TCS Metal Oxide Solutions Database (TCOX14)

Technical Information

Available Starting with Thermo-Calc Version 2025a

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Contents

About the TCS Metal Oxide Solutions Database (TCOX)

TCS Metal Oxide Solutions Database (TCOX) is a thermodynamic database for slags and oxides. The database integrates thermodynamic data plus properties data for molar volume, viscosity for ionic liquids, surface tension, electrical conductivity for ionic liquid, and thermal conductivity for the ionic liquid.

The properties data for molar volume and viscosity for ionic liquids are included with TCS Metal Oxide Solutions Database (TCOX) starting with version 10 (TCOX10). Surface tension is included as of version 11 (TCOX11). Electrical conductivity of ionic liquid is included as of version 13 (TCOX13). Thermal conductivity of ionic liquid is included as of version 14 (TCOX14).

Carbides and nitrides are included in the database. However, neither intermetallic compounds and phases, nor ordered BCC, FCC, and HCP, are included.

TCOX: TCS Metal Oxide Solutions Database Revision History. The current version of the database is TCOX14. See the link for any subversion release details.

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.

The TCOX database, which was first released in 1992, is the result of a long-term collaboration with academia. For some historical information, see TCOX: TCS Metal Oxide Solutions Database Revision History.

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

Use Case Examples

There are examples available to both demonstrate the *validation* of the database and to showcase the types of *calculations* that can be used for different materials or application area such as process metallurgy, heat treatment, and more depending on the database.

Some use case examples of how the TCOX14 database can be used include the following.

- The intended application is for solid and liquid ionized materials, e.g. oxides or sulfides. This could be development of ceramics, slags, refractories, metallurgical processing (e.g. slag and liquid metal interactions), ESR slags, materials corrosion, Thermal Barrier Coatings (TBC), Yttria-Stabilised-Zirconia (YSZ), solid oxide fuel cell materials, sulfide formation, dephosphorization and desulfurization.
- This database can be used for fluoride and sulfide systems without oxygen.
- The liquid phase is described from liquid metal to oxide and/or fluoride, i.e. no pure liquid oxygen or fluorine is modeled.
- For sulfur, the liquid phase is described all the way from metal to sulfur.
- The database is compatible with the Process Metallurgy Module, which is used for advanced calculations involving slag, metal, and gas.

Go to the Metal Slag and Oxides Database page on our website where you can access a Validation and Calculation Examples Collection and the Technical Information plus learn about its many applications with the Process Metallurgy Module. Also explore further applications of Thermo-Calc to Refractory Oxides and Slags including links to resources such as examples, publications, and more.

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 Metal Oxide Solutions Database (TCOX) 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 Metal Oxide Solutions Database (TCOX) Technical Information* PDF document contains version specific information such as the binary, ternary, and higher-order assessed systems, phases, and models. It also includes a list of the included elements, details about the properties (e.g. viscosity, molar volume, etc.), and a summary of the database revision history by version.
- The *TCS Metal Oxide Solutions Database (TCOX) Validation and Calculation Examples Collection* PDF document contains a series of validation examples using experimental data, and a set of calculation examples showing some of the ways the database can be used. Additional examples are available on the website.

Go to the Metal Slag and Oxides Database page on our website where you can access a Validation and Calculation Examples Collection and the Technical Information plus learn about its many applications with the Process Metallurgy Module. Also explore further applications of Thermo-Calc to Refractory Oxides and Slags including links to resources such as examples, publications, and more.

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

TCOX14 Elements, Systems, Phases, and Properties

Included Elements

There are 34 elements included in the most recent version of the database.

Included Elements									
Al	Ar*	B	Ba	C	Ca	Co	Cr	Cu	F
Fe	Gd	H*	Hf	K	La	Li	Mg	Mn	Mo
N	Na	Nb	Ni	O	P	S	Si	Ti	V
W	Y	Yb	Zr						

** Ar and H are only included in the gas phase.*

Assessed Systems

The most recent version of the database contains assessments of these systems:

- 433 binary and 557 ternary systems in the 34 element framework.
- 294 quaternary systems and 33 higher order systems.

Carbides and nitrides are included in the database. However, neither intermetallic compounds and phases, nor ordered BCC, FCC, and HCP, are included.

For those intermetallic phases not included, and in order for the metallic systems to be accurate to the full range of composition and temperature, phases need to be appended from another database. See TCOX14 Assessed Metallic Systems for suggestions.

The most accurate calculations are obtained in or near these sub-systems and composition ranges.

Assessed Phases

The most recent version of the database contains 744 phases in total.

TCOX14 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 often represent the metallic and ionized liquid phases. 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.

Common Phases for the TCOX Database

OTHER PHASES

The TCOX14 database also contains solid oxides, silicates, fluorides, sulfides, carbides and nitrides, a gaseous mixture phase and solid solution alloy phases (FCC_A1, BCC_A2 etc). Many phases are modeled as solution phases (in all cases where it is meaningful). The solid solution phases such as spinel, mullite, corundum, halite, olivine, fluorite, etc. are modeled within the framework of the Compound Energy Formalism (CEF) [2001Hil].

Properties Data Theory and Assessed Systems

The assessed, partially assessed, or estimated systems related to the properties data are included in this document.

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.

As detailed in each section, parameters for the thermophysical properties are assessed or estimated for the ionic liquid phase:

- **Viscosity**: TCOX14 Viscosity for Ionic Liquids: Assessed or Estimated Systems.
- **Molar Volume**: TCOX14 Molar Volume: Assessed or Estimated Phases.
- **Surface Tension**: TCOX14 Surface Tension for Oxide Slag: Assessed Systems.
- **Electrical Conductivity**: TCOX14 Electrical Conductivity/Resistivity for Ionic Liquids: Assessed or Estimated Systems.
- **Thermal Conductivity**: TCOX14 Thermal Conductivity/Resistivity for Ionic Liquids: Assessed or Estimated Systems.

Parameters and Variables

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 the SDKs (i.e. TC-Python or TC-Toolbox for MATLAB®)*
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
Electrical conductivity/resistivity	ELQ, ELRS	`ELCD/ELRS` for a system; `ELCD/ELRS(PHI)` for phase PHI
Thermal conductivity/resistivity	THCD	`THCD/THRS` for a system; `THCD/THRS(PHI)` for phase PHI

References

[1985Hil] M. Hillert, B. Jansson, B. Sundman, and J. Ågren, “A two-sublattice model for molten solutions with different tendency for ionization,” Metall. Trans. A, vol. 16(1), 261–266, 1985.

[1991Sun] B. Sundman, “Modification of the two-sublattice model for liquids,”Calphad, vol. 15(2), 109–119, 1991.

[2001Hil] M. Hillert, “The compound energy formalism,” J. Alloys Compd., vol. 320(2), 161–176, 2001.

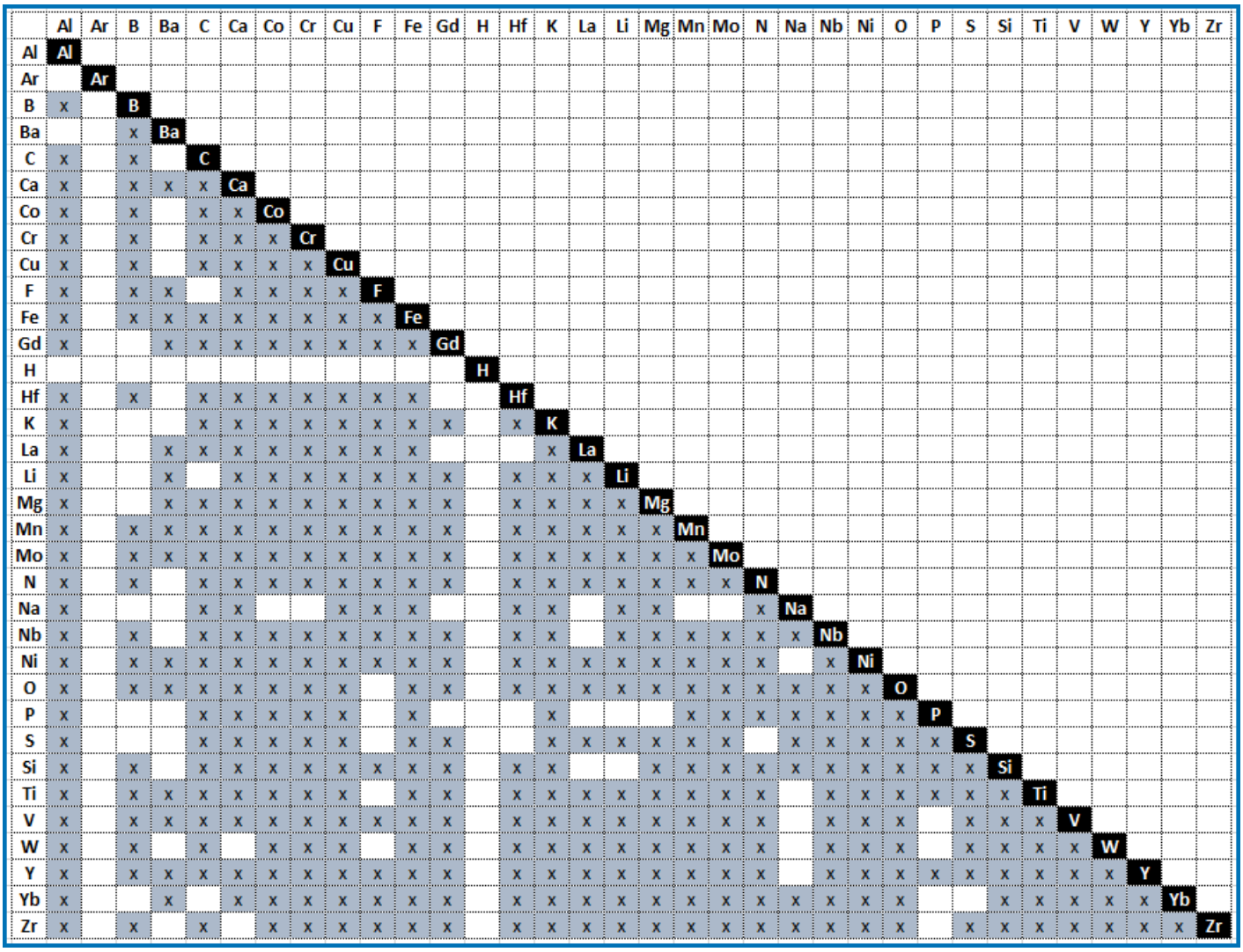
[2021Zha] R. Zhang, S. Hallström, H. Mao, L. Kjellqvist, Q. Chen, Accurate Viscosity Prediction for Molten Slags: A New Model and Database. ISIJ Int. 61, 1379–1388 (2021).

TCOX14 Systems

In this section:

TCOX14 Assessed Binary Systems

These are the assessed binary systems for the metallic, oxide, fluoride, and sulfide systems.



	Al	Ar	B	Ba	C	Ca	Co	Cr	Cu	F	Fe	Gd	H	Hf	K	La	Li	Mg	Mn	Mo	N	Na	Nb	Ni	O	P	S	Si	Ti	V	W	Y	Yb	Zr
Al	Al																																	
Ar		Ar																																
B	x		B																														
Ba			x	Ba																														
C	x		x		C																													
Ca	x		x	x	x	Ca																												
Co	x		x		x	x	Co																											
Cr	x		x		x	x	x	Cr																										
Cu	x		x		x	x	x	x	Cu																									
F	x		x	x		x	x	x	x	F																								
Fe	x		x	x	x	x	x	x	x	x	Fe																							
Gd	x			x	x	x	x	x	x	x	x	Gd																						
H													H																					
Hf	x		x		x	x	x	x	x	x	x			Hf																				
K	x				x	x	x	x	x	x	x	x		x	K																			
La	x			x	x	x	x	x	x	x	x				x	La																		
Li	x			x		x	x	x	x	x	x	x		x	x	x	Li																	
Mg	x			x	x	x	x	x	x	x	x	x		x	x	x	x	Mg																
Mn	x		x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	Mn															
Mo	x		x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	Mo														
N	x		x		x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	N													
Na	x				x	x			x	x	x			x	x		x	x			x	Na												
Nb	x		x		x	x	x	x	x	x	x	x		x	x		x	x	x	x	x	x	Nb											
Ni	x		x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x		x	Ni										
O	x		x	x	x	x	x	x	x		x	x		x	x	x	x	x	x	x	x	x	x	x	O									
P	x				x	x	x	x	x		x				x				x	x	x	x	x	x	x	P								
S	x				x	x	x	x	x		x	x			x	x	x	x	x	x		x	x	x	x	x	S							
Si	x		x		x	x	x	x	x	x	x	x		x	x			x	x	x	x	x	x	x	x	x	x	Si						
Ti	x		x	x	x	x	x	x	x		x	x		x	x	x	x	x	x	x	x		x	x	x	x	x	x	Ti					
V	x		x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x		x	x	x		x	x	x	V				
W	x		x		x		x	x	x		x	x		x	x	x	x	x	x	x	x		x	x	x		x	x	x	x	W			
Y	x		x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x	Y		
Yb	x			x		x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x			x	x	x	x	x	Yb	
Zr	x		x		x		x	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	Zr

TCOX14 Assessed Metallic Systems

Carbides and nitrides are included in the database. However, neither intermetallic compounds and phases, nor ordered BCC, FCC, and HCP, are included.

TCOX14 Assessed Binary Systems. Many ternary metallic systems are also assessed but not listed here.

If needed, more solid phases can be appended from TCS Steel and Fe-alloys Database (TCFE), TCS Ni-based Superalloys Database (TCNI), TCS Al-based Alloy Database (TCAL), or other appropriate databases. However, combining different databases should always be done with caution, since not always the same assessments of subsystems are used.

TCOX14 Assessed Oxide Systems

These are the assessed oxide systems for ternary, quaternary, and higher order systems in the full range of composition and temperature.

TCOX14 Assessed Binary Systems

Assessed Ternary Oxide Systems, Me1-Me2-O

	Al	Ar	B	Ba	C	Ca	Co	Cr	Cu	F	Fe	Gd	H	Hf	K	La	Li	Mg	Mn	Mo	N	Na	Nb	Ni	O	P	S	Si	Ti	V	W	Y	Yb	Zr
Al	Al		x	x		x	x	x	x	x	x	x		x	x	x	x	x	x	x		x	x	x		x	x	x	x	x	x	x	x	x
Ar		Ar																																
B			B	x		x	x		x		x	x			x	x	x	x	x			x	x	x		x		x	x	x	x	x	x	x
Ba				Ba	x	x		x		x	x	x		x		x	x	x			x			x		x		x	x			x	x	x
C					C	x		x			x				x	x	x	x				x		x					x	x				x
Ca						Ca	x	x	x	x	x	x		x		x	x	x	x		x		x	x		x	x	x	x	x	x	x	x	x
Co							Co	x	x		x	x				x	x	x	x				x	x		x	x	x	x	x	x	x		x
Cr								Cr	x		x	x				x	x	x	x			x	x	x		x	x	x	x	x		x		x
Cu									Cu	x	x	x			x	x	x	x	x	x		x	x	x		x	x	x	x			x		
F										F		x					x	x																
Fe											Fe	x			x	x	x	x	x	x		x	x	x		x	x	x	x	x	x	x	x	x
Gd												Gd		x		x		x	x					x		x		x	x			x		x
H													H																					
Hf														Hf		x		x										x	x		x	x	x	x
K															K											x		x	x					
La																La			x				x	x		x		x	x		x	x	x	x
Li																	Li	x	x		x				x		x	x			x		x
Mg																		Mg	x		x		x	x		x	x	x	x	x	x	x	x	x
Mn																			Mn				x	x		x	x	x	x	x	x	x		x
Mo																				Mo						x					x			
N																					N	x												
Na																						Na				x		x	x	x				
Nb																							Nb	x		x		x	x	x		x		x
Ni																								Ni		x		x	x	x	x	x		x
O																									O									
P																										P		x	x	x	x	x		x
S																											S	x						
Si																												Si	x	x	x	x	x	x
Ti																													Ti	x	x	x	x	x
V																														V		x		x
W																															W	x		x
Y																																Y	x	x
Yb																																	Yb	x
Zr																																		Zr

Assessed Quaternary Oxide Systems

Assessed Quaternary Oxide Systems, Me1-Me2-Me3-O						
Al-B-Ba-O	Al-B-Ca-O	Al-B-K-O	Al-B-Mg-O	Al-B-Na-O	Al-B-O-Si	Al-Ba-Ca-O
Al-Ba-Mg-O	Al-Ba-O-Si	Al-Ca-Co-O	Al-Ca-Cr-O	Al-Ca-Fe-O	Al-Ca-Gd-O	Al-Ca-K-O
Al-Ca-Li-O	Al-Ca-Mg-O	Al-Ca-Mn-O	Al-Ca-Na-O	Al-Ca-Nb-O	Al-Ca-Ni-O	Al-Ca-O-P
Al-Ca-O-Si	Al-Ca-O-Ti	Al-Ca-O-Y	Al-Ca-O-Yb	Al-Ca-O-Zr	Al-Co-O-Si	Al-Co-O-Ti
Al-Cr-Fe-O	Al-Cr-Mg-O	Al-Cr-O-Si	Al-Cr-O-Ti	Al-Cr-O-Y	Al-Cu-O-Si	Al-Fe-K-O
Al-Fe-Li-O	Al-Fe-Mg-O	Al-Fe-Mn-O	Al-Fe-Na-O	Al-Fe-O-Si	Al-Fe-O-Ti	Al-Fe-O-Y
Al-Gd-Hf-O	Al-Gd-O-Zr	Al-Hf-O-Y	Al-Hf-O-Yb	Al-K-Mg-O	Al-K-O-Si	Al-La-O-Y
Al-La-O-Zr	Al-Li-Mg-O	Al-Li-Na-O	Al-Li-O-Si	Al-Mg-O-P	Al-Mg-O-Si	Al-Mg-O-Ti
Al-Mg-O-Y	Al-Mg-O-Zr	Al-Mn-O-Si	Al-Mn-O-Ti	Al-Na-O-P	Al-Na-O-Si	Al-Ni-O-Ti
Al-O-P-Si	Al-O-Si-Ti	Al-O-Si-Y	Al-O-Si-Yb	Al-O-Si-Zr	Al-O-Ti-Zr	Al-O-Y-Zr
B-Ba-Ca-O	B-Ba-K-O	B-Ba-Li-O	B-Ba-Na-O	B-Ba-O-Si	B-Ca-Fe-O	B-Ca-O-Si
B-Fe-Na-O	B-K-Mg-O	B-K-Na-O	B-K-O-Si	B-Li-Na-O	B-Li-O-Si	B-Na-O-Si
Ba-C-Li-O	Ba-C-Na-O	Ba-Ca-Fe-O	Ba-Ca-N-O	Ba-Ca-O-P	Ba-Ca-O-Si	Ba-Ca-O-Y
Ba-Fe-O-P	Ba-Fe-O-Si	Ba-K-N-O	Ba-K-O-Si	Ba-Li-N-O	Ba-Li-O-Si	Ba-Mg-O-Si
Ba-Na-O-Si	Ba-O-Si-Ti	Ba-O-Y-Zr	C-Ca-Fe-O	C-Ca-Mg-O	C-Fe-Mg-O	C-K-Li-O
C-K-N-O	C-K-Na-O	C-Li-N-O	C-Li-Na-O	C-N-Na-O	Ca-Co-O-Si	Ca-Cr-Fe-O
Ca-Cr-O-Si	Ca-Cu-Fe-O	Ca-Cu-O-Si	Ca-Fe-Mg-O	Ca-Fe-Mn-O	Ca-Fe-O-P	Ca-Fe-O-Si
Ca-Fe-O-Ti	Ca-Gd-O-Si	Ca-Gd-O-Zr	Ca-Hf-O-Si	Ca-Hf-O-Y	Ca-Hf-O-Zr	Ca-K-N-O
Ca-K-O-Si	Ca-Li-N-O	Ca-Li-O-Si	Ca-Mg-Mn-O	Ca-Mg-N-O	Ca-Mg-O-P	Ca-Mg-O-Si
Ca-Mg-O-Ti	Ca-Mg-O-Zr	Ca-Mn-O-P	Ca-Mn-O-Si	Ca-Mn-O-Y	Ca-N-Na-O	Ca-Na-O-Si
Ca-Nb-O-Si	Ca-Ni-O-Si	Ca-O-P-Si	Ca-O-Si-Ti	Ca-O-Si-V	Ca-O-Si-Y	Ca-O-Si-Yb

Assessed Quaternary Oxide Systems, Me1-Me2-Me3-O						
Ca-O-Si-Zr	Ca-O-Y-Zr	Co-Cr-O-Si	Co-Cr-O-Ti	Co-Cu-La-O	Co-Cu-O-Si	Co-Fe-La-O
Co-Fe-Mn-O	Co-Fe-O-P	Co-Fe-O-Si	Co-La-Ni-O	Co-Mg-O-Si	Co-Mn-O-Si	Co-Mn-O-Y
Co-Ni-O-Si	Cr-Fe-Mn-O	Cr-Fe-Ni-O	Cr-Fe-O-Si	Cr-Fe-O-Ti	Cr-Fe-O-Y	Cr-La-Mn-O
Cr-Mg-O-Si	Cr-Mg-O-Ti	Cr-Mn-Ni-O	Cr-Mn-O-Si	Cr-Mn-O-Ti	Cr-Ni-O-Si	Cr-Ni-O-Ti
Cu-Fe-O-Si	Cu-Mg-O-Si	Fe-K-O-Si	Fe-Mg-O-Si	Fe-Mg-O-Ti	Fe-Mn-O-Si	Fe-Mn-O-Ti
Fe-Na-O-Si	Fe-Ni-O-Si	Fe-Ni-O-Ti	Fe-O-Si-Ti	Gd-La-O-Si	Gd-O-Si-Y	Gd-O-Si-Yb
Gd-O-Si-Zr	Hf-La-O-Zr	Hf-Mg-O-Zr	K-Li-N-O	K-Mg-N-O	K-Mg-O-Si	K-N-Na-O
K-Na-O-Si	La-O-Y-Zr	La-O-Yb-Zr	Li-Mg-N-O	Li-Mg-O-Si	Li-N-Na-O	Li-Na-O-Si
Mg-Mn-O-Si	Mg-Mn-O-Ti	Mg-N-Na-O	Mg-Na-O-Si	Mg-Ni-O-Si	Mg-O-P-Si	Mg-O-Si-Ti
Mg-O-Si-V	Mg-O-Si-Y	Mg-O-Si-Zr	Mg-O-Y-Zr	Mn-Ni-O-V	Mn-O-Y-Zr	Na-O-P-Si
O-Si-Y-Yb	O-Ti-Y-Zr	O-Y-Yb-Zr				

Assessed Higher Order Oxide Systems

Assessed Higher Order Oxide Systems					
Al-Ca-Co-O-Si	Al-Ca-Fe-O-Si	Al-Ca-K-O-Si	Al-Ca-Mg-O-Si	Al-Ca-Mg-O-Ti	Al-Ca-Mg-O-Zr
Al-Ca-Na-O-Si	Al-Ca-O-Si-Y	Al-Fe-K-Na-O-Si	Al-Fe-K-O-Si	Al-Fe-Mg-O-Si	Al-Fe-Mn-O-Si
Al-Fe-Na-O-Si	Al-Gd-O-Y-Zr	Al-K-Mg-Na-O-Si	Al-K-Mg-O-Si	Al-K-Na-O-Si	Al-La-O-Y-Zr
Al-Mg-Na-O-Si	Ba-Ca-Mg-O-Si	C-Cr-Fe-Mn-Ni-O	Ca-Fe-Mg-O-Si	Ca-Mg-Ni-O-Si	Ca-Mg-O-P-Si
Fe-K-Mg-Na-O-Si	Fe-K-Mg-O-Si	Gd-La-O-Y-Zr			

TCOX14 Assessed Sulfide Systems

These are the assessed sulfide systems for the ternary, quaternary, and higher order systems in the full range of composition and temperature.

TCOX14 Assessed Binary Systems

Assessed Ternary Sulfide Systems, Me1-Me2-S

	Al	Ar	B	Ba	C	Ca	Co	Cr	Cu	F	Fe	Gd	H	Hf	K	La	Li	Mg	Mn	Mo	N	Na	Nb	Ni	O	P	S	Si	Ti	V	W	Y	Yb	Zr
Al	Al								x		x					x								x	x										
Ar		Ar																																
B			B																															
Ba				Ba																														
C					C						x																							
Ca						Ca			x		x							x	x						x							x		
Co							Co	x	x		x								x					x	x									
Cr								Cr	x		x								x					x	x									
Cu									Cu		x					x		x	x					x	x			x						
F										F																								
Fe											Fe	x				x		x	x				x	x	x				x					x
Gd												Gd						x																
H													H																					
Hf														Hf																				
K															K																			
La																La		x																
Li																	Li																	
Mg																		Mg	x						x									
Mn																			Mn				x	x	x				x	x				x
Mo																				Mo														
N																					N													
Na																						Na												
Nb																							Nb											
Ni																								Ni										
O																									O			x						
P																										P								
S																											S							
Si																												Si						
Ti																													Ti					
V																														V				
W																															W			
Y																																Y		
Yb																																	Yb	
Zr																																		Zr

Assessed Oxy-sulfide Quaternary Systems

Assessed Oxy-sulfide Quaternary Systems				
Al-Ca-O-S	Al-Mg-O-S	Al-Mn-O-S	Ca-Fe-O-S	Ca-Mg-O-S
Ca-O-S-Si	C-K-O-S	C-Na-O-S	Cu-Fe-O-S	Fe-O-S-Si
Mg-O-S-Si	Mn-O-S-Si			

Assessed Oxy-sulfide Higher Order System

Assessed Oxy-sulfide Higher Order System
Al-Ca-Mn-O-S

TCOX14 Assessed Fluoride Systems

These are the assessed fluoride systems for the ternary, quaternary, and higher order systems in the full range of composition and temperature.

TCOX14 Assessed Binary Systems

Assessed Ternary Fluoride Systems

	Al	Ar	B	Ba	C	Ca	Co	Cr	Cu	F	Fe	Gd	H	Hf	K	La	Li	Mg	Mn	Mo	N	Na	Nb	Ni	O	P	S	Si	Ti	V	W	Y	Yb	Zr
Al	Al					x									x			x				x			x										x
Ar		Ar																																
B			B																															
Ba				Ba		x									x		x	x				x			x									x
C					C																													
Ca						Ca	x	x			x	x			x	x	x	x	x			x			x									
Co							Co					x						x						x										
Cr								Cr																										
Cu									Cu																x									
F										F																								
Fe											Fe													x										
Gd												Gd						x							x							x		
H													H																					
Hf														Hf																				
K															K		x	x				x												
La																La		x																x
Li																	Li	x				x			x									x
Mg																		Mg	x			x			x							x		
Mn																			Mn															
Mo																				Mo														
N																					N													
Na																						Na						x						
Nb																							Nb											
Ni																								Ni										
O																									O									
P																										P								
S																											S							
Si																												Si						
Ti																													Ti					
V																														V				
W																															W			
Y																																Y		
Yb																																	Yb	
Zr																																		Zr

Assessed Oxy-Fluoride Quaternary Systems

Assessed Oxy-Fluoride Quaternary Systems				
Al-Ca-F-O	Al-F-O-Si	B-Ba-F-O	Ba-Cr-F-O	C-F-K-O
C-F-Li-O	C-F-Na-O	Ca-Cr-F-O	Ca-F-Fe-O	Ca-F-Mg-O
Ca-F-O-P	Ca-F-O-Si	Ca-F-O-Ti	F-K-N-O	F-Li-N-O
F-Mg-O-Si	F-N-Na-O			

Assessed Oxy-Fluoride Higher Order Systems

Assessed Oxy-Fluoride Higher Order Systems				
Al-Ca-F-Mg-O	Al-Ca-F-O-Si	Ca-F-Fe-O-Si	Ca-F-K-O-Si	Ca-F-Na-O-Si

TCOX14 Properties Data

These sections list the assessed or estimated 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:

TCOX14 Viscosity for Ionic Liquids: Assessed or Estimated Systems

Using the CALPHAD approach, viscosity of oxide slags is critically assessed based on the evaluation of unary, binary, ternary and important higher order systems. By coupling to TCOX14, a two-sublattice ionic liquid viscosity model is employed to describe the ionic behavior of the oxide melts. It enables predicting viscosity of the oxide slags for various industrial applications, for example, iron-making and steel-making. The predicted viscosity is connected to the distribution and connectivity of species in the oxide melts, which gives predictions in the whole compositional range and a broad range of temperatures.

A system is estimated based on other predictions and data of ternaries. If it is estimated, it is marked with an asterisk (*) in the applicable table.

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.

Assessed or Estimated Unary Systems

Assessed or Estimated Unary Systems (Viscosity)							
Al_2O_3	B_2O_3	BaO*	CaF_2	CaO*	CaS*	Cr_2O_3*	CuO_x
FeO_x	Gd_2O_3*	K_2O	La_2O_3*	Li_2O*	MgO	MnO	MoO_2*
MoO_3*	Na_2O	Nb_2O_5*	NbO*	NiO	P_2O_5	SiO_2	TiO_2
V_2O_5	Y_2O_3*	Yb_2O_3*	ZrO_2*				

* Estimated

Assessed or Estimated Pseudo Binary Systems

Assessed or Estimated Pseudo Binary Systems (Viscosity)					
Al_2O_3-Gd_2O_3	Al_2O_3-La_2O_3	Al_2O_3-Na_2O	Al_2O_3-SiO_2	B_2O_3-SiO_2	BaO-Al_2O_3*
BaO-SiO_2*	CaF_2-Al_2O_3	CaF_2-MgO	CaF_2-SiO_2	CaF_2-TiO_2	CaF_2-V_2O_5

Assessed or Estimated Pseudo Binary Systems (Viscosity)					
$CaO-Al_2O_3$	$CaO-P_2O_5$	$CaO-SiO_2$	$CuxO-SiO_2$	Fe_xO-CaO	Fe_xO-Na_2O
Fe_xO-SiO_2	Fe_xO-TiO_2	$K_2O-Al_2O_3$	K_2O-FeO_x	K_2O-SiO_2	Li_2O-SiO_2
$MgO-Al_2O_3$	$MgO-SiO_2$	$MnO-SiO_2$	$MnO-TiO_2$	$Na_2O-P_2O_5$	Na_2O-SiO_2
$Na_2O-V_2O_5$	$NiO-SiO_2$	$SiO_2-Yb_2O_3$			

* Estimated

Assessed Pseudo Ternary Systems

Assessed Pseudo Ternary Systems (Viscosity)				
$Al_2O_3-MgO-SiO_2$	$CaF_2-Al_2O_3-TiO_2$	$CaF_2-Al_2O_3-V_2O_5$	$CaF_2-CaO-Al_2O_3$	$CaF_2-CaO-Cr_2O_3$
$CaO-Al_2O_3-SiO_2$	$CaO-Al_2O_3-ZrO_2$	$CaO-CaS-SiO_2$	$CaO-Cr_2O_3-SiO_2$	$CaO-MgO-SiO_2$
$CaO-NiO-SiO_2$	$CaO-SiO_2$	$CaO-SiO_2-Cr_2O_3$	$CaO-SiO_2-TiO_2$	$Cu_xO-Al_2O_3-SiO_2$
$Fe_2O_3-Al_2O_3-SiO_2$	$Fe_2O_3-Na_2O-SiO_2$	$Fe_xO-CaO-Al_2O_3$	$Fe_xO-CaO-SiO_2$	$Fe_xO-MgO-SiO_2$
$K_2O-Al_2O_3-SiO_2$	$K_2O-FeO_x-SiO_2$	$K_2O-Na_2O-SiO_2$	$Li_2O-SiO_2-TiO_2$	$MgO-SiO_2-TiO_2$
$MnO-SiO_2-TiO_2$	$Na_2O-Al_2O_3-SiO_2$	$Na_2O-CaO-SiO_2$	$Na_2O-MgO-SiO_2$	

Assessed Pseudo Quaternary Systems

Assessed Pseudo Quaternary Systems (Viscosity)			
$CaO-CuO_x-MgO-SiO_2$	$CaO-MgO-Al_2O_3-SiO_2$	$Fe_xO-CaO-Al_2O_3-SiO_2$	$Fe_xO-CaO-MgO-SiO_2$
$Fe_xO-CaO-SiO_2-CaF_2$	$Na_2O-CaO-Al_2O_3-SiO_2$		

Assessed Pseudo Quinary Systems

Assessed Pseudo Quinary Systems (Viscosity)			
$CaO-MgO-Al_2O_3-SiO_2-Na_2O$	$CaO-MgO-Al_2O_3-SiO_2-Yb_2O_3$	$Fe_xO-CaO-MgO-Al_2O_3-SiO_2$	$Fe_xO-CaO-SiO_2-Al_2O_3-CaF_2$

TCOX14 Molar Volume: Assessed or Estimated Phases

For the molar volume properties data included with the TCS Metal Oxide Solutions Database (TCOX), the molar volume parameters have been assessed or estimated as indicated. Molar volume is included with the database starting with version 10 (TCOX10).

A system is estimated based on other predictions and data of ternaries. If it is estimated, it is marked with an asterisk (*) in the applicable table.

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.

Assessed or Estimated Liquid Solution Phases

This lists the unary, binary, and ternary systems for the liquid solution phases and whether the molar volume has been assessed or estimated. If it is estimated, it is marked with an asterisk (*) in the table.

Assessed or Estimated Liquid Solution Phases (Molar Volume)*				
Al_2O_3	Al_2O_3-B_2O_3-CaF_2	Al_2O_3-B_2O_3-CaO	Al_2O_3-CaO	Al_2O_3-MgO
Al_2O_3-MgO-SiO_2	Al_2O_3-SiO_2	Al_2O_3-TiO_2-SiO_2	B_2O_3	BaO*
BaO-Al_2O_3*	BaO-SiO_2*	CaF_2	CaF_2-Al_2O_3	CaF_2-Al_2O_3-MgO-SiO_2
CaF_2-Al_2O_3-TiO_2	CaF_2-CaO	CaF_2-CaO-Al_2O_3	CaF_2-CaO-MgO-Al_2O_3	CaF_2-CaO-SiO_2
CaF_2-MgF_2	CaF_2-MgO	CaF_2-MgO-Al_2O_3	CaF_2-SiO_2	CaF_2-TiO_2
CaO	CaO-Al_2O_3-MnO-SiO_2	CaO-Al_2O_3-SiO_2	CaO-Al_2O_3-TiO_2	CaO-MgO-Al_2O_3-SiO_2
CaO-MgO-Al_2O_3	CaO-MgO-SiO_2	CaO-MnO-SiO_2	CaO-SiO_2	CaO-SiO_2-TiO_2
CaS*	CoO*	Cr_2O_3*	FeO	Fe_2O_3
Fe_xO-CaO	Fe_xO-SiO_2	Fe_xO-Al_2O_3-SiO_2	Fe_xO-CaO-Al_2O_3	Fe_xO-CaO-Al_2O_3-SiO_2
Fe_xO-CaO-MgO	Fe_xO-CaO-MgO-SiO_2	Fe_xO-CaO-MgO-Al_2O_3-SiO_2	Fe_xO-CaO-MnO-SiO_2	Fe_xO-CaO-SiO_2

Assessed or Estimated Liquid Solution Phases (Molar Volume)*				
Fe_xO-MgO-SiO_2	Fe_xO-MnO-SiO_2	K_2O	K_2O-SiO_2	La_2O_3*
Li_2O	Li_2O-SiO_2	Li_2O-Na_2O-SiO_2	Li_2O-MgO-SiO_2	Li_2O-CaO-SiO_2
MgF_2	MgO	MgO-SiO_2	MnO*	MnO-SiO_2
MoO_3*	Nb_2O_5*	NiO*	P_2O_5*	SiO_2
TiO_2	V_2O_5*	WO_3*	Yb_2O_3	ZrO_2*

* Estimated

TCOX14 Surface Tension for Oxide Slag: Assessed Systems

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.

Assessed Unary Systems

Assessed Unary Systems (Surface Tension)						
Al_2O_3	B_2O_3	BaO	CaF_2	CaO	CaS	CoO
Co_2O_3	Cr_2O_3	CrO	CuO	Cu_2O	FeO	Fe_2O_3
Gd_2O_3	K_2O	La_2O_3	Li_2O	MgF_2	MgO	MoO_2
MoO_3	NiO	NbO	Nb_2O_5	Na_2O	P_2O_5	SiO_2
TiO_2	V_2O_5	WO_3	Y_2O_3	ZrO_2		

Assessed Pseudo Binary Systems

Assessed Pseudo Binary Systems (Surface Tension)					
Al_2O_3-CaF_2	Al_2O_3-CaO	Al_2O_3-Cr_2O_3	Al_2O_3-MgO	Al_2O_3-SiO_2	Al_2O_3-TiO_2
B_2O_3-CaO	BaO-Al_2O_3	BaO-SiO_2	CaF_2-CaO	CaF_2-MgO	CaF_2-SiO_2
CaF_2-TiO_2	CaF_2-V_2O_5	CaO-CuO_x	CaO-FeO_x	CaO-P_2O_5	CaO-SiO_2
CaO-V_2O_5	FeO_x-MnO	FeO_x-Na_2O	FeO_x-P_2O_5	FeO_x-SiO_2	FeO_x-TiO_2
K_2O-SiO_2	Li_2O-SiO_2	MgO-SiO_2	MnO-SiO_2	Na_2O-SiO_2	

Assessed Pseudo Ternary Systems

Assessed Pseudo Ternary Systems (Surface Tension)					
Al_2O_3-B_2O_3-CaF_2	Al_2O_3-B_2O_3-CaO	Al_2O_3-CaF_2-CaO	Al_2O_3-CaF_2-MgO	Al_2O_3-CaF_2-TiO_2	Al_2O_3-CaF_2-V_2O_5

Assessed Pseudo Ternary Systems (Surface Tension)					
Al_2O_3-CaO-Cr_2O_3	Al_2O_3-CaO-Fe_2O_3	Al_2O_3-CaO-Li_2O	Al_2O_3-CaO-MgO	Al_2O_3-CaO-Na_2O	Al_2O_3-CaO-SiO_2
Al_2O_3-CaO-TiO_2	Al_2O_3-CaO-V_2O_5	Al_2O_3-CaO-ZrO_2	Al_2O_3-FeO_x-SiO_2	Al_2O_3-MgO-SiO_2	Al_2O_3-MnO-SiO_2
Al_2O_3-Na_2O-SiO_2	Al_2O_3-SiO_2-TiO_2	CaF_2-CaO-SiO_2	CaO-CaS-SiO_2	CaO-Cr_2O_3-SiO_2	CaO-FeO_x-SiO_2
CaO-MgO-SiO_2	CaO-MnO-SiO_2	CaO-Na_2O-SiO_2	CaO-P_2O_5-SiO_2	CaO-SiO_2-V_2O_5	FeO_x-MgO-SiO_2
FeO_x-MnO-SiO_2	K_2O-CaO-Al_2O_3	MgO-Na_2O-SiO_2			

Assessed Pseudo Quaternary Systems

Assessed Pseudo Quaternary Systems (Surface Tension)			
Al_2O_3-CaF_2-CaO-SiO_2	Al_2O_3-CaF_2-CaO-V_2O_5	Al_2O_3-CaF_2-K_2O-SiO_2	Al_2O_3-CaF_2-MgO-SiO_2
Al_2O_3-CaO-MnO-SiO_2	Al_2O_3-CaO-Na_2O-SiO_2	Al_2O_3-CaO-SiO_2-TiO_2	CaO-MgO-Al_2O_3-SiO_2
CaO-MgO-Na_2O-SiO_2	FeO_x-CaO-Al_2O_3-SiO_2	FeO_x-CaO-MgO-SiO_2	FeO_x-MgO-Al_2O_3-SiO_2

TCOX14 Electrical Conductivity/Resistivity for Ionic Liquids: Assessed or Estimated Systems

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.

A system is estimated based on other predictions and data of ternaries. If it is estimated, it is marked with an asterisk (*) in the applicable table.

Assessed or Estimated Unary Systems

Assessed or Estimated Unary Systems (Electrical Conductivity/Resistivity for Ionic Liquids)							
Al_2O_3	B_2O_3*	BaO*	CaO	CaF_2	Cr_2O_3*	CuO_x*	FeO_x
K_2O*	LaF_3*	La_2O_3*	Li_2O*	MgF_2	MgO	MnO_x	MoO_3*
Na_2O*	Nb_2O_5*	NiO*	P_2O_5*	SiO_2	TiO_2*	V_2O_5	Y_2O_3*
YF_3*	ZrO_2*						

*Estimated

Assessed or Estimated Pseudo Binary Systems

Assessed or Estimated Pseudo Binary Systems (Electrical Conductivity/Resistivity for Ionic Liquids)			
Al_2O_3-SiO_2	B_2O_3-CaF_2	BaO-SiO_2*	BaO-Al_2O_3*
BaO-MgO*	CaF_2-Al_2O_3	CaF_2-CaO	CaF_2-MgO
CaF_2-SiO_2	CaO-Al_2O_3	CaO-SiO_2	Fe-O-Al_2O_3
Fe-O-CaO	Fe-O-Na_2O	Fe-O-SiO_2	K_2O-SiO_2
La_2O_3-CaF_2	Li_2O-SiO_2	MgO-Al_2O_3	MgO-SiO_2

Assessed or Estimated Pseudo Binary Systems (Electrical Conductivity/Resistivity for Ionic Liquids)			
$MnO-Al_2O_3$	$MnO-SiO_2$	Na_2O-SiO_2	TiO_2-CaF_2
TiO_2-Fe-O	TiO_2-MnO	$Y_2O_3-CaF_2$	

*Estimated

Assessed Pseudo Ternary Systems

Assessed Pseudo Ternary Systems (Electrical Conductivity/Resistivity for Ionic Liquids)			
$Al_2O_3-MgO-SiO_2$	$CaO-Al_2O_3-SiO_2$	$CaO-MgO-SiO_2$	$Cr_2O_3-CaO-SiO_2$
Fe-O-$CaO-SiO_2$	Fe-O-$MgO-SiO_2$	Fe-O-$Al_2O_3-SiO_2$	$Li_2O-SiO_2-TiO_2$
$Li_2O-MgO-TiO_2$	$MnO-Al_2O_3-SiO_2$	$MnO-CaO-SiO_2$	$MnO-MgO-SiO_2$
$MoO_3-Fe_2O_3-P_2O_5$	$Na_2O-Al_2O_3-SiO_2$	$Nb_2O_5-Na_2O-P_2O_5$	$P_2O_5-CaO-SiO_2$
$TiO_2-CaO-Al_2O_3$	$TiO_2-CaO-SiO_2$	TiO_2-Fe-O-MnO	TiO_2-Fe-O-SiO_2
$TiO_2-MgO-SiO_2$	$TiO_2-MnO-SiO_2$	$TiO_2-Na_2O-SiO_2$	ZrO_2-CaF_2-CaO
$ZrO_2-CaO-Al_2O_3$			

Assessed Pseudo Quaternary Systems

Assessed Pseudo Quaternary Systems (Electrical Conductivity/Resistivity for Ionic Liquids)			
$CaF_2-CaO-MgO-SiO_2$	$CaF_2-CaO-Al_2O_3-SiO_2$	$CaF_2-CaO-MgO-Al_2O_3$	$CaO-MgO-Al_2O_3-SiO_2$
Fe-O-$CaO-Al_2O_3-SiO_2$	Fe-O-$MgO-Al_2O_3-SiO_2$	Fe-O-$CaO-MgO-SiO_2$	$MnO-CaO-Al_2O_3-SiO_2$
$MnO-CaO-MgO-SiO_2$	$TiO_2-Al_2O_3-Na_2O-SiO_2$	$TiO_2-CaO-Al_2O_3-SiO_2$	TiO_2-Fe-O-Na_2O-SiO_2
TiO_2-Fe-O-$CaO-SiO_2$			

Assessed Higher Order Systems

Assessed Higher Order Systems (Electrical Conductivity/Resistivity for Ionic Liquids)			
CaF_2-CMAS	Fe-O-CMAS	MnO-CMAS	TiO_2-CMAS
Fe-Mn-O-CaF_2-CMAS			

TCOX14 Thermal Conductivity/Resistivity for Ionic Liquids: Assessed or Estimated Systems

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.

A system is estimated based on other predictions and data of ternaries. If it is estimated, it is marked with an asterisk (*) in the applicable table.

Assessed or Estimated Unary Systems

Assessed or Estimated Unary Systems (Thermal Conductivity/Resistivity for Ionic Liquids)							
Al_2O_3*	$BO_{3/2}$	BaO*	CaF_2*	CaO*	CoO*	$CrO_{3/2}$*	CrO*
CuO*	Cu_2O*	$FeO_{3/2}$*	FeO*	Gd_2O_3*	HfO_2*	K_2O*	La_2O_3*
Li_2O*	MgO*	$MnO_{3/2}$*	MnO*	MoO_3*	MoO_2	Na_2O*	$NbO_{5/2}$*
NbO*	NiO*	$PO_{5/2}$*	SiO_2*	TiO_2*	$TiO_{3/2}$*	TiO*	VO_2*
$VO_{3/2}$*	$VO_{5/2}$*	VO*	WO_3*	Y_2O_3*	Yb_2O_3*	ZrO*	

*Estimated

Assessed or Estimated Pseudo Binary Systems

Assessed or Estimated Pseudo Binary Systems (Thermal Conductivity/Resistivity for Ionic Liquids)				
$CaO\text{-}SiO_2$	$CaO\text{-}Al_2O_3$	$Na_2O\text{-}SiO_2$*	$B_2O_3\text{-}SiO_2$	$Na_2O\text{-}B_2O_3$
$Li_2O\text{-}SiO_2$	$K_2O\text{-}SiO_2$			

*Estimated

Assessed Pseudo Ternary Systems

Assessed Pseudo Ternary Systems (Thermal Conductivity/Resistivity for Ionic Liquids)		
$CaO-Al_2O_3-SiO_2$	$Li_2O-CaO-SiO_2$	$Na_2O-CaO-SiO_2$
$K_2O-CaO-SiO_2$	$FeO_x-CaO-SiO_2$	

Assessed Pseudo Quaternary Systems

Assessed Pseudo Quaternary Systems (Thermal Conductivity/Resistivity for Ionic Liquids)
$CaO-MgO-Al_2O_3-SiO_2$

TCOX14 Phases

In this section:

Common Phases for the TCOX Database

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key oxides.

Name in the Database	*Common Name and Description*
CORUNDUM	Corundum (Al_2O_3), Eskolaite (Cr_2O_3), Hematite (Fe_2O_3), Karelianite (V_2O_3), Tistarite (Ti_2O_3), $CoTiO_3$, Ilmenite ($FeTiO_3$), Geikielite ($MgTiO_3$), Pyrophanite ($MnTiO_3$), $NiTiO_3$. The ilmenite ($(Co,Fe,Mg,Mn,Ni)TiO_3$) crystal structure consists of an ordered derivative of the corundum structure. In corundum all cations are identical, but in ilmenite Me+2 and Ti+4 occupy different sublattices. Both the disordered and ordered end-members are described in the CORUNDUM phase in the database. Anti-site occupancy in the ilmenite structure is not modeled.
HALITE	Lime (CaO), CoO, Wustite (FeO), Periclase (MgO), Manganosite (MnO), Bunsenite (NiO), Baria (BaO).
ALABANDITE	Alabandite (MnS), Oldhamite (CaS), MgS, GdS, LaS, ZrS, BaS.
GARNET	Grossular ($Ca_3Al_2(SiO_4)_3$), Uvarovite ($Ca_3Cr_2(SiO_4)_3$), Spessartine ($Mn_3Al_2(SiO_4)_3$), Goldmanite ($Ca_3V_3(SiO_4)_3$). Other minerals part of the Garnet structure, such as Pyrope and Almandine, are not part of the database since they are not stable at ambient pressure. Included in the GARNET model are also the $(Gd,Y,Yb)_3(Al,Fe)_5O_{12}$ descriptions.
M2O3A	This is the hexagonal La_2O_3 and Gd_2O_3 modifications.
M2O3B	This is monoclinic Gd_2O_3.
M2O3C	This is Bixbyite (Mn_2O_3) and cubic Gd_2O_3 , Y_2O_3 and Yb_2O_3.
M2O3H	This is hexagonal La_2O_3, Gd_2O_3, Y_2O_3 and Yb_2O_3.
M2O3X	This is x-La_2O_3 and high-temperature cubic Gd_2O_3.
MELILITE	Gehlenite ($Ca_2Al_2SiO_7$), Fe-Gehlenite ($Ca_2Fe_2SiO_7$), Åkermanite ($Ca_2MgSi_2O_7$), Fe-Åkermanite ($Ca_2FeSi_2O_7$), $CaCoSi_2O_7$, Bennesherite ($Ba_2FeSi_2O_7$), and $Ba_2MgSi_2O_7$.
OLIVINE	Calcio-olivine (Ca_2SiO_4), Co_2SiO_4, Fayalite (Fe_2SiO_4), Forsterite (Mg_2SiO_4), Tephroite (Mn_2SiO_4), Ni_2SiO_4, Kirschsteinite ($CaFeSiO_4$), Monitcellite ($CaMgSiO_4$), Glaucochroite ($CaMnSiO_4$), Liebenbergite (Ni_2SiO_4)
PSEUDO_ BROOKITE	Pseudobrookite (Fe_2TiO_5), Karrooite ($MgTi_2O_5$), Ti_3O_5, Al_2TiO_5, $CoTi_2O_5$, Armalcolite ($(Fe,Mg)Ti_2O_5$), $MnTi_2O_5$.
LOWCLINO_ PYROXENE	Low clino-enstatite ($MgSiO_3$), low clino-diopside ($CaMgSi_2O_6$).
CLINO_ PYROXENE	Clino-enstatite ($MgSiO_3$), clino-ferrosilite ($FeSiO_3$), diopside ($CaMgSi_2O_6$), Niopside ($CaNiSi_2O_6$), Pigeonite ($(Mg,Fe,Ca)Si_2O_6$), Hedenbergite ($CaFeSi_2O_6$).

Name in the Database	*Common Name and Description*
ORTHO_ PYROXENE	Enstatite ($MgSiO_3$), ortho-Diopside ($CaMgSi_2O_6$).
PROTO_ PYROXENE	Proto-enstatite ($MgSiO_3$), proto-diopside ($CaMgSi_2O_6$).
PYRRHOTITE	Pyrrhoitite (FeS), CoS, CrS, NbS, NiS, TiS, VS.
RUTILE	Rutile (TiO_2), Pyrolusite (MnO_2), high-temperature VO_2.
ALPHA_SPINEL	Tetragonal Hausmannite (Mn_3O_4).
SPINEL	The cubic AB2O4-type spinel. Many end-members, solid solutions and combinations are described in the SPINEL phase: Magnetite (Fe_3O_4), cubic Hausmannite (Mn_3O_4), Guite (Co_3O_4), Spinel ($MgAl_2O_4$), Cuprospinel ($CrFe_2O_4$), Chromite ($FeCr_2O_4$), Hercynite ($FeAl_2O_4$), Coulsonite (FeV_2O_4), Vuorelainenite (MnV_2O_4), Magnesiocoulsonite (MgV_2O_4), CoV_2O_4, NiV_2O_4, Galaxite ($MnAl_2O_4$), Jacobsite ($MnFe_2O_4$), Magnesiochromite ($MgCr_2O_4$), Magnesioferrite ($MgFe_2O_4$), Manganochromite ($MnCr_2O_4$), Thermaerogenite ($CuAl_2O_4$), Ulvöspinel ($TiFe_2O_4$), Trevorite ($NiFe_2O_4$), $NiAl_2O_4$, $CoAl_2O_4$, $CoFe_2O_4$, $FeCo_2O_4$, $CoMn_2O_4$, $CuMn_2O_4$, $MgMn_2O_4$, $NiMn_2O_4$, Co_2TiO_4, Mg_2TiO_4, $MgTi_2O_4$, $MnTi_2O_4$, Mn_2TiO_4, Ni_2TiO_4, $LiAl_5O_8$, $LiFe_5O_8$, $LiMn_2O_4$, $Li_4Mn_5O_{12}$, and $Li_4Ti_5O_{12}$.
ZIRCON	Zircon ($ZrSiO_4$), Xenotime (YPO_4), $GdPO_4$, $LaPO_4$, $HfSiO_4$.

TCOX14 Models for the Included Phases

Also see the listing at the end for Gas and IONIC_LIQ Phase.

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
A1C1F2	Unknown Structure				This is Al2O3.CaO.2Fe2O3	5	(CA+2)1(AL+3)1(FE+3)2(AL+3, FE+3)3(O-2)10
AF	FeGaO3		oP40	(33, Pna2_1)	This is Al2O3.Fe2O3.	3	(AL+3)2(FE+3)2(O-2)6
AL18B4O33	Al5BO9		oS60	(36, Cmc2_1)		3	(AL+3)18(B+3)4(O-2)33
AL2P6SI4O26	Unknown Structure					4	(AL+3)2(P+5)6(SI+4)4(O-2)26
AL2S3	alpha-Al2S3		hP30	(169, P6_1)		2	(AL)2(S)3
AL2SIO4F	Unknown Structure					4	(AL+3)2(SI+4)1(O-2)4(F-1)2
AL3PO7	Unknown Structure					3	(AL+3)3(P+5)1(O-2)7
AL4B2O9	Al4B1.5[BO3]0.5O7.5		mS124	(12, C2/m)		3	(AL+3)4(B+3)2(O-2)9
AL4C3_D71	Al4C3 (D71)	D71	hR7	(166, R-3m)		2	(AL, SI)4(C)3
ALABANDITE	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is CaS (oldhamite), MnS (alabandite), (Ba,Mg,Gd,La,Zr)S.	2	(BA, CA, CO, CR, CU, FE, GD, LA, MG, MN, Y, ZR)1(S)1
ALBITE_LOW	Albite (NaAlSi3O8, S68)	S68	aP26	(2, P-1)	This is low temperature albite (NaAlSi3O8).	4	(NA+1)1(AL+3)1(SI+4)3(O-2)8
ALBITE_MONO	Sanidine (KAlSi3O8, S67)	S67	mS52	(12, C2/m)	This is monoclinic albite (NaAlSi3O8).	4	(NA+1)1(AL+3)1(SI+4)3(O-2)8
ALF3_S2	AlF3		oS48	(63, Cmcm)		2	(AL+3)1(F-1)3
ALNB11O29	(Ti0.17Nb0.83)12O29		mS82	(12, C2/m)		3	(AL+3)1(NB+5)11(O-2)29
ALNB49O124	Unknown Structure					3	(AL+3)1(NB+5)49(O-2)124

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)		2	(AL)1(N)1
ALP3O9	AlP3O9		mS156	(9, Cc)	This is (Al,Cr,Fe)P3O9	2	(AL+3, CR+3, FE+3)1(PO3-1)3
ALPHA_SPINEL	Hausmannite (Mn3O4)		tI28	(141, I4_ 1/amd)	With solubility of Al, Co, Cr, Cu, Fe, Mg and Ni.	4	(CO+2, CU+2, MG+2, MN+2, MN+3, NI+2)1(AL+3, CR+3, FE+3, MN+2, MN+3, VA)2(MN+2, VA)2(O-2)4
ALPO4_S1	Al[AsO4]		hP18	(152, P3_121)	This is (Al,Fe, Mn)PO4 with SiO2 solubility.	2	(AL+3, FE+3, MN+3, SI+4)1(PO4-3, SIO4-4)1
ALPO4_S2	Al[PO4]		hP18	(180, P6_222)	This is AlPO4 with SiO2 solubility.	2	(AL+3, SI+4)1(PO4-3, SIO4-4)1
ALPO4_S3	AlPO4 low cristobalite type		oS24	(20, C222_1)	This is AlPO4 with SiO2 solubility.	2	(AL+3, SI+4)1(PO4-3, SIO4-4)1
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	(58, Pnnm)	This is a high-pressure phase	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
ANHYDRITE	Anhydrite (CaSO4, H01)	H01	oS24	(63, Cmcm)	This is (Ca,Cu,Fe,Mg,Mn,Ni)(SO4).	2	(CA+2, CO+2, CU+2, FE+2, MG+2, MN+2, NI+2)1(SO4-2)1
ANILITE	Cu7S4		oP44	(62, Pnma)	This is Cu7S4, orthorhombic structure.	2	(CU)1.75(S)1
ANORTHITE	Ca(Al0.5Si0.5)4O8		aP104	(2, P-1)	This is high temp albite (NaAlSi3O8), KAlSi3O8 and anorthite (CaAl2Si2O8)	5	(CA+2, K+1, NA+1)1(AL+3)1(AL+3, SI+4)1 (SI+4)2(O-2)8
APATITE	Fluorapatite [Ca5F(PO4)3, H57]	H57	hP42	(176, P6_3/m)	This is Ca2(Gd,Y)8(SiO4)6O2 and Mg2 (Gd,Y)8(SiO4)6O2	4	(CA+2, GD+3, MG+2, VA, Y+3, YB+3, ZR+4)4(GD+3, Y+3, YB+3)6(SIO4-4)6(O-2, VA)2
B2O3	B2O3		hP15	(152, P3_121)		2	(B+3)2(O-2)3
B4C_D1G	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		2	(B11C, B12)1(B2, C2B, CB2)1
BA2AL2B8O17	Unknown Structure					4	(BA+2)2(AL+3)2(B+3)8(O-2)17
BA2B10O17	Ba2B10O17		aP58	(2, P-1)		3	(BA+2)2(B+3)10(O-2)17
BA2B2O5	BaB2O5		mP171	(2, P-1)		3	(BA+2)2(B+3)2(O-2)5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
BA2CA4SI3O12	Unknown Structure					4	(BA+2)2(CA+2)4(SI+4)3(O-2)12
BA2CA6SI4O16	Unknown Structure					4	(BA+2)2(CA+2)6(SI+4)4(O-2)16
BA2CASI2O8	Unknown Structure				This is Ba2Ca(Ba,Ca)Si2O8 solid solution.	5	(BA+2)2(CA+2)1(BA+2, CA+2)1(SI+4)2(O-2)8
BA2FE2O5	Ba2Fe2O5		mP126	(14, P2_1/c)		3	(BA+2)2(FE+3)2(O-2)5
BA2FE6O11	Ba2Fe6O11		oP76	(58, Pnnm)		3	(BA+2)2(FE+3)6(O-2)11
BA2P2O7_A	Sr2[P2O7]		oP44	(62, Pnma)		2	(BA+2)2(P2O7-4)1
BA2SI3O8	Ba2Si3O8		mP52	(14, P2_1/c)		3	(BA+2)2(SI+4)3(O-2)8
BA2SIO4	Arcanite (K2SO4, H16)	H16	oP28	(62, Pnma)		2	(BA+2, CA+2)2(SIO4-4)1
BA2TI9O20	Ba2Ti9O20		aP124	(2, P-1)		3	(BA+2)2(TI+4)9(O-2)20
BA2TIO4	Ca2[SiO4]		mP28	(14, P2_1/c)		3	(BA+2)2(TI+4)1(O-2)4
BA2Y2ZRO7	Unknown Structure					4	(BA+2)2(Y+3)2(ZR+4)1(O-2)7
BA2ZRF8	Ba2ZrF8		oP44	(62, Pnma)		3	(BA+2)2(ZR+4)1(F-1)8
BA2ZRO4	K2NiF4		tI14	(139, I4/mmm)		3	(BA+2)2(ZR+4)1(O-2)4
BA3AL2O6	Ba3Al2O6		cP264	(198, P2_13)		3	(BA+2, CA+2)3(AL+3)2(O-2)6
BA3AL4B4O15	Unknown Structure					4	(BA+2)3(AL+3)4(B+3)4(O-2)15
BA3B2O6	Ba3[BO3]2		oP196	(55, Pbam)		3	(BA+2)3(B+3)2(O-2)6
BA3B6SI2O16	Ba3(sI0.33B0.67)6b2O16		aP29	(2, P-1)		4	(BA+2)3(B+3)6(SI+4)2(O-2)16
BA3CR2O6	Unknown Structure					3	(BA+2)3(CR+3)2(O-2)6

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
BA3FE2O6	Unknown Structure					3	(BA+2)3(FE+3)2(O-2)6
BA3GD4O9	Unknown Structure					3	(BA+2)3(GD+3)4(O-2)9
BA3NIO4	Ba3NiO4		hR48	(167, R-3c)		3	(BA+2)3(NI+2)1(O-2)4
BA3P2O8_A	Ba3[PO4]2		hR39	(166, R-3m)		2	(BA+2, CA+2)3(PO4-3)2
BA3P4O13_LT	Ba3P4O13		aP40	(2, P-1)		3	(BA+2)3(PO3-1)4(O-2)1
BA3SI5O13	Ba3Si5O13		mP84	(14, P2_1/c)		3	(BA+2)3(SI+4)5(O-2)13
BA3SIO5	Cs3CoCl5 (K31)	K31	tI36	(140, I4/mcm)		3	(BA+2)3(SI+4)1(O-2)5
BA3YB4O9	Ba3Yb4O9		hR48	(146, R3)		3	(BA+2)3(Y+3, YB+3)4(O-2)9
BA3ZR2O7	Unknown Structure					3	(BA+2)3(ZR+4)2(O-2)7
BA3ZRF10	Ba3ZrF10		oS56	(63, Cmcm)		3	(BA+2)3(ZR+4)1(F-1)10
BA4AL2O7	Ba4Al2O7		oS208	(64, Cmce)		3	(BA+2, CA+2)4(AL+3)2(O-2)7
BA4B2O7	Unknown Structure					3	(BA+2)4(B+3)2(O-2)7
BA4P2O9	Unknown Structure					3	(BA+2)4(PO4-3)2(O-2)1
BA4TI13O30	Ba4Ti13O30		oS188	(64, Cmce)		3	(BA+2)4(TI+4)13(O-2)30
BA4Y2ZR2O11	Unknown Structure					4	(BA+2)4(Y+3)2(ZR+4)2(O-2)11
BA5AL4B12O29	Unknown Structure					4	(BA+2)5(AL+3)4(B+3)12(O-2)29
BA5B4O11	Ba5B2[BO3]2O5		oP240	(19, P2_12_12_1)		3	(BA+2)5(B+3)4(O-2)11
BA5SI8O21	Ba5Si8O21		mS136	(15, C2/c)		3	(BA+2)5(SI+4)8(O-2)21

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
BA6TI17O40	Ba6Ti17O40		mS252	(15, C2/c)		3	(BA+2)6(TI+4)17(O-2)40
BA7AL2O10	Ba7Al2O10		oP19	(62, Pnma)		3	(BA+2)7(AL+3)2(O-2)10
BAAL2B2O7	BaAl2[BO3]2O		hR36	(155, R32)		4	(BA+2)1(AL+3)2(B+3)2(O-2)7
BAAL2B4O10	Unknown Structure					4	(BA+2)1(AL+3)2(B+3)4(O-2)10
BAAL2O4	BaAl2O4		hP56	(173, P6_3)		3	(BA+2, CA+2)1(AL+3)2(O-2)4
BAAL2SI2O8	SrGa2[SiO4]2		mS104	(15, C2/c)		4	(BA+2)1(AL+3)2(SI+4)2(O-2)8
BAB2O4_A	BaB2O4		hR126	(161, R3c)		3	(BA+2)1(B+3)2(O-2)4
BAB2O4_B	BaB2O4		hR126	(167, R-3c)		3	(BA+2)1(B+3)2(O-2)4
BAB4O7	BaB4O7		mP96	(14, P2_1/c)		3	(BA+2)1(B+3)4(O-2)7
BAB8O13	BaB8O13		tP88	(91, P4_122)		3	(BA+2, CA+2)1(B+3)8(O-2)13
BACA2AL8O15	Unknown Structure					4	(BA+2)1(CA+2)2(AL+3)8(O-2)15
BACA2MGSI2O8	BaAg2Mn[VO4]2		hP14	(147, P-3)		5	(BA+2, CA+2)1(BA+2, CA+2)2(MG+2)1 (SI+4)2(O-2)8
BACA2SI3O9	BaCa2Si3O9		aP30	(2, P-1)	This is (Ba, Ca)CaSi3O9 solid solution.	5	(BA+2, CA+2)1(BA+2, CA+2)1(CA+2)1 (SI+4)3(O-2)9
BACO3_S1	Ca[CO3]-a		oP20	(62, Pnma)		2	(BA+2)1(CO3-2)1
BACO3_S2	K[NO3]		hR15	(160, R3m)		2	(BA+2)1(CO3-2)1
BACO3_S3	Rb[NO3]		cF184	(225, Fm-3m)		2	(BA+2)1(CO3-2)1
BAFE2O4	BaFe2O4		oS56	(36, Cmc2_1)		3	(BA+2)1(FE+3)2(O-2)4
BAMG2SI2O7	BaCo2[Si2O7]		mS96	(15, C2/c)		4	(BA+2)1(MG+2)2(SI+4)2(O-2)7

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
BAMG3AL14O25	Unknown Structure					4	(BA+2)1(MG+2)3(AL+3)14(O-2)25
BAMGF4	BaZnF4		oS24	(36, Cmc2_1)		3	(BA+2)1(MG+2)1(F-1)4
BAMGSI3O8	Unknown Structure					4	(BA+2)1(MG+2)1(SI+4)3(O-2)8
BAMGSIO4	BaZn[GeO4]		hP42	(173, P6_3)		3	(BA+2)1(MG+2)1(SIO4-4)1
BANIO2	BaNiO2		oS16	(63, Cmcm)		3	(BA+2)1(NI+2)1(O-2)2
BAO2	CaC2-I (C11a)	C11a	tI6	(139, I4/mmm)		2	(BA+4)1(O-2)2
BAP2O6	BaP2O6		oP36	(19, P2_12_12_1)		2	(BA+2)1(PO3-1)2
BASI2O5	BaSi2O5		oP32	(62, Pnma)		3	(BA+2)1(SI+4)2(O-2)5
BASIO3	BaGeO3		oP20	(19, P2_12_12_1)	BaSiO3 with Ca solubility	3	(BA+2, CA+2)1(SI+4)1(O-2)3
BATI4O9	BaTi4O9		oP28	(59, Pmmn)		3	(BA+2)1(TI+4)4(O-2)9
BATIO3_C	BaTiO3		tP5	(99, P4mm)		3	(BA+2, VA)1(TI+4)1(O-2, VA)3
BATIO3_H	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(BA+2, VA)1(TI+4)1(O-2, VA)3
BAZR2F10_A	BaZr2F10		aP104	(2, P-1)		3	(BA+2)1(ZR+4)2(F-1)10
BAZR2F10_B	BaZr2F10		mS52	(15, C2/c)		3	(BA+2)1(ZR+4)2(F-1)10
BAZRF6_A	BaZrF6		mP32	(14, P2_1/c)		3	(BA+2)1(ZR+4)1(F-1)6
BAZRF6_B	ZrPbF6		oS32	(67, Cmme)		3	(BA+2)1(ZR+4)1(F-1)6
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)		2	(AL, BA, CA, CO, CR, CU, FE, GD, HF, K, LA, LI, MG, MN, MO, NA, NB, NI, P, S, SI, TI, V, W, Y, YB, ZR)1(B, C, N, O, VA)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
BCY	Unknown Structure					4	(BA+2, VA)0.1111(CA+2, Y+3)0.2222 (Y+3)0.6667(O-2)1.3333
BETA_RHOMBO_B	beta-B (R-105)		hR105	(166, R-3m)		2	(B)93(B, C, SI)12
BETA_V_O	CoO		tI4	(139, I4/mmm)		2	(V)1(O, VA)1
BPO4	BPO4 (H07)	H07	tI12	(82, I-4)		3	(B+3)1(P+5)1(O-2)4
BRONZE	Unknown Structure					3	(V+4, V+5)2(O-2)5(CA+2, FE+2, VA)1
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)	Not stable under anhydrous conditions.	4	(CA+2)6(AL+3)6(AL+3, FE+3)1(O-2)16.5
C13A6Z2	Ca7ZrAl6O18		oP104	(31, Pmn2_1)	This is 13CaO.3Al2O3.2ZrO2.	4	(CA+2)13(AL+3)12(ZR+4)2(O-2)35
C1A1	Al2CaO4		mP84	(14, P2_1/c)	This is CaO.Al2O3 with solubility of Ba and Fe	4	(BA+2, CA+2)3(AL+3)5(AL+3, FE+3)1(O-2)12
C1A2	Al4CaO7		mS48	(15, C2/c)	This is CaO.2Al2O3 with solubility of Fe	4	(CA+2)1(AL+3)3(AL+3, FE+3)1(O-2)7
C1A6	BaFe12O19		hP66	(194, P6_ 3/mmc)	This is BaO.6Al2O3, BaO.6Fe2O3 and CaO.6Al2O3 with solubility of Fe	3	(BA+2, CA+2)1(AL+3, FE+3)12(O-2)19
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	Unknown Structure				This is 2CaO.14Al2O3.2MgO	4	(CA+2)2(AL+3)28(MG+2)2(O-2)46
C2F	Ca2Fe2O5		oP36	(62, Pnma)	This is 2CaO.Fe2O3 with solubility of Al.	3	(CA+2)2(AL+3, FE+3)2(O-2)5
C3A1	Ca3Al2O6		cP264	(205, Pa-3)	This is 3CaO.Al2O3 with solubility of Fe	3	(CA+2)3(AL+3, FE+3)2(O-2)6
C3A2M1	3CaO.2Al2O3.MgO		oP72	(57, Pbcm)	This is 3CaO.2Al2O3.MgO	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

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C4WF4	Ca4Fe9O17		mS60	(5, C2)	This is 4CaO.FeO.4Fe2O3.	4	(CA+2)4(FE+2)1(FE+3)8(O-2)17
C4WF8	Sr2Fe2O5		oI44	(74, Imma)	This is 4CaO.FeO.8Fe2O3	4	(CA+2)4(FE+2)1(FE+3)16(O-2)29
CA10P6O25	Unknown Structure				This is Ca10(PO4)6O.	3	(CA+2)10(PO4-3)6(O-2)1
CA10SI3O15F2	Unknown Structure				This is 9CaO.3SiO2.CaF2	4	(CA+2)10(SI+4)3(O-2)15(F-1)2
CA10V6O19	Unknown Structure					3	(CA+2)5(V+3)3(O-2)9.5
CA11B2SI4O22_HT	Unknown Structure					4	(CA+2)11(B+3)2(SI+4)4(O-2)22
CA11B2SI4O22_LT	Unknown Structure					4	(CA+2)11(B+3)2(SI+4)4(O-2)22
CA15CU18O35	Ca4.8Cu6O11.6		mP92	(13, P2/c)		4	(CA+2)15(CU+2)14(CU+3)4(O-2)35
CA2AL2B2O8	Unknown Structure					4	(CA+2)2(AL+3)2(B+3)2(O-2)8
CA2ALF7	Ca2AlF7		oP40	(62, Pnma)		3	(CA+2)2(AL+3)1(F-1)7
CA2ALNBO6	Ca2AlNbO6		mP24	(14, P2_1/c)		4	(CA+2)2(AL+3)1(NB+5)1(O-2)6
CA2B2O5_S1	b-Mg2B2O5		mP36	(14, P2_1/c)		3	(CA+2)2(B+3)2(O-2)5
CA2B2O5_S2	Ca2B2O5		oP36	(19, P2_12_12_1)		3	(CA+2)2(B+3)2(O-2)5
CA2CUO3	Sr2CuO3		oI12	(71, Immm)		3	(CA+2)2(CU+2)1(O-2)3
CA2GD2ZRO7	Unknown Structure					4	(CA+2)2(GD+3)2(ZR+4)1(O-2)7
CA2HF7O16	Ca2Hf7O16		hR25	(148, R-3)		3	(CA+2)2(HF+4)7(O-2)16
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

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CA2NB2O7	La2Ti2O7		mP44	(4, P2_1)		3	(CA+2)2(NB+5)2(O-2)7
CA2P2O7_A	Ce2Si2O7		mP44	(14, P2_1/c)	This is alpha- Ca2(P2O7).	2	(CA+2, MG+2)2(P2O7-4)1
CA2P2O7_B	beta-Ca2[P2O7]		tP88	(76, P4_1)	This is beta- Ca2(P2O7).	2	(CA+2, MG+2)2(P2O7-4)1
CA2P2O7_G	Unknown Structure				This is gamma- Ca2(P2O7).	2	(CA+2, MG+2)2(P2O7-4)1
CA2P6O17	Ca2P6O17		mP56	(14, P2_1/c)	This is Ca2(P2O5)3O2.	3	(CA+2)2(P+5)6(O-2)17
CA2SIO4_ALPHA_A	Ca2SiO4		hP24	(194, P6_ 3/mmc)	This is 2CaO.SiO2 and 3CaO.P2O5.	3	(BA+2, CA+2, GD+3, LI2+2, MG+2, MN+2, Y+3)3(CA+2, VA)1(BO3-3, PO4-3, SIO4-4)2
CA2SIO4_ALPHA_ PRIME	K2CoCl4		oP84	(33, Pna2_1)	This is Ca2SiO4.	3	(BA+2, CA+2, FE+2, GD+3, LI2+2, MG+2, MN+2, Y+3)3(CA+2, VA)1(BO3-3, PO4-3, SIO4-4)2
CA2V2O7	Sr2V2O7		aP	(2, P-1)		3	(CA+2)2(V+5)2(O-2)7
CA2YB2O5	Unknown Structure					3	(CA+2)2(YB+3)2(O-2)5
CA2ZRSI4O12	cyclosilicate (Ca2ZrSi4O12)		mP38	(11, P2_1/m)		4	(CA+2)2(SI+4)4(ZR+4)1(O-2)12
CA3B2O6	Ca3[BO3]2		hR22	(167, R-3c)		3	(CA+2)3(B+3)2(O-2)6
CA3CO2O6	Ca3Co2O6		hR22	(167, R-3c)		3	(CA+2)3(CO+3, CU+2)2(O-2, VA)6
CA3CO4O9	Ca3Co4O9		mS30	(12, C2/m)		3	(CA+2)3(CO+3, CU+2)4(O-2, VA)9
CA3COAL4O10	Ca3ZnAl4O10		oP72	(29, Pca2_1)		4	(CA+2)3(CO+2)1(AL+3)4(O-2)10
CA3MG3P4O16	Unknown Structure				This is Ca3Mg3(PO4)4 solid solution.	3	(CA+2, MG+2)3(MG+2)3(PO4-3)4
CA3NA2SI6O16	Na2Ca3Si6O16		aP54	(2, P-1)		4	(CA+2)3(NA+1)2(SI+4)6(O-2)16
CA3NB2O8	Unknown Structure					3	(CA+2)3(NB+5)2(O-2)8
CA3P2O8_A	Ca3[PO4]2		mP312	(14, P2_1/c)	This is alpha- Ca3(PO4)2 with solubility of	3	(BA+2, CA+2, MG+2)3(CA+2, VA)1(PO4-3,

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					Ba, Mg and Si.		SIO4-4)2
CA3P2O8_B	Ca3[AsO4]2		hR92	(161, R3c)	This is beta- Ca3(PO4)2 with solubility of Ba and Mg.	2	(BA+2, CA+2, MG+2)3(PO4-3)2
CA3S3FE4OX	Unknown Structure				This is 3CaS.4FeO and 3CaS.4Fe2O3.	4	(CA+2)3(S-2)3(FE+2, FE+3)4(O-2, VA)6
CA3TI2O7	Ca3Ti2O7		oS48	(36, Cmc2_1)		3	(CA+2)3(TI+4)2(O-2)7
CA3TI8AL12O37	Unknown Structure					4	(CA+2)3(TI+4)8(AL+3)12(O-2)37
CA3V2O8	K2PbS2O8		hR273	(161, R3c)		3	(CA+2)3(V+5)2(O-2)8
CA3WO6	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)		3	(CA+2)3(W+6)1(O-2)6
CA3Y2SI3O12	Ca3Y2Si3O12		oP100	(62, Pnma)	This is 3CaO.(Gd,Y,Yb)2O3.3SiO2.	4	(CA+2)3(GD+3, Y+3, YB+3)2(SI+4)3(O-2)12
CA3Y2SI6O18	Ca0.6Y0.4Si6O18		mS116	(15, C2/c)	This is 3CaO.(Gd,Y,Yb)2O3.6SiO2.	4	(CA+2)3(GD+3, Y+3, YB+3)2(SI+4)6(O-2)18
CA3YB2O6	Unknown Structure					3	(CA+2)3(YB+3)2(O-2)6
CA3ZRSI2O9	Ca3Hf(Si2O7)O2		mP60	(14, P2_1/c)		4	(CA+2)3(SI+4)2(ZR+4)1(O-2)9
CA4MG2P6O21	Unknown Structure					3	(CA+2)4(MG+2)2(P2O7-4)3
CA4NB2O9_HT11	Ca4Nb2O9		mP20	(14, P2_1/c)		5	(CA+2)6(CA+2, NB+5)3(NB+5)3(O-2, VA)3 (O-2)15
CA4NB2O9_LT21	Ca4Nb2O9-lt		mP60	(14, P2_1/c)		5	(CA+2)6(CA+2, NB+5)4(CA+2)2(O-2, VA)3 (O-2)15
CA4P2O9_A	Ca4[PO4]2O		mP60	(4, P2_1)	This is alpha- Ca4(PO4)2O.	3	(CA+2)4(PO4-3)2(O-2)1
CA4P2O9_B	beta-Ca4(PO4)2O		oP60	(17, P222_1)	This is beta-Ca4(PO4)2O.	3	(CA+2)4(PO4-3)2(O-2)1
CA4P6O19	Ca4P6O19		aP58	(2, P-1)	This is Ca4(PO3)5(PO4).	3	(CA+2)4(PO3-1)5(PO4-3)1

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CA4TI3O10	Ca4Ti3O10		oP68	(61, Pbca)		3	(CA+2)4(TI+4)3(O-2)10
CA4V2O9	Ca4V2O9		oF	(22, F222)		3	(CA+2)4(V+5)2(O-2)9
CA5BA2B10O22	Unknown Structure					4	(CA+2)5(BA+2)2(B+3)10(O-2)22
CA5P2SIO12	Unknown Structure					3	(CA+2, VA)5(PO4-3)2(SIO4-4, VA)1
CA5SI2O8F2	Unknown Structure				This is 4CaO.2SiO2.CaF2	4	(CA+2)5(SI+4)2(O-2)8(F-1)2
CA6HF19O44	Ca6Hf19O44		hR138	(167, R-3c)		3	(CA+2)6(HF+4)19(O-2)44
CA6ZR19O44	Ca6Hf19O44		hR138	(167, R-3c)		3	(CA+2)6(ZR+4)19(O-2)44
CA7P2SI2O16	Ca7[(Si0.5P0.5)O4]4		hP180	(169, P6_1)		3	(CA+2)7(PO4-3)2(SIO4-4)2
CA9V6O18	Unknown Structure					3	(CA+2)9(V+3)6(O-2)18
CAAL2B2O7	Unknown Structure					4	(CA+2)1(AL+3)2(B+3)2(O-2)7
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
CAB2O4	CaB2O4 I (E32)	E32	oP28	(60, Pbcn)		3	(CA+2)1(B+3)2(O-2)4
CAB4O7	CaB4O7		mP96	(14, P2_1/c)		3	(CA+2)1(B+3)4(O-2)7
CABA2B2O6	Unknown Structure					4	(CA+2)1(BA+2)2(B+3)2(O-2)6
CABA2B6O12	Unknown Structure					4	(CA+2)1(BA+2)2(B+3)6(O-2)12
CAC2_BETA	CaC2		cF36	(225, Fm-3m)		2	(CA+2)1(C2-2)1
CAC2_C11A	CaC2-I (C11a)	C11a	tI6	(139, I4/mmm)		2	(CA+2)1(C2-2)1

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CACO3	Calcite (CaCO3, G01)	G01	hR30	(167, R-3c)	This is (Ca,Fe,Mg)CO3.	2	(CA+2, FE+2, MG+2)1(CO3-2)1
CACR2O4_A	SrCr2O4		oP28	(59, Pmmn)	With solubility of Al and Fe.	3	(BA+2, CA+2)1(AL+3, CR+3, FE+3)2(O-2)4
CACRSI4O10	gillespite (BaFeSi4O10)		tP64	(130, P4/ncc)	This is CaO.CrO.4SiO2, Gillespite	4	(CA+2)1(CR+2)1(SI+4)4(O-2)10
CACU2O3	Shcherbinaite (V2O5) (Revised)		oP14	(59, Pmmn)		3	(CA+2)1(CU+2)2(O-2)3
CAF2_S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is low temperature CaF2.	2	(BA+2, CA+2, MG+2, MN+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, MN+2)1(F-1, O-2, VA)2
CAMG3O16S4	Unknown Structure				This is CaMg3(SO4)4.	3	(CA+2)1(MG+2)3(SO4-2)4
CAMN2O4	CaMn2O4		oP28	(57, Pbcm)		3	(CA+2)1(MN+3)2(O-2)4
CAMO3	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)	This is CaHfO3, CaMnO3, CaTiO3, lt CaZrO3.	3	(CA+2, GD+3, Y+3)1(GD+3, HF+4, MN+4, TI+4, Y+3, ZR+4)1(O-2)3
CAN2O6	Pb(NO3)2 (G21)	G21	cP36	(205, Pa-3)	This is (Ba, Ca, Mg)(NO3)2 solid solution.	2	(BA+2, CA+2, MG+2)1(NO3-1)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
CAP2O6_A	CaP2O6		mS72	(9, Cc)	This is alpha-Ca(PO3)2.	2	(CA+2)1(PO3-1)2
CAP2O6_B	PbP2O6		mP72	(14, P2_1/c)	This is beta-Ca(PO3)2.	2	(CA+2)1(PO3-1)2
CAP2O6_G	CaP2O6		mP72	(9, Cc)	This is gamma-Ca(PO3)2.	2	(CA+2)1(PO3-1)2
CAP4O11_A	CaP4O11		oS128	(41, Aea2)	This is alpha- Ca(P2O5)2O.	3	(CA+2)1(P+5)4(O-2)11

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CAP4O11_B	CaP4O11		mP64	(14, P2_1/c)	This is beta- Ca(P2O5)2O.	3	(CA+2)1(P+5)4(O-2)11
CARNEGIEITE_A	alpha-Carnegieite (NaAlSiO4, S65)	S65	cP28	(198, P2_13)	This is NaAlSiO4 with solubility of Fe and Si.	3	(NAAL+4, NAFE+4, SI+4)4(SI+4)4(O-2)16
CARNEGIEITE_B	NaAl[SiO4]		oP56	(29, Pca2_1)	This is NaAlSiO4 with solubility of Fe and Si.	3	(NAAL+4, NAFE+4, SI+4)4(SI+4)4(O-2)16
CASFEO	Unknown Structure				This is CaS.FeO and CaS.Fe2O3.	4	(CA+2)2(S-2)2(FE+2, FE+3)2(O-2, VA)3
CASO4_HT	CePO4		hP18	(180, P6_222)	This is high- temperature (Ca,Co,Mg)SO4.	2	(CA+2, CO+2, MG+2)1(SO4-2)1
CAV2O4	CaV2O4		oP28	(62, Pnma)	This is CaO.Fe2O3, b-CaCr2O4, Ca(V,Y,Yb)2O4, Ba(Gd,La,Y)2O4.	3	(BA+2, CA+2)1(AL+3, CR+3, FE+3, GD+3, LA+3, V+3, Y+3, YB+3)2(O-2)4
CAV2O5	CaV2O5		oP16	(59, Pmmn)		3	(CA+2)1(V+4)2(O-2)5
CAV2O6	ThTi2O6		mS18	(12, C2/m)	This is CaV2O6, CoV2O6, MgV2O6, MnV2O6 and NiV2O6.	3	(CA+2, CO+2, MG+2, MN+2, NI+2)1(V+5)2(O-2)6
CAV3O7	CaV3O7		oP44	(62, Pnma)		3	(CA+2)1(V+4)3(O-2)7
CAV4O9	CaV4O9		tP9	(85, P4/n)		3	(CA+2)1(V+4)4(O-2)9
CAVO3	Unknown Structure					3	(CA+2)1(V+4)1(O-2)3
CAWO4	Scheelite (CaWO4, H04)	H04	tI24	(88, I4_1/a)		3	(CA+2)1(W+6)1(O-2)4
CAY4O7	(Ca0.25Gd0.75)4GdO7		mS48	(12, C2/m)	This is CaY4O7 and CaGd4O7.	3	(CA+2)1(GD+3, Y+3)4(O-2)7
CAYAL3O7	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_1m)	This is CaYAl3O7, CaYbAl3O7 and CaGdAl3O7	4	(CA+2)1(GD+3, Y+3, YB+3)1(AL+3)3(O-2)7
CAYALO4	K2NiF4		tI14	(139, I4/mmm)	This is CaYAlO4, CaYbAlO4 and CaGdAlO4	4	(CA+2)1(GD+3, Y+3, YB+3)1(AL+3)1(O-2)4
CAZR4O9	CaZr4O9		mS224	(15, C2/c)		3	(CA+2)1(ZR+4)4(O-2)9

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CAZRO3_C	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	Ba(Hf,Zr)O3 and High-temperature Ca (Hf,Zr)O3.	3	(BA+2, CA+2, Y+3)1(HF+4, Y+3, ZR+4)1(O-2)3
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(AL, CO, CR, CU, FE, MG, MN, MO, NB, NI, SI, TI, V, ZR)1(B, C, N, VA)1
CEMENTITE_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(AL, CO, CR, FE, MN, MO, NB, NI, SI, V, W)3(B, C, N)1
CF2	Ca3.5Fe14O24.5		mS172	(5, C2)	This is CaO.2Fe2O3	3	(CA+2)1(FE+3)4(O-2)7
CHALCOCITE_ALPHA	Cu2S-alpha		mP144	(14, P2_1/c)	This is Cu2S.	2	(CU)2(S)1
CHALCOCITE_BETA	Cu2S-beta		hP16	(194, P6_ 3/mmc)	This is Cu2S.	2	(CU)2(S)1
CHALCOPYRITE	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)	This is high-temperature nonstoichiometric CuFeS2.	3	(CU, FE, VA)1(CU, VA)1(S)1
CLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)	This is clino-enstatite (MgSiO3), clino-ferrosilit (FeSiO3), diopside (CaMgSi2O6), niopside (CaNiSi2O6), pigeonite ((Mg,Fe,Ca)Si2O6), hedenbergite (CaFeSi2O6) dissolving Co.	4	(CA+2, FE+2, MG+2, NI+2)1(CO+2, FE+2, MG+2, NI+2)1(SI+4)2(O-2)6
CO1LA2O4	La2CoO4		oP36	(55, Pbam)		3	(LA+3)2(CO+2)1(O-2)4
CO3LA4O10	Nd4Co3O10		mP68	(14, P2_1/c)		4	(LA+3)4(CO+2)1(CO+3)2(O-2)10
CO3P2O8	Co3[PO4]2		mP26	(14, P2_1/c)	This is (Co,Fe, Mg,Ni)3P2O8 with solubility of Ca.	2	(CA+2, CO+2, FE+2, MG+2, NI+2)3(PO4-3)2
CO9S8	Co9S8 (D89)	D89	cF68	(225, Fm-3m)		2	(CO, FE, NI)9(S)8
COLUMBITE	Columbite (FeNb2O6, E51)	E51	oP36	(60, Pbcn)	This is (Ca,Co,Fe,Mg,Mn)Nb2O6 with excess FeO and MgO.	3	(CA+2, CO+2, FE+2, MG+2, MN+2)1(FE+2, MG+2, NB+5)2(O-2, VA)6
CORDIERITE	Na0.04 (Mg0.5Fe0.5)2Al4Si5O18		oS120	(66, Cccm)	This is 2Al2O3.2MgO.5SiO2, 2Al2O3.2MnO.5SiO2 and 2Al2O3.2FeO.5SiO2	4	(AL+3)4(FE+2, MG+2, MN+2)2(SI+4)5(O-2)18

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CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	(167, R-3c)	This is Al2O3, Cr2O3, Fe2O3, Ti2O3, V2O3 + (Co,Fe,Mg,Mn,Ni)TiO3 Ilmenite.	2	(AL+3, CO+2, CR+3, FE+2, FE+3, MG+2, MN+2, MN+3, NI+2, TI+3, TI+4, V+3, V+4, VA)2(O-2)3
COVELLITE	Covellite (CuS, B18)	B18	hP12	(194, P6_ 3/mmc)	This is CuS.	2	(CU)1(S)1
CR1S1	CrS		mS8	(15, C2/c)	This is low-temp CrS.	2	(CR)1.03(S)1
CR2P4O13	Cr2P4O13		mP76	(14, P2_1/c)	This is Cr2P4O13, Cr2V4O13 and Fe2V4O13.	3	(CR+3, FE+3)2(P+5, V+5)4(O-2)13
CR2S3	Dolomite [MgCa(CO3)2, G11]	G11	hR10	(148, R-3)		2	(CR, FE)2(S)3
CR2TI2O7	Unknown Structure				with solubility of Al2O3 and Fe2O3.	3	(AL+3, CR+3, FE+3)2(TI+4)2(O-2)7
CR3P2O8	Unknown Structure					2	(CR+2)3(PO4-3)2
CR3PO7	Unknown Structure					3	(CR+3)3(P+5)1(O-2)7
CR3S4	Brezinaite (Cr3S4)		mS14	(12, C2/m)		2	(CR, FE, MN, NI)3(S)4
CR4P6O21	Unknown Structure					2	(CR+3)4(P2O7-4)3
CR5PO10	Unknown Structure					3	(CR+3)5(P+5)1(O-2)10
CR5S6	Cr5S6		hP22	(163, P-31c)		2	(CR)5(S)6
CR7S8	Cr7Se8		mS30	(12, C2/m)		2	(CR)7(S)8
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	(227, Fd-3m)	SiO2 with AlPO4 solubility.	2	(AL+3, SI+4)1(PO4-3, SIO4-4)1
CRNB25O64	Unknown Structure					3	(CR+3)1(NB+5)25(O-2)64
CRNB49O124	Unknown Structure					3	(CR+3)1(NB+5)49(O-2)124
CRNB9O24	Unknown Structure					3	(CR+3)1(NB+5)9(O-2)24

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CRNBO4	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)		3	(CR+3, VA)1(CR+3, NB+5)1(O-2, VA)4
CRPO4	Cr[PO4]		oI72	(74, Imma)		2	(CR+3)1(PO4-3)1
CRVO4	MgSO4		oS24	(63, Cmcm)		3	(CR+3)1(V+5)1(O-2)4
CRYOLITE	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)	This is (K,Na)3AlF6 solid solution.	2	(K+1, LI+1, NA+1, VA)3(ALF4-1, ALF6-3)1
CU2B4O7	Unknown Structure					3	(CU+1)2(B+3)4(O-2)7
CU2COO3	CaCu2O3		oP12	(59, Pmmn)		3	(CO+2)1(CU+2)2(O-2)3
CU2P2O7	alpha-Zn2V2O7		mS44	(15, C2/c)		2	(CU+2)2(P2O7-4)1
CU2SO4	Thenardite [Na2SO4 (V), H17]	H17	oF56	(70, Fddd)		2	(CU+1)2(SO4-2)1
CU2SO5	Cu2[SO4]O		mS32	(12, C2/m)		1	(CU2O5S1)1
CU2Y2O5	Cu2Ho2O5		oP36	(33, Pna2_1)		3	(CU+2)2(Y+3)2(O-2)5
CU3B2O6	Cu3B2O6		aP110	(2, P-1)		3	(CU+2)3(B+3)2(O-2)6
CU3NB2O8	Cu3(Ta0.5Nb0.5)2O8		aP13	(2, P-1)		3	(CU+2)3(NB+5)2(O-2)8
CU3P2O8	Unknown Structure					2	(CU+2)3(PO4-3)2
CUB2O4	CuB2O4		tI84	(122, I-42d)		3	(CU+2)1(B+3)2(O-2)4
CUB8O13	Unknown Structure					3	(CU+2)1(B+3)8(O-2)13
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		2	(AL, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, SI, TI, V, ZR)1(B, C, N, VA)1
CUCRS2	CuCrS2-b		hR4	(160, R3m)		3	(CU)1(CR)1(S)2
CUF1	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(CU+1)1(F-1)1

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CUF2	CuF2		mP6	(14, P2_1/c)	This is CrF2 and CuF2.	2	(CR+2, CU+2)1(F-1)2
CUFES2_LT	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)	This is stoichiometric low- temperature CuFeS2.	3	(CU)1(FE)1(S)2
CUGD2O4	CuNd2O4		tI14	(139, I4/mmm)		3	(CU+2)1(GD+3)2(O-2)4
CULA2O4	CuLa2O4		oS28	(64, Cmce)	With solubility of Co.	3	(CO+2, CU+2)1(LA+3)2(O-2)4
CUNB2O6	CuNb2O6		mP36	(14, P2_1/c)		3	(CU+2)1(NB+5)2(O-2)6
CUO	Tenorite (CuO, B26)	B26	mS8	(15, C2/c)		2	(CO+2, CU+2)1(O-2)1
CUP2O6	CuP2O6		mS72	(15, C2/c)	This is (Co,Cu,Fe,Mg, Mn,Ni)P2O6.	2	(CO+2, CU+2, FE+2, MG+2, MN+2, NI+2)1 (PO3-1)2
CUPO3	Unknown Structure					2	(CU+1)1(PO3-1)1
CUPRITE	Cuprite (Cu2O, C3)	C3	cP6	(224, Pn-3m)	This is Cu2O with solubility of Na.	2	(CU+1, NA+1)2(O-2)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
CW3F	CaFe5O7		oS52	(63, Cmcm)	This is CaO.3FeO.Fe2O3.	4	(CA+2)1(FE+2)3(FE+3)2(O-2)7
CWF	CaFe3O5		oS36	(63, Cmcm)	This is CaO.FeO.Fe2O3.	4	(CA+2)1(FE+2)1(FE+3)2(O-2)5
DANBURITE	Danburite (CaB2Si2O8, S63)	S63	oP52	(62, Pnma)		4	(CA+2)1(B+3)2(SI+4)2(O-2)8
DELAFOSSITE	Rhombohedral Delafossite (CuFeO2)		hR4	(166, R-3m)	This is Cu(Al,B,Cr,Fe,La,Mn,Y)O2	3	(CU+1)1(AL+3, B+3, CR+3, FE+3, LA+3, MN+3, Y+3)1(O-2)2
DHCP	alpha-La (A3')	A3'	hP4	(194, P6_ 3/mmc)		2	(AL, CA, CU, GD, LA, MG, MN, NI, Y)1(O, VA)0.5
DIAMOND_FCC_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	This is Silicon	2	(AL, B, C, MN, NA, P, SI)1(O, VA)1
DIGENITE	Cu2Se		cF44	(225, Fm-3m)	This is Cu2S with solubility of Fe, Mg and Mn.	3	(CU, FE, MG, MN, VA)2(CU, VA)1(S)1

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DJURLEITE	Cu31S16		mP376	(14, P2_1/c)	This is Cu31S16.	2	(CU)1.93(S)1
DYMN2O5	HoMn2O5		oP32	(55, Pbam)	This is Mn2(Gd, Y)O5.	4	(GD+3, Y+3)1(MN+3)1(MN+4)1(O-2)5
ETA_M5SIN	Fe3W3C (E93)	E93	cF112	(227, Fd-3m)		4	(CR, MO)3(FE, NI)2(SI)1(N)1
F6NA2SI1_A	Na2SiF6		hP27	(150, P321)		3	(NA+1)2(SI+4)1(F-1)6
F6NA2SI1_B	K2PtCl6 (J11)	J11	cF36	(225, Fm-3m)		3	(NA+1)2(SI+4)1(F-1)6
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	This is FCC_A1 solid solution and TiO and VO cubic oxides.	2	(AL, BA, CA, CO, CR, CU, FE, GD, HF, K, LA, LI, MG, MN, MO, NA, NB, NI, P, S, SI, TI, V, VA, W, Y, YB, ZR)1(B, C, N, O, VA)1
FE18P2O24	Fe4(Fe0.5P0.5)O6		oS44	(65, Cmmm)		4	(FE+2)16(FE+3)2(PO4-3)2(O-2)16
FE2O12S3	Fe2[SO4]3		hR34	(148, R-3)	This is (Al,Cr, Fe)2(SO4)3	2	(AL+3, CR+3, FE+3)2(SO4-2)3
FE2P2O7	Fe2[P2O7]		aP11	(2, P-1)		2	(FE+2)2(P2O7-4)1
FE2PO5	Fe2[PO4]O		mS32	(15, C2/c)		4	(FE+2)1(FE+3)1(PO4-3)1(O-2)1
FE3BO5	Fe3[BO3]O2		oP36	(55, Pbam)		4	(FE+2)2(FE+3)1(B+3)1(O-2)5
FE3BO6	Norbergite [Mg(F,OH)2 . Mg2SiO4, S07]	S07	oP40	(62, Pnma)		3	(FE+3)3(B+3)1(O-2)6
FE3P4O14	Unknown Structure					3	(FE+2)1(FE+3)2(P2O7-4)2
FE3PO7	Fe3PO7		hR11	(160, R3m)		3	(FE+3)3(P+5)1(O-2)7
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	(221, Pm-3m)		2	(CO, CR, FE, MN, NI)4(C, N, VA)1
FE4P6O21	Fe4[P2O7]3		mP124	(14, P2_1/c)		2	(FE+3)4(P2O7-4)3
FE7P6O24	Fe7[PO4]6		aP37	(2, P-1)		3	(FE+2)3(FE+3)4(PO4-3)6

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FE7P8O28	Unknown Structure					3	(FE+2)5(FE+3)2(P2O7-4)4
FE8SI2C	Mn8Si2C		aP*	(1, P1)		3	(FE, MN)8(SI)2(C)1
FEAL2S4	ZnIn2S4		hR7	(160, R3m)		3	(FE)1(AL)2(S)4
FEB4O7	ZnB4O7		oS48	(63, Cmcm)		3	(FE+2)1(B+3)4(O-2)7
FEBO3	Calcite (CaCO3, G01)	G01	hR10	(167, R-3c)		3	(FE+3)1(B+3)1(O-2)3
FEF3	FeF3 (D012)	D012	hR8	(167, R-3c)	This is (Al,Co,Cr, Fe)F3.	2	(AL+3, CO+3, CR+3, FE+3)1(F-1)3
FENB14O36	Unknown Structure				This is (Co, Fe)Nb14O36	3	(CO+2, FE+2)1(NB+5)14(O-2)36
FENB25O64	Unknown Structure					3	(FE+3)1(NB+5)25(O-2)64
FENB36O91	Unknown Structure				This is (Co, Fe)Nb36O91	3	(CO+2, FE+2)1(NB+5)36(O-2)91
FENB49O124	Unknown Structure					3	(FE+3)1(NB+5)49(O-2)124
FENB68O171	Unknown Structure				This is (Co, Fe)Nb68O171	3	(CO+2, FE+2)1(NB+5)68(O-2)171
FENB9O24	Unknown Structure					3	(FE+3)1(NB+5)9(O-2)24
FEV2O6	Unknown Structure					3	(FE+2)1(V+5)2(O-2)6
FEVO4	Zn[MoO4]		aP36	(2, P-1)	This is FeVO4 and AlVO4.	3	(AL+3, FE+3)1(V+5)1(O-2)4
FLUORAPATITE	Fluorapatite [Ca5F(PO4)3, H57]	H57	hP42	(176, P6_3/m)		3	(CA+2)10(PO4-3)6(F-1)2
FLUORITE	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is cubic high temp HfO2 and ZrO2	2	(AL+3, BA+2, CA+2, CR+3, FE+2, GD+3, HF+4, LA+3, MG+2, MN+2, MN+3, NB+5, NI+2, SI+4, TI+4, VA, Y+3, YB+3, ZR, ZR+4)2(O-2, VA)4
GARNET	Orthorhombic Garnet		oF320	(70, Fddd)	This is Grossular, Uvarovite, Spessartine and Goldmanite Garnets and (Gd, Y,Yb)3 (Al,Fe)5O12.	4	(CA+2, FE+2, GD+3, LA+3, MG+2, MN+2, Y+3, YB+3)3(AL+3, CR+3, FE+3, MG+2, V+3)2(AL+3, CR+3, FE+3, SI+4)3(O-2)12

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GD2SI2O7	Ce2Si2O7		mP44	(14, P2_1/c)	This is (Gd, La)2Si2O7	3	(GD+3, LA+3)1(GD+3, LA+3)1(SI2O7-6)1
GD2SIO5	Gd2SiO5 (RE2SiO5 X1)		mP32	(14, P2_1/c)	This is (Gd,La)2SiO5	4	(GD+3, LA+3)1(GD+3, LA+3)1(SIO4-4)1(O-2)1
GDBO3	GdBO3		hR30	(155, R32)	This is (Gd,La)BO3 solid solution.	3	(GD+3, LA+3)1(B+3)1(O-2)3
GDF3	H3Ho		hP24	(165, P-3c1)	This is high temp (Gd, Y,Yb)F3.	2	(GD+3, Y+3, YB+3)1(F-1)3
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_3/mmc)	Graphite	1	(B, C)1
GUGGENITE	CaCu2O3		oP12	(59, Pmmn)		3	(MG+2)0.825(CU+2)2.175(O-2)3
HALITE	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is BaO, CaO, CoO, FeO, MgO, MnO and NiO	2	(AL+3, BA+2, CA+2, CO+2, CO+3, CR+3, CU+2, FE+2, FE+3, GD+3, LIAL1/2+2, MG+2, MN+2, MN+3, NA+1, NI+2, NI+3, TI+4, V+3, VA, Y+3, YB+3, ZR+4)1(O-2)1
HATRURITE	Ca3(SiO4)O-b		hR81	(160, R3m)	This is 3CaO.SiO2	3	(CA+2, GD+3, VA, Y+3)3(SIO4-4)1(O-2)1
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)	HCP_A3 also describes hexagonal carbides and nitrades.	2	(AL, BA, CA, CO, CR, CU, FE, GD, HF, K, LA, LI, MG, MN, MO, NA, NB, NI, SI, TI, V, W, Y, YB, ZR)1(B, C, N, O, VA)0.5
HEAZLEWOODITE_B1	Cu1.9S		cF12	(216, F-43m)	This is non- stoichiometric high temperature Ni3S2.	2	(CO, FE, NI, VA)2(S)1
HEAZLEWOODITE_B2	Unknown Structure				This is non- stoichiometric high temperature Ni4S3.	2	(FE, NI, VA)2(S)1
HFW2O8	Zr[WO4]2		cP44	(198, P2_13)		3	(HF+4)1(W+6)2(O-2)8
K10MG5SI11O32	Unknown Structure					4	(K+1)10(MG+2)5(SI+4)11(O-2)32
K2BA3SI8O20	Unknown Structure					4	(K+1)2(BA+2)3(SI+4)8(O-2)20
K2CA2SI2O7	K2Ca2[Si2O7]		hP108	(176, P6_3/m)		4	(K+1)2(CA+2)2(SI+4)2(O-2)7

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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
K2CO3_S1	K2[CO3]		mP24	(14, P2_1/c)	With solubility of Na.	2	(K+1, NA+1)2(CO3-2)1
K2FE2SI6O16	Unknown Structure					4	(K+1)2(FE+3)2(SI+4)6(O-2)16
K2FESI3O8	Unknown Structure					4	(K+1)2(FE+2)1(SI+4)3(O-2)8
K2FESI5O12	K16Mg8Si40O96		mP160	(14, P2_1/c)		4	(K+1)2(FE+2)1(SI+4)5(O-2)12
K2MG3B2O7	Unknown Structure					4	(K+1)2(MG+2)3(B+3)2(O-2)7
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)		3	(MG+2)1(K+1)2(F-1)4
K2MGN4O12	Unknown Structure					3	(K+1)2(MG+2)1(NO3-1)4
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
K2S2	Na2O2		hP12	(189, P-62m)		2	(K)2(S)2
K2S3	K2S3		oS20	(36, Cmc2_1)		2	(K)2(S)3
K2S4	Unknown Structure					2	(K)2(S)4
K2S5	Tl2S5		oP28	(19, P2_12_12_1)		2	(K)2(S)5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
K2S6	Unknown Structure					2	(K)2(S)6
K2SI4O9_ALPHA	K2Si4O9		aP30	(2, P-1)	Low-temp K2Si4O9	3	(K+1)2(SI+4)4(O-2)9
K2SI4O9_BETA	K2Si4O9		hP30	(176, P6_3/m)	High-temp K2Si4O9	3	(K+1)2(SI+4)4(O-2)9
K2TI3O7	Unknown Structure					3	(K+1)2(TI+4)3(O-2)7
K2TI6O13	Na2Ti6O13		mS42	(12, C2/m)		3	(K+1)2(TI+4)6(O-2)13
K2TIO3	Cs2PbO3		oS24	(63, Cmcm)		3	(K+1)2(TI+4)1(O-2)3
K3FCO3	Unknown Structure					3	(K+1)3(F-1)1(CO3-2)1
K3PO4_ALPHA	Unknown Structure				low-temp	2	(K+1)3(PO4-3)1
K3PO4_BETA	Unknown Structure				mid-temp	2	(K+1)3(PO4-3)1
K3PO4_GAMMA	K3[PO4]-ht		cF32	(202, Fm-3)	high-temp	2	(K+1)3(PO4-3)1
K4AL22O35	K2Al10.67O17		hR30	(166, R-3m)	This is Beta double prime-Al2O3 K4 (AL,Fe)22O35 solid solution.	6	(K+1, VA)1(K+1, VA)1(AL+3, FE+3, MG+2)2 (O-2, VA)1(AL+3, FE+3)9(O-2)17
K4B6O11	Unknown Structure					3	(K+1)4(B+3)6(O-2)11
K4BASI3O9	K4SrSi3O9		oS68	(40, Ama2)		4	(K+1)4(BA+2)1(SI+4)3(O-2)9
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
K4FE4SI3O14	Unknown Structure					4	(K+1)4(FE+3)4(SI+4)3(O-2)14
K4FEO3	Unknown Structure					3	(K+1)4(FE+2)1(O-2)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
K4MG2SI5O14	Unknown Structure					4	(K+1)4(MG+2)2(SI+4)5(O-2)14
K4P2O7_ALPHA	K4[P2O7]		hP234	(169, P6_1)		2	(K+1)4(P2O7-4)1
K4P2O7_BETA	K4[P2O7]		hP26	(194, P6_ 3/mmc)		2	(K+1)4(P2O7-4)1
K4P2O7_DELTA	Unknown Structure					2	(K+1)4(P2O7-4)1
K4P2O7_GAMMA	Unknown Structure					2	(K+1)4(P2O7-4)1
K4SIO4	Cs4SnO4		mP36	(14, P2_1/c)		3	(K+1)4(SI+4)1(O-2)4
K4TIO4	Unknown Structure					3	(K+1)4(TI+4)1(O-2)4
K5B19O31	K5B19O31		mS220	(15, C2/c)		3	(K+1)5(B+3)19(O-2)31
K5P3O10_ALPHA	Unknown Structure					3	(K+1)5(P+5)3(O-2)10
K5P3O10_BETA	Unknown Structure					3	(K+1)5(P+5)3(O-2)10
K8BASI10O25	Unknown Structure		hR*			4	(K+1)8(BA+2)1(SI+4)10(O-2)25
K8CASI10O25	Unknown Structure					4	(K+1)8(CA+2)1(SI+4)10(O-2)25
K8TI5O14	Unknown Structure					3	(K+1)8(TI+4)5(O-2)14
KAL11O17	beta-Alumina (Al2O3, D56)	D56	hP60	(194, P6_ 3/mmc)	This is Beta-Al2O3 K(Al,Fe)11O17 solid solution.	6	(K+1, VA)1(K+1, VA)1(AL+3, FE+3, MG+2)2 (O-2, VA)1(AL+3, FE+3)9(O-2)17
KALSI2O6	K8(Al0.33Si0.67)24O48		tI160	(88, I4_1/a)	This is KAlSi2O6-KFeSi2O6-K2MgSi5O12 solid solution.	5	(K+1)2(AL+3, FE+3, MG+2)1(AL+3, FE+3, SI+4)1(SI+4)4(O-2)12
KALSIO4_HT	KLi[SO4]		hP14	(159, P31c)	This is high temperature KAlSiO4-K2MgSi3O8 ss. with SiO2 solubility	4	(K2MG+4, KAL+4)1(KAL+4, SI+4)1(SI+4)2 (O-2)8
KAPPA_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(AL)1(FE, MN)3(C, VA)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
KB9O14	Unknown Structure					3	(K+1)1(B+3)9(O-2)14
KBSI2O6	K(Si0.67B0.33)3O6		cI160	(220, I-43d)	Lisitsynite	4	(K+1)1(B+3)1(SI+4)2(O-2)6
KBSI3O8	Danburite (CaB2Si2O8, S63)	S63	oP52	(62, Pnma)		4	(K+1)1(B+3)1(SI+4)3(O-2)8
KCAF3	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(CA+2, MG+2)1(K+1)1(F-1)3
KFESIO4	Unknown Structure					4	(K+1)2(FE+3)2(SI+4)2(O-2)8
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
KMG2AL15O25	Unknown Structure					4	(K+1)1(MG+2)2(AL+3)15(O-2)25
KNO3_S1	alpha-Potassium Nitrate (KNO3) I		oP20	(62, Pnma)	This is lt-KNO3 with solubility of Na.	2	(K+1, NA+1)1(NO3-1)1
KPO3_ALPHA	KPO3		mP40	(14, P2_1/c)		2	(K+1)1(PO3-1)1
KPO3_BETA	alpha-Potassium Nitrate (KNO3) I		oP20	(62, Pnma)		2	(K+1)1(PO3-1)1
KPO3_GAMMA	KPO3		oS32	(63, Cmcm)		2	(K+1)1(PO3-1)1
KSI_CARBIDE	Mo6Fe11C5		mS44	(12, C2/m)		2	(CR, FE, MO, W)3(C)1
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	(2, P-1)	This is Al2O3.SiO2	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
LA1S2	CeSe2		mP12	(14, P2_1/c)		2	(LA)1(S)2
LA2CR3O12	Unknown Structure					3	(LA+3)2(CR+6)3(O-2)12
LA2CRO6	Unknown Structure					3	(LA+3)2(CR+6)1(O-2)6
LA2MNO4	K2NiF4		tI14	(139,	La2(Mn,Ni)O4 with Co solubility.	3	(LA+3)2(CO+2, MN+2, NI+2)1(O-2)4

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				I4/mmm)			
LA2NB12O33	Unknown Structure					3	(LA+3)2(NB+5)12(O-2)33
LA2S3	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)	This is (Gd,La)2S3.	2	(GD, LA)2(S)3
LA2TI3O9	Unknown Structure					3	(LA+3)2(TI+4)3(O-2)9
LA3BO6	Unknown Structure				This is (Gd, La)3BO6 solid solution.	3	(GD+3, LA+3)3(B+3)1(O-2)6
LA3NBO7	La3NbO7		oP44	(62, Pnma)		3	(LA+3)3(NB+5)1(O-2)7
LA3NI2O7	Sr3Sn2O7		oS48	(63, Cmcm)		4	(LA+3)3(CO+2, NI+2)1(NI+3)1(O-2)7
LA4NI3O10	La4Ni3O10		oS68	(64, Cmce)	La4Ni3O10 with Co solubility.	4	(LA+3)4(NI+2)1(CO+3, NI+3)2(O-2)10
LA4SI3O12	Unknown Structure					2	(LA+3)4(SIO4-4)3
LA4TI3O12	La4Ti3O12		hR19	(148, R-3)		3	(LA+3)4(TI+4)3(O-2)12
LA4TI9O24	Nd4Ti9O24		oF592	(70, Fddd)		3	(LA+3)4(TI+4)9(O-2)24
LAAL11O18	La0.83Al11.83O19		hP86	(194, P6_ 3/mmc)		3	(LA+3)1(AL+3)11(O-2)18
LAAP	PrNiO3		hR10	(167, R-3c)	This is Rhombohedral Perovskite: La (Al,Co)O3 with solubility of Ca, Cu, Ni, Y	3	(CA+2, LA+3, Y+3)1(AL+3, CO+3, CU+2, FE+3, NI+2)1(O-2, VA)3
LAB3O6	LaB3O6		mS40	(15, C2/c)	This is (Gd,La)B3O6 solid solution.	3	(GD+3, LA+3)1(B+3)3(O-2)6
LAF3	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	This is low temp (Gd,La,Y,Yb)F3.	2	(GD+3, LA+3, Y+3, YB+3)1(F-1)3
LAFE12O19	Unknown Structure					4	(LA+3)1(FE+2)1(FE+3)11(O-2)19
LANB3O9	La0.67Nb2O6-b		oS36	(65, Cmmm)		3	(LA+3)1(NB+5)3(O-2)9
LANBO4	LaNbO4		mS24	(15, C2/c)		3	(LA+3)1(NB+5)1(O-2)4

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LANIO3	PrNiO3		hR10	(167, R-3c)	This is a rhombohedral perovskite	3	(LA+3)1(NI+3)1(O-2)3
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
LAYP	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)	This is an Orthorhombic Perovskite, La (Y,Yb)O3.	3	(LA+3, Y+3, YB+3)1(LA+3, VA, Y+3, YB+3, ZR+4)1(O-2)3
LI2B4O7	Li2B4O7		tI104	(110, I4_1cd)		3	(LI+1)2(B+3)4(O-2)7
LI2B8O13	Unknown Structure					3	(LI+1)2(B+3)8(O-2)13
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
LI2CO3	Li2[CO3]		mS24	(15, C2/c)		2	(LI+1)2(CO3-2)1
LI2CUO2	Li2CuO2		oI10	(71, Immm)		3	(LI+1)2(CU+2)1(O-2)2
LI2FE3O5	Unknown Structure					4	(LI+1)2(FE+3)2(FE+2)1(O-2)5
LI2MNO3	Li2MnO3		mS24	(12, C2/m)		3	(LI+1)2(MN+4)1(O-2)3
LI2O2	Li2O2		hP8	(194, P6_ 3/mmc)		2	(LI+1)2(O2-2)1
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
LI2ZRF6	Rosiaite (PbSb2O6)		hP9	(162, P-31m)		3	(LI+1)2(ZR+4)1(F-1)6

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LI2ZRO3	Li2ZrO3		mS24	(15, C2/c)		3	(LI+1)2(ZR+4)1(O-2)3
LI3ALF6_S1	Li3VF6		mS120	(15, C2/c)		2	(LI+1)3(ALF6-3)1
LI3BO3	Li3[BO3]		mP28	(14, P2_1/c)		3	(LI+1)6(B+3)2(O-2)6
LI3N1	Li3N		hP4	(191, P6/mmm)		2	(LI)3(N)1
LI3NASIO4	Unknown Structure					4	(LI+1)3(NA+1)1(SI+4)1(O-2)4
LI3PO4_A	Enargite (AsCu3S4, H25)	H25	oP16	(31, Pmn2_1)		2	(LI+1)3(PO4-3)1
LI3ZR4F19	Zr4F19		aP52	(2, P-1)	P-1	3	(LI+1)3(ZR+4)4(F-1)19
LI3ZRF7	Unknown Structure					3	(LI+1)3(ZR+4)1(F-1)7
LI4B10O17	Unknown Structure					3	(LI+1)4(B+3)10(O-2)17
LI4B2O5_A	Li4B2O5		oP88	(29, Pca2_1)		3	(LI+1)4(B+3)2(O-2)5
LI4B2O5_B	Li4B2O5		mS44	(15, C2/c)		3	(LI+1)4(B+3)2(O-2)5
LI4P2O7_A	Li4[P2O7]		mP52	(14, P2_1/c)		2	(LI+1)4(P2O7-4)1
LI4P2O7_B	Li4[P2O7]		aP26	(2, P-1)		2	(LI+1)4(P2O7-4)1
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
LI4ZRF8	Li4TbF8		oP52	(62, Pnma)		3	(LI+1)4(ZR+4)1(F-1)8
LI5ALO4	Li5AlO4		oP20	(59, Pmmn)		3	(LI+1)5(AL+3, FE+3)1(O-2)4
LI6B4O9	Li6B4O9		mP76	(14, P2_1/c)		3	(LI+1)6(B+3)4(O-2)9
LI6BA2B4O11	Unknown Structure					4	(LI+1)6(BA+2)2(B+3)4(O-2)11

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LI6SI2O7	Li6[Si2O7]		tP30	(113, P-42_1m)		3	(LI+1)6(SI+4)2(O-2)7
LI6ZR2O7	Li6Zr2O7		mS60	(15, C2/c)		3	(LI+1)6(ZR+4)2(O-2)7
LI8SIO6	Li8CoO6		hP30	(185, P6_3cm)		3	(LI+1)8(SI+4)1(O-2)6
LI8ZRO6	Li8SnO6		hR45	(148, R-3)		3	(LI+1)8(ZR+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
LIALO2_A	NaFeO2		hR12	(166, R-3m)	This is LiCrO2, LiFeO2 and low-temp LiAlO2.	2	(LIAL+4, LICO+4, LICR+4, LIFE+4, SI+4)1(O-2)2
LIALSI2O6_HT	Li(Al0.33Si0.67)3O6		tP44	(92, P4_12_12)		3	(LIAL+4, SI+4)1(SI+4)2(O-2)6
LIALSI2O6_LT	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)		3	(LIAL+4)1(SI+4)2(O-2)6
LIALSI4O10	LiAlSi4O10		mP32	(13, P2/c)		3	(LIAL+4)1(SI+4)4(O-2)10
LIALSIO4_HT	LiAl[SiO4]		hP21	(180, P6_222)		3	(LIAL+4, SI+4)1(SI+4)1(O-2)4
LIALSIO4_LT	Be2[SiO4]		hR126	(148, R-3)		3	(LIAL+4, SI+4)1(SI+4)1(O-2)4
LIB3O5	LiB3O5		oP36	(33, Pna2_1)		3	(LI+1)2(B+3)6(O-2)10
LIBA2B5O10	LiBa2B5O10		mP36	(11, P2_1/m)		4	(LI+1)1(BA+2)2(B+3)5(O-2)10
LIBAB9O15	LiBaB9O15		hR156	(167, R-3c)		4	(LI+1)1(BA+2)1(B+3)9(O-2)15
LIBAF3	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(BA+2)1(LI+1)1(F-1)3
LIBO2	LiBO2		mP16	(14, P2_1/c)		3	(LI+1)2(B+3)2(O-2)4
LIMNO2	NaMnO2		oP8	(59, Pmmn)		3	(LI+1)1(MN+3)1(O-2)2

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LINO3	CaCO3		hR30	(167, R-3c)		2	(LI+1)1(NO3-1)1
LIPO3	LiPO3		mP100	(13, P2/c)		2	(LI+1)1(PO3-1)1
LIYO2	LiFeO2		tI16	(141, I4_ 1/amd)		3	(LI+1)1(Y+3)1(O-2)2
LOWCLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)	This is low clino-enstatite (MgSiO3) and low clino-diopside (CaMgSi2O6).	4	(CA+2, MG+2)1(MG+2)1(SI+4)2(O-2)6
M12C	Fe6W6C		cF104	(227, Fd-3m)		3	(CO)6(W)6(C)1
M23C6_D84	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)		3	(CO, CR, FE, MN, NI, V)20(CO, CR, FE, MN, MO, NI, V, W)3(B, C)6
M2O3A	La2O3 (D52)	D52	hP5	(164, P-3m1)	A-LA2O3. Also hexagonal A-type structure of Gd2O3.	3	(BA+2, CA+2, GD+3, HF+4, LA+3, MG+2, Y+3, YB+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3B	B-Sm2O3		mS30	(12, C2/m)	This is monoclinic B-type structure of R2O3	3	(AL+3, CA+2, CO+3, GD+3, HF+4, LA+3, MG+2, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3C	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)	This is also cubic Gd2O3, Y2O3 and Yb2O3	3	(AL+3, CA+2, CO+3, CR+3, FE+3, GD+3, HF+4, LA+3, MG+2, MN+3, NI+2, TI+4, Y, Y+3, YB+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3H	La2O3 (D52)	D52	hP5	(164, P-3m1)	H-La2O3. This is also hexagonal (Gd,Y,Yb)2O3.	3	(BA+2, CA+2, GD+3, HF+4, LA+3, MG+2, MN+3, Y, Y+3, YB+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3X	Nd2O3		cI26	(229, Im-3m)	X-LA2O3. This is also HT cubic X-type structure of Gd2O3.	3	(BA+2, CA+2, GD+3, HF+4, LA+3, MG+2, Y+3, YB+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M3C2_D510	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(CO, CR, MO, V, W)3(C)2
M4O7	Ti4O7-a		aP22	(2, P-1)	This is Ti4O7 and V4O7 with solubility of Al and Mn.	2	(AL, MN, TI, V)4(O)7
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(FE, MN, NB, V)5(C, N)2
M6C_E93	Fe3W3C (E93)	E93	cF112	(227, Fd-3m)		4	(CO, FE, NI)2(MO, NB, W)2(CO, CR, FE,

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							MO, NB, NI, SI, V, W)2(C)1
M6O11	Ti6O11		aP34	(2, P-1)	This is Ti6O11 and V6O11.	2	(TI, V)6(O)11
M7C3_D101	C3Cr7 (D101)	D101	oP40	(62, Pnma)		2	(AL, CO, CR, FE, MN, MO, NB, NI, SI, V, W)7(B, C)3
M7O13	Ti7O13		aP40	(2, P-1)	This is Ti7O13 and V7O13.	2	(TI, V)7(O)13
M8O15	Ti8O15		aP46	(2, P-1)	This is Ti8O15 and V8O15.	2	(TI, V)8(O)15
MALINKOITE	BaZn[GeO4]		hP42	(173, P6_3)	NaBSiO4 with SiO2 solubility	2	(NAB+4, SI+4)1(SIO4-4)1
MC_ETA	CMo		hP12	(194, P6_ 3/mmc)		2	(MO, TI, V, W)1(C, VA)1
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	(187, P-6m2)		2	(MO, W)1(C, N)1
MELILITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_ 1m)	This is gehlenite, akermanite, Fe-akermanite, bennesherite, Ba2MgSi2O7 and 2CaO.CoO.2SiO2.	5	(BA+2, CA+2, NA+1)2(AL+3, CO+2, FE+2, FE+3, MG+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 and 3BaO.MgO.2SiO2.	4	(BA+2, CA+2)3(MG+2)1(SI+4)2(O-2)8
MG2B2O5	Co2B2O5		aP18	(2, P-1)	This is (Co,Fe,Mg, Ni)2B2O5	3	(CO+2, FE+2, MG+2, NI+2)2(B+3)2(O-2)5
MG2C3	Mg2C3		oP10	(58, Pnnm)		2	(MG)2(C)3
MG2HF5O12	UY6O12		hR19	(148, R-3)		3	(MG+2)2(HF+4)5(O-2)12
MG2NA2SI6O15	Na2Mg2Si6O15		oS200	(64, Cmce)		4	(MG+2)2(NA+1)2(SI+4)6(O-2)15
MG2NB34O87	Unknown Structure					3	(MG+2)2(NB+5)34(O-2)87
MG2P2O7_A	Unknown Structure				This is alpha- Mg2(P2O7).	2	(CA+2, MG+2)2(P2O7-4)1
MG2P2O7_B	Mg2[P2O7]		mP44	(14, P2_1/c)	This is beta- Mg2(P2O7) and (Co,Ni)2P2O7.	2	(CA+2, CO+2, MG+2, NI+2)2(P2O7-4)1

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MG2V2O7	Co2[V2O7]		mP44	(14, P2_1/c)	This is Co2V2O7, Mg2V2O7 and Ni2V2O7.	3	(CO+2, MG+2, NI+2)2(V+5)2(O-2)7
MG3N2_D53	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)		2	(CA, MG)3(N)2
MG3V2O8	Ni3[VO4]2		oS52	(64, Cmce)	This is Co3V2O8, Mg3V2O8 and Ni3V2O8.	3	(CO+2, MG+2, NI+2)3(V+5)2(O-2)8
MG5NB4O15	Ta3N5		oS32	(63, Cmcm)		3	(MG+2)5(NB+5)4(O-2)15
MGB4O7	CdB4O7		oP96	(61, Pbca)		3	(MG+2)1(B+3)4(O-2)7
MGC2	MgC2		tP6	(136, P4_2/mnm)		2	(MG)1(C)2
MGF2	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mnm)	This is (Co,Fe,Mg,Mn,Ni,V)F2.	2	(CO+2, FE+2, LI2+2, MG+2, MN+2, NI+2, V+2)1(F-1)2
MGNA2SI4O10	Unknown Structure					4	(MG+2)1(NA+1)2(SI+4)4(O-2)10
MGP4O11	MgP4O11		mP64	(14, P2_1/c)		3	(MG+2)1(P+5)4(O-2)11
MGWO4_TYPE	Huanzalaite (MgWO4, H06)	H06	mP12	(13, P2/c)	This is (Al,Fe)NbO4 and (Co,Fe,Mg,Mn,Ni)WO4.	3	(AL+3, CO+2, FE+2, FE+3, MG+2, MN+2, NB+5, NI+2, VA)1(NB+5, W+6)1(O-2)4
MN2B4O9	Unknown Structure					3	(MN+3)2(B+3)4(O-2)9
MN2P2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	(12, C2/m)		2	(MN+2)2(P2O7-4)1
MN2V2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	(12, C2/m)		3	(MN+2)2(V+5)2(O-2)7
MN3N2	Mn3N2		tI10	(139, I4/mmm)		2	(MN)3(N)2
MN3P2O8	Unknown Structure					2	(MN+2)3(PO4-3)2
MN4NB2O9	Nb2Mn4O9		hP30	(165, P-3c1)	This is (Co,Fe, Mg,Mn)4Nb2O9.	3	(CO+2, FE+2, MG+2, MN+2)4(NB+5)2(O-2)9

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MN5SIC	Mn5SiC		oS56	(36, Cmc2_1)		3	(MN)0.714(SI)0.143(C)0.143
MN6N5	CoO		tI4	(139, I4/mmm)		2	(MN)6(N)5
MN9SI3O14S1	Unknown Structure				This is 8MnO.3SiO2.MnS	4	(MN+2)9(SI+4)3(O-2)14(S-2)1
MNB2O4	Unknown Structure					3	(MN+2)1(B+3)2(O-2)4
MNB3O6	Unknown Structure					3	(MN+3)1(B+3)3(O-2)6
MNB4O7	Unknown Structure					3	(MN+2)1(B+3)4(O-2)7
MNB6O10	Unknown Structure					3	(MN+2)1(B+3)6(O-2)10
MNBO3	Unknown Structure					3	(MN+3)1(B+3)1(O-2)3
MNF2_S1	Unknown Structure					2	(MN+2)1(F-1)2
MNF3	MnF3		mS48	(15, C2/c)		2	(MN+3)1(F-1)3
MNYO3_HEX	LuMnO3		hP30	(185, P6_3cm)		3	(Y+3)1(MN+3)1(O-2)3
MO1S2	Molybdenite (MoS2, C7)	C7	hP6	(194, P6_3/mmc)	This is MoS2 and WS2.	2	(MO, W)1(S)2
MO2S3	Mo2S3		mP10	(11, P2_1/m)		2	(MO)2(S)3
MO4O11	Mo4O11		oP60	(33, Pna2_1)		3	(MO+4)1(MO+6)3(O-2)11
MO8O23	High-Temperature Mo8O23		mP62	(13, P2/c)		3	(MO+4)1(MO+6)7(O-2)23
MO9O26	Mo9O26		mP70	(13, P2/c)		3	(MO+4)1(MO+6)8(O-2)26
MOF4	Unknown Structure					2	(MO+4)1(F-1)4
MONOCLINIC_S	beta-S		mP48	(14, P2_1/c)		1	(S)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MOO3	gamma-WO3		mP32	(14, P2_1/c)		2	(MO+6)1(O-2)3
MULLITE	Al(Al0.7Si0.3)2O4.8		oP24	(55, Pbam)	With solubility of B, Cr and Fe.	4	(AL+3)1(AL+3, CR+3, FE+3)1(AL+3, B+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 with solubility of Fe.	3	(NA+1)2(AL+3, FE+3)12(O-2)19
NA2AL2B2O7	Na2Ga2[BO3]2O		hP30	(163, P-31c)		4	(NA+1)2(AL+3)2(B+3)2(O-2)7
NA2B4O7	Na2B4O7		aP52	(2, P-1)	This is (K, Na)2B4O7.	3	(K+1, NA+1)2(B+3)4(O-2)7
NA2B8O13	Na2B8O13		mP92	(14, P2_1/c)		3	(NA+1)2(B+3)8(O-2)13
NA2BA2SI2O7	Unknown Structure					4	(NA+1)2(BA+2)2(SI+4)2(O-2)7
NA2BA4SI10O25	Unknown Structure					4	(NA+1)2(BA+2)4(SI+4)10(O-2)25
NA2BASI2O6	Na2BaSi2O6		mP22	(4, P2_1)		4	(NA+1)2(BA+2)1(SI+4)2(O-2)6
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, NA+1)2(CO3-2)1
NA2CO3_S2	Na2[CO3]		hP12	(194, P6_ 3/mmc)	This is (K, Na)2CO3 solid solution.	2	(K+1, LI+1, NA+1)2(CO3-2, S-2)1
NA2FEO2	Unknown Structure					3	(NA+1)2(FE+2)1(O-2)2
NA2FESIO4	Unknown Structure					4	(NA+1)2(FE+2)1(SI+4)1(O-2)4

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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
NA2S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is (K,Li,Na)2S.	2	(K, LI, NA)2(S)1
NA2SI2O5_ALPHA	Na2Si2O5-a		mP36	(14, P2_1/c)	This is lt-(K, Na)2Si2O5 solid solution.	3	(K+1, LI+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, LI+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, LI+1, NA+1)2(SI+4)2(O-2)5
NA2SIO3	Na2SiO3		oS24	(36, Cmc2_1)	This is (K, Li, Na)2SiO3 solid solution.	3	(K+1, LI+1, NA+1)2(SI+4)1(O-2)3
NA2TI3O7	Na2Ti3O7		mP24	(11, P2_1/m)		3	(NA+1)2(TI+4)3(O-2)7
NA2TI6O13	Na2Ti6O13		mS42	(12, C2/m)		3	(NA+1)2(TI+4)6(O-2)13
NA2TIO3_S1	Na2TiO3		mS24	(12, C2/m)		3	(NA+1)2(TI+4)1(O-2)3
NA2TIO3_S2	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		3	(NA+1)2(TI+4)1(O-2)3
NA2V2O6	LiVO3		mS40	(9, Cc)		3	(NA+1)2(V+5)2(O-2)6
NA3ALF6_S1	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)		3	(NA+1)3(AL+3)1(F-1)6
NA3BO3	NaB3O5-a		mP108	(14, P2_1/c)	This is (K, Na)3BO3.	3	(K+1, NA+1)3(B+3)1(O-2)3
NA3FE5O9	Na3Fe5O9		mS68	(15, C2/c)		3	(NA+1)3(FE+3)5(O-2)9
NA3FEO3	Na3FeO3		mP28	(14, P2_1/c)		3	(NA+1)3(FE+3)1(O-2)3
NA3PO4	Na3[PO4]		cF988	(225, Fm-3m)	This is Na3(PO4, VO4)	2	(NA+1)3(PO4-3, VO4-3)1

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NA4B2O5	Na4B2O5		mS44	(15, C2/c)	This is (K, Na)4B2O5.	3	(K+1, NA+1)4(B+3)2(O-2)5
NA4FE6O11	Unknown Structure					3	(NA+1)4(FE+3)6(O-2)11
NA4FEO3	Na4FeO3		mS32	(9, Cc)		3	(NA+1)4(FE+2)1(O-2)3
NA4P2O7	Na4[P2O7]		oP52	(19, P2_12_12_1)		2	(NA+1)4(P2O7-4)1
NA4SIO4	K4SnO4		aP18	(2, P-1)		4	(LI2+2, NA2+2)1(LI2+2, NA2+2)1(SI+4)1(O-2)4
NA4TIO4	K4SnO4		aP18	(2, P-1)		3	(NA+1)4(TI+4)1(O-2)4
NA4V2O7	Na4[V2O7]		mS208	(15, C2/c)		3	(NA+1)4(V+5)2(O-2)7
NA5AL3F14	Chiolite (Na5Al3F14, K75)	K75	tP44	(128, P4/mnc)		3	(NA+1)5(AL+3)3(F-1)14
NA5FEO4	Na5GaO4		oP80	(61, Pbca)		3	(NA+1)5(FE+3)1(O-2)4
NA5FESI4O12	Unknown Structure					4	(NA+1)5(FE+3)1(SI+4)4(O-2)12
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	(LI+1, NA+1)6(SI+4)8(O-2)19
NA8FE2O7	Na8Ga2O7		mP68	(14, P2_1/c)		3	(NA+1)8(FE+3)2(O-2)7
NA8FE6SI15O40	Unknown Structure					4	(NA+1)8(FE+2)6(SI+4)15(O-2)40
NA8TI5O14	Na8Ti5O14		aP54	(2, P-1)		3	(NA+1)8(TI+4)5(O-2)14
NAAL11O17	NaAl11O17		hP58	(194, P6_3/mmc)	This is Beta-Al2O3 (Li,Na)Al11O17 solid solution.	5	(LI+1, NA+1)2(NA+1, VA)2(AL+3)22(O-2)34(O-2, VA)1
NAALO2_D	LiGaO2		oP16	(33, Pna2_1)		2	(NAAL+4, SI+4)1(O-2)2

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NAB3O5	NaB3O5-a		mP108	(14, P2_1/c)	This is (K, Na)B3O5.	3	(K+1, NA+1)1(B+3)3(O-2)5
NAB5O8_A	Unknown Structure					3	(NA+1)1(B+3)5(O-2)8
NAB5O8_B	Unknown Structure					3	(NA+1)1(B+3)5(O-2)8
NAB5O8_G	KB5O8-a		oP112	(61, Pbca)	This is ht-NaB5O8 and KB5O8.	3	(K+1, NA+1)1(B+3)5(O-2)8
NAB9O14_A	Unknown Structure					3	(NA+1)1(B+3)9(O-2)14
NAB9O14_B	Unknown Structure					3	(NA+1)1(B+3)9(O-2)14
NAB9O14_G	Unknown Structure					3	(NA+1)1(B+3)9(O-2)14
NABO2_A	KBO2 (F513)	F513	hR24	(167, R-3c)	This is ht-NaBO2 and KBO2.	3	(K+1, NA+1)1(B+3)1(O-2)2
NABO2_B	Unknown Structure				rt-NaBO2	3	(NA+1)1(B+3)1(O-2)2
NAF1	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is (K,Li,Na)F.	2	(K+1, LI+1, MG+2, NA+1, VA)1(F-1)1
NAFE2O3	NaFe2O3		hP6	(164, P-3m1)		4	(NA+1)1(FE+2)1(FE+3)1(O-2)3
NAFEO2_A	Caswellsilverite (CrNaS2, F51)	F51	hR4	(166, R-3m)	This is also NaCrO2.	3	(NA+1)1(CR+3, FE+3)1(O-2)2
NAFEO2_B	LiGaO2		oP16	(33, Pna2_1)	This is low-temp K(Al,Fe)O2 + NaAlO2 and mid-temp NaFeO2 solid solutions.	2	(KAL+4, KFE+4, NAAL+4, NAFE+4, SI+4)1 (O-2)2
NAFEO2_G	LiAlO2		tP16	(92, P4_12_ 12)	This is high-temp K(Al,Fe)O2, LiAlO2 + NaFeO2 and mid-temp NaAlO2 solid solutions.	2	(KAL+4, KFE+4, LIAL+4, NAAL+4, NAFE+4, SI+4)1(O-2)2
NAFESI2O6	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)		4	(NA+1)1(FE+3)1(SI+4)2(O-2)6
NAMGF3	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)		3	(NA+1)1(MG+2)1(F-1)3
NANO3_S1	Calcite (CaCO3, G01)	G01	hR10	(167, R-3c)	With solubility of K.	2	(K+1, NA+1)1(NO3-1)1

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NANO3_S2	Rb[NO3]		hR9	(166, R-3m)	This is ht-(K, Na)(NO3) solid solution.	2	(K+1, NA+1)1(NO3-1)1
NAPO3	NaAsO3		aP30	(2, P-1)		2	(NA+1)1(PO3-1)1
NAS2	NaS2		tI48	(122, I-42d)		2	(NA)1(S)2
NB2O5	Nb2O5		mP99	(10, P2/m)		2	(MG+2, NB+5, V+5, ZR+4)2(O-2, VA)5
NB3BO9	Unknown Structure					3	(NB+5)3(B+3)1(O-2)9
NBF5	MoF5		mS48	(12, C2/m)		2	(NB+5)1(F-1)5
NBO1	NbO		cP6	(221, Pm-3m)		2	(NB+2)1(O-2)1
NBO2	alpha-NbO2		tI96	(88, I4_1/a)	This is NbO2	2	(FE+2, NB+4, NB+5)1(O-2)2
NEPHELINE_A	Unknown Structure				This is NaAlSiO4 with solubility of Si.	4	(NAAL+4)4(NAAL+4, SI+4)4(SI+4)8(O-2)32
NEPHELINE_B	Unknown Structure				This is NaAlSiO4 with solubility of Si.	4	(NAAL+4)4(NAAL+4, SI+4)4(SI+4)8(O-2)32
NEPHELINE_G	KLi[SO4]		hP18	(173, P6_3)	This is low temperature NaAlSiO4-KAlSiO4, K2MgSi3O8 dissolving SiO2, Fe.	4	(K2MG+4, KAL+4, NAAL+4)4(KAL+4, NAAL+4, NAFE+4, SI+4)4(SI+4)8(O-2)32
NI3B2O6	Kotoite (Mg3(BO3)2)		oP22	(58, Pnnm)	This is (Co,Mg,Ni)3B2O6	3	(CO+2, MG+2, NI+2)3(B+3)2(O-2)6
NI3S2_LT	Hazelwoodite (Ni3S2, D5e)	D5e	hR5	(155, R32)		2	(NI)3(S)2
NI4NB2O9	Nb2Ni4O9		oF480	(43, Fdd2)		3	(NI+2)4(NB+5)2(O-2)9
NI6MNO8_TYPE	Mg6MnO8		cF60	(225, Fm-3m)	This is (Mg, Ni)6MnO8, with an ordered NaCl-type structure.	3	(MG+2, NI+2)6(MN+4)1(O-2)8
NI7S6	Unknown Structure		t**			2	(FE, NI)7(S)6
NI9S8	Ni9S8		oS68	(21, C222)		2	(FE, NI)9(S)8
NIMNO3	Ilmenite (FeTiO3, E22)	E22	hR10	(148, R-3)	This is NiMnO3 with Ilmenite structure	2	(MN+3, MN+4, NI+2)2(O-2)3

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NINB14O36	Unknown Structure					3	(NI+2)1(NB+5)14(O-2)36
NINB2O6	Columbite (FeNb2O6, E51)	E51	oP36	(60, Pbcn)		3	(NB+5, NI+2, VA)1(NB+5, NI+2)2(O-2, VA)6
NINB36O91	Unknown Structure					3	(NI+2)1(NB+5)36(O-2)91
NINB68O171	Unknown Structure					3	(NI+2)1(NB+5)68(O-2)171
NIOCALITE_C10NS6	Niocalite		oS114	(21, C222)	This is 10CaO.Nb2O5.6SiO2.	4	(CA+2)10(NB+5)2(SI+4)6(O-2)27
NIS_LT	Millerite (NiS, B13)	B13	hR6	(160, R3m)	This is low temperature NiS.	2	(NI)1(S)1
OKAYAMALITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_ 1m)		4	(CA+2)2(B+3)2(SI+4)1(O-2)7
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	oP28	(62, Pnma)	This is Calcio-olivine (Ca2SiO4) - Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephroite (Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4) solid solution dissolving Cr and Cu.	4	(CA+2, CO+2, CR+2, CU+2, FE+2, LI2+2, MG+2, MN+2, NI+2)1(CA+2, CO+2, CR+2, CU+2, FE+2, LI2+2, MG+2, MN+2, NI+2)1 (SI+4)1(O-2)4
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	(70, Fddd)		1	(S)1
ORTHO_PYROXENE	Enstatite (MgSiO3, S43)	S43	oP80	(61, Pbca)	This is enstatite (MgSiO3) and ortho-diopside (CaMgSi2O6) with Fe solubility.	4	(CA+2, FE+2, MG+2)1(FE+2, MG+2)1 (SI+4)2(O-2)6
P2O5_H	P2O5		hR28	(161, R3c)		2	(P+5)2(O-2)5
P2O5_OO	P2O5		oP56	(43, Fdd2)		2	(P+5)2(O-2)5
P2O5_OP	P2O5		oP28	(62, Pnma)		2	(P+5)2(O-2)5
P2S5	P2S5		aP28	(2, P-1)		2	(P)2(S)5
PENTLANDITE	Co9S8 (D89)	D89	cF68	(225, Fm-3m)		3	(FE, NI)8(FE, NI)1(S)8
PEROVSKITE	PrNiO3		hR10	(167, R-3c)	This is (Cr,Fe, Mn)LaO3. Also includes	3	(LA+3, MN+3, VA)1(CO+3, CR+3, CR+4,

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					(Cr,Fe,Mn)LaO3 O-Perovskite.		FE+2, FE+3, FE+4, MN+2, MN+3, MN+4, VA)1(O-2, VA)3
PI_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		3	(CR)12.8(FE, NI, SI)7.2(N)4
PROTO_PYROXENE	MgSiO3		oP40	(60, Pbcn)	This is proto- enstatite (MgSiO3) and proto-diopside (CaMgSi2O6) dissolving Co, Cr, and Fe.	3	(CA+2, CO+2, CR+2, FE+2, MG+2, NI+2)1 (SI+4)1(O-2)3
PSEUDO_BROOKITE	Pseudobrookite (Fe2TiO5, E41)	E41	oS32	(63, Cmcm)	This is Fe2TiO5, Ti3O5, Al2TiO5 and (Co,Fe,Mg,Mn)Ti2O5.	3	(AL+3, CO+2, FE+2, FE+3, MG+2, MN+2, NI+2, SI+4, TI+3, TI+4, V+3)1(AL+3, FE+3, SI+4, TI+3, TI+4)2(O-2)5
PSEUDO_ WOLLASTONITE	CaSiO3		mS120	(15, C2/c)	This is CaO.SiO2 with Ba solubility	3	(BA+2, CA+2)1(SI+4)1(O-2)3
PYRITE	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)	This is Cattierite (CoS2), Pyrite (FeS2) - Hauerite (MnS2) - Vaesite (NiS2).	2	(CO, FE, MN, NI)1(S)2
PYROCHLORE	Cubic Pyrochlore (Eu2Ir2O7, E81)	E81	cF88	(227, Fd-3m)	This is (Gd,La)2(Hf,Zr)2O7 and (Gd,La,Y,Yb)2Ti2O7.	5	(GD+3, HF+4, LA+3, TI+4, Y+3, YB+3, ZR+4)2(GD+3, HF+4, LA+3, TI+4, Y+3, YB+3, ZR+4)2(O-2, VA)6(O-2)1(O-2, VA)1
PYRRHOTITE	NiAs (B81)	B81	hP4	(194, P6_ 3/mmc)	This is (Co,Cr, Fe,Nb,Ni,Ti,V)S.	2	(AL, CO, CR, CU, FE, GD, MG, MN, NB, NI, TI, V, VA, ZR)1(S)1
QUARTZ	alpha-Quartz (low Quartz)		hP9	(152, P3_121)	SiO2 with AlPO4 solubility.	2	(AL+3, SI+4)1(PO4-3, SIO4-4)1
Q_ALMGZRO	Unknown Structure					4	(MG+2)4.68(AL+3)2.64(ZR+4)1.68(O-2)12
RANKINITE	3CaO.2SiO2		mP48	(14, P2_1/c)		3	(CA+2)3(SI+4)2(O-2)7
RED_P	Unknown Structure				This is pure phosphorus.	1	(P)1
RHODONITE	Rhodonite (MnSiO3-b)		aP50	(2, P-1)	This is MnO.SiO2	3	(CA+2, CO+2, FE+2, MG+2, MN+2)1 (SI+4)1(O-2)3
RUTILE	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)	This is MnO2, TiO2 and ht-VO2.	2	(AL+3, HF+4, MN+4, TI+3, TI+4, V+4, ZR+4)1(O-2, VA)2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SAPPHIRINE	CaMg3Si3O10		aP68	(2, P-1)	This is 9Al2O3.7MgO.3SiO2	4	(AL+3)18(MG+2)7(SI+4)3(O-2)40
SI3N4	Nierite (alpha-Si3N4)		hP28	(159, P31c)		2	(SI)3(N)4
SI3P4O16	Unknown Structure					2	(SI+4)3(PO4-3)4
SIC_B3	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(SI)1(C)1
SILLIMANITE	Sillimanite (Al2SiO5, S03)	S03	oP32	(62, Pnma)	This is a high-pressure phase	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
SIP2O7_CUB	Si[P2O7]		cP1080	(205, Pa-3)	This is cubic (Si, Ti)P2O7.	2	(SI+4, TI+4)1(P2O7-4)1
SIP2O7_MONO	Si[P2O7]-a		mP40	(14, P2_1/c)		2	(SI+4)1(P2O7-4)1
SIP2O7_TETR	Unknown Structure					2	(SI+4)1(P2O7-4)1
SIS2	SiS2 (C42)	C42	oI12	(72, Ibam)		2	(SI)1(S)2
SPHENE	CaTi[SiO4]O		mP32	(14, P2_1/c)		4	(CA+2)1(TI+4)1(SI+4)1(O-2)5
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)	This is MgAl2O4, Fe3O4, Mn3O4 (ht) and many more.	4	(AL+3, CO+2, CO+3, CR+2, CR+3, CU+2, FE+2, FE+3, LI+1, MG+2, MN+2, NI+2)1 (AL+3, CA+2, CO+2, CO+3, CR+3, CU+2, FE+2, FE+3, LI+1, MG+2, MN+2, MN+3, MN+4, MO+4, NA+1, NI+2, TI+3, TI+4, V+3, VA)2(CR+2, FE+2, MG+2, MN+2, VA)2(O-2)4
THIOSPINEL	Spinel (Co3O4, D72)	D72	cF56	(227, Fd-3m)	This is a sulphur spinel: (Cu,Fe,Mn)Cr2S4, Co3S4, FeNi2S4 and Ni3S4.	3	(CO, CU, FE, MN, NI)1(CO, CR, NI)2(S)4
TI10O19	Unknown Structure					2	(TI)10(O)19
TI20O39	Ti20O39		aP118	(2, P-1)		2	(TI)20(O)39
TI2NB10O29	(Ti0.17Nb0.83)12O29		mS82	(12, C2/m)		3	(TI+4)2(NB+5)10(O-2)29
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)		2	(TI)2(C, N)1

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TI2S	Ta2P		oP36	(58, Pnnm)		2	(TI)2(S)1
TI3O2	(Ti3O2)		hP5	(191, P6/mmm)		3	(TI+2)2(TI)1(O-2)2
TI4C2S2	AlCCr2		hP8	(194, P6_ 3/mmc)		3	(TI)4(C)2(S)2
TI5O9	Ti5O9		aP28	(2, P-1)	Ti5O9 with solubility of V.	2	(TI, V)5(O)9
TI5P6O25	Unknown Structure					3	(TI+4)5(P+5)6(O-2)25
TI8S10	Ti0.81S		hP20	(194, P6_ 3/mmc)		2	(TI)8(S)10
TI8S3	Ti8S3		mS88	(12, C2/m)		2	(TI)8(S)3
TI8S9	TiS		hR18	(166, R-3m)		2	(TI)8(S)9
TI9O17	Ti9O17		aP52	(2, P-1)		2	(TI)9(O)17
TINB24O62	(Ti0.04Nb0.96)25O62		mS174	(5, C2)		3	(TI+4)1(NB+5)24(O-2)62
TINB2O7	(Ti0.33Nb0.67)3O7		mS60	(12, C2/m)		3	(TI+4)1(NB+5)2(O-2)7
TIO_ALPHA	alpha-TiO		mS20	(12, C2/m)		2	(TI+2)1(O-2)1
TIS2	CdI2		hP3	(164, P-3m1)		2	(TI)1(S)2
TIS3	ZrSe3		mP8	(11, P2_1/m)		2	(TI)1(S)3
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	(9, Cc)	SiO2 with AlPO4 solubility.	2	(AL+3, SI+4)1(PO4-3, SIO4-4)1
V2O5	Shcherbinaite (V2O5) (Revised)		oP14	(59, Pmmn)		2	(V+5)2(O-2)5
V2O_SS	V7O3		mS20	(12, C2/m)		2	(V)1(O, VA)0.5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
V3O5_HT	V3O5-ht		mS32	(15, C2/c)	This is ht-V3O5 with solubility of Al, Cr, Mg, Mn and Ti.	2	(AL, CR, MG, MN, TI, V)3(O)5
V3O5_LT	V3O5-lt		mP32	(13, P2/c)		2	(V)3(O)5
V3O7	V3O7		mS120	(15, C2/c)		2	(V)3(O)7
V52O64	V13O16		tI116	(141, I4_ 1/amd)		2	(V)52(O)64
V5O9	Ti5O9		aP28	(2, P-1)	V5O9 with solubility of Ti.	2	(TI, V)5(O)9
V6O13	V6O13		mS38	(12, C2/m)		2	(V)6(O)13
VO2_LT	VO2		mP12	(14, P2_1/c)	This is lt-VO2, MoO2 and WO2.	2	(MO+4, V+4, W+4)1(O-2)2
WHITE_P	Unknown Structure				This is pure phosphorus. Not stable at normal conditions.	1	(P)1
WO2_72	Unknown Structure					1	(O2_72W1)1
WO2_90	Unknown Structure					1	(O2_90W1)1
WO2_96	Unknown Structure					1	(O2_96W1)1
WO3_HT	WO2.95		tP16	(113, P-42_ 1m)		2	(W+6)1(O-2)3
WO3_LT	WO3		oP32	(60, Pbcn)		2	(W+6)1(O-2)3
WOLLASTONITE	Wollastonite (CaSiO3)		aP30	(2, P-1)	This is CaO.SiO2 with Ba, Fe, Mg and Mn solubility	3	(BA+2, CA+2, FE+2, MG+2, MN+2)1(SI+4)1 (O-2)3
Y15C19_ALPHA	alpha-Y15C19		oP18	(55, Pbam)		2	(C)19(Y)15
Y15C19_BETA	Unknown Structure					2	(C)19(Y)15
Y2C3_ALPHA	Sc3C4		tP70	(128, P4/mnc)		3	(Y)2(C)2(C, VA)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
Y2C3_BETA	Unknown Structure					3	(Y)2(C)2(C, VA)1
Y2S2A_Y2SI2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	(12, C2/m)	Y2Si2O7	3	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2B_Y2SI2O7	La4Ge3[GeO4]O10		aP44	(2, P-1)	(Y,Yb)2Si2O7 solid solution.	2	(Y+3, YB+3)2(SI2O7-6)1
Y2S2D_Y2SI2O7	Possible delta-Y2Si2O7		oP44	(62, Pnma)	Y2Si2O7 with Yb solubility.	2	(Y+3, YB+3)2(SI2O7-6)1
Y2S2G_Y2SI2O7	Y2Si2O7-b		mP22	(14, P2_1/c)	Y2Si2O7-b with Yb solubility.	2	(Y+3, YB+3)2(SI2O7-6)1
Y2SIO5	Y2SiO5 (RE2SiO5 X2)		mS64	(15, C2/c)	This is (Y,Yb)2SiO5	3	(Y+3, YB+3)2(SIO4-4)1(O-2)1
Y2TIO5	La2TiO5		oP32	(62, Pnma)	This is (Gd,La, Y)2TiO5	3	(GD+3, LA+3, Y+3)2(TI+4)1(O-2)5
Y3NBO7	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		3	(NB+5, VA, Y+3)3(NB+5, Y+3)1(O-2, VA)7
YAM	Y4Al2O9		mP60	(14, P2_1/c)	This is Y4Al2O9, Gd4Al2O9 and Ca2Y2Si2O9 (Cuspidine)	4	(AL+3, SI+4)2(CA+2, GD+3, LA+3, Y+3, YB+3)4(O-2, VA)1(O-2)9
YAP	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)	This is Y(Al,Co,Cr,Fe)O3, YbFeO3 and Gd (Al,Co,Cr,Fe)O3.	3	(AL+3, CO+3, CR+3, FE+3, MN+3)1(CA+2, GD+3, LA+3, Y+3, YB+3)1(O-2, VA)3
YB2TIO5	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		3	(YB+3)2(TI+4)1(O-2)5
YB6HFO11	Unknown Structure				Yb6HfO11 solid solution	4	(HF+4, YB+3)2(YB+3)6(O-2)12(O-2, VA)1
YBO3	Unknown Structure				This is (Y, Yb)BO3 solid solution.	3	(Y+3, YB+3)1(B+3)1(O-2)3
YC_B1	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		2	(Y)1(C, C2, VA)1
YNBO4	LaNbO4		mS24	(15, C2/c)		3	(NB+5, VA, Y+3)1(NB+5, Y+3)1(O-2, VA)4
ZIRCON	Zircon (ZrSiO4, S11)	S11	tI24	(141, I4_1/amd)	This is HfSiO4, ZrSiO4, GdPO4, LaPO4 and YPO4.	3	(P+5, SI+4)1(GD+3, HF+4, LA+3, Y+3, ZR+4)1(O-2, VA)4
ZR11NB4O32	Unknown Structure					3	(ZR+4)11(NB+5)4(O-2)32

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZR13NB4O36	Unknown Structure					3	(ZR+4)13(NB+5)4(O-2)36
ZR15NB4O40	Unknown Structure					3	(ZR+4)15(NB+5)4(O-2)40
ZR2P2O9	Zr2[PO4]2O		mS52	(12, C2/m)		3	(ZR+4)2(P+5)2(O-2)9
ZR3Y4O12	UY6O12		hR19	(148, R-3)	Zr3(Y,Yb)4O12 and Hf3Yb4O12.	3	(HF+4, ZR+4)3(Y+3, YB+3)4(O-2)12
ZR5NB2O15	Unknown Structure					3	(ZR+4)5(NB+5)2(O-2)15
ZR6NB2O17	Nb2Zr6O17		oI100	(46, Ima2)		3	(ZR+4)6(NB+5)2(O-2)17
ZR7NB2O19	Unknown Structure					3	(ZR+4)7(NB+5)2(O-2)19
ZR8NB2O21	Unknown Structure					3	(ZR+4)8(NB+5)2(O-2)21
ZRF4	ZrF4		mS60	(15, C2/c)	This is (Hf,Zr)F4.	2	(HF+4, ZR+4)1(F-1)4
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	(14, P2_1/c)	This is Monoclinic HfO2 and ZrO2	2	(AL+3, CA+2, CR+3, GD+3, HF+4, LA+3, TI+4, Y+3, YB+3, ZR+4)2(O-2, VA)4
ZRO2_TETR	HgI2 (C13)	C13	tP6	(137, P4_ 2/nmc)	This is Tetragonal HfO2 and ZrO2	2	(AL+3, BA+2, CA+2, CR+3, FE+2, GD+3, HF+4, LA+3, MG+2, MN+2, MN+3, NB+5, NI+2, TI+4, VA, Y+3, YB+3, ZR+4)2(O-2, VA)4
ZRO8S2	Zr[SO4]2		oP44	(62, Pnma)		2	(ZR+4)1(SO4-2)2
ZRS2	CdI2		hP3	(164, P-3m1)		2	(ZR)1(S)2
ZRTI2O6	Columbite (FeNb2O6, E51)	E51	oP36	(60, Pbcn)		3	(ZR+4)1(TI+4)2(O-2)6
ZRTIO4_ALPHA	Unknown Structure					3	(ZR+4)1(TI+4)1(O-2)4
ZRTIO4_BETA	zeta-Fe2N		oP12	(60, Pbcn)	This is (Hf, Zr)TiO4 solid solution with Al solubility.	3	(AL+3, HF+4, TI+4, ZR+4)2(AL+3, VA)1(O-2)4
Z_PHASE	CrNbN		tP6	(129, P4/nmm)		3	(CR, FE)1(MO, NB, V)1(N, VA)1

Gas and IONIC_LIQ Phase

Name	Prototype	Note	Sublattices	Formula Unit
GAS	Gas		1	(AL, AL1B1O2, AL1B3H12, AL1C1, AL1C2, AL1CU1, AL1CU1S1, AL1CU1S2, AL1F1, AL1F1H1, AL1F1H1O1, AL1F1H2, AL1F1H2O2, AL1F1O1, AL1F2, AL1F2H1, AL1F2H1O1, AL1F2NA1O1, AL1F2O1, AL1F3, AL1F4K1, AL1F4LI1, AL1F4NA1, AL1H1, AL1H1O1_ALOH, AL1H1O1_HALO, AL1H1O2, AL1H2, AL1H2O2, AL1H3, AL1H3O3, AL1N1, AL1O1, AL1O2, AL1P1, AL1P2, AL1S1, AL1S2, AL2, AL2C2, AL2C6H18, AL2F6, AL2F8NA2, AL2O1, AL2O2, AL2O3, AL2S1, AL2S2, AR, B, B10H14, B1BA1O2, B1C1, B1C1H3O1, B1C2, B1C2H7O2, B1C3H9, B1C3H9O3, B1C6H15, B1F1, B1F1H1, B1F1H1O1, B1F1H2, B1F1H2O2, B1F1O1, B1F2, B1F2H1, B1F2H1O1, B1F2O1, B1F3, B1F4K1, B1H1, B1H1O1_BOH, B1H1O1_HBO, B1H1O2, B1H1S1, B1H2, B1H2O1, B1H2O2, B1H3, B1H3O1, B1H3O2, B1H3O3, B1H6N1, B1K1O2, B1LI1O2, B1N1, B1NA1O2, B1O1, B1O2, B1S1, B1S2, B2, B2C1, B2F4, B2F4O1, B2H4O4, B2H6, B2O1, B2O2, B2O3, B2S1, B2S2, B2S3, B3F1H2O3, B3F2H1O3, B3F3O3, B3H3O3, B3H3O6, B3H6N3, B4S6, B5H9, BA, BA1F1, BA1F1H1O1, BA1F2, BA1H1, BA1H1O1, BA1H2O2, BA1MO1O4, BA1O1, BA1S1, BA2, BA2O1, BA2O2, C, C1F1, C1F1H1, C1F1H1O1, C1F1H2, C1F1H3, C1F1H4P1, C1F1N1, C1F1O1, C1F2, C1F2H1, C1F2H2, C1F2H3O1P1_1, C1F2H3O1P1_2, C1F2H3O1P1S1_O, C1F2H3O2P1, C1F2H3P1, C1F2H3P1S1_1, C1F2H3P1S1_2, C1F2N1P1, C1F2O1, C1F3, C1F3H1, C1F3H3SI1, C1F4, C1F4O1, C1F8S1, C1H1, C1H1N1_HCN, C1H1N1_HNC, C1H1N1O1, C1H1N1S1, C1H1O1, C1H1O2, C1H1P1, C1H1SI1_1, C1H1SI1_2, C1H2, C1H2N4, C1H2O1, C1H2O2_CIS, C1H2O2_DIOXIRANE, C1H2O2_TRANS, C1H2SI1_1, C1H2SI1_2, C1H3, C1H3O1_CH2OH, C1H3O1_CH3O, C1H3P1, C1H3SI1_1, C1H3SI1_2, C1H3SI1_3, C1H3SI1_4, C1H4, C1H4N2O1, C1H4O1, C1H4S1, C1H4SI1_1, C1H4SI1_2, C1H4SI1_3, C1H5N1, C1H5O1P1, C1H5O3P1, C1H5P1, C1H5P1S1, C1H5SI1_1, C1H5SI1_2, C1H6N1P1_N, C1H6N1P1_P, C1H6P2, C1H6SI1, C1K1N1, C1K2O3, C1N1, C1N1NA1, C1N1O1, C1N1O1_NCO, C1N2_CNN, C1N2_NCN, C1O1, C1O1S1, C1O2, C1P1, C1P1SI1, C1P1SI2, C1P2, C1S1, C1S2, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2F1, C2F1H1, C2F1H3, C2F1H5, C2F1H6P1, C2F2, C2F2H2_1_1C2H2F2, C2F2H2_CIS, C2F2H2_TRANS, C2F2H4, C2F2H6N1P1, C2F3, C2F3H1, C2F3H3, C2F3N1, C2F4, C2F4H2, C2F5, C2F5H1, C2F6, C2H1, C2H10SI2, C2H1N1, C2H1SI1, C2H2, C2H2O1, C2H2SI1, C2H3, C2H3SI1_1, C2H3SI1_2, C2H4, C2H4O1_ACETALDEHYDE, C2H4O1_OXIRANE, C2H4O2_ACETICACID, C2H4O2_DIOXETANE, C2H4O3_123TRIOXOLANE, C2H4O3_124TRIOXOLANE, C2H4SI1_1, C2H4SI1_2, C2H5, C2H5SI1, C2H6, C2H6O1_1, C2H6O1_2, C2H6O1SI1, C2H6O2, C2H6SI1_1, C2H6SI1_2, C2H6SI1_3, C2H7O1P1, C2H7O3P1, C2H7P1_1, C2H7P1_2, C2H7P1S1, C2H7SI1_1, C2H7SI1_2, C2H8N1P1_N, C2H8N1P1_P, C2H8SI1, C2H8SI1_2, C2K2N2, C2N1_CCN, C2N1_CNC, C2N2, C2N2NA2, C2O1, C2P1, C2P2, C2SI1, C2SI2, C2SI3, C3, C3H1, C3H10SI1, C3H1N1, C3H4_1, C3H4_2, C3H6_1, C3H6_2, C3H6O1_1, C3H6O1_2, C3H8, C3H8SI1, C3H9SI1_1, C3H9SI1_2, C3N1, C3O2, C4, C4H1, C4H10_1, C4H10_2, C4H11SI1, C4H12SI1_1, C4H12SI1_2, C4H2_1, C4H2_2, C4H4_1, C4H4_2, C4H6_1, C4H6_2, C4H6_3, C4H6_4, C4H6_5, C4H8_1, C4H8_2, C4H8_3, C4H8_4, C4H8_5, C4H8_6, C4N1, C4N2, C4NI1O4, C5, C5FE1O5, C5H1N1, C5N1, C60, C6H6, C6H6O1, C6MO1O6, C6N1, C6N2, C9N1, CA, CA1F1, CA1F1H1O1, CA1F2, CA1H1, CA1H1O1, CA1H2O2, CA1O1, CA1S1, CA2, CO, CO1F1, CO1F2, CO1F3, CO1H1, CO1H1O1, CO1H2O2, CO1O1, CO1S1, CO2, CO2F4, CR, CR1F1, CR1F1O1, CR1F1O2, CR1F2, CR1F2O1, CR1F2O2, CR1F3, CR1F3O1, CR1F4, CR1F4O1, CR1F5, CR1F6, CR1H1, CR1H1O1, CR1H1O2, CR1H1O3, CR1H2O2, CR1H2O3, CR1H2O4, CR1H3O3, CR1H3O4, CR1H4O4, CR1H4O5, CR1N1, CR1O1, CR1O2, CR1O3, CR1S1, CR1S2, CR2, CR2O1, CR2O2, CR2O3, CU, CU1F1, CU1F2, CU1H1, CU1H1O1, CU1O1, CU1S1, CU2, CU2F2, CU2F4, CU2S1, CU3F3, CU4F4, F, F10MO2, F10S2, F15MO3, F1FE1, F1H1, F1H1N1, F1H1O1, F1H1O3S1, F1H1SI1, F1H2N1, F1H3SI1, F1K1, F1LI1, F1LI1O1, F1MG1, F1MN1, F1MN1O3, F1MO1, F1MO1O1, F1MO1O2, F1N1, F1N1O1, F1N1O2, F1N1O3, F1NA1, F1NI1, F1O1, F1O1S1, F1O1TI1, F1O1W1, F1O2_1, F1O2_2, F1O2_OFO, F1O2W1, F1P1, F1P1S1, F1S1, F1SI1, F1TI1, F1W1, F1Y1, F1YB1, F1ZR1, F2, F2FE1, F2H1N1, F2H2, F2H2SI1, F2K2, F2LI2, F2MG1, F2MN1, F2MO1, F2MO1O1, F2MO1O2, F2N1, F2N2_CIS, F2N2_TRANS, F2NA2, F2NI1, F2O1, F2O1S1, F2O1SI1, F2O1TI1, F2O1W1, F2O2, F2O2_FOOF, F2O2S1, F2O2W1, F2P1, F2S1, F2S2_FSSF, F2S2_SSF2, F2SI1, F2TI1, F2V1, F2W1, F2ZR1, F3FE1, F3GD1, F3H1SI1, F3H3, F3LA1, F3LI3, F3MN1, F3MO1, F3MO1O1, F3N1, F3N1O1, F3NA3, F3NB1O1, F3NI1, F3O1P1, F3O1V1, F3O1W1, F3P1, F3P1S1, F3S1, F3SI1, F3TI1, F3V1, F3W1, F3Y1, F3YB1, F3ZR1, F4FE2, F4H4, F4HF1, F4MG2, F4MN1, F4MO1, F4MO1O1, F4N2_GAUCH, F4N2_TRANS, F4NI2, F4O1S1, F4O1W1, F4S1, F4SI1, F4TI1, F4V1, F4W1, F4ZR1, F5H5, F5MO1, F5NB1, F5P1, F5S1, F5V1, F5W1, F6FE2, F6H6, F6MO1, F6S1, F6W1, F7H7, FE, FE1H1, FE1H1O1, FE1H1O2, FE1H2O2, FE1O1, FE1O2, FE1S1, FE2, GD, GD1O1, GD1S1, H, H1K1, H1K1O1, H1LI1, H1LI1O1, H1MG1, H1MG1O1, H1MN1, H1MN1O1, H1MO1O1, H1MO1O2, H1MO3, H1N1, H1N1O1, H1N1O2_CIS, H1N1O2_TRANS, H1N1O3, H1N3, H1NA1, H1NA1O1, H1NI1, H1NI1O1, H1O1, H1O1P1, H1O1S1_HSO, H1O1S1_SOH, H1O1W1, H1O2, H1O2W1, H1P1, H1S1, H1SI1, H1YB1, H1ZR1, H2, H2K2O2, H2LI2O2, H2MG1O2, H2MO1O2, H2MO1O3, H2MO1O4, H2N1, H2N2_1_1N2H2, H2N2_CIS, H2N2_TRANS, H2N2O2, H2NA2O2, H2NI1O2, H2O1, H2O1S1_H2SO, H2O1S1_HSOH, H2O2, H2O2W1, H2O3SI1, H2O3W1, H2O4S1, H2O4W1, H2P1, H2S1, H2S2, H2SI1, H3N1, H3N1O1, H3P1, H3SI1, H4N2, H4O4SI1, H4SI1, H6SI2, HF, HF1O1, HF1O2, K, K1LI1, K1N1O2, K1N1O3, K1NA1, K1O1, K1S1, K2, K2O1, K2O2, K2O4S1, K2S1, LA, LA1O1, LA1S1, LA2O1, LA2O2, LI, LI1N1, LI1N1O1, LI1N1O2, LI1N1O3, LI1NA1, LI1NA1O1, LI1O1, LI2, LI2O1, LI2O2, LI2O4S1, MG, MG1N1, MG1O1, MG1S1, MG2, MN, MN1O1, MN1O2, MN1S1, MO, MO1N1, MO1O1, MO1O2, MO1O3, MO1S1, MO1S2, MO2, MO2O6, MO3O9, MO4O12, MO5O15, N, N1NA1O2, N1NA1O3, N1NB1, N1O1, N1O2, N1O3, N1P1, N1S1, N1SI1, N1SI2, N1TI1, N1V1, N1ZR1, N2, N2O1, N2O2, N2O3, N2O4, N2O5, N3, NA, NA1O1, NA2, NA2O1, NA2O2, NA2O4S1, NB, NB1O1, NB1O2, NB1S1, NI, NI1O1, NI1S1, NI2, O, O10P4, O10V4, O12W4, O15W5, O1P1, O1S1, O1S2, O1SI1, O1TI1, O1V1, O1W1, O1Y1, O1Y2, O1YB1, O1ZR1, O2, O2P1, O2S1, O2SI1, O2SI2, O2TI1, O2V1, O2W1, O2Y1, O2Y2, O2ZR1, O3, O3P2, O3S1, O3W1, O4P2, O5P2, O6P3, O6P4, O6W2, O7P4, O8P4, O8W3, O9P4, O9W3, P, P1S1, P1SI1, P1SI2, P2, P2SI2, P3, P4, P4S3, S, S1SI1, S1TI1, S1V1, S1W1, S1Y1, S1YB1, S1ZR1, S2, S2SI1, S2TI1, S2W1, S2ZR1, S3, S4, S5, S6, S7, S8, SI, SI2, SI3, TI, TI2, V, W, Y, YB, ZR, ZR2)1

Name	*Prototype*	*Note*	*Sublattices*	*Formula Unit*
IONIC_LIQ	Liquid	Liquid metal and slag mixture	2	(AL+3, BA+2, CA+2, CO+2, CR+2, CU+1, FE+2, GD+3, HF+4, K+1, LA+3, LI+1, MG+2, MN+2, MO+4, NA+1, NB+2, NI+2, P+5, SI+4, TI+2, V+2, W+6, Y+3, YB+3, ZR+4)P (ALN, ALO2-1, B, BO3-3, BO3/2, C, C3S2Z_1/6, CO3-2, COF3, COO3/2, CRF3, CRO3/2, CUF2, CUO, F-1, FEF3, FEO3/2, M3S2Z_1/6, MNO3/2, MOO3, N, NBF5, NBO5/2, NO3-1, O-2, PO4-3, PO5/2, S, S-2, SIO2, SIO4-4, TIO2, TIO3/2, VA, VO2, VO3/2, VO5/2)Q

TCOX: TCS Metal Oxide Solutions Database Revision History

Current Database Version

Database name (acronym):	**TCS Metal Oxide Solutions Database (TCOX)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**14.0**
First release:	**TCOX was released in 1992 under the name ION**

Changes in the Most Recent Database Release

TCOX13 to TCOX14

Software release version 2025a (January 2025)

New Elements and Phases

- Two new elements: Barium (Ba) and Lithium (Li) (for a total of 34 elements).
  - Ba is for glass ceramics, cathode, and potential applications in metallurgy. The BaO-containing systems are important for the glass industry, in particular for TV panel glasses and glasses used for nuclear waste disposal.
  - Li is for glass ceramics, metallurgical processes, semiconductor, electrode industry, and lithium from Li-ion battery recycling slags. Note that low temperature phases relevant for cathode or anode battery development are not included in TCOX.
- 138 new phases (744 phases in total).

Added Thermophysical Properties for the New Elements

- For both Ba and Li: Molar volume, viscosity, surface tension, electrical conductivity/resistivity and thermal conductivity/resistivity are included for the new additions.

Added Thermal Conductivity for Ionic Liquids and Electrical Conductivity for the Solids

- Thermal conductivity/resistivity is included for the ionic liquids and solids.
- Electrical conductivity/resistivity is included for the solids. ELCD/ELRS of ionic liquids already included with TCOX13.

New Systems

- 41 new binary systems are assessed: Ba-B, Ba-Ca, Ba-F, Ba-Fe, Ba-Gd, Ba-La, Ba-Li, Ba-Mg, Ba-Mn, Ba-Mo, Ba-Ni, Ba-O, Ba-Ti, Ba-V, Ba-Y, Ba-Yb, Li-Al, Li-Ca, Li-Co, Li-Cr, Li-Cu, Li-F, Li-Fe, Li-Gd, Li-Hf, Li-K, Li-La, Li-Mg, Li-Mn, Li-Mo, Li-N, Li-Na, Li-Nb, Li-Ni, Li-O, Li-S, Li-Ti, Li-V, Li-W, Li-Y, Li-Yb, Li-Zr.
- 49 new ternary systems are assessed: Al-Ba-O, B-Ba-O, Ba-C-O, Ba-Ca-O, Ba-Cr-O, Ba-F-O, Ba-Fe-O, Ba-Gd-O, Ba-Hf-O, Ba-La-O, Ba-Li-O, Ba-Mg-O, Ba-N-O, Ba-Ni-O, Ba-O-P, Ba-O-Si, Ba-O-Ti, Ba-O-Y, Ba-O-Yb, Ba-O-Zr, Al-Li-O, B-Li-O, C-Li-O, Ca-Li-O, Co-Li-O, Cr-Li-O, Cu-Li-O, F-Li-O, Fe-Li-O, Li-Mg-O, Li-Mn-O, Li-N-O, Li-O-P, Li-O-Si, Li-O-Ti, Li-O-Y, Li-O-Zr, Ba-Ca-F, Ba-F-K, Ba-F-Li, Ba-F-Mg, Ba-F-Na, Ba-F-Zr, Ca-F-Li, F-K-Li, F-Li-Mg, F-Li-Na, F-Li-Zr, Al-Li-Mg.
- 48 new quaternary systems are assessed: Al-B-Ba-O, Al-Ba-Ca-O, Al-Ba-Mg-O, Al-Ba-O-Si, Al-Ca-Li-O, Al-Fe-Li-O, Al-Li-Mg-O, Al-Li-Na-O, Al-Li-O-Si, B-Ba-Ca-O, B-Ba-F-O, B-Ba-K-O, B-Ba-Li-O, B-Ba-Na-O, B-Ba-O-Si, B-Li-Na-O, B-Li-O-Si, Ba-C-Li-O, Ba-C-Na-O, Ba-Ca-Fe-O, Ba-Ca-N-O, Ba-Ca-O-P, Ba-Ca-O-Si, Ba-Ca-O-Y, Ba-Cr-F-O, Ba-Fe-O-P, Ba-Fe-O-Si, Ba-K-N-O, Ba-K-O-Si, Ba-Li-N-O, Ba-Li-O-Si, Ba-Mg-O-Si, Ba-Na-O-Si, Ba-O-Si-Ti, Ba-O-Y-Zr, C-F-Li-O, C-K-Li-O, C-Li-N-O, C-Li-Na-O, Ca-Li-N-O, Ca-Li-O-Si, F-K-Li-Na, F-Li-N-O, K-Li-N-O, Li-Mg-N-O, Li-Mg-O-Si, Li-N-Na-O, Li-Na-O-Si.
- 1 new higher order system is assessed: Ba-Ca-Mg-O-Si.

Previous Releases

TCOX12.0 to TCOX13.0

Software release 2024a (December 2023/January 2024)

New Thermophysical Property Added

- Addition of Electrical Conductivity of Ionic Liquid.

One New System Added

- C-Ca

Reassessed Systems

- Al-Fe, Fe-Si
- Al-C-Fe, Al-Fe-Mn, Al-Fe-Nb, Al-Fe-Ni, Al-Fe-P, B-Fe-Si, C-Fe-Si, Co-Fe-Si, Fe-Cr-Si, Fe-Mn-Si, Fe-Ni-Si, Fe-P-Si, and C-Fe-O
- Fe-Cr-Ni-O
- Al_2O_3-CaO, Al_2O_3-CaO-Fe-O, Al_2O_3-CaO-MgO, Al_2O_3-CaO-SiO_2, Al_2O_3-CaO-Y_2O_3, Al_2O_3-CaO-MgO-SiO_2
- Al_2O_3-CrO_x-SiO_2, Al_2O_3-MnO-FeO-SiO_2

Improvements

- Much of the work related to reassessed systems and new systems are those for the Al/Si distribution between steel and slag.
- Fe-Al was reassessed and a different Fe-Si assessment was used. The ternary Fe-Al-Me and Fe-Si-Me systems are all reassessed (where Me = any metal).

Surface Tension Re-assessed

The surface tension of metallic liquid was re-assessed based on the Redlich-Kister-Muggianu (R-K-M) sub-regular solution model.

TCOX11.1 to TCOX12.0

Software release version: 2023a (December 2022/January 2023)

New Elements and Binary, Ternary, and Higher Order Systems

- Added three new elements: B, Hf, and Yb
- Added Hf: Assessed or added from literature 24 binary, 11 ternary, and 8 higher order systems.
- Added Yb: Assessed or added from literature 24 binary, 10 ternary, and 8 higher order systems.
- Added B: Assessed or added from literature 20 binary, 21 ternary, and 12 higher order systems.

New Assessed Systems

The following systems are assessed:

- Cu-F-O, Cu-K-O, F-Na-O-Si, F-K-O-Si, Ca-F-Fe-O-Si, Ca-F-K-O-Si, Ca-F-Na-O-Si, $NaF-SiF_4$, Na-Si-F-O, $CaCO_3$-$MgCO_3$, $CaCO_3$-$FeCO_3$, $FeCO_3$-$MgCO_3$, Nb_2O_5-ZrO_2, Al_2O_3-TiO_2-ZrO_2, Gd_2O_3-La_2O_3-ZrO_2, Cr_2O_3-MgO-SiO_2, MnO-SiO_2-TiO_2, TiO_2-Y_2O_3-ZrO_2, CaO-Gd_2O_3-ZrO_2, Al_2O_3-CaO-Gd_2O_3, Al_2O_3-Fe-O-Y_2O_3, Al_2O_3-CaO-SiO_2-Y_2O_3.

Reassessed Systems

The following systems are reassessed:

- Al_2O_3-CaO, Al_2O_3-CaO-SiO_2, Al_2O_3-CaO-FeO_x, Al_2O_3-CaO-MgO Al_2O_3-CaO-Y_2O_3, Al_2O_3-Na_2O-SiO_2, Al_2O_3-CaO-FeO_x-SiO_2, Al_2O_3-CaO-MgO-SiO_2, Al_2O_3-CaO-Na_2O-SiO_2, Cu-F, Ca-F-Mn, Al-O-V, Fe-Na-O, Al_2O_3-SiO_2-TiO_2.

- Reassessed ZrO_2-mono/tetra T0 for ZrO_2-Al_2O_3, ZrO_2-Gd_2O_3, ZrO_2-Y_2O_3.

Other Changes

- Extended the GARNET phase description.
- Included complete gas description.

TCOX10.1 to TCOX10.2 and TCOX11 to TCOX11.1

Software release version: 2022a (December 2021/January 2022)

- Fixed an error in molar volume of FCC_A1 and BCC_A2 phases.

TCOX10.1 to TCOX11.0

Software release version: 2021b (June 2021)

New Element

- Addition of K

Binary, Ternary and Higher Order System Updates

- K: Assessed or added from literature 24 binary, 13 ternary and 14 higher order systems.
- Added carbide and nitride phases.
- The following systems have been assessed: Al_2O_3-CaO-MgO.
- The following systems have been reassessed: Al_2O_3-CaO-MgO-SiO_2.
- Reassessed Fe-solubility in $MgSiO_3$ (ortho-pyroxene).
- Updated all metallic systems to be the same as in the TCFE database.

Thermophysical Properties

- Addition of surface tension of the ionic liquid phase.
- Addition of viscosity of the ionic liquid phase for the systems containing K.

TCOX10.0 to TCOX10.1

Software release version: 2021a (December 2020/January 2021)

Thermophysical Properties

- Added viscosity for the liquid oxides of MoO_2, MoO_3, NbO, Nb_2O_5 and Y_2O_3.
- Replaced the molar volumes of metallic liquid with the unified molar volumes, which is now consistent with all the other databases.

- Added molar volumes for both liquid and solid phases which had missing values in the previous version.

Binary, Ternary, and Higher Order Systems

- N: Added NO_3^{-1} to the liquid phase.
- Fixed a bug in NiO that made the function not continuous at T=1800 K. These systems are reassessed due to the change in NiO description: Ca-Ni-O, Gd-Ni-O, La-Ni-O, Nb-Ni-O, Ni-O-P, Ni-O-Si, Ni-O-Ti, Ni-O-V, Ni-O-Y, CaO-NiO-SiO_2, MgO-NiO-SiO_2, Co-La-Ni-O.
- Updated NbO_2 to the latest description.
- Decreased stability of $FeSiO_3$ ortho-pyroxene (should not be stable, but was in version 10.0).
- The following systems are assessed: AlF_3-NaF, $Ca(NO_3)_2$, $Mg(NO_3)_2$, MgF_2-NaF, $NaNO_3$, NaF-Na_2CO_3, $NaNO_3$-Na_2CO_3, Na_2CO_3-Na_2S, $Ca(NO_3)_2$-$Mg(NO_3)_2$, $Ca(NO_3)_2$-$NaNO_3$, $NaNO_3$-NaF, $Mg(NO_3)_2$-$NaNO_3$. Estimations: Al_2O_3-Na_2O-ZrO_2, Na_2O-SiO_2-ZrO_2.
- The following systems have been reassessed: Updated liquid AlF3 to [2013 Lambotte]. AlF_3-CaF_2, AlF_3-MgF_2. Reassessed solubility of Al in V3O5_HT and M4O7. Reassessed solubility of Mg in V3O5_HT.
- Assessed a separation between liquid NaF and oxides in the following NaF-MeO_x systems: MeO_x= CuO, $FeO_{3/2}$, $MnO_{3/2}$, $NbO_{5/2}$, SiO_2.

TCOX9.0 to TCOX10.0

Software release version: 2020b (June 2020)

New Thermophysical Properties

- Added/assessed molar volumes to the database, both for solid and liquid oxides and metals.
- Assessed viscosity for the liquid oxides. Included oxides: FeO, Fe_2O_3, CaO, MgO, Al_2O_3, SiO_2, CaF_2, Cr_2O_3, Na_2O, MnO, TiO_2, ZrO_2, P_2O_5, Gd_2O_3, La_2O_3, V_2O_5, NiO, CuO_x.

New Elements

- Addition of three new elements: N, Na, H (Hydrogen only in gas).

Binary, Ternary and Higher Order System Updates

- N: Added description of 17 binary and 28 ternary systems. Nitrogen is only assessed in metallic systems, so for example SiAlONs are not described in this database.
- Na: Assessed or added from literature eight binary metallic systems. Added Na-O from literature and assessed the Na-S system. Assessed eight ternary Me-Na-O and 11 higher order oxide systems.

- The following systems have been assessed: C-Ca-O and C-Mg-O.
- The following systems have been reassessed: Cr-O, Ca-Cr-O, Cr-Si-O, Ca-Cr-Si-O.
- Minor changes to the following systems: Co-Ni-O, Co-Fe-Ni-O, Co-Fe-Ti-O, Mo-O, Al-Mo-O, Mg-Mo-O, Mn-Mo-O, Mo-Ni-O, Nb-O, La-P-O, P-Zr-O, Ti-Zr-O.
- Assessed a separation between liquid metal and SiO_2 in the following Me-O-Si systems: Me = Ca, Gd, La, Mg, Mo, Nb, Ni, P, Ti, V, W, Y, Zr.

Other Updates and Improvements

- H: Added H, H_2, C_1H_4 and H_2O to the gas phase.
- Reassessed the vacancy fraction on the FCC metallic sublattice to get a Va-fraction of 1e-5 at liquidus (this was earlier 1e-4).

TCOX8.0 TO TCOX9.0

Software release version: 2019b (June 2019)

- Addition of Ti: Assessed or added from literature all binary and a few ternary metallic systems. Assessed Ti-O and Ti-S binary systems. Assessed 19 ternary Me-Ti-O, two Me-Ti-S and 23 higher order oxide systems as indicated in the TCOX information sheet. Ti+2/+3/+4 is included in the liquid oxide, so the correct distribution of oxidation states in the slag can be calculated.
- The following systems have been assessed for version 9: CaO-SiO_2-VO_x. The correct distribution of oxidation states in the slag (+3/+4/+5) can now be calculated.
- The following systems have been reassessed for version 9: Ca-O-V, Mg-O-V, O-Si-V, and CaO-SiO_2-Y_2O_3.
- The following systems have been estimated for version 9: MgO-SiO_2-VO_x, MnS-NbS, MnS-VS.
- Changed model for VO solid solution, from Halite to FCC_A1 to be consistent with cubic TiO. Reassessed solubility of V_2O_3 in CaO/CoO/FeO/MgO/MnO/NiO Halite due to change of model for VO. Assessed C-V-O, modeling complete solid solution between VC_x and VO_y (same applies to the C-Ti-O system).
- Merged CoV_2O_6 and NiV_2O_6 compounds to the CaV_2O_6 phase.
- Removed the SO_4^{-2} species in the liquid phase.
- Minor changes to the following systems: W-O, Al-Cr-O, Ca-Ni-O, Co-O-V, Cr-Cu-O, Mg-Mn-O, Co-Mn-O, Co-Mo-O, Co-O-P, Nb-O-P, Ni-O-Si, Ni-O-V, Al-Ca-Ni-O, Al-Ni-O-Y, Ca-Co-Cu-O, Ca-Co-Ni-O, Co-Mn-O-Y, Fe-La-Ni-O, Gd-Mn-O-Si.

TCOX7.0 to TCOX8.0

Software release version: 2018b (June 2018)

- Addition of 6 new elements: Co, Mo, P, V, W, Ar (only in gas).
- Co: Assessed or added from literature all binary and a few ternary metallic systems. Added/Assessed Co-F, Co-O and Co-S. Assessed 29 ternary Co-Me_2-O, Co-Me_2-S and Co-Me_2-F systems and 13 higher order oxide systems as indicated in the TCOX information sheet.
- Mo: Assessed or added from literature all binary and a few ternary metallic systems. Added/Assessed Mo-O and Mo-S. Assessed 6 ternary Me1-Mo-O and Me1-Mo-S systems as indicated in the TCOX information sheet.
- P: Assessed or added from literature all binary and a few ternary metallic systems except F-P, Gd-P, La-P, Mg-P, P-V, P-W and P-Zr. Assessed 18 ternary Me1-O-P systems and 11 higher order oxide and oxy-fluoride systems as indicated in the TCOX information sheet.
- V: Assessed or added from literature all binary and a few ternary metallic systems except P-V. Assessed 13 ternary Me1-V-O systems as indicated in the TCOX information sheet.
- W: Assessed or added from literature all binary and a few ternary metallic systems except Ca-W, F-W and P-W. Assessed 13 ternary Me1-W-O systems as indicated in the TCOX information sheet.
- The following systems have been assessed for version 8: CaF_2-CoF_2/CrF_3/MnF_2, CoF_2-GdF_3/MgF_2/NiF_2, FeF_3-NiF_2, GdF_3-YF_3, LaF_3-ZrF_4, Al-Cu-S, Al-La-S, Ca-Y-S, Al-Ni-S and Cr-Ni-S.
- The following systems have been reassessed for version 8: F-Fe, Mg-Ni-O-Si, CaO-NiO-SiO_2, Mn-Ni-O, Al-Ni-O, Mn-Si-O, Al-Mn-Si-O, Al-Fe-Mn-Si-O, Ca-Mn-Si-O, Ni-Si-O, Ca-Ni-Si-O, Mg-Ni-Si-O, Al-Cu-O, Al-Cu-Si-O.
- The following systems have been estimated for version 8: La-Mg-S, Mn-Zr-S, Gd-Mg-S, Fe-Zr-S, Fe-Gd-S, Fe-La-S, Cu-La-S, Cu-Si-S, Nb-S, Fe-Nb-S
- The large complex gaseous phase has been removed. A reduced gaseous mixture is used including only the important species. If a complete gas is needed, it should be appended from the SGTE substance database.
- α-Ca_2SiO_4 and α'-$Ca_3P_2O_8$ is merged into one phase. Reassessed solubility of Fe, Gd, Mg, Mn and Y due to change of models.
- Removed Ni-solubility in Corundum.

TCOX6.0 to TCOX7.0

Software release version: 2017a (March 2017).

- Addition of 6 new elements: Cu, F, S, Gd, La and Nb.
- Cu: Added all binary and a few ternary metallic systems. Added Cu-O and Cu-S. Assessed Al_2O_3-Cu-O, CaO-Cu-O, Cu-Cr-O, Cu-Fe-O, Cu-O-La_2O_3, Cu-O-MgO, Cu-Mn-O, Cu-Nb-O, Cu-Ni-O, Cu-Si-O, Cu-Y-O, Al_2O_3-Cu-O-SiO_2, CaO-Cu-Fe-O, CaO-Cu-O-SiO_2, Cu-Fe-O-SiO_2, Cu-O-MgO-SiO_2, Cu-Cr-S, Cu-Fe-S, Cu-Mg-S, Cu-Mn-S, Cu-Ni-S, Cu-O-S, Cu-Fe-O-S.

- F: Added liquid and solid AlF_3, CaF_2, CrF_2, CrF_3, CuF, CuF_2, FeF_2, FeF_3, GdF_3, LaF_3, MgF_2, MnF_2, NbF_2, NbF_5, NiF_2, SiF_4, YF_3, ZrF_4. Assessed Ca-CaF_2, CaF_2-CaO, GdF_3-Gd_2O_3, MgF_2-MgO, AlF_3-CaF_2, AlF_3-MgF_2, AlF_3-ZrF_4, CaF_2-FeF_2, CaF_2-GdF_3, CaF_2-LaF_3, CaF_2-MgF_2, MgF_2-GdF_3, MgF_2-LaF_3, MgF_2-YF_3, AlF_3-Al_2O_3-CaF_2-CaO, CaF_2-CaO-MgF_2-MgO, CaF_2-Cr_2O_3, CaF_2-CaO-FeO-Fe_2O_3-FeF_2, CaF_2-SiO_2-CaO-SiF_4, Al_2O_3-CaF_2-MgO, Al_2O_3-CaF_2-SiO_2, MgF_2-MgO-SiO_2. Estimated CaF_2-CaS, CaF_2-$CaSO_4$, AlF_3-SiO_2.
- S: Assessed or added from literature: Al-S, Ca-S, Cr-S, Cu-S, Fe-S, Mg-S, Mn-S, Ni-S, Si-S, Y-S, Al-Fe-S, Ca-Fe-S, Ca-Mg-S, Ca-Mn-S, Cr-Fe-S, Cu-Cr-S, Cu-Fe-S, Cu-Mg-S, Cu-Mn-S, Cu-Ni-S, Fe-Mg-S, Fe-Mn-S, Fe-Ni-S, Mg-Mn-S, Al-O-S, Ca-O-S, Cu-O-S, Fe-O-S, Mg-O-S, Mn-O-S, Si-O-S, CuS-SiO_2, FeS-SiO_2, MnS-SiO_2, Al_2O_3-CaO-CaS, Al_2O_3-MgO-MgS, Al_2O_3-MnO-MnS, CaO-SiO_2-CaS, MgS-SiO_2, Al_2O_3-CaO-CaS-MnO-MnS, Cu-Fe-O-S, CaF_2-CaS. Estimated Gd-S, La-S, CaF_2-CaS, CaF_2-$CaSO_4$.
- Gd: Added all binary metallic systems except Gd-La. Added Gd-O and estimated Gd-S. Assessed Al_2O_3-Gd_2O_3, CaO-Gd_2O_3, Cr_2O_3-Gd_2O_3, Fe_2O_3-Gd_2O_3, Gd_2O_3-MgO, Gd_2O_3-NiO, Gd_2O_3-SiO_2, Gd_2O_3-ZrO_2, Al_2O_3-Gd_2O_3-ZrO_2, CaO-Gd_2O_3-SiO_2, Gd_2O_3-SiO_2-ZrO_2.
- La: Added all binary metallic systems except Gd-La, La-Nb and La-Si. Added La-O and estimated La-S. Assessed Al_2O_3-La_2O_3, CaO-La_2O_3, Cr_2O_3-La_2O_3, Cu-O-La_2O_3, Fe-O-La_2O_3, La_2O_3-Mn-O, La_2O_3-Nb_2O_5, La_2O_3-NiO, La_2O_3-SiO_2, La_2O_3-ZrO_2, Al_2O_3-La_2O_3-Y_2O_3, Al_2O_3-La_2O_3-ZrO_2.
- Nb: Added all binary metallic systems except La-Nb. Assessed Nb-O. Assessed Al_2O_3-Nb_2O_5, CaO-Nb_2O_5, Cr_2O_3-Nb_2O_5, CuO-Nb_2O_5, Fe-Nb-O, La_2O_3-Nb_2O_5, MgO-Nb_2O_5, MnO-Nb_2O_5, Nb_2O_5-NiO, Nb_2O_5-SiO_2, CaO-Nb_2O_5-SiO_2.
- The following systems have been assessed for version 7: Al_2O_3-CaO-Cr_2O_3, SiO_2-Fe-Mn-O, CaO-FeO-MnO, Al_2O_3-Fe-Mn-O, SiO_2-Al_2O_3-Fe-Mn-O.
- The following systems have been estimated for version 7: CaO-Mn-O-Y_2O_3, Fe-O-NiO-SiO_2.
- Added assessment of Mg-Mn-O and Cr_2O_3-MgO-SiO_2 from literature.
- The following systems have been reassessed for version 7: CaO-SiO_2-ZrO_2, CaO-SiO_2-Y_2O_3, Al_2O_3-CaO-SiO_2-Y_2O_3.
- modeled Fe_2O_3 solubility in MULLITE.
- modeled ZrO_2 solubility in APATITE.
- modeled Y_2O_3 solubility in ZIRCON.
- Merging CF ($CaO.Fe_2O_3$), α-$CACR_2O_4$ and CAY_2O_4 to one phase: CAV2O4.

TCOX5.1 to TCOX6.0

Software release version: 2015a (June 2015)

The following systems have been assessed for version 6: Al-Ca-Fe-Si-O, Al-Ca-Mg-Zr-O, Al-Ca-Y-O, Al-Fe-Mg-O, Al-Mg-Y-O, Al-Mn-Si-O, Al-Si-Zr-O, Ca-Fe-Mg-O, Ca-Fe-Mg-Si-O, Ca-Mg-Zr-O, Ca-Si-Y-O, Ca-Si-Zr-O, Ca-Y-Zr-O, Fe-Mg-Si-O, Mg-Si-Y-O and Mg-Y-Zr-O.

- Added assessments of Mg-Y and Mg-Zr from literature.
- The following systems have been reassessed for version 6: Al-Ca-Zr-O, Al-Cr-Zr-O, Al-Mg-Zr-O, Al-Ni-O, Al-Zr-O, Fe-Mg-O, Fe-Mg-Si-O, Fe-Y-O, Fe-Zr-O, Mn-Si-O and Ni-Si-O.
- The following systems have been estimated for version 6: Al-Ca-Si-Y-O, C-Ca, C-Mg, Ca-Cr, Ca-Mn, Ca-Y, Ca-Mg-Mn-O, Ca-Ni-Si-O, Mg-Ni-Si-O and Mg-Si-Zr-O.
- Added interaction for Ca-Fe in HCP identical to FCC and BCC. This makes the HCP phase not stable in the binary phase diagram. Reassessed liquid phase.
- Modified Al-Fe-O CORUNDUM.
- modeled CaO solubility in ORTHO_PYROXENE.
- Estimation of Al-Fe-Mn-O to fit a Mn/Si steel in Fe-Al-Mn-Si-O.
- Added a parameter in liquid Al-Si-O to get rid of a miscibility gap at high SiO_2 in Al-Mn-Si-O in equilibrium with Mn.
- Added $Ca_2FeSi_2O_7$ (MELILITE) and estimated the “binaries” $Ca_2FeSi_2O_7$-$Ca_2MgSi_2O_7$ and $Ca_2FeSi_2O_7$-$Ca_2AlFeSiO_7$.
- Merged YAM and CUSPIDINE phases to get complete solubility between Y4Al2O9 and Ca2Si2Y2O9.
- Corrected a misprint in liquid Al-Ca-Zr-O, so the miscibility gap was removed.
- Changed back to the old description for ANORTHITE.

TCOX4.0 TO TCOX5.1

TCOX5 released in October 2012 and TCOX5.1 released in January 2013.

- Included Y_2O_3 and ZrO_2. Also added available descriptions for Y-O and Zr-O from literature, with small modifications due to model compatibility with TCOX. Many binary and ternary systems with these two new components are assessed for TCOX5.
- Al_2O_3-CaO-Fe-O, Al_2O_3-CaO-MnO, Al_2O_3-Fe-O-SiO_2, CaO-Cr-O-SiO_2, CaO-MnO-SiO_2, MgO-Al_2O_3-CrO-Cr_2O_3, FeO-Fe_2O_3-MgO-SiO_2 have been added from published assessments or assessed for TCOX5.
- Merged phases Mn_2O_3 and cubic Y_2O_3 to one single phase: M2O3C.
- Removed all intermetallic phases and carbides. Updated metallic liquid, fcc, bcc etc. to the latest available descriptions.
- Changed model for oxygen in DIAMOND_FCC_A4. Oxygen is now modeled as an interstitial element, instead of using a substitutional model as before. This change was done due to computational problems with the DIAMOND_FCC_A4 phase when Si was not defined in the system.
- Modification of the ANORTHITE phase stability in the Al_2O_3-CaO-MgO-SiO_2 system.
- Simplified the model for the ALPHA_SPINEL phase due to computational problems.
- Reassessed Al-Cr-O and Cr-O due to an unwanted miscibility gap in the Al_2O_3-Cr_2O_3 system close to Cr-O.

- Removed charged species from the gas phase.
- Al_2O_3-CaO-NiO, Al_2O_3-NiO, CaO-Cr-O, CaO-Mn-O, Cr-O-MgO, Cr-O-SiO_2 and MgO-NiO are reassessed.
- Added Ca to the SPINEL phase. Solubility of Ca in Fe_3O_4 and Mn_3O_4 has been assessed.
- Added ASSESSED_SYSTEMS. It is now possible to calculate the Me-O binaries using the BINARY module in Thermo-Calc.