TCS Metal Oxide Solutions Database (TCOX13)

Technical Information

Available Starting with Thermo-Calc Version 2024a

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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, and electrical conductivity for 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).

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 TCOX13. 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.

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 TCOX13 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 an 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) 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 an 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.

TCOX13 Elements, Systems, Phases, and Properties

Included Elements

There are 32 elements included in the most recent version of the database.

Al	Ar*	B	C	Ca	Co	Cr	Cu	F	Fe
Gd	H*	Hf	K	La	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:

- 392 binary and 508 ternary systems in the 32 element framework.
- 246 quaternary systems and 32 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 TCOX13 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 606 phases in total.

TCOX13 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 TCOX13 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 Assessed Systems

The assessed systems related to the properties data are included in this document.

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

Molar Volume

For the molar volume properties data, the molar volume parameters have been assessed or estimated as detailed in TCOX13 Molar Volume Assessed Systems and Phases.

Viscosity

For the viscosity properties data, the parameters have been assessed for the ionic liquid phase. The assessed systems are detailed in TCOX13 Viscosity for Ionic Liquids Assessed Systems.

Surface Tension

For the surface tension properties data, the parameters have been assessed for the ionic liquid phase. The assessed systems are detailed in TCOX13 Surface Tension Assessed Systems.

Electrical Conductivity

For the electrical conductivity properties data, the parameters have been assessed for the ionic liquid phase.

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 the TC-Python SDK. More details are described in the online help.

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

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).

TCOX13 Systems

In this section:

TCOX13 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.

- All metal-metal binaries are assessed except for B-Gd, B-K, B-La, B-Mg, B-Na, B-P, B-S, B-Yb, C-Yb, Ca-W, Ca-Zr, Co-Na, Cr-Na, F-Hf, F-Na, Gd-Hf, Gd-La, Gd-Na, Gd-P, Hf-P, Hf-S, La-Na, La-Nb, La-P, La-Si, Mg-P, Mn-Na, Mo-Na, Na-Ni, Na-Ti, Na-V, Na-W, Na-Y, P-V, P-W, P-Yb, P-Zr, and S-Yb
- Many ternary metallic systems are also assessed.

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.

TCOX13 Assessed Oxide Systems

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

Assessed Binary Oxide Systems

Assessed Binary Oxide Systems							
Al-O	B-O	Ca-O	Co-O	Cr-O	Cu-O	Fe-O	Gd-O
Hf-O	K-O	La-O	Mg-O	Mn-O	Mo-O	Na-O	Nb-O
Ni-O	P-O	Si-O	Ti-O	V-O	W-O	Yb-O	Y-O
Zr-O							

Assessed Quaternary Oxide Systems

Assessed Quaternary Oxide Systems, Me1-Me2-Me3-O				
Al-B-Ca-O	Al-B-K-O	Al-B-Mg-O	Al-B-Na-O	Al-B-O-Si
Al-Ca-Co-O	Al-Ca-Cr-O	Al-Ca-Fe-O	Al-Ca-Gd-O	Al-Ca-K-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-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-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

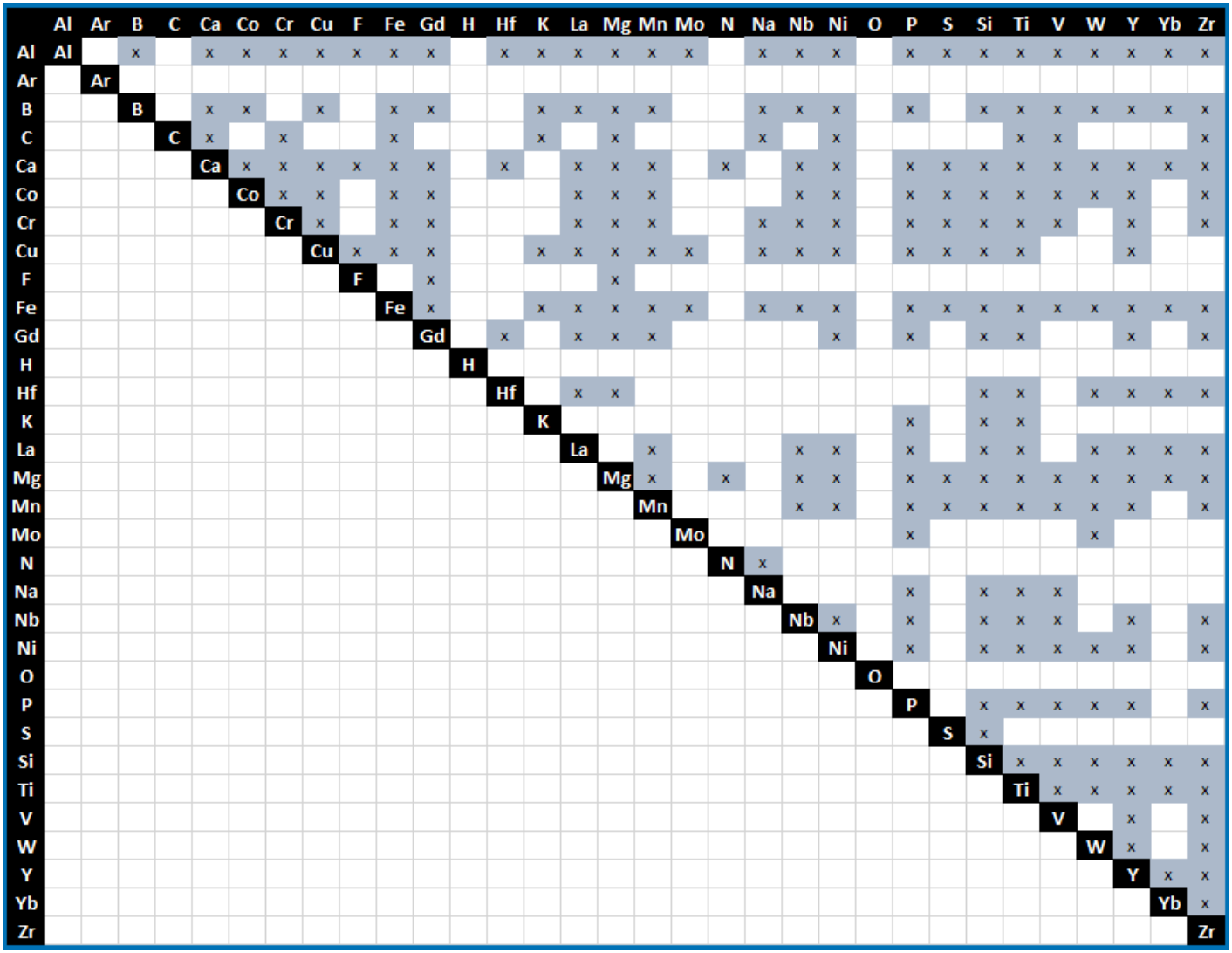
Assessed Quaternary Oxide Systems, Me1-Me2-Me3-O				
Al-O-Y-Zr	B-Ca-Fe-O	B-Ca-O-Si	B-Fe-Na-O	B-K-Mg-O
B-K-Na-O	B-K-O-Si	B-Na-O-Si	C-Ca-Fe-O	C-Ca-Mg-O
C-F-K-O	C-F-Na-O	C-Fe-Mg-O	C-K-N-O	C-K-Na-O
C-N-Na-O	Ca-Co-O-Si	Ca-Cr-Fe-O	Ca-Cr-O-Si	Ca-Cu-Fe-O
Ca-Cu-O-Si	Ca-Fe-Mg-O	Ca-Fe-Mn-O	Ca-Fe-O-P	Ca-Fe-O-Si
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-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	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-Mg-N-O	K-Mg-O-Si	K-N-Na-O	K-Na-O-Si
La-O-Y-Zr	La-O-Yb-Zr	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

Assessed Quaternary Oxide Systems, Me1-Me2-Me3-O				
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-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-Mg-O-Si	Al-Fe-Mn-O-Si	Al-Fe-Na-O-Si
Al-Gd-O-Y-Zr	Al-La-O-Y-Zr	Al-Mg-Na-O-Si	C-Cr-Fe-Mn-Ni-O	Ca-Fe-Mg-O-Si
Ca-Mg-Ni-O-Si	Ca-Mg-O-P-Si	Gd-La-O-Y-Zr		

Assessed Ternary Oxide Systems, Me1-Me2-O



TCOX13 Assessed Sulfide Systems

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

Assessed Binary Sulfide Systems

Assessed Binary Sulfide Systems							
Al-S	Ca-S	Co-S	Cr-S	Cu-S	Fe-S	Gd-S	K-S
La-S	Mg-S	Mn-S	Mo-S	Na-S	Nb-S	Ni-S	Si-S
Ti-S	V-S	W-S	Y-S	Zr-S			

Assessed Oxy-sulfide Ternary Systems

Assessed Oxy-sulfide Ternary Systems				
Al-O-S	Ca-O-S	Co-O-S	Cr-O-S	Cu-O-S
Fe-O-S	Mg-O-S	Mn-O-S	O-S-Si	

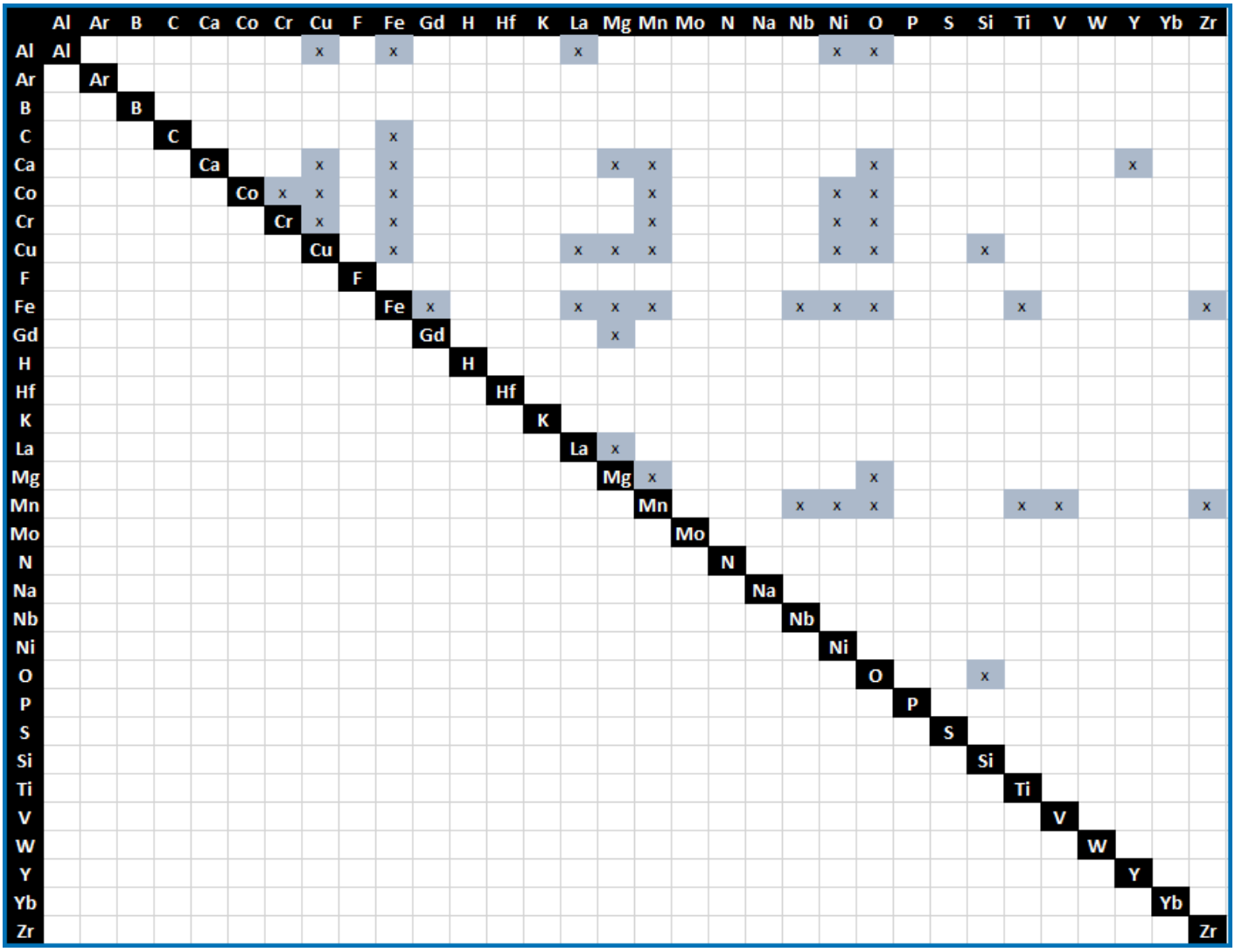
Assessed Oxy-sulfide Quaternary Systems

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

Assessed Ternary Sulfide Systems, Me1-Me2-S



TCOX13 Assessed Fluoride Systems

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

Assessed Binary Fluoride Systems

Assessed Binary Fluoride Systems					
AlF_3	Ca-F	CoF_2	CoF_3	CrF_2	CrF_3
CuF	CuF_2	FeF_2	FeF_3	GdF_3	HfF_4
KF	LaF_3	MgF_2	MnF_2	MoF_4	NaF
NbF_2	NbF_5	NiF_2	SiF_4	VF_2	YbF_3
YF_3	ZrF_4				

Assessed Oxy-fluoride Systems

Assessed Oxy-Fluoride Ternary Systems				
Al-F-O	Ca-F-O	Cu-F-O	F-Mg-O	Fe-Gd-O

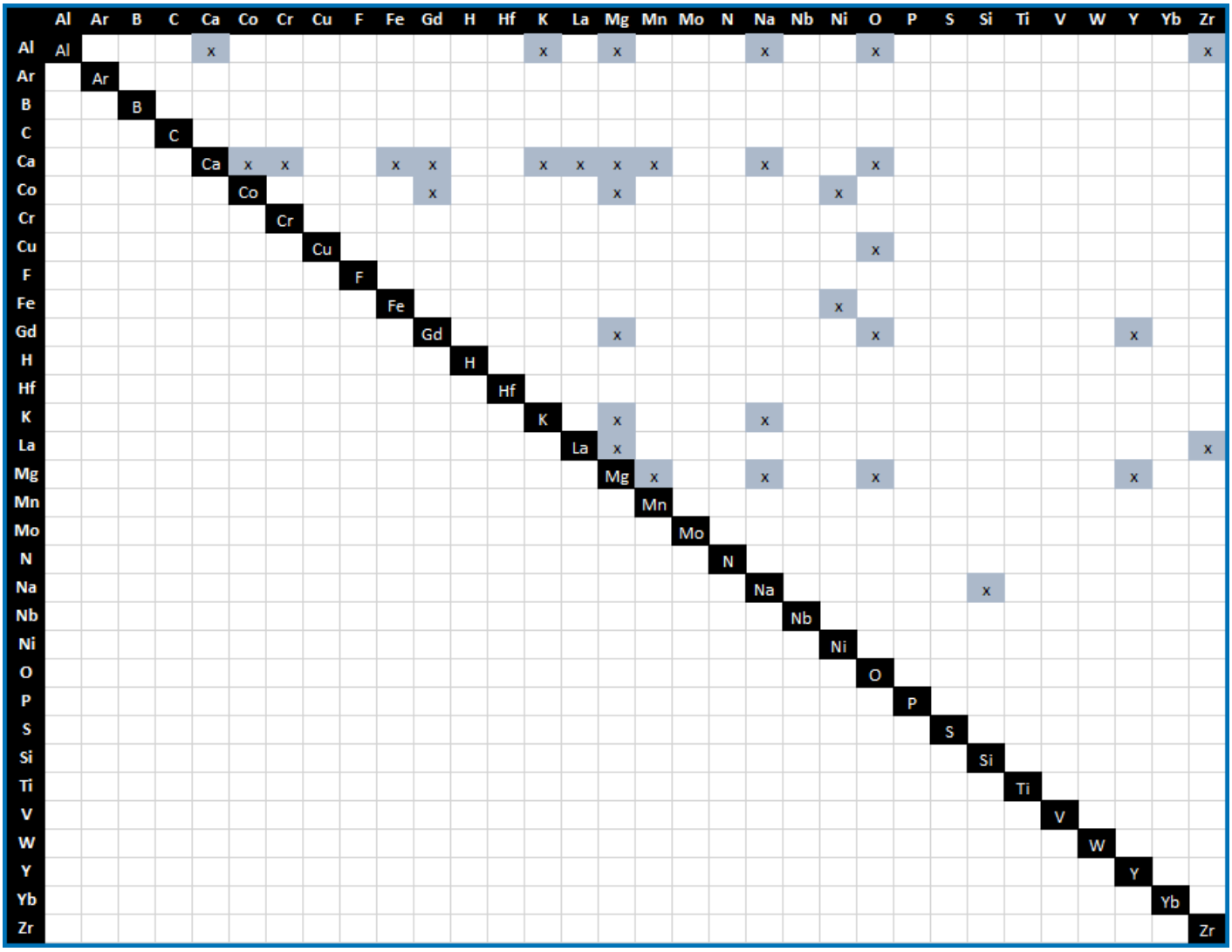
Assessed Oxy-Fluoride Quaternary Systems

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

Assessed Ternary Fluoride Systems



TCOX13 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).
ALABANDITE	Alabandite (MnS), Oldhamite (CaS), MgS, GdS, LaS, ZrS.
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 ($Ca_2FeSi_2O_7$), and $CaCoSi_2O_7$.
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.
ZIRCON	Zircon ($ZrSiO_4$), Xenotime (YPO_4), $GdPO_4$, $LaPO_4$, $HfSiO_4$ and YPO_4.

TCOX13 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)1.0(AL+3)1.0(FE+3)2.0(AL+3, FE+3)3.0(O-2)10.0
AF	FeGaO3		oP40	(33, Pna2_1)	This is Al2O3.Fe2O3.	3	(AL+3)2.0(FE+3)2.0(O-2)6.0
AL18B4O33	Al5BO9		oS60	(36, Cmc2_1)		3	(AL+3)18.0(B+3)4.0(O-2)33.0
AL2P6SI4O26	Unknown Structure					4	(AL+3)2.0(P+5)6.0(SI+4)4.0(O-2)26.0
AL2S3	alpha-Al2S3		hP30	(169, P6_1)		2	(AL)2.0(S)3.0
AL2SIO4F	Unknown Structure					4	(AL+3)2.0(SI+4)1.0(O-2)4.0(F-1)2.0
AL3PO7	Unknown Structure					3	(AL+3)3.0(P+5)1.0(O-2)7.0
AL4B2O9	Al4B1.5[BO3]0.5O7.5		mS124	(12, C2/m)		3	(AL+3)4.0(B+3)2.0(O-2)9.0
AL4C3_D71	Al4C3 (D71)	D71	hR7	(166, R-3m)		2	(AL, SI)4.0(C)3.0
ALABANDITE	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is CaS (oldhamite), MnS (alabandite), (Mg,Gd,La,Zr)S.	2	(CA, CO, CR, CU, FE, GD, LA, MG, MN, Y, ZR)1.0(S)1.0
ALBITE_LOW	Albite (NaAlSi3O8, S68)	S68	aP26	(2, P-1)	This is low temperature albite (NaAlSi3O8).	4	(NA+1)1.0(AL+3)1.0(SI+4)3.0(O-2)8.0
ALBITE_MONO	Sanidine (KAlSi3O8, S67)	S67	mS52	(12, C2/m)	This is monoclinic albite (NaAlSi3O8).	4	(NA+1)1.0(AL+3)1.0(SI+4)3.0(O-2)8.0
ALF3_S2	AlF3		oS48	(63, Cmcm)		2	(AL+3)1.0(F-1)3.0
ALNB11O29	(Ti0.17Nb0.83)12O29		mS82	(12, C2/m)		3	(AL+3)1.0(NB+5)11.0(O-2)29.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALNB49O124	Unknown Structure					3	(AL+3)1.0(NB+5)49.0(O-2)124.0
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)		2	(AL)1.0(N)1.0
ALP3O9	AlP3O9		mS156	(9, Cc)	This is (Al,Cr,Fe)P3O9	2	(AL+3, CR+3, FE+3)1.0(PO3-1)3.0
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)1.0(AL+3, CR+3, FE+3, MN+2, MN+3, VA)2.0(MN+2, VA)2.0(O-2)4.0
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)1.0(PO4-3, SIO4-4)1.0
ALPO4_S2	Al[PO4]		hP18	(180, P6_222)	This is AlPO4 with SiO2 solubility.	2	(AL+3, SI+4)1.0(PO4-3, SIO4-4)1.0
ALPO4_S3	AlPO4 low cristobalite type		oS24	(20, C222_1)	This is AlPO4 with SiO2 solubility.	2	(AL+3, SI+4)1.0(PO4-3, SIO4-4)1.0
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	(58, Pnnm)	This is a high-pressure phase	4	(AL+3)1.0(AL+3)1.0(SI+4)1.0(O-2)5.0
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)1.0(SO4-2)1.0
ANILITE	Cu7S4		oP44	(62, Pnma)	This is Cu7S4, orthorhombic structure.	2	(CU)1.75(S)1.0
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)1.0(AL+3)1.0(AL+3, SI+4)1.0(SI+4)2.0(O-2)8.0
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)4.0(GD+3, Y+3, YB+3)6.0(SIO4-4)6.0 (O-2, VA)2.0
B2O3	B2O3		hP15	(152, P3_121)		2	(B+3)2.0(O-2)3.0
B4C_D1G	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		2	(B11C, B12)1.0(B2, C2B, CB2)1.0
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)		2	(AL, CA, CO, CR, CU, FE, GD, HF, K, LA, MG, MN, MO, NA, NB, NI, P, S, SI, TI, V, W, Y, YB, ZR)1.0(B, C, N, O, VA)3.0

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BETA_RHOMBO_B	beta-B (R-105)		hR105	(166, R-3m)		2	(B)93.0(B, C, SI)12.0
BETA_V_O	CoO		tI4	(139, I4/mmm)		2	(V)1.0(O, VA)1.0
BPO4	BPO4 (H07)	H07	tI12	(82, I-4)		3	(B+3)1.0(P+5)1.0(O-2)4.0
BRONZE	Unknown Structure					3	(V+4, V+5)2.0(O-2)5.0(CA+2, FE+2, VA)1.0
C11A7F	Ca6Al7O16F		cI152	(220, I-43d)	This is 11CaO.7Al2O3.CaF2	4	(AL+3)14.0(CA+2)12.0(F-1)2.0(O-2)32.0
C12A7	Mayenite (12CaO.7Al2O3, K74, C12A7)	K74	cI152	(220, I-43d)	Not stable under anhydrous conditions.	4	(CA+2)6.0(AL+3)6.0(AL+3, FE+3)1.0(O-2)16.5
C13A6Z2	Ca7ZrAl6O18		oP104	(31, Pmn2_1)	This is 13CaO.3Al2O3.2ZrO2.	4	(CA+2)13.0(AL+3)12.0(ZR+4)2.0(O-2)35.0
C1A1	Al2CaO4		mP84	(14, P2_1/c)	This is CaO.Al2O3 (mP84, P121/c1) with solubility of Fe	4	(CA+2)3.0(AL+3)5.0(AL+3, FE+3)1.0(O-2)12.0
C1A2	Al4CaO7		mS48	(15, C2/c)	This is CaO.2Al2O3 (mS48, C12/c1) with solubility of Fe	4	(CA+2)1.0(AL+3)3.0(AL+3, FE+3)1.0(O-2)7.0
C1A6	Magnetoplumbite (PbFe12O19)		hP64	(194, P6_3/mmc)	This is CaO.6Al2O3 with solubility of Fe	3	(CA+2)1.0(AL+3, FE+3)12.0(O-2)19.0
C1A8M2	CaMg2Al16O27		hP94	(187, P-6m2)	This is CaO.8Al2O3.2MgO	4	(CA+2)1.0(AL+3)16.0(MG+2)2.0(O-2)27.0
C2A14M2	Unknown Structure				This is 2CaO.14Al2O3.2MgO	4	(CA+2)2.0(AL+3)28.0(MG+2)2.0(O-2)46.0
C2F	Ca2Fe2O5		oP36	(62, Pnma)	This is 2CaO.Fe2O3 with solubility of Al.	3	(CA+2)2.0(AL+3, FE+3)2.0(O-2)5.0
C3A1	Ca3Al2O6		cP264	(205, Pa-3)	This is 3CaO.Al2O3 with solubility of Fe	3	(CA+2)3.0(AL+3, FE+3)2.0(O-2)6.0
C3A2M1	3CaO.2Al2O3.MgO		oP72	(57, Pbcm)	This is 3CaO.2Al2O3.MgO	4	(CA+2)3.0(AL+3)4.0(MG+2)1.0(O-2)10.0
C3A3F	Unknown Structure				This is 3CaO.3Al2O3.CaF2	4	(AL+3)6.0(CA+2)4.0(F-1)2.0(O-2)12.0
C4WF4	Ca4Fe9O17		mS60	(5, C2)	This is 4CaO.FeO.4Fe2O3.	4	(CA+2)4.0(FE+2)1.0(FE+3)8.0(O-2)17.0

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C4WF8	Sr2Fe2O5		oI44	(74, Imma)	This is 4CaO.FeO.8Fe2O3	4	(CA+2)4.0(FE+2)1.0(FE+3)16.0(O-2)29.0
CA10P6O25	Unknown Structure				This is Ca10(PO4)6O.	3	(CA+2)10.0(PO4-3)6.0(O-2)1.0
CA10SI3O15F2	Unknown Structure				This is 9CaO.3SiO2.CaF2	4	(CA+2)10.0(SI+4)3.0(O-2)15.0(F-1)2.0
CA10V6O19	Unknown Structure					3	(CA+2)5.0(V+3)3.0(O-2)9.5
CA11B2SI4O22_HT	Unknown Structure					4	(CA+2)11.0(B+3)2.0(SI+4)4.0(O-2)22.0
CA11B2SI4O22_LT	Unknown Structure					4	(CA+2)11.0(B+3)2.0(SI+4)4.0(O-2)22.0
CA15CU18O35	Ca4.8Cu6O11.6		mP92	(13, P2/c)		4	(CA+2)15.0(CU+2)14.0(CU+3)4.0(O-2)35.0
CA2AL2B2O8	Unknown Structure					4	(CA+2)2.0(AL+3)2.0(B+3)2.0(O-2)8.0
CA2ALF7	Ca2AlF7		oP40	(62, Pnma)		3	(CA+2)2.0(AL+3)1.0(F-1)7.0
CA2ALNBO6	Ca2AlNbO6		mP24	(14, P2_1/c)		4	(CA+2)2.0(AL+3)1.0(NB+5)1.0(O-2)6.0
CA2B2O5_S1	b-Mg2B2O5		mP36	(14, P2_1/c)		3	(CA+2)2.0(B+3)2.0(O-2)5.0
CA2B2O5_S2	Ca2B2O5		oP36	(19, P2_12_12_1)		3	(CA+2)2.0(B+3)2.0(O-2)5.0
CA2CUO3	Sr2CuO3		oI12	(71, Immm)		3	(CA+2)2.0(CU+2)1.0(O-2)3.0
CA2GD2ZRO7	Unknown Structure					4	(CA+2)2.0(GD+3)2.0(ZR+4)1.0(O-2)7.0
CA2HF7O16	Ca2Hf7O16		hR25	(148, R-3)		3	(CA+2)2.0(HF+4)7.0(O-2)16.0
CA2NA2SI2O7	Na2Ca2Si2O7		mS208	(15, C2/c)		4	(CA+2)2.0(NA+1)2.0(SI+4)2.0(O-2)7.0
CA2NA2SI3O9	Na(Na0.5Ca0.5)2CaSi3O9		hP102	(152, P3_121)		4	(CA+2)2.0(NA+1)2.0(SI+4)3.0(O-2)9.0
CA2NB2O7	La2Ti2O7		mP44	(4, P2_1)		3	(CA+2)2.0(NB+5)2.0(O-2)7.0

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CA2P2O7_A	Ce2Si2O7		mP44	(14, P2_1/c)	This is alpha- Ca2(P2O7).	2	(CA+2, MG+2)2.0(P2O7-4)1.0
CA2P2O7_B	beta-Ca2[P2O7]		tP88	(76, P4_1)	This is beta- Ca2(P2O7).	2	(CA+2, MG+2)2.0(P2O7-4)1.0
CA2P2O7_G	Unknown Structure				This is gamma- Ca2(P2O7).	2	(CA+2, MG+2)2.0(P2O7-4)1.0
CA2P6O17	Ca2P6O17		mP56	(14, P2_1/c)	This is Ca2(P2O5)3O2.	3	(CA+2)2.0(P+5)6.0(O-2)17.0
CA2SIO4_ALPHA_A	Ca2SiO4		hP24	(194, P6_ 3/mmc)	This is 2CaO.SiO2 and 3CaO.P2O5.	3	(CA+2, GD+3, MG+2, MN+2, Y+3)3.0 (CA+2, VA)1.0(BO3-3, PO4-3, SIO4-4)2.0
CA2SIO4_ALPHA_ PRIME	K2CoCl4		oP84	(33, Pna2_1)	This is 2CaO.SiO2.	3	(CA+2, FE+2, GD+3, MG+2, MN+2, Y+3)3.0(CA+2, VA)1.0(BO3-3, PO4-3, SIO4-4)2.0
CA2V2O7	Sr2V2O7		aP	(2, P-1)		3	(CA+2)2.0(V+5)2.0(O-2)7.0
CA2YB2O5	Unknown Structure					3	(CA+2)2.0(YB+3)2.0(O-2)5.0
CA2ZRSI4O12	cyclosilicate (Ca2ZrSi4O12)		mP38	(11, P2_1/m)		4	(CA+2)2.0(SI+4)4.0(ZR+4)1.0(O-2)12.0
CA3B2O6	Ca3[BO3]2		hR22	(167, R-3c)		3	(CA+2)3.0(B+3)2.0(O-2)6.0
CA3CO2O6	Ca3Co2O6		hR22	(167, R-3c)		3	(CA+2)3.0(CO+3, CU+2)2.0(O-2, VA)6.0
CA3CO4O9	Ca3Co4O9		mS30	(12, C2/m)		3	(CA+2)3.0(CO+3, CU+2)4.0(O-2, VA)9.0
CA3COAL4O10	Ca3ZnAl4O10		oP72	(29, Pca2_1)		4	(CA+2)3.0(CO+2)1.0(AL+3)4.0(O-2)10.0
CA3MG3P4O16	Unknown Structure				This is Ca3Mg3(PO4)4 solid solution.	3	(CA+2, MG+2)3.0(MG+2)3.0(PO4-3)4.0
CA3NA2SI6O16	Na2Ca3Si6O16		aP54	(2, P-1)		4	(CA+2)3.0(NA+1)2.0(SI+4)6.0(O-2)16.0
CA3NB2O8	Unknown Structure					3	(CA+2)3.0(NB+5)2.0(O-2)8.0
CA3P2O8_A	Ca3[PO4]2		mP312	(14, P2_1/c)	This is alpha- Ca3(PO4)2 with solubility of Mg and Si.	3	(CA+2, MG+2)3.0(CA+2, VA)1.0(PO4-3, SIO4-4)2.0

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CA3P2O8_B	Ca3[AsO4]2		hR92	(161, R3c)	This is beta- Ca3(PO4)2 with solubility of Mg.	2	(CA+2, MG+2)3.0(PO4-3)2.0
CA3S3FE4OX	Unknown Structure				This is 3CaS.4FeO and 3CaS.4Fe2O3.	4	(CA+2)3.0(S-2)3.0(FE+2, FE+3)4.0(O-2, VA)6.0
CA3TI2O7	Ca3Ti2O7		oS48	(36, Cmc2_1)		3	(CA+2)3.0(TI+4)2.0(O-2)7.0
CA3TI8AL12O37	Unknown Structure					4	(CA+2)3.0(TI+4)8.0(AL+3)12.0(O-2)37.0
CA3V2O8	K2PbS2O8		hR273	(161, R3c)		3	(CA+2)3.0(V+5)2.0(O-2)8.0
CA3WO6	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)		3	(CA+2)3.0(W+6)1.0(O-2)6.0
CA3Y2SI3O12	Ca3Y2Si3O12		oP100	(62, Pnma)	This is 3CaO.(Gd,Y,Yb)2O3.3SiO2.	4	(CA+2)3.0(GD+3, Y+3, YB+3)2.0(SI+4)3.0(O-2)12.0
CA3Y2SI6O18	Ca0.6Y0.4Si6O18		mS116	(15, C2/c)	This is 3CaO.(Gd,Y,Yb)2O3.6SiO2.	4	(CA+2)3.0(GD+3, Y+3, YB+3)2.0(SI+4)6.0(O-2)18.0
CA3YB2O6	Unknown Structure					3	(CA+2)3.0(YB+3)2.0(O-2)6.0
CA3ZRSI2O9	Ca3Hf(Si2O7)O2		mP60	(14, P2_1/c)		4	(CA+2)3.0(SI+4)2.0(ZR+4)1.0(O-2)9.0
CA4MG2P6O21	Unknown Structure					3	(CA+2)4.0(MG+2)2.0(P2O7-4)3.0
CA4NB2O9_HT11	Ca4Nb2O9		mP20	(14, P2_1/c)		5	(CA+2)6.0(CA+2, NB+5)3.0(NB+5)3.0(O-2, VA)3.0(O-2)15.0
CA4NB2O9_LT21	Ca4Nb2O9-lt		mP60	(14, P2_1/c)		5	(CA+2)6.0(CA+2, NB+5)4.0(CA+2)2.0(O-2, VA)3.0(O-2)15.0
CA4P2O9_A	Ca4[PO4]2O		mP60	(4, P2_1)	This is alpha- Ca4(PO4)2O.	3	(CA+2)4.0(PO4-3)2.0(O-2)1.0
CA4P2O9_B	beta-Ca4(PO4)2O		oP60	(17, P222_1)	This is beta-Ca4(PO4)2O.	3	(CA+2)4.0(PO4-3)2.0(O-2)1.0
CA4P6O19	Ca4P6O19		aP58	(2, P-1)	This is Ca4(PO3)5(PO4).	3	(CA+2)4.0(PO3-1)5.0(PO4-3)1.0
CA4TI3O10	Ca4Ti3O10		oP68	(61, Pbca)		3	(CA+2)4.0(TI+4)3.0(O-2)10.0

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CA4V2O9	Ca4V2O9		oF	(22, F222)		3	(CA+2)4.0(V+5)2.0(O-2)9.0
CA5P2SIO12	Unknown Structure					3	(CA+2, VA)5.0(PO4-3)2.0(SIO4-4, VA)1.0
CA5SI2O8F2	Unknown Structure				This is 4CaO.2SiO2.CaF2	4	(CA+2)5.0(SI+4)2.0(O-2)8.0(F-1)2.0
CA6HF19O44	Ca6Hf19O44		hR138	(167, R-3c)		3	(CA+2)6.0(HF+4)19.0(O-2)44.0
CA6ZR19O44	Ca6Hf19O44		hR138	(167, R-3c)		3	(CA+2)6.0(ZR+4)19.0(O-2)44.0
CA7P2SI2O16	Ca7[(Si0.5P0.5)O4]4		hP180	(169, P6_1)		3	(CA+2)7.0(PO4-3)2.0(SIO4-4)2.0
CA9V6O18	Unknown Structure					3	(CA+2)9.0(V+3)6.0(O-2)18.0
CAAL2B2O7	Unknown Structure					4	(CA+2)1.0(AL+3)2.0(B+3)2.0(O-2)7.0
CAALF5_S1	CrMnF5		mS28	(15, C2/c)		3	(CA+2)1.0(AL+3)1.0(F-1)5.0
CAALF5_S2	CrMnF5		mP28	(14, P2_1/c)		3	(CA+2)1.0(AL+3)1.0(F-1)5.0
CAB2O4	CaB2O4 I (E32)	E32	oP28	(60, Pbcn)		3	(CA+2)1.0(B+3)2.0(O-2)4.0
CAB4O7	CaB4O7		mP96	(14, P2_1/c)		3	(CA+2)1.0(B+3)4.0(O-2)7.0
CAC2_BETA	CaC2		cF36	(225, Fm-3m)		2	(CA+2)1.0(C2-2)1.0
CAC2_C11A	CaC2-I (C11a)	C11a	tI6	(139, I4/mmm)		2	(CA+2)1.0(C2-2)1.0
CACO3	Calcite (CaCO3, G01)	G01	hR10	(167, R-3c)	This is (Ca,Fe,Mg)CO3.	2	(CA+2, FE+2, MG+2)1.0(CO3-2)1.0
CACR2O4_A	SrCr2O4		oP28	(59, Pmmn)	With solubility of Al and Fe.	3	(CA+2)1.0(AL+3, CR+3, FE+3)2.0(O-2)4.0
CACRSI4O10	gillespite (BaFeSi4O10)		tP64	(130, P4/ncc)	This is CaO.CrO.4SiO2, Gillespite	4	(CA+2)1.0(CR+2)1.0(SI+4)4.0(O-2)10.0
CACU2O3	Shcherbinaite (V2O5) (Revised)		oP14	(59, Pmmn)		3	(CA+2)1.0(CU+2)2.0(O-2)3.0

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CAF2_S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is low temperature CaF2.	2	(CA+2, MG+2, MN+2)1.0(F-1, O-2, VA)2.0
CAF2_S2	Cotunnite (PbCl2, C23)	C23	oP12	(62, Pnma)	This is high temperature CaF2.	2	(CA+2, MG+2, MN+2)1.0(F-1, O-2, VA)2.0
CAMG3O16S4	Unknown Structure				This is CaMg3(SO4)4.	3	(CA+2)1.0(MG+2)3.0(SO4-2)4.0
CAMN2O4	CaMn2O4		oP28	(57, Pbcm)		3	(CA+2)1.0(MN+3)2.0(O-2)4.0
CAMO3	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)	This is CaHfO3, CaMnO3, CaTiO3, lt CaZrO3.	3	(CA+2, GD+3, Y+3)1.0(GD+3, HF+4, MN+4, TI+4, Y+3, ZR+4)1.0(O-2)3.0
CAN2O6	Pb(NO3)2 (G21)	G21	cP36	(205, Pa-3)	This is (Ca, Mg)(NO3)2 solid solution.	2	(CA+2, MG+2)1.0(NO3-1)2.0
CANA2SI5O12	Unknown Structure					4	(CA+2)1.0(NA+1)2.0(SI+4)5.0(O-2)12.0
CANA2SIO4	Na2CaSiO4 (S66)	S66	cP32	(198, P2_13)		4	(CA+2)1.0(NA+1)2.0(SI+4)1.0(O-2)4.0
CANA4SI3O9	K4SrGe3O9		cP272	(205, Pa-3)		4	(CA+2)1.0(NA+1)4.0(SI+4)3.0(O-2)9.0
CAP2O6_A	CaP2O6		mS72	(9, Cc)	This is alpha-Ca(PO3)2.	2	(CA+2)1.0(PO3-1)2.0
CAP2O6_B	PbP2O6		mP72	(14, P2_1/c)	This is beta-Ca(PO3)2.	2	(CA+2)1.0(PO3-1)2.0
CAP2O6_G	CaP2O6		mP72	(9, Cc)	This is gamma-Ca(PO3)2.	2	(CA+2)1.0(PO3-1)2.0
CAP4O11_A	CaP4O11		oS128	(41, Aea2)	This is alpha- Ca(P2O5)2O.	3	(CA+2)1.0(P+5)4.0(O-2)11.0
CAP4O11_B	CaP4O11		mP64	(14, P2_1/c)	This is beta- Ca(P2O5)2O.	3	(CA+2)1.0(P+5)4.0(O-2)11.0
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)4.0(SI+4)4.0(O-2)16.0
CARNEGIEITE_B	NaAl[SiO4]		oP56	(29, Pca2_1)	This is NaAlSiO4 with solubility of Fe and Si.	3	(NAAL+4, NAFE+4, SI+4)4.0(SI+4)4.0(O-2)16.0
CASFEO	Unknown Structure				This is CaS.FeO and CaS.Fe2O3.	4	(CA+2)2.0(S-2)2.0(FE+2, FE+3)2.0(O-2, VA)3.0

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CASO4_HT	CePO4		hP18	(180, P6_222)	This is high- temperature (Ca,Co,Mg)SO4.	2	(CA+2, CO+2, MG+2)1.0(SO4-2)1.0
CAV2O4	CaV2O4		oP28	(62, Pnma)	This is CaO.Fe2O3, b-CaCr2O4 and Ca (V,Y,Yb)2O4.	3	(CA+2)1.0(AL+3, CR+3, FE+3, V+3, Y+3, YB+3)2.0(O-2)4.0
CAV2O5	CaV2O5		oP16	(59, Pmmn)		3	(CA+2)1.0(V+4)2.0(O-2)5.0
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)1.0 (V+5)2.0(O-2)6.0
CAV3O7	CaV3O7		oP44	(62, Pnma)		3	(CA+2)1.0(V+4)3.0(O-2)7.0
CAV4O9	CaV4O9		tP9	(85, P4/n)		3	(CA+2)1.0(V+4)4.0(O-2)9.0
CAVO3	Unknown Structure					3	(CA+2)1.0(V+4)1.0(O-2)3.0
CAWO4	Scheelite (CaWO4, H04)	H04	tI24	(88, I4_1/a)		3	(CA+2)1.0(W+6)1.0(O-2)4.0
CAY4O7	(Ca0.25Gd0.75)4GdO7		mS48	(12, C2/m)	This is CaY4O7 and CaGd4O7.	3	(CA+2)1.0(GD+3, Y+3)4.0(O-2)7.0
CAYAL3O7	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_ 1m)	This is CaYAl3O7, CaYbAl3O7 and CaGdAl3O7	4	(CA+2)1.0(GD+3, Y+3, YB+3)1.0(AL+3)3.0 (O-2)7.0
CAYALO4	K2NiF4		tI14	(139, I4/mmm)	This is CaYAlO4, CaYbAlO4 and CaGdAlO4	4	(CA+2)1.0(GD+3, Y+3, YB+3)1.0(AL+3)1.0 (O-2)4.0
CAZR4O9	CaZr4O9		mS224	(15, C2/c)		3	(CA+2)1.0(ZR+4)4.0(O-2)9.0
CAZRO3_C	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	High-temperature CaTiO3.	3	(CA+2, Y+3)1.0(HF+4, Y+3, ZR+4)1.0(O-2)3.0
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)1.0(B, C, N, VA)1.0
CEMENTITE_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(AL, CO, CR, FE, MN, MO, NB, NI, SI, V, W)3.0(B, C, N)1.0
CF2	Ca3.5Fe14O24.5		mS172	(5, C2)	This is CaO.2Fe2O3	3	(CA+2)1.0(FE+3)4.0(O-2)7.0

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CHALCOCITE_ALPHA	Cu2S-alpha		mP144	(14, P2_1/c)	This is Cu2S.	2	(CU)2.0(S)1.0
CHALCOCITE_BETA	Cu2S-beta		hP16	(194, P6_ 3/mmc)	This is Cu2S.	2	(CU)2.0(S)1.0
CHALCOPYRITE	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)	This is high-temperature nonstoichiometric CuFeS2.	3	(CU, FE, VA)1.0(CU, VA)1.0(S)1.0
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)1.0(CO+2, FE+2, MG+2, NI+2)1.0(SI+4)2.0(O-2)6.0
CO1LA2O4	La2CoO4		oP36	(55, Pbam)		3	(LA+3)2.0(CO+2)1.0(O-2)4.0
CO3LA4O10	Nd4Co3O10		mP68	(14, P2_1/c)		4	(LA+3)4.0(CO+2)1.0(CO+3)2.0(O-2)10.0
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)3.0(PO4-3)2.0
CO9S8	Co9S8 (D89)	D89	cF68	(225, Fm-3m)		2	(CO, FE, NI)9.0(S)8.0
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)1.0 (FE+2, MG+2, NB+5)2.0(O-2, VA)6.0
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)4.0(FE+2, MG+2, MN+2)2.0 (SI+4)5.0(O-2)18.0
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)2.0(O-2)3.0
COVELLITE	Covellite (CuS, B18)	B18	hP12	(194, P6_ 3/mmc)	This is CuS.	2	(CU)1.0(S)1.0
CR1S1	CrS		mS8	(15, C2/c)	This is low-temp CrS.	2	(CR)1.03(S)1.0
CR2P4O13	Cr2P4O13		mP76	(14, P2_1/c)	This is Cr2P4O13, Cr2V4O13 and	3	(CR+3, FE+3)2.0(P+5, V+5)4.0(O-2)13.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
					Fe2V4O13.		
CR2S3	Dolomite [MgCa(CO3)2, G11]	G11	hR10	(148, R-3)		2	(CR, FE)2.0(S)3.0
CR2TI2O7	Unknown Structure				with solubility of Al2O3 and Fe2O3.	3	(AL+3, CR+3, FE+3)2.0(TI+4)2.0(O-2)7.0
CR3P2O8	Unknown Structure					2	(CR+2)3.0(PO4-3)2.0
CR3PO7	Unknown Structure					3	(CR+3)3.0(P+5)1.0(O-2)7.0
CR3S4	Brezinaite (Cr3S4)		mS14	(12, C2/m)		2	(CR, FE, MN, NI)3.0(S)4.0
CR4P6O21	Unknown Structure					2	(CR+3)4.0(P2O7-4)3.0
CR5PO10	Unknown Structure					3	(CR+3)5.0(P+5)1.0(O-2)10.0
CR5S6	Cr5S6		hP22	(163, P-31c)		2	(CR)5.0(S)6.0
CR7S8	Cr7Se8		mS30	(12, C2/m)		2	(CR)7.0(S)8.0
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	(227, Fd-3m)	SiO2 with AlPO4 solubility.	2	(AL+3, SI+4)1.0(PO4-3, SIO4-4)1.0
CRNB25O64	Unknown Structure					3	(CR+3)1.0(NB+5)25.0(O-2)64.0
CRNB49O124	Unknown Structure					3	(CR+3)1.0(NB+5)49.0(O-2)124.0
CRNB9O24	Unknown Structure					3	(CR+3)1.0(NB+5)9.0(O-2)24.0
CRNBO4	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)		3	(CR+3, VA)1.0(CR+3, NB+5)1.0(O-2, VA)4.0
CRPO4	Cr[PO4]		oI72	(74, Imma)		2	(CR+3)1.0(PO4-3)1.0
CRVO4	MgSO4		oS24	(63, Cmcm)		3	(CR+3)1.0(V+5)1.0(O-2)4.0
CRYOLITE	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)	This is (K,Na)3AlF6 solid solution.	2	(K+1, NA+1, VA)3.0(ALF4-1, ALF6-3)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU2B4O7	Unknown Structure					3	(CU+1)2.0(B+3)4.0(O-2)7.0
CU2COO3	CaCu2O3		oP12	(59, Pmmn)		3	(CO+2)1.0(CU+2)2.0(O-2)3.0
CU2P2O7	alpha-Zn2V2O7		mS44	(15, C2/c)		2	(CU+2)2.0(P2O7-4)1.0
CU2SO4	Thenardite [Na2SO4 (V), H17]	H17	oF56	(70, Fddd)		2	(CU+1)2.0(SO4-2)1.0
CU2SO5	Cu2[SO4]O		mS32	(12, C2/m)		1	(CU2O5S1)1.0
CU2Y2O5	Cu2Ho2O5		oP36	(33, Pna2_1)		3	(CU+2)2.0(Y+3)2.0(O-2)5.0
CU3B2O6	Cu3B2O6		aP110	(2, P-1)		3	(CU+2)3.0(B+3)2.0(O-2)6.0
CU3NB2O8	Cu3(Ta0.5Nb0.5)2O8		aP13	(2, P-1)		3	(CU+2)3.0(NB+5)2.0(O-2)8.0
CU3P2O8	Unknown Structure					2	(CU+2)3.0(PO4-3)2.0
CUB2O4	CuB2O4		tI84	(122, I-42d)		3	(CU+2)1.0(B+3)2.0(O-2)4.0
CUB8O13	Unknown Structure					3	(CU+2)1.0(B+3)8.0(O-2)13.0
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)1.0(B, C, N, VA)1.0
CUCRS2	CuCrS2-b		hR4	(160, R3m)		3	(CU)1.0(CR)1.0(S)2.0
CUF1	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(CU+1)1.0(F-1)1.0
CUF2	CuF2		mP6	(14, P2_1/c)	This is CrF2 and CuF2.	2	(CR+2, CU+2)1.0(F-1)2.0
CUFES2_LT	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)	This is stoichiometric low- temperature CuFeS2.	3	(CU)1.0(FE)1.0(S)2.0
CUGD2O4	CuNd2O4		tI14	(139, I4/mmm)		3	(CU+2)1.0(GD+3)2.0(O-2)4.0

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CULA2O4	CuLa2O4		oS28	(64, Cmce)	With solubility of Co.	3	(CO+2, CU+2)1.0(LA+3)2.0(O-2)4.0
CUNB2O6	CuNb2O6		mP36	(14, P2_1/c)		3	(CU+2)1.0(NB+5)2.0(O-2)6.0
CUO	Tenorite (CuO, B26)	B26	mS8	(15, C2/c)		2	(CO+2, CU+2)1.0(O-2)1.0
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)1.0(PO3-1)2.0
CUPO3	Unknown Structure					2	(CU+1)1.0(PO3-1)1.0
CUPRITE	Cuprite (Cu2O, C3)	C3	cP6	(224, Pn-3m)	This is Cu2O with solubility of Na.	2	(CU+1, NA+1)2.0(O-2)1.0
CUSPIDINE	Ca4[Si2O7]([OH]0.25F0.75)2		mP60	(14, P2_1/c)	This is 3CaO.2SiO2.CaF2	4	(CA+2)4.0(SI+4)2.0(O-2)7.0(F-1)2.0
CW3F	CaFe5O7		oS52	(63, Cmcm)	This is CaO.3FeO.Fe2O3.	4	(CA+2)1.0(FE+2)3.0(FE+3)2.0(O-2)7.0
CWF	CaFe3O5		oS36	(63, Cmcm)	This is CaO.FeO.Fe2O3.	4	(CA+2)1.0(FE+2)1.0(FE+3)2.0(O-2)5.0
DANBURITE	Danburite (CaB2Si2O8, S63)	S63	oP52	(62, Pnma)		4	(CA+2)1.0(B+3)2.0(SI+4)2.0(O-2)8.0
DELAFOSSITE	Rhombohedral Delafossite (CuFeO2)		hR4	(166, R-3m)	This is Cu(Al,B,Cr,Fe,La,Mn,Y)O2	3	(CU+1)1.0(AL+3, B+3, CR+3, FE+3, LA+3, MN+3, Y+3)1.0(O-2)2.0
DHCP	alpha-La (A3')	A3'	hP4	(194, P6_ 3/mmc)		2	(AL, CA, CU, GD, LA, MG, MN, NI, Y)1.0 (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)1.0(O, VA)1.0
DIGENITE	Cu2Se		cF44	(225, Fm-3m)	This is Cu2S with solubility of Fe, Mg and Mn.	3	(CU, FE, MG, MN, VA)2.0(CU, VA)1.0 (S)1.0
DJURLEITE	Cu31S16		mP376	(14, P2_1/c)	This is Cu31S16.	2	(CU)1.93(S)1.0
DYMN2O5	HoMn2O5		oP32	(55, Pbam)	This is Mn2(Gd, Y)O5.	4	(GD+3, Y+3)1.0(MN+3)1.0(MN+4)1.0(O-2)5.0
ETA_M5SIN	Fe3W3C (E93)	E93	cF112	(227, Fd-3m)		4	(CR, MO)3.0(FE, NI)2.0(SI)1.0(N)1.0

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F6NA2SI1_A	Na2SiF6		hP27	(150, P321)		3	(NA+1)2.0(SI+4)1.0(F-1)6.0
F6NA2SI1_B	K2PtCl6 (J11)	J11	cF36	(225, Fm-3m)		3	(NA+1)2.0(SI+4)1.0(F-1)6.0
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, CA, CO, CR, CU, FE, GD, HF, K, LA, MG, MN, MO, NA, NB, NI, P, S, SI, TI, V, VA, W, Y, YB, ZR)1.0(B, C, N, O, VA)1.0
FE18P2O24	Fe4(Fe0.5P0.5)O6		oS44	(65, Cmmm)		4	(FE+2)16.0(FE+3)2.0(PO4-3)2.0(O-2)16.0
FE2O12S3	Fe2[SO4]3		hR34	(148, R-3)	This is (Al,Cr, Fe)2(SO4)3	2	(AL+3, CR+3, FE+3)2.0(SO4-2)3.0
FE2P2O7	Fe2[P2O7]		aP11	(2, P-1)		2	(FE+2)2.0(P2O7-4)1.0
FE2PO5	Fe2[PO4]O		mS32	(15, C2/c)		4	(FE+2)1.0(FE+3)1.0(PO4-3)1.0(O-2)1.0
FE3BO5	Fe3[BO3]O2		oP36	(55, Pbam)		4	(FE+2)2.0(FE+3)1.0(B+3)1.0(O-2)5.0
FE3BO6	Norbergite [Mg(F,OH)2 . Mg2SiO4, S07]	S07	oP40	(62, Pnma)		3	(FE+3)3.0(B+3)1.0(O-2)6.0
FE3P4O14	Unknown Structure					3	(FE+2)1.0(FE+3)2.0(P2O7-4)2.0
FE3PO7	Fe3PO7		hR11	(160, R3m)		3	(FE+3)3.0(P+5)1.0(O-2)7.0
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	(221, Pm-3m)		2	(CO, CR, FE, MN, NI)4.0(C, N, VA)1.0
FE4P6O21	Fe4[P2O7]3		mP124	(14, P2_1/c)		2	(FE+3)4.0(P2O7-4)3.0
FE7P6O24	Fe7[PO4]6		aP37	(2, P-1)		3	(FE+2)3.0(FE+3)4.0(PO4-3)6.0
FE7P8O28	Unknown Structure					3	(FE+2)5.0(FE+3)2.0(P2O7-4)4.0
FE8SI2C	Mn8Si2C		aP*	(1, P1)		3	(FE, MN)8.0(SI)2.0(C)1.0
FEAL2S4	ZnIn2S4		hR7	(160, R3m)		3	(FE)1.0(AL)2.0(S)4.0

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FEB4O7	ZnB4O7		oS48	(63, Cmcm)		3	(FE+2)1.0(B+3)4.0(O-2)7.0
FEBO3	Calcite (CaCO3, G01)	G01	hR10	(167, R-3c)		3	(FE+3)1.0(B+3)1.0(O-2)3.0
FEF3	FeF3 (D012)	D012	hR8	(167, R-3c)	This is (Al,Co,Cr, Fe)F3.	2	(AL+3, CO+3, CR+3, FE+3)1.0(F-1)3.0
FENB14O36	Unknown Structure				This is (Co, Fe)Nb14O36	3	(CO+2, FE+2)1.0(NB+5)14.0(O-2)36.0
FENB25O64	Unknown Structure					3	(FE+3)1.0(NB+5)25.0(O-2)64.0
FENB36O91	Unknown Structure				This is (Co, Fe)Nb36O91	3	(CO+2, FE+2)1.0(NB+5)36.0(O-2)91.0
FENB49O124	Unknown Structure					3	(FE+3)1.0(NB+5)49.0(O-2)124.0
FENB68O171	Unknown Structure				This is (Co, Fe)Nb68O171	3	(CO+2, FE+2)1.0(NB+5)68.0(O-2)171.0
FENB9O24	Unknown Structure					3	(FE+3)1.0(NB+5)9.0(O-2)24.0
FEV2O6	Unknown Structure					3	(FE+2)1.0(V+5)2.0(O-2)6.0
FEVO4	Zn[MoO4]		aP36	(2, P-1)	This is FeVO4 and AlVO4.	3	(AL+3, FE+3)1.0(V+5)1.0(O-2)4.0
FLUORITE	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is cubic high temp HfO2 and ZrO2	2	(AL+3, 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)2.0 (O-2, VA)4.0
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)3.0(AL+3, CR+3, FE+3, MG+2, V+3)2.0(AL+3, CR+3, FE+3, SI+4)3.0(O-2)12.0
GD2SI2O7	Ce2Si2O7		mP44	(14, P2_1/c)	This is (Gd, La)2Si2O7	3	(GD+3, LA+3)1.0(GD+3, LA+3)1.0(SI2O7-6)1.0
GD2SIO5	Gd2SiO5 (RE2SiO5 X1)		mP32	(14, P2_1/c)	This is (Gd,La)2SiO5	4	(GD+3, LA+3)1.0(GD+3, LA+3)1.0(SIO4-4)1.0(O-2)1.0

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GDBO3	GdBO3		hR30	(155, R32)	This is (Gd,La)BO3 solid solution.	3	(GD+3, LA+3)1.0(B+3)1.0(O-2)3.0
GDF3	H3Ho		hP24	(165, P-3c1)	This is high temp (Gd, Y,Yb)F3.	2	(GD+3, Y+3, YB+3)1.0(F-1)3.0
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_ 3/mmc)	Graphite	1	(B, C)1.0
GUGGENITE	CaCu2O3		oP12	(59, Pmmn)		3	(MG+2)0.825(CU+2)2.175(O-2)3.0
HALITE	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is CaO, CoO, FeO, MgO, MnO and NiO	2	(AL+3, CA+2, CO+2, CO+3, CR+3, CU+2, FE+2, FE+3, GD+3, MG+2, MN+2, MN+3, NA+1, NI+2, NI+3, TI+4, V+3, VA, Y+3, YB+3, ZR+4)1.0(O-2)1.0
HATRURITE	Ca3(SiO4)O-b		hR81	(160, R3m)	This is 3CaO.SiO2	3	(CA+2, GD+3, VA, Y+3)3.0(SIO4-4)1.0(O-2)1.0
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	HCP_A3 also describes hexagonal carbides and nitrades.	2	(AL, CA, CO, CR, CU, FE, GD, HF, K, LA, MG, MN, MO, NA, NB, NI, SI, TI, V, W, Y, YB, ZR)1.0(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)2.0(S)1.0
HEAZLEWOODITE_B2	Unknown Structure				This is non- stoichiometric high temperature Ni4S3.	2	(FE, NI, VA)2.0(S)1.0
HFW2O8	Zr[WO4]2		cP44	(198, P2_13)		3	(HF+4)1.0(W+6)2.0(O-2)8.0
K10MG5SI11O32	Unknown Structure					4	(K+1)10.0(MG+2)5.0(SI+4)11.0(O-2)32.0
K2CA2SI2O7	K2Ca2[Si2O7]		hP108	(176, P6_3/m)		4	(K+1)2.0(CA+2)2.0(SI+4)2.0(O-2)7.0
K2CA2SI9O21	Unknown Structure					4	(K+1)2.0(CA+2)2.0(SI+4)9.0(O-2)21.0
K2CA3SI6O16	Unknown Structure					4	(K+1)2.0(CA+2)3.0(SI+4)6.0(O-2)16.0
K2CA6SI4O15	K2Ca6Si4O15		mP54	(13, P2/c)		4	(K+1)2.0(CA+2)6.0(SI+4)4.0(O-2)15.0

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K2CASIO4	Unknown Structure					4	(K+1)2.0(CA+2)1.0(SI+4)1.0(O-2)4.0
K2CO3_S1	K2[CO3]		mP24	(14, P2_1/c)	With solubility of Na.	2	(K+1, NA+1)2.0(CO3-2)1.0
K2FE2SI6O16	Unknown Structure					4	(K+1)2.0(FE+3)2.0(SI+4)6.0(O-2)16.0
K2FESI3O8	Unknown Structure					4	(K+1)2.0(FE+2)1.0(SI+4)3.0(O-2)8.0
K2FESI5O12	K16Mg8Si40O96		mP160	(14, P2_1/c)		4	(K+1)2.0(FE+2)1.0(SI+4)5.0(O-2)12.0
K2MG3B2O7	Unknown Structure					4	(K+1)2.0(MG+2)3.0(B+3)2.0(O-2)7.0
K2MG5SI12O30	K2Mg5Si12O30		hP100	(192, P6/mcc)		4	(K+1)2.0(MG+2)5.0(SI+4)12.0(O-2)30.0
K2MGF4	K2NiF4		tI14	(139, I4/mmm)		3	(MG+2)1.0(K+1)2.0(F-1)4.0
K2MGN4O12	Unknown Structure					3	(K+1)2.0(MG+2)1.0(NO3-1)4.0
K2MGSIO4_HT	Unknown Structure					2	(K2MG+4, SI+4)1.0(SIO4-4)1.0
K2MGSIO4_LT	Na2Be[SiO4]		oP64	(29, Pca2_1)		2	(K2MG+4, SI+4)1.0(SIO4-4)1.0
K2S2	Na2O2		hP12	(189, P-62m)		2	(K)2.0(S)2.0
K2S3	K2S3		oS20	(36, Cmc2_1)		2	(K)2.0(S)3.0
K2S4	Unknown Structure					2	(K)2.0(S)4.0
K2S5	Tl2S5		oP28	(19, P2_12_12_1)		2	(K)2.0(S)5.0
K2S6	Unknown Structure					2	(K)2.0(S)6.0
K2SI4O9_ALPHA	K2Si4O9		aP30	(2, P-1)	Low-temp K2Si4O9	3	(K+1)2.0(SI+4)4.0(O-2)9.0
K2SI4O9_BETA	K2Si4O9		hP30	(176, P6_3/m)	High-temp K2Si4O9	3	(K+1)2.0(SI+4)4.0(O-2)9.0

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K2TI3O7	Unknown Structure					3	(K+1)2.0(TI+4)3.0(O-2)7.0
K2TI6O13	Na2Ti6O13		mS42	(12, C2/m)		3	(K+1)2.0(TI+4)6.0(O-2)13.0
K2TIO3	Cs2PbO3		oS24	(63, Cmcm)		3	(K+1)2.0(TI+4)1.0(O-2)3.0
K3FCO3	Unknown Structure					3	(K+1)3.0(F-1)1.0(CO3-2)1.0
K3PO4_ALPHA	Unknown Structure				low-temp	2	(K+1)3.0(PO4-3)1.0
K3PO4_BETA	Unknown Structure				mid-temp	2	(K+1)3.0(PO4-3)1.0
K3PO4_GAMMA	K3[PO4]-ht		cF32	(202, Fm-3)	high-temp	2	(K+1)3.0(PO4-3)1.0
K4AL22O35	K2Al10.67O17		hR30	(166, R-3m)	This is Beta double prime-Al2O3 K4 (AL,Fe)22O35 solid solution.	6	(K+1, VA)1.0(K+1, VA)1.0(AL+3, FE+3, MG+2)2.0(O-2, VA)1.0(AL+3, FE+3)9.0(O-2)17.0
K4B6O11	Unknown Structure					3	(K+1)4.0(B+3)6.0(O-2)11.0
K4CAN6O18	Unknown Structure					3	(K+1)4.0(CA+2)1.0(NO3-1)6.0
K4CASI3O9	K4SrGe3O9		cP272	(205, Pa-3)		4	(K+1)4.0(CA+2)1.0(SI+4)3.0(O-2)9.0
K4CASI6O15	Unknown Structure					4	(K+1)4.0(CA+2)1.0(SI+4)6.0(O-2)15.0
K4FE4SI3O14	Unknown Structure					4	(K+1)4.0(FE+3)4.0(SI+4)3.0(O-2)14.0
K4FEO3	Unknown Structure					3	(K+1)4.0(FE+2)1.0(O-2)3.0
K4MG2SI5O14	Unknown Structure					4	(K+1)4.0(MG+2)2.0(SI+4)5.0(O-2)14.0
K4P2O7_ALPHA	K4[P2O7]		hP234	(169, P6_1)		2	(K+1)4.0(P2O7-4)1.0
K4P2O7_BETA	K4[P2O7]		hP26	(194, P6_ 3/mmc)		2	(K+1)4.0(P2O7-4)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
K4P2O7_DELTA	Unknown Structure					2	(K+1)4.0(P2O7-4)1.0
K4P2O7_GAMMA	Unknown Structure					2	(K+1)4.0(P2O7-4)1.0
K4SIO4	Cs4SnO4		mP36	(14, P2_1/c)		3	(K+1)4.0(SI+4)1.0(O-2)4.0
K4TIO4	Unknown Structure					3	(K+1)4.0(TI+4)1.0(O-2)4.0
K5B19O31	K5B19O31		mS220	(15, C2/c)		3	(K+1)5.0(B+3)19.0(O-2)31.0
K5P3O10_ALPHA	Unknown Structure					3	(K+1)5.0(P+5)3.0(O-2)10.0
K5P3O10_BETA	Unknown Structure					3	(K+1)5.0(P+5)3.0(O-2)10.0
K8CASI10O25	Unknown Structure					4	(K+1)8.0(CA+2)1.0(SI+4)10.0(O-2)25.0
K8TI5O14	Unknown Structure					3	(K+1)8.0(TI+4)5.0(O-2)14.0
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)1.0(K+1, VA)1.0(AL+3, FE+3, MG+2)2.0(O-2, VA)1.0(AL+3, FE+3)9.0(O-2)17.0
KALSI2O6	K8(Al0.33Si0.67)24O48		tI160	(88, I4_1/a)	This is KAlSi2O6-KFeSi2O6-K2MgSi5O12 solid solution.	5	(K+1)2.0(AL+3, FE+3, MG+2)1.0(AL+3, FE+3, SI+4)1.0(SI+4)4.0(O-2)12.0
KALSIO4_HT	KLi[SO4]		hP14	(159, P31c)	This is high temperature KAlSiO4-K2MgSi3O8 ss. with SiO2 solubility	4	(K2MG+4, KAL+4)1.0(KAL+4, SI+4)1.0 (SI+4)2.0(O-2)8.0
KAPPA_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(AL)1.0(FE, MN)3.0(C, VA)1.0
KB9O14	Unknown Structure					3	(K+1)1.0(B+3)9.0(O-2)14.0
KBSI2O6	K(Si0.67B0.33)3O6		cI160	(220, I-43d)	Lisitsynite	4	(K+1)1.0(B+3)1.0(SI+4)2.0(O-2)6.0
KBSI3O8	Danburite (CaB2Si2O8, S63)	S63	oP52	(62, Pnma)		4	(K+1)1.0(B+3)1.0(SI+4)3.0(O-2)8.0
KCAF3	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(CA+2, MG+2)1.0(K+1)1.0(F-1)3.0

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KFESIO4	Unknown Structure					4	(K+1)2.0(FE+3)2.0(SI+4)2.0(O-2)8.0
KMG2AL15O25	Unknown Structure					4	(K+1)1.0(MG+2)2.0(AL+3)15.0(O-2)25.0
KNO3_S1	alpha-Potassium Nitrate (KNO3) I		oP20	(62, Pnma)	This is lt-KNO3 with solubility of Na.	2	(K+1, NA+1)1.0(NO3-1)1.0
KPO3_ALPHA	KPO3		mP40	(14, P2_1/c)		2	(K+1)1.0(PO3-1)1.0
KPO3_BETA	alpha-Potassium Nitrate (KNO3) I		oP20	(62, Pnma)		2	(K+1)1.0(PO3-1)1.0
KPO3_GAMMA	KPO3		oS32	(63, Cmcm)		2	(K+1)1.0(PO3-1)1.0
KSI_CARBIDE	Mo6Fe11C5		mS44	(12, C2/m)		2	(CR, FE, MO, W)3.0(C)1.0
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	(2, P-1)	This is Al2O3.SiO2	4	(AL+3)1.0(AL+3)1.0(SI+4)1.0(O-2)5.0
LA1S2	CeSe2		mP12	(14, P2_1/c)		2	(LA)1.0(S)2.0
LA2CR3O12	Unknown Structure					3	(LA+3)2.0(CR+6)3.0(O-2)12.0
LA2CRO6	Unknown Structure					3	(LA+3)2.0(CR+6)1.0(O-2)6.0
LA2MNO4	K2NiF4		tI14	(139, I4/mmm)	La2(Mn,Ni)O4 with Co solubility.	3	(LA+3)2.0(CO+2, MN+2, NI+2)1.0(O-2)4.0
LA2NB12O33	Unknown Structure					3	(LA+3)2.0(NB+5)12.0(O-2)33.0
LA2S3	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)	This is (Gd,La)2S3.	2	(GD, LA)2.0(S)3.0
LA2TI3O9	Unknown Structure					3	(LA+3)2.0(TI+4)3.0(O-2)9.0
LA3BO6	Unknown Structure				This is (Gd, La)3BO6 solid solution.	3	(GD+3, LA+3)3.0(B+3)1.0(O-2)6.0
LA3NBO7	La3NbO7		oP44	(62, Pnma)		3	(LA+3)3.0(NB+5)1.0(O-2)7.0
LA3NI2O7	Sr3Sn2O7		oS48	(63, Cmcm)		4	(LA+3)3.0(CO+2, NI+2)1.0(NI+3)1.0(O-

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							2)7.0
LA4NI3O10	La4Ni3O10		oS68	(64, Cmce)	La4Ni3O10 with Co solubility.	4	(LA+3)4.0(NI+2)1.0(CO+3, NI+3)2.0(O-2)10.0
LA4SI3O12	Unknown Structure					2	(LA+3)4.0(SIO4-4)3.0
LA4TI3O12	La4Ti3O12		hR19	(148, R-3)		3	(LA+3)4.0(TI+4)3.0(O-2)12.0
LA4TI9O24	Nd4Ti9O24		oF592	(70, Fddd)		3	(LA+3)4.0(TI+4)9.0(O-2)24.0
LAAL11O18	La0.83Al11.83O19		hP86	(194, P6_3/mmc)		3	(LA+3)1.0(AL+3)11.0(O-2)18.0
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)1.0(AL+3, CO+3, CU+2, FE+3, NI+2)1.0(O-2, VA)3.0
LAB3O6	LaB3O6		mS40	(15, C2/c)	This is (Gd,La)B3O6 solid solution.	3	(GD+3, LA+3)1.0(B+3)3.0(O-2)6.0
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)1.0(F-1)3.0
LAFE12O19	Unknown Structure					4	(LA+3)1.0(FE+2)1.0(FE+3)11.0(O-2)19.0
LANB3O9	La0.67Nb2O6-b		oS36	(65, Cmmm)		3	(LA+3)1.0(NB+5)3.0(O-2)9.0
LANBO4	LaNbO4		mS24	(15, C2/c)		3	(LA+3)1.0(NB+5)1.0(O-2)4.0
LANIO3	PrNiO3		hR10	(167, R-3c)	This is a rhombohedral perovskite	3	(LA+3)1.0(NI+3)1.0(O-2)3.0
LARNITE	Parawollastonite (CaSiO3, S33(II))	S33(II)	mP60	(14, P2_1/c)	This is 2CaO.SiO2 (metastable at 1 atm)	3	(CA+2)2.0(SI+4)1.0(O-2)4.0
LAYP	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)	This is an Orthorhombic Perovskite, La(Y,Yb)O3.	3	(LA+3, Y+3, YB+3)1.0(LA+3, VA, Y+3, YB+3, ZR+4)1.0(O-2)3.0
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)1.0(MG+2)1.0(SI+4)2.0(O-2)6.0
M12C	Fe6W6C		cF104	(227, Fd-3m)		3	(CO)6.0(W)6.0(C)1.0

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M23C6_D84	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)		3	(CO, CR, FE, MN, NI, V)20.0(CO, CR, FE, MN, MO, NI, V, W)3.0(B, C)6.0
M2O3A	La2O3 (D52)	D52	hP5	(164, P-3m1)	A-LA2O3. Also hexagonal A-type structure of Gd2O3.	3	(CA+2, GD+3, HF+4, LA+3, MG+2, Y+3, YB+3, ZR+4)2.0(O-2, VA)3.0(O-2, VA)1.0
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)2.0(O-2, VA)3.0(O-2, VA)1.0
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)2.0(O-2, VA)3.0(O-2, VA)1.0
M2O3H	La2O3 (D52)	D52	hP5	(164, P-3m1)	H-La2O3. This is also hexagonal (Gd,Y,Yb)2O3.	3	(CA+2, GD+3, HF+4, LA+3, MG+2, MN+3, Y, Y+3, YB+3, ZR+4)2.0(O-2, VA)3.0(O-2, VA)1.0
M2O3X	Nd2O3		cI26	(229, Im-3m)	X-LA2O3. This is also HT cubic X-type structure of Gd2O3.	3	(CA+2, GD+3, HF+4, LA+3, MG+2, Y+3, YB+3, ZR+4)2.0(O-2, VA)3.0(O-2, VA)1.0
M3C2_D510	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(CO, CR, MO, V, W)3.0(C)2.0
M4O7	Ti4O7-a		aP22	(2, P-1)	This is Ti4O7 and V4O7 with solubility of Al and Mn.	2	(AL, MN, TI, V)4.0(O)7.0
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(FE, MN, NB, V)5.0(C, N)2.0
M6C_E93	Fe3W3C (E93)	E93	cF112	(227, Fd-3m)		4	(CO, FE, NI)2.0(MO, NB, W)2.0(CO, CR, FE, MO, NB, NI, SI, V, W)2.0(C)1.0
M6O11	Ti6O11		aP34	(2, P-1)	This is Ti6O11 and V6O11.	2	(TI, V)6.0(O)11.0
M7C3_D101	C3Cr7 (D101)	D101	oP40	(62, Pnma)		2	(AL, CO, CR, FE, MN, MO, NB, NI, SI, V, W)7.0(B, C)3.0
M7O13	Ti7O13		aP40	(2, P-1)	This is Ti7O13 and V7O13.	2	(TI, V)7.0(O)13.0
M8O15	Ti8O15		aP46	(2, P-1)	This is Ti8O15 and V8O15.	2	(TI, V)8.0(O)15.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MALINKOITE	BaZn[GeO4]		hP42	(173, P6_3)	NaBSiO4 with SiO2 solubility	2	(NAB+4, SI+4)1.0(SIO4-4)1.0
MC_ETA	CMo		hP12	(194, P6_ 3/mmc)		2	(MO, TI, V, W)1.0(C, VA)1.0
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	(187, P-6m2)		2	(MO, W)1.0(C, N)1.0
MELILITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_ 1m)	This is gehlenite, akermanite, Fe-akermanite and 2CaO.CoO.2SiO2.	5	(CA+2, NA+1)2.0(AL+3, CO+2, FE+2, FE+3, MG+2)1.0(AL+3, SI+4)1.0(SI+4)1.0(O-2)7.0
MERWINITE	Ca3Mg(SiO4)2		mP56	(14, P2_1/c)	This is 3CaO.MgO.2SiO2	4	(CA+2)3.0(MG+2)1.0(SI+4)2.0(O-2)8.0
MG2B2O5	Co2B2O5		aP18	(2, P-1)	This is (Co,Fe,Mg, Ni)2B2O5	3	(CO+2, FE+2, MG+2, NI+2)2.0(B+3)2.0(O-2)5.0
MG2C3	Mg2C3		oP10	(58, Pnnm)		2	(MG)2.0(C)3.0
MG2HF5O12	UY6O12		hR19	(148, R-3)		3	(MG+2)2.0(HF+4)5.0(O-2)12.0
MG2NA2SI6O15	Na2Mg2Si6O15		oS200	(64, Cmce)		4	(MG+2)2.0(NA+1)2.0(SI+4)6.0(O-2)15.0
MG2NB34O87	Unknown Structure					3	(MG+2)2.0(NB+5)34.0(O-2)87.0
MG2P2O7_A	Unknown Structure				This is alpha- Mg2(P2O7).	2	(CA+2, MG+2)2.0(P2O7-4)1.0
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)2.0(P2O7-4)1.0
MG2V2O7	Co2[V2O7]		mP44	(14, P2_1/c)	This is Co2V2O7, Mg2V2O7 and Ni2V2O7.	3	(CO+2, MG+2, NI+2)2.0(V+5)2.0(O-2)7.0
MG3N2_D53	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)		2	(CA, MG)3.0(N)2.0
MG3V2O8	Ni3[VO4]2		oS52	(64, Cmce)	This is Co3V2O8, Mg3V2O8 and Ni3V2O8.	3	(CO+2, MG+2, NI+2)3.0(V+5)2.0(O-2)8.0
MG5NB4O15	Ta3N5		oS32	(63, Cmcm)		3	(MG+2)5.0(NB+5)4.0(O-2)15.0
MGB4O7	CdB4O7		oP96	(61, Pbca)		3	(MG+2)1.0(B+3)4.0(O-2)7.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MGC2	MgC2		tP6	(136, P4_ 2/mnm)		2	(MG)1.0(C)2.0
MGF2	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)	This is (Co,Fe,Mg,Mn,Ni,V)F2.	2	(CO+2, FE+2, MG+2, MN+2, NI+2, V+2)1.0(F-1)2.0
MGNA2SI4O10	Unknown Structure					4	(MG+2)1.0(NA+1)2.0(SI+4)4.0(O-2)10.0
MGP4O11	MgP4O11		mP64	(14, P2_1/c)		3	(MG+2)1.0(P+5)4.0(O-2)11.0
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)1.0(NB+5, W+6)1.0(O-2)4.0
MN2B4O9	Unknown Structure					3	(MN+3)2.0(B+3)4.0(O-2)9.0
MN2P2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	(12, C2/m)		2	(MN+2)2.0(P2O7-4)1.0
MN2V2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	(12, C2/m)		3	(MN+2)2.0(V+5)2.0(O-2)7.0
MN3N2	Mn3N2		tI10	(139, I4/mmm)		2	(MN)3.0(N)2.0
MN3P2O8	Unknown Structure					2	(MN+2)3.0(PO4-3)2.0
MN4NB2O9	Nb2Mn4O9		hP30	(165, P-3c1)	This is (Co,Fe, Mg,Mn)4Nb2O9.	3	(CO+2, FE+2, MG+2, MN+2)4.0(NB+5)2.0(O-2)9.0
MN5SIC	Mn5SiC		oS56	(36, Cmc2_1)		3	(MN)0.714(SI)0.143(C)0.143
MN6N5	CoO		tI4	(139, I4/mmm)		2	(MN)6.0(N)5.0
MN9SI3O14S1	Unknown Structure				This is 8MnO.3SiO2.MnS	4	(MN+2)9.0(SI+4)3.0(O-2)14.0(S-2)1.0
MNB2O4	Unknown Structure					3	(MN+2)1.0(B+3)2.0(O-2)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MNB3O6	Unknown Structure					3	(MN+3)1.0(B+3)3.0(O-2)6.0
MNB4O7	Unknown Structure					3	(MN+2)1.0(B+3)4.0(O-2)7.0
MNB6O10	Unknown Structure					3	(MN+2)1.0(B+3)6.0(O-2)10.0
MNBO3	Unknown Structure					3	(MN+3)1.0(B+3)1.0(O-2)3.0
MNF2_S1	Unknown Structure					2	(MN+2)1.0(F-1)2.0
MNF3	MnF3		mS48	(15, C2/c)		2	(MN+3)1.0(F-1)3.0
MNYO3_HEX	LuMnO3		hP30	(185, P6_3cm)		3	(Y+3)1.0(MN+3)1.0(O-2)3.0
MO1S2	Molybdenite (MoS2, C7)	C7	hP6	(194, P6_ 3/mmc)	This is MoS2 and WS2.	2	(MO, W)1.0(S)2.0
MO2S3	Mo2S3		mP10	(11, P2_1/m)		2	(MO)2.0(S)3.0
MO4O11	Mo4O11		oP60	(33, Pna2_1)		3	(MO+4)1.0(MO+6)3.0(O-2)11.0
MO8O23	High-Temperature Mo8O23		mP62	(13, P2/c)		3	(MO+4)1.0(MO+6)7.0(O-2)23.0
MO9O26	Mo9O26		mP70	(13, P2/c)		3	(MO+4)1.0(MO+6)8.0(O-2)26.0
MOF4	Unknown Structure					2	(MO+4)1.0(F-1)4.0
MONOCLINIC_S	beta-S		mP48	(14, P2_1/c)		1	(S)1.0
MOO3	gamma-WO3		mP32	(14, P2_1/c)		2	(MO+6)1.0(O-2)3.0
MULLITE	Al(Al0.7Si0.3)2O4.8		oP24	(55, Pbam)	With solubility of B, Cr and Fe.	4	(AL+3)1.0(AL+3, CR+3, FE+3)1.0(AL+3, B+3, SI+4)1.0(O-2, VA)5.0
NA10SIO7	Unknown Structure					3	(NA+1)10.0(SI+4)1.0(O-2)7.0
NA2AL12O19	Na0.5Al3O4.75		oP24	(55, Pbam)	This is Beta double prime-Al2O3 Na2Al12O19 with solubility of Fe.	3	(NA+1)2.0(AL+3, FE+3)12.0(O-2)19.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NA2AL2B2O7	Na2Ga2[BO3]2O		hP30	(163, P-31c)		4	(NA+1)2.0(AL+3)2.0(B+3)2.0(O-2)7.0
NA2B4O7	Na2B4O7		aP52	(2, P-1)	This is (K, Na)2B4O7.	3	(K+1, NA+1)2.0(B+3)4.0(O-2)7.0
NA2B8O13	Na2B8O13		mP92	(14, P2_1/c)		3	(NA+1)2.0(B+3)8.0(O-2)13.0
NA2CA3AL16O28	Unknown Structure					4	(NA+1)2.0(CA+2)3.0(AL+3)16.0(O-2)28.0
NA2CA8AL6O18	Unknown Structure					4	(NA+1)2.0(CA+2)8.0(AL+3)6.0(O-2)18.0
NA2CAAL4O8	Unknown Structure				This is (K, Na)2CaAl4O8 solid solution.	4	(K+1, NA+1, VA)1.0(CA+2, K+1, NA+1)1.0 (AL+3)2.0(O-2)4.0
NA2CO3_S1	Na2[CO3]-b		mS24	(12, C2/m)	With solubility of K.	2	(K+1, NA+1)2.0(CO3-2)1.0
NA2CO3_S2	Na2[CO3]		hP12	(194, P6_ 3/mmc)	This is (K, Na)2CO3 solid solution.	2	(K+1, NA+1)2.0(CO3-2, S-2)1.0
NA2FEO2	Unknown Structure					3	(NA+1)2.0(FE+2)1.0(O-2)2.0
NA2FESIO4	Unknown Structure					4	(NA+1)2.0(FE+2)1.0(SI+4)1.0(O-2)4.0
NA2O1_S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is rt (K,Na)2O.	2	(K+1, NA+1)2.0(O-2)1.0
NA2O1_S2	Unknown Structure				This is ht1 (K, Na)2O.	2	(K+1, NA+1)2.0(O-2)1.0
NA2O1_S3	Unknown Structure				This is ht2 (K, Na)2O.	2	(K+1, NA+1)2.0(O-2)1.0
NA2S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is (K,Na)2S.	2	(K, NA)2.0(S)1.0
NA2SI2O5_ALPHA	Na2Si2O5-a		mP36	(14, P2_1/c)	This is lt-(K, Na)2Si2O5 solid solution.	3	(K+1, NA+1)2.0(SI+4)2.0(O-2)5.0
NA2SI2O5_BETA	Na2Si2O5-b		mP36	(14, P2_1/c)	This is intermediat-temp (K,Na)2Si2O5 solid solution.	3	(K+1, NA+1)2.0(SI+4)2.0(O-2)5.0
NA2SI2O5_GAMMA	Na2Si2O5		oP36	(60, Pbcn)	This is ht-(K, Na)2Si2O5 solid solution.	3	(K+1, NA+1)2.0(SI+4)2.0(O-2)5.0

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NA2SIO3	Na2SiO3		oS24	(36, Cmc2_1)	This is (K, Na)2SiO3 solid solution.	3	(K+1, NA+1)2.0(SI+4)1.0(O-2)3.0
NA2TI3O7	Na2Ti3O7		mP24	(11, P2_1/m)		3	(NA+1)2.0(TI+4)3.0(O-2)7.0
NA2TI6O13	Na2Ti6O13		mS42	(12, C2/m)		3	(NA+1)2.0(TI+4)6.0(O-2)13.0
NA2TIO3_S1	Na2TiO3		mS24	(12, C2/m)		3	(NA+1)2.0(TI+4)1.0(O-2)3.0
NA2TIO3_S2	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		3	(NA+1)2.0(TI+4)1.0(O-2)3.0
NA2V2O6	LiVO3		mS40	(9, Cc)		3	(NA+1)2.0(V+5)2.0(O-2)6.0
NA3ALF6_S1	Cryolite (Na3AlF6, J26)	J26	mP20	(14, P2_1/c)		3	(NA+1)3.0(AL+3)1.0(F-1)6.0
NA3BO3	NaB3O5-a		mP108	(14, P2_1/c)	This is (K, Na)3BO3.	3	(K+1, NA+1)3.0(B+3)1.0(O-2)3.0
NA3FE5O9	Na3Fe5O9		mS68	(15, C2/c)		3	(NA+1)3.0(FE+3)5.0(O-2)9.0
NA3FEO3	Na3FeO3		mP28	(14, P2_1/c)		3	(NA+1)3.0(FE+3)1.0(O-2)3.0
NA3PO4	Na3[PO4]		cF988	(225, Fm-3m)	This is Na3(PO4, VO4)	2	(NA+1)3.0(PO4-3, VO4-3)1.0
NA4B2O5	Na4B2O5		mS44	(15, C2/c)	This is (K, Na)4B2O5.	3	(K+1, NA+1)4.0(B+3)2.0(O-2)5.0
NA4FE6O11	Unknown Structure					3	(NA+1)4.0(FE+3)6.0(O-2)11.0
NA4FEO3	Na4FeO3		mS32	(9, Cc)		3	(NA+1)4.0(FE+2)1.0(O-2)3.0
NA4P2O7	Na4[P2O7]		oP52	(19, P2_12_12_1)		2	(NA+1)4.0(P2O7-4)1.0
NA4SIO4	K4SnO4		aP18	(2, P-1)		3	(NA+1)4.0(SI+4)1.0(O-2)4.0
NA4TIO4	K4SnO4		aP18	(2, P-1)		3	(NA+1)4.0(TI+4)1.0(O-2)4.0
NA4V2O7	Na4[V2O7]		mS208	(15, C2/c)		3	(NA+1)4.0(V+5)2.0(O-2)7.0

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NA5AL3F14	Chiolite (Na5Al3F14, K75)	K75	tP44	(128, P4/mnc)		3	(NA+1)5.0(AL+3)3.0(F-1)14.0
NA5FEO4	Na5GaO4		oP80	(61, Pbca)		3	(NA+1)5.0(FE+3)1.0(O-2)4.0
NA5FESI4O12	Unknown Structure					4	(NA+1)5.0(FE+3)1.0(SI+4)4.0(O-2)12.0
NA6SI2O7	Na6[Si2O7]		aP120	(2, P-1)		3	(NA+1)6.0(SI+4)2.0(O-2)7.0
NA6SI8O19	Na6Si8O19		mP132	(14, P2_1/c)		3	(NA+1)6.0(SI+4)8.0(O-2)19.0
NA8FE2O7	Na8Ga2O7		mP68	(14, P2_1/c)		3	(NA+1)8.0(FE+3)2.0(O-2)7.0
NA8FE6SI15O40	Unknown Structure					4	(NA+1)8.0(FE+2)6.0(SI+4)15.0(O-2)40.0
NA8TI5O14	Na8Ti5O14		aP54	(2, P-1)		3	(NA+1)8.0(TI+4)5.0(O-2)14.0
NAAL11O17	NaAl11O17		hP58	(194, P6_ 3/mmc)	This is Beta-Al2O3 NaAl11O17 solid solution.	5	(NA+1)2.0(NA+1, VA)2.0(AL+3)22.0(O-2)34.0(O-2, VA)1.0
NAALO2_D	LiGaO2		oP16	(33, Pna2_1)		2	(NAAL+4, SI+4)1.0(O-2)2.0
NAB3O5	NaB3O5-a		mP108	(14, P2_1/c)	This is (K, Na)B3O5.	3	(K+1, NA+1)1.0(B+3)3.0(O-2)5.0
NAB5O8_A	Unknown Structure					3	(NA+1)1.0(B+3)5.0(O-2)8.0
NAB5O8_B	Unknown Structure					3	(NA+1)1.0(B+3)5.0(O-2)8.0
NAB5O8_G	KB5O8-a		oP112	(61, Pbca)	This is ht-NaB5O8 and KB5O8.	3	(K+1, NA+1)1.0(B+3)5.0(O-2)8.0
NAB9O14_A	Unknown Structure					3	(NA+1)1.0(B+3)9.0(O-2)14.0
NAB9O14_B	Unknown Structure					3	(NA+1)1.0(B+3)9.0(O-2)14.0
NAB9O14_G	Unknown Structure					3	(NA+1)1.0(B+3)9.0(O-2)14.0
NABO2_A	KBO2 (F513)	F513	hR24	(167, R-3c)	This is ht-NaBO2 and KBO2.	3	(K+1, NA+1)1.0(B+3)1.0(O-2)2.0

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NABO2_B	Unknown Structure				rt-NaBO2	3	(NA+1)1.0(B+3)1.0(O-2)2.0
NAF1	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is (K,Na)F.	2	(K+1, NA+1)1.0(F-1)1.0
NAFE2O3	NaFe2O3		hP6	(164, P-3m1)		4	(NA+1)1.0(FE+2)1.0(FE+3)1.0(O-2)3.0
NAFEO2_A	Caswellsilverite (CrNaS2, F51)	F51	hR4	(166, R-3m)	This is also NaCrO2.	3	(NA+1)1.0(CR+3, FE+3)1.0(O-2)2.0
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)1.0(O-2)2.0
NAFEO2_G	LiAlO2		tP16	(92, P4_12_12)	This is high-temp K(Al,Fe)O2 + NaFeO2 and mid-temp NaAlO2 solid solutions.	2	(KAL+4, KFE+4, NAAL+4, NAFE+4, SI+4)1.0(O-2)2.0
NAFESI2O6	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)		4	(NA+1)1.0(FE+3)1.0(SI+4)2.0(O-2)6.0
NAMGF3	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)		3	(NA+1)1.0(MG+2)1.0(F-1)3.0
NANO3_S1	Calcite (CaCO3, G01)	G01	hR10	(167, R-3c)	With solubility of K.	2	(K+1, NA+1)1.0(NO3-1)1.0
NANO3_S2	Rb[NO3]		hR9	(166, R-3m)	This is ht-(K, Na)(NO3) solid solution.	2	(K+1, NA+1)1.0(NO3-1)1.0
NAPO3	NaAsO3		aP30	(2, P-1)		2	(NA+1)1.0(PO3-1)1.0
NAS2	NaS2		tI48	(122, I-42d)		2	(NA)1.0(S)2.0
NB2O5	Nb2O5		mP99	(10, P2/m)		2	(MG+2, NB+5, V+5, ZR+4)2.0(O-2, VA)5.0
NB3BO9	Unknown Structure					3	(NB+5)3.0(B+3)1.0(O-2)9.0
NBF5	MoF5		mS48	(12, C2/m)		2	(NB+5)1.0(F-1)5.0
NBO1	NbO		cP6	(221, Pm-3m)		2	(NB+2)1.0(O-2)1.0
NBO2	alpha-NbO2		tI96	(88, I4_1/a)	This is NbO2	2	(FE+2, NB+4, NB+5)1.0(O-2)2.0
NEPHELINE_A	Unknown Structure				This is NaAlSiO4 with solubility of Si.	4	(NAAL+4)4.0(NAAL+4, SI+4)4.0(SI+4)8.0 (O-2)32.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NEPHELINE_B	Unknown Structure				This is NaAlSiO4 with solubility of Si.	4	(NAAL+4)4.0(NAAL+4, SI+4)4.0(SI+4)8.0 (O-2)32.0
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)4.0(KAL+4, NAAL+4, NAFE+4, SI+4)4.0(SI+4)8.0(O-2)32.0
NI3B2O6	Kotoite (Mg3(BO3)2)		oP22	(58, Pnnm)	This is (Co,Mg,Ni)3B2O6	3	(CO+2, MG+2, NI+2)3.0(B+3)2.0(O-2)6.0
NI3S2_LT	Hazelwoodite (Ni3S2, D5e)	D5e	hR5	(155, R32)		2	(NI)3.0(S)2.0
NI4NB2O9	Nb2Ni4O9		oF480	(43, Fdd2)		3	(NI+2)4.0(NB+5)2.0(O-2)9.0
NI6MNO8_TYPE	Mg6MnO8		cF60	(225, Fm-3m)	This is (Mg, Ni)6MnO8, with an ordered NaCl-type structure.	3	(MG+2, NI+2)6.0(MN+4)1.0(O-2)8.0
NI7S6	Unknown Structure		t**			2	(FE, NI)7.0(S)6.0
NI9S8	Ni9S8		oS68	(21, C222)		2	(FE, NI)9.0(S)8.0
NIMNO3	Ilmenite (FeTiO3, E22)	E22	hR10	(148, R-3)	This is NiMnO3 with Ilmenite structure	2	(MN+3, MN+4, NI+2)2.0(O-2)3.0
NINB14O36	Unknown Structure					3	(NI+2)1.0(NB+5)14.0(O-2)36.0
NINB2O6	Columbite (FeNb2O6, E51)	E51	oP36	(60, Pbcn)		3	(NB+5, NI+2, VA)1.0(NB+5, NI+2)2.0(O-2, VA)6.0
NINB36O91	Unknown Structure					3	(NI+2)1.0(NB+5)36.0(O-2)91.0
NINB68O171	Unknown Structure					3	(NI+2)1.0(NB+5)68.0(O-2)171.0
NIOCALITE_C10NS6	Niocalite		oS114	(21, C222)	This is 10CaO.Nb2O5.6SiO2.	4	(CA+2)10.0(NB+5)2.0(SI+4)6.0(O-2)27.0
NIS_LT	Millerite (NiS, B13)	B13	hR6	(160, R3m)	This is low temperature NiS.	2	(NI)1.0(S)1.0
OKAYAMALITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_1m)		4	(CA+2)2.0(B+3)2.0(SI+4)1.0(O-2)7.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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, MG+2, MN+2, NI+2)1.0(CA+2, CO+2, CR+2, CU+2, FE+2, MG+2, MN+2, NI+2)1.0 (SI+4)1.0(O-2)4.0
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	(70, Fddd)		1	(S)1.0
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)1.0(FE+2, MG+2)1.0 (SI+4)2.0(O-2)6.0
P2O5_H	P2O5		hR28	(161, R3c)		2	(P+5)2.0(O-2)5.0
P2O5_OO	P2O5		oP56	(43, Fdd2)		2	(P+5)2.0(O-2)5.0
P2O5_OP	P2O5		oP28	(62, Pnma)		2	(P+5)2.0(O-2)5.0
P2S5	P2S5		aP28	(2, P-1)		2	(P)2.0(S)5.0
PENTLANDITE	Co9S8 (D89)	D89	cF68	(225, Fm-3m)		3	(FE, NI)8.0(FE, NI)1.0(S)8.0
PEROVSKITE	PrNiO3		hR10	(167, R-3c)	This is (Cr,Fe, Mn)LaO3. Also includes (Cr,Fe,Mn)LaO3 O-Perovskite.	3	(LA+3, MN+3, VA)1.0(CO+3, CR+3, CR+4, FE+2, FE+3, FE+4, MN+2, MN+3, MN+4, VA)1.0(O-2, VA)3.0
PI_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		3	(CR)12.8(FE, NI, SI)7.2(N)4.0
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)1.0(SI+4)1.0(O-2)3.0
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)1.0(AL+3, FE+3, SI+4, TI+3, TI+4)2.0(O-2)5.0
PSEUDO_ WOLLASTONITE	CaSiO3		mS120	(15, C2/c)	This is CaO.SiO2	3	(CA+2)1.0(SI+4)1.0(O-2)3.0
PYRITE	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)	This is Cattierite (CoS2), Pyrite (FeS2) -	2	(CO, FE, MN, NI)1.0(S)2.0

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					Hauerite (MnS2) - Vaesite (NiS2).		
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)2.0(GD+3, HF+4, LA+3, TI+4, Y+3, YB+3, ZR+4)2.0(O-2, VA)6.0(O-2)1.0(O-2, VA)1.0
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)1.0(S)1.0
QUARTZ	alpha-Quartz (low Quartz)		hP9	(152, P3_121)	SiO2 with AlPO4 solubility.	2	(AL+3, SI+4)1.0(PO4-3, SIO4-4)1.0
Q_ALMGZRO	Unknown Structure					4	(MG+2)4.68(AL+3)2.64(ZR+4)1.68(O-2)12.0
RANKINITE	3CaO.2SiO2		mP48	(14, P2_1/c)		3	(CA+2)3.0(SI+4)2.0(O-2)7.0
RED_P	Unknown Structure				This is pure phosphorus.	1	(P)1.0
RHODONITE	Rhodonite (MnSiO3-b)		aP50	(2, P-1)	This is MnO.SiO2	3	(CA+2, CO+2, FE+2, MG+2, MN+2)1.0 (SI+4)1.0(O-2)3.0
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)1.0(O-2, VA)2.0
SAPPHIRINE	CaMg3Si3O10		aP68	(2, P-1)	This is 9Al2O3.7MgO.3SiO2	4	(AL+3)18.0(MG+2)7.0(SI+4)3.0(O-2)40.0
SI3N4	Nierite (alpha-Si3N4)		hP28	(159, P31c)		2	(SI)3.0(N)4.0
SI3P4O16	Unknown Structure					2	(SI+4)3.0(PO4-3)4.0
SIC_B3	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(SI)1.0(C)1.0
SILLIMANITE	Sillimanite (Al2SiO5, S03)	S03	oP32	(62, Pnma)	This is a high-pressure phase	4	(AL+3)1.0(AL+3)1.0(SI+4)1.0(O-2)5.0
SIP2O7_CUB	Si[P2O7]		cP1080	(205, Pa-3)	This is cubic (Si, Ti)P2O7.	2	(SI+4, TI+4)1.0(P2O7-4)1.0
SIP2O7_MONO	Si[P2O7]-a		mP40	(14, P2_1/c)		2	(SI+4)1.0(P2O7-4)1.0

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SIP2O7_TETR	Unknown Structure					2	(SI+4)1.0(P2O7-4)1.0
SIS2	SiS2 (C42)	C42	oI12	(72, Ibam)		2	(SI)1.0(S)2.0
SPHENE	CaTi[SiO4]O		mP32	(14, P2_1/c)		4	(CA+2)1.0(TI+4)1.0(SI+4)1.0(O-2)5.0
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, MG+2, MN+2, NI+2)1.0 (AL+3, CA+2, CO+2, CO+3, CR+3, CU+2, FE+2, FE+3, MG+2, MN+2, MN+3, MN+4, MO+4, NI+2, TI+3, TI+4, V+3, VA)2.0 (CR+2, FE+2, MG+2, MN+2, VA)2.0(O-2)4.0
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)1.0(CO, CR, NI)2.0 (S)4.0
TI10O19	Unknown Structure					2	(TI)10.0(O)19.0
TI20O39	Ti20O39		aP118	(2, P-1)		2	(TI)20.0(O)39.0
TI2NB10O29	(Ti0.17Nb0.83)12O29		mS82	(12, C2/m)		3	(TI+4)2.0(NB+5)10.0(O-2)29.0
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mnm)		2	(TI)2.0(C, N)1.0
TI2S	Ta2P		oP36	(58, Pnnm)		2	(TI)2.0(S)1.0
TI3O2	(Ti3O2)		hP5	(191, P6/mmm)		3	(TI+2)2.0(TI)1.0(O-2)2.0
TI4C2S2	AlCCr2		hP8	(194, P6_3/mmc)		3	(TI)4.0(C)2.0(S)2.0
TI5O9	Ti5O9		aP28	(2, P-1)	Ti5O9 with solubility of V.	2	(TI, V)5.0(O)9.0
TI5P6O25	Unknown Structure					3	(TI+4)5.0(P+5)6.0(O-2)25.0
TI8S10	Ti0.81S		hP20	(194, P6_3/mmc)		2	(TI)8.0(S)10.0

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TI8S3	Ti8S3		mS88	(12, C2/m)		2	(TI)8.0(S)3.0
TI8S9	TiS		hR18	(166, R-3m)		2	(TI)8.0(S)9.0
TI9O17	Ti9O17		aP52	(2, P-1)		2	(TI)9.0(O)17.0
TINB24O62	(Ti0.04Nb0.96)25O62		mS174	(5, C2)		3	(TI+4)1.0(NB+5)24.0(O-2)62.0
TINB2O7	(Ti0.33Nb0.67)3O7		mS60	(12, C2/m)		3	(TI+4)1.0(NB+5)2.0(O-2)7.0
TIO_ALPHA	alpha-TiO		mS20	(12, C2/m)		2	(TI+2)1.0(O-2)1.0
TIS2	CdI2		hP3	(164, P-3m1)		2	(TI)1.0(S)2.0
TIS3	ZrSe3		mP8	(11, P2_1/m)		2	(TI)1.0(S)3.0
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	(9, Cc)	SiO2 with AlPO4 solubility.	2	(AL+3, SI+4)1.0(PO4-3, SIO4-4)1.0
V2O5	Shcherbinaite (V2O5) (Revised)		oP14	(59, Pmmn)		2	(V+5)2.0(O-2)5.0
V2O_SS	V7O3		mS20	(12, C2/m)		2	(V)1.0(O, VA)0.5
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)3.0(O)5.0
V3O5_LT	V3O5-lt		mP32	(13, P2/c)		2	(V)3.0(O)5.0
V3O7	V3O7		mS120	(15, C2/c)		2	(V)3.0(O)7.0
V52O64	V13O16		tI116	(141, I4_1/amd)		2	(V)52.0(O)64.0
V5O9	Ti5O9		aP28	(2, P-1)	V5O9 with solubility of Ti.	2	(TI, V)5.0(O)9.0
V6O13	V6O13		mS38	(12, C2/m)		2	(V)6.0(O)13.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
VO2_LT	VO2		mP12	(14, P2_1/c)	This is lt-VO2, MoO2 and WO2.	2	(MO+4, V+4, W+4)1.0(O-2)2.0
WHITE_P	Unknown Structure				This is pure phosphorus. Not stable at normal conditions.	1	(P)1.0
WO2_72	Unknown Structure					1	(O2_72W1)1.0
WO2_90	Unknown Structure					1	(O2_90W1)1.0
WO2_96	Unknown Structure					1	(O2_96W1)1.0
WO3_HT	WO2.95		tP16	(113, P-42_ 1m)		2	(W+6)1.0(O-2)3.0
WO3_LT	WO3		oP32	(60, Pbcn)		2	(W+6)1.0(O-2)3.0
WOLLASTONITE	Wollastonite (CaSiO3)		aP30	(2, P-1)	This is CaO.SiO2	3	(CA+2, FE+2, MG+2, MN+2)1.0(SI+4)1.0 (O-2)3.0
Y15C19_ALPHA	alpha-Y15C19		oP18	(55, Pbam)		2	(C)19.0(Y)15.0
Y15C19_BETA	Unknown Structure					2	(C)19.0(Y)15.0
Y2C3_ALPHA	Sc3C4		tP70	(128, P4/mnc)		3	(Y)2.0(C)2.0(C, VA)1.0
Y2C3_BETA	Unknown Structure					3	(Y)2.0(C)2.0(C, VA)1.0
Y2S2A_Y2SI2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	(12, C2/m)	Y2Si2O7	3	(Y+3)1.0(Y+3)1.0(SI2O7-6)1.0
Y2S2B_Y2SI2O7	La4Ge3[GeO4]O10		aP44	(2, P-1)	(Y,Yb)2Si2O7 solid solution.	2	(Y+3, YB+3)2.0(SI2O7-6)1.0
Y2S2D_Y2SI2O7	Possible delta-Y2Si2O7		oP44	(62, Pnma)	Y2Si2O7 with Yb solubility.	2	(Y+3, YB+3)2.0(SI2O7-6)1.0
Y2S2G_Y2SI2O7	Y2Si2O7-b		mP22	(14, P2_1/c)	Y2Si2O7-b with Yb solubility.	2	(Y+3, YB+3)2.0(SI2O7-6)1.0
Y2SIO5	Y2SiO5 (RE2SiO5 X2)		mS64	(15, C2/c)	This is (Y,Yb)2SiO5	3	(Y+3, YB+3)2.0(SIO4-4)1.0(O-2)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
Y2TIO5	La2TiO5		oP32	(62, Pnma)	This is (Gd,La, Y)2TiO5	3	(GD+3, LA+3, Y+3)2.0(TI+4)1.0(O-2)5.0
Y3NBO7	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		3	(NB+5, VA, Y+3)3.0(NB+5, Y+3)1.0(O-2, VA)7.0
YAM	Y4Al2O9		mP60	(14, P2_1/c)	This is Y4Al2O9, Gd4Al2O9 and Ca2Y2Si2O9 (Cuspidine)	4	(AL+3, SI+4)2.0(CA+2, GD+3, LA+3, Y+3, YB+3)4.0(O-2, VA)1.0(O-2)9.0
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)1.0 (CA+2, GD+3, LA+3, Y+3, YB+3)1.0(O-2, VA)3.0
YB2TIO5	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		3	(YB+3)2.0(TI+4)1.0(O-2)5.0
YB6HFO11	Unknown Structure				Yb6HfO11 solid solution	4	(HF+4, YB+3)2.0(YB+3)6.0(O-2)12.0(O-2, VA)1.0
YBO3	Unknown Structure				This is (Y, Yb)BO3 solid solution.	3	(Y+3, YB+3)1.0(B+3)1.0(O-2)3.0
YC_B1	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		2	(Y)1.0(C, C2, VA)1.0
YNBO4	LaNbO4		mS24	(15, C2/c)		3	(NB+5, VA, Y+3)1.0(NB+5, Y+3)1.0(O-2, VA)4.0
ZIRCON	Zircon (ZrSiO4, S11)	S11	tI24	(141, I4_1/amd)	This is HfSiO4, ZrSiO4, GdPO4, LaPO4 and YPO4.	3	(P+5, SI+4)1.0(GD+3, HF+4, LA+3, Y+3, ZR+4)1.0(O-2, VA)4.0
ZR11NB4O32	Unknown Structure					3	(ZR+4)11.0(NB+5)4.0(O-2)32.0
ZR13NB4O36	Unknown Structure					3	(ZR+4)13.0(NB+5)4.0(O-2)36.0
ZR15NB4O40	Unknown Structure					3	(ZR+4)15.0(NB+5)4.0(O-2)40.0
ZR2P2O9	Zr2[PO4]2O		mS52	(12, C2/m)		3	(ZR+4)2.0(P+5)2.0(O-2)9.0
ZR3Y4O12	UY6O12		hR19	(148, R-3)	Zr3(Y,Yb)4O12 and Hf3Yb4O12.	3	(HF+4, ZR+4)3.0(Y+3, YB+3)4.0(O-2)12.0
ZR5NB2O15	Unknown Structure					3	(ZR+4)5.0(NB+5)2.0(O-2)15.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZR6NB2O17	Nb2Zr6O17		oI100	(46, Ima2)		3	(ZR+4)6.0(NB+5)2.0(O-2)17.0
ZR7NB2O19	Unknown Structure					3	(ZR+4)7.0(NB+5)2.0(O-2)19.0
ZR8NB2O21	Unknown Structure					3	(ZR+4)8.0(NB+5)2.0(O-2)21.0
ZRF4	ZrF4		mS60	(15, C2/c)	This is (Hf,Zr)F4.	2	(HF+4, ZR+4)1.0(F-1)4.0
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)2.0(O-2, VA)4.0
ZRO2_TETR	HgI2 (C13)	C13	tP6	(137, P4_ 2/nmc)	This is Tetragonal HfO2 and ZrO2	2	(AL+3, 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)2.0(O-2, VA)4.0
ZRO8S2	Zr[SO4]2		oP44	(62, Pnma)		2	(ZR+4)1.0(SO4-2)2.0
ZRS2	CdI2		hP3	(164, P-3m1)		2	(ZR)1.0(S)2.0
ZRTI2O6	Columbite (FeNb2O6, E51)	E51	oP36	(60, Pbcn)		3	(ZR+4)1.0(TI+4)2.0(O-2)6.0
ZRTIO4_ALPHA	Unknown Structure					3	(ZR+4)1.0(TI+4)1.0(O-2)4.0
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)2.0(AL+3, VA)1.0 (O-2)4.0
Z_PHASE	CrNbN		tP6	(129, P4/nmm)		3	(CR, FE)1.0(MO, NB, V)1.0(N, VA)1.0

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,

Name	Prototype	Note	Sublattices	Formula Unit
				AL1F2H1O1, AL1F2NA1O1, AL1F2O1, AL1F3, AL1F4K1, 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, 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, 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, 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, C1H2, C1H2N4, C1H2O1, C1H2O2_CIS, C1H2O2_DIOXIRANE, C1H2O2_TRANS, C1H3, C1H3O1_CH2OH, C1H3O1_CH3O, C1H3P1, C1H4, C1H4N2O1, C1H4O1, C1H4S1, C1H5N1, C1H5O1P1, C1H5O3P1, C1H5P1, C1H5P1S1, C1H6N1P1_N, C1H6N1P1_P, C1H6P2, 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, C2H1N1, C2H2, C2H2O1, C2H3, C2H4, C2H4O1_ACETALDEHYDE, C2H4O1_OXIRANE, C2H4O2_ACETICACID, C2H4O2_DIOXETANE, C2H4O3_123TRIOXOLANE, C2H4O3_124TRIOXOLANE, C2H5, C2H6, C2H6O1_1, C2H6O1_2, C2H6O1SI1, C2H6O2, C2H7O1P1, C2H7O3P1, C2H7P1_1, C2H7P1_2, C2H7P1S1, C2H8N1P1_N, C2H8N1P1_P, C2H8SI1, C2K2N2, C2N1_CCN, C2N1_CNC, C2N2, C2N2NA2, C2O1, C2P1, C2P2, C2SI1, C2SI2, C2SI3, C3, C3H1, C3H1N1, C3H4_1, C3H4_2, C3H6_1, C3H6_2, C3H6O1_1, C3H6O1_2, C3H8, C3N1, C3O2, C4, C4H1, C4H10_1, C4H10_2, C4H12SI1, 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, 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, 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, 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, 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, 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, K1N1O2, K1N1O3, K1NA1, K1O1, K1S1, K2, K2O1, K2O2, K2O4S1, K2S1, LA, LA1O1, LA1S1, LA2O1, LA2O2, 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)1.0
IONIC_LIQ	Liquid	Liquid metal and slag mixture	2	(AL+3, CA+2, CO+2, CR+2, CU+1, FE+2, GD+3, HF+4, K+1, LA+3, 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)1.0(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)1.0

TCOX13 Properties Data and Assessed Systems

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

For more information about the various thermophysical 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:

TCOX13 Viscosity for Ionic Liquids Assessed 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 TCOX13, 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.

Model Description

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

Included Oxides

Included Oxides Assessed for Viscosity							
Al_2O_3	CaF_2	CaO	Cr_2O_3	CuO_x	FeO	Fe_2O_3	Gd_2O_3
K_2O	La_2O_3	MgO	MnO	MoO_2	MoO_3	Na_2O	NbO
Nb_2O_5	NiO	P_2O_5	SiO_2	TiO_2	V_2O_5	Y_2O_3	ZrO_2

Assessed or Estimated Unary Systems

A system is estimated based on other predictions and data of ternaries.

System	*Status*	*System*	*Status*	*System*	*Status*
Al_2O_3	Assessed	B_2O_3	Assessed	CaF_2	Assessed
CaO	Estimated	CaS	Estimated	Cr_2O_3	Estimated
CuO_x	Assessed	FeO_x	Assessed	Gd_2O_3	Estimated
K_2O	Assessed	La_2O_3	Estimated	MgO	Assessed

System	Status	System	Status	System	Status
MnO	Assessed	MoO_2	Estimated	MoO_3	Estimated
Na_2O	Assessed	Nb_2O_5	Estimated	NbO	Estimated
NiO	Assessed	P_2O_5	Assessed	SiO_2	Assessed
TiO_2	Assessed	V_2O_5	Assessed	Y_2O_3	Estimated
Yb_2O_3	Estimated	ZrO_2	Estimated		

Assessed Pseudo Binary Systems

Pseudo Binary Systems Assessed for 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	CaF_2-Al_2O_3	CaF_2-MgO
CaF_2-SiO_2	CaF_2-TiO_2	CaF_2-V_2O_5	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
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					

Assessed Pseudo Ternary Systems

Pseudo Ternary Systems Assessed for Viscosity					
Al_2O_3-MgO-SiO_2	CaF_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
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

Pseudo Quaternary Systems Assessed for 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

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

TCOX13 Molar Volume Assessed Systems and 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 in these sections. Molar volume is included with the database starting with version 10 (TCOX10).

Model Description

For more information about the various thermophysical 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.

System	*Status*	*System*	*Status*	*System*	*Status*
B_2O_3	Assessed	Yb_2O_3	Assessed	CaO	Assessed
MgO	Assessed	Al_2O_3	Assessed	SiO_2	Assessed
MnO	Estimated	FeO	Assessed	Fe_2O_3	Assessed
CaF_2	Assessed	MgF_2	Assessed	TiO_2	Assessed
K_2O	Assessed	Cr_2O_3	Estimated	V_2O_5	Estimated
ZrO_2	Estimated	P_2O_5	Estimated	Nb_2O_5	Estimated
NiO	Estimated	WO_3	Estimated	La_2O_3	Estimated
CoO	Estimated	MoO_3	Estimated	CaS	Estimated
Al_2O_3-CaO	Assessed	Al_2O_3-MgO	Assessed	Al_2O_3-SiO_2	Assessed
CaF_2-Al_2O_3	Assessed	CaF_2-CaO	Assessed	CaF_2-MgO	Assessed
CaF_2-MgF_2	Assessed	CaF_2-SiO_2	Assessed	CaF_2-TiO_2	Assessed
CaO-SiO_2	Assessed	Fe_xO-CaO	Assessed	Fe_xO-SiO_2	Assessed
K_2O-SiO_2	Assessed	MgO-SiO_2	Assessed	MnO-SiO_2	Assessed

System	Status	System	Status	System	Status
Al_2O_3-B_2O_3-CaF_2	Assessed	Al_2O_3-B_2O_3-CaO	Assessed	Al_2O_3-MgO-SiO_2	Assessed
Al_2O_3-TiO_2-SiO_2	Assessed	CaF_2-Al_2O_3-TiO_2	Assessed	CaF2-CaO-Al2O3	Assessed
CaF_2-CaO-SiO_2	Assessed	CaF_2-MgO-Al_2O_3	Assessed	CaO-Al_2O_3-SiO_2	Assessed
CaO-Al_2O_3-TiO_2	Assessed	CaO-MgO-Al_2O_3	Assessed	CaO-MgO-SiO_2	Assessed
CaO-MnO-SiO_2	Assessed	CaO-SiO_2-TiO_2	Assessed	Fe_xO-Al_2O_3-SiO_2	Assessed
Fe_xO-CaO-Al_2O_3	Assessed	Fe_xO-CaO-MgO	Assessed	Fe_xO-CaO-SiO_2	Assessed
Fe_xO-MgO-SiO_2	Assessed	Fe_xO-MnO-SiO_2	Assessed	CaF_2-Al_2O_3-MgO-SiO_2	Assessed
CaF_2-CaO-MgO-Al_2O_3	Assessed	CaO-Al_2O_3-MnO-SiO_2	Assessed	CaO-MgO-Al_2O_3-SiO_2	Assessed
Fe_xO-CaO-Al_2O_3-SiO_2	Assessed	Fe_xO-CaO-MgO-SiO_2	Assessed	Fe_xO-CaO-MgO-Al_2O_3-SiO_2	Assessed
Fe_xO-CaO-MnO-SiO_2	Assessed				

Assessed or Estimated Solid Solution and Alloy Phases

This lists the solid solution phases and alloys phases and the associated system and indicates whether the molar volume has been assessed or estimated.

Phase	System	Status	Phase	System	Status
Alabandite	Ca-S	Assessed	Alabandite	Co-S	Assessed
Alabandite	Cr-S	Assessed	Alabandite	Cu-S	Assessed
Alabandite	Fe-S	Assessed	Alabandite	Gd-S	Assessed
Alabandite	La-S	Assessed	Alabandite	Mg-S	Assessed
Alabandite	Mn-S	Assessed	Alabandite	S-Y	Estimated
Alabandite	S-Zr	Assessed	AlPO4	Al-O-P	Assessed
Anhydrite	Ca-O-S	Assessed	Anhydrite	Co-O-S	Assessed

Phase	*System*	*Status*	*Phase*	*System*	*Status*
Anhydrite	Cu-O-S	Assessed	Anhydrite	Fe-O-S	Assessed
Anhydrite	Mg-O-S	Assessed	Anhydrite	Mn-O-S	Assessed
Anhydrite	Ni-O-S	Assessed	Anorthite	Al-Ca-O-Si	Assessed
Anorthite	Al-Na-O-Si	Assessed	Apatite	Gd-O-Si	Assessed
Apatite	O-Si-Y	Estimated	BCC_A2	Al	Assessed
BCC_A2	Ca	Estimated	BCC_A2	Co	Assessed
BCC_A2	Cr	Assessed	BCC_A2	Cu	Assessed
BCC_A2	Fe	Assessed	BCC_A2	Mg	Assessed
BCC_A2	Mn	Assessed	BCC_A2	Mo	Assessed
BCC_A2	Nb	Assessed	BCC_A2	Ni	Assessed
BCC_A2	P	Assessed	BCC_A2	S	Assessed
BCC_A2	Si	Assessed	BCC_A2	Ti	Assessed
BCC_A2	V	Assessed	BCC_A2	W	Assessed
BCC_A2	Y	Assessed	BCC_A2	Zr	Assessed
BCC_A2	Al-C	Assessed	BCC_A2	C-Ca	Estimated
BCC_A2	C-Co	Assessed	BCC_A2	C-Cr	Assessed
BCC_A2	C-Cu	Assessed	BCC_A2	C-Fe	Assessed
BCC_A2	C-Gd	Assessed	BCC_A2	C-Mg	Assessed
BCC_A2	C-Mn	Assessed	BCC_A2	C-Mo	Assessed
BCC_A2	C-Nb	Assessed	BCC_A2	C-Ni	Assessed
BCC_A2	C-P	Assessed	BCC_A2	C-S	Assessed
BCC_A2	C-Si	Assessed	BCC_A2	C-Ti	Assessed

Phase	System	Status	Phase	System	Status
BCC_A2	C-V	Assessed	BCC_A2	C-W	Assessed
BCC_A2	C-Y	Estimated	BCC_A2	C-Zr	Estimated
BCC_A2	Ca-O	Estimated	BCC_A2	Co-O	Assessed
BCC_A2	Cr-O	Estimated	BCC_A2	Cu-O	Assessed
BCC_A2	Fe-O	Estimated	BCC_A2	Gd-O	Estimated
BCC_A2	La-O	Estimated	BCC_A2	Mg-O	Assessed
BCC_A2	Mn-O	Assessed	BCC_A2	Ni-O	Estimated
BCC_A2	Ni-Ti	Assessed	BCC_A2	Ni-V	Assessed
BCC_A2	O-P	Estimated	BCC_A2	O-S	Assessed
BCC_A2	O-Si	Estimated	BCC_A2	O-Ti	Estimated
BCC_A2	O-V	Estimated	BCC_A2	O-W	Estimated
BCC_A2	O-Y	Estimated	BCC_A2	O-Zr	Estimated
BCC_A2	Ti-Zr	Assessed	Bronze	Ca-O-V	Assessed
Bronze	Fe-O-V	Estimated	Ca2P2O7 (α, β, and γ)	Ca-O-P	Assessed
Ca2P2O7 (α, β, and γ)	Mg-O-P	Assessed	Ca2SiO4 (α and α')	Ca-O-P	Assessed
Ca2SiO4 (α and α')	Ca-O-Si	Assessed	Ca2SiO4 (α and α')	Fe-O-P	Assessed
Ca2SiO4 (α and α')	Gd-O-Si	Estimated	Ca2SiO4 (α and α')	Mg-O-P	Assessed
Ca2SiO4 (α and α')	Mn-O-P	Assessed	Ca2SiO4 (α and α')	O-Si-Y	Estimated
Ca3Co2O6	Ca-Co	Estimated	Ca3Co2O6	Ca-Cu	Estimated
Ca3Co2O6	Ca-Co-O	Assessed	Ca3Co2O6	Ca-Cu-O	Estimated
Ca3Co4O9	Ca-Co	Estimated	Ca3Co4O9	Ca-Cu	Estimated
Ca3Co4O9	Ca-Co-O	Estimated	Ca3Co4O9	Ca-Cu-O	Estimated

Phase	*System*	*Status*	*Phase*	*System*	*Status*
Ca3P2O8 (α and β)	Ca-O-P	Assessed	Ca3P2O8 (α and β)	Ca-O-Si	Estimated
Ca3P2O8 (α and β)	Mg-O-P	Assessed	Ca3S3Fe4Ox	Ca-Fe-S	Estimated
Ca4Nb2O9_HT11	Ca-Nb-O	Estimated	Ca4Nb2O9_LT21	Ca-O	Assessed
Ca4Nb2O9_LT21	Ca-Nb-O	Estimated	CaCr2O4_A	Al-Ca-O	Estimated
CaCr2O4_A	Ca-Cr-O	Estimated	CaCr2O4_A	Ca-Fe-O	Assessed
CaF2_S1	Ca	Estimated	CaF2_S1	Mg	Estimated
CaF2_S1	Ca-F	Assessed	CaF2_S2	Ca	Estimated
CaF2_S2	Cu	Estimated	CaF2_S2	Mg	Estimated
CaF2_S2	Ca-F	Assessed	Calcium Ferro-aluminates	C3A1:Al-Ca-O	Assessed
Calcium Ferro-aluminates	C3A1:Ca-Fe-O	Estimated	Calcium Ferro-aluminates	C12A7:Al-Ca-O	Estimated
Calcium Ferro-aluminates	C1A1:Al-Ca-O	Assessed	Calcium Ferro-aluminates	C1A2:Al-Ca-O	Assessed
Calcium Ferro-aluminates	C1A6:Al-Ca-O	Assessed	Calcium Ferro-aluminates	C2F:Al-Ca-O	Assessed
Calcium Ferro-aluminates	C2F:Ca-Fe-O	Assessed	CaMO3	O-Y	Estimated
CaMO3	Ca-Mn-O	Assessed	CaMO3	Ca-O-Ti	Assessed
CaMO3	Ca-O-Y	Assessed	CaMO3	Ca-O-Zr	Assessed
CaMO3	Mn-O-Y	Assessed	CaMO3	O-Ti-Y	Assessed
CaMO3	O-Y-Zr	Assessed	Carnegieite (α and β)	Al-Na-O-Si	Assessed
Carnegieite (α and β)	Fe-Na-O-Si	Assessed	CaSFeO	Ca-Fe-S	Estimated
CaSO4_HT	Ca-O-S	Assessed	CaSO4_HT	Co-O-S	Assessed
CaSO4_HT	Mg-O-S	Assessed	CaV2O4	Al-Ca-O	Assessed
CaV2O4	Ca-Cr-O	Assessed	CaV2O4	Ca-Fe-O	Assessed

Phase	System	Status	Phase	System	Status
CaV2O4	Ca-O-V	Assessed	CaV2O4	Ca-O-Y	Assessed
CaV2O6	Ca-O-V	Assessed	CaV2O6	Co-O-V	Assessed
CaV2O6	Mg-O-V	Assessed	CaV2O6	Mn-O-V	Assessed
CaV2O6	Ni-O-V	Assessed	CaY4O7	Ca-Gd-O	Assessed
CaY4O7	Ca-O-Y	Estimated	CaZrO3_C	O-Y	Estimated
CaZrO3_C	Ca-O-Y	Assessed	CaZrO3_C	Ca-O-Zr	Assessed
CBCC_A12	Al	Estimated	CBCC_A12	Co	Estimated
CBCC_A12	Cr	Estimated	CBCC_A12	Cu	Estimated
CBCC_A12	Fe	Estimated	CBCC_A12	Mg	Estimated
CBCC_A12	Mn	Assessed	CBCC_A12	Mo	Estimated
CBCC_A12	Nb	Estimated	CBCC_A12	Ni	Estimated
CBCC_A12	Si	Estimated	CBCC_A12	Ti	Estimated
CBCC_A12	V	Estimated	CBCC_A12	Zr	Estimated
CBCC_A12	Al-C	Estimated	CBCC_A12	C-Co	Estimated
CBCC_A12	C-Cr	Estimated	CBCC_A12	C-Cu	Estimated
CBCC_A12	C-Mg	Estimated	CBCC_A12	C-Mn	Estimated
CBCC_A12	C-Mo	Estimated	CBCC_A12	C-Nb	Estimated
CBCC_A12	C-Ni	Estimated	CBCC_A12	C-Si	Estimated
CBCC_A12	C-Ti	Estimated	CBCC_A12	C-V	Assessed
CBCC_A12	C-Zr	Estimated	Chalcopyrite	S	Estimated
Chalcopyrite	Cu-S	Assessed	Chalcopyrite	Fe-S	Estimated
Chalcopyrite	Cu-Fe-S	Assessed	c-M2O3	Al-O	Estimated

Phase	System	Status	Phase	System	Status
c-M2O3	Ca-O	Assessed	c-M2O3	Co-O	Assessed
c-M2O3	Cr-O	Assessed	c-M2O3	Fe-O	Estimated
c-M2O3	Gd-O	Estimated	c-M2O3	La-O	Estimated
c-M2O3	Mn-O	Estimated	c-M2O3	Ni-O	Estimated
c-M2O3	Y-O	Assessed	c-M2O3	Zr-O	Estimated
Co9S8	Co-S	Estimated	Co9S8	Fe-S	Estimated
Co9S8	Ni-S	Estimated	Co9S8	Co-Mg	Assessed
Columbite	Fe	Estimated	Columbite	Ca-Fe	Estimated
Columbite	Ca-Mg	Estimated	Columbite	Ca-Nb	Estimated
Columbite	Co-Fe	Assessed	Columbite	Co-Mg	Assessed
Columbite	Co-Nb	Assessed	Columbite	Ca-Fe-O	Estimated
Columbite	Co-Mg-O	Estimated	Columbite	Co-Nb-O	Assessed
Columbite	Fe-Mg-O	Estimated	Columbite	Fe-Nb-O	Assessed
Columbite	Mg-Mn-O	Estimated	Columbite	Mg-Nb-O	Assessed
Columbite	Mn-Nb-O	Assessed	Cordierite	Al-Fe-O-Si	Assessed
Cordierite	Al-Mg-O-Si	Assessed	Cordierite	Al-Mn-O-Si	Assessed
Corundum	Al-O	Assessed	Corundum	Co-O	Assessed
Corundum	Cr-O	Assessed	Corundum	Fe-O	Assessed
Corundum	Mg-O	Assessed	Corundum	Mn-O	Assessed
Corundum	Ni-O	Assessed	Corundum	O-Ti	Assessed
Corundum	O-V	Assessed	Corundum	Al-Cr-O	Assessed
Corundum	Al-Fe-O	Estimated	Corundum	Al-Ni-O	Estimated

Phase	*System*	*Status*	*Phase*	*System*	*Status*
Corundum	Cr-Fe-O	Assessed	Corundum	Cr-Mn-O	Estimated
Corundum	Cr-O-Ti	Estimated	Corundum	Cr-O-V	Estimated
Corundum	Fe-Mn-O	Estimated	Corundum	Fe-Ni-O	Estimated
Corundum	Fe-O-Ti	Estimated	Corundum	Fe-O-V	Estimated
Cr2P4O13	Cr-O-P	Estimated	Cr2P4O13	Cr-O-V	Estimated
Cr2P4O13	Fe-O-P	Estimated	Cr2P4O13	Fe-O-V	Assessed
Cr2S3	Cr-S	Assessed	Cr2S3	Fe-S	Assessed
Cr2Ti2O7	Al-O-Ti	Estimated	Cr2Ti2O7	Cr-O-Ti	Estimated
Cr2Ti2O7	Fe-O-Ti	Estimated	Cr3S4	Cr-S	Assessed
Cr3S4	Fe-S	Assessed	Cr3S4	Mn-S	Estimated
Cristobalite	O-Si	Assessed	Cristobalite	Al-O-P	Assessed
CrNbO4	Cr	Assessed	CrNbO4	Nb	Assessed
CrNbO4	Cr-Nb	Assessed	CrNbO4	Cr-O	Assessed
CrNbO4	Nb-O	Estimated	CrNbO4	Cr-Nb-O	Estimated
CUB_A13	Al	Estimated	CUB_A13	Co	Estimated
CUB_A13	Cr	Estimated	CUB_A13	Cu	Estimated
CUB_A13	Fe	Estimated	CUB_A13	Mg	Estimated
CUB_A13	Mn	Assessed	CUB_A13	Mo	Estimated
CUB_A13	Nb	Estimated	CUB_A13	Ni	Estimated
CUB_A13	Si	Estimated	CUB_A13	Ti	Estimated
CUB_A13	V	Estimated	CUB_A13	Zr	Estimated
CUB_A13	Al-C	Estimated	CUB_A13	C-Co	Estimated

Phase	System	Status	Phase	System	Status
CUB_A13	C-Cr	Estimated	CUB_A13	C-Cu	Estimated
CUB_A13	C-Mg	Estimated	CUB_A13	C-Mn	Estimated
CUB_A13	C-Mo	Estimated	CUB_A13	C-Nb	Estimated
CUB_A13	C-Ni	Estimated	CUB_A13	C-Si	Estimated
CUB_A13	C-Ti	Estimated	CUB_A13	C-V	Assessed
CUB_A13	C-Zr	Estimated	CuF2	Cr-F	Assessed
CuF2	Cu-F	Assessed	CuLa2O4	Co-La-O	Assessed
CuLa2O4	Cu-La-O	Assessed	CuO	Cu-O	Assessed
CuO	Co-O	Assessed	CuO	Co-Cu-O	Assessed
CuP2O6	Co-O-P	Assessed	CuP2O6	Cu-O-P	Estimated
CuP2O6	Ni-O-P	Assessed	Cuprite	Cu-O	Assessed
Cuprite	Na-O	Assessed	Delafossite	Al-Cu-O	Assessed
Delafossite	Cr-Cu-O	Assessed	Delafossite	Cu-Fe-O	Assessed
Delafossite	Cu-Mn-O	Assessed	Delafossite	Cu-O-Y	Assessed
DHCP	Al	Estimated	DHCP	Ca	Estimated
DHCP	Cu	Estimated	DHCP	Mg	Estimated
DHCP	Mn	Estimated	DHCP	Ni	Estimated
DHCP	Y	Estimated	DHCP	Al-O	Estimated
DHCP	Cu-O	Estimated	DHCP	Gd-O	Estimated
DHCP	La-O	Estimated	DIAMOND_FCC_A4	Al	Estimated
DIAMOND_FCC_A4	C	Estimated	DIAMOND_FCC_A4	P	Estimated
DIAMOND_FCC_A4	Al-O	Assessed	DIAMOND_FCC_A4	O-P	Estimated

Phase	*System*	*Status*	*Phase*	*System*	*Status*
Digenite	Cu-S	Assessed	Digenite	Fe-S	Assessed
Digenite	Mg-S	Estimated	Digenite	Mn-S	Assessed
Digenite	Cu-Fe-S	Estimated	Digenite	Cu-Mg-S	Estimated
Digenite	Cu-Mn-S	Assessed	DyMn2O5	Gd-Mn-O	Assessed
DyMn2O5	Mn-O-Y	Assessed	δ-NaAlO2	Al-Na-O	Assessed
δ-NaAlO2	Al-Na-O-Si	Assessed	FCC_A1	Al	Assessed
FCC_A1	Ca	Assessed	FCC_A1	Co	Assessed
FCC_A1	Cr	Assessed	FCC_A1	Cu	Assessed
FCC_A1	Fe	Assessed	FCC_A1	Mg	Assessed
FCC_A1	Mo	Assessed	FCC_A1	Nb	Assessed
FCC_A1	Ni	Assessed	FCC_A1	P	Assessed
FCC_A1	S	Assessed	FCC_A1	Si	Assessed
FCC_A1	Ti	Assessed	FCC_A1	V	Assessed
FCC_A1	W	Assessed	FCC_A1	Zr	Assessed
FCC_A1	Al-C	Assessed	FCC_A1	Al-O	Estimated
FCC_A1	C-Ca	Estimated	FCC_A1	C-Co	Assessed
FCC_A1	C-Cr	Assessed	FCC_A1	C-Cu	Assessed
FCC_A1	C-Fe	Assessed	FCC_A1	C-Gd	Assessed
FCC_A1	C-Mg	Assessed	FCC_A1	C-Mn	Assessed
FCC_A1	C-Mo	Assessed	FCC_A1	C-Nb	Assessed
FCC_A1	C-Ni	Assessed	FCC_A1	C-P	Assessed
FCC_A1	C-S	Assessed	FCC_A1	C-Si	Assessed

Phase	System	Status	Phase	System	Status
FCC_A1	C-Ti	Assessed	FCC_A1	C-V	Assessed
FCC_A1	C-W	Assessed	FCC_A1	C-Y	Estimated
FCC_A1	C-Zr	Assessed	FCC_A1	Ca-O	Estimated
FCC_A1	Co-O	Estimated	FCC_A1	Cr-O	Estimated
FCC_A1	Cu-O	Estimated	FCC_A1	Fe-O	Estimated
FCC_A1	Gd-O	Estimated	FCC_A1	La-O	Estimated
FCC_A1	Mg-O	Assessed	FCC_A1	Mn-Ni	Assessed
FCC_A1	Mn-O	Assessed	FCC_A1	Mo-O	Assessed
FCC_A1	Nb-O	Assessed	FCC_A1	Ni-O	Estimated
FCC_A1	Ni-Si	Assessed	FCC_A1	Ni-Ti	Assessed
FCC_A1	Ni-V	Assessed	FCC_A1	Ni-W	Assessed
FCC_A1	O-P	Estimated	FCC_A1	O-S	Assessed
FCC_A1	O-Si	Estimated	FCC_A1	O-Ti	Estimated
FCC_A1	O-V	Estimated	FCC_A1	O-W	Assessed
FCC_A1	O-Y	Estimated	FCC_A1	O-Zr	Estimated
Fe2O12S3	Al-O-S	Assessed	Fe2O12S3	Cr-O-S	Assessed
Fe2O12S3	Fe-O-S	Assessed	FeF3	Al-F	Assessed
FeF3	Co-F	Assessed	FeF3	Cr-F	Assessed
FeF3	F-Fe	Assessed	FeNb14O36	Co-Nb-O	Estimated
FeNb14O36	Fe-Nb-O	Estimated	FeNb36O91	Co-Nb-O	Estimated
FeNb36O91	Fe-Nb-O	Estimated	FeNb68O171	Co-Nb-O	Estimated
FeNb68O171	Fe-Nb-O	Estimated	FePO4	Fe-O-P	Assessed

Phase	*System*	*Status*	*Phase*	*System*	*Status*
FePO4	Mn-O-P	Assessed	FeVO4	Al-O-V	Assessed
FeVO4	Fe-O-V	Assessed	Fluorite	Al	Estimated
Fluorite	Ca	Estimated	Fluorite	Cr	Estimated
Fluorite	Fe	Estimated	Fluorite	Mg	Estimated
Fluorite	Mn	Estimated	Fluorite	Ni	Estimated
Fluorite	Si	Estimated	Fluorite	Y	Estimated
Fluorite	Zr	Estimated	Fluorite	Al-O	Estimated
Fluorite	Ca-O	Assessed	Fluorite	Cr-O	Assessed
Fluorite	Gd-O	Estimated	Fluorite	La-O	Estimated
Fluorite	O-Y	Estimated	Fluorite	O-Zr	Assessed
Garnet	Al-Ca-O-Si	Assessed	Gd2Si2O7	Gd-O-Si	Assessed
Gd2Si2O7	La-O-Si	Assessed	Gd2SiO5	Gd-O-Si	Assessed
Gd2SiO5	La-O-Si	Assessed	GdF3	F-Gd	Assessed
GdF3	F-Y	Assessed	Halite	O	Estimated
Halite	Al-O	Estimated	Halite	Ca-O	Assessed
Halite	Co-O	Assessed	Halite	Cr-O	Estimated
Halite	Cu-O	Estimated	Halite	Fe-O	Estimated
Halite	Gd-O	Estimated	Halite	Mg-O	Assessed
Halite	Mn-O	Assessed	Halite	Na-O	Assessed
Halite	Ni-O	Assessed	Halite	Ti-O	Assessed
Halite	V-O	Estimated	Halite	Ca-Mn-O	Assessed
Halite	Fe-Mg-O	Assessed	Halite	Fe-Ni-O	Assessed

Phase	*System*	*Status*	*Phase*	*System*	*Status*
Hatrurite	Ca-O-Si	Assessed	Hatrurite	Gd-O-Si	Estimated
Hatrurite	O-Si-Y	Estimated	HCP_A3	Al	Assessed
HCP_A3	Co	Assessed	HCP_A3	Cr	Assessed
HCP_A3	Cu	Assessed	HCP_A3	Fe	Assessed
HCP_A3	Mg	Assessed	HCP_A3	Mn	Assessed
HCP_A3	Mo	Assessed	HCP_A3	Nb	Assessed
HCP_A3	Ni	Assessed	HCP_A3	Si	Assessed
HCP_A3	Ti	Assessed	HCP_A3	V	Assessed
HCP_A3	W	Assessed	HCP_A3	Y	Assessed
HCP_A3	Zr	Assessed	HCP_A3	Al-C	Assessed
HCP_A3	Al-O	Estimated	HCP_A3	C-Ca	Estimated
HCP_A3	C-Co	Assessed	HCP_A3	C-Cr	Assessed
HCP_A3	C-Cu	Estimated	HCP_A3	Fe-C	Assessed
HCP_A3	C-Gd	Estimated	HCP_A3	C-Mg	Estimated
HCP_A3	C-Mn	Estimated	HCP_A3	C-Mo	Assessed
HCP_A3	C-Nb	Assessed	HCP_A3	C-Ni	Estimated
HCP_A3	C-Si	Estimated	HCP_A3	C-Ti	Assessed
HCP_A3	C-V	Assessed	HCP_A3	C-W	Assessed
HCP_A3	C-Y	Estimated	HCP_A3	C-Zr	Assessed
HCP_A3	Ca-O	Estimated	HCP_A3	Cr-O	Estimated
HCP_A3	Cu-O	Estimated	HCP_A3	Fe-O	Estimated
HCP_A3	Gd-O	Estimated	HCP_A3	La-O	Estimated

Phase	System	Status	Phase	System	Status
HCP_A3	Mn-O	Estimated	HCP_A3	Mo-O	Estimated
HCP_A3	Nb-O	Estimated	HCP_A3	Ni-O	Estimated
HCP_A3	O-Si	Estimated	HCP_A3	O-Ti	Estimated
HCP_A3	O-V	Estimated	HCP_A3	O-W	Estimated
HCP_A3	O-Y	Estimated	HCP_A3	O-Zr	Estimated
h-M2O3	Ca-O	Assessed	h-M2O3	Gd-O	Assessed
h-M2O3	La-O	Assessed	h-M2O3	Y-O	Estimated
h-M2O3	Zr-O	Estimated	La2MnO4	Co-La-O	Assessed
La2MnO4	La-Mn-O	Estimated	La2MnO4	La-Ni-O	Assessed
La2S3	Gd-S	Assessed	La2S3	La-S	Assessed
La3Ni2O7	La-Ni-O	Assessed	La4Ni3O10	La-Ni-O	Assessed
LaAP	Al-Ca-O	Assessed	LaAP	Al-La-O	Assessed
LaAP	Al-O-Y	Assessed	LaAP	Ca-Co-O	Assessed
LaAP	Ca-Cu-O	Assessed	LaAP	Ca-Fe-O	Assessed
LaAP	Ca-Ni-O	Assessed	LaAP	Co-La-O	Assessed
LaAP	Co-O-Y	Assessed	LaAP	Cu-La-O	Assessed
LaAP	Cu-O-Y	Assessed	LaAP	Fe-La-O	Assessed
LaAP	Fe-O-Y	Assessed	LaAP	La-Ni-O	Assessed
LaAP	Ni-O-Y	Assessed	LaF3	F-Gd	Assessed
LaF3	F-La	Assessed	LaF3	F-Y	Assessed
LaYP	La-O	Assessed	LaYP	Y-O	Assessed
LaYP	La-O-Y	Assessed	M4O7	Ti-O	Assessed

Phase	*System*	*Status*	*Phase*	*System*	*Status*
M4O7	V-O	Assessed	M4O7	Al-O-V	Estimated
M4O7	Mn-O-V	Estimated	M6O11	Ti-O	Assessed
M6O11	V-O	Assessed	M7O13	Ti-O	Assessed
M7O13	V-O	Assessed	Mg2P2O7 (α and β)	Ca-O-P	Assessed
Mg2P2O7 (α and β)	Mg-O-P	Assessed	Mg2V2O7	Co-O-V	Estimated
Mg2V2O7	Mg-O-V	Assessed	Mg2V2O7	Ni-O-V	Estimated
Mg3P2O8	Ca-O-P	Assessed	Mg3P2O8	Mg-O-P	Assessed
Mg3V2O8	Co-O-V	Assessed	Mg3V2O8	Mg-O-V	Assessed
Mg3V2O8	Ni-O-V	Assessed	MgF2	Co-F	Assessed
MgF2	F-Fe	Assessed	MgF2	F-Mg	Assessed
MgF2	F-Mn	Assessed	MgF2	F-Ni	Assessed
MgF2	F-V	Assessed	MgWO4-type	Al-Nb-O	Assessed
MgWO4-type	Al-O-W	Assessed	MgWO4-type	Co-Nb-O	Assessed
MgWO4-type	Co-O-W	Assessed	MgWO4-type	Fe-Nb-O	Assessed
MgWO4-type	Fe-O-W	Assessed	MgWO4-type	Mg-Nb-O	Assessed
MgWO4-type	Mg-O-W	Assessed	MgWO4-type	Mn-Nb-O	Assessed
MgWO4-type	Mn-O-W	Assessed	MgWO4-type	Nb-Ni-O	Assessed
MgWO4-type	Nb-O-W	Assessed	MgWO4-type	Ni-O-W	Assessed
Mn4Nb2O9	Co-Nb-O	Assessed	Mn4Nb2O9	Fe-Nb-O	Estimated
Mn4Nb2O9	Mg-Nb-O	Assessed	Mn4Nb2O9	Mn-Nb-O	Assessed
MoS2	Mo-S	Estimated	MoS2	S-W	Estimated
Mullite	Al-O-Si	Estimated	m-ZrO2	Al-O	Estimated

Phase	*System*	*Status*	*Phase*	*System*	*Status*
m-ZrO2	Ca-O	Assessed	m-ZrO2	Cr-O	Assessed
m-ZrO2	Gd-O	Estimated	m-ZrO2	La-O	Estimated
m-ZrO2	Y-O	Estimated	m-ZrO2	O-Zr	Assessed
Na2Al12O19	Al-Na-O	Estimated	NaAl11O17	Al-Na-O	Assessed
Nb2O5	Mg-O	Estimated	Nb2O5	Nb-O	Assessed
Nb2O5	V-O	Estimated	NbO2	Nb-O	Assessed
Nepheline (α and β)	Na-Al-Si-O	Assessed	Ni6MnO8-type	Mg-Mn-O	Assessed
Ni6MnO8-type	Mn-Ni-O	Estimated	Ni7S6	Fe-S	Estimated
Ni7S6	Ni-S	Estimated	Ni9S8	Fe-S	Estimated
Ni9S8	Ni-S	Estimated	NiMnO3	Mn-O	Estimated
NiMnO3	Ni-O	Estimated	NiNb2O6	Nb-Ni-O	Assessed
Olivine	Ca-O-Si	Assessed	Olivine	Co-O-Si	Assessed
Olivine	Cr-O-Si	Assessed	Olivine	Cu-O-Si	Estimated
Olivine	Fe-O-Si	Assessed	Olivine	Mg-O-Si	Assessed
Olivine	Mn-O-Si	Assessed	Olivine	Ni-O-Si	Assessed
Pentlandite	Fe-S	Estimated	Pentlandite	Ni-S	Estimated
Pentlandite	Fe-Ni-S	Assessed	Perovskite	Co-La	Assessed
Perovskite	Co-Mn	Assessed	Perovskite	Co-O	Assessed
Perovskite	Cr-La	Assessed	Perovskite	Cr-Mn	Assessed
Perovskite	Cr-O	Assessed	Perovskite	Fe-La	Assessed
Perovskite	La-O	Assessed	Perovskite	Co-La-O	Assessed
Perovskite	Cr-La-O	Assessed	Perovskite	Fe-La-O	Assessed

Phase	System	Status	Phase	System	Status
Perovskite	La-Mn-O	Assessed	Pseudo-brookite	Al-O-Ti	Assessed
Pseudo-brookite	Al-O-V	Assessed	Pseudo-brookite	Co-O-Ti	Assessed
Pseudo-brookite	Mg-O-Ti	Assessed	Pseudo-brookite	Mn-O-Ti	Estimated
Pseudo-brookite	Ni-O-Ti	Estimated	Pyrite	Co-S	Assessed
Pyrite	Fe-S	Assessed	Pyrite	Mn-S	Assessed
Pyrite	Ni-S	Assessed	Pyrite	Cu-Fe-S	Assessed
Pyrochlore	Gd-O	Assessed	Pyrochlore	La-O	Assessed
Pyrochlore	Zr-O	Assessed	Pyrochlore	Gd-La-O	Estimated
Pyrochlore	Gd-O-Ti	Partly Assessed	Pyrochlore	Gd-O-Y	Estimated
Pyrochlore	Gd-O-Zr	Estimated	Pyrochlore	La-O-Ti	Partly Assessed
Pyrochlore	La-O-Y	Estimated	Pyrochlore	La-O-Zr	Estimated
Pyrochlore	O-Ti-Y	Partly Assessed	Pyrochlore	O-Ti-Zr	Estimated
Pyrochlore	O-Y-Zr	Partly Assessed	Pyroxenes: Clino-pyroxene	Fe-O-Si	Assessed
Pyroxenes: Clino-pyroxene	Mg-O-Si	Assessed	Pyroxenes: Clino-pyroxene	Ni-O-Si	Assessed
Pyroxenes: Clino-pyroxene	Ca-Mg-O-Si	Assessed	Pyroxenes: Low clino-pyroxene	Mg-O-Si	Assessed
Pyroxenes: Ortho-pyroxene	Fe-O-Si	Assessed	Pyroxenes: Ortho-pyroxene	Mg-O-Si	Assessed
Pyroxenes: Ortho-pyroxene	Ca-Mg-O-Si	Assessed	Pyroxenes: Proto-pyroxene	Ca-O-Si	Assessed
Pyroxenes: Proto-pyroxene	Co-O-Si	Assessed	Pyroxenes: Proto-pyroxene	Cr-O-Si	Assessed
Pyroxenes: Proto-	Fe-O-Si	Assessed	Pyroxenes: Proto-pyroxene	Mg-O-Si	Assessed

Phase	*System*	*Status*	*Phase*	*System*	*Status*
pyroxene					
Pyroxenes: Proto-pyroxene	Ni-O-Si	Assessed	Pyrrhotite	Al-S	Estimated
Pyrrhotite	Co-S	Assessed	Pyrrhotite	Cr-S	Assessed
Pyrrhotite	Cu-S	Assessed	Pyrrhotite	Fe-S	Assessed
Pyrrhotite	Gd-S	Assessed	Pyrrhotite	Mg-S	Estimated
Pyrrhotite	Mn-S	Assessed	Pyrrhotite	Nb-S	Estimated
Pyrrhotite	Ni-S	Assessed	Pyrrhotite	S-Ti	Assessed
Pyrrhotite	S-V	Estimated	Pyrrhotite	S-Zr	Assessed
Quartz	O-Si	Assessed	Quartz	Al-O-P	Assessed
Rhodonite	Ca-O-Si	Assessed	Rhodonite	Co-O-Si	Assessed
Rhodonite	Fe-O-Si	Assessed	Rhodonite	Mg-O-Si	Assessed
Rhodonite	Mn-O-Si	Assessed	Rutile	Mn-O	Assessed
Rutile	O-Ti	Assessed	Rutile	O-Zr	Assessed
Rutile	Al-O-Ti	Assessed	Spinel	Al-O	Assessed
Spinel	Co-O	Estimated	Spinel	Cr-O	Estimated
Spinel	Cu-O	Assessed	Spinel	Fe-O	Estimated
Spinel	Mg-O	Estimated	Spinel	Mn-O	Estimated
Spinel	Ni-O	Estimated	Spinel	Al-Co-O	Estimated
Spinel	Al-Cr-O	Estimated	Spinel	Al-Cu-O	Assessed
Spinel	Al-Fe-O	Estimated	Spinel	Al-Mn-O	Estimated
Spinel	Al-Ni-O	Assessed	Spinel	Al-O-Ti	Assessed

Phase	*System*	*Status*	*Phase*	*System*	*Status*
Spinel	Al-O-V	Assessed	Spinel	Ca-Co-O	Assessed
Spinel	Ca-Cr-O	Assessed	Spinel	Ca-Cu-O	Assessed
Spinel	Ca-Fe-O	Assessed	Spinel	Ca-Mg-O	Assessed
Spinel	Ca-Ni-O	Assessed	Spinel	Co-Cr-O	Estimated
Spinel	Co-Cu-O	Assessed	Spinel	Co-Fe-O	Estimated
Spinel	Co-Mg-O	Estimated	Spinel	Co-Mn-O	Estimated
Spinel	Co-Mo-O	Assessed	Spinel	Co-Ni-O	Assessed
Spinel	Co-O-Ti	Assessed	Spinel	Cr-Cu-O	Assessed
Spinel	Cr-Fe-O	Estimated	Spinel	Cr-Mg-O	Estimated
Spinel	Cr-Mn-O	Estimated	Spinel	Cr-Mo-O	Assessed
Spinel	Cr-Ni-O	Estimated	Spinel	Cr-O-Ti	Estimated
Spinel	Cr-O-V	Estimated	Spinel	Cu-Fe-O	Estimated
Spinel	Cu-Mg-O	Estimated	Spinel	Cu-Mn-O	Estimated
Spinel	Cu-Mo-O	Assessed	Spinel	Cu-Ni-O	Assessed
Spinel	Cu-O-Ti	Estimated	Spinel	Cu-O-V	Estimated
Spinel	Fe-Mg-O	Estimated	Spinel	Fe-Mn-O	Estimated
Spinel	Fe-Mo-O	Estimated	Spinel	Fe-Ni-O	Estimated
Spinel	Fe-O-Ti	Estimated	Spinel	Fe-O-V	Estimated
Spinel	Mg-Mn-O	Estimated	Spinel	Mg-Mo-O	Estimated
Spinel	Mg-Ni-O	Estimated	Spinel	Mg-O-Ti	Assessed
Spinel	Mg-O-V	Assessed	Spinel	Mn-Mo-O	Assessed
Spinel	Mn-Ni-O	Estimated	Spinel	Mn-O-Ti	Assessed

Phase	*System*	*Status*	*Phase*	*System*	*Status*
Spinel	Mn-O-V	Assessed	Spinel	Mo-Ni-O	Assessed
Spinel	Ni-O-Ti	Assessed	Spinel	Ni-O-V	Assessed
Thio-spinel	Co-S	Assessed	Thio-spinel	Ni-S	Assessed
Thio-spinel	Co-Cr-S	Assessed	Thio-spinel	Co-Cu-S	Assessed
Thio-spinel	Co-Fe-S	Assessed	Thio-spinel	Co-Mn-S	Assessed
Thio-spinel	Co-Ni-S	Assessed	Thio-spinel	Cr-Cu-S	Assessed
Thio-spinel	Cr-Fe-S	Assessed	Thio-spinel	Cr-Mn-S	Assessed
Thio-spinel	Cr-Ni-S	Assessed	Thio-spinel	Cu-Ni-S	Estimated
Thio-spinel	Fe-Ni-S	Assessed	Thio-spinel	Mn-Ni-S	Assessed
Ti5O9	O-Ti	Assessed	Ti5O9	O-V	Assessed
Tridymite	O-Si	Assessed	Tridymite	Al-O-P	Assessed
t-ZrO2	Ca-O	Assessed	t-ZrO2	Cr-O	Assessed
t-ZrO2	Gd-O	Estimated	t-ZrO2	La-O	Estimated
t-ZrO2	Y-O	Estimated	t-ZrO2	O-Zr	Assessed
V2O_SS	O-V	Estimated	V3O5-HT	O-Ti	Assessed
V3O5-HT	O-V	Assessed	V3O5-HT	Al-O-V	Estimated
V3O5-HT	Cr-O-V	Assessed	V5O9	O-Ti	Assessed
V5O9	O-V	Assessed	VO2-LT	O-V	Assessed
VO2-LT	O-W	Assessed	Wollastonite	Ca-O-Si	Assessed
Wollastonite	Fe-O-Si	Assessed	Wollastonite	Mg-O-Si	Assessed
Wollastonite	Mn-O-Si	Assessed	x-M2O3	Ca-O	Assessed
x-M2O3	Gd-O	Assessed	x-M2O3	La-O	Assessed

Phase	System	Status	Phase	System	Status
x-M2O3	Y-O	Assessed	x-M2O3	Zr-O	Estimated
Y2TiO5	Gd-Ti-O	Assessed	Y2TiO5	La-Ti-O	Assessed
Y2TiO5	Y-Ti-O	Assessed	Y3NbO7	Nb-O-Y	Assessed
YAG	Al-Gd-O	Estimated	YAG	Al-La-O	Estimated
YAG	Al-O-Y	Assessed	YAG	Cr-Gd-O	Estimated
YAG	Cr-La-O	Estimated	YAG	Cr-O-Y	Estimated
YAG	Fe-Gd-O	Estimated	YAG	Fe-La-O	Estimated
YAG	Fe-O-Y	Assessed	YAM	Al-Gd-O	Estimated
YAM	Al-La-O	Estimated	YAM	Al-O-Y	Estimated
YAM	Ca-O-Si	Assessed	YAM	Gd-O-Si	Assessed
YAM	La-O-Si	Assessed	YAM	O-Si-Y	Assessed
YAP	Al-Ca	Assessed	YAP	Al-Gd	Assessed
YAP	Al-La	Assessed	YAP	Al-Y	Assessed
YAP	Ca-Co	Assessed	YAP	Ca-Cr	Assessed
YAP	Ca-Fe	Assessed	YAP	Ca-Mn	Estimated
YAP	Co-Gd	Assessed	YAP	Co-La	Assessed
YAP	Co-Y	Assessed	YAP	Cr-Gd	Assessed
YAP	Cr-La	Assessed	YAP	Cr-Y	Assessed
YAP	Fe-Gd	Estimated	YAP	Fe-La	Assessed
YAP	Al-Gd-O	Assessed	YAP	Al-La-O	Assessed
YAP	Al-O-Y	Assessed	YAP	Ca-Co-O	Assessed
YAP	Ca-Cr-O	Assessed	YAP	Ca-Fe-O	Assessed

Phase	*System*	*Status*	*Phase*	*System*	*Status*
YAP	Co-Gd-O	Assessed	YAP	Co-La-O	Assessed
YAP	Co-O-Y	Assessed	YAP	Cr-Gd-O	Assessed
YAP	Cr-La-O	Assessed	YAP	Cr-Y-O	Assessed
YAP	Fe-Gd-O	Assessed	YAP	Fe-La-O	Assessed
YAP	Fe-O-Y	Assessed	YAP	Gd-Mn-O	Assessed
YAP	La-Mn-O	Assessed	YAP	Mn-O-Y	Assessed
YNbO4	Nb-O-Y	Assessed	Zircon	Gd-Si	Assessed
Zircon	Gd-O-P	Assessed	Zircon	Gd-O-Si	Assessed
Zircon	O-P-Y	Assessed	Zircon	O-Si-Y	Estimated
Zircon	O-Si-Zr	Assessed	α-M2O3	Gd-O	Assessed
α-M2O3	La-O	Assessed	α-M2O3	Y-O	Assessed
α-M2O3	Zr-O	Estimated	α-NaFeO2	Cr-Na-O	Assessed
α-NaFeO2	Fe-Na-O	Assessed	α-Spinel	Co-O	Estimated
α-Spinel	Cu-O	Estimated	α-Spinel	Mn-O	Estimated
α-Spinel	Ni-O	Estimated	α-Spinel	Al-Co-O	Estimated
α-Spinel	Al-Cu-O	Assessed	α-Spinel	Al-Mn-O	Estimated
α-Spinel	Al-Ni-O	Assessed	α-Spinel	Co-Cr-O	Estimated
α-Spinel	Co-Fe-O	Estimated	α-Spinel	Co-Mn-O	Estimated
α-Spinel	Cr-Cu-O	Assessed	α-Spinel	Cr-Mg-O	Estimated
α-Spinel	Cr-Mn-O	Estimated	α-Spinel	Cr-Ni-O	Estimated
α-Spinel	Cu-Fe-O	Estimated	α-Spinel	Cu-Mn-O	Estimated
α-Spinel	Fe-Mg-O	Estimated	α-Spinel	Fe-Mn-O	Estimated

Phase	System	Status	Phase	System	Status
α-Spinel	Fe-Ni-O	Estimated	α-Spinel	Mg-Mn-O	Estimated
α-Spinel	Ni-Mn-O	Estimated	β1-Heazlewoodite	S	Estimated
β1-Heazlewoodite	Co-S	Assessed	β1-Heazlewoodite	Fe-S	Estimated
β1-Heazlewoodite	Ni-S	Estimated	β2-Heazlewoodite	S	Estimated
β2-Heazlewoodite	Fe-S	Estimated	β2-Heazlewoodite	Ni-S	Estimated
β-M2O3	Al-O	Assessed	β-M2O3	Ca-O	Assessed
β-M2O3	Co-O	Assessed	β-M2O3	Gd-O	Assessed
β-M2O3	La-O	Assessed	β-M2O3	Y-O	Assessed
β-M2O3	Zr-O	Estimated	β-NaFeO2	O-Si	Assessed
β-NaFeO2	Al-Na-O	Assessed	β-NaFeO2	Fe-Na-O	Assessed
β-ZrTiO4	O-Ti-Zr	Assessed	γ-NaFeO2	O-Si	Assessed
γ-NaFeO2	Al-Na-O	Assessed	γ-NaFeO2	Fe-Na-O	Assessed
γ-Nepheline	Na-Al-Si-O	Assessed	γ-Nepheline	Na-Fe-Si-O	Assessed

Assessed or Estimated Stoichiometric Compounds

This lists the stoichiometric compounds and whether the molar volume has been assessed or estimated.

Stoichiometric Compound	Status	Stoichiometric Compound	Status	Stoichiometric Compound	Status
AF	Assessed	AL2P6SI4O26	Estimated	AL2S3	Assessed
AL2SIO4F	Assessed	AL3PO7	Estimated	ALBITE_LOW	Assessed
ALBITE_MONO	Assessed	ALF3_S2	Assessed	ALNB11O29	Estimated
ALNB49O124	Estimated	ALN_B4	Assessed	ALP3O9	Assessed

Stoichiometric Compound	*Status*	*Stoichiometric Compound*	*Status*	*Stoichiometric Compound*	*Status*
ANDALUSITE	Assessed	ANILITE	Assessed	C11A7F	Estimated
C13A6Z2	Estimated	C1A8M2	Estimated	C2A14M2	Estimated
C3A2M1	Estimated	C3A3F	Estimated	C4WF4	Assessed
C4WF8	Estimated	CA10P6O25	Estimated	CA10SI3O15F2	Estimated
CA10V6O19	Estimated	CA15CU18O35	Estimated	CA2ALF7	Estimated
CA2ALNBO6	Assessed	CA2CUO3	Assessed	CA2NA2SI2O7	Estimated
CA2NA2SI3O9	Estimated	CA2NB2O7	Assessed	CA2P6O17	Estimated
CA2V2O7	Assessed	CA2ZRSI4O12	Estimated	CA3COAL4O10	Assessed
CA3NA2SI6O16	Assessed	CA3NB2O8	Estimated	CA3TI2O7	Assessed
CA3TI8AL12O37	Estimated	CA3V2O8	Assessed	CA3WO6	Estimated
CA3ZRSI2O9	Assessed	CA4MG2P6O21	Estimated	CA4P2O9_A	Assessed
CA4P2O9_B	Assessed	CA4P6O19	Estimated	CA4TI3O10	Assessed
CA4V2O9	Estimated	CA5SI2O8F2	Estimated	CA6ZR19O44	Estimated
CA7P2SI2O16	Estimated	CA9V6O18	Estimated	CAALF5_S1	Estimated
CAALF5_S2	Estimated	CACO3	Assessed	CACRSI4O10	Estimated
CACU2O3	Assessed	CAMG3O16S4	Estimated	CAMN2O4	Assessed
CANA2SI5O12	Estimated	CANA2SIO4	Assessed	CANA4SI3O9	Estimated
CAP2O6_A	Assessed	CAP2O6_B	Assessed	CAP2O6_G	Assessed
CAP4O11_A	Assessed	CAP4O11_B	Assessed	CAV2O5	Assessed
CAV3O7	Assessed	CAV4O9	Estimated	CAVO3	Assessed
CAWO4	Assessed	CAZR4O9	Estimated	CF2	Estimated

Stoichiometric Compound	Status	Stoichiometric Compound	Status	Stoichiometric Compound	Status
CHALCOCITE_ALPHA	Assessed	CHALCOCITE_BETA	Assessed	CO1LA2O4	Assessed
CO2P2O7	Assessed	CO3LA4O10	Assessed	CO3P2O8	Assessed
COVELLITE	Assessed	CR1S1	Assessed	CR3P2O8	Estimated
CR3PO7	Estimated	CR4P6O21	Estimated	CR5PO10	Estimated
CR5S6	Assessed	CR7S8	Estimated	CRNB25O64	Estimated
CRNB49O124	Estimated	CRNB9O24	Estimated	CRP3O9	Assessed
CRPO4	Assessed	CRVO4	Assessed	CU2COO3	Assessed
CU2P2O7	Assessed	CU2SO4	Assessed	CU2SO5	Assessed
CU2Y2O5	Assessed	CU3NB2O8	Estimated	CU3P2O8	Assessed
CUCRS2	Assessed	CUF	Assessed	CUFES2_LT	Assessed
CUGD2O4	Assessed	CUNB2O6	Assessed	CUPO3	Estimated
CUSPIDINE	Assessed	CW3F	Assessed	CWF	Assessed
DJURLEITE	Assessed	FE18P2O24	Estimated	FE2P2O7	Assessed
FE2PO5	Assessed	FE3P2O8	Assessed	FE3P4O14	Estimated
FE3PO7	Assessed	FE4P6O21	Estimated	FE7P6O24	Estimated
FE7P8O28	Estimated	FEAL2S4	Assessed	FENB25O64	Estimated
FENB49O124	Estimated	FENB9O24	Estimated	FEP2O6	Assessed
FEP3O9	Estimated	FEV2O6	Estimated	GUGGENITE	Assessed
K10MG5SI11O32	Estimated	K2CA2SI2O7	Estimated	K2CA2SI9O21	Estimated
K2CA3SI6O16	Estimated	K2CA6SI4O15	Estimated	K2CASIO4	Estimated
K2FE2SI6O16	Estimated	K2FESI3O8	Estimated	K2FESI5O12	Estimated

Stoichiometric Compound	Status	Stoichiometric Compound	Status	Stoichiometric Compound	Status
K2MG5SI12O30	Estimated	K2MGF4	Estimated	K2MGN4O12	Estimated
K2S2	Estimated	K2S3	Estimated	K2S4	Estimated
K2S5	Estimated	K2S6	Estimated	K2SI4O9_ALPHA	Estimated
K2SI4O9_BETA	Estimated	K2TI3O7	Estimated	K2TI6O13	Estimated
K2TIO3	Estimated	K3ALF6	Estimated	K3FCO3	Estimated
K3PO4_ALPHA	Estimated	K3PO4_BETA	Estimated	K3PO4_GAMMA	Estimated
K4CAN6O18	Estimated	K4CASI3O9	Estimated	K4CASI6O15	Estimated
K4FE4SI3O14	Estimated	K4FEO3	Estimated	K4MG2SI5O14	Estimated
K4P2O7_ALPHA	Estimated	K4P2O7_BETA	Estimated	K4P2O7_DELTA	Estimated
K4P2O7_GAMMA	Estimated	K4SIO4	Estimated	K4TIO4	Estimated
K5P3O10_ALPHA	Estimated	K5P3O10_BETA	Estimated	K8CASI10O25	Estimated
K8TI5O14	Estimated	KCAF3	Estimated	KFESIO4	Estimated
KMG2AL15O25	Estimated	KMGF3	Estimated	KPO3_ALPHA	Estimated
KPO3_BETA	Estimated	KPO3_GAMMA	Estimated	KYANITE	Assessed
LA1S2	Assessed	LA2CR3O12	Estimated	LA2CRO6	Assessed
LA2NB12O33	Estimated	LA2TI3O9	Estimated	LA3NBO7	Assessed
LA4SI3O12	Estimated	LA4TI3O12	Estimated	LA4TI9O24	Estimated
LAAL11O18	Estimated	LAFE12O19	Estimated	LANB3O9	Estimated
LANBO4	Assessed	LANIO3	Assessed	LARNITE	Assessed
M12C	Assessed	MERWINITE	Assessed	MG2C3	Estimated
MG2NA2SI6O15	Estimated	MG2NB34O87	Estimated	MG5NB4O15	Estimated

Stoichiometric Compound	Status	Stoichiometric Compound	Status	Stoichiometric Compound	Status
MGC2	Estimated	MGCO3	Assessed	MGNA2SI4O10	Estimated
MGP2O6	Assessed	MGP4O11	Assessed	MN2P2O7	Assessed
MN2V2O7	Assessed	MN3N2	Assessed	MN3P2O8	Assessed
MN5SIC	Estimated	MN6N5	Estimated	MN9SI3O14S1	Estimated
MNF2_S1	Assessed	MNF3	Assessed	MNP2O6	Assessed
MNYO3_HEX	Assessed	MO2S3	Estimated	MO4O11	Estimated
MO8O23	Estimated	MO9O26	Assessed	MOF4	Estimated
MOO3	Estimated	NA10SIO7	Estimated	NA2CA3AL16O28	Estimated
NA2CA8AL6O18	Estimated	NA2FEO2	Estimated	NA2FESIO4	Estimated
NA2TI3O7	Assessed	NA2TI6O13	Assessed	NA2TIO3_S1	Assessed
NA2TIO3_S2	Assessed	NA2V2O6	Assessed	NA3ALF6_S1	Estimated
NA3FE5O9	Assessed	NA3FEO3	Assessed	NA3PO4	Estimated
NA4FE6O11	Estimated	NA4FEO3	Assessed	NA4P2O7	Assessed
NA4SIO4	Assessed	NA4TIO4	Assessed	NA4V2O7	Assessed
NA5AL3F14	Estimated	NA5FEO4	Assessed	NA5FESI4O12	Estimated
NA6SI2O7	Assessed	NA6SI8O19	Assessed	NA6V2O8	Estimated
NA8FE2O7	Estimated	NA8FE6SI15O40	Estimated	NA8TI5O14	Assessed
NAFE2O3	Assessed	NAFESI2O6	Assessed	NAMGF3	Estimated
NAPO3	Assessed	NAS2	Assessed	NBF5	Assessed
NBO1	Assessed	NI2P2O7	Assessed	NI3P2O8	Assessed
NI3S2_LT	Assessed	NI4NB2O9	Estimated	NINB14O36	Estimated

Stoichiometric Compound	*Status*	*Stoichiometric Compound*	*Status*	*Stoichiometric Compound*	*Status*
NINB36O91	Estimated	NINB68O171	Estimated	NIOCALITE_C10NS6	Estimated
NIS_LT	Estimated	P2O5_H	Assessed	P2O5_O	Assessed
P2O5_OP	Assessed	P2S5	Assessed	PSEUDO_ WOLLASTONITE	Assessed
Q_ALMGZRO	Estimated	RANKINITE	Assessed	SAPPHIRINE	Estimated
SI3N4	Estimated	SI3P4O16	Estimated	SIC_B3	Assessed
SILLIMANITE	Assessed	SIP2O7_CUB	Assessed	SIP2O7_MONO	Assessed
SIP2O7_TETR	Assessed	SIS2	Assessed	SPHENE	Assessed
TI10O19	Estimated	TI20O39	Assessed	TI2NB10O29	Estimated
TI2S	Assessed	TI3O2	Estimated	TI4C2S2	Assessed
TI5P6O25	Estimated	TI8S10	Estimated	TI8S3	Estimated
TI8S9	Estimated	TI9O17	Assessed	TINB24O62	Estimated
TINB2O7	Estimated	TIO_ALPHA	Estimated	TIP2O7	Assessed
TIS2	Assessed	TIS3	Assessed	V2O5	Assessed
V3O5_LT	Assessed	V3O7	Assessed	V52O64	Assessed
V6O13	Assessed	WO2_72	Assessed	WO2_90	Assessed
WO2_96	Assessed	WO3_HT	Assessed	WO3_LT	Assessed
Y15C19_ALPHA	Estimated	Y15C19_BETA	Estimated	Y2S2A_Y2SI2O7	Assessed
Y2S2B_Y2SI2O7	Assessed	Y2S2D_Y2SI2O7	Assessed	Y2S2G_Y2SI2O7	Assessed
Y2SIO5	Assessed	ZR11NB4O32	Estimated	ZR13NB4O36	Estimated
ZR15NB4O40	Estimated	ZR2P2O9	Assessed	ZR3Y4O12	Assessed
ZR5NB2O15	Estimated	ZR6NB2O17	Estimated	ZR7NB2O19	Estimated

Stoichiometric Compound	*Status*	*Stoichiometric Compound*	*Status*	*Stoichiometric Compound*	*Status*
ZR8NB2O21	Estimated	ZRF4	Assessed	ZRO8S2	Assessed
ZRS2	Assessed	ZRTI2O6	Assessed	ZRTIO4_ALPHA	Estimated

TCOX13 Surface Tension Assessed Systems

Model Description

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

Included Oxides

Included Oxides Assessed for Surface Tension							
Al_2O_3	B_2O_3	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
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

Pseudo Binary Systems Assessed for 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
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	MgO-SiO_2	MnO-SiO_2	Na_2O-SiO_2		

Assessed Pseudo Ternary Systems

Pseudo Ternary Systems Assessed for 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
Al_2O_3-CaO-Cr_2O_3	Al_2O_3-CaO-Fe_2O_3	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

Pseudo Ternary Systems Assessed for Surface Tension					
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

Pseudo Quaternary Systems Assessed for 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

TCOX13 Electrical Conductivity for Ionic Liquids Assessed Systems

Model Description

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

Included Oxides and Fluorides

Included Oxides and Fluorides for Electrical Conductivity					
Al_2O_3	B_2O_3	CaF_2	CaO	Cr_2O_3	CuO_x
FeO_x	K_2O	LaF_3	La_2O_3	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

Assessed or Estimated Unary Systems

A system is estimated based on other predictions and data of ternaries.

System	*Status*	*System*	*Status*
Al_2O_3	Assessed	B_2O_3	Estimated
CaO	Assessed	CaF_2	Assessed
Cr_2O_3	Estimated	CuO_x	Estimated
FeO_x	Assessed	K_2O	Estimated
LaF_3	Estimated	La_2O_3	Estimated
MgF_2	Assessed	MgO	Assessed

System	Status	System	Status
MnO_x	Assessed	MoO_3	Estimated
Na_2O	Estimated	Nb_2O_5	Estimated
NiO	Estimated	P_2O_5	Estimated
SiO_2	Assessed	TiO_2	Estimated
V_2O_5	Assessed	Y_2O_3	Estimated
YF_3	Estimated	ZrO_2	Estimated

Assessed Pseudo Binary Systems

Pseudo Binary Systems Assessed for Electrical Conductivity of Ionic Liquid			
Al_2O_3-SiO_2	B_2O_3-CaF_2	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	MgO-Al_2O_3	MgO-SiO_2
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	

Assessed Pseudo Ternary Systems

Pseudo Ternary Systems Assessed for Electrical Conductivity of Ionic Liquid			
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	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

Pseudo Quaternary Systems Assessed for Electrical Conductivity of Ionic Liquid			
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

Higher Order Systems Assessed for Electrical Conductivity of Ionic Liquid			
CaF_2-CMAS	Fe-O-CMAS	MnO-CMAS	TiO_2-CMAS
Fe-Mn-O-CaF_2-CMAS			

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:	**13.0**
First release:	**TCOX was released in 1992 under the name ION**

Changes in the Most Recent Database Release

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.

Previous Releases

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.