

TCS Salt Database (TCSALT1)

Technical Information

Available Starting with Thermo-Calc Version 2024a



Contents

About the TCS Salt Database (TCSALT)	3
TCS Salt Database (TCSALT) Resources	4
TCSALT1 Elements, Systems, and Phases	5
Included Elements	5
Assessed Systems	5
Assessed Phases	5
TCSALT1 Systems	7
TCSALT1 Assessed Pseudo-Binary Systems	8
TCSALT1 Assessed Pseudo-Ternary Systems	10
TCSALT1 Assessed Higher Order Systems	12
TCSALT1 Assessed Mixed Systems	13
TCSALT1 Phases	14
TCSALT1 Models for the Included Phases	15

About the TCS Salt Database (TCSALT)

TCS Salt 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.

The current version of the database is TCSALT1.

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.

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 Salt 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 Salt 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.



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.

TCSALT1 Elements, Systems, and Phases

Included Elements

There are 11 elements included in the database.

Al	Ca	Cl	F	K	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

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

Pseudo-Ternary

- 12 Assessed Systems with Chloride (Cl)
- 11 Assessed Systems with Fluoride (F)
- 18 Assessed Systems with Oxygen (O)

Higher Order

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

Mixed

- 28 Assessed Mixed Systems

Assessed Phases

The most recent version of the database contains 159 phases in total.



[TCSALT1 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.

Different composition sets also describe miscibility gaps frequently found in e.g. silicate 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.

TCSALT1 Systems

In this section:

TCSALT1 Assessed Pseudo-Binary Systems	8
TCSALT1 Assessed Pseudo-Ternary Systems	10
TCSALT1 Assessed Higher Order Systems	12
TCSALT1 Assessed Mixed Systems	13

TCSALT1 Assessed Pseudo-Binary Systems

These are the assessed pseudo-binary systems with F (18 total), Cl (21 total), and O (18) in the full range of composition and temperature.

Assessed Pseudo-Binary Systems with Chloride (Cl)

	AlCl ₃	CaCl ₂	KCl	MgCl ₂	NaCl	SiCl ₄	SrCl ₂	ZnCl ₂
AlCl ₃	AlCl₃	x	x	x	x	x		x
CaCl ₂		CaCl₂	x	x	x		x	x
KCl			KCl	x	x		x	x
MgCl ₂				MgCl₂	x		x	x
NaCl					NaCl		x	x
SiCl ₄						SiCl₄		
SrCl ₂							SrCl₂	x
ZnCl ₂								ZnCl₂

Assessed Pseudo-Binary Systems with Fluoride (F)

	AlF ₃	CaF ₂	KF	MgF ₂	NaF	SiF ₄	SrF ₂	ZnF ₂
AlF ₃	AlF₃	x	x	x	x			
CaF ₂		CaF₂	x	x	x		x	
KF			KF	x	x	x	x	x
MgF ₂				MgF₂	x		x	
NaF					NaF	x	x	x
SiF ₄						SiF₄		
SrF ₂							SrF₂	
ZnF ₂								ZnF₂

TCSALT1 Assessed Pseudo-Ternary Systems

These are the assessed pseudo-ternary systems with Cl (12 total), F (11 total), and O (18 total) in the full range of composition and temperature.

Assessed Pseudo-Ternary Systems with Chloride (Cl)

<i>Assessed Pseudo-Ternary Systems with Cl</i>	
$\text{AlCl}_3\text{-KCl-MgCl}_2$	$\text{AlCl}_3\text{-KCl-NaCl}$
$\text{AlCl}_3\text{-MgCl}_2\text{-NaCl}$	$\text{CaCl}_2\text{-KCl-MgCl}_2$
$\text{CaCl}_2\text{-KCl-NaCl}$	$\text{CaCl}_2\text{-KCl-ZnCl}_2$
$\text{CaCl}_2\text{-MgCl}_2\text{-NaCl}$	$\text{CaCl}_2\text{-NaCl-SrCl}_2$
$\text{KCl-MgCl}_2\text{-NaCl}$	KCl-NaCl-SrCl_2
KCl-NaCl-ZnCl_2	

Assessed Pseudo-Ternary Systems with Fluoride (F)

<i>Assessed Pseudo-Ternary Systems with F</i>	
$\text{AlF}_3\text{-CaF}_2\text{-NaF}$	$\text{AlF}_3\text{-KF-NaF}$
$\text{AlF}_3\text{-MgF}_2\text{-NaF}$	$\text{CaF}_2\text{-KF-MgF}_2$
$\text{CaF}_2\text{-KF-NaF}$	$\text{CaF}_2\text{-KF-SrF}_2$
$\text{CaF}_2\text{-MgF}_2\text{-NaF}$	$\text{CaF}_2\text{-NaF-SrF}_2$
$\text{KF-MgF}_2\text{-NaF}$	$\text{KF-MgF}_2\text{-ZnF}_2$
KF-NaF-SrF_2	

Assessed Pseudo-Ternary Systems with Oxygen (O)

<i>Assessed Pseudo-Ternary Systems with O</i>	
$\text{Al}_2\text{O}_3\text{-CaO-K}_2\text{O}$	$\text{Al}_2\text{O}_3\text{-CaO-MgO}$
$\text{Al}_2\text{O}_3\text{-CaO-Na}_2\text{O}$	$\text{Al}_2\text{O}_3\text{-CaO-SiO}_2$
$\text{Al}_2\text{O}_3\text{-CaO-SrO}$	$\text{Al}_2\text{O}_3\text{-K}_2\text{O-MgO}$
$\text{Al}_2\text{O}_3\text{-MgO-SiO}_2$	$\text{Al}_2\text{O}_3\text{-MgO-ZnO}$
$\text{CaO-K}_2\text{O-SiO}_2$	CaO-MgO-SiO_2
CaO-MgO-ZnO	$\text{CaO-Na}_2\text{O-SiO}_2$
$\text{CaO-SiO}_2\text{-SrO}$	$\text{CaO-SiO}_2\text{-ZnO}$
$\text{K}_2\text{O-MgO-SiO}_2$	$\text{K}_2\text{O-Na}_2\text{O-SiO}_2$
$\text{MgO-Na}_2\text{O-SiO}_2$	$\text{MgO-SiO}_2\text{-ZnO}$

TCSALT1 Assessed Higher Order Systems

These are the assessed higher order systems with Cl (1 total), F (1 total), and O (4 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	
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Assessed Higher Order Systems with Fluoride (F)

Assessed Higher Order Systems with F

K ₂ SiF ₆ -K ₃ AlF ₆ -Na ₂ SiF ₆ -Na ₃ AlF ₆	
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TCSALT1 Assessed Mixed Systems

These are the 28 assessed mixed systems in the full range of composition and temperature.

<i>Assessed Mixed Systems</i>	
$\text{Al}_2\text{O}_3\text{-CaF}_2$	$\text{Al}_2\text{O}_3\text{-CaF}_2\text{-CaO}$
$\text{Al}_2\text{O}_3\text{-CaF}_2\text{-SiO}_2$	$\text{AlCl}_3\text{-AlF}_3\text{-KCl-KF}$
$\text{AlCl}_3\text{-AlF}_3\text{-NaCl-NaF}$	$\text{CaCl}_2\text{-CaF}_2$
$\text{CaCl}_2\text{-CaF}_2\text{-CaO}$	$\text{CaCl}_2\text{-CaF}_2\text{-KCl-KF}$
$\text{CaCl}_2\text{-CaF}_2\text{-MgCl}_2\text{-MgF}_2$	$\text{CaCl}_2\text{-CaF}_2\text{-NaCl-NaF}$
$\text{CaCl}_2\text{-CaF}_2\text{-SrCl}_2\text{-SrF}_2$	$\text{CaCl}_2\text{-CaO}$
$\text{CaF}_2\text{-CaO}$	$\text{CaF}_2\text{-KF-SiO}_2$
$\text{CaF}_2\text{-NaF-SiO}_2$	$\text{CaF}_2\text{-SiO}_2$
$\text{K}_2\text{SiF}_6\text{-KCl}$	$\text{K}_2\text{SiF}_6\text{-KCl-Na}_2\text{SiF}_6\text{-NaCl}$
KCl-KF	KCl-KF-NaCl-NaF
$\text{KCl-KF-SrCl}_2\text{-SrF}_2$	$\text{MgCl}_2\text{-MgF}_2$
$\text{MgCl}_2\text{-MgF}_2\text{-NaCl-NaF}$	$\text{MgF}_2\text{-SiO}_2$
NaCl-NaF	$\text{NaCl-NaF-SrCl}_2\text{-SrF}_2$
$\text{SrCl}_2\text{-SrF}_2$	$\text{SrCl}_2\text{-SrO}$

TCSALT1 Phases

In this section:

TCSALT1 Models for the Included Phases	15
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TCSALT1 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)2.0(Si+4)1.0(O-2)4.0(F-1)2.0
AL2SR4O7_A	Unknown Structure					3	(AL+3)2.0(SR+2)4.0(O-2)7.0
AL2SR4O7_B	Unknown Structure					3	(AL+3)2.0(SR+2)4.0(O-2)7.0
AL2SRO4_H	BaAl2O4 (H28)	H28	hP18	(182, P6_322)		3	(AL+3)2.0(CA+2, SR+2)1.0(O-2)4.0
AL2SRO4_L	SrAl2O4		mP28	(4, P2_1)		3	(AL+3)2.0(SR+2)1.0(O-2)4.0
ALCL3	AlCl3		mS16	(12, C2/m)		2	(AL+3)1.0(CL-1)3.0
ALF3_S1	FeF3 (D012)	D012	hR8	(167, R-3c)		2	(AL+3)1.0(F-1)3.0
ALF3_S2	AlF3		oS48	(63, Cmc _m)		2	(AL+3)1.0(F-1)3.0
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	(58, Pnnm)	This is a high-pressure phase (Al2O3.SiO2)	4	(AL+3)1.0(AL+3)1.0(Si+4)1.0(O-2)5.0
ANORTHITE	Ca(Al0.5Si0.5)4O8		aP104	(2, P-1)	This is anorthite (CaAl2Si2O8)	5	(CA+2)1.0(AL+3)1.0(AL+3)1.0(Si+4)2.0(O-2)8.0
C11A7F	Ca6Al7O16F		cI152	(220, I-43d)	This is 11CaO.7Al2O3.CaF2	4	(AL+3)14.0(CA+2)12.0(F-1)2.0(O-2)32.0
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)6.0(AL+3)6.0(AL+3)1.0(O-2)16.5
C1A1	Al2CaO4		mP84	(14, P2_1/c)	This is CaO.Al2O3	4	(CA+2, SR+2)3.0(AL+3)5.0(AL+3)1.0(O-2)12.0
C1A2	Al4CaO7		mS48	(15, C2/c)	This is CaO.2Al2O3 and SrO.2Al2O3	4	(CA+2, SR+2)1.0(AL+3)3.0(AL+3)1.0(O-2)7.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
C1A6	Magnetoplumbite (PbFe12O19)		hP64	(194, P6 ₃ /mmc)	This is CaO.6Al2O3 and SrO.6Al2O3	3	(CA+2, SR+2)1.0(AL+3)12.0(O-2)19.0
C1A8M2	CaMg2Al16O27		hP94	(187, P-6m2)	This is CaO.8Al2O3.2MgO	4	(CA+2)1.0(AL+3)16.0(MG+2)2.0(O-2)27.0
C2A14M2	BaFe15O23		hR78	(166, R-3m)	This is 2CaO.14Al2O3.2MgO	4	(CA+2)2.0(AL+3)28.0(MG+2)2.0(O-2)46.0
C3A1	Ca3Al2O6		cP264	(205, Pa-3)	This is 3CaO.Al2O3 and 3SrO.Al2O3	3	(CA+2, SR+2)3.0(AL+3)2.0(O-2)6.0
C3A2M1	3CaO.2Al2O3.MgO		oP72	(57, Pbcm)	This is 3CaO.2Al2O3.MgO (oP72, Pbcm or Pca21);	4	(CA+2)3.0(AL+3)4.0(MG+2)1.0(O-2)10.0
C3A3F	Unknown Structure				This is 3CaO.3Al2O3.CaF2	4	(AL+3)6.0(CA+2)4.0(F-1)2.0(O-2)12.0
CA10Si3O15F2	Unknown Structure				This is 9CaO.3SiO2.CaF2	4	(CA+2)10.0(Si+4)3.0(O-2)15.0(F-1)2.0
CA2AlF7	Ca2AlF7		oP40	(62, Pnma)		3	(CA+2)2.0(AL+3)1.0(F-1)7.0
CA2NA2Si2O7	Na2Ca2Si2O7		mS208	(15, C2/c)		4	(CA+2)2.0(NA+1)2.0(Si+4)2.0(O-2)7.0
CA2NA2Si3O9	Na(Na0.5Ca0.5)2CaSi3O9		hP102	(152, P3 ₁₂₁)		4	(CA+2)2.0(NA+1)2.0(Si+4)3.0(O-2)9.0
CA2SiO4_ALPHA_A	Ca2SiO4		hP24	(194, P6 ₃ /mmc)		3	(CA+2, MG+2, ZN+2)3.0(CA+2)1.0(SiO4-4)2.0
CA2SiO4_ALPHA_PRIME	K2CoCl4		oP84	(33, Pna2 ₁)		3	(CA+2, MG+2, ZN+2)3.0(CA+2)1.0(SiO4-4)2.0
CA3NA2Si6O16	Na2Ca3Si6O16		aP54	(2, P-1)		4	(CA+2)3.0(NA+1)2.0(Si+4)6.0(O-2)16.0
CA4Cl6O	Ba4Cl6O		hP22	(186, P6 ₃ mc)		3	(CA+2, SR+2)4.0(CL-1)6.0(O-2)1.0
CA5Si2O8F2	Unknown Structure				This is 4CaO.2SiO2.CaF2	4	(CA+2)5.0(Si+4)2.0(O-2)8.0(F-1)2.0
CAALCL5	Unknown Structure					3	(CA+2)1.0(AL+3)1.0(CL-1)5.0
CAALF5_S1	CrMnF5		mS28	(15, C2/c)		3	(CA+2)1.0(AL+3)1.0(F-1)5.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CAALF5_S2	CrMnF5		mP28	(14, P2_1/c)		3	(CA+2)1.0(AL+3)1.0(F-1)5.0
CACL2	Hydrophilite (CaCl2, C35)	C35	oP6	(58, Pnnm)	This is CaCl2 and low temperature SrCl2	2	(CA+2, MG+2, SR+2)1.0(CL-1)2.0
CACLF	Matlockite (PbFCl, E01)	E01	tP6	(129, P4/nmm)		3	(CA+2, SR+2)1.0(CL-1)1.0(F-1)1.0
CAF2_S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is SrF2 and low temperature CaF2.	2	(CA+2, MG+2, SR+2)1.0(F-1, O-2, VA)2.0
CAF2_S2	Cotunnite (PbCl2, C23)	C23	oP12	(62, Pnma)	This is high temperature CaF2.	2	(CA+2, MG+2, SR+2)1.0(F-1, O-2, VA)2.0
CANA2SI5O12	Unknown Structure					4	(CA+2)1.0(NA+1)2.0(Si+4)5.0(O-2)12.0
CANA2SiO4	Na2CaSiO4 (S66)	S66	cP32	(198, P2_13)		4	(CA+2)1.0(NA+1)2.0(Si+4)1.0(O-2)4.0
CANA4Si3O9	K4SrGe3O9		cP272	(205, Pa-3)		4	(CA+2)1.0(NA+1)4.0(Si+4)3.0(O-2)9.0
CLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)	clinoenstatite and diopside.	4	(CA+2, MG+2)1.0(MG+2)1.0(Si+4)2.0(O-2)6.0
CORDIERITE	Na0.04 (Mg0.5Fe0.5)2Al4Si5O18		oS120	(66, Cccm)	This is 2Al2O3.2MgO.5SiO2.	4	(AL+3)4.0(MG+2)2.0(Si+4)5.0(O-2)18.0
CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	(167, R-3c)	This is Al2O3	2	(AL+3)2.0(O-2)3.0
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	(227, Fd-3m)		2	(Si+4)1.0(SiO4-4)1.0
CRYOLITE	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)	This is (K,Na)3AlF6 solid solution.	2	(CA+2, K+1, NA+1, VA)3.0(ALF4-1, ALF6-3)1.0
CUSPIDINE	Ca4[Si2O7]([OH]0.25F0.75)2		mP60	(14, P2_1/c)	This is 3CaO.2SiO2.CaF2	4	(CA+2)4.0(Si+4)2.0(O-2)7.0(F-1)2.0
CAZNSI3O8	CAZNSI3O8		aP52	(2, P-1)		4	(CA+2)1.0(ZN+2)1.0(Si+4)3.0(O-2)8.0
GARNET	Orthorhombic Garnet		oF320	(70, Fddd)	This is Grossular, Uvarovite, Spessartine and Goldmanite Garnets.	4	(CA+2, MG+2)3.0(AL+3)2.0(Si+4)3.0(O-2)12.0
HALITE_B1	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is (K,Na)(Cl,F) solid solution.	2	(CA+2, K+1, NA+1, VA)1.0(CL-1, F-1)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
HALITE_OX	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is CaO, MgO and SrO.	2	(AL+3, CA+2, MG+2, NA+1, SR+2, VA, ZN+2)1.0(O-2)1.0
HATRURITE	Ca ₃ (SiO ₄)O-b		hR81	(160, R3m)	This is 3CaO.SiO ₂ .	3	(CA+2, ZN+2)3.0(SiO4-4)1.0(O-2)1.0
K10MG5SI11O32	Unknown Structure					4	(K+1)10.0(MG+2)5.0(Si+4)11.0(O-2)32.0
K2ALF5	Rb ₂ MnF ₅		tP8	(123, P4/mmm)		3	(K+1)2.0(AL+3)1.0(F-1)5.0
K2CA2SI2O7	K ₂ Ca ₂ [Si ₂ O ₇]		hP108	(176, P6 ₃ /m)		4	(K+1)2.0(CA+2)2.0(Si+4)2.0(O-2)7.0
K2CA2SI9O21	Unknown Structure					4	(K+1)2.0(CA+2)2.0(Si+4)9.0(O-2)21.0
K2CA3SI6O16	Unknown Structure					4	(K+1)2.0(CA+2)3.0(Si+4)6.0(O-2)16.0
K2CA6SI4O15	K ₂ Ca ₆ Si ₄ O ₁₅		mP54	(13, P2/c)		4	(K+1)2.0(CA+2)6.0(Si+4)4.0(O-2)15.0
K2CASIO4	Unknown Structure					4	(K+1)2.0(CA+2)1.0(Si+4)1.0(O-2)4.0
K2MG5SI12O30	K ₂ Mg ₅ Si ₁₂ O ₃₀		hP100	(192, P6/mcc)		4	(K+1)2.0(MG+2)5.0(Si+4)12.0(O-2)30.0
K2MGF4	K ₂ NiF ₄		tI14	(139, I4/mmm)	This is K ₂ ZnF ₄ and K ₂ Mg(Cl,F) ₄ solid solution.	3	(K+1, NA+1)2.0(MG+2, ZN+2)1.0(CL-1, F-1)4.0
K2MGSI04_HT	Unknown Structure					2	(K2MG+4, Si+4)1.0(SiO4-4)1.0
K2MGSI04_LT	Na ₂ Be[SiO ₄]		oP64	(29, Pca2 ₁)		2	(K2MG+4, Si+4)1.0(SiO4-4)1.0
K2NAALF6	Double Perovskite (Ba ₂ MnWO ₆)		cF40	(225, Fm-3m)		3	(K+1)2.0(NA+1)1.0(ALF6-3)1.0
K2Si4O9_ALPHA	K ₂ Si ₄ O ₉		aP30	(2, P-1)	Low-temp K ₂ Si ₄ O ₉ (tricl)	3	(K+1)2.0(Si+4)4.0(O-2)9.0
K2Si4O9_BETA	K ₂ Si ₄ O ₉		hP30	(176, P6 ₃ /m)	High-temp K ₂ Si ₄ O ₉ (hex)	3	(K+1)2.0(Si+4)4.0(O-2)9.0
K2SRCL4	Th ₃ P ₄ (D73)	D73	cl28	(220, I-43d)		3	(K+1)2.0(SR+2)1.0(CL-1)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
K2ZNCL4	Arcanite (K2SO4, H16)	H16	oP28	(62, Pnma)		3	(K+1)2.0(ZN+2)1.0(CL-1)4.0
K3MG2CL7	Sr3Ti2O7		tI24	(139, I4/mmm)		3	(K+1)3.0(MG+2)2.0(CL-1)7.0
K3SIF7	Unknown Structure					3	(K+1)3.0(SI+4)1.0(F-1)7.0
K4AL22O35	K2Al10.67O17		hR30	(166, R-3m)	This is Beta double prime-Al2O3 K4AL22O35.	6	(K+1, VA)1.0(K+1, VA)1.0(AL+3, MG+2)2.0 (O-2, VA)1.0(AL+3)9.0(O-2)17.0
K4CASI3O9	K4SrGe3O9		cP272	(205, Pa-3)		4	(K+1)4.0(CA+2)1.0(SI+4)3.0(O-2)9.0
K4CASI6O15	Unknown Structure					4	(K+1)4.0(CA+2)1.0(SI+4)6.0(O-2)15.0
K4MG2SI5O14	Unknown Structure					4	(K+1)4.0(MG+2)2.0(SI+4)5.0(O-2)14.0
K4SIO4	Cs4SnO4		mP36	(14, P2_1/c)		3	(K+1)4.0(SI+4)1.0(O-2)4.0
K5ZN4CL13	Unknown Structure					3	(K+1)5.0(ZN+2)4.0(CL-1)13.0
K8CASI10O25	Unknown Structure					4	(K+1)8.0(CA+2)1.0(SI+4)10.0(O-2)25.0
KAL11O17	beta-Alumina (Al2O3, D56)	D56	hP60	(194, P6_3/mmc)	This is Beta- Al2O3 KAl11O17.	6	(K+1, VA)1.0(K+1, VA)1.0(AL+3, MG+2)2.0 (O-2, VA)1.0(AL+3)9.0(O-2)17.0
KAL4F13	Unknown Structure					3	(K+1)1.0(AL+3)4.0(F-1)13.0
KALCL4	KAICl4		mP24	(4, P2_1)		3	(K+1)1.0(AL+3)1.0(CL-1)4.0
KALF4	RbAlF4		tP12	(127, P4/mbm)		3	(K+1)1.0(AL+3)1.0(F-1)4.0
K2MGSI5O12	K8(Al0.33Si0.67)24O48		tI160	(88, I4_1/a)		5	(K+1)2.0(MG+2)1.0(SI+4)1.0(SI+4)4.0(O-2)12.0
K2MGSI3O8	KLi[SO4]		hP14	(159, P31c)		4	(K2MG+4)1.0(SI+4)1.0(SI+4)2.0(O-2)8.0
KMG2AL15O25	Unknown Structure					4	(K+1)1.0(MG+2)2.0(AL+3)15.0(O-2)25.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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, NA+1)1.0(CA+2, MG+2, SR+2, ZN+2)1.0(CL-1, F-1)3.0
KSR2CL5	U ₂ PbSe ₅		mP32	(14, P2_1/c)		3	(K+1)1.0(SR+2)2.0(CL-1)5.0
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)1.0(AL+3)1.0(SI+4)1.0(O-2)5.0
KZN2CL5	Unknown Structure					3	(K+1)1.0(ZN+2)2.0(CL-1)5.0
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)2.0(SI+4)1.0(O-2)4.0
LOWCLINO_PYROXENE	Diopside [CaMg(SiO ₃) ₂ , S41]	S41	mS40	(15, C2/c)	This is low- clinoenstatite and low-clinodiopside	4	(CA+2, MG+2)1.0(MG+2)1.0(SI+4)2.0(O-2)6.0
MELILITE	Akermanite (Ca ₂ MgSi ₂ O ₇ , S53)	S53	tP24	(113, P-42_1m)	This is gehlenite and akermanite.	5	(CA+2)2.0(AL+3, MG+2, ZN+2)1.0(AL+3, SI+4)1.0(SI+4)1.0(O-2)7.0
MERWINITE	Ca ₃ Mg(SiO ₄) ₂		mP56	(14, P2_1/c)	This is 3CaO.MgO.2SiO ₂	4	(CA+2)3.0(MG+2)1.0(SI+4)2.0(O-2)8.0
MG2NA2SI6O15	Na ₂ Mg ₂ Si ₆ O ₁₅		oS200	(64, Cmce)		4	(MG+2)2.0(NA+1)2.0(SI+4)6.0(O-2)15.0
MGAL2CL8	CoAl ₂ Cl ₈		mS44	(15, C2/c)		3	(MG+2)1.0(AL+3)2.0(CL-1)8.0
MGAL2F8	Unknown Structure					3	(MG+2)1.0(AL+3)2.0(F-1)8.0
MGCL2	CdI ₂		hP3	(164, P-3m1)		2	(MG+2)1.0(CL-1)2.0
MGF2	Rutile (TiO ₂ , C4)	C4	tP6	(136, P4_2/mnm)	This is MgF ₂ and It- ZnF ₂ .	2	(MG+2, ZN+2)1.0(F-1)2.0
MGNA2SI4O10	Unknown Structure					4	(MG+2)1.0(NA+1)2.0(SI+4)4.0(O-2)10.0
MULLITE	Al(Al _{0.7} Si _{0.3}) ₂ O _{4.8}		oP24	(55, Pbam)		4	(AL+3)1.0(AL+3)1.0(AL+3, SI+4)1.0(O-2, VA)5.0
NA10SIO7	Unknown Structure					3	(NA+1)10.0(SI+4)1.0(O-2)7.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NA2AL12O19	Na0.5Al3O4.75		oP24	(55, Pbam)	This is Beta double prime-Al2O3 Na2Al12O19.	3	(NA+1)2.0(AL+3)12.0(O-2)19.0
NA2CA3AL16O28	Unknown Structure					4	(NA+1)2.0(CA+2)3.0(AL+3)16.0(O-2)28.0
NA2CA8AL6O18	Unknown Structure					4	(NA+1)2.0(CA+2)8.0(AL+3)6.0(O-2)18.0
NA2CAAL4O8	Unknown Structure				This is (K, Na)2CaAl4O8 solid solution.	4	(K+1, NA+1, VA)1.0(CA+2, K+1, NA+1)1.0 (AL+3)2.0(O-2)4.0
NA2MGCL4	Sr2PbO4		oP20	(55, Pbam)		3	(NA+1)2.0(MG+2)1.0(CL-1)4.0
NA2O1_S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is rt (K,Na)2O.	2	(K+1, NA+1)2.0(O-2)1.0
NA2O1_S2	Unknown Structure				This is ht1 (K, Na)2O.	2	(K+1, NA+1)2.0(O-2)1.0
NA2O1_S3	Unknown Structure				This is ht2 (K, Na)2O.	2	(K+1, NA+1)2.0(O-2)1.0
NA2SI2O5_ALPHA	Na2Si2O5-a		mP36	(14, P2_1/c)	This is lt-(K, Na)2Si2O5 solid solution.	3	(K+1, NA+1)2.0(SI+4)2.0(O-2)5.0
NA2SI2O5_BETA	Na2Si2O5-b		mP36	(14, P2_1/c)	This is intermediat-temp (K,Na)2Si2O5 solid solution.	3	(K+1, NA+1)2.0(SI+4)2.0(O-2)5.0
NA2SI2O5_GAMMA	Na2Si2O5		oP36	(60, Pbcn)	This is ht-(K, Na)2Si2O5 solid solution.	3	(K+1, NA+1)2.0(SI+4)2.0(O-2)5.0
NA2SIF6_S1	Na2SiF6		hP27	(150, P321)	low-temperature trigonal phase	2	(NA+1)2.0(SIF6-2)1.0
NA2SIF6_S2	K2PtCl6 (J11)	J11	cF36	(225, Fm-3m)	high-temperature cubic phase	2	(K+1, NA+1)2.0(SIF6-2)1.0
NA2SIO3	Na2SiO3		oS24	(36, Cmc2_1)	This is (K, Na)2SiO3 solid solution.	3	(K+1, NA+1)2.0(SI+4)1.0(O-2)3.0
NA2ZNCL4	Forsterite (Mg2SiO4, S12)	S12	oP28	(62, Pnma)		3	(NA+1)2.0(ZN+2)1.0(CL-1)4.0
NA3ALF6_S1	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)		3	(NA+1)3.0(AL+3)1.0(F-1)6.0
NA4SIO4	K4SnO4		aP18	(2, P-1)		3	(NA+1)4.0(SI+4)1.0(O-2)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NA5AL3F14	Chiolite (Na5Al3F14, K75)	K75	tP44	(128, P4/mnc)		3	(NA+1)5.0(AL+3)3.0(F-1)14.0
NA6Si2O7	Na6[Si2O7]		aP120	(2, P-1)		3	(NA+1)6.0(Si+4)2.0(O-2)7.0
NA6Si8O19	Na6Si8O19		mP132	(14, P2_1/c)		3	(NA+1)6.0(Si+4)8.0(O-2)19.0
NAAL11O17	NaAl11O17		hP58	(194, P6_3/mmc)	This is Beta- Al2O3 NaAl11O17 solid solution.	5	(NA+1)2.0(NA+1, VA)2.0(AL+3)22.0(O-2)34.0(O-2, VA)1.0
NAALCL4	NaAlCl4		oP24	(19, P2_12_12_1)		3	(NA+1)1.0(AL+3)1.0(CL-1)4.0
NAALO2_D	LiGaO2		oP16	(33, Pna2_1)		2	(NAAL+4)1.0(O-2)2.0
NACAALF6_S1	NaCaAlF6		mP72	(14, P2_1/c)		4	(NA+1)1.0(CA+2)1.0(AL+3)1.0(F-1)6.0
NACAALF6_S2	Unknown Structure					4	(NA+1)1.0(CA+2)1.0(AL+3)1.0(F-1)6.0
NACAALF6_S3	Unknown Structure					4	(NA+1)1.0(CA+2)1.0(AL+3)1.0(F-1)6.0
NAFE02_B	LiGaO2		oP16	(33, Pna2_1)	This is low-temp KAlO2 and NaAlO2 solid solutions.	2	(KAL+4, NAAL+4)1.0(O-2)2.0
NAFE02_G	LiAlO2		tP16	(92, P4_12_12)	This is high-temp KAlO2 and mid-temp NaAlO2 solid solutions.	2	(KAL+4, NAAL+4)1.0(O-2)2.0
NAMGCL3	Ilmenite (FeTiO3, E22)	E22	hR10	(148, R-3)		3	(NA+1)1.0(MG+2)1.0(CL-1)3.0
NAMGF3	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)		3	(NA+1)1.0(MG+2, ZN+2)1.0(F-1)3.0
NEPHELINE_G	KLi[SO4]		hP18	(173, P6_3)	This is K2MgSi3O8.	4	(K2MG+4)4.0(Si+4)4.0(Si+4)8.0(O-2)32.0
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	oP28	(62, Pnma)	This is 2CaO.SiO2, forsterite and monticellite[CaO.MgO.SiO2]	4	(CA+2, MG+2, ZN+2)1.0(CA+2, MG+2, ZN+2)1.0(Si+4)1.0(O-2)4.0
ORTHO_PYROXENE	Enstatite (MgSiO3, S43)	S43	oP80	(61, Pbca)	This is enstatite and orthodiopside	4	(CA+2, MG+2)1.0(MG+2)1.0(Si+4)2.0(O-2)6.0
PROTO_PYROXENE	MgSiO3		oP40	(60, Pbcn)	This is proto- enstatite and protodiopside.	3	(CA+2, MG+2, ZN+2)1.0(Si+4)1.0(O-2)3.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PSEUDO_WOLLASTONITE	CaSiO3		mS120	(15, C2/c)	This is CaO.SiO2	3	(CA+2, SR+2)1.0(SI+4)1.0(O-2)3.0
QUARTZ	alpha-Quartz (low Quartz)		hP9	(152, P3_121)		2	(SI+4)1.0(SIO4-4)1.0
RANKINITE	3CaO.2SiO2		mP48	(14, P2_1/c)	This is 3CaO.2SiO2	3	(CA+2)3.0(SI+4)2.0(O-2)7.0
SAPPHIRINE	CaMg3Si3O10		aP68	(2, P-1)	This is 9Al2O3.7MgO.3SiO2	4	(AL+3)18.0(MG+2)7.0(SI+4)3.0(O-2)40.0
SILLIMANITE	Sillimanite (Al2SiO5, S03)	S03	oP32	(62, Pnma)	This is a high-pressure phase (Al2O3.SiO2)	4	(AL+3)1.0(AL+3)1.0(SI+4)1.0(O-2)5.0
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)	This is MgAl2O4.	4	(AL+3, MG+2, ZN+2)1.0(AL+3, CA+2, MG+2, VA, ZN+2)2.0(MG+2, VA)2.0(O-2)4.0
SR2SIO4_ALPHA_A	Arcanite (K2SO4, H16)	H16	oP28	(62, Pnma)		3	(SR+2)2.0(SI+4)1.0(O-2)4.0
SR2SIO4_ALPHA_PRIME	Unknown Structure					3	(SR+2)2.0(SI+4)1.0(O-2)4.0
SR3SIO5	Sr3[SiO4]O		tP36	(130, P4/ncc)		3	(SR+2)3.0(SI+4)1.0(O-2)5.0
SRCL2_S2	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(CA+2, SR+2)1.0(CL-1)2.0
SRMGF4_S1	Bi[ReO4]		oS24	(63, Cmcm)		3	(MG+2)1.0(SR+2)1.0(F-1)4.0
SRMGF4_S2	Unknown Structure					3	(MG+2)1.0(SR+2)1.0(F-1)4.0
SRSIO3	SrSiO3		mS60	(15, C2/c)		3	(CA+2, SR+2)1.0(SI+4)1.0(O-2)3.0
SRZNCL4	Scheelite (CaWO4, H04)	H04	tI24	(88, I4_1/a)		3	(SR+2)1.0(ZN+2)1.0(CL-1)4.0
TRIDYMITITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	(9, Cc)		2	(SI+4)1.0(SIO4-4)1.0
WOLLASTONITE	Wollastonite (CaSiO3)		aP30	(2, P-1)	This is CaO.SiO2.	3	(CA+2, MG+2)1.0(SI+4)1.0(O-2)3.0
ZINCITE	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	This is ZnO with Ca and Mg solubility.	2	(CA+2, MG+2, ZN+2)1.0(O-2)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZN2SIO4	Phenakite (Be2SiO4, S13)	S13	hR42	(148, R-3)		4	(MG+2, ZN+2)1.0(MG+2, ZN+2)1.0 (SI+4)1.0(O-2)4.0
ZNCL2	ZnCl2		oP12	(33, Pna2_1)		2	(ZN+2)1.0(CL-1)2.0
ZNF2_S2	Unknown Structure					2	(ZN+2)1.0(F-1)2.0

Gas and IONIC_LIQ Phases

Name	Prototype	Info	Sublattices	Formula Unit
GAS	Gas		1	(AL, AL1CL1, AL1CL1F1, AL1CL1F2, AL1CL1O1, AL1CL2, AL1CL2F1, AL1CL2O1, AL1CL3, AL1F1, AL1F1O1, AL1F2, AL1F2NA1O1, AL1F2O1, AL1F3, AL1F4K1, AL1F4NA1, AL1O1, AL1O2, AL2, AL2CL6, AL2F6, AL2F8NA2, AL2O1, AL2O2, AL2O3, AL3CA1CL11, CA, CA1CL1, CA1CL2, CA1F1, CA1F2, CA1O1, CA2, CL, CL1F1, CL1F1MG1, CL1F1O3, CL1F1SI1, CL1F3, CL1F3SI1, CL1F5, CL1K1, CL1MG1, CL1NA1, CL1O1, CL1O2, CL1O3, CL1SI1, CL1SR1, CL1ZN1, CL2, CL2K2, CL2MG1, CL2NA2, CL2O1, CL2O1_1, CL2O1_2, CL2O2_1, CL2O2_2, CL2O2_3, CL2SI1, CL2SR1, CL2ZN1, CL3F1SI1, CL3NA3, CL3SI1, CL4MG2, CL4SI1, CL4ZN2, F, F1K1, F1MG1, F1NA1, F1O1, F1O2_1, F1O2_2, F1O2_OFO, F1SI1, F1SR1, F1ZN1, F2, F2K2, F2MG1, F2NA2, F2O1, F2O1SI1, F2O2, F2O2_FOOF, F2SI1, F2SR1, F2ZN1, F3NA3, F3SI1, F4MG2, F4SI1, F4ZN2, K, K1NA1, K1O1, K2, K2O1, K2O2, MG, MG1O1, MG2, NA, NA1O1, NA2, NA2O1, NA2O2, O, O1SI1, O1SR1, O1ZN1, O2, O2SI1, O2SI2, O3, SI, SI2, SI3, SR, SR2, ZN)1.0
IONIC_LIQ	Liquid	Liquid metal and slag mixture.	2	(CA+2, K+1, MG+2, NA+1, SR+2, ZN+2)P(ALCL4-1, ALF4-1, ALF6-3, CL-1, F-1, O-2, SIF6-2, SIO4-4, ALCL3, ALF3, ALO3/2, SICL4, SIF4, SIO2, ZNCL2, ZNF2)Q