TCS Metal Oxide Solutions Database (TCOX12)

Technical Information

Available Starting with Thermo-Calc Version 2023a

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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, and surface tension.

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).

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 TCOX12. 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 TCOX12 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.

TCOX12 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:

- 398 binary and 535 ternary systems in the 32 element framework.

> 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 TCOX12 Assessed Metallic Systems for suggestions.

- 141 pseudo-ternary oxide systems, 39 oxy-fluoride and oxy-sulfide systems, and some higher order systems.

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 604 phases in total.

TCOX12 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 TCOX12 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 TCOX12 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 TCOX12 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 TCOX12 Surface Tension Assessed Systems.

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

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).

TCOX12 Systems

In this section:

TCOX12 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.

TCOX12 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 Ternary Oxide Systems, Me1-Me2-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	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

Assessed Quaternary Oxide Systems, Me1-Me2-Me3-O							
Mg-O-Si-Ti	Mg-O-Si-V	Mg-O-Si-Y	Mg-O-Si-Zr	Mg-O-Y-Zr	Mn-Ni-O-V	Mn-O-Y-Zr	Na-O-P-Si
O-Si-Y-Yb	O-Ti-Y-Zr	O-Y-Yb-Zr					

Assessed Higher Order Oxide Systems

Assessed Higher Order Oxide Systems				
Al-Ca-Co-O-Si	Al-Ca-Fe-O-Si	Al-Ca-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		

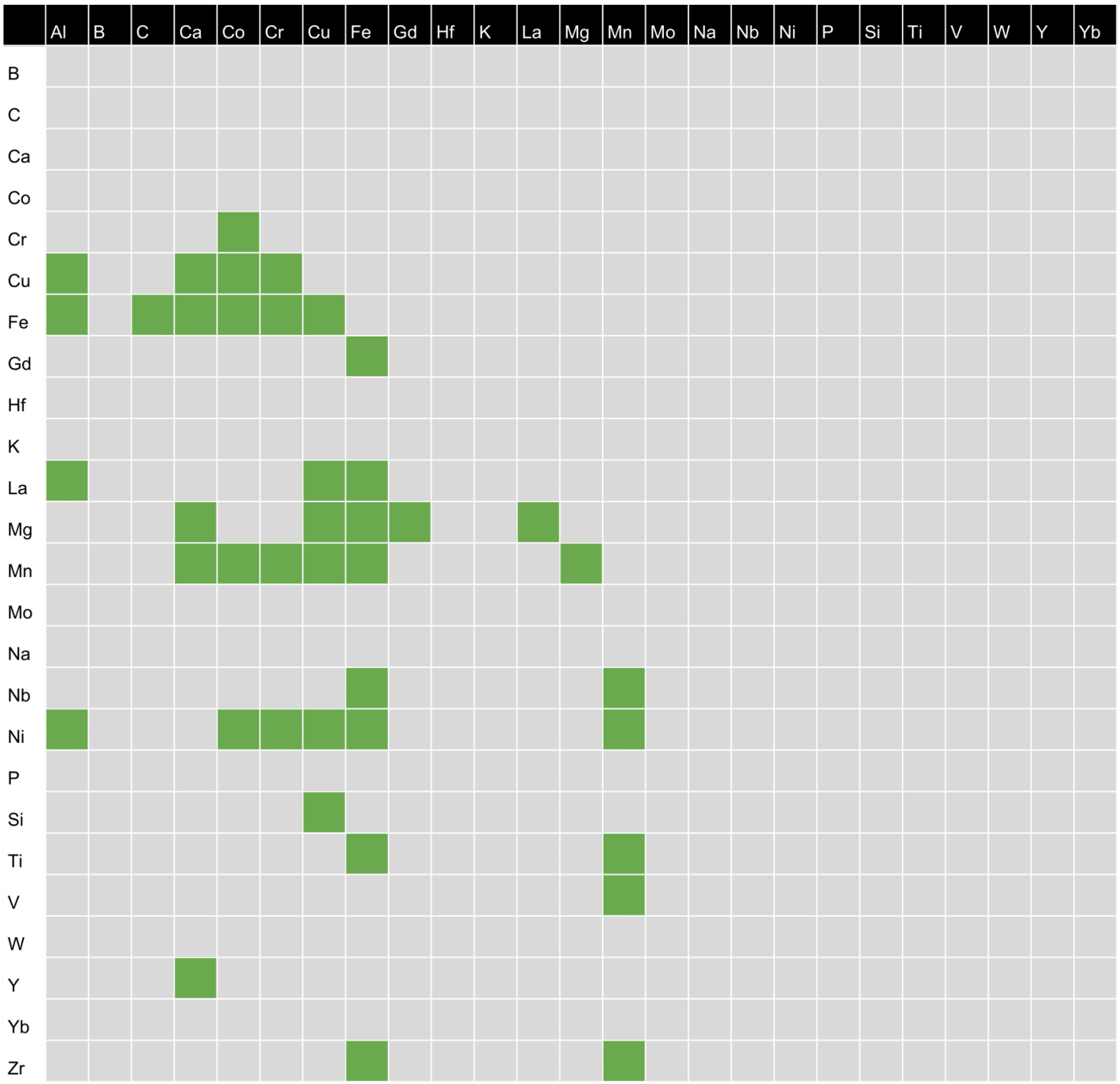
TCOX12 Assessed Sulfide Systems

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 Ternary Sulfide Systems, Me1-Me2-S



Assessed Oxy-sulfide 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				
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
Al-Ca-Mn-O-S

TCOX12 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 Ternary Fluoride Systems

Assessed Ternary Fluoride Systems					
Al-Ca-F	Al-F-K	Al-F-Mg	Al-F-Na	Al-F-Zr	Ca-Co-F
Ca-Cr-F	Ca-F-Fe	Ca-F-Gd	Ca-F-K	Ca-F-La	Ca-F-Mg
Ca-F-Mn	Ca-F-Na	Co-F-Gd	Co-F-Mg	Co-F-Ni	F-Fe-Ni
F-Gd-Mg	F-Gd-Y	F-K-Mg	F-K-Na	F-La-Mg	F-La-Zr
F-Mg-Mn	F-Mg-Na	F-Mg-Y	F-Na-Si		

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			
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			
Al-Ca-F-Mg-O	Al-Ca-F-O-Si	Ca-F-Fe-O-Si	Ca-F-Na-O-Si

TCOX12 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.

TCOX12 Models for the Included Phases

Also see the listing for Gas Phase.

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
IONIC_LIQ	Liquid					Liquid metal and slag mixture.	2	[1.0, 1.0]	(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(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
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	This is FCC_A1 solid solution and TiO and VO cubic oxides.	2	[1.0, 1.0]	(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(B, C, N, O, VA)1
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229		2	[1.0, 3.0]	(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(B, C, N, O, VA)3
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194	HCP_A3 also describes hexagonal carbides and nitrades.	2	[1.0, 0.5]	(AL, CA, CO, CR, CU, FE, GD, HF, K, LA, MG, MN, MO, NA, NB, NI, SI, TI, V, W, Y, YB, ZR)1

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									(B, C, N, O, VA)0.5
CUB_A13	beta-Mn (A13)	A13	cP20	P4_132	213		2	[1.0, 1.0]	(AL, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, SI, TI, V, ZR)1(B, C, N, VA)1
CBCC_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[1.0, 1.0]	(AL, CO, CR, CU, FE, MG, MN, MO, NB, NI, SI, TI, V, ZR)1(B, C, N, VA)1
DHCP	alpha-La (A3')	A3'	hP4	P6_3/mmc	194		2	[1.0, 0.5]	(AL, CA, CU, GD, LA, MG, MN, NI, Y)1(O, VA)0.5
BETA_RHOMBO_B	beta-B (R-105)		hR105	R-3m	166		2	[93.0, 12.0]	(B)93(B, C, SI)12
DIAMOND_FCC_A4	Diamond (A4)	A4	cF8	Fd-3m	227	This is Silicon	2	[1.0, 1.0]	(AL, B, C, MN, NA, P, SI)1(O, VA)1
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	P6_3/mmc	194	Graphite	1	[1.0]	(B, C)1
AL18B4O33	Al5BO9		oS60	Cmc2_1	36		3	[18.0, 4.0, 33.0]	(AL+3)18(B+3)4(O-2)33
AL4B2O9	Al4B1.5[BO3]0.5O7.5		mS124	C2/m	12		3	[4.0, 2.0, 9.0]	(AL+3)4(B+3)2(O-2)9
CAB4O7	CaB4O7		mP96	P2_1/c	14		3	[1.0, 4.0, 7.0]	(CA+2)1(B+3)4(O-2)7
CAB2O4	CaB2O4 I (E32)	E32	oP28	Pbcn	60		3	[1.0, 2.0, 4.0]	(CA+2)1(B+3)2(O-2)4
CA2B2O5_S1	b-Mg2B2O5		mP36	P2_1/c	14		3	[2.0, 2.0, 5.0]	(CA+2)2(B+3)2(O-2)5
CA2B2O5_S2	Ca2B2O5		oP36	P2_12_12_1	19		3	[2.0, 2.0, 5.0]	(CA+2)2(B+3)2(O-2)5

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
CA3B2O6	Ca3[BO3]2		hR22	R-3c	167		3	[3.0, 2.0, 6.0]	(CA+2)3(B+3)2(O-2)6
FEB4O7	ZnB4O7		oS48	Cmcm	63		3	[1.0, 4.0, 7.0]	(FE+2)1(B+3)4(O-2)7
FE3BO5	Fe3[BO3]O2		oP36	Pbam	55		4	[2.0, 1.0, 1.0, 5.0]	(FE+2)2(FE+3)1(B+3)1 (O-2)5
FEBO3	Calcite (CaCO3, G01)	G01	hR10	R-3c	167		3	[1.0, 1.0, 3.0]	(FE+3)1(B+3)1(O-2)3
FE3BO6	Norbergite [Mg(F,OH)2 . Mg2SiO4, S07]	S07	oP40	Pnma	62		3	[3.0, 1.0, 6.0]	(FE+3)3(B+3)1(O-2)6
MGB4O7	CdB4O7		oP96	Pbca	61		3	[1.0, 4.0, 7.0]	(MG+2)1(B+3)4(O-2)7
MG2B2O5	Co2B2O5		aP18	P-1	2	This is (Co,Fe,Mg,Ni)2B2O5	3	[2.0, 2.0, 5.0]	(CO+2, FE+2, MG+2, NI+2)2(B+3)2(O-2)5
NI3B2O6	Kotoite (Mg3(BO3)2)		oP22	Pnnm	58	This is (Co,Mg,Ni)3B2O6	3	[3.0, 2.0, 6.0]	(CO+2, MG+2, NI+2)3 (B+3)2(O-2)6
NABO2_A	KBO2 (F513)	F513	hR24	R-3c	167	This is ht-NaBO2 and KBO2.	3	[1.0, 1.0, 2.0]	(K+1, NA+1)1(B+3)1 (O-2)2
NABO2_B	Unknown Structure					rt-NaBO2	3	[1.0, 1.0, 2.0]	(NA+1)1(B+3)1(O-2)2
NAB3O5	NaB3O5-a		mP108	P2_1/c	14	This is (K,Na)B3O5.	3	[1.0, 3.0, 5.0]	(K+1, NA+1)1(B+3)3 (O-2)5
NAB5O8_A	Unknown Structure						3	[1.0, 5.0, 8.0]	(NA+1)1(B+3)5(O-2)8
NAB5O8_B	Unknown Structure						3	[1.0, 5.0, 8.0]	(NA+1)1(B+3)5(O-2)8

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
NAB5O8_G	KB5O8-a		oP112	Pbca	61	This is ht-NaB5O8 and KB5O8.	3	[1.0, 5.0, 8.0]	(K+1, NA+1)1(B+3)5 (O-2)8
NAB9O14_A	Unknown Structure						3	[1.0, 9.0, 14.0]	(NA+1)1(B+3)9(O-2)14
NAB9O14_B	Unknown Structure						3	[1.0, 9.0, 14.0]	(NA+1)1(B+3)9(O-2)14
NAB9O14_G	Unknown Structure						3	[1.0, 9.0, 14.0]	(NA+1)1(B+3)9(O-2)14
NA2B4O7	Na2B4O7		aP52	P-1	2	This is (K,Na)2B4O7.	3	[2.0, 4.0, 7.0]	(K+1, NA+1)2(B+3)4 (O-2)7
NA2B8O13	Na2B8O13		mP92	P2_1/c	14		3	[2.0, 8.0, 13.0]	(NA+1)2(B+3)8(O-2)13
NA3BO3	NaB3O5-a		mP108	P2_1/c	14	This is (K,Na)3BO3.	3	[3.0, 1.0, 3.0]	(K+1, NA+1)3(B+3)1 (O-2)3
NA4B2O5	Na4B2O5		mS44	C2/c	15	This is (K,Na)4B2O5.	3	[4.0, 2.0, 5.0]	(K+1, NA+1)4(B+3)2 (O-2)5
K4B6O11	Unknown Structure						3	[4.0, 6.0, 11.0]	(K+1)4(B+3)6(O-2)11
K5B19O31	K5B19O31		mS220	C2/c	15		3	[5.0, 19.0, 31.0]	(K+1)5(B+3)19(O-2)31
KB9O14	Unknown Structure						3	[1.0, 9.0, 14.0]	(K+1)1(B+3)9(O-2)14
YBO3	Unknown Structure					This is (Y,Yb)BO3 solid solution.	3	[1.0, 1.0, 3.0]	(Y+3, YB+3)1(B+3)1(O-2)3
GDBO3	GdBO3		hR30	R32	155	This is (Gd,La)BO3 solid solution.	3	[1.0, 1.0, 3.0]	(GD+3, LA+3)1(B+3)1 (O-2)3

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
LA3BO6	Unknown Structure					This is (Gd,La)3BO6 solid solution.	3	[3.0, 1.0, 6.0]	(GD+3, LA+3)3(B+3)1 (O-2)6
LAB3O6	LaB3O6		mS40	C2/c	15	This is (Gd,La)B3O6 solid solution.	3	[1.0, 3.0, 6.0]	(GD+3, LA+3)1(B+3)3 (O-2)6
CU3B2O6	Cu3B2O6		aP110	P-1	2		3	[3.0, 2.0, 6.0]	(CU+2)3(B+3)2(O-2)6
CUB2O4	CuB2O4		tI84	I-42d	122		3	[1.0, 2.0, 4.0]	(CU+2)1(B+3)2(O-2)4
CUB8O13	Unknown Structure						3	[1.0, 8.0, 13.0]	(CU+2)1(B+3)8(O-2)13
CU2B4O7	Unknown Structure						3	[2.0, 4.0, 7.0]	(CU+1)2(B+3)4(O-2)7
NB3BO9	Unknown Structure						3	[3.0, 1.0, 9.0]	(NB+5)3(B+3)1(O-2)9
BPO4	BPO4 (H07)	H07	tI12	I-4	82		3	[1.0, 1.0, 4.0]	(B+3)1(P+5)1(O-2)4
MNB2O4	Unknown Structure						3	[1.0, 2.0, 4.0]	(MN+2)1(B+3)2(O-2)4
MNB4O7	Unknown Structure						3	[1.0, 4.0, 7.0]	(MN+2)1(B+3)4(O-2)7
MNB6O10	Unknown Structure						3	[1.0, 6.0, 10.0]	(MN+2)1(B+3)6(O-2)10
MNBO3	Unknown Structure						3	[1.0, 1.0, 3.0]	(MN+3)1(B+3)1(O-2)3
MN2B4O9	Unknown Structure						3	[2.0, 4.0, 9.0]	(MN+3)2(B+3)4(O-2)9

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
MNB3O6	Unknown Structure						3	[1.0, 3.0, 6.0]	(MN+3)1(B+3)3(O-2)6
K2MG3B2O7	Unknown Structure						4	[2.0, 3.0, 2.0, 7.0]	(K+1)2(MG+2)3(B+3)2 (O-2)7
CAAL2B2O7	Unknown Structure						4	[1.0, 2.0, 2.0, 7.0]	(CA+2)1(AL+3)2(B+3)2 (O-2)7
CA2AL2B2O8	Unknown Structure						4	[2.0, 2.0, 2.0, 8.0]	(CA+2)2(AL+3)2(B+3)2 (O-2)8
NA2AL2B2O7	Na2Ga2[BO3]2O		hP30	P-31c	163		4	[2.0, 2.0, 2.0, 7.0]	(NA+1)2(AL+3)2(B+3)2 (O-2)7
MALINKOITE	BaZn[GeO4]		hP42	P6_3	173	NaBSiO4 with SiO2 solubility	2	[1.0, 1.0]	(NAB+4, SI+4)1(SIO4-4)1
KBSI2O6	K(Si0.67B0.33)3O6		cI160	I-43d	220	Lisitsynite	4	[1.0, 1.0, 2.0, 6.0]	(K+1)1(B+3)1(SI+4)2 (O-2)6
KBSI3O8	Danburite (CaB2Si2O8, S63)	S63	oP52	Pnma	62		4	[1.0, 1.0, 3.0, 8.0]	(K+1)1(B+3)1(SI+4)3 (O-2)8
DANBURITE	Danburite (CaB2Si2O8, S63)	S63	oP52	Pnma	62		4	[1.0, 2.0, 2.0, 8.0]	(CA+2)1(B+3)2(SI+4)2 (O-2)8
OKAYAMALITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	P-42_1m	113		4	[2.0, 2.0, 1.0, 7.0]	(CA+2)2(B+3)2(SI+4)1 (O-2)7
CA11B2SI4O22_LT	Unknown Structure						4	[11.0, 2.0, 4.0, 22.0]	(CA+2)11(B+3)2 (SI+4)4(O-2)22
CA11B2SI4O22_HT	Unknown Structure						4	[11.0, 2.0, 4.0, 22.0]	(CA+2)11(B+3)2 (SI+4)4(O-2)22
CEMENTITE_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(AL, CO, CR, FE, MN, MO, NB, NI, SI, V, W)3 (B, C, N)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
M23C6_D84	Cr23C6 (D84)	D84	cF116	Fm-3m	225		3	[20.0, 3.0, 6.0]	(CO, CR, FE, MN, NI, V)20(CO, CR, FE, MN, MO, NI, V, W)3(B, C)6
M7C3_D101	C3Cr7 (D101)	D101	oP40	Pnma	62		2	[7.0, 3.0]	(AL, CO, CR, FE, MN, MO, NB, NI, SI, V, W)7 (B, C)3
M6C_E93	Fe3W3C (E93)	E93	cF112	Fd-3m	227		4	[2.0, 2.0, 2.0, 1.0]	(CO, FE, NI)2(MO, NB, W)2(CO, CR, FE, MO, NB, NI, SI, V, W)2(C)1
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[5.0, 2.0]	(FE, MN, NB, V)5(C, N)2
M3C2_D510	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62		2	[3.0, 2.0]	(CO, CR, MO, V, W)3 (C)2
MC_ETA	CMo		hP12	P6_3/mmc	194		2	[1.0, 1.0]	(MO, TI, V, W)1(C, VA)1
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	P-6m2	187		2	[1.0, 1.0]	(MO, W)1(C, N)1
KSI_CARBIDE	Mo6Fe11C5		mS44	C2/m	12		2	[3.0, 1.0]	(CR, FE, MO, W)3(C)1
B4C_D1G	B13C2 B4C (D1g)	D1g	hR15	R-3m	166		2	[1.0, 1.0]	(B11C, B12)1(B2, C2B, CB2)1
KAPPA_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221		3	[1.0, 3.0, 1.0]	(AL)1(FE, MN)3(C, VA)1
AL4C3_D71	Al4C3 (D71)	D71	hR7	R-3m	166		2	[4.0, 3.0]	(AL, SI)4(C)3
M12C	Fe6W6C		cF104	Fd-3m	227		3	[6.0, 6.0, 1.0]	(CO)6(W)6(C)1
FE8SI2C	Mn8Si2C		aP*	P1	1		3	[8.0, 2.0, 1.0]	(FE, MN)8(SI)2(C)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
MGC2	MgC2		tP6	P4_2/mnm	136		2	[1.0, 2.0]	(MG)1(C)2
MG2C3	Mg2C3		oP10	Pnnm	58		2	[2.0, 3.0]	(MG)2(C)3
SIC_B3	Zincblende (ZnS, B3)	B3	cF8	F-43m	216		2	[1.0, 1.0]	(SI)1(C)1
MN5SIC	Mn5SiC		oS56	Cmc2_1	36		3	[0.714, 0.143, 0.143]	(MN)0.714(SI)0.143 (C)0.143
Y15C19_ALPHA	alpha-Y15C19		oP18	Pbam	55		2	[19.0, 15.0]	(C)19(Y)15
Y15C19_BETA	Unknown Structure						2	[19.0, 15.0]	(C)19(Y)15
Y2C3_ALPHA	Sc3C4		tP70	P4/mnc	128		3	[2.0, 2.0, 1.0]	(Y)2(C)2(C, VA)1
Y2C3_BETA	Unknown Structure						3	[2.0, 2.0, 1.0]	(Y)2(C)2(C, VA)1
YC_B1	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		2	[1.0, 1.0]	(Y)1(C, C2, VA)1
TI4C2S2	AlCCr2		hP8	P6_3/mmc	194		3	[4.0, 2.0, 2.0]	(TI)4(C)2(S)2
Z_PHASE	CrNbN		tP6	P4/nmm	129		3	[1.0, 1.0, 1.0]	(CR, FE)1(MO, NB, V)1 (N, VA)1
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	Pm-3m	221		2	[4.0, 1.0]	(CO, CR, FE, MN, NI)4 (C, N, VA)1
PI_A13	beta-Mn (A13)	A13	cP20	P4_132	213		3	[12.8, 7.2, 4.0]	(CR)12.8(FE, NI, SI)7.2 (N)4
ETA_M5SIN	Fe3W3C (E93)	E93	cF112	Fd-3m	227		4	[3.0, 2.0, 1.0, 1.0]	(CR, MO)3(FE, NI)2 (SI)1(N)1
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186		2	[1.0, 1.0]	(AL)1(N)1

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SI3N4	Nierite (alpha-Si3N4)		hP28	P31c	159		2	[3.0, 4.0]	(SI)3(N)4
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136		2	[2.0, 1.0]	(TI)2(C, N)1
MN3N2	Mn3N2		tI10	I4/mmm	139		2	[3.0, 2.0]	(MN)3(N)2
MN6N5	CoO		tI4	I4/mmm	139		2	[6.0, 5.0]	(MN)6(N)5
MG3N2_D53	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	206		2	[3.0, 2.0]	(CA, MG)3(N)2
RED_P	Unknown Structure					This is pure phosphorus.	1	[1.0]	(P)1
WHITE_P	Unknown Structure					This is pure phosphorus. Not stable at normal conditions.	1	[1.0]	(P)1
C1A1	Al2CaO4		mP84	P2_1/c	14	This is CaO.Al2O3 (mP84, P121/c1) with solubility of Fe	4	[3.0, 5.0, 1.0, 12.0]	(CA+2)3(AL+3)5(AL+3, FE+3)1(O-2)12
C1A2	Al4CaO7		mS48	C2/c	15	This is CaO.2Al2O3 (mS48, C12/c1) with solubility of Fe	4	[1.0, 3.0, 1.0, 7.0]	(CA+2)1(AL+3)3(AL+3, FE+3)1(O-2)7
C1A6	Magnetoplumbite (PbFe12O19)		hP64	P6_3/mmc	194	This is CaO.6Al2O3 with solubility of Fe	3	[1.0, 12.0, 19.0]	(CA+2)1(AL+3, FE+3)12(O-2)19
C3A1	Ca3Al2O6		cP264	Pa-3	205	This is 3CaO.Al2O3 with solubility of Fe	3	[3.0, 2.0, 6.0]	(CA+2)3(AL+3, FE+3)2 (O-2)6
C12A7	Mayenite (12CaO.7Al2O3, K74, C12A7)	K74	cI152	I-43d	220	Not stable under anhydrous conditions.	4	[6.0, 6.0, 1.0, 16.5]	(CA+2)6(AL+3)6(AL+3, FE+3)1(O-2)16.5
AF	FeGaO3		oP40	Pna2_1	33	This is Al2O3.Fe2O3.	3	[2.0, 2.0, 6.0]	(AL+3)2(FE+3)2(O-2)6
CACR2O4_A	SrCr2O4		oP28	Pmmn	59	With solubility of Al and Fe.	3	[1.0, 2.0, 4.0]	(CA+2)1(AL+3, CR+3, FE+3)2(O-2)4
CF2	Ca3.5Fe14O24.5		mS172	C2	5	This is CaO.2Fe2O3	3	[1.0, 4.0, 7.0]	(CA+2)1(FE+3)4(O-2)7

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C2F	Ca2Fe2O5		oP36	Pnma	62	This is 2CaO.Fe2O3 with solubility of Al.	3	[2.0, 2.0, 5.0]	(CA+2)2(AL+3, FE+3)2 (O-2)5
CWF	CaFe3O5		oS36	Cmcm	63	This is CaO.FeO.Fe2O3.	4	[1.0, 1.0, 2.0, 5.0]	(CA+2)1(FE+2)1 (FE+3)2(O-2)5
CW3F	CaFe5O7		oS52	Cmcm	63	This is CaO.3FeO.Fe2O3.	4	[1.0, 3.0, 2.0, 7.0]	(CA+2)1(FE+2)3 (FE+3)2(O-2)7
C4WF4	Ca4Fe9O17		mS60	C2	5	This is 4CaO.FeO.4Fe2O3.	4	[4.0, 1.0, 8.0, 17.0]	(CA+2)4(FE+2)1 (FE+3)8(O-2)17
C4WF8	Sr2Fe2O5		oI44	Imma	74	This is 4CaO.FeO.8Fe2O3	4	[4.0, 1.0, 16.0, 29.0]	(CA+2)4(FE+2)1 (FE+3)16(O-2)29
CAV2O4	CaV2O4		oP28	Pnma	62	This is CaO.Fe2O3, b-CaCr2O4 and Ca(V,Y,Yb)2O4.	3	[1.0, 2.0, 4.0]	(CA+2)1(AL+3, CR+3, FE+3, V+3, Y+3, YB+3)2(O-2)4
CAMN2O4	CaMn2O4		oP28	Pbcm	57		3	[1.0, 2.0, 4.0]	(CA+2)1(MN+3)2(O-2)4
CUO	Tenorite (CuO, B26)	B26	mS8	C2/c	15		2	[1.0, 1.0]	(CO+2, CU+2)1(O-2)1
CUPRITE	Cuprite (Cu2O, C3)	C3	cP6	Pn-3m	224	This is Cu2O with solubility of Na.	2	[2.0, 1.0]	(CU+1, NA+1)2(O-2)1
GUGGENITE	CaCu2O3		oP12	Pmmn	59		3	[0.825, 2.175, 3.0]	(MG+2)0.825 (CU+2)2.175(O-2)3
CACU2O3	Shcherbinaite (V2O5) (Revised)		oP14	Pmmn	59		3	[1.0, 2.0, 3.0]	(CA+2)1(CU+2)2(O-2)3
CA2CUO3	Sr2CuO3		oI12	Immm	71		3	[2.0, 1.0, 3.0]	(CA+2)2(CU+2)1(O-2)3
CU2COO3	CaCu2O3		oP12	Pmmn	59		3	[1.0, 2.0, 3.0]	(CO+2)1(CU+2)2(O-2)3

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
CA15CU18O35	Ca4.8Cu6O11.6		mP92	P2/c	13		4	[15.0, 14.0, 4.0, 35.0]	(CA+2)15(CU+2)14 (CU+3)4(O-2)35
CUGD2O4	CuNd2O4		tI14	I4/mmm	139		3	[1.0, 2.0, 4.0]	(CU+2)1(GD+3)2(O-2)4
CU2Y2O5	Cu2Ho2O5		oP36	Pna2_1	33		3	[2.0, 2.0, 5.0]	(CU+2)2(Y+3)2(O-2)5
DELAFOSSITE	Rhombohedral Delafossite (CuFeO2)		hR4	R-3m	166	This is Cu (Al,B,Cr,Fe,La,Mn,Y)O2	3	[1.0, 1.0, 2.0]	(CU+1)1(AL+3, B+3, CR+3, FE+3, LA+3, MN+3, Y+3)1(O-2)2
CULA2O4	CuLa2O4		oS28	Cmce	64	With solubility of Co.	3	[1.0, 2.0, 4.0]	(CO+2, CU+2)1(LA+3)2 (O-2)4
NIMNO3	Ilmenite (FeTiO3, E22)	E22	hR10	R-3	148	This is NiMnO3 with Ilmenite structure	2	[2.0, 3.0]	(MN+3, MN+4, NI+2)2 (O-2)3
NI6MNO8_TYPE	Mg6MnO8		cF60	Fm-3m	225	This is (Mg,Ni)6MnO8, with an ordered NaCl-type structure.	3	[6.0, 1.0, 8.0]	(MG+2, NI+2)6 (MN+4)1(O-2)8
P2O5_H	P2O5		hR28	R3c	161		2	[2.0, 5.0]	(P+5)2(O-2)5
P2O5_OP	P2O5		oP28	Pnma	62		2	[2.0, 5.0]	(P+5)2(O-2)5
P2O5_OO	P2O5		oP56	Fdd2	43		2	[2.0, 5.0]	(P+5)2(O-2)5
QUARTZ	alpha-Quartz (low Quartz)		hP9	P3_121	152	SiO2 with AlPO4 solubility.	2	[1.0, 1.0]	(AL+3, SI+4)1(PO4-3, SIO4-4)1
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	Cc	9	SiO2 with AlPO4 solubility.	2	[1.0, 1.0]	(AL+3, SI+4)1(PO4-3, SIO4-4)1
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	Fd-3m	227	SiO2 with AlPO4 solubility.	2	[1.0, 1.0]	(AL+3, SI+4)1(PO4-3, SIO4-4)1
CA2SIO4_ALPHA_A	Ca2SiO4		hP24	P6_3/mmc	194	This is 2CaO.SiO2 and 3CaO.P2O5.	3	[3.0, 1.0, 2.0]	(CA+2, GD+3, MG+2, MN+2, Y+3)3(CA+2,

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
									VA)1(BO3-3, PO4-3, SIO4-4)2
CA2SIO4_ALPHA_ PRIME	K2CoCl4		oP84	Pna2_1	33	This is 2CaO.SiO2.	3	[3.0, 1.0, 2.0]	(CA+2, FE+2, GD+3, MG+2, MN+2, Y+3)3 (CA+2, VA)1(BO3-3, PO4-3, SIO4-4)2
LARNITE	Parawollastonite (CaSiO3, S33(II))	S33(II)	mP60	P2_1/c	14	This is 2CaO.SiO2 (metastable at 1 atm)	3	[2.0, 1.0, 4.0]	(CA+2)2(SI+4)1(O-2)4
RANKINITE	3CaO.2SiO2		mP48	P2_1/c	14		3	[3.0, 2.0, 7.0]	(CA+2)3(SI+4)2(O-2)7
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	oP28	Pnma	62	This is Calcio-olivine (Ca2SiO4) - Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephroite (Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4) solid solution dissolving Cr and Cu.	4	[1.0, 1.0, 1.0, 4.0]	(CA+2, CO+2, CR+2, CU+2, FE+2, MG+2, MN+2, NI+2)1(CA+2, CO+2, CR+2, CU+2, FE+2, MG+2, MN+2, NI+2)1(SI+4)1(O-2)4
LOWCLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	C2/c	15	This is low clino-enstatite (MgSiO3) and low clino-diopside (CaMgSi2O6).	4	[1.0, 1.0, 2.0, 6.0]	(CA+2, MG+2)1 (MG+2)1(SI+4)2(O-2)6
CLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	C2/c	15	This is clino-enstatite (MgSiO3), clino-ferrosilit (FeSiO3), diopside (CaMgSi2O6), niopside (CaNiSi2O6), pigeonite ((Mg,Fe,Ca)Si2O6), hedenbergite (CaFeSi2O6) dissolving Co.	4	[1.0, 1.0, 2.0, 6.0]	(CA+2, FE+2, MG+2, NI+2)1(CO+2, FE+2, MG+2, NI+2)1(SI+4)2 (O-2)6
ORTHO_PYROXENE	Enstatite (MgSiO3, S43)	S43	oP80	Pbca	61	This is enstatite (MgSiO3) and ortho-diopside (CaMgSi2O6) with Fe solubility.	4	[1.0, 1.0, 2.0, 6.0]	(CA+2, FE+2, MG+2)1 (FE+2, MG+2)1(SI+4)2 (O-2)6
PROTO_PYROXENE	MgSiO3		oP40	Pbcn	60	This is proto-enstatite (MgSiO3) and proto-diopside (CaMgSi2O6) dissolving Co, Cr, and Fe.	3	[1.0, 1.0, 3.0]	(CA+2, CO+2, CR+2, FE+2, MG+2, NI+2)1 (SI+4)1(O-2)3

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WOLLASTONITE	Wollastonite (CaSiO3)		aP30	P-1	2	This is CaO.SiO2	3	[1.0, 1.0, 3.0]	(CA+2, FE+2, MG+2, MN+2)1(SI+4)1(O-2)3
PSEUDO_ WOLLASTONITE	CaSiO3		mS120	C2/c	15	This is CaO.SiO2	3	[1.0, 1.0, 3.0]	(CA+2)1(SI+4)1(O-2)3
HATRURITE	Ca3(SiO4)O-b		hR81	R3m	160	This is 3CaO.SiO2	3	[3.0, 1.0, 1.0]	(CA+2, GD+3, VA, Y+3)3(SIO4-4)1(O-2)1
MULLITE	Al(Al0.7Si0.3)2O4.8		oP24	Pbam	55	With solubility of B, Cr and Fe.	4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3, CR+3, FE+3)1(AL+3, B+3, SI+4)1(O-2, VA)5
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	Pnnm	58	This is a high-pressure phase	4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(SI+4)1 (O-2)5
SILLIMANITE	Sillimanite (Al2SiO5, S03)	S03	oP32	Pnma	62	This is a high-pressure phase	4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(SI+4)1 (O-2)5
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	P-1	2	This is Al2O3.SiO2	4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(SI+4)1 (O-2)5
RHODONITE	Rhodonite (MnSiO3-b)		aP50	P-1	2	This is MnO.SiO2	3	[1.0, 1.0, 3.0]	(CA+2, CO+2, FE+2, MG+2, MN+2)1(SI+4)1 (O-2)3
CORDIERITE	Na0.04 (Mg0.5Fe0.5)2Al4Si5O18		oS120	Cccm	66	This is 2Al2O3.2MgO.5SiO2, 2Al2O3.2MnO.5SiO2 and 2Al2O3.2FeO.5SiO2	4	[4.0, 2.0, 5.0, 18.0]	(AL+3)4(FE+2, MG+2, MN+2)2(SI+4)5(O-2)18
MELILITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	P-42_1m	113	This is gehlenite, akermanite, Fe-akermanite and 2CaO.CoO.2SiO2.	5	[2.0, 1.0, 1.0, 1.0, 7.0]	(CA+2)2(AL+3, CO+2, FE+2, FE+3, MG+2)1 (AL+3, SI+4)1(SI+4)1 (O-2)7
CA3COAL4O10	Ca3ZnAl4O10		oP72	Pca2_1	29		4	[3.0, 1.0, 4.0, 10.0]	(CA+2)3(CO+2)1 (AL+3)4(O-2)10
C3A2M1	3CaO.2Al2O3.MgO		oP72	Pbcm	57	This is 3CaO.2Al2O3.MgO	4	[3.0, 4.0, 1.0, 10.0]	(CA+2)3(AL+3)4 (MG+2)1(O-2)10

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
C1A8M2	CaMg2Al16O27		hP94	P-6m2	187	This is CaO.8Al2O3.2MgO	4	[1.0, 16.0, 2.0, 27.0]	(CA+2)1(AL+3)16 (MG+2)2(O-2)27
C2A14M2	Unknown Structure					This is 2CaO.14Al2O3.2MgO	4	[2.0, 28.0, 2.0, 46.0]	(CA+2)2(AL+3)28 (MG+2)2(O-2)46
CACRSI4O10	gillespite (BaFeSi4O10)		tP64	P4/ncc	130	This is CaO.CrO.4SiO2, Gillespite	4	[1.0, 1.0, 4.0, 10.0]	(CA+2)1(CR+2)1 (SI+4)4(O-2)10
SAPPHIRINE	CaMg3Si3O10		aP68	P-1	2	This is 9Al2O3.7MgO.3SiO2	4	[18.0, 7.0, 3.0, 40.0]	(AL+3)18(MG+2)7 (SI+4)3(O-2)40
ANORTHITE	Ca(Al0.5Si0.5)4O8		aP104	P-1	2	This is high temp albite (NaAlSi3O8), KAlSi3O8 and anorthite (CaAl2Si2O8)	5	[1.0, 1.0, 1.0, 2.0, 8.0]	(CA+2, K+1, NA+1)1 (AL+3)1(AL+3, SI+4)1 (SI+4)2(O-2)8
MERWINITE	Ca3Mg(SiO4)2		mP56	P2_1/c	14	This is 3CaO.MgO.2SiO2	4	[3.0, 1.0, 2.0, 8.0]	(CA+2)3(MG+2)1 (SI+4)2(O-2)8
CA2ZRSI4O12	cyclosilicate (Ca2ZrSi4O12)		mP38	P2_1/m	11		4	[2.0, 4.0, 1.0, 12.0]	(CA+2)2(SI+4)4 (ZR+4)1(O-2)12
CA3ZRSI2O9	Ca3Hf(Si2O7)O2		mP60	P2_1/c	14		4	[3.0, 2.0, 1.0, 9.0]	(CA+2)3(SI+4)2 (ZR+4)1(O-2)9
CA3TI8AL12O37	Unknown Structure						4	[3.0, 8.0, 12.0, 37.0]	(CA+2)3(TI+4)8 (AL+3)12(O-2)37
A1C1F2	Unknown Structure					This is Al2O3.CaO.2Fe2O3	5	[1.0, 1.0, 2.0, 3.0, 10.0]	(CA+2)1(AL+3)1 (FE+3)2(AL+3, FE+3)3 (O-2)10
FLUORITE	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	This is cubic high temperature HfO2 and ZrO2	2	[2.0, 4.0]	(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(O-2, VA)4

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ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	P2_1/c	14	This is Monoclinic HfO2 and ZrO2	2	[2.0, 4.0]	(AL+3, CA+2, CR+3, GD+3, HF+4, LA+3, TI+4, Y+3, YB+3, ZR+4)2(O-2, VA)4
ZRO2_TETR	HgI2 (C13)	C13	tP6	P4_2/nmc	137	This is Tetragonal HfO2 and ZrO2	2	[2.0, 4.0]	(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(O-2, VA)4
M2O3C	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	206	This is also cubic Gd2O3, Y2O3 and Yb2O3	3	[2.0, 3.0, 1.0]	(AL+3, CA+2, CO+3, CR+3, FE+3, GD+3, HF+4, LA+3, MG+2, MN+3, NI+2, TI+4, Y, Y+3, YB+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3H	La2O3 (D52)	D52	hP5	P-3m1	164	H-La2O3. This is also hexagonal (Gd,Y,Yb)2O3.	3	[2.0, 3.0, 1.0]	(CA+2, GD+3, HF+4, LA+3, MG+2, MN+3, Y, Y+3, YB+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3B	B-Sm2O3		mS30	C2/m	12	This is monoclinic B-type structure of R2O3	3	[2.0, 3.0, 1.0]	(AL+3, CA+2, CO+3, GD+3, HF+4, LA+3, MG+2, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3A	La2O3 (D52)	D52	hP5	P-3m1	164	A-LA2O3. Also hexagonal A-type structure of Gd2O3.	3	[2.0, 3.0, 1.0]	(CA+2, GD+3, HF+4, LA+3, MG+2, Y+3, YB+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3X	Nd2O3		cI26	Im-3m	229	X-LA2O3. This is also HT cubic X-type structure of Gd2O3.	3	[2.0, 3.0, 1.0]	(CA+2, GD+3, HF+4, LA+3, MG+2, Y+3, YB+3, ZR+4)2(O-2, VA)3(O-2, VA)1
PYROCHLORE	Cubic Pyrochlore (Eu2Ir2O7, E81)	E81	cF88	Fd-3m	227	This is (Gd,La)2(Hf,Zr)2O7 and (Gd,La,Y,Yb)2Ti2O7.	5	[2.0, 2.0, 6.0, 1.0, 1.0]	(GD+3, HF+4, LA+3, TI+4, Y+3, YB+3, ZR+4)2(GD+3, HF+4, LA+3, TI+4, Y+3, YB+3,

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									ZR+4)2(O-2, VA)6(O-2)1(O-2, VA)1
MNYO3_HEX	LuMnO3		hP30	P6_3cm	185		3	[1.0, 1.0, 3.0]	(Y+3)1(MN+3)1(O-2)3
DYMN2O5	HoMn2O5		oP32	Pbam	55	This is Mn2(Gd,Y)O5.	4	[1.0, 1.0, 1.0, 5.0]	(GD+3, Y+3)1(MN+3)1 (MN+4)1(O-2)5
YB2TIO5	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		3	[2.0, 1.0, 5.0]	(YB+3)2(TI+4)1(O-2)5
Y2TIO5	La2TiO5		oP32	Pnma	62	This is (Gd,La,Y)2TiO5	3	[2.0, 1.0, 5.0]	(GD+3, LA+3, Y+3)2 (TI+4)1(O-2)5
LA4TI3O12	La4Ti3O12		hR19	R-3	148		3	[4.0, 3.0, 12.0]	(LA+3)4(TI+4)3(O-2)12
LA2TI3O9	Unknown Structure						3	[2.0, 3.0, 9.0]	(LA+3)2(TI+4)3(O-2)9
LA4TI9O24	Nd4Ti9O24		oF592	Fddd	70		3	[4.0, 9.0, 24.0]	(LA+3)4(TI+4)9(O-2)24
YAM	Y4Al2O9		mP60	P2_1/c	14	This is Y4Al2O9, Gd4Al2O9 and Ca2Y2Si2O9 (Cuspidine)	4	[2.0, 4.0, 1.0, 9.0]	(AL+3, SI+4)2(CA+2, GD+3, LA+3, Y+3, YB+3)4(O-2, VA)1(O-2)9
GARNET	Orthorhombic Garnet		oF320	Fddd	70	This is Garnets and (Gd,Y,Yb)3 (Al,Fe)5O12.	4	[3.0, 2.0, 3.0, 12.0]	(CA+2, FE+2, GD+3, LA+3, MG+2, MN+2, Y+3, YB+3)3(AL+3, CR+3, FE+3, MG+2, V+3)2(AL+3, CR+3, FE+3, SI+4)3(O-2)12
YAP	CaTiO3 Pnma Perovskite		oP20	Pnma	62	This is Y(Al,Co,Cr,Fe)O3, YbFeO3 and Gd(Al,Co,Cr,Fe)O3.	3	[1.0, 1.0, 3.0]	(AL+3, CO+3, CR+3, FE+3, MN+3)1(CA+2, GD+3, LA+3, Y+3, YB+3)1(O-2, VA)3

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ZR3Y4O12	UY6O12		hR19	R-3	148	Zr3(Y,Yb)4O12 and Hf3Yb4O12.	3	[3.0, 4.0, 12.0]	(HF+4, ZR+4)3(Y+3, YB+3)4(O-2)12
LA2CR3O12	Unknown Structure						3	[2.0, 3.0, 12.0]	(LA+3)2(CR+6)3(O-2)12
LA2CRO6	Unknown Structure						3	[2.0, 1.0, 6.0]	(LA+3)2(CR+6)1(O-2)6
LA3NI2O7	Sr3Sn2O7		oS48	Cmcm	63		4	[3.0, 1.0, 1.0, 7.0]	(LA+3)3(CO+2, NI+2)1 (NI+3)1(O-2)7
LAFE12O19	Unknown Structure						4	[1.0, 1.0, 11.0, 19.0]	(LA+3)1(FE+2)1 (FE+3)11(O-2)19
CO1LA2O4	La2CoO4		oP36	Pbam	55		3	[2.0, 1.0, 4.0]	(LA+3)2(CO+2)1(O-2)4
CO3LA4O10	Nd4Co3O10		mP68	P2_1/c	14		4	[4.0, 1.0, 2.0, 10.0]	(LA+3)4(CO+2)1 (CO+3)2(O-2)10
LAAL11O18	La0.83Al11.83O19		hP86	P6_3/mmc	194		3	[1.0, 11.0, 18.0]	(LA+3)1(AL+3)11(O-2)18
LA2MNO4	K2NiF4		tI14	I4/mmm	139	La2(Mn,Ni)O4 with Co solubility.	3	[2.0, 1.0, 4.0]	(LA+3)2(CO+2, MN+2, NI+2)1(O-2)4
LA4NI3O10	La4Ni3O10		oS68	Cmce	64	La4Ni3O10 with Co solubility.	4	[4.0, 1.0, 2.0, 10.0]	(LA+3)4(NI+2)1(CO+3, NI+3)2(O-2)10
PEROVSKITE	PrNiO3		hR10	R-3c	167	This is (Cr,Fe,Mn)LaO3. Also includes (Cr,Fe,Mn)LaO3 O-Perovskite.	3	[1.0, 1.0, 3.0]	(LA+3, MN+3, VA)1 (CO+3, CR+3, CR+4, FE+2, FE+3, FE+4, MN+2, MN+3, MN+4, VA)1(O-2, VA)3
LAAP	PrNiO3		hR10	R-3c	167	This is Rhombohedral Perovskite: La(Al,Co)O3 with solubility of Ca, Cu, Ni, Y	3	[1.0, 1.0, 3.0]	(CA+2, LA+3, Y+3)1 (AL+3, CO+3, CU+2, FE+3, NI+2)1(O-2, VA)3

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
LAYP	CaTiO3 Pnma Perovskite		oP20	Pnma	62	This is an Orthorhombic Perovskite, La(Y,Yb)O3.	3	[1.0, 1.0, 3.0]	(LA+3, Y+3, YB+3)1 (LA+3, VA, Y+3, YB+3, ZR+4)1(O-2)3
LANIO3	PrNiO3		hR10	R-3c	167	This is a rhombohedral perovskite	3	[1.0, 1.0, 3.0]	(LA+3)1(NI+3)1(O-2)3
CAMO3	CaTiO3 Pnma Perovskite		oP20	Pnma	62	This is CaHfO3, CaMnO3, CaTiO3, lt CaZrO3.	3	[1.0, 1.0, 3.0]	(CA+2, GD+3, Y+3)1 (GD+3, HF+4, MN+4, TI+4, Y+3, ZR+4)1(O-2)3
CA6HF19O44	Ca6Hf19O44		hR138	R-3c	167		3	[6.0, 19.0, 44.0]	(CA+2)6(HF+4)19(O-2)44
CA2HF7O16	Ca2Hf7O16		hR25	R-3	148		3	[2.0, 7.0, 16.0]	(CA+2)2(HF+4)7(O-2)16
MG2HF5O12	UY6O12		hR19	R-3	148		3	[2.0, 5.0, 12.0]	(MG+2)2(HF+4)5(O-2)12
HFW2O8	Zr[WO4]2		cP44	P2_13	198		3	[1.0, 2.0, 8.0]	(HF+4)1(W+6)2(O-2)8
CA4TI3O10	Ca4Ti3O10		oP68	Pbca	61		3	[4.0, 3.0, 10.0]	(CA+2)4(TI+4)3(O-2)10
CA3TI2O7	Ca3Ti2O7		oS48	Cmc2_1	36		3	[3.0, 2.0, 7.0]	(CA+2)3(TI+4)2(O-2)7
GD2SI2O7	Ce2Si2O7		mP44	P2_1/c	14	This is (Gd,La)2Si2O7	3	[1.0, 1.0, 1.0]	(GD+3, LA+3)1(GD+3, LA+3)1(SI2O7-6)1
GD2SIO5	Gd2SiO5 (RE2SiO5 X1)		mP32	P2_1/c	14	This is (Gd,La)2SiO5	4	[1.0, 1.0, 1.0, 1.0]	(GD+3, LA+3)1(GD+3, LA+3)1(SIO4-4)1(O-2)1
Y2S2D_Y2SI2O7	Possible delta-Y2Si2O7		oP44	Pnma	62	Y2Si2O7 with Yb solubility.	2	[2.0, 1.0]	(Y+3, YB+3)2(SI2O7-6)1

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Y2S2G_Y2SI2O7	Y2Si2O7-b		mP22	P2_1/c	14	Y2Si2O7-b with Yb solubility.	2	[2.0, 1.0]	(Y+3, YB+3)2(SI2O7-6)1
Y2S2B_Y2SI2O7	La4Ge3[GeO4]O10		aP44	P-1	2	(Y,Yb)2Si2O7 solid solution.	2	[2.0, 1.0]	(Y+3, YB+3)2(SI2O7-6)1
Y2S2A_Y2SI2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	C2/m	12	Y2Si2O7	3	[1.0, 1.0, 1.0]	(Y+3)1(Y+3)1(SI2O7-6)1
Y2SIO5	Y2SiO5 (RE2SiO5 X2)		mS64	C2/c	15	This is (Y,Yb)2SiO5	3	[2.0, 1.0, 1.0]	(Y+3, YB+3)2(SIO4-4)1 (O-2)1
ZIRCON	Zircon (ZrSiO4, S11)	S11	tI24	I4_1/amd	141	This is HfSiO4, ZrSiO4, GdPO4, LaPO4 and YPO4.	3	[1.0, 1.0, 4.0]	(P+5, SI+4)1(GD+3, HF+4, LA+3, Y+3, ZR+4)1(O-2, VA)4
ZRTIO4_ALPHA	Unknown Structure						3	[1.0, 1.0, 4.0]	(ZR+4)1(TI+4)1(O-2)4
ZRTIO4_BETA	zeta-Fe2N		oP12	Pbcn	60	This is (Hf,Zr)TiO4 solid solution with Al solubility.	3	[2.0, 1.0, 4.0]	(AL+3, HF+4, TI+4, ZR+4)2(AL+3, VA)1(O-2)4
ZRTI2O6	Columbite (FeNb2O6, E51)	E51	oP36	Pbcn	60		3	[1.0, 2.0, 6.0]	(ZR+4)1(TI+4)2(O-2)6
CAZRO3_C	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221	High-temperature CaTiO3.	3	[1.0, 1.0, 3.0]	(CA+2, Y+3)1(HF+4, Y+3, ZR+4)1(O-2)3
CAZR4O9	CaZr4O9		mS224	C2/c	15		3	[1.0, 4.0, 9.0]	(CA+2)1(ZR+4)4(O-2)9
Q_ALMGZRO	Unknown Structure						4	[4.68, 2.64, 1.68, 12.0]	(MG+2)4.68 (AL+3)2.64(ZR+4)1.68 (O-2)12
CA6ZR19O44	Ca6Hf19O44		hR138	R-3c	167		3	[6.0, 19.0, 44.0]	(CA+2)6(ZR+4)19(O-2)44
C13A6Z2	Ca7ZrAl6O18		oP104	Pmn2_1	31	This is 13CaO.3Al2O3.2ZrO2.	4	[13.0, 12.0,	(CA+2)13(AL+3)12

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
								2.0, 35.0]	(ZR+4)2(O-2)35
LA4SI3O12	Unknown Structure						2	[4.0, 3.0]	(LA+3)4(SIO4-4)3
CAY4O7	(Ca0.25Gd0.75)4GdO7		mS48	C2/m	12	This is CaY4O7 and CaGd4O7.	3	[1.0, 4.0, 7.0]	(CA+2)1(GD+3, Y+3)4 (O-2)7
CAYALO4	K2NiF4		tI14	I4/mmm	139	This is CaYAlO4, CaYbAlO4 and CaGdAlO4	4	[1.0, 1.0, 1.0, 4.0]	(CA+2)1(GD+3, Y+3, YB+3)1(AL+3)1(O-2)4
CAYAL3O7	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	P-42_1m	113	This is CaYAl3O7, CaYbAl3O7 and CaGdAl3O7	4	[1.0, 1.0, 3.0, 7.0]	(CA+2)1(GD+3, Y+3, YB+3)1(AL+3)3(O-2)7
CA2YB2O5	Unknown Structure						3	[2.0, 2.0, 5.0]	(CA+2)2(YB+3)2(O-2)5
CA3YB2O6	Unknown Structure						3	[3.0, 2.0, 6.0]	(CA+2)3(YB+3)2(O-2)6
CA3Y2SI6O18	Ca0.6Y0.4Si6O18		mS116	C2/c	15	This is 3CaO. (Gd,Y,Yb)2O3.6SiO2.	4	[3.0, 2.0, 6.0, 18.0]	(CA+2)3(GD+3, Y+3, YB+3)2(SI+4)6(O-2)18
CA3Y2SI3O12	Ca3Y2Si3O12		oP100	Pnma	62	This is 3CaO. (Gd,Y,Yb)2O3.3SiO2.	4	[3.0, 2.0, 3.0, 12.0]	(CA+2)3(GD+3, Y+3, YB+3)2(SI+4)3(O-2)12
APATITE	Fluorapatite [Ca5F(PO4)3, H57]	H57	hP42	P6_3/m	176	This is Ca2(Gd,Y)8(SiO4)6O2 and Mg2(Gd,Y)8(SiO4)6O2	4	[4.0, 6.0, 6.0, 2.0]	(CA+2, GD+3, MG+2, VA, Y+3, YB+3, ZR+4)4 (GD+3, Y+3, YB+3)6 (SIO4-4)6(O-2, VA)2
YB6HFO11	Unknown Structure					Yb6HfO11 solid solution	4	[2.0, 6.0, 12.0, 1.0]	(HF+4, YB+3)2(YB+3)6 (O-2)12(O-2, VA)1
MO4O11	Mo4O11		oP60	Pna2_1	33		3	[1.0, 3.0, 11.0]	(MO+4)1(MO+6)3(O-2)11
MO8O23	High-Temperature Mo8O23		mP62	P2/c	13		3	[1.0, 7.0, 23.0]	(MO+4)1(MO+6)7(O-2)23

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
MO9O26	Mo9O26		mP70	P2/c	13		3	[1.0, 8.0, 26.0]	(MO+4)1(MO+6)8(O-2)26
MOO3	gamma-WO3		mP32	P2_1/c	14		2	[1.0, 3.0]	(MO+6)1(O-2)3
KNO3_S1	alpha-Potassium Nitrate (KNO3) I		oP20	Pnma	62	This is lt-KNO3 with solubility of Na.	2	[1.0, 1.0]	(K+1, NA+1)1(NO3-1)1
K4CAN6O18	Unknown Structure						3	[4.0, 1.0, 6.0]	(K+1)4(CA+2)1(NO3-1)6
K2MGN4O12	Unknown Structure						3	[2.0, 1.0, 4.0]	(K+1)2(MG+2)1(NO3-1)4
K4FEO3	Unknown Structure						3	[4.0, 1.0, 3.0]	(K+1)4(FE+2)1(O-2)3
KAL11O17	beta-Alumina (Al2O3, D56)	D56	hP60	P6_3/mmc	194	This is Beta-Al2O3 K (Al,Fe)11O17 solid solution.	6	[1.0, 1.0, 2.0, 1.0, 9.0, 17.0]	(K+1, VA)1(K+1, VA)1 (AL+3, FE+3, MG+2)2 (O-2, VA)1(AL+3, FE+3)9(O-2)17
K4AL22O35	K2Al10.67O17		hR30	R-3m	166	This is Beta double prime-Al2O3 K4(AL,Fe)22O35 solid solution.	6	[1.0, 1.0, 2.0, 1.0, 9.0, 17.0]	(K+1, VA)1(K+1, VA)1 (AL+3, FE+3, MG+2)2 (O-2, VA)1(AL+3, FE+3)9(O-2)17
KMG2AL15O25	Unknown Structure						4	[1.0, 2.0, 15.0, 25.0]	(K+1)1(MG+2)2 (AL+3)15(O-2)25
K4SIO4	Cs4SnO4		mP36	P2_1/c	14		3	[4.0, 1.0, 4.0]	(K+1)4(SI+4)1(O-2)4
K2SI4O9_ALPHA	K2Si4O9		aP30	P-1	2	Low-temp K2Si4O9	3	[2.0, 4.0, 9.0]	(K+1)2(SI+4)4(O-2)9
K2SI4O9_BETA	K2Si4O9		hP30	P6_3/m	176	High-temp K2Si4O9	3	[2.0, 4.0, 9.0]	(K+1)2(SI+4)4(O-2)9
K4TIO4	Unknown Structure						3	[4.0, 1.0,	(K+1)4(TI+4)1(O-2)4

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
								4.0]	
K2TIO3	Cs2PbO3		oS24	Cmcm	63		3	[2.0, 1.0, 3.0]	(K+1)2(TI+4)1(O-2)3
K8TI5O14	Unknown Structure						3	[8.0, 5.0, 14.0]	(K+1)8(TI+4)5(O-2)14
K2TI3O7	Unknown Structure						3	[2.0, 3.0, 7.0]	(K+1)2(TI+4)3(O-2)7
K2TI6O13	Na2Ti6O13		mS42	C2/m	12		3	[2.0, 6.0, 13.0]	(K+1)2(TI+4)6(O-2)13
K3PO4_ALPHA	Unknown Structure					low-temp	2	[3.0, 1.0]	(K+1)3(PO4-3)1
K3PO4_BETA	Unknown Structure					mid-temp	2	[3.0, 1.0]	(K+1)3(PO4-3)1
K3PO4_GAMMA	K3[PO4]-ht		cF32	Fm-3	202	high-temp	2	[3.0, 1.0]	(K+1)3(PO4-3)1
KPO3_ALPHA	KPO3		mP40	P2_1/c	14		2	[1.0, 1.0]	(K+1)1(PO3-1)1
KPO3_BETA	alpha-Potassium Nitrate (KNO3) I		oP20	Pnma	62		2	[1.0, 1.0]	(K+1)1(PO3-1)1
KPO3_GAMMA	KPO3		oS32	Cmcm	63		2	[1.0, 1.0]	(K+1)1(PO3-1)1
K5P3O10_ALPHA	Unknown Structure						3	[5.0, 3.0, 10.0]	(K+1)5(P+5)3(O-2)10
K5P3O10_BETA	Unknown Structure						3	[5.0, 3.0, 10.0]	(K+1)5(P+5)3(O-2)10
K4P2O7_ALPHA	K4[P2O7]		hP234	P6_1	169		2	[4.0, 1.0]	(K+1)4(P2O7-4)1
K4P2O7_BETA	K4[P2O7]		hP26	P6_3/mmc	194		2	[4.0, 1.0]	(K+1)4(P2O7-4)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
K4P2O7_GAMMA	Unknown Structure						2	[4.0, 1.0]	(K+1)4(P2O7-4)1
K4P2O7_DELTA	Unknown Structure						2	[4.0, 1.0]	(K+1)4(P2O7-4)1
KALSIO4_HT	KLi[SO4]		hP14	P31c	159	This is high temperature KAlSiO4-K2MgSi3O8 ss. with SiO2 solubility	4	[1.0, 1.0, 2.0, 8.0]	(K2MG+4, KAL+4)1 (KAL+4, SI+4)1(SI+4)2 (O-2)8
KALSI2O6	K8(Al0.33Si0.67)24O48		tI160	I4_1/a	88	This is KAlSi2O6-KFeSi2O6-K2MgSi5O12 solid solution.	5	[2.0, 1.0, 1.0, 4.0, 12.0]	(K+1)2(AL+3, FE+3, MG+2)1(AL+3, FE+3, SI+4)1(SI+4)4(O-2)12
K2CASIO4	Unknown Structure						4	[2.0, 1.0, 1.0, 4.0]	(K+1)2(CA+2)1(SI+4)1 (O-2)4
K2CA2SI2O7	K2Ca2[Si2O7]		hP108	P6_3/m	176		4	[2.0, 2.0, 2.0, 7.0]	(K+1)2(CA+2)2(SI+4)2 (O-2)7
K4CASI3O9	K4SrGe3O9		cP272	Pa-3	205		4	[4.0, 1.0, 3.0, 9.0]	(K+1)4(CA+2)1(SI+4)3 (O-2)9
K8CASI10O25	Unknown Structure						4	[8.0, 1.0, 10.0, 25.0]	(K+1)8(CA+2)1 (SI+4)10(O-2)25
K4CASI6O15	Unknown Structure						4	[4.0, 1.0, 6.0, 15.0]	(K+1)4(CA+2)1(SI+4)6 (O-2)15
K2CA3SI6O16	Unknown Structure						4	[2.0, 3.0, 6.0, 16.0]	(K+1)2(CA+2)3(SI+4)6 (O-2)16
K2CA2SI9O21	Unknown Structure						4	[2.0, 2.0, 9.0, 21.0]	(K+1)2(CA+2)2(SI+4)9 (O-2)21
K2CA6SI4O15	K2Ca6Si4O15		mP54	P2/c	13		4	[2.0, 6.0, 4.0, 15.0]	(K+1)2(CA+2)6(SI+4)4 (O-2)15
K2MG5SI12O30	K2Mg5Si12O30		hP100	P6/mcc	192		4	[2.0, 5.0, 12.0, 30.0]	(K+1)2(MG+2)5 (SI+4)12(O-2)30

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K4MG2SI5O14	Unknown Structure						4	[4.0, 2.0, 5.0, 14.0]	(K+1)4(MG+2)2(SI+4)5 (O-2)14
K10MG5SI11O32	Unknown Structure						4	[10.0, 5.0, 11.0, 32.0]	(K+1)10(MG+2)5 (SI+4)11(O-2)32
KFESIO4	Unknown Structure						4	[2.0, 2.0, 2.0, 8.0]	(K+1)2(FE+3)2(SI+4)2 (O-2)8
K2FE2SI6O16	Unknown Structure						4	[2.0, 2.0, 6.0, 16.0]	(K+1)2(FE+3)2(SI+4)6 (O-2)16
K4FE4SI3O14	Unknown Structure						4	[4.0, 4.0, 3.0, 14.0]	(K+1)4(FE+3)4(SI+4)3 (O-2)14
K2FESI3O8	Unknown Structure						4	[2.0, 1.0, 3.0, 8.0]	(K+1)2(FE+2)1(SI+4)3 (O-2)8
K2FESI5O12	K16Mg8Si40O96		mP160	P2_1/c	14		4	[2.0, 1.0, 5.0, 12.0]	(K+1)2(FE+2)1(SI+4)5 (O-2)12
NA2O1_S1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	This is rt (K,Na)2O.	2	[2.0, 1.0]	(K+1, NA+1)2(O-2)1
NA2O1_S2	Unknown Structure					This is ht1 (K,Na)2O.	2	[2.0, 1.0]	(K+1, NA+1)2(O-2)1
NA2O1_S3	Unknown Structure					This is ht2 (K,Na)2O.	2	[2.0, 1.0]	(K+1, NA+1)2(O-2)1
NAAL11O17	NaAl11O17		hP58	P6_3/mmc	194	This is Beta-Al2O3 NaAl11O17 solid solution.	5	[2.0, 2.0, 22.0, 34.0, 1.0]	(NA+1)2(NA+1, VA)2 (AL+3)22(O-2)34(O-2, VA)1
NA2AL12O19	Na0.5Al3O4.75		oP24	Pbam	55	This is Beta double prime-Al2O3 Na2Al12O19 with solubility of Fe.	3	[2.0, 12.0, 19.0]	(NA+1)2(AL+3, FE+3)12(O-2)19
CACO3	Calcite (CaCO3, G01)	G01	hR10	R-3c	167	This is (Ca,Fe,Mg)CO3.	2	[1.0, 1.0]	(CA+2, FE+2, MG+2)1 (CO3-2)1
NA2CO3_S1	Na2[CO3]-b		mS24	C2/m	12	With solubility of K.	2	[2.0, 1.0]	(K+1, NA+1)2(CO3-2)1

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NA2CO3_S2	Na2[CO3]		hP12	P6_3/mmc	194	This is (K,Na)2CO3 solid solution.	2	[2.0, 1.0]	(K+1, NA+1)2(CO3-2, S-2)1
K2CO3_S1	K2[CO3]		mP24	P2_1/c	14	With solubility of Na.	2	[2.0, 1.0]	(K+1, NA+1)2(CO3-2)1
K3FCO3	Unknown Structure						3	[3.0, 1.0, 1.0]	(K+1)3(F-1)1(CO3-2)1
CAN2O6	Pb(NO3)2 (G21)	G21	cP36	Pa-3	205	This is (Ca,Mg)(NO3)2 solid solution.	2	[1.0, 2.0]	(CA+2, MG+2)1(NO3-1)2
NANO3_S1	Calcite (CaCO3, G01)	G01	hR10	R-3c	167	With solubility of K.	2	[1.0, 1.0]	(K+1, NA+1)1(NO3-1)1
NANO3_S2	Rb[NO3]		hR9	R-3m	166	This is ht-(K,Na)(NO3) solid solution.	2	[1.0, 1.0]	(K+1, NA+1)1(NO3-1)1
NA3FE5O9	Na3Fe5O9		mS68	C2/c	15		3	[3.0, 5.0, 9.0]	(NA+1)3(FE+3)5(O-2)9
NA4FE6O11	Unknown Structure						3	[4.0, 6.0, 11.0]	(NA+1)4(FE+3)6(O-2)11
NA8FE2O7	Na8Ga2O7		mP68	P2_1/c	14		3	[8.0, 2.0, 7.0]	(NA+1)8(FE+3)2(O-2)7
NA3FEO3	Na3FeO3		mP28	P2_1/c	14		3	[3.0, 1.0, 3.0]	(NA+1)3(FE+3)1(O-2)3
NA5FEO4	Na5GaO4		oP80	Pbca	61		3	[5.0, 1.0, 4.0]	(NA+1)5(FE+3)1(O-2)4
NAFEO2_A	Caswellsilverite (CrNaS2, F51)	F51	hR4	R-3m	166	This is also NaCrO2.	3	[1.0, 1.0, 2.0]	(NA+1)1(CR+3, FE+3)1(O-2)2
NAFEO2_B	LiGaO2		oP16	Pna2_1	33	This is low-temp K(Al,Fe)O2 + NaAlO2 and mid-temp NaFeO2 solid solutions.	2	[1.0, 2.0]	(KAL+4, KFE+4, NAAL+4, NAFE+4, SI+4)1(O-2)2
K2MGSIO4_LT	Na2Be[SiO4]		oP64	Pca2_1	29		2	[1.0, 1.0]	(K2MG+4, SI+4)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
									(SIO4-4)1
K2MGSIO4_HT	Unknown Structure						2	[1.0, 1.0]	(K2MG+4, SI+4)1 (SIO4-4)1
NAFEO2_G	LiAlO2		tP16	P4_12_12	92	This is high-temp K(Al,Fe)O2 + NaFeO2 and mid-temp NaAlO2 solid solutions.	2	[1.0, 2.0]	(KAL+4, KFE+4, NAAL+4, NAFE+4, SI+4)1(O-2)2
NAALO2_D	LiGaO2		oP16	Pna2_1	33		2	[1.0, 2.0]	(NAAL+4, SI+4)1(O-2)2
NA2FEO2	Unknown Structure						3	[2.0, 1.0, 2.0]	(NA+1)2(FE+2)1(O-2)2
NA4FEO3	Na4FeO3		mS32	Cc	9		3	[4.0, 1.0, 3.0]	(NA+1)4(FE+2)1(O-2)3
NAFE2O3	NaFe2O3		hP6	P-3m1	164		4	[1.0, 1.0, 1.0, 3.0]	(NA+1)1(FE+2)1 (FE+3)1(O-2)3
NA10SIO7	Unknown Structure						3	[10.0, 1.0, 7.0]	(NA+1)10(SI+4)1(O-2)7
NA4SIO4	K4SnO4		aP18	P-1	2		3	[4.0, 1.0, 4.0]	(NA+1)4(SI+4)1(O-2)4
NA6SI2O7	Na6[Si2O7]		aP120	P-1	2		3	[6.0, 2.0, 7.0]	(NA+1)6(SI+4)2(O-2)7
NA2SIO3	Na2SiO3		oS24	Cmc2_1	36	This is (K,Na)2SiO3 solid solution.	3	[2.0, 1.0, 3.0]	(K+1, NA+1)2(SI+4)1 (O-2)3
NA2SI2O5_ALPHA	Na2Si2O5-a		mP36	P2_1/c	14	This is lt-(K,Na)2Si2O5 solid solution.	3	[2.0, 2.0, 5.0]	(K+1, NA+1)2(SI+4)2 (O-2)5
NA2SI2O5_BETA	Na2Si2O5-b		mP36	P2_1/c	14	This is intermediat-temp (K,Na)2Si2O5 solid solution.	3	[2.0, 2.0, 5.0]	(K+1, NA+1)2(SI+4)2 (O-2)5
NA2SI2O5_GAMMA	Na2Si2O5		oP36	Pbcn	60	This is ht-(K,Na)2Si2O5 solid	3	[2.0, 2.0,	(K+1, NA+1)2(SI+4)2

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
						solution.		5.0]	(O-2)5
NA6SI8O19	Na6Si8O19		mP132	P2_1/c	14		3	[6.0, 8.0, 19.0]	(NA+1)6(SI+4)8(O-2)19
NAPO3	NaAsO3		aP30	P-1	2		2	[1.0, 1.0]	(NA+1)1(PO3-1)1
NA3PO4	Na3[PO4]		cF988	Fm-3m	225	This is Na3(PO4,VO4)	2	[3.0, 1.0]	(NA+1)3(PO4-3, VO4-3)1
NA4P2O7	Na4[P2O7]		oP52	P2_12_12_1	19		2	[4.0, 1.0]	(NA+1)4(P2O7-4)1
NA4TIO4	K4SnO4		aP18	P-1	2		3	[4.0, 1.0, 4.0]	(NA+1)4(TI+4)1(O-2)4
NA2TI3O7	Na2Ti3O7		mP24	P2_1/m	11		3	[2.0, 3.0, 7.0]	(NA+1)2(TI+4)3(O-2)7
NA2TIO3_S1	Na2TiO3		mS24	C2/m	12		3	[2.0, 1.0, 3.0]	(NA+1)2(TI+4)1(O-2)3
NA2TIO3_S2	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		3	[2.0, 1.0, 3.0]	(NA+1)2(TI+4)1(O-2)3
NA8TI5O14	Na8Ti5O14		aP54	P-1	2		3	[8.0, 5.0, 14.0]	(NA+1)8(TI+4)5(O-2)14
NA2TI6O13	Na2Ti6O13		mS42	C2/m	12		3	[2.0, 6.0, 13.0]	(NA+1)2(TI+4)6(O-2)13
NA2V2O6	LiVO3		mS40	Cc	9		3	[2.0, 2.0, 6.0]	(NA+1)2(V+5)2(O-2)6
NA4V2O7	Na4[V2O7]		mS208	C2/c	15		3	[4.0, 2.0, 7.0]	(NA+1)4(V+5)2(O-2)7
NA2FESIO4	Unknown Structure						4	[2.0, 1.0, 1.0, 4.0]	(NA+1)2(FE+2)1 (SI+4)1(O-2)4

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
NA8FE6SI15O40	Unknown Structure						4	[8.0, 6.0, 15.0, 40.0]	(NA+1)8(FE+2)6 (SI+4)15(O-2)40
NA5FESI4O12	Unknown Structure						4	[5.0, 1.0, 4.0, 12.0]	(NA+1)5(FE+3)1 (SI+4)4(O-2)12
NAFESI2O6	Diopside [CaMg(SiO3)2, S41]	S41	mS40	C2/c	15		4	[1.0, 1.0, 2.0, 6.0]	(NA+1)1(FE+3)1 (SI+4)2(O-2)6
NA2CA3AL16O28	Unknown Structure						4	[2.0, 3.0, 16.0, 28.0]	(NA+1)2(CA+2)3 (AL+3)16(O-2)28
NA2CA8AL6O18	Unknown Structure						4	[2.0, 8.0, 6.0, 18.0]	(NA+1)2(CA+2)8 (AL+3)6(O-2)18
NA2CAAL4O8	Unknown Structure					This is (K,Na)2CaAl4O8 solid solution.	4	[1.0, 1.0, 2.0, 4.0]	(K+1, NA+1, VA)1 (CA+2, K+1, NA+1)1 (AL+3)2(O-2)4
NEPHELINE_A	Unknown Structure					This is NaAlSiO4 with solubility of Si.	4	[4.0, 4.0, 8.0, 32.0]	(NAAL+4)4(NAAL+4, SI+4)4(SI+4)8(O-2)32
NEPHELINE_B	Unknown Structure					This is NaAlSiO4 with solubility of Si.	4	[4.0, 4.0, 8.0, 32.0]	(NAAL+4)4(NAAL+4, SI+4)4(SI+4)8(O-2)32
NEPHELINE_G	KLi[SO4]		hP18	P6_3	173	This is low temperature NaAlSiO4-KAlSiO4, K2MgSi3O8 dissolving SiO2, Fe.	4	[4.0, 4.0, 8.0, 32.0]	(K2MG+4, KAL+4, NAAL+4)4(KAL+4, NAAL+4, NAFE+4, SI+4)4(SI+4)8(O-2)32
CARNEGIEITE_A	alpha-Carnegieite (NaAlSiO4, S65)	S65	cP28	P2_13	198	This is NaAlSiO4 with solubility of Fe and Si.	3	[4.0, 4.0, 16.0]	(NAAL+4, NAFE+4, SI+4)4(SI+4)4(O-2)16
CARNEGIEITE_B	NaAl[SiO4]		oP56	Pca2_1	29	This is NaAlSiO4 with solubility of Fe and Si.	3	[4.0, 4.0, 16.0]	(NAAL+4, NAFE+4, SI+4)4(SI+4)4(O-2)16
ALBITE_LOW	Albite (NaAlSi3O8, S68)	S68	aP26	P-1	2	This is low temperature albite (NaAlSi3O8).	4	[1.0, 1.0, 3.0, 8.0]	(NA+1)1(AL+3)1 (SI+4)3(O-2)8
ALBITE_MONO	Sanidine (KAlSi3O8, S67)	S67	mS52	C2/m	12	This is monoclinic albite	4	[1.0, 1.0,	(NA+1)1(AL+3)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
						(NaAlSi3O8).		3.0, 8.0]	(SI+4)3(O-2)8
NB2O5	Nb2O5		mP99	P2/m	10		2	[2.0, 5.0]	(MG+2, NB+5, V+5, ZR+4)2(O-2, VA)5
NBO1	NbO		cP6	Pm-3m	221		2	[1.0, 1.0]	(NB+2)1(O-2)1
TI3O2	(Ti3O2)		hP5	P6/mmm	191		3	[2.0, 1.0, 2.0]	(TI+2)2(TI)1(O-2)2
TIO_ALPHA	alpha-TiO		mS20	C2/m	12		2	[1.0, 1.0]	(TI+2)1(O-2)1
M4O7	Ti4O7-a		aP22	P-1	2	This is Ti4O7 and V4O7 with solubility of Al and Mn.	2	[4.0, 7.0]	(AL, MN, TI, V)4(O)7
TI5O9	Ti5O9		aP28	P-1	2	Ti5O9 with solubility of V.	2	[5.0, 9.0]	(TI, V)5(O)9
M6O11	Ti6O11		aP34	P-1	2	This is Ti6O11 and V6O11.	2	[6.0, 11.0]	(TI, V)6(O)11
M7O13	Ti7O13		aP40	P-1	2	This is Ti7O13 and V7O13.	2	[7.0, 13.0]	(TI, V)7(O)13
M8O15	Ti8O15		aP46	P-1	2	This is Ti8O15 and V8O15.	2	[8.0, 15.0]	(TI, V)8(O)15
TI9O17	Ti9O17		aP52	P-1	2		2	[9.0, 17.0]	(TI)9(O)17
TI10O19	Unknown Structure						2	[10.0, 19.0]	(TI)10(O)19
TI20O39	Ti20O39		aP118	P-1	2		2	[20.0, 39.0]	(TI)20(O)39
TI5P6O25	Unknown Structure						3	[5.0, 6.0, 25.0]	(TI+4)5(P+5)6(O-2)25
PSEUDO_BROOKITE	Pseudobrookite (Fe2TiO5, E41)	E41	oS32	Cmcm	63	This is Fe2TiO5, Ti3O5, Al2TiO5 and (Co,Fe,Mg,Mn)Ti2O5.	3	[1.0, 2.0, 5.0]	(AL+3, CO+2, FE+2, FE+3, MG+2, MN+2, NI+2, SI+4, TI+3, TI+4, V+3)1(AL+3, FE+3, SI+4, TI+3, TI+4)2(O-2)5

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
RUTILE	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136	This is MnO2, TiO2 and ht-VO2.	2	[1.0, 2.0]	(AL+3, HF+4, MN+4, TI+3, TI+4, V+4, ZR+4)1(O-2, VA)2
NBO2	alpha-NbO2		tI96	I4_1/a	88	This is NbO2	2	[1.0, 2.0]	(FE+2, NB+4, NB+5)1 (O-2)2
BETA_V_O	CoO		tI4	I4/mmm	139		2	[1.0, 1.0]	(V)1(O, VA)1
BRONZE	Unknown Structure					This is (Ca,Fe)xV2O5 bronze.	3	[2.0, 5.0, 1.0]	(V+4, V+5)2(O-2)5 (CA+2, FE+2, VA)1
V2O_SS	V7O3		mS20	C2/m	12		2	[1.0, 0.5]	(V)1(O, VA)0.5
V2O5	Shcherbinaite (V2O5) (Revised)		oP14	Pmmn	59		2	[2.0, 5.0]	(V+5)2(O-2)5
V3O5_HT	V3O5-ht		mS32	C2/c	15	This is ht-V3O5 with solubility of Al, Cr, Mg, Mn and Ti.	2	[3.0, 5.0]	(AL, CR, MG, MN, TI, V)3(O)5
V3O5_LT	V3O5-lt		mP32	P2/c	13		2	[3.0, 5.0]	(V)3(O)5
V3O7	V3O7		mS120	C2/c	15		2	[3.0, 7.0]	(V)3(O)7
V52O64	V13O16		tI116	I4_1/amd	141		2	[52.0, 64.0]	(V)52(O)64
V5O9	Ti5O9		aP28	P-1	2	V5O9 with solubility of Ti.	2	[5.0, 9.0]	(TI, V)5(O)9
V6O13	V6O13		mS38	C2/m	12		2	[6.0, 13.0]	(V)6(O)13
VO2_LT	VO2		mP12	P2_1/c	14	This is lt-VO2, MoO2 and WO2.	2	[1.0, 2.0]	(MO+4, V+4, W+4)1 (O-2)2
CA2V2O7	Sr2V2O7		aP	P-1	2		3	[2.0, 2.0, 7.0]	(CA+2)2(V+5)2(O-2)7
CA3V2O8	K2PbS2O8		hR273	R3c	161		3	[3.0, 2.0, 8.0]	(CA+2)3(V+5)2(O-2)8

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
CA4V2O9	Ca4V2O9		oF	F222	22		3	[4.0, 2.0, 9.0]	(CA+2)4(V+5)2(O-2)9
CA10V6O19	Unknown Structure						3	[5.0, 3.0, 9.5]	(CA+2)5(V+3)3(O-2)9.5
CA9V6O18	Unknown Structure						3	[9.0, 6.0, 18.0]	(CA+2)9(V+3)6(O-2)18
CAV2O5	CaV2O5		oP16	Pmmn	59		3	[1.0, 2.0, 5.0]	(CA+2)1(V+4)2(O-2)5
CAV3O7	CaV3O7		oP44	Pnma	62		3	[1.0, 3.0, 7.0]	(CA+2)1(V+4)3(O-2)7
CAV4O9	CaV4O9		tP9	P4/n	85		3	[1.0, 4.0, 9.0]	(CA+2)1(V+4)4(O-2)9
CAVO3	Unknown Structure						3	[1.0, 1.0, 3.0]	(CA+2)1(V+4)1(O-2)3
CAV2O6	ThTi2O6		mS18	C2/m	12	This is CaV2O6, CoV2O6, MgV2O6, MnV2O6 and NiV2O6.	3	[1.0, 2.0, 6.0]	(CA+2, CO+2, MG+2, MN+2, NI+2)1(V+5)2(O-2)6
MG2V2O7	Co2[V2O7]		mP44	P2_1/c	14	This is Co2V2O7, Mg2V2O7 and Ni2V2O7.	3	[2.0, 2.0, 7.0]	(CO+2, MG+2, NI+2)2(V+5)2(O-2)7
MG3V2O8	Ni3[VO4]2		oS52	Cmce	64	This is Co3V2O8, Mg3V2O8 and Ni3V2O8.	3	[3.0, 2.0, 8.0]	(CO+2, MG+2, NI+2)3(V+5)2(O-2)8
MN2V2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	C2/m	12		3	[2.0, 2.0, 7.0]	(MN+2)2(V+5)2(O-2)7
CRVO4	MgSO4		oS24	Cmcm	63		3	[1.0, 1.0, 4.0]	(CR+3)1(V+5)1(O-2)4
FEVO4	Zn[MoO4]		aP36	P-1	2	This is FeVO4 and AlVO4.	3	[1.0, 1.0, 4.0]	(AL+3, FE+3)1(V+5)1(O-2)4

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
FEV2O6	Unknown Structure						3	[1.0, 2.0, 6.0]	(FE+2)1(V+5)2(O-2)6
WO2_72	Unknown Structure						1	[1.0]	(O2_72W1)1
WO2_90	Unknown Structure						1	[1.0]	(O2_90W1)1
WO2_96	Unknown Structure						1	[1.0]	(O2_96W1)1
WO3_HT	WO2.95		tP16	P-42_1m	113		2	[1.0, 3.0]	(W+6)1(O-2)3
WO3_LT	WO3		oP32	Pbcn	60		2	[1.0, 3.0]	(W+6)1(O-2)3
ALNB11O29	(Ti0.17Nb0.83)12O29		mS82	C2/m	12		3	[1.0, 11.0, 29.0]	(AL+3)1(NB+5)11(O-2)29
ALNB49O124	Unknown Structure						3	[1.0, 49.0, 124.0]	(AL+3)1(NB+5)49(O-2)124
CA2NB2O7	La2Ti2O7		mP44	P2_1	4		3	[2.0, 2.0, 7.0]	(CA+2)2(NB+5)2(O-2)7
CA3NB2O8	Unknown Structure						3	[3.0, 2.0, 8.0]	(CA+2)3(NB+5)2(O-2)8
FENB49O124	Unknown Structure						3	[1.0, 49.0, 124.0]	(FE+3)1(NB+5)49(O-2)124
FENB25O64	Unknown Structure						3	[1.0, 25.0, 64.0]	(FE+3)1(NB+5)25(O-2)64
FENB9O24	Unknown Structure						3	[1.0, 9.0, 24.0]	(FE+3)1(NB+5)9(O-2)24
MG2NB34O87	Unknown Structure						3	[2.0, 34.0, 87.0]	(MG+2)2(NB+5)34(O-2)87
MG5NB4O15	Ta3N5		oS32	Cmcm	63		3	[5.0, 4.0, 15.0]	(MG+2)5(NB+5)4(O-2)15

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
CA2ALNBO6	Ca2AlNbO6		mP24	P2_1/c	14		4	[2.0, 1.0, 1.0, 6.0]	(CA+2)2(AL+3)1 (NB+5)1(O-2)6
CANA2SIO4	Na2CaSiO4 (S66)	S66	cP32	P2_13	198		4	[1.0, 2.0, 1.0, 4.0]	(CA+2)1(NA+1)2 (SI+4)1(O-2)4
CANA4SI3O9	K4SrGe3O9		cP272	Pa-3	205		4	[1.0, 4.0, 3.0, 9.0]	(CA+2)1(NA+1)4 (SI+4)3(O-2)9
CANA2SI5O12	Unknown Structure						4	[1.0, 2.0, 5.0, 12.0]	(CA+2)1(NA+1)2 (SI+4)5(O-2)12
CA2NA2SI2O7	Na2Ca2Si2O7		mS208	C2/c	15		4	[2.0, 2.0, 2.0, 7.0]	(CA+2)2(NA+1)2 (SI+4)2(O-2)7
CA2NA2SI3O9	Na(Na0.5Ca0.5)2CaSi3O9		hP102	P3_121	152		4	[2.0, 2.0, 3.0, 9.0]	(CA+2)2(NA+1)2 (SI+4)3(O-2)9
CA3NA2SI6O16	Na2Ca3Si6O16		aP54	P-1	2		4	[3.0, 2.0, 6.0, 16.0]	(CA+2)3(NA+1)2 (SI+4)6(O-2)16
MGNA2SI4O10	Unknown Structure						4	[1.0, 2.0, 4.0, 10.0]	(MG+2)1(NA+1)2 (SI+4)4(O-2)10
MG2NA2SI6O15	Na2Mg2Si6O15		oS200	Cmce	64		4	[2.0, 2.0, 6.0, 15.0]	(MG+2)2(NA+1)2 (SI+4)6(O-2)15
NIOCALITE_C10NS6	Niocalite		oS114	C222	21	This is 10CaO.Nb2O5.6SiO2.	4	[10.0, 2.0, 6.0, 27.0]	(CA+2)10(NB+5)2 (SI+4)6(O-2)27
CU3NB2O8	Cu3(Ta0.5Nb0.5)2O8		aP13	P-1	2		3	[3.0, 2.0, 8.0]	(CU+2)3(NB+5)2(O-2)8
CUNB2O6	CuNb2O6		mP36	P2_1/c	14		3	[1.0, 2.0, 6.0]	(CU+2)1(NB+5)2(O-2)6
NINB68O171	Unknown Structure						3	[1.0, 68.0, 171.0]	(NI+2)1(NB+5)68(O-2)171

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
NINB36O91	Unknown Structure						3	[1.0, 36.0, 91.0]	(NI+2)1(NB+5)36(O-2)91
NINB14O36	Unknown Structure						3	[1.0, 14.0, 36.0]	(NI+2)1(NB+5)14(O-2)36
NI4NB2O9	Nb2Ni4O9		oF480	Fdd2	43		3	[4.0, 2.0, 9.0]	(NI+2)4(NB+5)2(O-2)9
ZR8NB2O21	Unknown Structure						3	[8.0, 2.0, 21.0]	(ZR+4)8(NB+5)2(O-2)21
ZR15NB4O40	Unknown Structure						3	[15.0, 4.0, 40.0]	(ZR+4)15(NB+5)4(O-2)40
ZR7NB2O19	Unknown Structure						3	[7.0, 2.0, 19.0]	(ZR+4)7(NB+5)2(O-2)19
ZR13NB4O36	Unknown Structure						3	[13.0, 4.0, 36.0]	(ZR+4)13(NB+5)4(O-2)36
ZR6NB2O17	Nb2Zr6O17		oI100	Ima2	46		3	[6.0, 2.0, 17.0]	(ZR+4)6(NB+5)2(O-2)17
ZR11NB4O32	Unknown Structure						3	[11.0, 4.0, 32.0]	(ZR+4)11(NB+5)4(O-2)32
ZR5NB2O15	Unknown Structure						3	[5.0, 2.0, 15.0]	(ZR+4)5(NB+5)2(O-2)15
CRNB49O124	Unknown Structure						3	[1.0, 49.0, 124.0]	(CR+3)1(NB+5)49(O-2)124
CRNB25O64	Unknown Structure						3	[1.0, 25.0, 64.0]	(CR+3)1(NB+5)25(O-2)64
CRNB9O24	Unknown Structure						3	[1.0, 9.0, 24.0]	(CR+3)1(NB+5)9(O-2)24

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
LA3NBO7	La3NbO7		oP44	Pnma	62		3	[3.0, 1.0, 7.0]	(LA+3)3(NB+5)1(O-2)7
LANBO4	LaNbO4		mS24	C2/c	15		3	[1.0, 1.0, 4.0]	(LA+3)1(NB+5)1(O-2)4
LANB3O9	La0.67Nb2O6-b		oS36	Cmmm	65		3	[1.0, 3.0, 9.0]	(LA+3)1(NB+5)3(O-2)9
LA2NB12O33	Unknown Structure						3	[2.0, 12.0, 33.0]	(LA+3)2(NB+5)12(O-2)33
TINB2O7	(Ti0.33Nb0.67)3O7		mS60	C2/m	12		3	[1.0, 2.0, 7.0]	(TI+4)1(NB+5)2(O-2)7
TI2NB10O29	(Ti0.17Nb0.83)12O29		mS82	C2/m	12		3	[2.0, 10.0, 29.0]	(TI+4)2(NB+5)10(O-2)29
TINB24O62	(Ti0.04Nb0.96)25O62		mS174	C2	5		3	[1.0, 24.0, 62.0]	(TI+4)1(NB+5)24(O-2)62
CA4NB2O9_HT11	Ca4Nb2O9		mP20	P2_1/c	14		5	[6.0, 3.0, 3.0, 3.0, 15.0]	(CA+2)6(CA+2, NB+5)3 (NB+5)3(O-2, VA)3(O-2)15
CA4NB2O9_LT21	Ca4Nb2O9-lt		mP60	P2_1/c	14		5	[6.0, 4.0, 2.0, 3.0, 15.0]	(CA+2)6(CA+2, NB+5)4 (CA+2)2(O-2, VA)3(O-2)15
FENB14O36	Unknown Structure					This is (Co,Fe)Nb14O36	3	[1.0, 14.0, 36.0]	(CO+2, FE+2)1 (NB+5)14(O-2)36
FENB68O171	Unknown Structure					This is (Co,Fe)Nb68O171	3	[1.0, 68.0, 171.0]	(CO+2, FE+2)1 (NB+5)68(O-2)171
FENB36O91	Unknown Structure					This is (Co,Fe)Nb36O91	3	[1.0, 36.0, 91.0]	(CO+2, FE+2)1 (NB+5)36(O-2)91
COLUMBITE	Columbite (FeNb2O6, E51)	E51	oP36	Pbcn	60	This is (Ca,Co,Fe,Mg,Mn)Nb2O6 with excess FeO and MgO.	3	[1.0, 2.0, 6.0]	(CA+2, CO+2, FE+2, MG+2, MN+2)1(FE+2,

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
									MG+2, NB+5)2(O-2, VA)6
MGWO4_TYPE	Huanzalaite (MgWO4, H06)	H06	mP12	P2/c	13	This is (Al,Fe)NbO4 and (Co,Fe,Mg,Mn,Ni)WO4.	3	[1.0, 1.0, 4.0]	(AL+3, CO+2, FE+2, FE+3, MG+2, MN+2, NB+5, NI+2, VA)1 (NB+5, W+6)1(O-2)4
CAWO4	Scheelite (CaWO4, H04)	H04	tI24	I4_1/a	88		3	[1.0, 1.0, 4.0]	(CA+2)1(W+6)1(O-2)4
CA3WO6	Cryolite (Na3AlF6, J26)	J26	mP20	P2_1/c	14		3	[3.0, 1.0, 6.0]	(CA+2)3(W+6)1(O-2)6
MN4NB2O9	Nb2Mn4O9		hP30	P-3c1	165	This is (Co,Fe,Mg,Mn)4Nb2O9.	3	[4.0, 2.0, 9.0]	(CO+2, FE+2, MG+2, MN+2)4(NB+5)2(O-2)9
NINB2O6	Columbite (FeNb2O6, E51)	E51	oP36	Pbcn	60		3	[1.0, 2.0, 6.0]	(NB+5, NI+2, VA)1 (NB+5, NI+2)2(O-2, VA)6
YNBO4	LaNbO4		mS24	C2/c	15		3	[1.0, 1.0, 4.0]	(NB+5, VA, Y+3)1 (NB+5, Y+3)1(O-2, VA)4
Y3NBO7	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		3	[3.0, 1.0, 7.0]	(NB+5, VA, Y+3)3 (NB+5, Y+3)1(O-2, VA)7
CRNBO4	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136		3	[1.0, 1.0, 4.0]	(CR+3, VA)1(CR+3, NB+5)1(O-2, VA)4
CA3CO2O6	Ca3Co2O6		hR22	R-3c	167		3	[3.0, 2.0, 6.0]	(CA+2)3(CO+3, CU+2)2(O-2, VA)6
CA3CO4O9	Ca3Co4O9		mS30	C2/m	12		3	[3.0, 4.0, 9.0]	(CA+2)3(CO+3, CU+2)4(O-2, VA)9
CR2TI2O7	Unknown Structure					with solubility of Al2O3 and Fe2O3.	3	[2.0, 2.0, 7.0]	(AL+3, CR+3, FE+3)2 (TI+4)2(O-2)7

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
CA2GD2ZRO7	Unknown Structure						4	[2.0, 2.0, 1.0, 7.0]	(CA+2)2(GD+3)2 (ZR+4)1(O-2)7
SPHENE	CaTi[SiO4]O		mP32	P2_1/c	14		4	[1.0, 1.0, 1.0, 5.0]	(CA+2)1(TI+4)1(SI+4)1 (O-2)5
CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	R-3c	167	This is Al2O3, Cr2O3, Fe2O3, Ti2O3, V2O3 + (Co,Fe,Mg,Mn,Ni)TiO3 Ilmenite.	2	[2.0, 3.0]	(AL+3, CO+2, CR+3, FE+2, FE+3, MG+2, MN+2, MN+3, NI+2, TI+3, TI+4, V+3, V+4, VA)2(O-2)3
HALITE	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225	This is CaO, CoO, FeO, MgO, MnO and NiO	2	[1.0, 1.0]	(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(O-2)1
ALPHA_SPINEL	Hausmannite (Mn3O4)		tI28	I4_1/amd	141	With solubility of Al, Co, Cr, Cu, Fe, Mg and Ni.	4	[1.0, 2.0, 2.0, 4.0]	(CO+2, CU+2, MG+2, MN+2, MN+3, NI+2)1 (AL+3, CR+3, FE+3, MN+2, MN+3, VA)2 (MN+2, VA)2(O-2)4
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	Fd-3m	227	This is MgAl2O4, Fe3O4, Mn3O4 (ht) and many more.	4	[1.0, 2.0, 2.0, 4.0]	(AL+3, CO+2, CO+3, CR+2, CR+3, CU+2, FE+2, FE+3, MG+2, MN+2, NI+2)1(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(CR+2, FE+2, MG+2, MN+2, VA)2(O-2)4
ALF3_S2	AlF3		oS48	Cmcm	63		2	[1.0, 3.0]	(AL+3)1(F-1)3
CUF1	Zincblende (ZnS, B3)	B3	cF8	F-43m	216		2	[1.0, 1.0]	(CU+1)1(F-1)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
MNF2_S1	Unknown Structure						2	[1.0, 2.0]	(MN+2)1(F-1)2
MNF3	MnF3		mS48	C2/c	15		2	[1.0, 3.0]	(MN+3)1(F-1)3
MOF4	Unknown Structure						2	[1.0, 4.0]	(MO+4)1(F-1)4
NAF1	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225	This is (K,Na)F.	2	[1.0, 1.0]	(K+1, NA+1)1(F-1)1
NBF5	MoF5		mS48	C2/m	12		2	[1.0, 5.0]	(NB+5)1(F-1)5
ZRF4	ZrF4		mS60	C2/c	15	This is (Hf,Zr)F4.	2	[1.0, 4.0]	(HF+4, ZR+4)1(F-1)4
NAMGF3	CaTiO3 Pnma Perovskite		oP20	Pnma	62		3	[1.0, 1.0, 3.0]	(NA+1)1(MG+2)1(F-1)3
CA2ALF7	Ca2AlF7		oP40	Pnma	62		3	[2.0, 1.0, 7.0]	(CA+2)2(AL+3)1(F-1)7
CAALF5_S1	CrMnF5		mS28	C2/c	15		3	[1.0, 1.0, 5.0]	(CA+2)1(AL+3)1(F-1)5
CAALF5_S2	CrMnF5		mP28	P2_1/c	14		3	[1.0, 1.0, 5.0]	(CA+2)1(AL+3)1(F-1)5
NA5AL3F14	Chiolite (Na5Al3F14, K75)	K75	tP44	P4/mnc	128		3	[5.0, 3.0, 14.0]	(NA+1)5(AL+3)3(F-1)14
NA3ALF6_S1	Cryolite (Na3AlF6, J26)	J26	mP20	P2_1/c	14		3	[3.0, 1.0, 6.0]	(NA+1)3(AL+3)1(F-1)6
CRYOLITE	Cryolite (Na3AlF6, J26)	J26	mP20	P2_1/c	14	This is (K,Na)3AlF6 solid solution.	2	[3.0, 1.0]	(K+1, NA+1, VA)3 (ALF4-1, ALF6-3)1
KCAF3	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221		3	[1.0, 1.0, 3.0]	(CA+2, MG+2)1(K+1)1 (F-1)3
K2MGF4	K2NiF4		tI14	I4/mmm	139		3	[1.0, 2.0, 4.0]	(MG+2)1(K+1)2(F-1)4

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F6NA2SI1_A	Na2SiF6		hP27	P321	150		3	[2.0, 1.0, 6.0]	(NA+1)2(SI+4)1(F-1)6
F6NA2SI1_B	K2PtCl6 (J11)	J11	cF36	Fm-3m	225		3	[2.0, 1.0, 6.0]	(NA+1)2(SI+4)1(F-1)6
CAF2_S1	Unknown Structure					This is low temperature CaF2.	2	[1.0, 2.0]	(CA+2, MG+2, MN+2)1 (F-1, O-2, VA)2
CAF2_S2	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	This is high temperature CaF2.	2	[1.0, 2.0]	(CA+2, MG+2, MN+2)1 (F-1, O-2, VA)2
MGF2	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136	This is (Co,Fe,Mg,Mn,Ni,V)F2.	2	[1.0, 2.0]	(CO+2, FE+2, MG+2, MN+2, NI+2, V+2)1(F-1)2
CUF2	CuF2		mP6	P2_1/c	14	This is CrF2 and CuF2.	2	[1.0, 2.0]	(CR+2, CU+2)1(F-1)2
FEF3	FeF3 (D012)	D012	hR8	R-3c	167	This is (Al,Co,Cr,Fe)F3.	2	[1.0, 3.0]	(AL+3, CO+3, CR+3, FE+3)1(F-1)3
GDF3	H3Ho		hP24	P-3c1	165	This is high temp (Gd,Y,Yb)F3.	2	[1.0, 3.0]	(GD+3, Y+3, YB+3)1(F-1)3
LAF3	Cementite (Fe3C, D011)	D011	oP16	Pnma	62	This is low temp (Gd,La,Y,Yb)F3.	2	[1.0, 3.0]	(GD+3, LA+3, Y+3, YB+3)1(F-1)3
C3A3F	Unknown Structure					This is 3CaO.3Al2O3.CaF2	4	[6.0, 4.0, 2.0, 12.0]	(AL+3)6(CA+2)4(F-1)2 (O-2)12
C11A7F	Ca6Al7O16F		cI152	I-43d	220	This is 11CaO.7Al2O3.CaF2	4	[14.0, 12.0, 2.0, 32.0]	(AL+3)14(CA+2)12(F-1)2(O-2)32
AL2SIO4F	Unknown Structure						4	[2.0, 1.0, 4.0, 2.0]	(AL+3)2(SI+4)1(O-2)4 (F-1)2
CUSPIDINE	Ca4[Si2O7]([OH]0.25F0.75)2		mP60	P2_1/c	14	This is 3CaO.2SiO2.CaF2	4	[4.0, 2.0, 7.0, 2.0]	(CA+2)4(SI+4)2(O-2)7 (F-1)2

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CA5SI2O8F2	Unknown Structure					This is 4CaO.2SiO2.CaF2	4	[5.0, 2.0, 8.0, 2.0]	(CA+2)5(SI+4)2(O-2)8 (F-1)2
CA10SI3O15F2	Unknown Structure					This is 9CaO.3SiO2.CaF2	4	[10.0, 3.0, 15.0, 2.0]	(CA+2)10(SI+4)3(O-2)15(F-1)2
MONOCLINIC_S	beta-S		mP48	P2_1/c	14		1	[1.0]	(S)1
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	Fddd	70		1	[1.0]	(S)1
AL2S3	alpha-Al2S3		hP30	P6_1	169		2	[2.0, 3.0]	(AL)2(S)3
CR1S1	CrS		mS8	C2/c	15	This is low-temp CrS.	2	[1.03, 1.0]	(CR)1.03(S)1
CR7S8	Cr7Se8		mS30	C2/m	12		2	[7.0, 8.0]	(CR)7(S)8
CR5S6	Cr5S6		hP22	P-31c	163		2	[5.0, 6.0]	(CR)5(S)6
CR3S4	Brezinaite (Cr3S4)		mS14	C2/m	12		2	[3.0, 4.0]	(CR, FE, MN, NI)3(S)4
CR2S3	Dolomite [MgCa(CO3)2, G11]	G11	hR10	R-3	148		2	[2.0, 3.0]	(CR, FE)2(S)3
LA1S2	CeSe2		mP12	P2_1/c	14		2	[1.0, 2.0]	(LA)1(S)2
NIS_LT	Millerite (NiS, B13)	B13	hR6	R3m	160	This is low temperature NiS.	2	[1.0, 1.0]	(NI)1(S)1
NI3S2_LT	Hazelwoodite (Ni3S2, D5e)	D5e	hR5	R32	155		2	[3.0, 2.0]	(NI)3(S)2
CUCRS2	CuCrS2-b		hR4	R3m	160		3	[1.0, 1.0, 2.0]	(CU)1(CR)1(S)2
FEAL2S4	ZnIn2S4		hR7	R3m	160		3	[1.0, 2.0, 4.0]	(FE)1(AL)2(S)4
SIS2	SiS2 (C42)	C42	oI12	Ibam	72		2	[1.0, 2.0]	(SI)1(S)2
ZRS2	CdI2		hP3	P-3m1	164		2	[1.0, 2.0]	(ZR)1(S)2

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
ANILITE	Cu7S4		oP44	Pnma	62	This is Cu7S4, orthorhombic structure.	2	[1.75, 1.0]	(CU)1.75(S)1
CHALCOCITE_ALPHA	Cu2S-alpha		mP144	P2_1/c	14	This is Cu2S.	2	[2.0, 1.0]	(CU)2(S)1
CHALCOCITE_BETA	Cu2S-beta		hP16	P6_3/mmc	194	This is Cu2S.	2	[2.0, 1.0]	(CU)2(S)1
COVELLITE	Covellite (CuS, B18)	B18	hP12	P6_3/mmc	194	This is CuS.	2	[1.0, 1.0]	(CU)1(S)1
DJURLEITE	Cu31S16		mP376	P2_1/c	14	This is Cu31S16.	2	[1.93, 1.0]	(CU)1.93(S)1
CUFES2_LT	Chalcopyrite (CuFeS2, E11)	E11	tI16	I-42d	122	This is stoichiometric low-temperature CuFeS2.	3	[1.0, 1.0, 2.0]	(CU)1(FE)1(S)2
MO2S3	Mo2S3		mP10	P2_1/m	11		2	[2.0, 3.0]	(MO)2(S)3
MO1S2	Molybdenite (MoS2, C7)	C7	hP6	P6_3/mmc	194	This is MoS2 and WS2.	2	[1.0, 2.0]	(MO, W)1(S)2
NAS2	NaS2		tI48	I-42d	122		2	[1.0, 2.0]	(NA)1(S)2
NA2S1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	This is (K,Na)2S.	2	[2.0, 1.0]	(K, NA)2(S)1
TIS3	ZrSe3		mP8	P2_1/m	11		2	[1.0, 3.0]	(TI)1(S)3
TIS2	CdI2		hP3	P-3m1	164		2	[1.0, 2.0]	(TI)1(S)2
TI8S10	Ti0.81S		hP20	P6_3/mmc	194		2	[8.0, 10.0]	(TI)8(S)10
TI8S9	TiS		hR18	R-3m	166		2	[8.0, 9.0]	(TI)8(S)9
TI2S	Ta2P		oP36	Pnnm	58		2	[2.0, 1.0]	(TI)2(S)1
TI8S3	Ti8S3		mS88	C2/m	12		2	[8.0, 3.0]	(TI)8(S)3
K2S2	Na2O2		hP12	P-62m	189		2	[2.0, 2.0]	(K)2(S)2

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K2S3	K2S3		oS20	Cmc2_1	36		2	[2.0, 3.0]	(K)2(S)3
K2S4	Unknown Structure						2	[2.0, 4.0]	(K)2(S)4
K2S5	Tl2S5		oP28	P2_12_12_1	19		2	[2.0, 5.0]	(K)2(S)5
K2S6	Unknown Structure						2	[2.0, 6.0]	(K)2(S)6
LA2S3	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62	This is (Gd,La)2S3.	2	[2.0, 3.0]	(GD, LA)2(S)3
HEAZLEWOODITE_B1	Cu1.9S		cF12	F-43m	216	This is non- stoichiometric high temperature Ni3S2.	2	[2.0, 1.0]	(CO, FE, NI, VA)2(S)1
HEAZLEWOODITE_B2	Unknown Structure					This is non- stoichiometric high temperature Ni4S3.	2	[2.0, 1.0]	(FE, NI, VA)2(S)1
NI7S6	Unknown Structure		t**				2	[7.0, 6.0]	(FE, NI)7(S)6
NI9S8	Ni9S8		oS68	C222	21		2	[9.0, 8.0]	(FE, NI)9(S)8
THIOSPINEL	Spinel (Co3O4, D72)	D72	cF56	Fd-3m	227	This is a sulphur spinel: (Cu,Fe,Mn)Cr2S4, Co3S4, FeNi2S4 and Ni3S4.	3	[1.0, 2.0, 4.0]	(CO, CU, FE, MN, NI)1 (CO, CR, NI)2(S)4
ALABANDITE	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225	This is CaS (oldhamite), MnS (alabandite), (Mg,Gd,La,Zr)S.	2	[1.0, 1.0]	(CA, CO, CR, CU, FE, GD, LA, MG, MN, Y, ZR)1(S)1
PYRRHOTITE	NiAs (B81)	B81	hP4	P6_3/mmc	194	This is (Co,Cr,Fe,Nb,Ni,Ti,V)S.	2	[1.0, 1.0]	(AL, CO, CR, CU, FE, GD, MG, MN, NB, NI, TI, V, VA, ZR)1(S)1
PYRITE	Pyrite (FeS2, C2)	C2	cP12	Pa-3	205	This is Cattierite (CoS2), Pyrite (FeS2) - Hauerite (MnS2) - Vaesite (NiS2).	2	[1.0, 2.0]	(CO, FE, MN, NI)1(S)2
CO9S8	Co9S8 (D89)	D89	cF68	Fm-3m	225		2	[9.0, 8.0]	(CO, FE, NI)9(S)8
PENTLANDITE	Co9S8 (D89)	D89	cF68	Fm-3m	225		3	[8.0, 1.0,	(FE, NI)8(FE, NI)1(S)8

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
								8.0]	
DIGENITE	Cu2Se		cF44	Fm-3m	225	This is Cu2S with solubility of Fe, Mg and Mn.	3	[2.0, 1.0, 1.0]	(CU, FE, MG, MN, VA)2(CU, VA)1(S)1
CHALCOPYRITE	Chalcopyrite (CuFeS2, E11)	E11	tI16	I-42d	122	This is high-temperature nonstoichiometric CuFeS2.	3	[1.0, 1.0, 1.0]	(CU, FE, VA)1(CU, VA)1(S)1
FE2O12S3	Fe2[SO4]3		hR34	R-3	148	This is (Al,Cr,Fe)2(SO4)3	2	[2.0, 3.0]	(AL+3, CR+3, FE+3)2 (SO4-2)3
ZRO8S2	Zr[SO4]2		oP44	Pnma	62		2	[1.0, 2.0]	(ZR+4)1(SO4-2)2
ANHYDRITE	Anhydrite (CaSO4, H01)	H01	oS24	Cmcm	63	This is (Ca,Cu,Fe,Mg,Mn,Ni) (SO4).	2	[1.0, 1.0]	(CA+2, CO+2, CU+2, FE+2, MG+2, MN+2, NI+2)1(SO4-2)1
CASO4_HT	CePO4		hP18	P6_222	180	This is high-temperature (Ca,Co,Mg)SO4.	2	[1.0, 1.0]	(CA+2, CO+2, MG+2)1 (SO4-2)1
CAMG3O16S4	Unknown Structure					This is CaMg3(SO4)4.	3	[1.0, 3.0, 4.0]	(CA+2)1(MG+2)3(SO4-2)4
CU2SO4	Thenardite [Na2SO4 (V), H17]	H17	oF56	Fddd	70		2	[2.0, 1.0]	(CU+1)2(SO4-2)1
CU2SO5	Cu2[SO4]O		mS32	C2/m	12		1	[1.0]	(CU2O5S1)1
CASFEO	Unknown Structure					This is CaS.FeO and CaS.Fe2O3.	4	[2.0, 2.0, 2.0, 3.0]	(CA+2)2(S-2)2(FE+2, FE+3)2(O-2, VA)3
CA3S3FE4OX	Unknown Structure					This is 3CaS.4FeO and 3CaS.4Fe2O3.	4	[3.0, 3.0, 4.0, 6.0]	(CA+2)3(S-2)3(FE+2, FE+3)4(O-2, VA)6
MN9SI3O14S1	Unknown Structure					This is 8MnO.3SiO2.MnS	4	[9.0, 3.0, 14.0, 1.0]	(MN+2)9(SI+4)3(O-2)14(S-2)1
ALPO4_S1	Al[AsO4]		hP18	P3_121	152	This is (Al,Fe,Mn)PO4 with SiO2 solubility.	2	[1.0, 1.0]	(AL+3, FE+3, MN+3, SI+4)1(PO4-3, SIO4-4)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
ALPO4_S2	Al[PO4]		hP18	P6_222	180	This is AlPO4 with SiO2 solubility.	2	[1.0, 1.0]	(AL+3, SI+4)1(PO4-3, SIO4-4)1
ALPO4_S3	AlPO4 low cristobalite type		oS24	C222_1	20	This is AlPO4 with SiO2 solubility.	2	[1.0, 1.0]	(AL+3, SI+4)1(PO4-3, SIO4-4)1
AL3PO7	Unknown Structure						3	[3.0, 1.0, 7.0]	(AL+3)3(P+5)1(O-2)7
ALP3O9	AlP3O9		mS156	Cc	9	This is (Al,Cr,Fe)P3O9	2	[1.0, 3.0]	(AL+3, CR+3, FE+3)1 (PO3-1)3
CA4P2O9_A	Ca4[PO4]2O		mP60	P2_1	4	This is alpha-Ca4(PO4)2O.	3	[4.0, 2.0, 1.0]	(CA+2)4(PO4-3)2(O-2)1
CA4P2O9_B	beta-Ca4(PO4)2O		oP60	P222_1	17	This is beta-Ca4(PO4)2O.	3	[4.0, 2.0, 1.0]	(CA+2)4(PO4-3)2(O-2)1
CA10P6O25	Unknown Structure					This is Ca10(PO4)6O.	3	[10.0, 6.0, 1.0]	(CA+2)10(PO4-3)6(O-2)1
CA3P2O8_A	Ca3[PO4]2		mP312	P2_1/c	14	This is alpha-Ca3(PO4)2 with solubility of Mg and Si.	3	[3.0, 1.0, 2.0]	(CA+2, MG+2)3(CA+2, VA)1(PO4-3, SIO4-4)2
CA3P2O8_B	Ca3[AsO4]2		hR92	R3c	161	This is beta-Ca3(PO4)2 with solubility of Mg.	2	[3.0, 2.0]	(CA+2, MG+2)3(PO4-3)2
CA2P2O7_A	Ce2Si2O7		mP44	P2_1/c	14	This is alpha-Ca2(P2O7).	2	[2.0, 1.0]	(CA+2, MG+2)2(P2O7-4)1
CA2P2O7_B	beta-Ca2[P2O7]		tP88	P4_1	76	This is beta-Ca2(P2O7).	2	[2.0, 1.0]	(CA+2, MG+2)2(P2O7-4)1
CA2P2O7_G	Unknown Structure					This is gamma-Ca2(P2O7).	2	[2.0, 1.0]	(CA+2, MG+2)2(P2O7-4)1
CA4P6O19	Ca4P6O19		aP58	P-1	2	This is Ca4(PO3)5(PO4).	3	[4.0, 5.0, 1.0]	(CA+2)4(PO3-1)5(PO4-3)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
CAP2O6_A	CaP2O6		mS72	Cc	9	This is alpha-Ca(PO3)2.	2	[1.0, 2.0]	(CA+2)1(PO3-1)2
CAP2O6_B	PbP2O6		mP72	P2_1/c	14	This is beta-Ca(PO3)2.	2	[1.0, 2.0]	(CA+2)1(PO3-1)2
CAP2O6_G	CaP2O6		mP72	Cc	9	This is gamma-Ca(PO3)2.	2	[1.0, 2.0]	(CA+2)1(PO3-1)2
CA2P6O17	Ca2P6O17		mP56	P2_1/c	14	This is Ca2(P2O5)3O2.	3	[2.0, 6.0, 17.0]	(CA+2)2(P+5)6(O-2)17
CAP4O11_A	CaP4O11		oS128	Aea2	41	This is alpha- Ca(P2O5)2O.	3	[1.0, 4.0, 11.0]	(CA+2)1(P+5)4(O-2)11
CAP4O11_B	CaP4O11		mP64	P2_1/c	14	This is beta- Ca(P2O5)2O.	3	[1.0, 4.0, 11.0]	(CA+2)1(P+5)4(O-2)11
CO3P2O8	Co3[PO4]2		mP26	P2_1/c	14	This is (Co,Fe,Mg,Ni)3P2O8 with solubility of Ca.	2	[3.0, 2.0]	(CA+2, CO+2, FE+2, MG+2, NI+2)3(PO4-3)2
CR3P2O8	Unknown Structure						2	[3.0, 2.0]	(CR+2)3(PO4-3)2
CR2P4O13	Cr2P4O13		mP76	P2_1/c	14	This is Cr2P4O13, Cr2V4O13 and Fe2V4O13.	3	[2.0, 4.0, 13.0]	(CR+3, FE+3)2(P+5, V+5)4(O-2)13
CR4P6O21	Unknown Structure						2	[4.0, 3.0]	(CR+3)4(P2O7-4)3
CRPO4	Cr[PO4]		oI72	Imma	74		2	[1.0, 1.0]	(CR+3)1(PO4-3)1
CR3PO7	Unknown Structure						3	[3.0, 1.0, 7.0]	(CR+3)3(P+5)1(O-2)7
CR5PO10	Unknown Structure						3	[5.0, 1.0, 10.0]	(CR+3)5(P+5)1(O-2)10
FE4P6O21	Fe4[P2O7]3		mP124	P2_1/c	14		2	[4.0, 3.0]	(FE+3)4(P2O7-4)3
FE3PO7	Fe3PO7		hR11	R3m	160		3	[3.0, 1.0, 7.0]	(FE+3)3(P+5)1(O-2)7

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
FE2P2O7	Fe2[P2O7]		aP11	P-1	2		2	[2.0, 1.0]	(FE+2)2(P2O7-4)1
FE18P2O24	Fe4(Fe0.5P0.5)O6		oS44	Cmmm	65		4	[16.0, 2.0, 2.0, 16.0]	(FE+2)16(FE+3)2(PO4-3)2(O-2)16
FE7P6O24	Fe7[PO4]6		aP37	P-1	2		3	[3.0, 4.0, 6.0]	(FE+2)3(FE+3)4(PO4-3)6
FE2PO5	Fe2[PO4]O		mS32	C2/c	15		4	[1.0, 1.0, 1.0, 1.0]	(FE+2)1(FE+3)1(PO4-3)1(O-2)1
FE7P8O28	Unknown Structure						3	[5.0, 2.0, 4.0]	(FE+2)5(FE+3)2(P2O7-4)4
FE3P4O14	Unknown Structure						3	[1.0, 2.0, 2.0]	(FE+2)1(FE+3)2(P2O7-4)2
MG2P2O7_A	Unknown Structure					This is alpha- Mg2(P2O7).	2	[2.0, 1.0]	(CA+2, MG+2)2(P2O7-4)1
MG2P2O7_B	Mg2[P2O7]		mP44	P2_1/c	14	This is beta- Mg2(P2O7) and (Co,Ni)2P2O7.	2	[2.0, 1.0]	(CA+2, CO+2, MG+2, NI+2)2(P2O7-4)1
MGP4O11	MgP4O11		mP64	P2_1/c	14		3	[1.0, 4.0, 11.0]	(MG+2)1(P+5)4(O-2)11
MN3P2O8	Unknown Structure						2	[3.0, 2.0]	(MN+2)3(PO4-3)2
MN2P2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	C2/m	12		2	[2.0, 1.0]	(MN+2)2(P2O7-4)1
CU3P2O8	Unknown Structure						2	[3.0, 2.0]	(CU+2)3(PO4-3)2
CUPO3	Unknown Structure						2	[1.0, 1.0]	(CU+1)1(PO3-1)1
CU2P2O7	alpha-Zn2V2O7		mS44	C2/c	15		2	[2.0, 1.0]	(CU+2)2(P2O7-4)1
CUP2O6	CuP2O6		mS72	C2/c	15	This is (Co,Cu,Fe,Mg,Mn,Ni)P2O6.	2	[1.0, 2.0]	(CO+2, CU+2, FE+2, MG+2, MN+2, NI+2)1

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
									(PO3-1)2
SI3P4O16	Unknown Structure						2	[3.0, 4.0]	(SI+4)3(PO4-3)4
SIP2O7_MONO	Si[P2O7]-a		mP40	P2_1/c	14		2	[1.0, 1.0]	(SI+4)1(P2O7-4)1
SIP2O7_TETR	Unknown Structure						2	[1.0, 1.0]	(SI+4)1(P2O7-4)1
SIP2O7_CUB	Si[P2O7]		cP1080	Pa-3	205	This is cubic (Si,Ti)P2O7.	2	[1.0, 1.0]	(SI+4, TI+4)1(P2O7-4)1
P2S5	P2S5		aP28	P-1	2		2	[2.0, 5.0]	(P)2(S)5
AL2P6SI4O26	Unknown Structure						4	[2.0, 6.0, 4.0, 26.0]	(AL+3)2(P+5)6(SI+4)4 (O-2)26
CA3MG3P4O16	Unknown Structure					This is Ca3Mg3(PO4)4 solid solution.	3	[3.0, 3.0, 4.0]	(CA+2, MG+2)3 (MG+2)3(PO4-3)4
CA4MG2P6O21	Unknown Structure						3	[4.0, 2.0, 3.0]	(CA+2)4(MG+2)2 (P2O7-4)3
CA7P2SI2O16	Ca7[(Si0.5P0.5)O4]4		hP180	P6_1	169		3	[7.0, 2.0, 2.0]	(CA+2)7(PO4-3)2 (SIO4-4)2
CA5P2SIO12	Unknown Structure						3	[5.0, 2.0, 1.0]	(CA+2, VA)5(PO4-3)2 (SIO4-4, VA)1
ZR2P2O9	Zr2[PO4]2O		mS52	C2/m	12		3	[2.0, 2.0, 9.0]	(ZR+4)2(P+5)2(O-2)9
B2O3	B2O3		hP15	P3_121	152		2	[2.0, 3.0]	(B+3)2(O-2)3

Gas Phase

Name	*Prototype*	*Sublattice*	*Sites*	*Formula Unit*
GAS	Gas	1	[1.0]	(AL, AL1B1O2, AL1B3H12, AL1C1, AL1C2, AL1CU1, AL1CU1S1, AL1CU1S2, AL1F1, AL1F1H1, AL1F1H1O1, AL1F1H2, AL1F1H2O2, AL1F1O1, AL1F2, AL1F2H1, 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

TCOX12 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:

TCOX12 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 TCOX12, 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*
Al2O3	Assessed	B2O3	Assessed	CaF2	Assessed
CaO	Estimated	CaS	Estimated	Cr2O3	Estimated
CuOx	Assessed	FeOx	Assessed	Gd2O3	Estimated
K2O	Assessed	La2O3	Estimated	MgO	Assessed

System	Status	System	Status	System	Status
MnO	Assessed	MoO2	Estimated	MoO3	Estimated
Na2O	Assessed	Nb2O5	Estimated	NbO	Estimated
NiO	Assessed	P2O5	Assessed	SiO2	Assessed
TiO2	Assessed	V2O5	Assessed	Y2O3	Estimated
Yb2O3	Estimated	ZrO2	Estimated		

Assessed Pseudo Binary Systems

Pseudo Binary Systems Assessed for Viscosity						
Al2O3-Gd2O3	Al2O3-La2O3	Al2O3-Na2O	Al2O3-SiO2	B2O3-SiO2	CaF2-Al2O3	CaF2-MgO
CaF2-SiO2	CaF2-TiO2	CaF2-V2O5	CaO-Al2O3	CaO-P2O5	CaO-SiO2	CuxO-SiO2
FexO-CaO	FexO-Na2O	FexO-SiO2	FexO-TiO2	K2O-Al2O3	K2O-FeOx	K2O-SiO2
MgO-Al2O3	MgO-SiO2	MnO-SiO2	MnO-TiO2	Na2O-P2O5	Na2O-SiO2	Na2O-V2O5
NiO-SiO2	SiO2-Yb2O3					

Assessed Pseudo Ternary Systems

Pseudo Ternary Systems Assessed for Viscosity					
Al2O3-MgO-SiO2	CaF2	CaF2-Al2O3-TiO2	CaF2-Al2O3-V2O5	CaF2-CaO-Al2O3	CaF2-CaO-Cr2O3
CaO-Al2O3-SiO2	CaO-Al2O3-ZrO2	CaO-CaS-SiO2	CaO-Cr2O3-SiO2	CaO-MgO-SiO2	CaO-NiO-SiO2
CaO-SiO2	CaO-SiO2-Cr2O3	CaO-SiO2-TiO2	CuxO-Al2O3-SiO2	Fe2O3-Al2O3-SiO2	Fe2O3-Na2O-SiO2
FexO-CaO-Al2O3	FexO-CaO-SiO2	FexO-MgO-SiO2	K2O-Al2O3-SiO2	K2O-FeOx-SiO2	K2O-Na2O-SiO2
MgO-SiO2-TiO2	MnO-SiO2-TiO2	Na2O-Al2O3-SiO2	Na2O-CaO-SiO2	Na2O-MgO-SiO2	

Assessed Pseudo Quaternary Systems

Pseudo Quaternary Systems Assessed for Viscosity			
CaO-CuOx-MgO-SiO2	CaO-MgO-Al2O3-SiO2	FexO-CaO-Al2O3-SiO2	FexO-CaO-MgO-SiO2
FexO-CaO-SiO2-CaF2	Na2O-CaO-Al2O3-SiO2		

Assessed Pseudo Quinary Systems

Pseudo Quinary Systems Assessed for Viscosity			
CaO-MgO-Al2O3-SiO2-Na2O	CaO-MgO-Al2O3-SiO2-Yb2O3	FexO-CaO-MgO-Al2O3-SiO2	FexO-CaO-SiO2-Al2O3-CaF2

TCOX12 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*
B2O3	Assessed	Yb2O3	Assessed	CaO	Assessed
MgO	Assessed	Al2O3	Assessed	SiO2	Assessed
MnO	Estimated	FeO	Assessed	Fe2O3	Assessed
CaF2	Assessed	MgF2	Assessed	TiO2	Assessed
K2O	Assessed	Cr2O3	Estimated	V2O5	Estimated
ZrO2	Estimated	P2O5	Estimated	Nb2O5	Estimated
NiO	Estimated	WO3	Estimated	La2O3	Estimated
CoO	Estimated	MoO3	Estimated	CaS	Estimated
Al2O3-CaO	Assessed	Al2O3-MgO	Assessed	Al2O3-SiO2	Assessed
CaF2-Al2O3	Assessed	CaF2-CaO	Assessed	CaF2-MgO	Assessed
CaF2-MgF2	Assessed	CaF2-SiO2	Assessed	CaF2-TiO2	Assessed
CaO-SiO2	Assessed	FexO-CaO	Assessed	FexO-SiO2	Assessed
K2O-SiO2	Assessed	MgO-SiO2	Assessed	MnO-SiO2	Assessed

System	Status	System	Status	System	Status
Al2O3-B2O3-CaF2	Assessed	Al2O3-B2O3-CaO	Assessed	Al2O3-MgO-SiO2	Assessed
Al2O3-TiO2-SiO2	Assessed	CaF2-Al2O3-TiO2	Assessed	CaF2-CaO-Al2O3	Assessed
CaF2-CaO-SiO2	Assessed	CaF2-MgO-Al2O3	Assessed	CaO-Al2O3-SiO2	Assessed
CaO-Al2O3-TiO2	Assessed	CaO-MgO-Al2O3	Assessed	CaO-MgO-SiO2	Assessed
CaO-MnO-SiO2	Assessed	CaO-SiO2-TiO2	Assessed	FexO-Al2O3-SiO2	Assessed
FexO-CaO-Al2O3	Assessed	FexO-CaO-MgO	Assessed	FexO-CaO-SiO2	Assessed
FexO-MgO-SiO2	Assessed	FexO-MnO-SiO2	Assessed	CaF2-Al2O3-MgO-SiO2	Assessed
CaF2-CaO-MgO-Al2O3	Assessed	CaO-Al2O3-MnO-SiO2	Assessed	CaO-MgO-Al2O3-SiO2	Assessed
FexO-CaO-Al2O3-SiO2	Assessed	FexO-CaO-MgO-SiO2	Assessed	FexO-CaO-MgO-Al2O3-SiO2	Assessed
FexO-CaO-MnO-SiO2	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

TCOX12 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						
Al2O3-CaF2	Al2O3-CaO	Al2O3-Cr2O3	Al2O3-MgO	Al2O3-SiO2	Al2O3-TiO2	B2O3-CaO
CaF2-CaO	CaF2-MgO	CaF2-SiO2	CaF2-TiO2	CaF2-V2O5	CaO-CuOx	CaO-FeOx
CaO-P2O5	CaO-SiO2	CaO-V2O5	FeOx-MnO	FeOx-Na2O	FeOx-P2O5	FeOx-SiO2
FeOx-TiO2	K2O-SiO2	MgO-SiO2	MnO-SiO2	Na2O-SiO2		

Assessed Pseudo Ternary Systems

Pseudo Ternary Systems Assessed for Surface Tension					
Al2O3-B2O3-CaF2	Al2O3-B2O3-CaO	Al2O3-CaF2-CaO	Al2O3-CaF2-MgO	Al2O3-CaF2-TiO2	Al2O3-CaF2-V2O5
Al2O3-CaO-Cr2O3	Al2O3-CaO-Fe2O3	Al2O3-CaO-MgO	Al2O3-CaO-Na2O	Al2O3-CaO-SiO2	Al2O3-CaO-TiO2
Al2O3-CaO-V2O5	Al2O3-CaO-ZrO2	Al2O3-FeOx-SiO2	Al2O3-MgO-SiO2	Al2O3-MnO-SiO2	Al2O3-Na2O-SiO2

Pseudo Ternary Systems Assessed for Surface Tension					
Al2O3-SiO2-TiO2	CaF2-CaO-SiO2	CaO-CaS-SiO2	CaO-Cr2O3-SiO2	CaO-FeOx-SiO2	CaO-MgO-SiO2
CaO-MnO-SiO2	CaO-Na2O-SiO2	CaO-P2O5-SiO2	CaO-SiO2-V2O5	FeOx-MgO-SiO2	FeOx-MnO-SiO2
K2O-CaO-Al2O3	MgO-Na2O-SiO2				

Assessed Pseudo Quaternary Systems

Pseudo Quaternary Systems Assessed for Surface Tension			
Al2O3-CaF2-CaO-SiO2	Al2O3-CaF2-CaO-V2O5	Al2O3-CaF2-K2O-SiO2	Al2O3-CaF2-MgO-SiO2
Al2O3-CaO-MnO-SiO2	Al2O3-CaO-Na2O-SiO2	Al2O3-CaO-SiO2-TiO2	CaO-MgO-Al2O3-SiO2
CaO-MgO-Na2O-SiO2	FeOx-CaO-Al2O3-SiO2	FeOx-CaO-MgO-SiO2	FeOx-MgO-Al2O3-SiO2

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:	**12.0**
First release:	**TCOX was released in 1992 under the name ION**

Changes in the Most Recent Database Release

TCOX11.1 to TCOX12

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.

Previous Releases

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

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.