorimetry [11]

Table 49.4. Heat capacity

Binary eutectic (mol % Li_2SO_4)	C_p (cal $K^{-1}mol^{-1}$)	Temp. range (K)	Uncertainty
58.1	32.6	763-874	∿ ± 2%

Reference [11].

11. Volume Change on Melting (ΔV_f)

No data; but see LiCl, NaCl, KCl, NaCl-KCl, etc., for guidelines.

12. Vapor Pressure (p_{vap})

No vaporization studies reported.

13. Thermal Conductivity (liquid) (λ_ℓ)

No thermal conductivity studies reported.

14. Thermal Conductivity (solid) (λ_s)

No thermal conductivity studies reported.

15. Cryoscopic Constant (k_f)

Measurement method: calc'd., from ΔH_f° [12]

Table 49.5. Cryoscopic constant

k_f (K $mol^{-1} kg^{-1}$)	Uncertainty
5.6	∿ ± 2%

References [11,12].

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The present work provides selected data with value judgements for a set of 49 salt systems of interest as candidate materials for thermal energy storage sub-systems and for electrochemical energy storage systems. The physical properties assessed are: melting points; phase diagrams; eutectic compositions; density; surface tension; viscosity; electrical conductivity; diffusion constants for ions; heat of fusion; heat capacity; volume change on fusion; vapor pressure; thermal conductivity (liquid and solid); and cryoscopic constant. The status of corrosion studies in the form of annotated bibliographic summaries, and salient observations on safety and hazards are also reported. A summarizing series of tables is provided as index to the data-gaps status for this set of candidate materials.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)*
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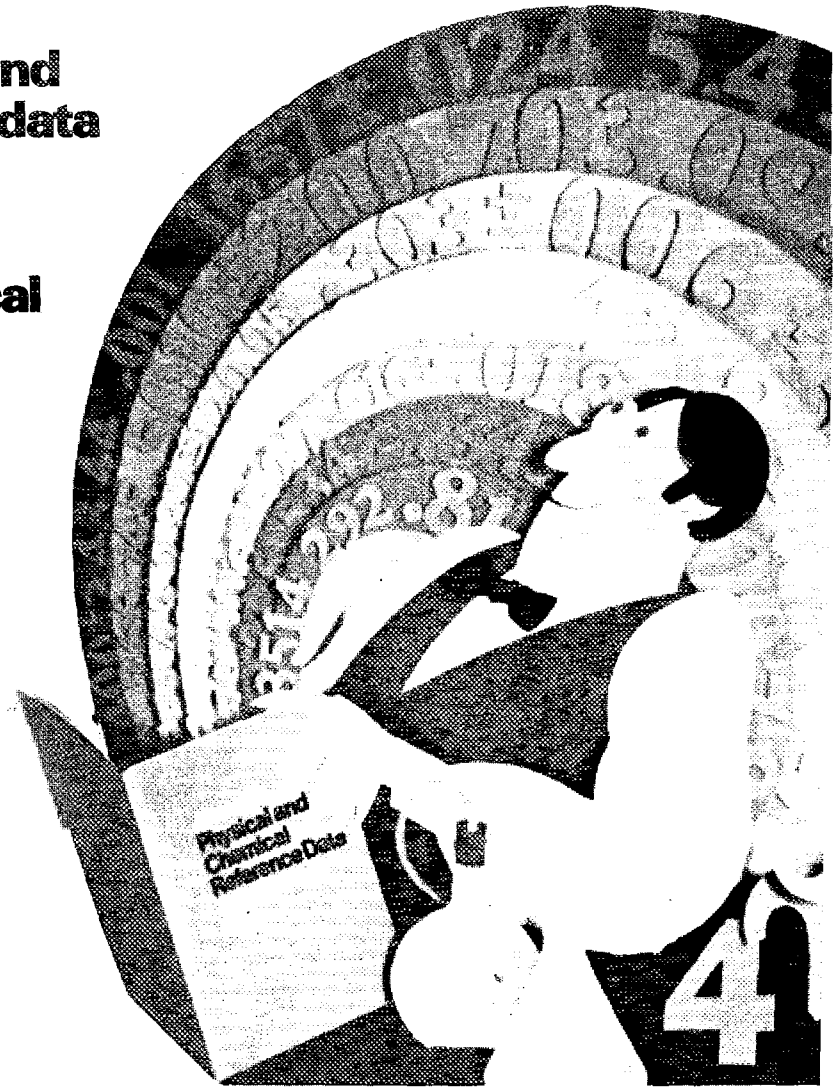

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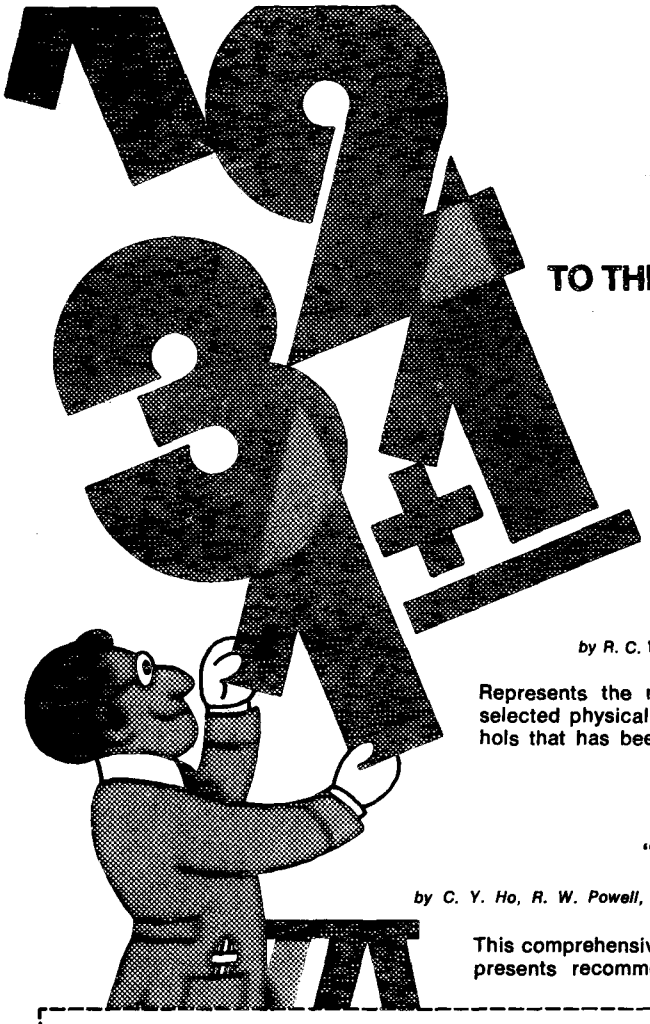

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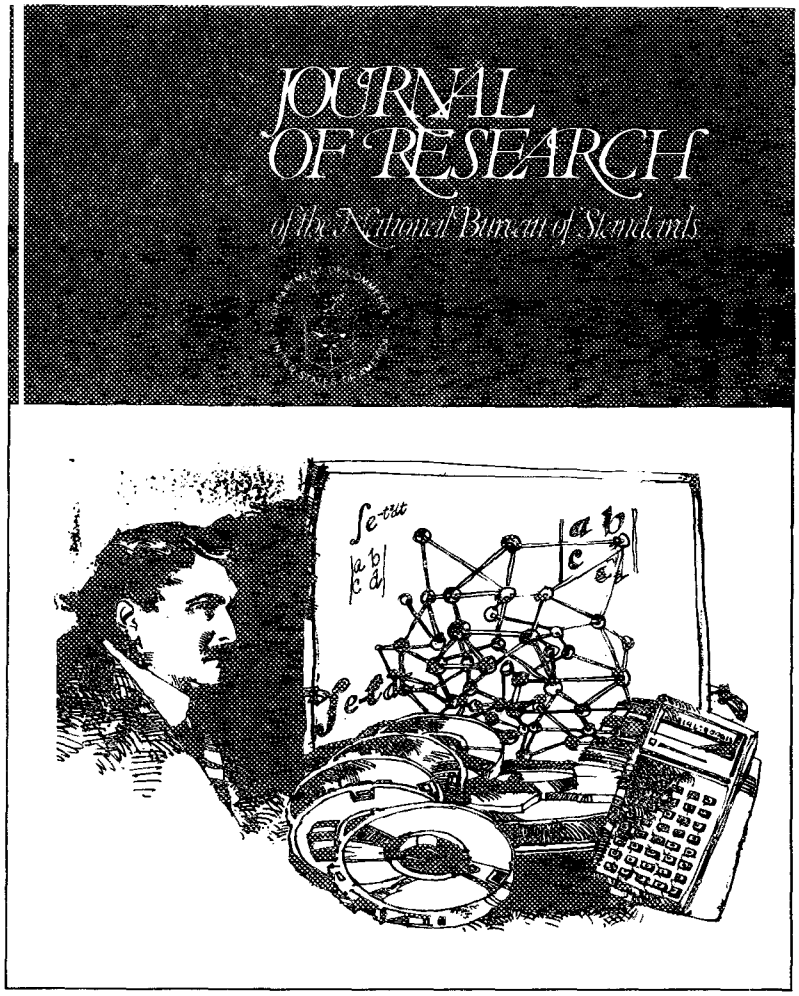

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