TCS Metal Oxide Solutions Database (TCOX11)

Technical Information

Available Starting with Thermo-Calc Version 2021b

Document created 11/15/2021

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).

Intermetallic compounds, except carbides and nitrides, are not included in the database.

TCS Metal Oxide Solutions Database (TCOX) Revision History. The current version of the database is TCOX11.

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 TCS Metal Oxide Solutions Database (TCOX) 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 TCOX11 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 plus 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 plus 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.

TCOX11 Elements, Systems, Phases, and Properties

Included Elements

There are 29 elements included in the most recent version of the database.

Al	Ar*	C	Ca	Co	Cr	Cu	F	Fe	Gd
H*	K	La	Mg	Mn	Mo	N	Na	Nb	Ni
O	P	S	Si	Ti	V	W	Y	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:

- 324 binary and 327 ternary systems to the full range of composition and temperature in the 29 element framework.
- 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 550 phases in total.

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 TCOX11 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 TCOX11 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 TCOX11 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 TCOX11 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).

TCOX11 Systems

In this section:

TCOX11 Assessed Metallic Systems

No intermetallic phases, except carbides and nitrides, are included in the database.

- All metal-metal binaries are assessed except for Ca-W, Ca-Zr, Co-Na, Cr-Na, F-Na, Gd-La, Gd-Na, Gd-P, 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, and P-Zr.
- Many ternary metallic systems are also assessed.
- If needed, more solid phases can be appended from TCFE (TCS Steel and Fe-alloys Database), TCNI (TCS Ni-based Superalloys Database), TCAL (TCS Al-based Alloy Database) or other appropriate databases. However, combining different databases should always be done with caution, since not always the same assessments of subsystems are used in the different databases.

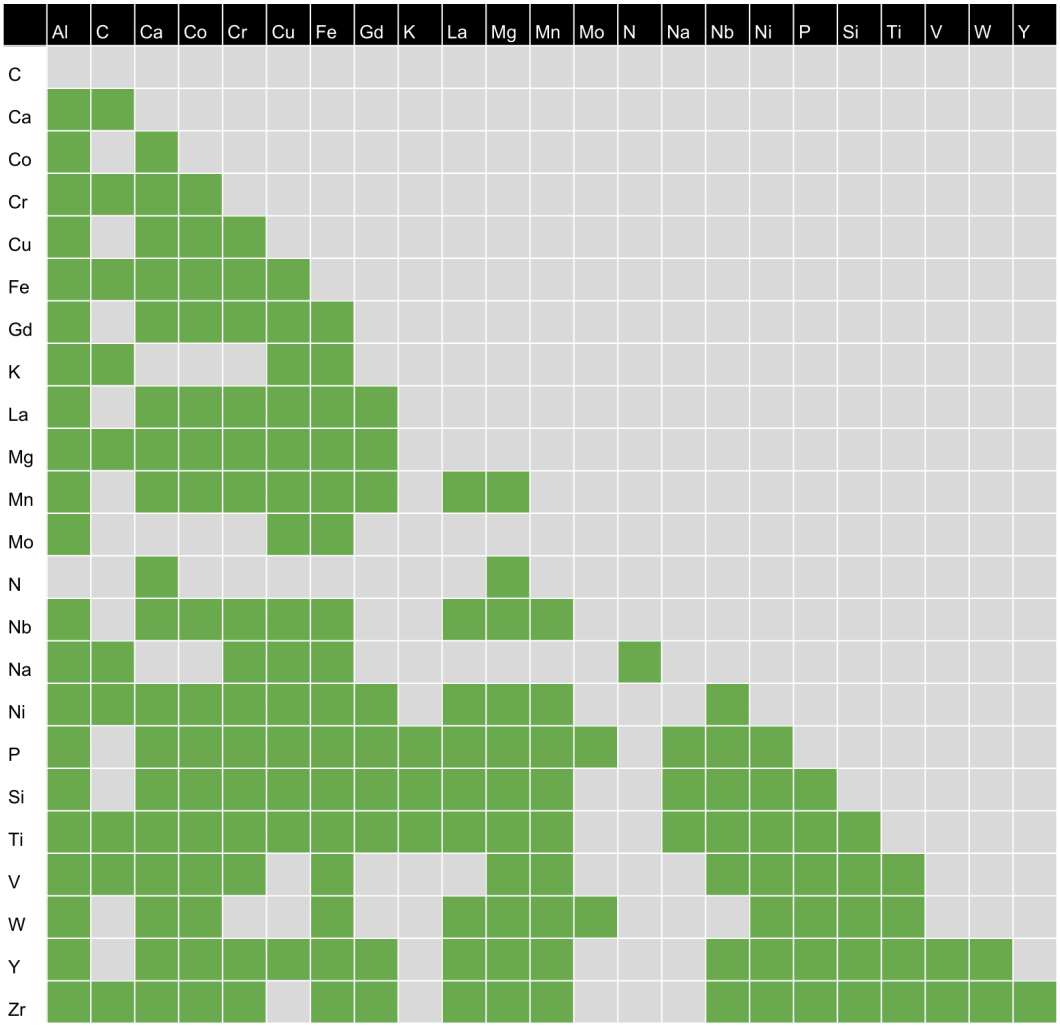
TCOX11 Assessed Oxide Systems

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

Assessed Binary Oxide Systems

Al-O	Ca-O	Co-O	Cr-O	Cu-O	Fe-O	Gd-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
Y-O	Zr-O								

Assessed Ternary Oxide Systems, Me1-Me2-O



Assessed Quaternary Oxide Systems, Me1-Me2-Me3-O

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-Zr
Al-Co-O-Si	Al-Co-O-Ti	Al-Cr-Fe-O	Al-Cr-Mg-O	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-O-Zr
Al-K-O-Si	Al-La-O-Y	Al-La-O-Zr	Al-Mg-K-O	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-Zr	Al-O-Y-Zr	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-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-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-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-Zr	K-Mg-N-O	K-N-Na-O	K-Na-O-Si
La-O-Y-Zr	Mg-Mn-O-Si	Mg-Mn-O-Ti	Mg-N-Na-O	Mg-Na-O-Si
Mg-Ni-O-Si	Mg-O-P-Si	Mg-O-Si-Ti	Mg-O-Si-V	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-Ti-Y-Zr				

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	Ca-Fe-Mg-O-Si	Ca-Mg-Ni-O-Si	Ca-Mg-O-P-Si
Gd-La-O-Y-Zr	C-Cr-Fe-Mn-Ni-O		

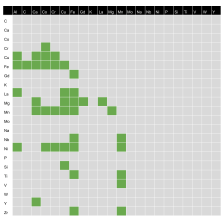
TCOX11 Assessed Sulfide Systems

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

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

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	Al-Ca-O-S	Al-Mg-O-S	Al-Mn-O-S
C-K-O-S	C-Na-O-S	Ca-Fe-O-S	Ca-Mg-O-S	Ca-O-S-Si	Cu-Fe-O-S
Fe-O-S-Si	Mg-O-S-Si	Mn-O-S-Si	Al-Ca-Mn-O-S		

TCOX11 Assessed Fluoride Systems

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

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	KF	LaF_3	MgF_2	MnF_2	MoF_4
NaF	NbF_2	NbF_5	NiF_2	SiF_4	VF_2	YF_3	ZrF_4

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-Fe-F	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	Fe-F-Ni	F-Gd-Mg	F-Gd-Y	F-K-Mg
F-La-Zr	F-Mg-La	F-Mg-Na	F-Mg-Y			

Assessed Oxy-fluoride Systems

Al-F-O	Ca-F-O	Co-F-O	F-Mg-O	Al-Ca-F-O	C-F-K-O
C-F-Na-O	C-K-N-O	Ca-F-Mg-O	Ca-Fe-F-O	Ca-F-O-P	Ca-F-O-Si
F-K-N-O	F-Mg-O-Si	F-N-Na-O	Al-Ca-F-Mg-O	Al-Ca-F-O-Si	

TCOX11 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.
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 and Y_2O_3.
M2O3H	This is hexagonal La_2O_3, Gd_2O_3, and Y_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 ($CaFeSi_2O_6$).
ORTHO_ PYROXENE	Enstatite ($MgSiO_3$), ortho-Diopside ($CaMgSi_2O_6$).

Name in the Database	*Common Name and Description*
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), $GdPO_4$, $LaPO_4$.

TCOX11 Liquid Solution Phases

The liquid phase contains all elements in the TCOX11 database except Ar and H. The ionic two-sublattice liquid model is used. The model may thus be used to describe liquid metal, oxides, sulfides, sulfur, fluoride, silicates etc. with the following formula:

$(Al^{+3}, Ca^{+2}, Co^{+2}, Cr^{+2}, Cu^{+1}, Fe^{+2}, Gd^{+3}, K^{+1}, La^{+3}, Mg^{+2}, Mn^{+2}, Mo^{+4}, Na^{+1}, Nb^{+2}, Ni^{+2}, P^{+5}, Si^{+4}, Ti^{+2}, V^{+2}, W^{+6}, Y^{+3}, Zr^{+4})_P$ $(AlO_2^{-1}, CO_3^{-2}, F^{-1}, NO_3^{-1}, O^{-2}, PO_4^{-3}, S^{-2}, SiO_4^{-4}, Va, AlN, C, C_3S_2Z_{1/6}, CoF_3, CoO_{3/2}, CrF_3, CrO_{3/2}, CuF_2, CuO, FeF_3, FeO_{3/2}, M_3S_2Z_{1/6}, MnO_{3/2}, MoO_3, N, NbF_5, NbO_{5/2}, PO_{5/2}, S, SiO_2, TiO_{3/2}, TiO_2, VO_2, VO_{3/2}, VO_{5/2})_Q$

TCOX11 Alloy Phases

BCC_A2

Containing Al, Ca, Co, Cr, Cu, Fe, Gd, K, La, Mg, Mn, Mo, Na, Nb, Ni, P, S, Si, Ti, V, W, Y, and Zr with C, O and N modeled interstitially.

FCC_A1

Containing Al, Ca, Co, Cr, Cu, Fe, Gd, K, La, Mg, Mn, Mo, Na, Nb, Ni, P, S, Si, Ti, V, W, Y, and Zr with C, O and N modeled interstitially. FCC_A1 also describes cubic carbides and nitrades, and the two cubic oxides TiO and VO solid solutions.

HCP_A3

Containing Al, Ca, Co, Cr, Cu, Fe, Gd, K, La, Mg, Mn, Mo, Na, Nb, Ni, Si, Ti, V, W, Y, and Zr with C, N, and O modeled interstitially. HCP_A3 also describes hexagonal carbides and nitrades.

DHCP

La phase dissolving Al, Ca, Cu, Gd, Mg, Mn, Ni, and Y with O modeled interstitially.

CUB_A13

β-Mn, containing Al, Co, Cr, Cu, Fe, Mg, Mo, Nb, Ni, Si, Ti, V, and Zr with C and N modeled interstitially.

CBCC_A12

α-Mn, containing Al, Co, Cr, Cu, Fe, Mg, Mo, Nb, Ni, Si, Ti, V, and Zr with C and N modeled interstitially.

DIAMOND_FCC_A4

Diamond structure based on Si containing Al, C, Mn, Na, and P with O modeled interstitially.

GRAPHITE

This is pure carbon.

RED_P, WHITE_P

This is pure phosphorus. Phosphorus exists in two modifications: white (not stable at normal conditions) and red (up to the melting temperature of 579° C).

ORTHORHOMBIC_S, MONOCLINIC_S

This is pure sulfur. Sulfur exists in two modifications: orthorhombic (up to 95° C) and monoclinic (up to the melting temperature of 115° C).

TCOX11 Gas Phase

A reduced gas phase containing AL1F3, AR, CA, C1H4, C1O1, C1O2, CA1F2, F, F2, H, H2, H2O1, K, K1N1O3, K2, K2O1, K2O2, MG, MO, MO1O1, MO1O2, MO1O3, MO2O6, MO3O9, MO4O12, MO5O15, N, N1NA1O3, N2, NA, NA2, NA1O1, NA2O1, O, O10P4, O1P1, O2P1, O1S1, O1SI1, O2, O2S1, O3S1, O5P2, O1TI1, O6W2, O8W3, O9W3, O12W4, P2, P4, S2, Ti and V.

TCOX11 Solid Solutions Phases

The solid solution phases are modeled within the framework of the Compound Energy Formalism (CEF) [3]. These models take into account distribution of cations between sublattices, defects such as vacancies, anti-sites and ordering. 211 solutions are modeled in the database.

Al_4C_3_D71

This is Al_4C_3 with solubility of Si.

Alabandite

This is CaS (oldhamite), MnS (alabandite), MgS, GdS, LaS, and ZrS solid solution, with solubility of Co, Cr, Cu, Fe, and Y.

$AlPO_4$

There are three modifications (S1, S2, and S3)of $AlPO_4$ with solubility of SiO_2.

Anhydrite

This is $(Ca,Co,Cu,Fe,Mg,Mn,Ni)SO_4$.

Anorthite

This is high-temperature albite ($NaAlSi_3O_8$), $KAlSi_3O_8$ and Anorthite ($CaO.Al_2O_3.2SiO_2$) solid solution.

Apatite

This is $(Ca,Mg)_2(Gd,Y)_8(SiO_4)_6O_2$ solid solution dissolving Zr.

β-V-O

This is β-V-O.

Bronze

This is $(Ca,Fe)_xV_2O_5$ bronze.

Calcium Ferro-aluminates

- C3A1: This is $Ca_3Al_2O_6$ dissolving ferric Fe.
- C12A7: This is $Ca_{12}Al_{14}O_{32}$ dissolving ferric Fe. C12A7 is not stable in the anhydrous $CaO\text{-}Al_2O_3$ system. It is, however, important in practice, and included in the database. In the optimization it was treated as if it does not contain any water.
- C1A1: This is $CaAl_2O_4$ dissolving ferric Fe.
- C1A2: This is $CaAl_4O_7$ dissolving ferric Fe.
- C1A6: This is $CaAl_{12}O_{19}$ dissolving ferric Fe.
- A1C1F2: This is $Al_2CaFe_4O_{10}$ with a variation in Al/Fe: $CaAlFe_2(Al,Fe)_3O_{10}$.
- C2F: This is $Ca_2Fe_2O_5$ dissolving Al.

$Ca_2P_2O_7$ (α, β and γ)

α, β and γ-$Ca_2P_2O_7$ dissolving Mg.

Ca_2SiO_4 (α and α')

α-Ca_2SiO_4- α'-$Ca_3P_2O_8$ dissolving Gd, Mg, Mn, Y, and α'-Ca_2SiO_4 dissolving Fe, Gd, Mg, Mn, P, and Y.

$Ca_3Co_2O_6$

This is $Ca_3Co_2O_6$ dissolving Cu.

$Ca_3Co_4O_9$

This is $Ca_3Co_4O_9$ dissolving Cu.

$Ca_3Mg_3P_4O_{16}$

This is $Ca_3Mg_3P_4O_{16}$.

$Ca_3P_2O_8$ (α and β)

α-$Ca_3P_2O_8$ dissolving Mg and Si and β-$Ca_3P_2O_8$ dissolving Mg.

$Ca_3S_3Fe_4O_x$

This is the oxy-sulfide 3CaS.4FeO-3CaS.4Fe_2O_3.

$Ca_3Y_2Si_3O_{12}$

This is $Ca_3(Gd,Y)_2(SiO_4)_3$.

$Ca_3Y_2Si_6O_{18}$

This is 3CaO.$(Gd,Y)_2O_3$.6SiO_2.

$Ca_4Nb_2O_9$_HT11

This is the high-temperature $Ca_4Nb_2O_9$ phase with excess CaO.

$Ca_4Nb_2O_9$_LT21

This is the low-temperature $Ca_4Nb_2O_9$ phase with excess CaO.

$Ca_5P_2SiO_{12}$

This is $Ca_5P_2SiO_{12}$.

$CaCr_2O_4$_A

This is the high-temperature $CaCr_2O_4$ dissolving Al and Fe.

CaF_2_S1

This is low-temperature CaF_2 dissolving CaO and MgF_2.

CaF_2_S2

This is high-temperature CaF_2 and CuF_2 dissolving CaO and MgF_2.

$CaMO_3$

This is $CaMnO_3$, $CaTiO_3$ and low-temperature $CaZrO_3$ dissolving Y.

CaN_2O_6

This is $(Ca,Mg)(NO_3)_2$ solid solution.

Carnegieite (α and β)

This is $NaAlSiO_4$ with solubility of Fe and Si.

CaSFeO

This is the oxy-sulfide $CaS.FeO$-$CaS.Fe_2O_3$.

$CaSO_4$_HT

This is $(Ca,Co,Mg)SO_4$.

CaV_2O_4

This is $CaFe_2O_4$, β-$CaCr_2O_4$, CaV_2O_4 and CaY_2O_4 solid solution dissolving Al. Prototype phase is CaV_2O_4.

CaV_2O_6

This is $(Ca,Co,Mg,Mn,Ni)V_2O_6$.

CaY_4O_7

This is $Ca(Gd,Y)_4O_7$.

$CaYAl_3O_7$

This is $Ca(Gd,Y)Al_3O_7$.

$CaYAlO_4$

This is $Ca(Gd,Y)AlO_4$.

$CaZrO_3\_C$

This is the cubic high-temperature $CaZrO_3$ phase dissolving Y.

Cementite

Fe_3C, Mn_3C with solubility of Al, Co, Cr, Mo, Nb, Ni, Si, V, W, N.

Chalcopyrite

This is an intermediate solid solution phase in the Cu-Fe-S system around the composition $CuFeS_2$.

Co_9S_8

This is Co_9S_8 dissolving Fe and Ni.

Columbite

This is $(Ca,Co,Fe,Mg,Mn)Nb_2O_6$ with excess FeO and MgO.

Cordierite

This is $Al_4(Fe,Mg,Mn)_2Si_5O_8$.

Corundum

This is Corundum (Al_2O_3), Eskolaite (Cr_2O_3), Hematite (Fe_2O_3), Karelianite (V_2O_3), Tistarite (Ti_2O_3), and $(Co,Fe,Mg,Mn,Ni)TiO_3$ Ilmenite solid solution.

$Cr_2P_4O_{13}$

This is $Cr_2P_4O_{13}$ and $(Cr,Fe)_2V_4O_{13}$.

Cr_2S_3

This is Cr_2S_3 dissolving Fe.

$Cr_2Ti_2O_7$

This is $Cr_2Ti_2O_7$ with solubility of Al and Fe.

Cr_3S_4

This is Cr_3S_4 dissolving Fe, Mn, and Ni.

$CrNbO_4$

This is $CrNbO_4$ solid solution with excess Cr_2O_3 and Nb_2O_5.

Cristobalite

This is SiO_2 with solubility of $AlPO_4$.

Cryolite

This is β-Na_3AlF_6 solid solution.

CuF_2

This is CrF_2 and low temperature CuF_2.

$CuLa_2O_4$

This is $CuLa_2O_4$ with solubility of Co.

CuO

This is CuO with solubility of Co.

CuP_2O_6

This is $(Co,Cu,Ni)P_2O_6$.

Cuprite

This is Cu_2O with solubility of Na.

Delafossite

This is $Cu(Al,Cr,Fe,La,Mn,Y)O_2$.

Digenite

This is Cu_2S solid solution with excess S and solubility of Fe, Mg, and Mn.

$DyMn_2O_5$

This is $Mn_2(Gd,Y)O_5$ solid solution. Prototype phase is $DyMn_2O_5$.

ETA_M5Si5

This is Cr_3Ni_2SiN with solubility of Mo, Fe.

$Fe_2O_{12}S_3$

This is the oxy-sulfides $(Al,Cr,Fe)_2(SO_4)_3$.

Fe_4N_LP1

This is Fe_4N with solubility of Co, Cr, Mn, Ni, C.

Fe_8Si_2C

This is Fe_8Si_2C with solubility of Mn.

FeF_3

This is $(Al,Co,Cr,Fe)F_3$.

$FeNb_{14}O_{36}$

This is $(Co,Fe)Nb_{14}O_{36}$.

$FeNb_{36}O_{91}$

This is $(Co,Fe)Nb_{36}O_{91}$.

$FeNb_{68}O_{171}$

This is $(Co,Fe)Nb_{68}O_{171}$.

$FePO_4$

This is $(Fe,Mn)PO_4$.

$FeVO_4$

This is $(Al,Fe)VO_4$.

Fluorite

This is high-temperature ZrO_2 solid solution with solubility of Al, Ca, Cr, Fe, Gd, La, Mg, Mn, Ni, Si, Ti, and Y.

Garnet

This is grossular ($Ca_3Al_2Si_3O_{12}$), uvarovite ($Ca_3Cr_2Si_3O_{12}$), spessartine ($Mn_3Al_2Si_3O_{12}$), and goldmanite ($Ca_3V_2Si_3O_{12}$).

$Gd_2Si_2O_7$

This is $(Gd,La)_2Si_2O_7$.

Gd_2SiO_5

This is $(Gd,La)_2SiO_5$.

GdF_3

This is high temperature $(Gd,Y)F_3$.

Halite

This is Lime (CaO), CoO, Wustite (FeO), Periclase (MgO), Manganosite (MnO), bunsenite (NiO) solid solution dissolving also Al, Cu, Cr, Gd, Na, Ti, V, Y, and Zr.

Hatrurite

This is Ca_3SiO_5 dissolving Gd and Y.

β1-Heazlewoodite

This is non-stoichiometric high-temperature Ni_3S_2 dissolving Co and Fe.

β2-Heazlewoodite

This is non-stoichiometric high-temperature Ni_4S_3 dissolving Fe.

K_2CO_3_S1

This is low temperature K_2CO_3 with solubility of Na.

K_2MgSiO_4 (lt and ht)

This is K_2MgSiO_4 with excess SiO_2.

$K_4Al_{22}O_{35}$

This is β''-Al_2O_3 $K_4(Al,Fe)_{22}O_{35}$ solid solution.

$KAl_{11}O_{17}$

This is β-Al_2O_3 $K(Al,Fe)_{11}O_{17}$ solid solution.

$KAlSi_2O_6$

This is $KAlSi_2O_6$-$KFeSi_2O_6$-$K_2MgSi_5O_{12}$ solid solution.

ht-$KAlSiO_4$

This is $KAlSiO_4$-$K_2MgSi_3O_8$ solid solution with SiO_2 solubility.

Kappa_E21

This is $Al(Fe,Mn)_3C$ solid solution.

KNO_3_S1

This is low temperature KNO_3 with solubility of Na.

KSI_Carbide

This is $Mo_6Fe_{11}C_5$ with solubility of Cr, W.

La_2MnO_4

This is $La_2(Mn,Ni)O_4$ solid solution dissolving Co.

La_2S_3

This is $(Gd,La)_2S_3$.

$La_3Ni_2O_7$

This is $La_3Ni_2O_7$ dissolving Co.

$La_4Ni_3O_{10}$

This is $La_4Ni_3O_{10}$ dissolving Co.

LaAP

This is a rhombohedral perovskite, $La(Al,Co)O_3$ dissolving Ca, Cu, Ni, and Y.

LaF_3

This is low temperature $(Gd,La,Y)F_3$.

LaYP

This is the orthorhombic perovskite, $LaYO_3$ solid solution.

$M_{23}C_6$_D84

This is $M_{23}C_6$ carbides, such as $Cr_{23}C_6$ and $Mn_{23}C_6$.

α-M_2O_3

This is hexagonal α-La_2O_3 and Gd_2O_3 solid solution dissolving Ca, Mg, Y, and Zr.

β-M_2O_3

This is monoclinic β-Gd_2O_3 dissolving Al, Ca, Co, La, Mg, Y, and Zr.

c-M_2O_3

This is Mn_2O_3, cubic Gd_2O_3 and Y_2O_3 solid solution dissolving Al, Ca, Co, Cr, Fe, La, Mg, Ni, Ti, Y, and Zr.

h-M_2O_3

This is hexagonal La_2O_3, Gd_2O_3 and Y_2O_3 solid solution dissolving Ca, Mg, Mn, and Zr.

x-M_2O_3

This is x-La_2O_3 and high-temperature cubic Gd_2O_3 solid solution dissolving Ca, Mg, Y, and Zr.

M_3C_2_D510

This is M_3C_2 carbide Cr_3C_2 dissolving Co, Mo, V, W.

M_4O_7

This is $(Ti,V)_4O_7$ solid solution dissolving Al and Mn.

M_5C_2

This is M_5C_2 carbide Mn_5C_2 dissolving Fe, N, Nb, V.

M_6C_E93

This is M_6C carbide, such as W_3Fe_3C dissolving Co, Cr, Mo, Nb, Ni, Si, V.

M_6O_{11}

This is $(Ti,V)_6O_{11}$ solid solution.

M_7C_3_D101

This is M_7C_3 carbides, such as Mn_7C_3 and Cr_7C_3, dissolving Al, Co, Fe, Mo, Nb, Ni, Si, V, W.

M_7O_{13}

This is $(Ti,V)_7O_{13}$ solid solution.

M_8O_{15}

This is $(Ti,V)_8O_{15}$ solid solution.

MC_Eta

This is MoC_{1-x} dissolving Ti, V, W.

MC_SHP

This is MoC, WC dissolving N.

Melilite

This is Gehlenite ($Ca_2Al_2SiO_7$), Fe-Gehlenite ($Ca_2Fe_2SiO_7$), Åkermanite ($Ca_2MgSi_2O_7$), Fe-Åkermanite ($Ca_2FeSi_2O_7$), and $Ca_2CoSi_2O_7$.

$Mg_2P_2O_7$ (α and β)

This is α and β-$Mg_2P_2O_7$ dissolving Ca.

$Mg_2V_2O_7$

This is $(Co,Mg,Ni)_2V_2O_7$.

Mg_3N_2_D53

This is $(Ca,Mg)N_2$.

$Mg_3P_2O_8$

This is $Mg_3P_2O_8$ dissolving Ca.

$Mg_3V_2O_8$

This is $(Co,Mg,Ni)_3V_2O_8$.

MgF_2

This is $(Co,Fe,Mg,Mn,Ni,V)F_2$.

$MgWO_4$-type

This is $(Al,Fe)NbO_4$ and $(Co,Fe,Mg,Mn,Ni)WO_4$ solid solution. Prototype $MgWO_4$.

$Mn_4Nb_2O_9$

This is $(Co,Fe,Mg,Mn)_4Nb_2O_9$.

MoS_2

This is $(Mo,W)S_2$ solid solution.

Mullite

Mullite (around $Al_6Si_2O_{13}$) solid solution dissolving Fe.

$Na_2Al_{12}O_{19}$

This is $Na_2Al_{12}O_{19}$ with solubility of Fe.

$Na_2CaAl_4O_8$

This is $(K,Na)_2CaAl_4O_8$ solid solution.

Na_2CO3-S1

This is low temperature Na_2CO_3 with solubility of K.

Na_2CO3-S2

This is high temperature $(K,Na)_2CO_3$ solid solution.

Na_2O (S1, S2, S3)

This is low, mid and high temperature $(K,Na)_2O$.

Na_2S

This is $(K,Na)_2S$.

$Na_2Si_2O_5$ (α, β, γ)

This is low, mid and high temperature $(K,Na)_2Si_2O_5$ solid solutions.

Na_2SiO_3

This is $(K,Na)_2SiO_3$ solid solution.

$NaAl_{11}O_{17}$

This is $NaAl_{11}O_{17}$ solid solution.

δ-$NaAlO_2$

This is high-temperature $NaAlO_2$ with solubility of Si.

NaF

This is (K,Na)F.

α-$NaFeO_2$

This is $NaCrO_2$ and low-temperature $NaFeO_2$.

β-$NaFeO_2$

This is low-temperature $K(Al,Fe)O_2$ and $NaAlO_2$ and mid-temperature $NaFeO_2$ solid solutions with solubility of Si.

γ-$NaFeO_2$

This is high-temperature $K(Al,Fe)O_2$ and $NaFeO_2$ and mid-temperature $NaAlO_2$ solid solutions with solubility of Si.

$NaNO_3$-S1

This is low-temperature $NaNO_3$ with solubility of K.

$NaNO_3$-S2

This is high-temperature $(K,Na)NO_3$.

Nb_2O_5

This is Nb_2O_5 dissolving Mg and V.

NbO_2

This is NbO_2 dissolving Fe.

Nepheline (α and β)

This is $NaAlSiO_4$ with solubility of Si.

γ-Nepheline

This is low-temperature $(K,Na)AlSiO_4$ and $K_2MgSi_3O_8$ solid solutions with solubility of Fe and Si.

Ni_6MnO_8-type

This is $(Mg,Ni)_6MnO_8$.

Ni_7S_6

This is Ni_7S_6 dissolving Fe.

Ni_9S_8

This is Ni_9S_8 dissolving Fe.

$NiMnO_3$

This is $NiMnO_3$ with Ilmenite structure.

$NiNb_2O_6$

This is $NiNb_2O_6$. This phase has the same structure as the Nb_2FeO_6 phase, but is modeled separately.

Olivine

This is Calcio-olivine (Ca_2SiO_4) – Co_2SiO_4 – Fayalite (Fe_2SiO_4) – Forsterite (Mg_2SiO_4) – Tephroite (Mn_2SiO_4) – Ni_2SiO_4 – Kirschsteinite ($CaFeSiO_4$) – Monticellite ($CaMgSiO_4$) solid solution dissolving Cr and Cu.

Pentlandite

This is ternary $(Fe,Ni)_9S_8$.

Perovskite

This is $(Cr,Fe,Mn)LaO_3$.

Pseudo-brookite

This is Fe_2TiO_5. This is also Ti_3O_5, Al_2TiO_5 and $(Co,Fe,Mg,Mn)Ti_2O_5$ with solubility of Ni and V.

Pyrite

This is Cattierite (CoS_2), Pyrite (FeS_2) – Hauerite (MnS_2) – Vaesite (NiS_2).

Pyrochlore

This is $(Gd,La)_2Zr_2O_7$ and $(Gd,La,Y)_2Ti_2O_7$ solid solution.

Pyroxenes

Modeling of low clino-pyroxene, clino-pyroxene, ortho-pyroxene, and proto-pyroxene solid solutions taking into account the distribution of cations between different sublattices.

- Low clino-pyroxene: This is low clino-enstatite ($MgSiO_3$) and low clino-diopside ($CaMgSi_2O_6$).
- Clino-pyroxene: This is clino-enstatite ($MgSiO_3$), clino-ferrosilit ($FeSiO_3$), diopside ($CaMgSi_2O_6$), niopside ($CaNiSi_2O_6$), pigeonite ($(Mg,Fe,Ca)Si_2O_6$), hedenbergite ($CaFeSi_2O_6$) dissolving Co.
- Ortho-pyroxene: This is enstatite ($MgSiO_3$) and ortho-diopside ($CaMgSi_2O_6$) with Fe solubility.
- Proto-pyroxene: This is proto-enstatite ($MgSiO_3$) and proto-diopside ($CaMgSi_2O_6$) dissolving Co, Cr, and Fe.

Pyrrhotite

This is Pyrrhotite (FeS) – CoS – CrS– NbS – NiS – TiS – VS solid solution dissolving Al, Cu, Gd, Mg, Mn, and Zr.

Quartz

This is SiO_2 with solubility of $AlPO_4$.

Rhodonite

This is $MnO.SiO_2$ dissolving Ca, Co, Fe, and Mg.

Rutile

This is MnO_2 – TiO_2 – high temperature VO_2 solid solution dissolving Al and Zr.

α-Spinel

This is low-temperature tetragonal Mn_3O_4 solid solution dissolving Al, Co, Cr, Cu, Fe, Mg and Ni. Distribution of cations between tetrahedral and octahedral sites, as well as vacancies on the octahedral sites to model deviation from the ideal stoichiometry toward higher oxygen potential and interstitial Mn to model deviation toward excess manganese are taken into account.

Spinel

This is the cubic AB_2O_4-type spinel solid solution containing Al-Ca-Co-Cr-Cu-Fe-Mg-Mn-Ni-Ti-O. Distribution of cations between tetrahedral and octahedral sites, as well as vacancies on the octahedral sites to model deviation from the ideal stoichiometry toward higher oxygen potential and interstitial Fe to model deviation toward excess iron are taken into account.

This is Spinel ($MgAl_2O_4$), Magnetite (Fe_3O_4), Cuprospinel ($CrFe_2O_4$), Hercynite ($FeAl_2O_4$), and many more.

Thio-spinel

This is the sulfur spinel. This has the same structure as the oxygen-spinel, but is modeled as a separate phase. This is $(Cu,Fe,Mn)Cr_2S_4$ – Co_3S_4 – $FeNi_2S_4$ – Ni_3S_4.

Ti_2N_C4

This is Ti_2N with solubility of C. Prototype TiO_2.

Ti_5O_9

This is Ti_5O_9 dissolving V.

Tridymite

This is SiO_2 with solubility of $AlPO_4$.

V_2O_SS

This is V_2O solid solution.

V_3O_5-HT

This is high temperature V_3O_5 dissolving Al, Cr, Mn, and Ti.

V_5O_9

This is V_5O_9 dissolving Ti.

VO_2-LT

This is low temperature VO_2, MoO_2, and WO_2.

Wollastonite

This is $CaSiO_3$ dissolving Fe, Mg, and Mn.

α-Y_2C_3

This is Y_2C_3 solid solution. Prototype Sc_3C_4.

β-Y_2C_3

This is Y_2C_3 solid solution.

Y_2TiO_5

This is $(Gd,La,Y)_2TiO_5$ solid solution.

Y_3NbO_7

This is Y_3NbO_7 solid solution with excess Nb_2O_5 and Y_2O_3.

YAG

This is $(Gd,Y)_3(Al,Fe)_5O_{12}$ solid solution dissolving Cr and La.

YAM

This is $(Gd,Y)_4Al_2O_9$ and Cuspidine ($Ca_2Y_2Si_2O_9$) solid solution dissolving La.

YAP

This is $(Gd,Y)(Al,Co,Cr,Fe)O_3$ solid solution dissolving Ca, Mn, and La.

YC_B1

This is YC solid solution. Prototype NaCl.

$YNbO_4$

This is $YNbO_4$ solid solution with excess Y_2O_3.

Zircon

This is Zircon ($ZrSiO_4$) and $(Gd,La,Y)PO_4$ solid solution.

m-ZrO_2

This is monoclinic ZrO_2 solid solution dissolving Al, Ca, Cr, Gd, La, Ti, and Y.

t-ZrO_2

This is tetragonal ZrO_2 solid solution dissolving Al, Ca, Cr, Fe, Gd, La, Mg, Mn, Ni, Ti, and Y.

β-$ZrTiO_4$

This is $ZrTiO_4$ with solubility of Al.

Z_PHASE

This is ZrNbN with solubility of Fe, Mo, V.

TCOX11 Stoichiometric Compounds

339 stoichiometric compounds are modeled in the database. The **Status** column indicates whether the molar volume has been **Assessed**, **Estimated** or **Unassessed**. Molar volume is included with the database starting with version 10 (TCOX10). Also see TCOX11 Molar Volume Assessed Systems and Phases.

Stoichiometric Compound	*Molar Volume 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	*Molar Volume 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

Stoichiometric Compound	*Molar Volume Status*
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

Stoichiometric Compound	*Molar Volume Status*
CAV2O5	Assessed
CAV3O7	Assessed
CAV4O9	Estimated
CAVO3	Assessed
CAWO4	Assessed
CAZR4O9	Estimated
CF2	Estimated
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

Stoichiometric Compound	*Molar Volume Status*
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

Stoichiometric Compound	*Molar Volume Status*
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
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

Stoichiometric Compound	*Molar Volume Status*
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

Stoichiometric Compound	*Molar Volume Status*
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
MGC2	Estimated
MGCO3	Assessed
MGNA2SI4O10	Estimated
MGP2O6	Assessed
MGP4O11	Assessed
MN2P2O7	Assessed
MN2V2O7	Assessed

Stoichiometric Compound	*Molar Volume Status*
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

Stoichiometric Compound	*Molar Volume Status*
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	*Molar Volume 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

Stoichiometric Compound	*Molar Volume Status*
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

Stoichiometric Compound	*Molar Volume Status*
ZR13NB4O36	Estimated
ZR15NB4O40	Estimated
ZR2P2O9	Assessed
ZR3Y4O12	Assessed
ZR5NB2O15	Estimated
ZR6NB2O17	Estimated
ZR7NB2O19	Estimated
ZR8NB2O21	Estimated
ZRF4	Assessed
ZRO8S2	Assessed
ZRS2	Assessed
ZRTI2O6	Assessed
ZRTIO4_ALPHA	Estimated

TCOX11 Properties Data and Assessed Systems

You can find information on our website about the thermophysical 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.

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.

In this section:

TCOX11 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 TCOX11, 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

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.

Unary Assessed Systems

The ^{E} subscript indicates a system is estimated based on other predictions and data of ternaries.

Al_2O_3

CaF_2, CaO^E, CaS^E, $Cr_2O_3^E$, CuO_x

FeO_x

$Gd_2O_3^E$

K_2O

$La_2O_3^E$

MgO, MnO, MoO_2^E, MoO_3^E

Na_2O, NbO^E, $Nb_2O_5^E$, NiO

P_2O_5

SiO_2

TiO_2

V_2O_5

Y_2O_3[E]

ZrO_2[E]

Binary Assessed Systems

Al_2O_3-Gd_2O_3, Al_2O_3-La_2O_3, Al_2O_3-Na_2O, Al_2O_3-SiO_2

CaF_2-Al_2O_3, CaF_2-MgO, CaF_2-SiO_2, CaF_2-TiO_2, CaF_2-V_2O_5, CaO-Al_2O_3, CaO-P_2O_5

CaO-SiO_2, Cu_xO-SiO_2

Fe_xO-Na_2O, Fe_xO-TiO_2, Fe_xO-CaO, Fe_xO-SiO_2

K_2O-FeO_x, K_2O-Al_2O_3, K_2O-SiO_2

MgO-Al_2O_3, MgO-SiO_2, MnO-SiO_2, MnO-TiO_2

Na_2O-P_2O_5, Na_2O-SiO_2, Na_2O-V_2O_5, NiO-SiO_2

Ternary Assessed Systems

Al_2O_3-MgO-SiO_2

CaF_2-Al_2O_3-TiO_2, CaF_2-Al_2O_3-V_2O_5, CaF_2-CaO-Al_2O_3, CaF_2-CaO-Cr_2O_3,

CaF_2,-CaO-SiO_2, CaO-Al_2O_3-SiO_2, CaO-Al_2O_3-ZrO_2, CaO-CaS-SiO_2

CaO-Cr_2O_3-SiO_2, CaO-MgO-SiO_2, CaO-NiO-SiO_2, CaO-SiO_2-Cr_2O_3

CaO-SiO_2-TiO_2, Cu_xO-Al_2O_3-SiO_2

Fe_2O_3-Na_2O-SiO_2, Fe_2O_3-Al_2O_3-SiO_2, Fe_xO-CaO-Al_2O_3, Fe_xO-CaO-SiO_2

Fe_xO-MgO-SiO_2

K_2O-FeO_x-SiO_2, K_2O-Al_2O_3-SiO_2, K_2O-Na_2O-SiO_2

MnO-SiO_2-TiO_2

Na_2O-Al_2O_3-SiO_2, Na_2O-CaO-SiO_2, Na_2O-MgO-SiO_2, MgO-SiO_2-TiO_2

TCOX11 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. Below is the list of the status of the systems and phases that the estimated ones are marked with a subscript of E, otherwise they are assessed.

Also see TCOX11 Stoichiometric Compounds.

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.

Liquid Solution Phases

Unary Systems

CaO, MgO, Al_2O_3, SiO_2, MnO ^{E}, FeO, Fe_2O_3, CaF_2, MgF_2, TiO_2, K_2O, Cr_2O_3 ^{E}, V_2O_5 ^{E}, ZrO_2 ^{E}, P_2O_5 ^{E}, Nb_2O_5 ^{E}, NiO ^{E}, WO_3 ^{E}, La_2O_3 ^{E}, CoO ^{E}, MoO_3 ^{E} and CaS ^{E}

Binary Systems

Al_2O_3-CaO, Al_2O_3-MgO, Al_2O_3-SiO_2, CaF_2-Al_2O_3, CaF_2-CaO, CaF_2-MgO, CaF_2-MgF_2, CaF_2-SiO_2, CaF_2-TiO_2, CaO-SiO_2, Fe_xO-CaO, Fe_xO-SiO_2, K_2O-SiO_2, MgO-SiO_2, MnO-SiO_2

Ternary Systems

Al_2O_3-MgO-SiO_2, Al_2O_3-TiO_2-SiO_2, CaF_2-Al_2O_3-TiO_2, CaF_2-CaO-Al_2O_3, CaF_2-CaO-SiO_2, CaF_2-MgO-Al_2O_3, CaO-Al_2O_3-SiO_2, CaO-Al_2O_3-TiO_2, CaO-MgO-Al_2O_3, CaO-MgO-SiO_2, CaO-MnO-SiO_2, CaO-SiO_2-TiO_2, Fe_xO-Al_2O_3-SiO_2, Fe_xO-CaO-Al_2O_3, Fe_xO-CaO-MgO, Fe_xO-CaO-SiO_2, Fe_xO-MgO-SiO_2, Fe_xO-MnO-SiO_2

Quaternary and Quinary Systems

CaF_2-Al_2O_3-MgO-SiO_2, CaF_2-CaO-MgO-Al_2O_3, CaO-Al_2O_3-MnO-SiO_2, CaO-MgO-Al_2O_3-SiO_2, Fe_xO-CaO-Al_2O_3-SiO_2, Fe_xO-CaO-MgO-SiO_2, Fe_xO-CaO-MgO-Al_2O_3-SiO_2, Fe_xO-CaO-MnO-SiO_2

Alloy Phases

BCC_A2

Al, Ca ^{E}, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, P, S, Si, Ti, V, W, Y, Zr

Al-C, C-Ca [E], C-Co, C-Cr, C-Cu, C-Fe, C-Gd, C-Mg, C-Mn, C-Mo, C-Nb, C-Ni, C-P, C-S, C-Si, C-Ti, C-V, C-W, C-Y [E], C-Zr [E], Ca-O [E], Co-O, Cr-O [E], Cu-O, Fe-O [E], Gd-O [E], La-O [E], Mg-O, Mn-O, Ni-O [E], Ni-Ti, Ni-V, O-P [E], O-S, O-Si [E], O-Ti [E], O-V [E], O-W [E], O-Y [E], O-Zr [E], Ti-Zr

FCC_A1

Al, Ca, Co, Cr, Cu, Fe, Mg, Mo, Nb, Ni, P, S, Si, Ti, V, W, Zr

Al-C, Al-O [E], C-Ca [E], C-Co, C-Cr, C-Cu, C-Fe, C-Gd, C-Mg, C-Mn, C-Mo, C-Nb, C-Ni, C-P, C-S, C-Si, C-Ti, C-V, C-W, C-Y [E], C-Zr, Ca-O [E], Co-O [E], Cr-O [E], Cu-O [E], Fe-O [E], Gd-O [E], La-O [E], Mg-O, Mn-Ni, Mn-O, Mo-O, Nb-O, Ni-O [E], Ni-Si, Ni-Ti, Ni-V, Ni-W, O-P [E], O-S, O-Si [E], O-Ti [E], O-V [E], O-W, O-Y [E], O-Zr [E]

HCP_A3

Al, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, Si, Ti, V, W, Y, Zr

Al-C, Al-O [E], C-Ca [E], C-Co, C-Cr,C-Cu [E], Fe-C, C-Gd [E], C-Mg [E], C-Mn [E], C-Mo, C-Nb, C-Ni [E], C-Si [E], C-Ti, C-V, C-W, C-Y [E], C-Zr, Ca-O [E], Cr-O [E], Cu-O [E], Fe-O [E], Gd-O [E], La-O [E], Mn-O [E], Mo-O [E], Nb-O [E], Ni-O [E], O-Si [E], O-Ti [E], O-V [E], O-W [E], O-Y [E], O-Zr [E]

DHCP

Al [E], Ca [E], Cu [E], Mg [E], Mn [E], Ni [E], Y [E]

Al-O [E], Cu-O [E], Gd-O [E], La-O [E]

CUB_A13

Al [E], Co [E], Cr [E], Cu [E], Fe [E], Mg [E], Mn, Mo [E], Nb [E], Ni [E], Si [E], Ti [E], V [E], Zr [E]

Al-C [E], C-Co [E], C-Cr [E], C-Cu [E], C-Mg [E], C-Mn [E], C-Mo [E], C-Nb [E], C-Ni [E], C-Si [E], C-Ti [E], C-V, C-Zr [E]

CBCC_A12

Al [E], Co [E], Cr [E], Cu [E], Fe [E], Mg [E], Mn, Mo [E], Nb [E], Ni [E], Si [E], Ti [E], V [E], Zr [E]

Al-C [E], C-Co [E], C-Cr [E], C-Cu [E], C-Mg [E], C-Mn [E], C-Mo [E], C-Nb [E], C-Ni [E], C-Si [E], C-Ti [E], C-V, C-Zr [E]

DIAMOND_FCC_A4

Al [E], C [E], P [E], Al-O, O-P [E]

Solid Solution Phases

Anorthite

Al-Ca-O-Si, Al-Na-O-Si

Alabandite

Ca-S, Co-S, Cr-S, Cu-S, Fe-S, Gd-S, La-S, Mg-S, Mn-S, S-Y [E], S-Zr

$AlPO_4$

Al-O-P

Anhydrite

Ca-O-S, Co-O-S, Cu-O-S, Fe-O-S, Mg-O-S, Mn-O-S, Ni-O-S

Apatite

Gd-O-Si, O-Si-Y [E]

Bronze

Ca-O-V, Fe-O-V [E]

Calcium Ferro-aluminates

C3A1: Al-Ca-O, Ca-Fe-O [E]

C12A7: Al-Ca-O [E]

C1A1: Al-Ca-O

C1A2: Al-Ca-O

C1A6: Al-Ca-O

C2F: Al-Ca-O, Ca-Fe-O

$Ca_3P_2O_8$ (α and β)

Ca-O-P, Ca-O-Si [E], Mg-O-P

$Ca_2P_2O_7$ (α, β and γ)

Ca-O-P, Mg-O-P

Ca_2SiO_4 (α and α')

Ca-O-P, Ca-O-Si, Fe-O-P, Gd-O-Si [E], Mg-O-P, Mn-O-P, O-Si-Y [E]

$Ca_3S_3Fe_4O_x$

Ca-Fe-S [E], Ca-Fe-S-O (not assessed)

$Ca_4Nb_2O_9$_HT11

Ca-Nb-O [E]

$Ca_4Nb_2O_9$_LT21

Ca-O, Ca-Nb-O [E]

$Ca_3Co_2O_6$

Ca-Co [E], Ca-Cu [E], Ca-Co-O, Ca-Cu-O [E]

$Ca_3Co_4O_9$

This is $Ca_3Co_4O_9$ dissolving Cu.

Ca-Co [E], Ca-Cu [E], Ca-Co-O [E], Ca-Cu-O [E]

$CaCr_2O_4$_A

Al-Ca-O [E], Ca-Cr-O [E], Ca-Fe-O

CaF_2_S1

Ca [E], Mg [E], Ca-F

CaF_2_S2

Ca [E], Cu [E], Mg [E], Ca-F

$CaMO_3$

O-Y [E], Ca-Mn-O, Ca-O-Ti, Ca-O-Y, Ca-O-Zr, Mn-O-Y, O-Ti-Y, O-Y-Zr

Carnegieite (α and β)

Al-Na-O-Si, Fe-Na-O-Si

CaSFeO

Ca-Fe-S [E]

$CaSO_4$_HT

Ca-O-S, Co-O-S, Mg-O-S

CaV_2O_4

Al-Ca-O, Ca-Cr-O, Ca-Fe-O, Ca-O-V, Ca-O-Y

CaV_2O_6

Ca-O-V, Co-O-V, Mg-O-V, Mn-O-V, Ni-O-V

CaY_4O_7

Ca-Gd-O, Ca-O-Y [E]

$CaZrO_3$_C

O-Y [E], Ca-O-Y, Ca-O-Zr

Chalcopyrite

S [E], Cu-S, Fe-S [E], Cu-Fe-S

Co_9S_8

Co-S [E], Fe-S [E], Ni-S [E], Co-Mg,

Columbite

Fe E, Ca-Fe [E], Ca-Mg [E], Ca-Nb [E], Co-Fe, Co-Mg, Co-Nb, Ca-Fe-O [E], Co-Mg-O [E], Co-Nb-O, Fe-Mg-O [E], Fe-Nb-O, Mg-Mn-O [E], Mg-Nb-O, Mn-Nb-O

Cordierite

Al-Fe-O-Si, Al-Mg-O-Si, Al-Mn-O-Si

Corundum

Al-O, Co-O, Cr-O, Fe-O, Mg-O, Mn-O, Ni-O, O-Ti, O-V

Al-Cr-O, Al-Fe-O [E], Al-Ni-O [E], Cr-Fe-O, Cr-Mn-O [E], Cr-O-Ti [E], Cr-O-V [E], Fe-Mn-O [E], Fe-Ni-O [E], Fe-O-Ti [E], Fe-O-V [E]

Cr_2S_3

Cr-S, Fe-S

Cr_3S_4

Cr-S, Fe-S, Mn-S [E]

$CrNbO_4$

Cr, Nb, Cr-Nb, Cr-O, Nb-O [E], Cr-Nb-O [E]

$Cr_2P_4O_{13}$

Cr-O-P [E], Cr-O-V [E], Fe-O-P [E], Fe-O-V

$Cr_2Ti_2O_7$

Al-O-Ti [E], Cr-O-Ti [E], Fe-O-Ti [E]

CuF_2

Cr-F, Cu-F

$CuLa_2O_4$

Co-La-O, Cu-La-O

CuP_2O_6

Co-O-P, Cu-O-P [E], Ni-O-P

CuO

Cu-O, Co-O, Co-Cu-O

Cuprite

Cu-O, Na-O

Cristobalite

O-Si, Al-O-P

Delafossite

Al-Cu-O, Cr-Cu-O, Cu-Fe-O, Cu-Mn-O, Cu-O-Y

Digenite

Cu-S, Fe-S, Mg-S [E], Mn-S, Cu-Fe-S [E], Cu-Mg-S [E], Cu-Mn-S

$DyMn_2O_5$

Gd-Mn-O, Mn-O-Y

FeF_3

Al-F, Co-F, Cr-F, F-Fe

$Fe_2O_{12}S_3$

Al-O-S, Cr-O-S, Fe-O-S

$FeNb_{14}O_{36}$

Co-Nb-O [E], Fe-Nb-O [E]

$FeNb_{36}O_{91}$

Co-Nb-O [E], Fe-Nb-O [E]

$FeNb_{68}O_{171}$

Co-Nb-O [E], Fe-Nb-O [E]

$FePO_4$

Fe-O-P, Mn-O-P

$FeVO_4$

Al-O-V, Fe-O-V

Fluorite

Al [E], Ca [E], Cr [E], Fe [E], Mg [E], Mn [E], Ni [E], Si [E], Y [E], Zr [E]

Al-O [E], Ca-O, Cr-O, Gd-O [E], La-O [E], O-Y [E], O-Zr

Garnet

Al-Ca-O-Si

GdF_3

F-Gd, F-Y

$Gd_2Si_2O_7$

Gd-O-Si, La-O-Si

Gd_2SiO_5

Gd-O-Si, La-O-Si

Halite

O [E], Al-O [E], Ca-O, Co-O, Cr-O [E], Cu-O [E], Fe-O [E], Gd-O [E], Mg-O, Mn-O, Na-O, Ni-O, Ti-O, V-O [E]

Ca-Mn-O, Fe-Mg-O, Fe-Ni-O

Hatrurite

Ca-O-Si, Gd-O-Si [E], O-Si-Y [E]

β1-Heazlewoodite

S [E], Co-S, Fe-S [E], Ni-S [E],

β2-Heazlewoodite

S [E], Fe-S [E], Ni-S [E],

LaF_3

F-Gd, F-La, F-Y

La_2S_3

Gd-S, La-S

La_2MnO_4

Co-La-O, La-Mn-O [E], La-Ni-O

$La_3Ni_2O_7$

La-Ni-O

$La_4Ni_3O_{10}$

La-Ni-O

LaAP

Al-Ca-O, Al-La-O, Al-O-Y, Ca-Co-O, Ca-Cu-O, Ca-Fe-O, Ca-Ni-O, Co-La-O, Co-O-Y, Cu-La-O, Cu-O-Y, Fe-La-O, Fe-O-Y, La-Ni-O, Ni-O-Y,

LaYP

La-O, Y-O, La-O-Y

α-M_2O_3

Gd-O, La-O, Y-O, Zr-O [E]

β-M_2O_3

Al-O, Ca-O, Co-O, Gd-O, La-O, Y-O, Zr-O [E]

c-M_2O_3

Al-O [E], Ca-O, Co-O, Cr-O, Fe-O [E], Gd-O [E], La-O [E], Mn-O [E], Ni-O [E], Y-O, Zr-O [E]

h-M_2O_3

Ca-O, Gd-O, La-O, Y-O [E], Zr-O [E]

x-M_2O_3

Ca-O, Gd-O, La-O, Y-O, Zr-O [E]

M_4O_7

Ti-O, V-O, Al-O-V [E], Mn-O-V [E]

M_6O_{11}

Ti-O, V-O

M_7O_{13}

Ti-O, V-O

MgF_2

Co-F, F-Fe, F-Mg, F-Mn, F-Ni, F-V

$Mg_2P_2O_7$ (α and β)

Ca-O-P, Mg-O-P

$Mg_2V_2O_7$

Co-O-V [E], Mg-O-V, Ni-O-V [E]

$Mg_3P_2O_8$

Ca-O-P, Mg-O-P

$Mg_3V_2O_8$

Co-O-V, Mg-O-V, Ni-O-V

$MgWO_4$-type

Al-Nb-O, Al-O-W, Co-Nb-O, Co-O-W, Fe-Nb-O, Fe-O-W, Mg-Nb-O, Mg-O-W, Mn-Nb-O, Mn-O-W, Nb-Ni-O, Nb-O-W, Ni-O-W

$Mn_4Nb_2O_9$

Co-Nb-O, Fe-Nb-O [E], Mg-Nb-O, Mn-Nb-O

MoS_2

Mo-S [E], S-W [E]

Mullite

Al-O-Si [E]

$NaAl_{11}O_{17}$

Al-Na-O

$Na_2Al_{12}O_{19}$

Al-Na-O [E]

α-$NaFeO_2$

Cr-Na-O, Fe-Na-O

β-$NaFeO_2$

O-Si, Al-Na-O, Fe-Na-O

γ-$NaFeO_2$

O-Si, Al-Na-O, Fe-Na-O

δ-$NaAlO_2$

Al-Na-O, Al-Na-O-Si

NbO_2

Nb-O

Nb_2O_5

Mg-O [E], Nb-O, V-O [E]

Nepheline (α and β)

Na-Al-Si-O

γ-Nepheline

Na-Al-Si-O, Na-Fe-Si-O

Ni_6MnO_8-type

Mg-Mn-O, Mn-Ni-O [E]

Ni_7S_6

Fe-S [E], Ni-S [E]

Ni_9S_8

Fe-S [E], Ni-S [E]

$NiMnO_3$

Mn-O [E], Ni-O [E]

$NiNb_2O_6$

Nb-Ni-O

Olivine

Ca-O-Si, Co-O-Si, Cr-O-Si, Cu-O-Si E, Fe-O-Si, Mg-O-Si, Mn-O-Si, Ni-O-Si

Pentlandite

Fe-S E, Ni-S E, Fe-Ni-S

Perovskite

Co-La, Co-Mn, Co-O, Cr-La, Cr-Mn, Cr-O, Fe-La, La-O, Co-La-O, Cr-La-O, Fe-La-O, La-Mn-O

Pseudo-brookite

Al-O-Ti, Al-O-V, Co-O-Ti, Mg-O-Ti, Mn-O-Ti [E], Ni-O-Ti [E]

Pyrite

Co-S, Fe-S, Mn-S, Ni-S, Cu-Fe-S

Pyrochlore

Gd-O, La-O, Zr-O, Gd-La-O [E], Gd-O-Ti (partly assessed), Gd-O-Y [E], Gd-O-Zr [E], La-O-Ti (partly assessed), La-O-Y[E], La-O-Zr [E], O-Ti-Y (partly assessed), O-Ti-Zr [E], O-Y-Zr (partly assessed)

Pyroxenes

Low clino-pyroxene: Mg-O-Si

Clino-pyroxene: Fe-O-Si, Mg-O-Si, Ni-O-Si, Ca-Mg-O-Si

Ortho-pyroxene: Fe-O-Si, Mg-O-Si, Ca-Mg-O-Si

Proto-pyroxene: Ca-O-Si, Co-O-Si, Cr-O-Si, Fe-O-Si, Mg-O-Si, Ni-O-Si

Pyrrhotite

Al-S [E], Co-S, Cr-S, Cu-S, Fe-S, Gd-S, Mg-S [E], Mn-S, Nb-S [E], Ni-S, S-Ti, S-V [E], S-Zr,

Quartz

O-Si, Al-O-P

Rhodonite

Ca-O-Si, Co-O-Si, Fe-O-Si, Mg-O-Si, Mn-O-Si

Rutile

Mn-O, O-Ti, O-Zr, Al-O-Ti

α-Spinel

Co-O [E], Cu-O[E], Mn-O [E], Ni-O [E]

Al-Co-O [E], Al-Cu-O, Al-Mn-O [E], Al-Ni-O, Co-Cr-O [E], Co-Fe-O [E], Co-Mn-O [E], Cr-Cu-O, Cr-Mg-O [E], Cr-Mn-O [E], Cr-Ni-O [E], Cu-Fe-O [E], Cu-Mn-O [E], Fe-Mg-O [E], Fe-Mn-O [E], Fe-Ni-O [E], Mg-Mn-O [E], Ni-Mn-O [E]

Spinel

Al-O, Co-O [E], Cr-O [E], Cu-O, Fe-O [E], Mg-O [E], Mn-O [E], Ni-O [E]

Al-Co-O [E], Al-Cr-O [E], Al-Cu-O, Al-Fe-O [E], Al-Mn-O [E], Al-Ni-O, Al-O-Ti, Al-O-V, Ca-Co-O, Ca-Cr-O, Ca-Cu-O, Ca-Fe-O, Ca-Mg-O, Ca-Ni-O, Co-Cr-O [E], Co-Cu-O, Co-Fe-O [E], Co-Mg-O [E], Co-Mn-O [E], Co-Mo-O, Co-Ni-O, Co-O-Ti, Cr-Cu-O, Cr-Fe-O [E], Cr-Mg-O [E], Cr-Mn-O [E], Cr-Mo-O, Cr-Ni-O [E], Cr-O-Ti [E], Cr-O-V [E], Cu-Fe-O [E], Cu-Mg-O [E], Cu-Mn-O [E], Cu-Mo-O, Cu-Ni-O, Cu-O-Ti [E], Cu-O-V [E], Fe-Mg-O [E], Fe-Mn-O [E], Fe-Mo-O [E], Fe-Ni-O [E], Fe-O-Ti [E], Fe-O-V [E], Mg-Mn-O [E], Mg-Mo-O [E], Mg-Ni-O [E], Mg-O-Ti, Mg-O-V, Mn-Mo-O, Mn-Ni-O [E], Mn-O-Ti, Mn-O-V, Mo-Ni-O, Ni-O-Ti, Ni-O-V

Thio-spinel

Co-S, Ni-S

Co-Cr-S, Co-Cu-S, Co-Fe-S, Co-Mn-S, Co-Ni-S, Cr-Cu-S, Cr-Fe-S, Cr-Mn-S, Cr-Ni-S, Cu-Ni-S [E], Fe-Ni-S, Mn-Ni-S,

Ti_5O_9

O-Ti, O-V

Tridymite

O-Si, Al-O-P

V_2O_SS

O-V [E]

V_3O_5-HT

O-Ti, O-V, Al-O-V [E], Cr-O-V

V_5O_9

O-Ti, O-V

VO_2-LT

O-V, O-W

Wollastonite

Ca-O-Si, Fe-O-Si, Mg-O-Si, Mn-O-Si

YAG

Al-Gd-O [E], Al-La-O [E], Al-O-Y, Cr-Gd-O [E], Cr-La-O [E], Cr-O-Y [E], Fe-Gd-O [E], Fe-La-O [E], Fe-O-Y

YAM

Al-Gd-O [E], Al-La-O [E], Al-O-Y [E], Ca-O-Si, Gd-O-Si, La-O-Si, O-Si-Y

YAP

Al-Ca, Al-Gd, Al-La, Al-Y, Ca-Co, Ca-Cr, Ca-Fe, Ca-Mn [E], Co-Gd, Co-La, Co-Y, Cr-Gd, Cr-La, Cr-Y, Fe-Gd [E], Fe-La

Al-Gd-O, Al-La-O, Al-O-Y, Ca-Co-O, Ca-Cr-O, Ca-Fe-O, Co-Gd-O, Co-La-O, Co-O-Y, Cr-Gd-O, Cr-La-O, Cr-Y-O, Fe-Gd-O, Fe-La-O, Fe-O-Y, Gd-Mn-O, La-Mn-O, Mn-O-Y,

Y_2TiO_5

Gd-Ti-O, La-Ti-O, Y-Ti-O

Y_3NbO_7

Nb-O-Y

$YNbO_4$

Nb-O-Y

Zircon

Gd-Si, Gd-O-P, Gd-O-Si, O-P-Y, O-Si-Y [E], O-Si-Zr

m-ZrO_2

Al-O [E], Ca-O, Cr-O, Gd-O [E], La-O [E], Y-O [E], O-Zr

t-ZrO_2

Ca-O, Cr-O, Gd-O [E], La-O [E], Y-O [E], O-Zr,

β-$ZrTiO_4$

O-Ti-Zr

TCOX11 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

Al_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

Pseudo Binary Assessed Systems

Al_2O_3-CaF_2, Al_2O_3-CaO, Al_2O_3-Cr_2O_3, Al_2O_3-MgO, Al_2O_3-SiO_2, Al_2O_3-TiO_2

CaF_2-CaO, CaF_2-MgO, CaF_2-SiO_2, CaF_2-TiO_2, CaF_2-V_2O_5

CaO-FeO_x, CaO-CuO_x, CaO-P_2O_5, CaO-SiO_2, CaO-V_2O_5,

FeO_x-MnO, FeO_x-Na_2O, FeO_x-P_2O_5, FeO_x-SiO_2, FeO_x-TiO_2,

K_2O-SiO_2, MgO-SiO_2, MnO-SiO_2, Na_2O-SiO_2

Pseudo Ternary Assessed Systems

Al_2O_3-CaF_2-CaO, Al_2O_3-CaF_2-MgO, Al_2O_3-CaF_2-TiO_2, Al_2O_3-CaF_2-V_2O_5, Al_2O_3-CaO-Cr_2O_3, Al_2O_3-CaO-Fe_2O_3, Al_2O_3-CaO-Na_2O, Al_2O_3-CaO-MgO, Al_2O_3-CaO-SiO_2, Al_2O_3-CaO-TiO_2, Al_2O_3-CaO-V_2O_5, Al_2O_3-CaO-ZrO_2, Al_2O_3-FeO_x-SiO_2, Al_2O_3-MgO-SiO_2, Al_2O_3-MnO-SiO_2, Al_2O_3-Na_2O-SiO_2, Al_2O_3-SiO_2-TiO_2

CaF_2-CaO-SiO_2, CaO-CaS-SiO_2, CaO-Cr_2O_3-SiO_2, CaO-FeO_x-SiO_2, CaO-MgO-SiO_2, CaO-MnO-SiO_2, CaO-Na_2O-SiO_2, CaO-P_2O_5-SiO_2, CaO-SiO_2-V_2O_5

FeO_x-MgO-SiO_2, FeO_x-MnO-SiO_2, K_2O-CaO-Al_2O_3, MgO-Na_2O-SiO_2

Pseudo Quaternary Ternary Assessed Systems

Al_2O_3-CaF_2-CaO-SiO_2, Al_2O_3-CaF_2-CaO-V_2O_5, Al_2O_3-CaF_2-MgO-SiO_2, Al_2O_3-CaF_2-K_2O-SiO_2, Al_2O_3-CaO-MnO-SiO_2, Al_2O_3-CaO-Na_2O-SiO_2, Al_2O_3-CaO-SiO_2-TiO_2, CaO-MgO-Al_2O_3-SiO_2, CaO-MgO-Na_2O-SiO_2, FeO_x-CaO-Al_2O_3-SiO_2, FeO_x-CaO-MgO-SiO_2, FeO_x-MgO-Al_2O_3-SiO_2

TCS Metal Oxide Solutions Database (TCOX) Revision History

Current Database Version

Database name (acronym):	**TCS Metal Oxide Solutions Database (TCOX)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**11.1**
First release:	**TCOX was released in 1992 under the name ION**

Changes in the Most Recent Database Release

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.

Previous Releases

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, H2, C1H4 and H2O 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.