TCS Salt Database (TCSALT2)

Technical Information

Available Starting with Thermo-Calc Version 2025a

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Contents

About the TCS Molten Salts Database (TCSALT)

TCS Molten Salts Database (TCSALT) is a thermodynamic database for molten salts. The types of salts the database are designed for is fluorides (F) and chlorides (Cl) where the ionic two-sublattice liquid model is used for the molten salt. No metallic liquid is modeled. Several oxide (O) systems are also modeled and assessed.

The database can be used for a variety of applications, especially for 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 iconic liquids, and viscosity of the iconic liquids are added to the database as of version 2 (TCSALT2).

The current version of the database is TCSALT2. See the link for any subversion release details: TCSALT: TCS Molten Salts Database Revision History.

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.

For more learning resources about CALPHAD and our databases, visit the video tutorials on our website or our YouTube playlist.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

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.

TCS Molten Salts Database (TCSALT) Resources

Information about the database is available on our website and in the Thermo-Calc software online Help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online Help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCS Molten Salts Database (TCSALT) Technical Information* PDF document contains version specific information such as the assessed pseudo-binary, pseudo-ternary, higher order, and mixed systems, and the phase models, and summaries of the database revision history by version.

Go to the Molten Salt Databases page on our website where you can access the Technical Information. Also explore further applications of Thermo-Calc to molten salts on this page.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

TCSALT2 Elements, Systems, Phases, and Properties

Included Elements

There are 12 elements included in the database.

Included Elements					
Al	Ca	Cl	F	K	Li
Mg	Na	O	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

- 28 Assessed Systems with Chloride (Cl)
- 25 Assessed Systems with Fluoride (F)
- 25 Assessed Systems with Oxygen (O)

Pseudo-Ternary

- 21 Assessed Systems with Chloride (Cl)
- 22 Assessed Systems with Fluoride (F)
- 22 Assessed Systems with Oxygen (O)

Higher Order

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

Mixed

- 36 Assessed Mixed Systems

Assessed Phases

The most recent version of the database contains 177 phases in total.

TCSALT2 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.

Properties Data and Assessed Systems

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

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

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

Molar Volume

For the molar volume properties data, the molar volume parameters have been assessed as detailed in TCSALT2 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 TCSALT2 Surface Tension for IonicLiquids: Assessed Systems .

Viscosity

For the viscosity properties data, the parameters have been assessed for the ionic liquid phase. The assessed systems are detailed in TCSALT2 Viscosity for Ionic Liquids: Assessed Systems .

Below is a summary of the available parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode 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

TCSALT2 Systems

In this section:

TCSALT2 Assessed Pseudo-Binary Systems

These are the assessed pseudo-binary systems with F (25 total), Cl (28 total), and O (25) in the full range of composition and temperature.

Assessed Pseudo-Binary Systems with Chloride (Cl)

	$AlCl_3$	$CaCl_2$	KCl	LiCl	$MgCl_2$	NaCl	$SiCl_4$	$SrCl_2$	$ZnCl_2$
$AlCl_3$	$AlCl_3$	x	x	x	x	x	x		x
$CaCl_2$		$CaCl_2$	x	x	x	x		x	x
KCl			KCl	x	x	x		x	x
LiCl				LiCl	x	x		x	x
$MgCl_2$					$MgCl_2$	x		x	x
NaCl						NaCl		x	x
$SiCl_4$							$SiCl_4$		
$SrCl_2$								$SrCl_2$	x
$ZnCl_2$									$ZnCl_2$

Assessed Pseudo-Binary Systems with Fluoride (F)

	AlF_3	CaF_2	KF	LiF	MgF_2	NaF	SiF_4	SrF_2	ZnF_2
AlF_3	AlF_3	x	x	x	x	x			
CaF_2		CaF_2	x	x	x	x		x	
KF			KF	x	x	x	x	x	x
LiF				LiF	x	x		x	x
MgF_2					MgF_2	x		x	
NaF						NaF	x	x	x
SiF_4							SiF_4		
SrF_2								SrF_2	
ZnF_2									ZnF_2

Assessed Pseudo-Binary Systems with Oxygen (O)

	Al_2O_3	CaO	K_2O	Li_2O	MgO	Na_2O	SiO_2	SrO	ZnO
Al_2O_3	Al_2O_3	x	x	x	x	x	x	x	x
CaO		CaO		x	x		x	x	x
K_2O			K_2O	x			x		
Li_2O				Li_2O	x	x	x		x
MgO					MgO		x	x	x
Na_2O						Na_2O	x		
SiO_2							SiO_2	x	x
SrO								SrO	
ZnO									ZnO

TCSALT2 Assessed Pseudo-Ternary Systems

These are the assessed pseudo-ternary systems with Cl (21 total), F (22 total), and O (22 total) in the full range of composition and temperature.

Assessed Pseudo-Ternary Systems with Chloride (Cl)

Assessed Pseudo-Ternary Systems with Cl					
$AlCl_3$-$CaCl_2$-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-$SrCl_2$	$CaCl_2$-$MgCl_2$-NaCl
$CaCl_2$-NaCl-$SrCl_2$	KCl-LiCl-$MgCl_2$	KCl-LiCl-NaCl	KCl-LiCl-$SrCl_2$	KCl-LiCl-$ZnCl_2$	KCl-$MgCl_2$-NaCl
KCl-NaCl-$SrCl_2$	KCl-NaCl-$ZnCl_2$	LiCl-NaCl-$SrCl_2$			

Assessed Pseudo-Ternary Systems with Fluoride (F)

Assessed Pseudo-Ternary Systems with F					
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
CaF_2-KF-LiF	CaF_2-KF-MgF2	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	KF-NaF-SrF_2	LiF-MgF_2-NaF	LiF-MgF_2-SrF_2		

Assessed Pseudo-Ternary Systems with Oxygen (O)

Assessed Pseudo-Ternary Systems with O					
Al_2O_3-CaO-K_2O	Al_2O_3-CaO-MgO	Al_2O_3-CaO-Na_2O	Al_2O_3-CaO-SiO_2	Al_2O_3-CaO-SrO	Al_2O_3-K_2O-MgO
Al_2O_3-Li_2O-Na_2O	Al_2O_3-MgO-SiO_2	Al_2O_3-MgO-ZnO	CaO-K_2O-SiO_2	CaO-Li_2O-SiO_2	CaO-MgO-SiO_2
CaO-MgO-ZnO	CaO-Na_2O-SiO_2	CaO-SiO_2-SrO	CaO-SiO_2-ZnO	K_2O-MgO-SiO_2	K_2O-Na_2O-SiO_2
Li_2O-MgO-SiO_2	Li_2O-Na_2O-SiO_2	MgO-Na_2O-SiO_2	MgO-SiO_2-ZnO		

TCSALT2 Assessed Higher Order Systems

These are the assessed higher order systems with Cl (1 total) and F (1 total) in the full range of composition and temperature.

Assessed Higher Order Systems with Chloride (Cl)

Assessed Higher Order Systems with Cl
$AlCl_3$-KCl-$MgCl_2$-NaCl

Assessed Higher Order Systems with Fluoride (F)

Assessed Higher Order Systems with F
K_2SiF_6-K_3AlF_6-Na_2SiF_6-Na_3AlF_6

TCSALT2 Assessed Mixed Systems

These are the 36 assessed mixed systems in the full range of composition and temperature.

Assessed Mixed Systems				
Al_2O_3-CaF_2	Al_2O_3-CaF_2-CaO	Al_2O_3-CaF_2-SiO_2	$AlCl_3$-AlF_3-KCl-KF	$AlCl_3$-AlF_3-LiCl-LiF
$AlCl_3$-AlF_3-NaCl-NaF	$CaCl_2$-CaF_2	$CaCl_2$-CaF_2-CaO	$CaCl_2$-CaF_2-KCl-KF	$CaCl_2$-CaF_2-LiCl-LiF
$CaCl_2$-CaF_2-$MgCl_2$-MgF_2	$CaCl_2$-CaF_2-NaCl-NaF	$CaCl_2$-CaF_2-$SrCl_2$-SrF_2	$CaCl_2$-CaO	CaF_2-CaO
CaF_2-KF-SiO_2	CaF_2-NaF-SiO_2	CaF_2-SiO_2	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	Li_2O-LiCl
Li_2O-LiF	LiCl-LiF	LiCl-LiF-NaCl-NaF	LiCl-LiF-$SrCl_2$-SrF_2	$MgCl_2$-MgF_2
$MgCl_2$-MgF_2-NaCl-NaF	MgF_2-SiO_2	NaCl-NaF	NaCl-NaF-$SrCl_2$-SrF_2	$SrCl_2$-SrF_2
$SrCl_2$-SrO				

TCSALT2 Properties Data and Assessed Systems

This section lists the assessed systems for each of the properties.

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

In this section:

TCSALT2 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, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

Unary Systems

Assessed Unary Systems (Molar Volume)									
$AlCl_3$	AlF_3	$CaCl_2$	CaF_2	KCl	KF	Li_2O	Li_3AlF_6	LiCl	LiF
$MgCl_2$	MgF_2	Na_3AlF_6	NaCl	NaF	$SiCl_4$	SiF_4	$SrCl_2$	SrF_2	SrO
$ZnCl_2$	ZnF_2	ZnO							

Pseudo Binary Systems

Assessed Pseudo Binary Systems (Molar Volume)							
Al_2O_3-CaO	Al_2O_3-K_2O	Al_2O_3-MgO	Al_2O_3-Na_2O	Al_2O_3-SiO_2	Al_2O_3-SrO	Al_2O_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	$CaCl_2$-CaF_2	$CaCl_2$-CaO	$CaCl_2$-KCl
$CaCl_2$-LiCl	$CaCl_2$-$MgCl_2$	$CaCl_2$-NaCl	$CaCl_2$-$SrCl_2$	$CaCl_2$-$ZnCl_2$	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	K_2O-SiO_2
KCl-KF	KCl-LiCl	KCl-$MgCl_2$	KCl-NaCl	KCl-$SrCL_2$	KCl-$ZnCl_2$	KF-LiF	KF-MgF_2
KF-NaF	KF-SiF_4	KF-SrF_4	KF-ZnF_2	Li_2O-SIO_2	LiCl-LiF	LiCl-$MgCl_2$	LiCl-NaCl

Assessed Pseudo Binary Systems (Molar Volume)							
LiCl-$ZnCl_2$	LiF-NaF	$MgCl_2$-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_2O-SiO_2	NaCl-NaF	NaCl-$SrCl_2$	NaCl-$ZnCl_2$
NaF-SiF_4	NaF-SrF_2	NaF-ZnF_2	SiF_4-SrF_2	SiF_4-ZnF_2	SiO_2-SrO	SiO_2-ZnO	$SrCl_2$-SrF_2
$SrCl_2$-SrO	$SrCl_2$-$ZnCl_2$						

Higher Order Pseudo Systems

Assessed Higher Order Pseudo Systems (Molar Volume)					
Al_2O_3-KF-Na_3AlF_6	Al_2O_3-Na_3AlF_6	$AlCl_3$-LiCl-NaCl	$CaCl_2$-$MgCl_2$-NaCl	CaF_2-Na_3AlF_6	K_3AlF_6-Na_3AlF_6
Li_2O-CaO-SiO_2	Li_2O-MgO-SIO_2	Li_2O-Na_2O-SiO_2	Li_3AlF_6-Na_3AlF_6	LiF-Na_3AlF_6	Na_3AlF_6-KF
Al_2O_3-Li_3AlF_6	AlF_3-Na_3AlF_6	K_3AlF_6-Li_3AlF_6			

TCSALT2 Surface Tension for IonicLiquids: 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, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

Unary Systems

Assessed Unary Systems (Surface Tension)									
Al_2O_3	$AlCl_3$	AlF_3	$CaCl_2$	CaF_2	CaO	K_2O	KCl	KF	LiCl
LiF	$MgCl_2$	MgF_2	MgO	Na_2O	NaCl	NaF	$SiCl_4$	SiF_4	SiO_2
$SrCl_2$	SrF_2	SrO	$ZnCl_2$	ZnF_2	ZnO				

Pseudo Binary Systems

Assessed Pseudo Binary Systems (Surface Tension)							
Al_2O_3-CaO	Al_2O_3-K_2O	Al_2O_3-MgO	Al_2O_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	AlF_3-NaF
$CaCl_2$-KCl	$CaCl_2$-LiCl	$CaCl_2$-$MgCl_2$	$CaCl_2$-NaCl	CaF_2-CaO	CaF_2-SiF_4	CaO-SiO_2	K_2O-SiO_2
KCl-LiCl	KCl-$MgCl_2$	KCl-NaCl	KCl-$SrCl_2$	KCl-$ZnCl_2$	KF-LiF	KF-NaF	KF-SiF_4
LiCl-LiF	LiCl-$MgCl_2$	LiCl-NaCl	LiF-NaF	$MgCl_2$-NaCl	MgF_2-SiF_4	MgO-SiO_2	Na_2O-SiO_2
NaF-SiF_4	SiF_4-SrF_2	SiF_4-ZnF_2	SrO-SiO_2	ZnO-SiO_2			

Higher Order Pseudo Systems

Assessed Higher Order Pseudo Systems (Surface Tension)				
$CaCl_2$-KCl-$MgCl_2$	$CaCl_2$-$MgCl_2$-NaCl	KF-Na_3AlF_6	K_3AlF_6-Na_3AlF_6	Al_2O_3-KF-Na_3AlF_6

TCSALT2 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, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

Unary Assessed Systems

Assessed Unary Systems (Viscosity)									
Al_2O_3	$AlCl_3$	AlF_3	$CaCl_2$	CaF_2	CaO	K_2O	KCl	KF	Li_2O
Li_3AlF_6	LiCl	LiF	$MgCl_2$	MgF_2	MgO	Na_2O	Na_3AlF_6	NaCl	NaF
$SiCl_4$	SiF_4	SiO_2	$SrCl_2$	SrF_2	SrO	$ZnCl_2$	ZnF_2	ZnO	

Pseudo Binary Systems

Assessed Pseudo Binary Systems (Viscosity)							
Al_2O_3-CaO	Al_2O_3-K_2O	Al_2O_3-MgO	Al_2O_3-Na_2O	Al_2O_3-SiO_2	$AlCl_3$-$CaCl_2$	$AlCl_3$-KCl	$AlCl_3$-LiCl
$AlCl_3$-$MgCl_2$	$AlCl_3$-NaCl	$AlCl_3$-$SiCl_4$	$AlCl_3$-$SrCl_2$	$AlCl_3$-$ZnCl_2$	AlF_3-CaF_2	AlF_3-KF	AlF_3-LiF
AlF_3-MgF_2	AlF_3-Na_3AlF_6	AlF_3-NaF	AlF_3-SrF_2	AlF_3-ZnF_2	$CaCl_2$-NaCl	CaF_2-MgO	CaF_2-SiF_4
CaO-SiO_2	K_2O-SiO_2	KCl-LiCl	KCl-$MgCl_2$	KCl-NaCl	KCl-$ZnCl_2$	Li_2O-SiO_2	LiCl-$MgCl_2$
LiCl-$ZnCl_2$	LiF-Na_3AlF_6	LiF-NaF	$MgCl_2$-NaCl	MgF_2-SiF_4	MgO-SiO_2	Na_2O-SiO_2	NaCl-$ZnCl_2$
NaF-Na_3AlF_6	SiF_4-SrF_2	SiF_4-ZnF_2	SiO_2-SrO	SiO_2-ZnO			

Higher Order Pseudo Systems

Assessed Higher Order Psedo Systems (Viscosity)					
Al_2O_3-NaF-AlF_3-CaF_2	$AlCl_3$-LiCl-NaCl	CaF_2-Na_3AlF_6	KCl-NaCl-$ZnCl_2$	Li_3AlF_6-Na_3AlF_6	MgF_2-Na_3AlF_6

Assessed Higher Order Psedo Systems (Viscosity)					
NaCl-KCl-$MgCl_2$	NaCl-Na_3AlF_6	NaF-Na_3AlF_6			

TCSALT2 Phases

In this section:

TCSALT2 Models for the Included Phases

See the separate listing for Gas and IONIC_LIQ Phases below.

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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, Pnnm)	This is a high-pressure phase (Al2O3.SiO2)	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
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
C11A7F	Ca6Al7O16F		cI152	(220, I-43d)	This is 11CaO.7Al2O3.CaF2	4	(AL+3)14(CA+2)12(F-1)2(O-2)32
C12A7	Mayenite (12CaO.7Al2O3, K74, C12A7)	K74	cI152	(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
C1A1	Al2CaO4		mP84	(14, P2_1/c)	This is CaO.Al2O3	4	(CA+2, SR+2)3(AL+3)5(AL+3)1(O-2)12
C1A2	Al4CaO7		mS48	(15, C2/c)	This is CaO.2Al2O3 and SrO.2Al2O3	4	(CA+2, SR+2)1(AL+3)3(AL+3)1(O-2)7
C1A6	Magnetoplumbite (PbFe12O19)		hP64	(194, P6_ 3/mmc)	This is CaO.6Al2O3 and SrO.6Al2O3	3	(CA+2, SR+2)1(AL+3)12(O-2)19

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
C1A8M2	CaMg2Al16O27		hP94	(187, P-6m2)	This is CaO.8Al2O3.2MgO	4	(CA+2)1(AL+3)16(MG+2)2(O-2)27
C2A14M2	BaFe15O23		hR78	(166, R-3m)	This is 2CaO.14Al2O3.2MgO	4	(CA+2)2(AL+3)28(MG+2)2(O-2)46
C3A1	Ca3Al2O6		cP264	(205, Pa-3)	This is 3CaO.Al2O3 and 3SrO.Al2O3	3	(CA+2, SR+2)3(AL+3)2(O-2)6
C3A2M1	3CaO.2Al2O3.MgO		oP72	(57, Pbcm)	This is 3CaO.2Al2O3.MgO (oP72, Pbcm or Pca21);	4	(CA+2)3(AL+3)4(MG+2)1(O-2)10
C3A3F	Unknown Structure				This is 3CaO.3Al2O3.CaF2	4	(AL+3)6(CA+2)4(F-1)2(O-2)12
CA10SI3O15F2	Unknown Structure				This is 9CaO.3SiO2.CaF2	4	(CA+2)10(SI+4)3(O-2)15(F-1)2
CA2ALF7	Ca2AlF7		oP40	(62, Pnma)		3	(CA+2)2(AL+3)1(F-1)7
CA2NA2SI2O7	Na2Ca2Si2O7		mS208	(15, C2/c)		4	(CA+2)2(NA+1)2(SI+4)2(O-2)7
CA2NA2SI3O9	Na(Na0.5Ca0.5)2CaSi3O9		hP102	(152, P3_121)		4	(CA+2)2(NA+1)2(SI+4)3(O-2)9
CA2SIO4_ALPHA_A	Ca2SiO4		hP24	(194, P6_3/mmc)		3	(CA+2, LI2+2, MG+2, ZN+2)3(CA+2)1(SIO4-4)2
CA2SIO4_ALPHA_PRIME	K2CoCl4		oP84	(33, Pna2_1)		3	(CA+2, LI2+2, MG+2, ZN+2)3(CA+2)1(SIO4-4)2
CA3NA2SI6O16	Na2Ca3Si6O16		aP54	(2, P-1)		4	(CA+2)3(NA+1)2(SI+4)6(O-2)16
CA4CL6O	Ba4Cl6O		hP22	(186, P6_3mc)		3	(CA+2, SR+2)4(CL-1)6(O-2)1
CA5SI2O8F2	Unknown Structure				This is 4CaO.2SiO2.CaF2	4	(CA+2)5(SI+4)2(O-2)8(F-1)2
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

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CACL2	Hydrophilite (CaCl2, C35)	C35	oP6	(58, Pnnm)	This is CaCl2 and low temperature SrCl2	2	(CA+2, MG+2, SR+2)1(CL-1)2
CACLF	Matlockite (PbFCl, E01)	E01	tP6	(129, P4/nmm)		3	(CA+2, SR+2)1(CL-1)1(F-1)1
CAF2_S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is SrF2 and low temperature CaF2.	2	(CA+2, MG+2, SR+2)1(F-1, O-2, VA)2
CAF2_S2	Cotunnite (PbCl2, C23)	C23	oP12	(62, Pnma)	This is high temperature CaF2.	2	(CA+2, MG+2, SR+2)1(F-1, O-2, VA)2
CANA2SI5O12	Unknown Structure					4	(CA+2)1(NA+1)2(SI+4)5(O-2)12
CANA2SIO4	Na2CaSiO4 (S66)	S66	cP32	(198, P2_13)		4	(CA+2)1(NA+1)2(SI+4)1(O-2)4
CANA4SI3O9	K4SrGe3O9		cP272	(205, Pa-3)		4	(CA+2)1(NA+1)4(SI+4)3(O-2)9
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 (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
HALITE_B1	Rock Salt (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

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HALITE_OX	Rock Salt (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, SR+2, VA, ZN+2)1(O-2)1
HATRURITE	Ca3(SiO4)O-b		hR81	(160, R3m)	This is 3CaO.SiO2.	3	(CA+2, 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
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
K2CASIO4	Unknown Structure					4	(K+1)2(CA+2)1(SI+4)1(O-2)4
K2LIALF6	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
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
K2MGSIO4_HT	Unknown Structure					2	(K2MG+4, SI+4)1(SIO4-4)1
K2MGSIO4_LT	Na2Be[SiO4]		oP64	(29, Pca2_1)		2	(K2MG+4, SI+4)1(SIO4-4)1
K2NAALF6	Double Perovskite (Ba2MnWO6)		cF40	(225, Fm-3m)		3	(K+1)2(NA+1)1(ALF6-3)1

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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
K2SRCL4	Th3P4 (D73)	D73	cI28	(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
K3MG2CL7	Sr3Ti2O7		tI24	(139, I4/mmm)		3	(K+1)3(MG+2)2(CL-1)7
K3SIF7	Unknown Structure					3	(K+1)3(SI+4)1(F-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
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 (Al2O3, D56)	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	KAlCl4		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

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KMG2AL15O25	Unknown Structure					4	(K+1)1(MG+2)2(AL+3)15(O-2)25
KMGF3	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	This is KCa(Cl,F)3, K(Mg,Zn)F3, ht NaMgF3 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
KSR2CL5	U2PbSe5		mP32	(14, P2_1/c)		3	(K+1)1(SR+2)2(CL-1)5
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	(2, P-1)	This is Al2O3.SiO2 (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
LARNITE	Parawollastonite (CaSiO3, S33(II))	S33(II)	mP60	(14, P2_1/c)	This is 2CaO.SiO2 (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	Li2Ca2[Si2O7]		hP78	(178, P6_122)		4	(LI2+2)1(CA+2)2(SI+4)2(O-2)7
LI2CA3SI6O16	Unknown Structure					4	(LI2+2)1(CA+2)3(SI+4)6(O-2)16
LI2CA4SI4O13	Li2Ca4Si4O13		aP46	(2, P-1)		4	(LI2+2)1(CA+2)4(SI+4)4(O-2)13
LI2CASIO4	[NH4]Ag2AsS4		tI16	(121, I-42m)		4	(LI2+2)1(CA+2)1(SI+4)1(O-2)4
LI2SI2O5_HT	Unknown Structure					3	(LI+1, NA+1)2(SI+4)2(O-2)5
LI2SI2O5_LT	Li2Si2O5		oS36	(37, Ccc2)		3	(LI+1, NA+1)2(SI+4)2(O-2)5
LI2ZNCL4_LT	Spinel (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)	This is low temperature Li2ZnCl4.	3	(LI+1)2(ZN+2)1(CL-1)4
LI3ALF6_S1	Li3VF6		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	Li4[SiO4]		mP28	(11, P2_1/m)		4	(LI2+2, NA2+2)1(LI2+2, MG+2, NA2+2)1 (SI+4)1(O-2)4

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LI5ALO4	Li5AlO4		oP20	(59, Pmmn)		3	(LI+1)5(AL+3)1(O-2)4
LI6SI2O7	Li6[Si2O7]		tP30	(113, P-42_ 1m)		3	(LI+1)6(SI+4)2(O-2)7
LI8SIO6	Li8CoO6		hP30	(185, P6_3cm)		3	(LI+1)8(SI+4)1(O-2)6
LIAL5O8	LiFe5O8		cP56	(213, P4_132)	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
LIKMGCL4	Unknown Structure					4	(LI+1)1(K+1)1(MG+2)1(CL-1)4
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
MELILITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_ 1m)	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
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
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	(LI2+2, MG+2)1(CL-1)2
MGF2	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)	This is MgF2 and lt- ZnF2.	2	(LI2+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

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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
NA2LIALF6	Ca(Ca0.5Nd0.5)2NbO6		mP20	(14, P2_1/c)		3	(NA+1)2(LI+1)1(ALF6-3)1
NA2MGCL4	Sr2PbO4		oP20	(55, Pbam)		3	(NA+1)2(MG+2)1(CL-1)4
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
NA2ZNCL4	Forsterite (Mg2SiO4, S12)	S12	oP28	(62, Pnma)	This is Na2ZnCl4 and high temperature	3	(LI+1, NA+1)2(ZN+2)1(CL-1)4

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					Li2ZnCl4.		
NA3ALF6_S1	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)		3	(NA+1)3(AL+3)1(F-1)6
NA3LI3AL2F12	Garnet (Co3Al2Si3O12, S14)	S14	cI160	(230, Ia-3d)		3	(NA+1)3(LI+1)3(ALF6-3)2
NA4SIO4	K4SnO4		aP18	(2, P-1)		4	(LI2+2, NA2+2)1(LI2+2, NA2+2)1(SI+4)1(O-2)4
NA5AL3F14	Chiolite (Na5Al3F14, K75)	K75	tP44	(128, P4/mnc)		3	(NA+1)5(AL+3)3(F-1)14
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
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
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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NEPHELINE_G	KLi[SO4]		hP18	(173, P6_3)	This is K2MgSi3O8.	4	(K2MG+4)4(SI+4)4(SI+4)8(O-2)32
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	oP28	(62, Pnma)	This is 2CaO.SiO2, forsterite and monticellite[CaO.MgO.SiO2]	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 (MgSiO3, 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	MgSiO3		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	CaSiO3		mS120	(15, C2/c)	This is CaO.SiO2	3	(CA+2, SR+2)1(SI+4)1(O-2)3
QUARTZ	alpha-Quartz (low Quartz)		hP9	(152, P3_121)		2	(SI+4)1(SIO4-4)1
RANKINITE	3CaO.2SiO2		mP48	(14, P2_1/c)	This is 3CaO.2SiO2	3	(CA+2)3(SI+4)2(O-2)7
SAPPHIRINE	CaMg3Si3O10		aP68	(2, P-1)	This is 9Al2O3.7MgO.3SiO2	4	(AL+3)18(MG+2)7(SI+4)3(O-2)40
SILLIMANITE	Sillimanite (Al2SiO5, S03)	S03	oP32	(62, Pnma)	This is a high-pressure phase (Al2O3.SiO2)	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)	This is MgAl2O4.	4	(AL+3, LI+1, MG+2, ZN+2)1(AL+3, LI+1, MG+2, NA+1, VA, ZN+2)2(MG+2, VA)2(O-2)4
SR2SIO4_ALPHA_A	Arcanite (K2SO4, H16)	H16	oP28	(62, Pnma)		3	(SR+2)2(SI+4)1(O-2)4
SR2SIO4_ALPHA_ PRIME	Unknown Structure					3	(SR+2)2(SI+4)1(O-2)4
SR3SIO5	Sr3[SiO4]O		tP36	(130, P4/ncc)		3	(SR+2)3(SI+4)1(O-2)5
SRCL2_S2	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(CA+2, SR+2)1(CL-1)2
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
SRSIO3	SrSiO3		mS60	(15, C2/c)		3	(CA+2, SR+2)1(SI+4)1(O-2)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SRZNCL4	Scheelite (CaWO4, H04)	H04	tI24	(88, I4_1/a)		3	(SR+2)1(ZN+2)1(CL-1)4
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	(9, Cc)		2	(SI+4)1(SIO4-4)1
WOLLASTONITE	Wollastonite (CaSiO3)		aP30	(2, P-1)	This is CaO.SiO2.	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 (Be2SiO4, S13)	S13	hR42	(148, R-3)		4	(MG+2, ZN+2)1(MG+2, ZN+2)1(SI+4)1(O-2)4
ZNCL2	ZnCl2		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

Gas and IONIC_LIQ Phases

Name	Prototype	Info	Sublattices	Formula Unit
GAS	Gas		1	(AL, AL1CL1, AL1CL1F1, AL1CL1F2, AL1CL1O1, AL1CL2, AL1CL2F1, AL1CL2O1, AL1CL3, AL1CL4K1, AL1CL4NA1, AL1F1, AL1F1O1, AL1F2, AL1F2NA1O1, AL1F2O1, AL1F3, AL1F4K1, AL1F4LI1, AL1F4NA1, AL1O1, AL1O2, AL2, AL2CL6, AL2CL8K2, AL2CL8NA2, AL2F6, AL2F8NA2, AL2O1, AL2O2, AL2O3, AL3CA1CL11, CA, CA1CL1, CA1CL2, CA1F1, CA1F2, CA1O1, CA2, CL, CL1F1, CL1F1LI2, CL1F1MG1, CL1F1O3, CL1F1SI1, CL1F3, CL1F3SI1, CL1F5, CL1K1, CL1LI1, CL1LI1O1, CL1MG1, CL1NA1, CL1O1, CL1O2, CL1O3, CL1SI1, CL1SR1, CL1ZN1, CL2, CL2K2, CL2LI2, CL2MG1, CL2NA2, CL2O1, CL2O1_1, CL2O1_2, CL2O2_1, CL2O2_2, CL2O2_3, CL2SI1, CL2SR1, CL2ZN1, CL3F1SI1, CL3LI3, CL3NA3, CL3SI1, CL4MG2, CL4SI1, CL4ZN2, F, F1K1, F1LI1, F1LI1O1, F1MG1, F1NA1, F1O1, F1O2_1, F1O2_2, F1O2_OFO, F1SI1, F1SR1, F1ZN1, F2, F2K2, F2LI2, F2MG1, F2NA2, F2O1, F2O1SI1, F2O2, F2O2_FOOF, F2SI1, F2SR1, F2ZN1, F3LI3, F3NA3, F3SI1, F4MG2, F4SI1, F4ZN2, K, K1LI1, K1NA1, K1O1, K2, K2O1, K2O2, LI, LI1NA1, LI1NA1O1, LI1O1, LI2, LI2O1, LI2O2, MG, MG1O1, MG2, NA, NA1O1, NA2, NA2O1, NA2O2, O, O1SI1, O1SR1, O1ZN1, O2, O2SI1, O2SI2, O3, SI, SI2, SI3, SR, SR2, ZN)1
IONIC_LIQ	Liquid	Molten salt	2	(CA+2, K+1, LI+1, MG+2, NA+1, SR+2, ZN+2)P(ALCL3, ALCL4-1, ALF3, ALF4-1, ALF6-3, ALO3/2, CL-1, F-1, O-2, SICL4, SIF4, SIF6-2, SIO2, SIO4-4, ZNCL2, ZNF2)Q

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:	**2.0**
First release:	**TCSALT1 was released with 2024a**

Changes in the Most Recent Database Release

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: $AlCl_3$-LiCl, $CaCl_2$-LiCl, KCl-LiCl, LiCl-$MgCl_2$, LiCl-NaCl, LiCl-$SrCl_2$, LiCl-$ZnCl_2$, AlF_3-LiF, CaF_2-LiF, KF-LiF, LiF-MgF_2, LiF-NaF, LiF-SrF_2, LiF-ZnF_2, Al_2O_3-Li_2O, CaO-Li_2O, K_2O-Li_2O, Li_2O-MgO, Li_2O-Na_2O, Li_2O-SiO_2, Li_2O-ZnO.

- 24 new pseudo-ternary systems are assessed: $AlCl_3$-KCl-LiCl, $CaCl_2$-KCl-LiCl, $CaCl_2$-LiCl-NaCl, $CaCl_2$-LiCl-$SrCl_2$, KCl-LiCl-$MgCl_2$, KCl-LiCl-NaCl, KCl-LiCl-$SrCl_2$, KCl-LiCl-$ZnCl_2$, LiCl-NaCl-$SrCl_2$, AlF_3-CaF_2-LiF, AlF_3-KF-LiF, AlF_3-LiF-NaF, CaF_2-KF-LiF, CaF_2-LiF-MgF_2, CaF_2-LiF-NaF, CaF_2-LiF-SrF_2, KF-LiF-MgF_2, KF-LiF-NaF, LiF-MgF_2-NaF, LiF-MgF_2-SrF_2, Al_2O_3-Li_2O-Na_2O, CaO-Li_2O-SiO_2, Li_2O-MgO-SiO_2, Li_2O-Na_2O-SiO_2.

- 8 new mixed systems are assessed: $AlCl_3$-AlF_3-LiCl-LiF, $CaCl_2$-CaF_2-LiCl-LiF, KCl-KF-LiCl-LiF, Li_2O-LiCl, Li_2O-LiF, LiCl-LiF, LiCl-LiF-NaCl-NaF, LiCl-LiF-$SrCl_2$-SrF_2.

Thermophysical Properties Added

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