

TCS Salt Database (TCSALT3)

Technical Information

Available Starting with Thermo-Calc Version 2026b



Contents

About the TCS Molten Salts Database (TCSALT)	4
<i>Interconnectivity to Other Products</i>	4
<i>Use Case Examples</i>	5
<i>Combining Databases</i>	6
<i>Release History</i>	6
TCS Molten Salts Database (TCSALT) Resources	7
<i>About the CALPHAD Method</i>	7
<i>Learn More</i>	7
TCSALT3 Elements, Systems, and Phases	9
<i>Included Elements</i>	9
<i>Assessed Systems</i>	9
<i>Assessed Phases</i>	10
TCSALT3 Thermophysical Properties and Assessed Systems	12
<i>Molar Volume</i>	12
<i>Surface Tension</i>	12
<i>Viscosity</i>	12
<i>Thermophysical Parameters and Variables</i>	12
<i>Examples</i>	13
<i>Learn More</i>	13
<i>Reference</i>	13
TCSALT3 Systems	14
<i>TCSALT3 Assessed Pseudo-Binary Systems</i>	15
<i>TCSALT3 Assessed Pseudo-Ternary Systems</i>	19
<i>TCSALT3 Assessed Higher Order Systems</i>	22
<i>TCSALT3 Assessed Mixed Systems</i>	23

TCSALT3 Properties Data	26
<i>TCSALT3 Molar Volume for Ionic Liquids: Assessed Systems</i>	27
<i>TCSALT3 Surface Tension for Ionic Liquids: Assessed Systems</i>	30
<i>TCSALT3 Viscosity for Ionic Liquids: Assessed Systems</i>	32
TCSALT3 Phases	34
<i>TCSALT3 Models for the Included Phases</i>	35
TCSALT: TCS Molten Salts Database Revision History	53
<i>TCSALT2 to TCSALT3</i>	53
<i>TCSALT1 to TCSALT2</i>	55

About the TCS Molten Salts Database (TCSALT)

TCS Molten Salts Database (TCSALT) is a thermodynamic and properties database designed to be used for fluorides (F-1) and chlorides (Cl-1) where the ionic two-sublattice liquid model is used for the molten salt. Several oxide (O-2) systems are also modeled and assessed as well as carbonate (CO₃-2), nitrate (NO₃-1), nitrite (NO₂-1), and sulfate (SO₄-2) salts. No metallic liquid is modeled.

The database can be used for a variety of applications, for example, processes involved with recycling aluminium where fluxes are used. The database covers the most common fluxes and you can study the flux ability to dissolve inclusions, like oxides, removal of unwanted elements in the Al-melt and how this varies with flux composition and temperature.

The database can also be used to understand high temperature corrosion where molten salts can destroy the corrosion resistance.



Molar volume, surface tension of the ionic liquids, and viscosity of the ionic liquids are added to the database as of version 2 (TCSALT2).

Molten salts play a crucial role in numerous industrial applications, including nuclear reactors, thermal energy storage, and high-temperature electrochemical processes. Their thermophysical properties, such as viscosity, surface tension, and molar volume, are essential for optimizing performance and ensuring operational safety, as they govern heat transfer, fluid flow, and interfacial behavior in high-temperature environments.

Using the TCS Molten Salts Database (TCSALT), viscosity and surface tension can be directly predicted from the underlying ionic structure description of the melt, offering quantitative insights into species distribution, connectivity, and structural evolution across a wide range of temperatures and compositions. The database also includes molar volume descriptions for both liquid and solid phases, further enhancing its applicability in high-temperature material processing and engineering applications. The integration of these thermophysical properties within a unified computational thermodynamic framework provides a powerful tool for material design and process optimization.

Interconnectivity to Other Products

TCS Molten Salts Database (TCSALT) can be used with Thermo-Calc and all available SDKs. The database does not currently have a corresponding mobility database. It also cannot be used with the Additive Manufacturing (AM) Module.

Use Case Examples

The database can be used for a variety of applications, especially for processes involved with recycling aluminum where fluxes are used. The database covers the most common fluxes and you can study the flux ability to dissolve inclusions, like oxides, removal of unwanted elements in the Al-melt and how this varies with flux composition and temperature.

The database can also be used to understand high temperature corrosion where molten salts can destroy the corrosion resistance. Other applications include electrochemical processing, thermal energy storage, molten salt reactors, and catalysis (e.g., sulfuric acid production).

The database includes a variety of molten salts that can be used in a variety of contexts:

- Molten nitrate (NO₃-1) and nitrite (NO₂-1) salts are commonly used as high-temperature heat transfer fluids and thermal energy storage media.
- The sulfate (SO₄-2) molten salts, such as Na₂SO₄, K₂SO₄ and Mg(SO₄)₂, are high-temperature ionic liquids commonly used in solar energy storage, catalysis (e.g., sulfuric acid production), and as reaction media for synthesizing advanced ceramic or battery materials.
- Molten carbonate salts (containing CO₃-2) are high-temperature electrolytes primarily used for electrochemical capture/conversion into solid carbon, and as heat transfer fluids in concentrated solar power (CSP).

Molten salts used in metallurgical applications are often based on alkali-earth chloride fluoride mixtures. Such molten salts can be used as fluxes for metal treatment. You can also explore applications of molten salt reactions using Zn chloride with this database.

Some use case examples of how the database can be used include the following.

- Calculate the liquidus projection of molten salt
- Examine the interactions of a molten salt mixture such as NaCl-KCl-NaF-KF when used in applications such as electrochemical processing, thermal energy storage, and molten salt reactors.
- Investigate how flux composition influences element reduction
- Investigate the influence of oxyfluoride melts in geophysics or in the aluminium industry
- Examine the influence of oxygen in aluminum recycling
- Analyze chloroaluminate melts when used as electrolytes to produce aluminium
- Investigate electrodeposition of refractory metals such as tungsten and molybdenum using molten ZnCl₂-NaCl-KCl system as an electrolyte
- Use the thermophysical properties such as density, surface tension, and viscosity to investigate
XXXXXX

Combining Databases

It is possible to combine several databases to make calculations using Thermo-Calc. For more information related to a specific type of problem, contact one of our support specialists at info@thermocalc.com. The experts are available to make recommendations on the most suitable database to use for your needs.

Release History



[TCSALT: TCS Molten Salts Database Revision History](#). The current version of the database is TCSALT3. See the link for any subversion release details.

TCS Molten Salts Database (TCSALT) Resources

Database technical content and examples are available in different formats (html help files or PDFs).

Go to these locations to access the same content:

- **Locally Installed Help:** When in Thermo-Calc, press F1 to open the current version of the help in a local browser. You can also click **Online Help** from the **My Project** page to open the file. Then search or navigate to the **Databases** folder to browse the contents.
- **Web Help:** Go to the [Documentation](#) page to link to the most recent version of the web help. Then search or navigate to the **Databases** folder to browse the contents.
- **Website resources:** The individual database technical information and examples are also available in PDF format from the website. Download the *current version* of the PDFs for each database.

| About the CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.



Learn more on our website about the [CALPHAD Method](#) and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our [website](#) or our [YouTube playlist](#).

| Learn More



Go to the [Molten Salt Databases](#) page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information*. Also explore further applications of Thermo-Calc to molten salts on this page.



Read more on our website about applications for [Sustainability](#). The webpage highlights several examples demonstrating how Thermo-Calc has been applied to address key sustainability challenges.



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

TCSALT3 Elements, Systems, and Phases

This section summarizes the available elements, assessed systems, and assessed phases in the TCS Molten Salts Database (TCSALT).

Included Elements

There are 16 elements included in the database, with different types of salts (anions): chlorides (Cl-1), fluorides (F-1), oxides (O-2), carbonates (CO₃-2), nitrates (NO₃-1), nitrites (NO₂-1), and sulfates (SO₄-2).

Included Elements									
Al	C	Ca	Cl	F	K	Li	Mg	N	Na
Nd	O	S	Si	Sr	Zn				

Assessed Systems

The most accurate calculations are obtained in or near these sub-systems and composition ranges. The most recent version of the database contains assessments of these systems:

Pseudo-Binary

These are the assessed pseudo-binary systems in the full range of composition and temperature.

- 35 Assessed Systems with Chloride (Cl-1)
- 31 Assessed Systems with Fluoride (F-1)
- 29 Assessed Systems with Oxygen (O-2)
- 6 Assessed Systems with Carbonate (CO₃-2)
- 10 Assessed Systems with Nitrate (NO₃-1)
- 6 Assessed Systems with Nitrite (NO₂-1)
- 15 Assessed Systems with Sulfate (SO₄-2)

Pseudo-Ternary

These are the assessed pseudo-ternary systems in the full range of composition and temperature.

- 30 Assessed Systems with Chloride (Cl-1)
- 23 Assessed Systems with Fluoride (F-1)
- 28 Assessed Systems with Oxygen (O-2)
- 2 Assessed Systems with Carbonate (CO3-2)
- 10 Assessed Systems with Nitrate (NO3-1)
- 2 Assessed Systems with Sulfate (SO4-2)

Higher Order

These are the assessed higher order systems in the full range of composition and temperature.

- 1 Assessed Chloride (Cl-1) System
- 1 Assessed Fluoride (F-1) System

Mixed

These are the assessed mixed systems in the full range of composition and temperature.

- 118 Assessed Mixed Systems

Assessed Phases

The most recent version of the database contains 284 phases in total.



[TCSALT3 Models for the Included Phases](#)



When using Console Mode, phases and constituents can be listed in the DATABASE (TDB) module and the Gibbs (GES) module. To show models and constituents for the phases in a chosen system, use the command LIST_SYSTEM with the option CONSTITUENTS in the TDB module.

IONIC_LIQ Phase

The liquid metal and slag (IONIC_LIQ) is described with the ionic two-sublattice liquid model [1985Hil; 1991Sun].



The advantage with the ionic two-sublattice model is that it allows a continuous description of a liquid which changes in character with composition. The model has successfully been used to describe liquid oxides, silicates, sulfides, fluorides as well as liquid short range order, molten salts and ordinary metallic liquids. At low level of oxygen, the model becomes equivalent to a substitutional solution model between metallic atoms.

Different composition sets of IONIC_LIQ designated by #1, #2 etc. (e.g. IONIC_LIQ#1) may be observed, which represent miscibility gaps frequently found in some systems.

The #n suffix (where n is an integer) is generated dynamically by Thermo-Calc when using global minimization and therefore the identification of the phases should be determined from these compositions.

TCSALT3 Thermophysical Properties and Assessed Systems

A variety of properties data are included with the TCS Molten Salts Database (TCSALT).

Molar Volume

For the molar volume properties data, the molar volume parameters have been assessed as detailed in [TCSALT3 Molar Volume for Ionic Liquids: Assessed Systems](#). The molar volume of solids is also included in the database but not specifically listed.

Surface Tension

For the surface tension properties data, the parameters have been assessed for the ionic liquid phase. The assessed systems are detailed in [TCSALT3 Surface Tension for Ionic Liquids: Assessed Systems](#).

Viscosity

For the viscosity properties data, the parameters have been assessed for the ionic liquid phase. The assessed systems are detailed in [TCSALT3 Viscosity for Ionic Liquids: Assessed Systems](#).

Thermophysical Parameters and Variables

Below is a summary of the available thermophysical parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode (CM) versus Graphical Mode (GM) as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property	Model Parameters	Variables to Show or Plot in Console Mode and TC-Python
Surface tension	SIGM	SURF (ION)
Dynamic viscosity	VISC	DVIS (LIQUID) DVIS (ION)
Kinematic viscosity		KVIS (LIQUID) KVIS (ION)
Molar volume	V0, VA	VM for a system VM (PHI) for phase PHI

Examples

In Thermo-Calc, press F1 and search or navigate to the relevant database to discover the Validation and Calculation Examples Collection, which is also available in PDF format on our website.



Go to the [Molten Salt Databases](#) page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information*. Also explore further applications of Thermo-Calc to molten salts on this page.

Learn More



Molar volume, surface tension of the ionic liquids, and viscosity of the ionic liquids are added to the database as of version 2 (TCSALT2).



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

Reference

[2026Zha] R. Zhang, L. Kjellqvist, H. Mao, A. Markström, R. Naraghi, Q. Chen, Thermophysical Properties of Molten Salts: Insights from the TCSALT Database. *Int. J. Thermophys.* 47, 23 (2026).

TCSALT3 Systems

In this section:

TCSALT3 Assessed Pseudo-Binary Systems	15
TCSALT3 Assessed Pseudo-Ternary Systems	19
TCSALT3 Assessed Higher Order Systems	22
TCSALT3 Assessed Mixed Systems	23

TCSALT3 Assessed Pseudo-Binary Systems

These are the assessed pseudo-binary systems in the full range of composition and temperature.

- 35 Assessed Systems with Chloride (Cl-1)
- 31 Assessed Systems with Fluoride (F-1)
- 29 Assessed Systems with Oxygen (O-2)
- 6 Assessed Systems with Carbonate (CO3-2)
- 10 Assessed Systems with Nitrate (NO3-1)
- 6 Assessed Systems with Nitrite (NO2-1)
- 15 Assessed Systems with Sulfate (SO4-2)

Assessed Pseudo-Binary Systems with Chloride (Cl-1)

This shows the pseudo-binary chloride (Cl-1) systems that are assessed. Compounds are shown as rows and columns. An 'x' indicates an assessed system.

	AlCl ₃	CaCl ₂	KCl	LiCl	MgCl ₂	NaCl	NdCl ₃	SiCl ₄	SrCl ₂	ZnCl ₂
AlCl ₃	AlCl ₃									
CaCl ₂	x	CaCl ₂								
KCl	x	x	KCl							
LiCl	x	x	x	LiCl						
MgCl ₂	x	x	x	x	MgCl ₂					
NaCl	x	x	x	x	x	NaCl				
NdCl ₃	x	x	x	x	x	x	NdCl ₃			
SiCl ₄	x							SiCl ₄		
SrCl ₂		x	x	x	x	x	x		SrCl ₂	
ZnCl ₂	x	x	x	x	x	x			x	ZnCl ₂

Assessed Pseudo-Binary Systems with Fluoride (F-1)

This shows the pseudo-binary fluoride (F-1) systems that are assessed. Compounds are shown as rows and columns. An 'x' indicates an assessed system.

	AlF ₃	CaF ₂	KF	LiF	MgF ₂	NaF	NdF ₃	SiF ₄	SrF ₂	ZnF ₂
AlF ₃	AlF ₃									
CaF ₂	x	CaF ₂								
KF	x	x	KF							
LiF	x	x	x	LiF						
MgF ₂	x	x	x	x	MgF ₂					
NaF	x	x	x	x	x	NaF				
NdF ₃	x	x		x	x	x	NdF ₃			
SiF ₄			x			x		SiF ₄		
SrF ₂		x	x	x	x	x	x		SrF ₂	
ZnF ₂			x	x		x				ZnF ₂

Assessed Pseudo-Binary Systems with Oxygen (O-2)

This shows the pseudo-binary oxide (O-2) systems that are assessed. Compounds are shown as rows and columns. An 'x' indicates an assessed system.

	Al ₂ O ₃	CaO	K ₂ O	Li ₂ O	MgO	Na ₂ O	Nd ₂ O ₃	SiO ₂	SrO	ZnO
Al ₂ O ₃	Al ₂ O ₃									
CaO	x	CaO								
K ₂ O	x		K ₂ O							
Li ₂ O	x	x	x	Li ₂ O						
MgO	x	x		x	MgO					
Na ₂ O	x			x		Na ₂ O				
Nd ₂ O ₃	x	x			x		Nd ₂ O ₃			
SiO ₂	x	x	x	x	x	x	x	SiO ₂		
SrO	x	x			x			x	SrO	
ZnO	x	x		x	x			x		ZnO

Assessed Pseudo-Binary Systems with Carbonate (CO3-2)

This shows the pseudo-binary carbonate (CO3-2) systems that are assessed. Compounds are shown as rows and columns. An 'x' indicates an assessed system.

	CaCO ₃	K ₂ CO ₃	Li ₂ CO ₃	Na ₂ CO ₃
CaCO ₃	CaCO ₃			
K ₂ CO ₃	x	K ₂ CO ₃		
Li ₂ CO ₃	x	x	Li ₂ CO ₃	
Na ₂ CO ₃	x	x	x	Na ₂ CO ₃

Assessed Pseudo-Binary Systems with Nitrate (NO3-1)

This shows the pseudo-binary nitrate (NO3-1) systems that are assessed. Compounds are shown as rows and columns. An 'x' indicates an assessed system.

	Ca(NO ₃) ₂	KNO ₃	LiNO ₃	Mg(NO ₃) ₂	NaNO ₃
Ca(NO ₃) ₂	Ca(NO ₃) ₂				
KNO ₃	x	KNO ₃			
LiNO ₃	x	x	LiNO ₃		
Mg(NO ₃) ₂	x	x	x	Mg(NO ₃) ₂	
NaNO ₃	x	x	x	x	NaNO ₃

Assessed Pseudo-Binary Systems with Nitrite (NO2-1)

This shows the pseudo-binary nitrite (NO2-1) systems that are assessed. Compounds are shown as rows and columns. An 'x' indicates an assessed system.

	Ca(NO ₂) ₂	KNO ₂	LiNO ₂	NaNO ₂
Ca(NO ₂) ₂	Ca(NO ₂) ₂			
KNO ₂	x	KNO ₂		
LiNO ₂	x	x	LiNO ₂	
NaNO ₂	x	x	x	NaNO ₂

TCSALT3 Assessed Pseudo-Ternary Systems

These are the assessed pseudo-ternary systems in the full range of composition and temperature.

- 30 Assessed Systems with Chloride (Cl-1)
- 23 Assessed Systems with Fluoride (F-1)
- 28 Assessed Systems with Oxygen (O-2)
- 2 Assessed Systems with Carbonate (CO3-2)
- 10 Assessed Systems with Nitrate (NO3-1)
- 2 Assessed Systems with Sulfate (SO4-2)

Assessed Pseudo-Ternary Systems with Chloride (Cl-1)

<i>Assessed Pseudo-Ternary Systems with Chloride (Cl-1)</i>				
AlCl ₃ -CaCl ₂ -NaCl	AlCl ₃ -KCl-LiCl	AlCl ₃ -KCl-MgCl ₂	AlCl ₃ -KCl-NaCl	AlCl ₃ -MgCl ₂ -NaCl
CaCl ₂ -KCl-LiCl	CaCl ₂ -KCl-MgCl ₂	CaCl ₂ -KCl-NaCl	CaCl ₂ -KCl-ZnCl ₂	CaCl ₂ -LiCl-NaCl
CaCl ₂ -LiCl-SrCl ₂	CaCl ₂ -LiCl-NdCl ₃	CaCl ₂ -MgCl ₂ -NaCl	CaCl ₂ -MgCl ₂ -NdCl ₃	CaCl ₂ -NaCl-NdCl ₃
CaCl ₂ -NaCl-SrCl ₂	CaCl ₂ -NdCl ₃ -SrCl ₂	KCl-LiCl-MgCl ₂	KCl-LiCl-NaCl	KCl-LiCl-NdCl ₃
KCl-LiCl-SrCl ₂	KCl-LiCl-ZnCl ₂	KCl-MgCl ₂ -NaCl	KCl-MgCl ₂ -NdCl ₃	KCl-NaCl-SrCl ₂
KCl-NaCl-ZnCl ₂	LiCl-NaCl-SrCl ₂	LiCl-NdCl ₃ -SrCl ₂	MgCl ₂ -NdCl ₃ -SrCl ₂	NaCl-NdCl ₃ -SrCl ₂

Assessed Pseudo-Ternary Systems with Fluoride (F-1)

<i>Assessed Pseudo-Ternary Systems with Fluoride (F-1)</i>				
AlF ₃ -CaF ₂ -LiF	AlF ₃ -CaF ₂ -NaF	AlF ₃ -KF-LiF	AlF ₃ -KF-NaF	AlF ₃ -LiF-NaF
AlF ₃ -MgF ₂ -NaF	AlF ₃ -NaF-NdF ₃	CaF ₂ -KF-LiF	CaF ₂ -KF-MgF ₂	CaF ₂ -KF-NaF
CaF ₂ -KF-SrF ₂	CaF ₂ -LiF-MgF ₂	CaF ₂ -LiF-NaF	CaF ₂ -LiF-SrF ₂	CaF ₂ -MgF ₂ -NaF
CaF ₂ -NaF-SrF ₂	KF-LiF-MgF ₂	KF-LiF-NaF	KF-MgF ₂ -NaF	KF-MgF ₂ -ZnF ₂

Assessed Pseudo-Ternary Systems with Fluoride (F-1)

KF-NaF-SrF ₂	LiF-MgF ₂ -NaF	LiF-MgF ₂ -SrF ₂		
-------------------------	---------------------------	--	--	--

Assessed Pseudo-Ternary Systems with Oxygen (O-2)

Assessed Pseudo-Ternary Systems with Oxygen (O-2)

Al ₂ O ₃ -CaO-K ₂ O	Al ₂ O ₃ -CaO-MgO	Al ₂ O ₃ -CaO-Na ₂ O	Al ₂ O ₃ -CaO-Nd ₂ O ₃	Al ₂ O ₃ -CaO-SiO ₂
Al ₂ O ₃ -CaO-SrO	Al ₂ O ₃ -K ₂ O-MgO	Al ₂ O ₃ -Li ₂ O-Na ₂ O	Al ₂ O ₃ -MgO-Nd ₂ O ₃	Al ₂ O ₃ -MgO-SiO ₂
Al ₂ O ₃ -MgO-ZnO	Al ₂ O ₃ -Nd ₂ O ₃ -SiO ₂	CaO-K ₂ O-SiO ₂	CaO-Li ₂ O-SiO ₂	CaO-MgO-SiO ₂
CaO-MgO-ZnO	CaO-Na ₂ O-SiO ₂	CaO-Nd ₂ O ₃ -SiO ₂	CaO-SiO ₂ -SrO	CaO-SiO ₂ -ZnO
K ₂ O-MgO-SiO ₂	K ₂ O-Na ₂ O-SiO ₂	Li ₂ O-MgO-SiO ₂	Li ₂ O-Na ₂ O-SiO ₂	MgO-Na ₂ O-SiO ₂
MgO-Nd ₂ O ₃ -SiO ₂	MgO-SiO ₂ -ZnO	Nd ₂ O ₃ -SiO ₂ -SrO		

Assessed Pseudo-Ternary Systems with Carbonate (CO3-2)

Assessed Pseudo-Ternary Systems with Carbonate (CO3-2)

CaCO ₃ -K ₂ CO ₃ -Na ₂ CO ₃	K ₂ CO ₃ -Li ₂ CO ₃ -Na ₂ CO ₃
--	--

Assessed Pseudo-Ternary Systems with Nitrate (NO3-1)

Assessed Pseudo-Ternary Systems with Nitrate (NO3-1)

Ca(NO ₃) ₂ -KNO ₃ -LiNO ₃	Ca(NO ₃) ₂ -KNO ₃ -Mg(NO ₃) ₂	Ca(NO ₃) ₂ -KNO ₃ -NaNO ₃
Ca(NO ₃) ₂ -LiNO ₃ -NaNO ₃	Ca(NO ₃) ₂ -Mg(NO ₃) ₂ -NaNO ₃	Ca(NO ₃) ₂ -NaNO ₃ -Sr(NO ₃) ₂
KNO ₃ -LiNO ₃ -Mg(NO ₃) ₂	KNO ₃ -LiNO ₃ -NaNO ₃	KNO ₃ -Mg(NO ₃) ₂ -NaNO ₃
LiNO ₃ -Mg(NO ₃) ₂ -NaNO ₃		

Assessed Pseudo-Ternary Systems with Sulfate (SO4-2)

Assessed Pseudo-Ternary Systems with Sulfate (SO4-2)

CaSO₄-K₂SO₄-MgSO₄

K₂SO₄-Na₂SO₄-ZnSO₄

TCSALT3 Assessed Higher Order Systems

These are the assessed higher order systems in the full range of composition and temperature.

- 1 Assessed Chloride (Cl-1) System
- 1 Assessed Fluoride (F-1) System

Assessed Higher Order Systems with Chloride (Cl-1)

Assessed Higher Order Systems with Cl

$\text{AlCl}_3\text{-KCl-MgCl}_2\text{-NaCl}$

Assessed Higher Order Systems with Fluoride (F-1)

Assessed Higher Order Systems with F

$\text{K}_2\text{SiF}_6\text{-K}_3\text{AlF}_6\text{-Na}_2\text{SiF}_6\text{-Na}_3\text{AlF}_6$

TCSALT3 Assessed Mixed Systems

These are the assessed mixed systems in the full range of composition and temperature.

- 118 Assessed Mixed Systems

Assessed Mixed Systems

<i>Assessed Mixed Systems</i>		
$\text{Al}_2\text{O}_3\text{-CaF}_2$	$\text{Al}_2\text{O}_3\text{-CaF}_2\text{-CaO}$	$\text{Al}_2\text{O}_3\text{-CaF}_2\text{-SiO}_2$
$\text{AlCl}_3\text{-AlF}_3\text{-KCl-KF}$	$\text{AlCl}_3\text{-AlF}_3\text{-LiCl-LiF}$	$\text{AlCl}_3\text{-AlF}_3\text{-NaCl-NaF}$
$\text{Ca}(\text{NO}_2)_2\text{-Ca}(\text{NO}_3)_2\text{-KNO}_2\text{-KNO}_3$	$\text{Ca}(\text{NO}_2)_2\text{-Ca}(\text{NO}_3)_2\text{-LiNO}_2\text{-LiNO}_3$	$\text{Ca}(\text{NO}_2)_2\text{-Ca}(\text{NO}_3)_2\text{-NaNO}_2\text{-NaNO}_3$
$\text{Ca}_2\text{CO}_3\text{-CaF}_2$	$\text{CaCO}_3\text{-CaF}_2\text{-Na}_2\text{CO}_3\text{-NaF}$	$\text{CaCO}_3\text{-CaO}$
$\text{CaCO}_3\text{-CaSO}_4$	$\text{CaCl}_2\text{-CaF}_2$	$\text{CaCl}_2\text{-CaF}_2\text{-CaO}$
$\text{CaCl}_2\text{-CaF}_2\text{-CaSO}_4$	$\text{CaCl}_2\text{-CaF}_2\text{-KCl-KF}$	$\text{CaCl}_2\text{-CaF}_2\text{-LiCl-LiF}$
$\text{CaCl}_2\text{-CaF}_2\text{-MgCl}_2\text{-MgF}_2$	$\text{CaCl}_2\text{-CaF}_2\text{-NaCl-NaF}$	$\text{CaCl}_2\text{-CaF}_2\text{-SrCl}_2\text{-SrF}_2$
$\text{CaCl}_2\text{-CaO}$	$\text{CaCl}_2\text{-CaSO}_4$	$\text{CaCl}_2\text{-CaSO}_4\text{-K}_2\text{SO}_4\text{-KCl}$
$\text{CaCl}_2\text{-CaSO}_4\text{-Na}_2\text{SO}_4\text{-NaCl}$	$\text{CaCl}_2\text{-Nd}_2\text{O}_3\text{-NdCl}_3$	$\text{CaF}_2\text{-CaO}$
$\text{CaF}_2\text{-CaSO}_4$	$\text{CaF}_2\text{-CaSO}_4\text{-Li}_2\text{SO}_4\text{-LiF}$	$\text{CaF}_2\text{-KF-SiO}_2$
$\text{CaF}_2\text{-NaF-SiO}_2$	$\text{CaF}_2\text{-SiO}_2$	CaO-CaSO_4
$\text{K}_2\text{CO}_3\text{-K}_2\text{SO}_4$	$\text{K}_2\text{CO}_3\text{-K}_2\text{SO}_4\text{-KCl}$	$\text{K}_2\text{CO}_3\text{-K}_2\text{SO}_4\text{-KF}$
$\text{K}_2\text{CO}_3\text{-K}_2\text{SO}_4\text{-Na}_2\text{CO}_3\text{-Na}_2\text{SO}_4$	$\text{K}_2\text{CO}_3\text{-KCl}$	$\text{K}_2\text{CO}_3\text{-KCl-KF}$
$\text{K}_2\text{CO}_3\text{-KCl-Li}_2\text{CO}_3\text{-LiCl}$	$\text{K}_2\text{CO}_3\text{-KCl-Na}_2\text{CO}_3\text{-NaCl}$	$\text{K}_2\text{CO}_3\text{-KF}$
$\text{K}_2\text{CO}_3\text{-KNO}_3$	$\text{K}_2\text{SO}_4\text{-KCl}$	$\text{K}_2\text{SO}_4\text{-KCl-KF}$
$\text{K}_2\text{SO}_4\text{-KCl-Li}_2\text{SO}_4\text{-LiCl}$	$\text{K}_2\text{SO}_4\text{-KCl-MgCl}_2\text{-MgSO}_4$	$\text{K}_2\text{SO}_4\text{-KCl-Na}_2\text{SO}_4\text{-NaCl}$
$\text{K}_2\text{SO}_4\text{-KCl-SrCl}_2\text{-SrSO}_4$	$\text{K}_2\text{SO}_4\text{-KF}$	$\text{K}_2\text{SO}_4\text{-KF-Na}_2\text{SO}_4\text{-NaF}$

<i>Assessed Mixed Systems</i>		
K_2SO_4 - KNO_3 - Na_2SO_4 - $NaNO_3$	K_2SiF_6 -KCl	K_2SiF_6 -KCl- Na_2SiF_6 -NaCl
KCl-KF	KCl-KF-LiCl-LiF	KCl-KF-NaCl-NaF
KCl-KF-SrCl ₂ -SrF ₂	KCl-KNO ₃	KCl-KNO ₃ -Sr(NO ₃) ₂ -SrCl ₂
KF-KNO ₃	KNO ₂ -KNO ₃	KNO ₂ -KNO ₃ -NaNO ₂ -NaNO ₃
Li ₂ CO ₃ -Li ₂ O	Li ₂ CO ₃ -Li ₂ SO ₄	Li ₂ CO ₃ -LiCl
Li ₂ CO ₃ -LiCl- Na_2CO_3 -NaCl	Li ₂ CO ₃ -LiF	Li ₂ CO ₃ -LiNO ₃
Li ₂ O-LiCl	Li ₂ O-LiF	Li ₂ SO ₄ -LiCl
Li ₂ SO ₄ -LiCl- Na_2SO_4 -NaCl	Li ₂ SO ₄ -LiCl-SrCl ₂ -SrSO ₄	Li ₂ SO ₄ -LiCl-ZnCl ₂ -ZnSO ₄
Li ₂ SO ₄ -LiF	Li ₂ SO ₄ -LiF- Na_2SO_4 -NaF	Li ₂ SO ₄ -LiNO ₃
LiCl-LiF	LiCl-LiF-NaCl-NaF	LiCl-LiF-SrCl ₂ -SrF ₂
LiCl-LiNO ₃	LiCl-LiNO ₃ -Sr(NO ₃) ₂ -SrCl ₂	LiF-LiNO ₃
LiNO ₂ -LiNO ₃	LiNO ₂ -LiNO ₃ -NaNO ₂ -NaNO ₃	MgCl ₂ -MgF ₂
MgCl ₂ -MgF ₂ -NaCl-NaF	MgCl ₂ -MgO-Nd ₂ O ₃ -NdCl ₃	MgCl ₂ -MgSO ₄
MgCl ₂ -MgSO ₄ - Na_2SO_4 -NaCl	MgF ₂ -SiO ₂	Na ₂ CO ₃ -Na ₂ O
Na ₂ CO ₃ - Na_2SO_4 -NaCl	Na ₂ CO ₃ - Na_2SO_4 -NaF	Na ₂ CO ₃ -NaCl
Na ₂ CO ₃ -NaCl-NaF	Na ₂ CO ₃ -NaF	Na ₂ CO ₃ -NaNO ₃
Na ₂ SO ₄ -NaCO ₃	Na ₂ SO ₄ -NaCl	Na ₂ SO ₄ -NaCl-NaF
Na ₂ SO ₄ -NaCl-NaNO ₃	Na ₂ SO ₄ -NaCl-ZnSO ₄ -ZnSO ₄	Na ₂ SO ₄ -NaF
Na ₂ SO ₄ -NaNO ₃	NaCl-NaF	NaCl-NaF-SrCl ₂ -SrF ₂
NaCl-NaNO ₃	NaCl-NaNO ₃ -Sr(NO ₃) ₂ -SrCl ₂	NaF-NaNO ₃
NaNO ₂ -NaNO ₃	Nd ₂ O ₃ -NdCl ₃	Nd ₂ O ₃ -NdCl ₃ -SrCl ₂ -SrO
SrCO ₃ -SrCl ₂	SrCl ₂ -SrF ₂	SrCl ₂ -SrO

Assessed Mixed Systems

ZnCl ₂ -ZnSO ₄		
--------------------------------------	--	--

TCSALT3 Properties Data

In this section:

TCSALT3 Molar Volume for Ionic Liquids: Assessed Systems	27
TCSALT3 Surface Tension for Ionic Liquids: Assessed Systems	30
TCSALT3 Viscosity for Ionic Liquids: Assessed Systems	32

TCSALT3 Molar Volume for Ionic Liquids: Assessed Systems

Molar volume is included with the TCS Molten Salts Database (TCSALT) starting with version 2 (TCSALT2).



This section includes all the assessed systems for the ionic liquids. The molar volume of solids is also included in the database but not specifically listed.

Model Description



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

Unary Systems

Assessed Unary Systems (Molar Volume)

AlCl ₃	AlF ₃	CaCl ₂	CaF ₂	K ₂ CO ₃	K ₂ SO ₄
KCl	KF	KNO ₂	KNO ₃	Li ₂ CO ₃	Li ₂ O
Li ₂ SO ₄	Li ₃ AlF ₆	LiCl	LiF	LiNO ₃	MgCl ₂
MgF ₂	Na ₂ CO ₃	Na ₂ SO ₄	Na ₃ AlF ₆	NaCl	NaF
NaNO ₂	NaNO ₃	NdCl ₃	SiCl ₄	SiF ₄	SrCl ₂
SrF ₂	SrO	ZnCl ₂	ZnF ₂	ZnO	ZnSO ₄

Pseudo-Binary Systems

Assessed Pseudo-Binary Systems (Molar Volume)

Al ₂ O ₃ -CaO	Al ₂ O ₃ -K ₂ O	Al ₂ O ₃ -MgO	Al ₂ O ₃ -Na ₂ O	Al ₂ O ₃ -SiO ₂
-------------------------------------	--	-------------------------------------	---	--

Assessed Pseudo-Binary Systems (Molar Volume)

Al ₂ O ₃ -SrO	Al ₂ O ₃ -ZnO	AlCl ₃ -CaCl ₂	AlCl ₃ -KCl	AlCl ₃ -LiCl
AlCl ₃ -MgCl ₂	AlCl ₃ -NaCl	AlCl ₃ -SiCl ₄	AlCl ₃ -SrCl ₂	AlCl ₃ -ZnCl ₂
AlF ₃ -CaF ₂	AlF ₃ -KF	AlF ₃ -MgF ₂	AlF ₃ -NaF	AlF ₃ -SrF ₂
AlF ₃ -ZnF ₂	Ca(NO ₃) ₂ -KNO ₃	Ca(NO ₃) ₂ -NaNO ₃	CaCl ₂ -CaF ₂	CaCl ₂ -CaO
CaCl ₂ -KCl	CaCl ₂ -LiCl	CaCl ₂ -MgCl ₂	CaCl ₂ -NaCl	CaCl ₂ -SrCl ₂
CaCl ₂ -ZnCl ₂	CaCO ₃ -K ₂ CO ₃	CaF ₂ -CaO	CaF ₂ -KF	CaF ₂ -LiF
CaF ₂ -MgF ₂	CaF ₂ -NaF	CaF ₂ -SiF ₄	CaO-MgO	CaO-SiO ₂
CaO-SrO	CaO-ZnO	CaSO ₄ -Na ₂ SO ₄	K ₂ CO ₃ -LiCl	K ₂ CO ₃ -LiF
K ₂ CO ₃ -Na ₂ CO ₃	K ₂ O-SiO ₂	KCl-K ₂ CO ₃	KCl-K ₂ SO ₄	KCl-KF
KCl-KNO ₃	KCl-Li ₂ CO ₃	KCl-LiCl	KCl-MgCl ₂	KCl-Na ₂ CO ₃
KCl-NaCl	KCl-SrCl ₂	KCl-ZnCl ₂	KCl-ZnSO ₄	KF-Li ₂ CO ₃
KF-LiF	KF-MgF ₂	KF-NaF	KF-SiF ₄	KF-SrF ₄
KF-ZnF ₂	KNO ₂ -KNO ₃	KNO ₂ -NaNO ₂	KNO ₂ -NaNO ₃	KNO ₃ -LiNO ₃
KNO ₃ -Mg(NO ₃) ₂	KNO ₃ -NaNO ₃	KNO ₃ -Sr(NO ₃) ₂	Li ₂ CO ₃ -K ₂ CO ₃	Li ₂ CO ₃ -Na ₂ CO ₃
Li ₂ O-SiO ₂	Li ₂ SiO ₄ -Na ₂ SO ₄	Li ₂ SiO ₄ -ZnSO ₄	LiCl-Li ₂ CO ₃	LiCl-LiF
LiCl-LiNO ₃	LiCl-MgCl ₂	LiCl-NaCl	LiCl-ZnCl ₂	LiF-Li ₂ CO ₃
LiF-NaF	LiNO ₃ -NaNO ₃	MgCl ₂ -MgF ₂	MgCl ₂ -NaCl	MgCl ₂ -SrCl ₂
MgCl ₂ -ZnCl ₂	MgF ₂ -MgO	MgF ₂ -NaF	MgF ₂ -SiF ₄	MgF ₂ -SrF ₂
MgO-SiO ₂	MgO-SrO	Na ₂ O-SiO ₂	Na ₂ SO ₄ -ZnSO ₄	NaCl-Na ₂ CO ₃
NaCl-NaF	NaCl-NaNO ₃	NaCl-SrCl ₂	NaCl-ZnCl ₂	NaF-SiF ₄
NaF-SrF ₂	NaF-ZnF ₂	NaNO ₂ -NaNO ₃	SiF ₄ -SrF ₂	SiF ₄ -ZnF ₂
SiO ₂ -SrO	SiO ₂ -ZnO	SrCl ₂ -SrF ₂	SrCl ₂ -SrO	SrCl ₂ -ZnCl ₂

Pseudo-Ternary and Higher Order Systems

Assessed Pseudo-Ternary and Higher Order Systems (Molar Volume)

$\text{AlCl}_3\text{-LiCl-NaCl}$	$\text{AlF}_3\text{-Na}_3\text{AlF}_6$	$\text{Al}_2\text{O}_3\text{-KF-Na}_3\text{AlF}_6$	$\text{Al}_2\text{O}_3\text{-Na}_3\text{AlF}_6$
$\text{Al}_2\text{O}_3\text{-Li}_3\text{AlF}_6$	$\text{CaCl}_2\text{-MgCl}_2\text{-NaCl}$	$\text{CaF}_2\text{-Na}_3\text{AlF}_6$	$\text{Ca}(\text{NO}_3)_2\text{-KNO}_3\text{-NaNO}_3$
$\text{K}_3\text{AlF}_6\text{-Li}_3\text{AlF}_6$	$\text{K}_3\text{AlF}_6\text{-Na}_3\text{AlF}_6$	$\text{Li}_2\text{CO}_3\text{-K}_2\text{CO}_3\text{-Na}_2\text{CO}_3$	$\text{Li}_2\text{O-CaO-SiO}_2$
$\text{Li}_2\text{O-MgO-SiO}_2$	$\text{Li}_2\text{O-Na}_2\text{O-SiO}_2$	$\text{Li}_3\text{AlF}_6\text{-Na}_3\text{AlF}_6$	$\text{LiF-Na}_3\text{AlF}_6$
$\text{Na}_3\text{AlF}_6\text{-KF}$	$\text{NaNO}_3\text{-NaNO}_2\text{-KNO}_3$		

TCSALT3 Surface Tension for Ionic Liquids: Assessed Systems

Surface tension is included with the TCS Molten Salts Database (TCSALT) starting with version 2 (TCSALT2).

Model Description



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

Unary Systems

Assessed Unary Systems (Surface Tension)

Al ₂ O ₃	AlCl ₃	AlF ₃	Ca(NO ₃) ₂	CaCl ₂	CaF ₂
CaO	K ₂ CO ₃	K ₂ O	K ₂ SO ₄	KCl	KF
KNO ₂	KNO ₃	Li ₂ CO ₃	Li ₂ SO ₄	KCl	KF
LiCl	LiF	LiNO ₃	MgCl ₂	MgF ₂	MgO
Na ₂ CO ₃	Na ₂ O	Na ₂ SO ₄	NaCl	NaF	NaNO ₂
NaNO ₃	SiCl ₄	SiF ₄	SiO ₂	Sr(NO ₃) ₂	SrCl ₂
SrF ₂	SrO	ZnCl ₂	ZnF ₂	ZnO	

Pseudo-Binary Systems

Assessed Pseudo-Binary Systems (Surface Tension)

Al ₂ O ₃ -CaO	Al ₂ O ₃ -K ₂ O	Al ₂ O ₃ -MgO	Al ₂ O ₃ -SiO ₂	AlCl ₃ -CaCl ₂
AlCl ₃ -KCl	AlCl ₃ -MgCl ₂	AlCl ₃ -NaCl	AlCl ₃ -SrCl ₂	AlCl ₃ -ZnCl ₂
AlF ₂ -SrF ₂	AlF ₂ -ZnF ₂	AlF ₃ -CaF ₂	AlF ₃ -KF	AlF ₃ -MgF ₂

Assessed Pseudo-Binary Systems (Surface Tension)

AlF ₃ -NaF	Ca(NO ₃) ₂ -KNO ₃	Ca(NO ₃) ₂ -NaNO ₃	CaCl ₂ -KCl	CaCl ₂ -LiCl
CaCl ₂ -MgCl ₂	CaCl ₂ -NaCl	CaF ₂ -CaO	CaF ₂ -SiF ₄	CaO-SiO ₂
CaSO ₄ -Na ₂ SO ₄	K ₂ CO ₃ -Na ₂ CO ₃	K ₂ O-SiO ₂	K ₂ SO ₄ -Na ₂ SO ₄	KCl-K ₂ SO ₄
KCl-Li ₂ SO ₄	KCl-LiCl	KCl-MgCl ₂	KCl-NaCl	KCl-NaNO ₃
KCl-NdCl ₃	KCl-SrCl ₂	KCl-ZnCl ₂	KF-LiF	KF-NaF
KF-SiF ₄	KNO ₂ -KNO ₃	KNO ₃ -LiNO ₃	KNO ₃ -NaNO ₃	Li ₂ CO ₃ -Na ₂ CO ₃
Li ₂ SO ₄ -NaCl	LiCl-Li ₂ CO ₃	LiCl-LiF	LiCl-MgCl ₂	LiCl-NaCl
LiF-NaF	MgCl ₂ -NaCl	MgF ₂ -SiF ₄	MgO-SiO ₂	Na ₂ O-SiO ₂
NaCl-Na ₂ SO ₄	NaF-SiF ₄	NaNO ₂ -NaNO ₃	SiF ₄ -SrF ₂	SiF ₄ -ZnF ₂
SrO-SiO ₂	ZnO-SiO ₂			

Pseudo-Ternary and Higher Order Systems
Assessed Pseudo-Ternary and Higher Order Systems (Surface Tension)

Al ₂ O ₃ -KF-Na ₃ AlF ₆	CaCl ₂ -KCl-MgCl ₂	CaCl ₂ -MgCl ₂ -NaCl
K ₃ AlF ₆ -Na ₃ AlF ₆	KCl•NaCl-NdCl ₃	K ₂ CO ₃ -Li ₂ CO ₃ -Na ₂ CO ₃
KF-Na ₃ AlF ₆		

TCSALT3 Viscosity for Ionic Liquids: Assessed Systems

Viscosity is included with the TCS Molten Salts Database (TCSALT) starting with version 2 (TCSALT2).

Model Description



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

Unary Systems

Assessed Unary Systems (Viscosity)

Al ₂ O ₃	AlCl ₃	AlF ₃	Ca(NO ₃) ₂	CaCl ₂	CaF ₂
CaO	K ₂ CO ₃	K ₂ O	KCl	KF	KNO ₂
KNO ₃	Li ₂ CO ₃	Li ₂ O	Li ₃ AlF ₆	LiCl	LiF
LiNO ₂	LiNO ₃	MgCl ₂	MgF ₂	MgO	Na ₂ CO ₃
Na ₂ O	Na ₂ SO ₄	Na ₃ AlF ₆	NaCl	NaF	NaNO ₂
NaNO ₃	SiCl ₄	SiF ₄	SiO ₂	Sr(NO ₃) ₂	SrCl ₂
SrF ₂	SrO	ZnCl ₂	ZnF ₂	ZnO	

Pseudo-Binary Systems

Assessed Pseudo Binary Systems (Viscosity)

Al ₂ O ₃ -CaO	Al ₂ O ₃ -K ₂ O	Al ₂ O ₃ -MgO	Al ₂ O ₃ -Na ₂ O
Al ₂ O ₃ -SiO ₂	AlCl ₃ -CaCl ₂	AlCl ₃ -KCl	AlCl ₃ -LiCl
AlCl ₃ -MgCl ₂	AlCl ₃ -NaCl	AlCl ₃ -SiCl ₄	AlCl ₃ -SrCl ₂

Assessed Pseudo Binary Systems (Viscosity)

AlCl ₃ -ZnCl ₂	AlF ₃ -CaF ₂	AlF ₃ -KF	AlF ₃ -LiF
AlF ₃ -MgF ₂	AlF ₃ -Na ₃ AlF ₆	AlF ₃ -NaF	AlF ₃ -SrF ₂
AlF ₃ -ZnF ₂	Ca(NO ₃) ₂ -KNO ₃	Ca(NO ₃) ₂ -LiNO ₃	Ca(NO ₃) ₂ -NaNO ₃
CaCl ₂ -NaCl	CaF ₂ -MgO	CaF ₂ -SiF ₄	CaO-SiO ₂
K ₂ CO ₃ -Li ₂ CO ₃	K ₂ CO ₃ -Na ₂ CO ₃	K ₂ O-SiO ₂	KCl-LiCl
KCl-MgCl ₂	KCl-NaCl	KCl-ZnCl ₂	KNO ₂ -NaNO ₂
KNO ₃ -LiNO ₃	KNO ₃ -NaNO ₃	KNO ₃ -Sr(NO ₃) ₂	Li ₂ CO ₃ -Na ₂ CO ₃
Li ₂ O-SiO ₂	LiCl-Li ₂ CO ₃	LiCl-MgCl ₂	LiCl-ZnCl ₂
LiF-Na ₃ AlF ₆	LiF-NaF	LiNO ₃ -NaNO ₃	MgCl ₂ -NaCl
MgF ₂ -SiF ₄	MgO-SiO ₂	Na ₂ O-SiO ₂	NaCl-NaNO ₃
NaCl-ZnCl ₂	NaF-Na ₃ AlF ₆	SiF ₄ -SrF ₂	SiF ₄ -ZnF ₂
SiO ₂ -SrO	SiO ₂ -ZnO		

Pseudo-Ternary and High Order Systems
Assessed Pseudo-Ternary and Higher Order Systems (Viscosity)

Al ₂ O ₃ -NaF-AlF ₃ -CaF ₂	AlCl ₃ -LiCl-NaCl	CaF ₂ -Na ₃ AlF ₆
Ca(NO ₃) ₂ -KNO ₃ -NaNO ₃	K ₂ CO ₃ -Li ₂ CO ₃ -Na ₂ CO ₃	KCl•NaCl-NdCl ₃
KCl-NaCl-ZnCl ₂	Li ₃ AlF ₆ -Na ₃ AlF ₆	MgF ₂ -Na ₃ AlF ₆
NaCl-KCl-MgCl ₂	NaCl-Na ₃ AlF ₆	NaF-Na ₃ AlF ₆
NaNO ₃ -NaNO ₂ -KNO ₃		

TCSALT3 Phases

In this section:

TCSALT3 Models for the Included Phases	35
--	----

TCSALT3 Models for the Included Phases

 See the separate listing for [Gas and IONIC LIQ Phases](#) below.

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL2O12S3	Fe2[SO4]3	-	hR102	(148, R-3)	-	2	(AL+3)2(SO4-2)3
AL2SiO4F	Unknown Structure	-	-	-	-	4	(AL+3)2(Si+4)1(O-2)4(F-1)2
AL2SR4O7_A	Unknown Structure	-	-	-	-	3	(AL+3)2(SR+2)4(O-2)7
AL2SR4O7_B	Unknown Structure	-	-	-	-	3	(AL+3)2(SR+2)4(O-2)7
AL2SRO4_H	BaAl2O4 (H28)	H28	hP18	(182, P6_322)	-	3	(AL+3)2(CA+2, SR+2)1(O-2)4
AL2SRO4_L	SrAl2O4	-	mP28	(4, P2_1)	-	3	(AL+3)2(SR+2)1(O-2)4
ALCL3	AlCl3	-	mS16	(12, C2/m)	-	2	(AL+3)1(CL-1)3
ALF3_S1	FeF3 (D012)	D012	hR8	(167, R-3c)	-	2	(AL+3)1(F-1)3
ALF3_S2	AlF3	-	oS48	(63, Cmcm)	-	2	(AL+3)1(F-1)3
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	(58, Pnm)	This is a high-pressure phase (Al2O3.SiO2)	4	(AL+3)1(AL+3)1(Si+4)1(O-2)5
ANHYDRITE	Anhydrite (CaSO4, H01)	H01	oS24	(63, Cmcm)	This is low temperature (Ca, Mg)(SO4).	2	(CA+2, MG+2)1(SO4-2)1
ANORTHITE	Ca(Al0.5Si0.5)4O8	-	aP104	(2, P-1)	This is anorthite (CaAl2Si2O8)	5	(CA+2)1(AL+3)1(AL+3)1(Si+4)2(O-2)8
APATITE	Fluorapatite [Ca5F(PO4)3, H57]	H57	hP42	(176, P6_3/m)	This is Ca2Nf8(SiO4)6O2-Gd9.333(SiO4)6O2 solid solution	4	(CA+2, MG+2, ND+3, SR+2, VA)4(ND+3)6(SiO4-4)6(O-2)2
C11A7F	Ca6Al7O16F	-	cl152	(220, I-43d)	This is 11CaO.7Al2O3.CaF2	4	(AL+3)14(CA+2)12(F-1)2(O-2)32
C12A7	Mayenite (12 CaO.7Al2O3, K74, C12A7)	K74	cl152	(220, I-43d)	This is 12CaO.7Al2O3 (oS100, Cmc21), not stable under anhydrous conditions.	4	(CA+2)6(AL+3)6(AL+3)1(O-2)16.5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
C1A1	Al ₂ CaO ₄	-	mP84	(14, P2 ₁ /c)	This is CaO.Al ₂ O ₃	4	(CA+2, SR+2)3(AL+3)5(AL+3)1(O-2)12
C1A2	Al ₄ CaO ₇	-	mS48	(15, C2/c)	This is CaO.2Al ₂ O ₃ and SrO.2Al ₂ O ₃	4	(CA+2, SR+2)1(AL+3)3(AL+3)1(O-2)7
C1A6	Magnetoplumbite (PbFe ₁₂ O ₁₉)	-	hP64	(194, P6 ₃ /mmc)	This is CaO.6Al ₂ O ₃ and SrO.6Al ₂ O ₃	3	(CA+2, SR+2)1(AL+3)12(O-2)19
C1A8M2	CaMg ₂ Al ₁₆ O ₂₇	-	hP94	(187, P-6m2)	This is CaO.8Al ₂ O ₃ .2MgO	4	(CA+2)1(AL+3)16(MG+2)2(O-2)27
C2A14M2	BaFe ₁₅ O ₂₃	-	hR78	(166, R-3m)	This is 2CaO.14Al ₂ O ₃ .2MgO	4	(CA+2)2(AL+3)28(MG+2)2(O-2)46
C3A1	Ca ₃ Al ₂ O ₆	-	cP264	(205, Pa-3)	This is 3CaO.Al ₂ O ₃ and 3SrO.Al ₂ O ₃	3	(CA+2, SR+2)3(AL+3)2(O-2)6
C3A2M1	3CaO.2Al ₂ O ₃ .MgO	-	oP72	(57, Pbcm)	This is 3CaO.2Al ₂ O ₃ .MgO (oP72, Pbcm or Pca21);	4	(CA+2)3(AL+3)4(MG+2)1(O-2)10
C3A3F	Unknown Structure	-	-	-	This is 3CaO.3Al ₂ O ₃ .CaF ₂	4	(AL+3)6(CA+2)4(F-1)2(O-2)12
CA10Si ₃ O ₁₅ F ₂	Unknown Structure	-	-	-	This is 9CaO.3SiO ₂ .CaF ₂	4	(CA+2)10(Si+4)3(O-2)15(F-1)2
CA2AlF ₇	Ca ₂ AlF ₇	-	oP40	(62, Pnma)	-	3	(CA+2)2(AL+3)1(F-1)7
CA2NA ₂ Si ₂ O ₇	Na ₂ Ca ₂ Si ₂ O ₇	-	mS208	(15, C2/c)	-	4	(CA+2)2(NA+1)2(Si+4)2(O-2)7
CA2NA ₂ Si ₃ O ₉	Na(Na _{0.5} Ca _{0.5}) ₂ CaSi ₃ O ₉	-	hP102	(152, P3 ₁ 21)	-	4	(CA+2)2(NA+1)2(Si+4)3(O-2)9
CA2SiO ₄ _ALPHA_A	Ca ₂ SiO ₄	-	hP24	(194, P6 ₃ /mmc)	This is (Ca, Sr) ₂ SiO ₄	3	(CA+2, Li ₂ +2, MG+2, ND+3, SR+2, ZN+2)3 (CA+2, SR+2, VA)1(SiO ₄ -4)2
CA2SiO ₄ _ALPHA_PRIME	K ₂ CoCl ₄	-	oP84	(33, Pna2 ₁)	This is (Ca, Sr) ₂ SiO ₄	3	(CA+2, Li ₂ +2, MG+2, ND+3, SR+2, ZN+2)3 (CA+2, SR+2, VA)1(SiO ₄ -4)2
CA3NA ₂ Si ₆ O ₁₆	Na ₂ Ca ₃ Si ₆ O ₁₆	-	aP54	(2, P-1)	-	4	(CA+2)3(NA+1)2(Si+4)6(O-2)16
CA4Cl ₆ O	Ba ₄ Cl ₆ O	-	hP22	(186, P6 ₃ mc)	-	3	(CA+2, SR+2)4(CL-1)6(O-2)1
CA5Si ₂ O ₈ F ₂	Unknown Structure	-	-	-	This is 4CaO.2SiO ₂ .CaF ₂	4	(CA+2)5(Si+4)2(O-2)8(F-1)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CAALCL5	Unknown Structure	-	-	-	-	3	(CA+2)1(AL+3)1(CL-1)5
CAALF5_S1	CrMnF5	-	mS28	(15, C2/c)	-	3	(CA+2)1(AL+3)1(F-1)5
CAALF5_S2	CrMnF5	-	mP28	(14, P2_1/c)	-	3	(CA+2)1(AL+3)1(F-1)5
CACL2	Hydrophilite (CaCl ₂ , C35)	C35	oP6	(58, Pnnm)	This is CaCl ₂ and low temperature SrCl ₂	2	(CA+2, MG+2, SR+2)1(CL-1)2
CACLF	Matlockite (E01, PbCl)	E01	tP6	(129, P4/nmm)	-	3	(CA+2, SR+2)1(CL-1)1(F-1)1
CACO3	Calcite (CaCO ₃ , G01)	G01	hR10	(167, R-3c)	This is (Ca, Mg, Zn)CO ₃ .	2	(CA+2, MG+2, ZN+2)1(CO3-2)1
CAF2_S1	Fluorite (CaF ₂ , C1)	C1	cF12	(225, Fm-3m)	This is SrF ₂ and low temperature CaF ₂ .	2	(CA+2, MG+2, ND+3, SR+2, VA)1(F-1, O-2, VA)2
CAF2_S2	Cotunnite (PbCl ₂ , C23)	C23	oP12	(62, Pnma)	This is high temperature CaF ₂ .	2	(CA+2, MG+2, ND+3, SR+2, VA)1(F-1, O-2, VA)2
CAMG3O16S4	Unknown Structure	-	-	-	This is CaMg ₃ (SO ₄) ₄	3	(CA+2)1(MG+2)3(SO4-2)4
CAN2O4	Unknown Structure	-	-	-	-	2	(CA+2, SR+2)1(NO2-1)2
CAN2O6	Pb(NO ₃) ₂ (G21)	G21	cP36	(205, Pa-3)	This is (Ca, Mg, Sr)(NO ₃) ₂ solid solution.	2	(CA+2, MG+2, SR+2)1(NO3-1)2
CANA2Si5O12	Unknown Structure	-	-	-	-	4	(CA+2)1(NA+1)2(Si+4)5(O-2)12
CANA2SiO4	Na ₂ CaSiO ₄ (S66)	S66	cP32	(198, P2_13)	-	4	(CA+2)1(NA+1)2(Si+4)1(O-2)4
CANA4Si3O9	K ₄ SrGe ₃ O ₉	-	cP272	(205, Pa-3)	-	4	(CA+2)1(NA+1)4(Si+4)3(O-2)9
CANDAL3O7	Akermanite (Ca ₂ MgSi ₂ O ₇ , S53)	S53	tP24	(113, P-42_1m)	-	4	(AL+3)3(CA+2)1(ND+3)1(O-2)7
CANDALO4	K ₂ NiF ₄	-	tI14	(139, I4/mmm)	-	4	(AL+3)1(CA+2)1(ND+3)1(O-2)4
CASO4_S2	CePO ₄	-	hP18	(180, P6_222)	This is high- temperature (Ca, Mg)SO ₄ .	2	(CA+2, MG+2)1(SO4-2)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CAZNSI3O8	CAZNSI3O8	-	aP52	(2, P-1)	-	4	(CA+2)1(ZN+2)1(SI+4)3(O-2)8
CLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)	clinoenstatite and diopside.	4	(CA+2, MG+2)1(MG+2)1(SI+4)2(O-2)6
CORDIERITE	Na0.04 (Mg0.5Fe0.5)2Al4Si5O18	-	oS120	(66, Cccm)	This is 2Al2O3.2MgO.5SiO2.	4	(AL+3)4(MG+2)2(SI+4)5(O-2)18
CORUNDUM	Corundum (alpha-alumina, Al2O3, D51)	D51	hR10	(167, R-3c)	This is Al2O3	2	(AL+3)2(O-2)3
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	(227, Fd-3m)	-	2	(SI+4)1(SIO4-4)1
CRYOLITE	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)	This is (K, Li Na)3AlF6 ht solid solution.	2	(CA+2, K+1, LI+1, NA+1, VA)3(ALF4-1, ALF6-3)1
CUSPIDINE	Ca4[Si2O7]([OH]0.25F0.75)2	-	mP60	(14, P2_1/c)	This is 3CaO.2SiO2.CaF2	4	(CA+2)4(SI+4)2(O-2)7(F-1)2
GARNET	Orthorhombic Garnet	-	oF320	(70, Fddd)	This is Grossular, Uvarovite, Spessartine and Goldmanite Garnets.	4	(CA+2, MG+2)3(AL+3)2(SI+4)3(O-2)12
GLASERITE	K3Na[SO4]2	-	hP14	(164, P-3m1)	-	3	(K+1, NA+1)3(NA+1)1(SO4-2)2
GLAUBERITE	Na2Ca[SO4]2	-	mS52	(15, C2/c)	-	3	(NA+1)2(CA+2)1(SO4-2)2
HALITE_B1	Rock Salt/Halite (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is (K, Li, Na)(Cl, F) solid solution.	2	(CA+2, K+1, LI+1, MG+2, NA+1, VA, ZN+2)1 (CL-1, F-1)1
HALITE_OX	Rock Salt/Halite (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is CaO, MgO and SrO.	2	(AL+3, CA+2, LIAL1/2+2, MG+2, NA+1, ND+3, SR+2, VA, ZN+2)1(O-2)1
HATRURITE	Ca3(SiO4)O-b	-	hR81	(160, R3m)	This is 3CaO.SiO2.	3	(CA+2, ND+3, VA, ZN+2)3(SIO4-4)1(O-2)1
K10MG5SI11O32	Unknown Structure	-	-	-	-	4	(K+1)10(MG+2)5(SI+4)11(O-2)32
K2ALF5	Rb2MnF5	-	tP8	(123, P4/mmm)	-	3	(K+1)2(AL+3)1(F-1)5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
K2CA2C3O9	K2Ca2[CO3]3	-	hR96	(146, R3)	-	3	(K+1)2(CA+2)2(CO3-2)3
K2CA2SI2O7	K2Ca2[Si2O7]	-	hP108	(176, P6_3/m)	-	4	(K+1)2(CA+2)2(SI+4)2(O-2)7
K2CA2SI9O21	Unknown Structure	-	-	-	-	4	(K+1)2(CA+2)2(SI+4)9(O-2)21
K2CA3SI6O16	Unknown Structure	-	-	-	-	4	(K+1)2(CA+2)3(SI+4)6(O-2)16
K2CA6SI4O15	K2Ca6Si4O15	-	mP54	(13, P2/c)	-	4	(K+1)2(CA+2)6(SI+4)4(O-2)15
K2CAC2O6_S1	K2Ca[CO3]2	-	hR33	(166, R-3m)	-	3	(K+1)2(CA+2)1(CO3-2)2
K2CAC2O6_S2	K0.67Ca0.33[CO3]2	-	hP40	(194, P6_3/mmc)	This is (K, Na)2Ca(CO3)2 solid solution.	3	(K+1, NA+1)2(CA+2)1(CO3-2)2
K2CAN4O8	K2Ca[NO2]4	-	mS30	(12, C2/m)	-	3	(K+1)2(CA+2)1(NO2-1)4
K2CASIO4	Unknown Structure	-	-	-	-	4	(K+1)2(CA+2)1(SI+4)1(O-2)4
K2CO3_S1	K2[CO3]	-	mP24	(14, P2_1/c)	With solubility of Na and SO4.	2	(K+1, NA+1)2(CO3-2, SO4-2)1
K2LIALF6	-	-	hP30	(156, P3m1)	-	3	(K+1)2(LI+1)1(ALF6-3)1
K2MG5SI12O30	K2Mg5Si12O30	-	hP100	(192, P6/mcc)	-	4	(K+1)2(MG+2)5(SI+4)12(O-2)30
K2MGF4	K2NiF4	-	tI14	(139, I4/mmm)	This is K2ZnF4 and K2Mg(Cl, F)4 solid solution.	3	(K+1, NA+1)2(MG+2, ZN+2)1(CL-1, F-1)4
K2MGN4O12	Unknown Structure	-	-	-	-	3	(K+1)2(MG+2)1(NO3-1)4
K2MGSI3O8	KLi[SO4]	-	hP14	(159, P31c)	-	4	(K2MG+4)1(SI+4)1(SI+4)2(O-2)8
K2MGSI5O12	K8(Al0.33Si0.67)24O48	-	tI160	(88, I4_1/a)	-	5	(K+1)2(MG+2)1(SI+4)1(SI+4)4(O-2)12
K2MGSI04_S1	Na2Be[SiO4]	-	oP64	(29, Pca2_1)	-	2	(K2MG+4, SI+4)1(SIO4-4)1
K2MGSI04_S2	Unknown Structure	-	-	-	-	2	(K2MG+4, SI+4)1(SIO4-4)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
K2NAALF6	Double Perovskite (Ba2MnWO6)	-	cF40	(225, Fm-3m)	-	3	(K+1)2(NA+1)1(ALF6-3)1
K2NDCL5	K2PrCl5	-	oP32	(62, Pnma)	-	3	(K+1)2(ND+3)1(CL-1)5
K2NO3CL	K2[PO3F]	-	oP28	(62, Pnma)	-	3	(K+1)2(NO3-1)1(CL-1)1
K2Si4O9_ALPHA	K2Si4O9	-	aP30	(2, P-1)	Low-temp K2Si4O9 (tricl)	3	(K+1)2(Si+4)4(O-2)9
K2Si4O9_BETA	K2Si4O9	-	hP30	(176, P6_3/m)	High-temp K2Si4O9 (hex)	3	(K+1)2(Si+4)4(O-2)9
K2SO4_S1	Arcanite (K2SO4, H16)	H16	oP28	(62, Pnma)	-	2	(CA+2, K+1, MG+2, NA+1, VA)2(CO3-2, SO4-2)1
K2SR2S3O12_S1	Unknown Structure	-	-	-	-	3	(K+1)2(SR+2)2(SO4-2)3
K2SR2S3O12_S2	Unknown Structure	-	-	-	-	3	(K+1)2(SR+2)2(SO4-2)3
K2SRCL4	Th3P4 (D73)	D73	cl28	(220, I-43d)	-	3	(K+1)2(SR+2)1(CL-1)4
K2ZNCL4	Arcanite (K2SO4, H16)	H16	oP28	(62, Pnma)	-	3	(K+1)2(ZN+2)1(CL-1)4
K2ZNS2O8	Ba2Ni[PO4]2	-	mP52	(14, P2_1/c)	-	3	(K+1)2(ZN+2)1(SO4-2)2
K3FCO3	Unknown Structure	-	-	-	This is K3F(CO3, SO4) solid solution.	3	(K+1)3(F-1)1(CO3-2, SO4-2)1
K3MG2CL7	Sr3Ti2O7	-	tl24	(139, I4/mmm)	-	3	(K+1)3(MG+2)2(CL-1)7
K3NDCL6	Double Perovskite (Ba2MnWO6)	-	cF40	(225, Fm-3m)	-	3	(K+1)3(ND+3)1(CL-1)6
K3SIF7	Unknown Structure	-	-	-	-	3	(K+1)3(Si+4)1(F-1)7
K3SR2N7O14	Unknown Structure	-	-	-	-	3	(K+1)3(SR+2)2(NO2-1)7
K4AL22O35	K2Al10.67O17	-	hR30	(166, R-3m)	This is Beta double prime-Al2O3 K4AL22O35.	6	(K+1, VA)1(K+1, VA)1(AL+3, MG+2)2(O-2, VA)1(AL+3)9(O-2)17

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
K4CAS7O21	Unknown Structure	-	-	-	-	3	(K+1)4(CA+2)5(CO3-2)7
K4CAN6O18	Unknown Structure	-	-	-	-	3	(K+1)4(CA+2)1(NO3-1)6
K4CASI3O9	K4SrGe3O9	-	cP272	(205, Pa-3)	-	4	(K+1)4(CA+2)1(SI+4)3(O-2)9
K4CASI6O15	Unknown Structure	-	-	-	-	4	(K+1)4(CA+2)1(SI+4)6(O-2)15
K4MG2SI5O14	Unknown Structure	-	-	-	-	4	(K+1)4(MG+2)2(SI+4)5(O-2)14
K4SIO4	Cs4SnO4	-	mP36	(14, P2_1/c)	-	3	(K+1)4(SI+4)1(O-2)4
K5ZN4CL13	Unknown Structure	-	-	-	-	3	(K+1)5(ZN+2)4(CL-1)13
K8CASI10O25	Unknown Structure	-	-	-	-	4	(K+1)8(CA+2)1(SI+4)10(O-2)25
KAL11O17	beta-Alumina (D56, Al2O3)	D56	hP60	(194, P6_3/mmc)	This is Beta- Al2O3 KAl11O17.	6	(K+1, VA)1(K+1, VA)1(AL+3, MG+2)2(O-2, VA)1(AL+3)9(O-2)17
KAL4F13	Unknown Structure	-	-	-	-	3	(K+1)1(AL+3)4(F-1)13
KALCL4	KAICl4	-	mP24	(4, P2_1)	-	3	(K+1)1(AL+3)1(CL-1)4
KALF4	RbAlF4	-	tP12	(127, P4/mbm)	-	3	(K+1)1(AL+3)1(F-1)4
KLI3N4O8	Unknown Structure	-	-	-	-	3	(K+1)1(LI+1)3(NO2-1)4
KLICO3	LiBa[BO3]	-	mP24	(14, P2_1/c)	-	3	(K+1)1(LI+1)1(CO3-2)1
KLIN2O6	Unknown Structure	-	-	-	-	3	(K+1)1(LI+1)1(NO3-1)2
KLISO4_ALPHA	LiKSO4 (H14)	H14	hP14	(173, P6_3)	-	3	(K+1)1(LI+1)1(SO4-2)1
KLISO4_BETA	Li[NH4][SO4]	-	oP44	(62, Pnma)	-	3	(K+1, LI+1)1(LI+1)1(SO4-2)1
KLISO4_GAMMA	KLi[SO4]	-	hP24	(194, P6_3/mmc)	-	3	(K+1, LI+1)1(LI+1)1(SO4-2)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
KMG2AL15O25	Unknown Structure	-	-	-	-	4	(K+1)1(MG+2)2(AL+3)15(O-2)25
KMGCLSO4	Unknown Structure	-	-	-	-	4	(K+1)1(MG+2)1(CL-1)1(SO4-2)1
KMGF3	Cubic Perovskite (CaTiO ₃ , E21)	E21	cP5	(221, Pm-3m)	This is KCa(Cl, F) ₃ , K(Mg, Zn)F ₃ , ht NaMgF ₃ and KMg(Cl, F) ₃ solid solution.	3	(K+1, Li+1, NA+1)1(CA+2, MG+2, SR+2, ZN+2)1(CL-1, F-1)3
KND2CL7	Unknown Structure	-	-	-	-	3	(K+1)1(ND+3)2(CL-1)7
KNO2_S1	K[NO ₂]-b	-	hR57	(166, R-3m)	-	2	(K+1)1(NO2-1, NO3-1)1
KNO2_S2	K[NO ₂]	-	cF104	(225, Fm-3m)	-	2	(K+1)1(NO2-1, NO3-1)1
KNO3_S1	alpha-Potassium Nitrate (KNO ₃) I	-	oP20	(62, Pnma)	This is lt-KNO ₃ with solubility of Na and KNO ₂ .	2	(K+1, NA+1)1(NO2-1, NO3-1)1
KSR2CL5	U ₂ PbSe ₅	-	mP32	(14, P2_1/c)	-	3	(K+1)1(SR+2)2(CL-1)5
KYANITE	Kyanite (Al ₂ SiO ₅ , S01)	S01	aP32	(2, P-1)	This is Al ₂ O ₃ .SiO ₂ (oP32, Pnma)	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
KZN2CL5	Unknown Structure	-	-	-	-	3	(K+1)1(ZN+2)2(CL-1)5
LANGBEINITE_S1	K ₂ Mg ₂ [SO ₄] ₃	-	cP76	(198, P2_13)	This is K ₂ (Ca, Mg, Zn) ₂ [SO ₄] ₃ .	3	(K+1)2(CA+2, MG+2, ZN+2)2(SO4-2)3
LANGBEINITE_S2	Unknown Structure	-	-	-	This is mid temperature K ₂ Ca ₂ [SO ₄] ₃ .	3	(K+1)2(CA+2)2(SO4-2)3
LANGBEINITE_S3	Unknown Structure	-	-	-	This is high temperature K ₂ Ca ₂ [SO ₄] ₃ .	3	(K+1)2(CA+2)2(SO4-2)3
LARNITE	Parawollastonite (CaSiO ₃ , S33(II))	S33(II)	mP60	(14, P2_1/c)	This is 2CaO.SiO ₂ (metastable at 1 atm)	3	(CA+2)2(SI+4)1(O-2)4
LI12K2ZNCL16	Unknown Structure	-	-	-	-	4	(LI+1)12(K+1)2(ZN+2)1(CL-1)16
LI2CA2SI2O7	Li ₂ Ca ₂ [Si ₂ O ₇]	-	hP78	(178, P6_122)	-	4	(LI+2)1(CA+2)2(SI+4)2(O-2)7
LI2CA3SI6O16	Unknown Structure	-	-	-	-	4	(LI+2)1(CA+2)3(SI+4)6(O-2)16

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LI2CA4SI4O13	Li ₂ Ca ₄ Si ₄ O ₁₃	-	aP46	(2, P-1)	-	4	(Li ₂ +2)1(CA+2)4(SI+4)4(O-2)13
LI2CASIO4	[NH ₄]Ag ₂ As ₄	-	tI16	(121, I-42m)	-	4	(Li ₂ +2)1(CA+2)1(SI+4)1(O-2)4
LI2CO3	Li ₂ [CO ₃]	-	mS24	(15, C2/c)	-	2	(Li+1)2(CO3-2)1
LI2MG2S3O12	Li ₂ Fe ₂ [MoO ₄] ₃	-	oP76	(60, Pbcn)	-	3	(Li+1)2(MG+2)2(SO4-2)3
LI2SI2O5_S1	Li ₂ Si ₂ O ₅	-	oS36	(37, Ccc2)	-	3	(Li+1, NA+1)2(SI+4)2(O-2)5
LI2SI2O5_S2	Unknown Structure	-	-	-	-	3	(Li+1, NA+1)2(SI+4)2(O-2)5
LI2SO4_S1	Li ₂ [SO ₄]	-	mP28	(14, P2_1/c)	-	2	(Li+1)2(SO4-2)1
LI2SO4_S2	K ₂ [SO ₄]	-	cF12	(225, Fm-3m)	-	2	(K+1, Li+1, MG+2, NA+1, VA, ZN+2)2(CO3-2, SO4-2)1
LI2ZNCL4_S1	Spinel (Al ₂ MgO ₄ , H11)	H11	cF56	(227, Fd-3m)	This is low temperature Li ₂ ZnCl ₄ .	3	(Li+1)2(ZN+2)1(CL-1)4
LI2ZNS2O8	Li ₂ Ni[SO ₄] ₂	-	oP104	(61, Pbca)	-	3	(Li+1)2(ZN+2)1(SO4-2)2
LI3ALF6_S1	Li ₃ VF ₆	-	mS120	(15, C2/c)	-	2	(Li+1)3(ALF6-3)1
LI3K2ZN4CL13	Unknown Structure	-	-	-	-	4	(Li+1)3(K+1)2(ZN+2)4(CL-1)13
LI3NASIO4	Unknown Structure	-	-	-	-	4	(Li+1)3(NA+1)1(SI+4)1(O-2)4
LI4SIO4	Li ₄ [SiO ₄]	-	mP28	(11, P2_1/m)	-	4	(Li ₂ +2, NA ₂ +2)1(Li ₂ +2, MG+2, NA ₂ +2)1(SI+4)1(O-2)4
LI5ALO4	Li ₅ AlO ₄	-	oP20	(59, Pmmn)	-	3	(Li+1)5(AL+3)1(O-2)4
LI6SI2O7	Li ₆ [Si ₂ O ₇]	-	tP30	(113, P-42_1m)	-	3	(Li+1)6(SI+4)2(O-2)7
LI8SIO6	Li ₈ CoO ₆	-	hP30	(185, P6_3cm)	-	3	(Li+1)8(SI+4)1(O-2)6

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LIAL5O8	LiFe5O8	-	cP56	(213, P4 ₁ 32)	This is low-temp LiAl5O8.	3	(Li+1)1(AL+3)5(O-2)8
LIALCL4	LiAlCl4	-	mP24	(14, P2 ₁ /c)	-	3	(Li+1)1(AL+3)1(CL-1)4
LIALO2_A	NaFeO2	-	hR12	(166, R-3m)	This is low-temp LiAlO2.	2	(LIAL+4)1(O-2)2
LICACL3	Unknown Structure	-	-	-	-	3	(Li+1)1(CA+2)1(CL-1)3
LICAN3O6	Unknown Structure	-	-	-	-	3	(Li+1)1(CA+2)1(NO2-1)3
LIKMGCL4	Unknown Structure	-	-	-	-	4	(Li+1)1(K+1)1(MG+2)1(CL-1)4
LINASO4_S1	NaLi[SO4]	-	hP42	(159, P31c)	-	3	(Li+1)1(NA+1)1(SO4-2)1
LINASO4_S2	Unknown Structure	-	-	-	-	3	(Li+1, NA+1)1(Li+1, NA+1)1(SO4-2)1
LIND2CL7	Unknown Structure	-	-	-	-	3	(Li+1)1(ND+3)2(CL-1)7
LINO2_S1	Unknown Structure	-	-	-	-	2	(Li+1)1(NO2-1, NO3-1)1
LINO2_S2	Unknown Structure	-	-	-	-	2	(Li+1)1(NO2-1, NO3-1)1
LINO3	CaCO3	-	hR30	(167, R-3c)	-	2	(Li+1)1(NO3-1)1
LOWCLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)	This is low- clinoenstatite and low-clinodiopside	4	(CA+2, MG+2)1(MG+2)1(SI+4)2(O-2)6
M2O3A	La2O3 (D52)	D52	hP5	(164, P-3m1)	-	2	(ND+3, SR+2)2(O-2, VA)3
M2O3H	H-La2O3	-	hP10	(194, P6 ₃ /mmc)	-	2	(ND+3, SR+2)2(O-2, VA)3
M2O3X	Nd2O3	-	cl26	(229, Im-3m)	-	2	(ND+3, SR+2)2(O-2, VA)3
MELILITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42 ₁ m)	This is gehlenite and akermanite.	5	(CA+2)2(AL+3, MG+2, ZN+2)1(AL+3, SI+4)1(SI+4)1(O-2)7

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MERWINITE	Ca3Mg(SiO4)2	-	mP56	(14, P2_1/c)	This is 3CaO.MgO.2SiO2	4	(CA+2)3(MG+2)1(SI+4)2(O-2)8
MG2NA2Si6O15	Na2Mg2Si6O15	-	oS200	(64, Cmce)	-	4	(MG+2)2(NA+1)2(SI+4)6(O-2)15
MG3ND2O2CL8	Unknown Structure	-	-	-	-	4	(MG+2)3(ND+3)2(O-2)2(CL-1)8
MGAL2CL8	CoAl2Cl8	-	mS44	(15, C2/c)	-	3	(MG+2)1(AL+3)2(CL-1)8
MGAL2F8	Unknown Structure	-	-	-	-	3	(MG+2)1(AL+3)2(F-1)8
MGCL2	CdI2	-	hP3	(164, P-3m1)	-	2	(LI+2, MG+2)1(CL-1)2
MGF2	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mmm)	This is MgF2 and It- ZnF2.	2	(LI+2, MG+2, ZN+2)1(F-1)2
MGNA2Si4O10	Unknown Structure	-	-	-	-	4	(MG+2)1(NA+1)2(SI+4)4(O-2)10
MULLITE	Al(Al0.7Si0.3)2O4.8	-	oP24	(55, Pbam)	-	4	(AL+3)1(AL+3)1(AL+3, SI+4)1(O-2, VA)5
NA10SiO7	Unknown Structure	-	-	-	-	3	(NA+1)10(SI+4)1(O-2)7
NA2AL12O19	Na0.5Al3O4.75	-	oP24	(55, Pbam)	This is Beta double prime-Al2O3 Na2Al12O19.	3	(NA+1)2(AL+3)12(O-2)19
NA2CA3AL16O28	Unknown Structure	-	-	-	-	4	(NA+1)2(CA+2)3(AL+3)16(O-2)28
NA2CA8AL6O18	Unknown Structure	-	-	-	-	4	(NA+1)2(CA+2)8(AL+3)6(O-2)18
NA2CAAL4O8	Unknown Structure	-	-	-	This is (K, Na)2CaAl4O8 solid solution.	4	(K+1, NA+1, VA)1(CA+2, K+1, NA+1)1(AL+3)2(O-2)4
NA2CO3_S1	Na2[CO3]-b	-	mS24	(12, C2/m)	With solubility of K.	2	(K+1, LI+1, NA+1)2(CO3-2)1
NA2CO3_S2	Na2[CO3]	-	hP12	(194, P6_3/mmc)	This is high temperature K2CO3-Na2CO3-K2SO4-Na2SO4 solid solutions	2	(CA+2, K+1, LI+1, MG+2, NA+1, SR+2, VA, ZN+2)2(CO3-2, SO4-2)1
NA2LIALF6	Ca(Ca0.5Nd0.5)2NbO6	-	mP20	(14, P2_1/c)	-	3	(NA+1)2(LI+1)1(ALF6-3)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NA2MG3S4O16	NaCaFe3[PO4]4	-	oP200	(61, Pbca)	-	3	(NA+1)2(MG+2)3(SO4-2)4
NA2MGCL4	Sr2PbO4	-	oP20	(55, Pbam)	-	3	(NA+1)2(MG+2)1(CL-1)4
NA2MGS2O8_S1	Na2Mg[SO4]2	-	aP209	(2, P-1)	-	3	(NA+1)2(MG+2)1(SO4-2)2
NA2MGS2O8_S2	Unknown Structure	-	-	-	-	3	(NA+1)2(MG+2)1(SO4-2)2
NA2MGS2O8_S3	Unknown Structure	-	-	-	-	3	(NA+1)2(MG+2)1(SO4-2)2
NA2NO3NO2	Unknown Structure	-	-	-	-	3	(NA+1)2(NO3-1)1(NO2-1)1
NA2O1_S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is rt (K, Li, Na)2O.	2	(K+1, LI+1, NA+1)2(O-2)1
NA2O1_S2	Unknown Structure	-	-	-	This is ht1 (K, Na)2O.	2	(K+1, NA+1)2(O-2)1
NA2O1_S3	Unknown Structure	-	-	-	This is ht2 (K, Na)2O.	2	(K+1, NA+1)2(O-2)1
NA2Si2O5_ALPHA	Na2Si2O5-a	-	mP36	(14, P2_1/c)	This is lt-(K, Na)2Si2O5 solid solution.	3	(K+1, NA+1)2(SI+4)2(O-2)5
NA2Si2O5_BETA	Na2Si2O5-b	-	mP36	(14, P2_1/c)	This is intermediat-temp (K, Na)2Si2O5 solid solution.	3	(K+1, NA+1)2(SI+4)2(O-2)5
NA2Si2O5_GAMMA	Na2Si2O5	-	oP36	(60, Pbcn)	This is ht-(K, Na)2Si2O5 solid solution.	3	(K+1, NA+1)2(SI+4)2(O-2)5
NA2SiF6_S1	Na2SiF6	-	hP27	(150, P321)	low-temperature trigonal phase	2	(NA+1)2(SIF6-2)1
NA2SiF6_S2	K2PtCl6 (J11)	J11	cF36	(225, Fm-3m)	high- temperature cubic phase	2	(K+1, NA+1)2(SIF6-2)1
NA2SiO3	Na2SiO3	-	oS24	(36, Cmc2_1)	This is (K, Na)2SiO3 solid solution.	3	(K+1, LI+1, NA+1)2(SI+4)1(O-2)3
NA2SO4_S1	Thenardite [Na2SO4 (V), H17]	H17	oF56	(70, Fddd)	-	2	(K+1, NA+1)2(SO4-2)1
NA2SO4_S2	Na2CrO4 (H18)	H18	oS28	(63, Cmcn)	-	2	(K+1, NA+1)2(SO4-2)1
NA2ZN3S4O16	Unknown Structure	-	-	-	-	3	(NA+1)2(ZN+2)3(SO4-2)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NA2ZNCL4	Forsterite (Mg2SiO4, S12)	S12	oP28	(62, Pnma)	This is Na2ZnCl4 and high temperature Li2ZnCl4.	3	(Li+1, NA+1)2(ZN+2)1(CL-1)4
NA2ZNS2O8	Na2Zn[SO4]2	-	mP104	(13, P2/c)	-	3	(NA+1)2(ZN+2)1(SO4-2)2
NA3ALF6_S1	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)	-	3	(NA+1)3(AL+3)1(F-1)6
NA3LI3AL2F12	Garnet [S14, Co3Al2(SiO4)3]	S14	cl160	(230, Ia-3d)	-	3	(NA+1)3(LI+1)3(ALF6-3)2
NA3ND5CL18	Unknown Structure	-	-	-	-	3	(NA+1)3(ND+3)5(CL-1)18
NA3SO4F	Na3[SO4]F	-	mP108	(11, P2_1/m)	-	3	(NA+1)3(SO4-2)1(F-1)1
NA4SiO4	K4SnO4	-	aP18	(2, P-1)	-	4	(LI2+2, NA2+2)1(LI2+2, NA2+2)1(SI+4)1(O-2)4
NA4ZNS3O12	Unknown Structure	-	-	-	-	3	(NA+1)4(ZN+2)1(SO4-2)3
NA5AL3F14	Chiolite (Na5Al3F14, K75)	K75	tP44	(128, P4/mnc)	-	3	(NA+1)5(AL+3)3(F-1)14
NA5ND9F32	Unknown Structure	-	-	-	-	3	(NA+1)5(ND+3)9(F-1)32
NA6CAS4O16	Unknown Structure	-	-	-	-	3	(NA+1)6(CA+2)1(SO4-2)4
NA6MGS4O16	Na6Mg[SO4]4	-	mP54	(14, P2_1/c)	-	3	(NA+1)6(MG+2)1(SO4-2)4
NA6Si2O7	Na6[Si2O7]	-	aP120	(2, P-1)	-	3	(NA+1)6(SI+4)2(O-2)7
NA6Si8O19	Na6Si8O19	-	mP132	(14, P2_1/c)	-	3	(NA+1)6(SI+4)8(O-2)19
NA6ZNS4O16	Unknown Structure	-	-	-	-	3	(NA+1)6(ZN+2)1(SO4-2)4
NAAL11O17	NaAl11O17	-	hP58	(194, P6_3/mmc)	This is Beta- Al2O3 NaAl11O17 solid solution.	5	(LI+1, NA+1)2(NA+1, VA)2(AL+3)22(O-2)34(O-2, VA)1
NAALCL4	NaAlCl4	-	oP24	(19, P2_12_12_1)	-	3	(NA+1)1(AL+3)1(CL-1)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NAALO2_D	LiGaO2	-	oP16	(33, Pna2_1)	-	2	(NAAL+4)1(O-2)2
NACAALF6_S1	NaCaAlF6	-	mP72	(14, P2_1/c)	-	4	(NA+1)1(CA+2)1(AL+3)1(F-1)6
NACAALF6_S2	Unknown Structure	-	-	-	-	4	(NA+1)1(CA+2)1(AL+3)1(F-1)6
NACAALF6_S3	Unknown Structure	-	-	-	-	4	(NA+1)1(CA+2)1(AL+3)1(F-1)6
NAFEO2_B	LiGaO2	-	oP16	(33, Pna2_1)	This is low-temp KAlO2 and NaAlO2 solid solutions.	2	(KAL+4, NAAL+4)1(O-2)2
NAFEO2_G	LiAlO2	-	tP16	(92, P4_12_12)	This is high-temp KAlO2, LiAlO2 and mid-temp NaAlO2 solid solutions.	2	(KAL+4, LIAL+4, NAAL+4)1(O-2)2
NAKZNS2O8	Unknown Structure	-	-	-	-	4	(NA+1)1(K+1)1(ZN+2)1(SO4-2)2
NALICO3_S1	NaLi[CO3]	-	aP54	(1, P1)	-	3	(NA+1)1(LI+1)1(CO3-2)1
NALICO3_S2	NaLi[CO3]	-	hP54	(174, P-6)	-	3	(NA+1)1(LI+1)1(CO3-2)1
NALICO3_S3	NaLi[CO3]	-	hP21	(174, P-6)	-	3	(NA+1)1(LI+1)1(CO3-2)1
NAMGCL3	Ilmenite (FeTiO3, E22)	E22	hR10	(148, R-3)	-	3	(NA+1)1(MG+2)1(CL-1)3
NAMGF3	CaTiO3 Pnma Perovskite	-	oP20	(62, Pnma)	-	3	(NA+1)1(MG+2, ZN+2)1(F-1)3
NANO2	Na[NO2]	-	oI16	(17, P222_1)	-	2	(NA+1)1(NO2-1, NO3-1)1
NANO3_S1	Calcite (CaCO3, G01)	G01	hR10	(167, R-3c)	With solubility of K.	2	(K+1, NA+1)1(NO3-1)1
NANO3_S2	Rb[NO3]	-	hR9	(166, R-3m)	This is ht-(K, Na)(NO3) solid solution.	2	(K+1, NA+1)1(NO2-1, NO3-1)1
ND2S3O12	Nd2[SO4]3	-	mS68	(15, C2/c)	-	2	(ND+3)2(SO4-2)3
ND2SI2O7	beta-Ca2[P2O7]	-	tP88	(76, P4_1)	-	3	(ND+3)2(SI+4)2(O-2)7
ND2SIO5	Gd2SiO5 (RE2SIO5 X1)	-	mP32	(14, P2_1/c)	-	3	(ND+3)2(SI+4)1(O-2)5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NDAL11O18	La0.83Al11.83O19	-	hP84	(194, P6 ₃ /mmc)	-	3	(ND+3)1(AL+3)11(O-2)18
NDAL3CL12	Unknown Structure	-	-	-	-	3	(ND+3)1(AL+3)3(CL-1)12
NDAP	LaAlO ₃	-	hR30	(167, R-3c)	-	3	(ND+3)1(AL+3)1(O-2)3
NDCL3	UCl ₃	-	hP8	(176, P6 ₃ /m)	-	2	(ND+3)1(CL-1)3
NDF3	H3Ho	-	hP24	(165, P-3c1)	-	3	(CA+2, ND+3, SR+2)1(CA+2, SR+2, VA)1(F-1)3
NDNAF4	Na(Na0.5Nd0.5)NdF ₆	-	hP10	(174, P-6)	-	3	(NA+1)1(ND+3)1(F-1)4
NDOCL	Matlockite (E01, PbFCI)	E01	tP6	(129, P4/nmm)	-	3	(ND+3)1(O-2)1(CL-1)1
NEPHELINE_G	KLi[SO ₄]	-	hP18	(173, P6 ₃)	This is K ₂ MgSi ₃ O ₈ .	4	(K2MG+4)4(Si+4)4(Si+4)8(O-2)32
OLIVINE	Forsterite (Mg ₂ SiO ₄ , S12)	S12	oP28	(62, Pnma)	This is 2CaO.SiO ₂ , forsterite and monticellite[CaO.MgO.SiO ₂]	4	(CA+2, LI2+2, MG+2, ZN+2)1(CA+2, LI2+2, MG+2, ZN+2)1(Si+4)1(O-2)4
ORTHO_PYROXENE	Enstatite (MgSiO ₃ , S43)	S43	oP80	(61, Pbca)	This is enstatite and orthodiopside	4	(CA+2, MG+2)1(MG+2)1(Si+4)2(O-2)6
PROTO_PYROXENE	MgSiO ₃	-	oP40	(60, Pbcn)	This is proto- enstatite and protodiopside.	3	(CA+2, MG+2, ZN+2)1(Si+4)1(O-2)3
PSEUDO_WOLLASTONITE	CaSiO ₃	-	mS120	(15, C2/c)	This is CaO.SiO ₂	3	(CA+2, SR+2)1(Si+4)1(O-2)3
QUARTZ	alpha-Quartz (low Quartz)	-	hP9	(152, P3 ₁ 21)	-	2	(Si+4)1(SiO4-4)1
RANKINITE	3CaO.2SiO ₂	-	mP48	(14, P2 ₁ /c)	This is 3CaO.2SiO ₂	3	(CA+2)3(Si+4)2(O-2)7
SAPPHIRINE	CaMg ₃ Si ₃ O ₁₀	-	aP68	(2, P-1)	This is 9Al ₂ O ₃ .7MgO.3SiO ₂	4	(AL+3)18(MG+2)7(Si+4)3(O-2)40
SILLIMANITE	Sillimanite (Al ₂ SiO ₅ , S03)	S03	oP32	(62, Pnma)	This is a high-pressure phase (Al ₂ O ₃ .SiO ₂)	4	(AL+3)1(AL+3)1(Si+4)1(O-2)5
SPINEL	Spinel (Al ₂ MgO ₄ , H11)	H11	cF56	(227, Fd-3m)	This is MgAl ₂ O ₄ .	4	(AL+3, LI+1, MG+2, ZN+2)1(AL+3, LI+1,

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							MG+2, NA+1, VA, ZN+2)2(MG+2, VA)2(O-2)4
SR3ND4O9	(Sr0.5Nd0.5)6NdO9	-	mS64	(9, Cc)	-	3	(SR+2)3(ND+3)4(O-2)9
SR3NDCL9	Unknown Structure	-	-	-	-	3	(SR+2)3(ND+3)1(CL-1)9
SR3SiO5	Sr3[SiO4]O	-	tP36	(130, P4/ncc)	-	3	(SR+2)3(Si+4)1(O-2)5
SR5ND8O17	Unknown Structure	-	-	-	-	3	(SR+2)5(ND+3)8(O-2)17
SRCL2_S2	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	-	2	(CA+2, SR+2)1(CL-1)2
SRCO3_S1	Ca[CO3]-a	-	oP20	(62, Pnma)	-	2	(SR+2)1(CO3-2)1
SRCO3_S2	NaNO3	-	hR48	(167, R-3c)	-	2	(SR+2)1(CO3-2)1
SRMGF4_S1	Bi[ReO4]	-	oS24	(63, Cmcm)	-	3	(MG+2)1(SR+2)1(F-1)4
SRMGF4_S2	Unknown Structure	-	-	-	-	3	(MG+2)1(SR+2)1(F-1)4
SRND2O4	CaV2O4	-	oP28	(62, Pnma)	-	3	(SR+2)1(ND+3)2(O-2)4
SRND4O7	Unknown Structure	-	-	-	-	3	(SR+2)1(ND+3)4(O-2)7
SRSiO3	SrSiO3	-	mS60	(15, C2/c)	-	3	(CA+2, SR+2)1(Si+4)1(O-2)3
SRSO4_S1	Barite (BaSO4, H02)	H02	oP24	(62, Pnma)	low- temperature (Sr, Zn)SO4	2	(SR+2)1(SO4-2)1
SRSO4_S2	High-Temperature Cubic KClO4 (H05)	H05	cF24	(216, F-43m)	high-temperature (Sr, Zn)SO4	2	(SR+2)1(SO4-2)1
SRZNCL4	Scheelite (CaWO4, H04)	H04	tI24	(88, I4_1/a)	-	3	(SR+2)1(ZN+2)1(CL-1)4
TRIDYMITTE	Monoclinic (Cc) Low Tridymite (SiO2)	-	mS144	(9, Cc)	-	2	(Si+4)1(SiO4-4)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
WOLLASTONITE	Wollastonite (CaSiO ₃)	-	aP30	(2, P-1)	This is CaO.SiO ₂ .	3	(CA+2, MG+2)1(SI+4)1(O-2)3
ZINCITE	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	This is ZnO with Ca and Mg solubility.	2	(CA+2, MG+2, ZN+2)1(O-2)1
ZN2SIO4	Phenakite (Be2SiO ₄ , S13)	S13	hR42	(148, R-3)	-	4	(MG+2, ZN+2)1(MG+2, ZN+2)1(SI+4)1(O-2)4
ZN2SO4CL2	Unknown Structure	-	-	-	-	3	(ZN+2)2(SO4-2)1(CL-1)2
ZN4S3O12CL2	Unknown Structure	-	-	-	-	3	(ZN+2)4(SO4-2)3(CL-1)2
ZNCL2	ZnCl ₂	-	oP12	(33, Pna2_1)	-	2	(LI2+2, ZN+2)1(CL-1)2
ZNF2_S2	Unknown Structure	-	-	-	-	2	(LI2+2, ZN+2)1(F-1)2
ZNN2O6	Unknown Structure	-	-	-	-	2	(ZN+2)1(NO3-1)2
ZNSO4_S1	Chalcocyanite (CuSO ₄)	-	oP24	(62, Pnma)	-	2	(ZN+2)1(SO4-2)1
ZNSO4_S2	Zn[SO ₄]	-	cF24	(216, F-43m)	-	2	(ZN+2)1(SO4-2)1
ZNSO4_S3	Unknown Structure	-	-	-	-	2	(ZN+2)1(SO4-2)1

TCSALT: TCS Molten Salts Database Revision History

Current Database Version

Database name (acronym):	TCS Molten Salts Database (TCSALT)
Database owner:	Thermo-Calc Software AB
Database version:	3.0
First release:	TCSALT1 was released with 2024a

TCSALT2 to TCSALT3

Software release version: 2026b (June 2026)

New Elements and Phases

- Four new elements (for a total of 16).
- One new metal (cation): Neodymium (Nd).
- Four new types of salts (anions): Nitrate (NO₃-1), Nitrite (NO₂-1), Carbonate (CO₃-2), Sulfate (SO₄-2).
- 107 new phases (284 phases in total).

Systems

- 54 new pseudo-binary systems are assessed: AlCl₃-NdCl₃, CaCl₂-NdCl₃, KCl-NdCl₃, LiCl-NdCl₃, MgCl₂-NdCl₃, NaCl-NdCl₃, NdCl₃-SrCl₂, AlF₃-NdF₃, CaF₂-NdF₃, LiF-NdF₃, MgF₂-NdF₃, NaF-NdF₃, NdF₃-SrF₂, Al₂O₃-Nd₂O₃, CaO-Nd₂O₃, MgO-Nd₂O₃, Nd₂O₃-SiO₂, Ca(NO₂)₂-KNO₂, Ca(NO₂)₂-LiNO₂, Ca(NO₂)₂-NaNO₂, KNO₂-LiNO₂, KNO₂-NaNO₂, LiNO₂-NaNO₂, Ca(NO₃)₂-KNO₂, Ca(NO₃)₂-LiNO₃, Ca(NO₃)₂-Mg(NO₃)₂, Ca(NO₃)₂-NaNO₃, KNO₃-LiNO₃, KNO₃-Mg(NO₃)₂, KNO₃-NaNO₃, LiNO₃-Mg(NO₃)₂, LiNO₃-NaNO₃, Mg(NO₃)₂-NaNO₃, CaCO₃-K₂CO₃, CaCO₃-Li₂CO₃, CaCO₃-Na₂CO₃, K₂CO₃-Li₂CO₃, K₂CO₃-Na₂CO₃, Li₂CO₃-Na₂CO₃, CaSO₄-K₂SO₄, CaSO₄-Li₂SO₄, CaSO₄-MgSO₄, CaSO₄-Na₂SO₄, K₂SO₄-Li₂SO₄, K₂SO₄-MgSO₄, K₂SO₄-Na₂SO₄, K₂SO₄-SrSO₄, K₂SO₄-ZnSO₄, Li₂SO₄-MgSO₄, Li₂SO₄-Na₂SO₄, Li₂SO₄-SrSO₄, Li₂SO₄-ZnSO₄, MgSO₄-Na₂SO₄, Na₂SO₄-ZnSO₄.

- 30 new pseudo-ternary systems are assessed: CaCl₂-LiCl-NdCl₃, CaCl₂-MgCl₂-NdCl₃, CaCl₂-NaCl-NdCl₃, CaCl₂-NdCl₃-SrCl₂, KCl-LiCl-NdCl₃, KCl-MgCl₂-NdCl₃, LiCl-NdCl₃-SrCl₂, MgCl₂-NdCl₃-SrCl₂, NaCl-NdCl₃-SrCl₂, AlF₃-NaF-NdF₃, Al₂O₃-CaO-Nd₂O₃, Al₂O₃-MgO-Nd₂O₃, Al₂O₃-Nd₂O₃-SiO₂, CaO-Nd₂O₃-SiO₂, MgO-Nd₂O₃-SiO₂, Nd₂O₃-SiO₂-SrO, Ca(NO₃)₂-KNO₃-LiNO₃, Ca(NO₃)₂-KNO₃-Mg(NO₃)₂, Ca(NO₃)₂-KNO₃-NaNO₃, Ca(NO₃)₂-LiNO₃-NaNO₃, Ca(NO₃)₂-Mg(NO₃)₂-NaNO₃, Ca(NO₃)₂-NaNO₃-Sr(NO₃)₂, KNO₃-LiNO₃-Mg(NO₃)₂, KNO₃-LiNO₃-NaNO₃, KNO₃-Mg(NO₃)₂-NaNO₃, LiNO₃-Mg(NO₃)₂-NaNO₃, CaCO₃-K₂CO₃-Na₂CO₃, K₂CO₃-Li₂CO₃-Na₂CO₃, CaSO₄-K₂SO₄-MgSO₄, K₂SO₄-Na₂SO₄-ZnSO₄.
- 82 new mixed systems are assessed: Ca(NO₂)₂-Ca(NO₃)₂-KNO₂-KNO₃, Ca(NO₂)₂-Ca(NO₃)₂-LiNO₂-LiNO₃, Ca(NO₂)₂-Ca(NO₃)₂-NaNO₂-NaNO₃, Ca₂CO₃-CaF₂, CaCO₃-CaF₂-Na₂CO₃-NaF, CaCO₃-CaO, CaCO₃-CaSO₄, CaCl₂-CaF₂-CaSO₄, CaCl₂-CaSO₄, CaCl₂-CaSO₄-K₂SO₄-KCl, CaCl₂-CaSO₄-Na₂SO₄-NaCl, CaCl₂-Nd₂O₃-NdCl₃, CaF₂-CaSO₄, CaF₂-CaSO₄-Li₂SO₄-LiF, CaO-CaSO₄, K₂CO₃-K₂SO₄, K₂CO₃-K₂SO₄-KCl, K₂CO₃-K₂SO₄-KF, K₂CO₃-K₂SO₄-Na₂CO₃-Na₂SO₄, K₂CO₃-KCl, K₂CO₃-KCl-KF, K₂CO₃-KCl-Li₂CO₃-LiCl, K₂CO₃-KCl-Na₂CO₃-NaCl, K₂CO₃-KF, K₂CO₃-KNO₃, K₂SO₄-KCl, K₂SO₄-KCl-KF, K₂SO₄-KCl-Li₂SO₄-LiCl, K₂SO₄-KCl-MgCl₂-MgSO₄, K₂SO₄-KCl-Na₂SO₄-NaCl, K₂SO₄-KCl-SrCl₂-SrSO₄, K₂SO₄-KF, K₂SO₄-KF-Na₂SO₄-NaF, K₂SO₄-KNO₃-Na₂SO₄-NaNO₃, KCl-KNO₃, KCl-KNO₃-Sr(NO₃)₂-SrCl₂, KF-KNO₃, KNO₂-KNO₃, KNO₂-KNO₃-NaNO₂-NaNO₃, Li₂CO₃-Li₂O, Li₂CO₃-Li₂SO₄, Li₂CO₃-LiCl, Li₂CO₃-LiCl-Na₂CO₃-NaCl, Li₂CO₃-LiF, Li₂CO₃-LiNO₃, Li₂SO₄-LiCl, Li₂SO₄-LiCl-Na₂SO₄-NaCl, Li₂SO₄-LiCl-SrCl₂-SrSO₄, Li₂SO₄-LiCl-ZnCl₂-ZnSO₄, Li₂SO₄-LiF, Li₂SO₄-LiF-Na₂SO₄-NaF, Li₂SO₄-LiNO₃, LiCl-LiNO₃, LiCl-LiNO₃-Sr(NO₃)₂-SrCl₂, LiF-LiNO₃, LiNO₂-LiNO₃, LiNO₂-LiNO₃-NaNO₂-NaNO₃, MgCl₂-MgO-Nd₂O₃-NdCl₃, MgCl₂-MgSO₄, MgCl₂-MgSO₄-Na₂SO₄-NaCl, Na₂CO₃-Na₂O, Na₂CO₃-Na₂SO₄-NaCl, Na₂CO₃-Na₂SO₄-NaF, Na₂CO₃-NaCl, Na₂CO₃-NaCl-NaF, Na₂CO₃-NaF, Na₂CO₃-NaNO₃, Na₂SO₄-NaCO₃, Na₂SO₄-NaCl, Na₂SO₄-NaCl-NaF, Na₂SO₄-NaCl-NaNO₃, Na₂SO₄-NaCl-ZnSO₄-ZnSO₄, Na₂SO₄-NaF, Na₂SO₄-NaNO₃, NaCl-NaNO₃, NaCl-NaNO₃-Sr(NO₃)₂-SrCl₂, NaF-NaNO₃, NaNO₂-NaNO₃, Nd₂O₃-NdCl₃, Nd₂O₃-NdCl₃-SrCl₂-SrO, SrCO₃-SrCl₂, ZnCl₂-ZnSO₄.
- 1 system is reassessed: CaCl₂-CaO.

Thermophysical Properties

Molar volumes, surface tensions and viscosities were included with additions of new elements Nd and new types of salts of NO₃-1, NO₂-1, CO₃-2, and SO₄-2.

- Molar volume assessed systems: KNO₃, LiNO₃, NaNO₃, NdCl₃, K₂CO₃, Li₂CO₃, Na₂CO₃, K₂SO₄, Li₂SO₄, Na₂SO₄, ZnSO₄, KNO₂, NaNO₂, CaCO₃-K₂CO₃, Ca(NO₃)₂-KNO₃, Ca(NO₃)₂-NaNO₃, CaSO₄-Na₂SO₄, KCl-KNO₃, KCl-K₂CO₃, KCl-K₂SO₄, KCl-Li₂CO₃, KCl-Na₂CO₃, KCl-ZnSO₄, KF-Li₂CO₃, KNO₃-LiNO₃, KNO₃-Mg(NO₃)₂, KNO₃-NaNO₃, KNO₃-Sr(NO₃)₂, K₂CO₃-LiCl, K₂CO₃-LiF, K₂CO₃-Na₂CO₃, LiCl-LiNO₃, LiCl-Li₂CO₃, LiF-Li₂CO₃, LiNO₃-NaNO₃, Li₂CO₃-K₂CO₃, Li₂CO₃-Na₂CO₃, Li₂SiO₄-Na₂SO₄, Li₂SiO₄-ZnSO₄, NaCl-NaNO₃, NaCl-Na₂CO₃, Na₂SO₄-ZnSO₄, KNO₂-KNO₃, KNO₂-NaNO₂, KNO₂-NaNO₃, NaNO₂-NaNO₃, Ca(NO₃)₂-KNO₃-NaNO₃, Li₂CO₃-K₂CO₃-Na₂CO₃, NaNO₃-NaNO₂-KNO₃
- Surface tension assessed systems: Ca(NO₃)₂, KNO₃, LiNO₃, NaNO₃, Li₂SO₃, Li₂SO₄, K₂SO₄, Na₂SO₄, CaSO₃, MgSO₃, K₂CO₃, Li₂CO₃, Na₂CO₃, Sr(NO₃)₂, KNO₂, NaNO₂, Ca(NO₃)₂-KNO₃, Ca(NO₃)₂-

NaNO₃, CaSO₄-Na₂SO₄, K₂SO₄-Na₂SO₄, KCl-K₂SO₄, KCl-Li₂SO₄, KCl-NaNO₃, KCl-NdCl₃, LiCl-Li₂CO₃, NaCl-Na₂SO₄, KNO₃-LiNO₃, KNO₃-NaNO₃, K₂CO₃-Na₂CO₃, Li₂CO₃-Na₂CO₃, Li₂SO₄-NaCl, KNO₂-KNO₃, NaNO₂-NaNO₃, KCl*NaCl-NdCl₃, K₂CO₃-Li₂CO₃-Na₂CO₃

- Viscosity assessed systems: KNO₃, LiNO₃, NaNO₃, Ca(NO₃)₂, Na₂SO₄, K₂CO₃, Li₂CO₃, Na₂CO₃, Sr(NO₃)₂, LiNO₂, KNO₂, NaNO₂, Ca(NO₃)₂-KNO₃, Ca(NO₃)₂-LiNO₃, Ca(NO₃)₂-NaNO₃, KNO₃-LiNO₃, KNO₃-NaNO₃, KNO₃-Sr(NO₃)₂, LiNO₃-NaNO₃, K₂CO₃-Li₂CO₃, K₂CO₃-Na₂CO₃, LiCl-Li₂CO₃, Li₂CO₃-Na₂CO₃, NaCl-NaNO₃, KNO₂-NaNO₂, Ca(NO₃)₂-KNO₃-NaNO₃, KCl*NaCl-NdCl₃, K₂CO₃-Li₂CO₃-Na₂CO₃, NaNO₃-NaNO₂-KNO₃

TCSALT1 to TCSALT2

Software release version: 2025a (January 2025)

New Element and Phases

- One new element: Lithium (Li) (for a total of 12 elements).
- 23 new phases (177 phases in total).

Systems

- 21 new pseudo-binary systems are assessed: AlCl₃-LiCl, CaCl₂-LiCl, KCl-LiCl, LiCl-MgCl₂, LiCl-NaCl, LiCl-SrCl₂, LiCl-ZnCl₂, AlF₃-LiF, CaF₂-LiF, KF-LiF, LiF-MgF₂, LiF-NaF, LiF-SrF₂, LiF-ZnF₂, Al₂O₃-Li₂O, CaO-Li₂O, K₂O-Li₂O, Li₂O-MgO, Li₂O-Na₂O, Li₂O-SiO₂, Li₂O-ZnO.
- 24 new pseudo-ternary systems are assessed: AlCl₃-KCl-LiCl, CaCl₂-KCl-LiCl, CaCl₂-LiCl-NaCl, CaCl₂-LiCl-SrCl₂, KCl-LiCl-MgCl₂, KCl-LiCl-NaCl, KCl-LiCl-SrCl₂, KCl-LiCl-ZnCl₂, LiCl-NaCl-SrCl₂, AlF₃-CaF₂-LiF, AlF₃-KF-LiF, AlF₃-LiF-NaF, CaF₂-KF-LiF, CaF₂-LiF-MgF₂, CaF₂-LiF-NaF, CaF₂-LiF-SrF₂, KF-LiF-MgF₂, KF-LiF-NaF, LiF-MgF₂-NaF, LiF-MgF₂-SrF₂, Al₂O₃-Li₂O-Na₂O, CaO-Li₂O-SiO₂, Li₂O-MgO-SiO₂, Li₂O-Na₂O-SiO₂.
- 8 new mixed systems are assessed: AlCl₃-AlF₃-LiCl-LiF, CaCl₂-CaF₂-LiCl-LiF, KCl-KF-LiCl-LiF, Li₂O-LiCl, Li₂O-LiF, LiCl-LiF, LiCl-LiF-NaCl-NaF, LiCl-LiF-SrCl₂-SrF₂.

Thermophysical Properties Added

- Surface tension and viscosity of the ionic liquids.
- Molar volume of the ionic liquids and solids