Thermo-Calc Software

TCS Metal Oxide Solutions Database (TCOX10)

Thermo-Calc Version 2020b

Technical Information

Contents

About the TCS Metal Oxide Solutions Database (TCOX)

Current Database Version

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 and viscosity for ionic liquids.

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).

Intermetallic compounds and carbides are not included in the database.

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 in some cases, important higher order systems which 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.

CALPHAD is originally an abbreviation for *CALculation of PHAse Diagrams*, but was later expanded to refer to *computer coupling of phase diagrams and thermochemistry*. More about the CALPHAD methodology, including some of its history, is available on the Thermo-Calc Software website.

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 this 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.

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 *TCOX: TCS Metal Oxide Solutions Database 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 and molar volume), and summaries of the database revision history by version.
- The *TCOX: TCS Metal Oxide Solutions Database 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.
- Process Metallurgy on the Thermo-Calc website has a variety of information related to the use of this database with the Process Metallurgy Module.

TCOX10 Elements, Systems, and Phases

Included Elements

There are 28 elements included in the most recent version of the database.

Al	Ar*	C	Ca	Co	Cr	Cu	F	Fe	Gd
H*	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:

- 288 binary and 283 ternary systems to the full range of composition and temperature in the 28 element framework.
- 126 pseudo-ternary oxide systems, 32 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.

Molar Volume

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

Assessed Phases

The most recent version of the database contains 449 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 [1985, Hillert; 1991, Sundman].

> 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 their compositions.

Common Phases for the TCOX Database

Molar Volume

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

Other Phases

The TCOX10 database also contains solid oxides, silicates, fluorides and sulfides, 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) [2001, Hillert].

References

[1985, Hillert] 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.

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

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

TCOX10 Systems

In this section:

TCOX10 Assessed Metallic Systems

No intermetallic phases 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.

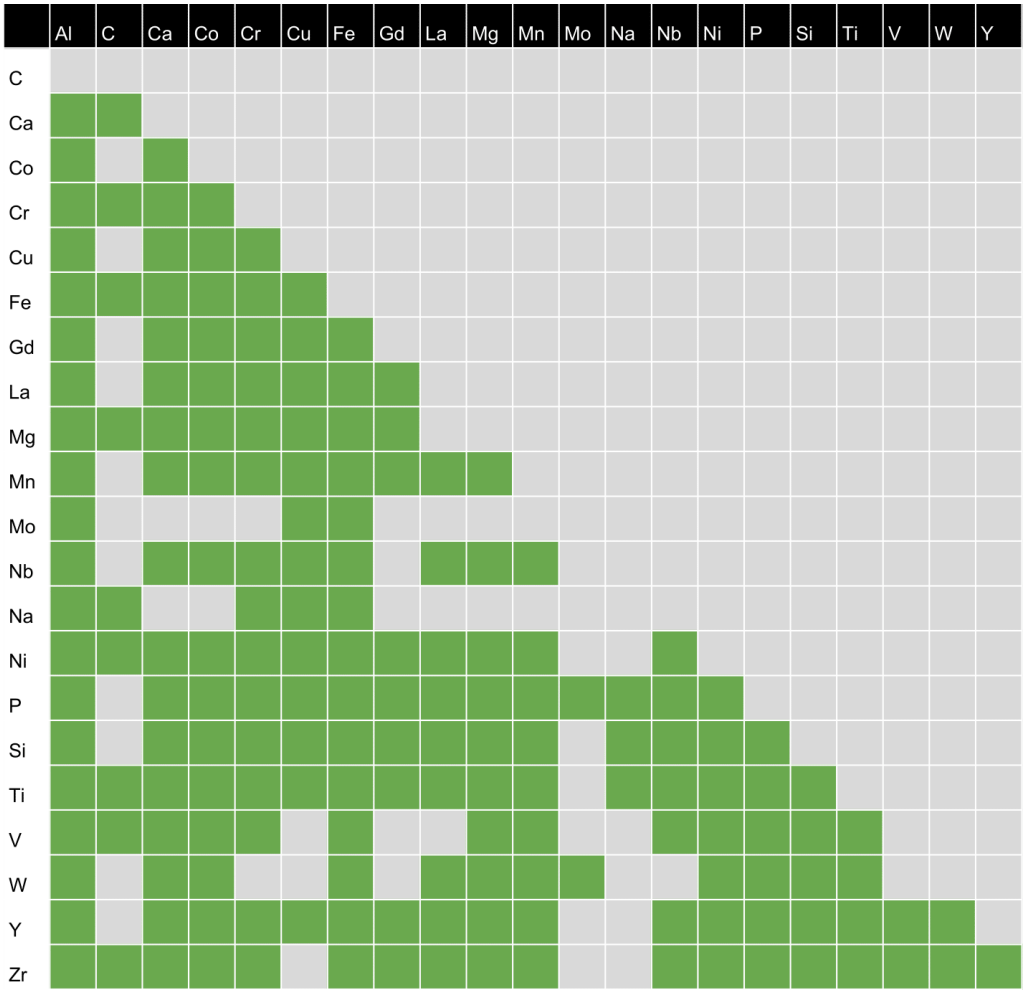
TCOX10 Assessed Oxide Systems

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	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-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-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-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-Zr	Al-O-Y-Zr
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-Mg-Mn-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-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-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	La-O-Y-Zr	Mg-Mn-O-Si	Mg-Mn-O-Ti	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		

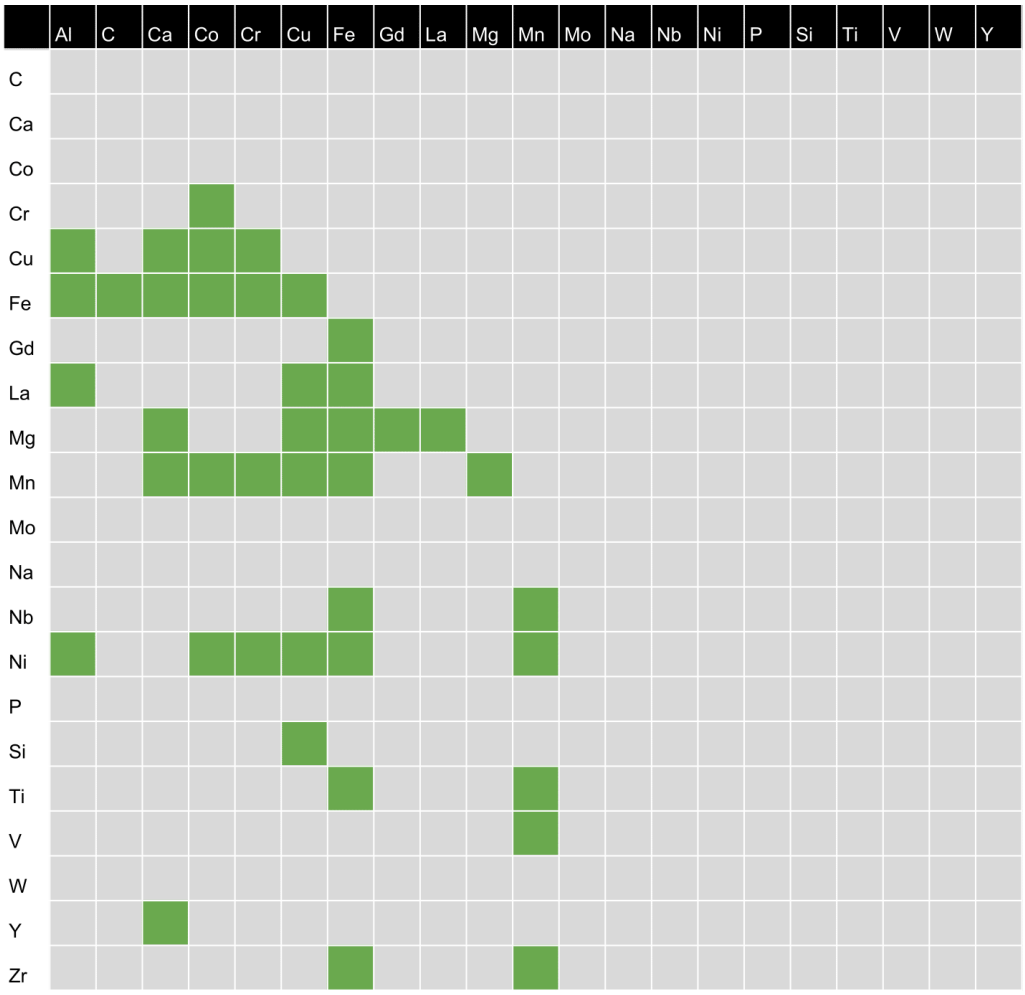
TCOX10 Assessed Sulfide Systems

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
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
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				

TCOX10 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	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-Mg	Al-F-Zr	Ca-Co-F	Ca-Cr-F	Ca-Fe-F	Ca-F-Gd
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-La-Zr	F-Mg-La	F-Mg-Y	

Assessed Oxy-fluoride Systems

Al-F-O	Ca-F-O	Co-F-O	F-Mg-O	Al-Ca-F-O	Ca-F-Mg-O
Ca-Fe-F-O	Ca-F-O-P	Ca-F-O-Si	F-Mg-O-Si	Al-Ca-F-Mg-O	Al-Ca-F-O-Si

TCOX10 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 (Al2O3), Eskolaite (Cr2O3), Hematite (Fe2O3), Karelianite (V2O3), Tistarite (Ti2O3), CoTiO3, Ilmenite (FeTiO3), Geikielite (MgTiO3), Pyrophanite (MnTiO3), NiTiO3. The ilmenite ((Co,Fe,Mg,Mn,Ni)TiO3) 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 modelled.
HALITE	Lime (CaO), CoO, Wustite (FeO), Periclase (MgO), Manganosite (MnO), Bunsenite (NiO).
ALABANDITE	Alabandite (MnS), Oldhamite (CaS), MgS, GdS, LaS, ZrS.
GARNET	Grossular (Ca3Al2(SiO4)3), Uvarovite (Ca3Cr2(SiO4)3), Spessartine (Mn3Al2(SiO4)3), Goldmanite (Ca3V3 (SiO4)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 La2O3 and Gd2O3 modifications.
M2O3B	This is monoclinic Gd2O3.
M2O3C	This is Bixbyite (Mn2O3) and cubic Gd2O3 and Y2O3.
M2O3H	This is hexagonal La2O3, Gd2O3 and Y2O3.
M2O3X	This is x-La2O3 and high-temperature cubic Gd2O3.
MELILITE	Gehlenite (Ca2Al2SiO7), Fe-Gehlenite (Ca2Fe2SiO7), Åkermanite (Ca2MgSi2O7), Fe-Åkermanite (Ca2FeSi2O7) and CaCoSi2O7.
OLIVINE	Calcio-olivine (Ca2SiO4), Co2SiO4, Fayalite (Fe2SiO4), Forsterite (Mg2SiO4), Tephroite (Mn2SiO4), Ni2SiO4, Kirschsteinite (CaFeSiO4), Monitcellite (CaMgSiO4), Glaucochroite (CaMnSiO4), Liebenbergite (Ni2SiO4)
PSEUDO_ BROOKITE	Pseudobrookite (Fe2TiO5), Karrooite (MgTi2O5), Ti3O5, Al2TiO5, CoTi2O5, Armalcolite ((Fe,Mg)Ti2O5), MnTi2O5.
LOWCLINO_ PYROXENE	Low clino-enstatite (MgSiO3), low clino-diopside (CaMgSi2O6).
CLINO_ PYROXENE	Clino-enstatite (MgSiO3), clino-ferrosilite (FeSiO3), diopside (CaMgSi2O6), Niopside (CaNiSi2O6), Pigeonite ((Mg,Fe,Ca)Si2O6), Hedenbergite (CaFeSi2O6).

Name in the Database	*Common Name and Description*
ORTHO_ PYROXENE	Enstatite (MgSiO3), ortho-Diopside (CaMgSi2O6).
PROTO_ PYROXENE	Proto-enstatite (MgSiO3), proto-diopside (CaMgSi2O6).
PYRRHOTITE	Pyrrhoitite (FeS), CoS, CrS, NbS, NiS, TiS, VS.
RUTILE	Rutile (TiO2), Pyrolusite (MnO2), high-temperature VO2.
ALPHA_ SPINEL	Tetragonal Hausmannite (Mn3O4).
SPINEL	The cubic AB2O4-type spinel. Many end-members, solid solutions and combinations are described in the SPINEL phase: Magnetite (Fe3O4), cubic Hausmannite (Mn3O4), Guite (Co3O4), Spinel (MgAl2O4), Cuprospinel (CrFe2O4), Chromite (FeCr2O4), Hercynite (FeAl2O4), Coulsonite (FeV2O4), Vuorelainenite (MnV2O4), Magnesiocoulsonite (MgV2O4), CoV2O4, NiV2O4, Galaxite (MnAl2O4), Jacobsite (MnFe2O4), Magnesiochromite (MgCr2O4), Magnesioferrite (MgFe2O4), Manganochromite (MnCr2O4), Thermaerogenite (CuAl2O4), Ulvöspinel (TiFe2O4), Trevorite (NiFe2O4), NiAl2O4, CoAl2O4, CoFe2O4, FeCo2O4, CoMn2O4, CuMn2O4, MgMn2O4, NiMn2O4, Co2TiO4, Mg2TiO4, MgTi2O4, MnTi2O4, Mn2TiO4, Ni2TiO4.
ZIRCON	Zircon (ZrSiO4), Xenotime (YPO4), GdPO4, LaPO4.

TCOX10 Liquid Solution Phases

The liquid phase contains all elements in the TCOX10 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:

$(Al^{+3}, Ca^{+2}, Co^{+2}, Cr^{+2}, Cu^{+1}, Fe^{+2}, Gd^{+3}, La^{+3}, Mg^{+2}, Mn^{+2}, Mo^{+4}, Na^{+1}, Nb^{+2}, Ni^{+2}, P^{+5}, Si^{+4}, Ti^{+2}, V^{+2}, W^{+6}, Y^{+3}, Zr^{+4})_P$ $(AlO_2^{-1}, CO_3^{-2}, F^{-1}, O^{-2}, PO_4^{-3}, S^{-2}, SiO_4^{-4}, SO_4^{-4}, Va, AlN, C, C_3S_2Z_{1/6}, CoF_3, CoO_{3/2}, CrF_3, CrO_{3/2}, CuF_2, CuO, FeF_3, FeO_{3/2}, M_3S_2Z_{1/6}, MnO_{3/2}, NbF_5, NbO_{5/2}, PO_{5/2}, S, SiO_2, TiO_{3/2}, TiO_2, VO_2, VO_{3/2}, VO_{5/2})_Q$

TCOX10 Alloy Phases

BCC_A2

Containing Al, Ca, Co, Cr, Cu, Fe, Gd, 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, 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 the two cubic oxides TiO and VO solid solutions.

HCP_A3

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

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, Fe, Mg, Mo, Nb, Ni, Si, Ti, V and Zr with C and N modeled interstitially.

CBCC_A12

α-Mn, containing Al, Co, Cr, 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, 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).

TCOX10 Gas Phase

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

TCOX10 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. 145 solutions are modeled in the database.

Anorthite

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

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

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.
- C1A1F2: 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.

$Ca_3P_2O_8$ (α and β)

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

$Ca_2P_2O_7$ (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.

$Ca_3S_3Fe_4O_x$

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 $Ca_3(Gd,Y)_2(SiO_4)_6$.

$Ca_4Nb_2O_9$_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.

$Ca_3Co_2O_6$

This is $Ca_3Co_2O_6$ dissolving Cu.

$Ca_3Co_4O_9$

This is $Ca_3Co_4O_9$ dissolving Cu.

$CaCr_2O_4$_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.

$Ca_3Mg_3P_4O_{16}$

This is $Ca_3Mg_3P_4O_{16}$.

$CaMO_3$

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

$Ca_5P_2SiO_{12}$

This is $Ca_5P_2SiO_{12}$.

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.

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_2S_3

This is Cr_2S_3 dissolving 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.

$Cr_2P_4O_{13}$

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

$Cr_2Ti_2O_7$

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

CuF_2

This is CrF_2 and low temperature CuF_2.

$CuLa_2O_4$

This is $CuLa_2O_4$ with solubility of Co.

CuP_2O_6

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

CuO

This is CuO with solubility of Co.

Cuprite

This is Cu_2O with solubility of Na.

Cristobalite

This is SiO_2 with solubility of $AlPO_4$.

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 $DyMn_2O_5$.

FeF_3

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

$Fe_2O_{12}S_3$

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

$FeNb_{14}O_{36}$

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 ($Ca_3V_2Si_3O_{12}$).

GdF_3

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

$Gd_2Si_2O_7$

This is $(Gd,La)_2Si_2O_7$.

Gd_2SiO_5

This is $(Gd,La)_2SiO_5$.

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.

LaF_3

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

La_2S_3

This is $(Gd,La)_2S_3$.

La_2MnO_4

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

$La_3Ni_2O_7$

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.

LaYP

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

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_4O_7

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

M_6O_{11}

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

M_7O_{13}

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

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 $Ca_2CoSi_2O_7$.

MgF_2

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

$Mg_2P_2O_7$ (α and β)

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

$Mg_2V_2O_7$

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

$Mg_3P_2O_8$

This is $Mg_3P_2O_8$ dissolving Ca.

$Mg_3V_2O_8$

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

$MgWO_4$-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.

$NaAl_{11}O_{17}$

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

$Na_2Al_{12}O_{19}$

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

α-$NaFeO_2$

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

β-$NaFeO_2$

This is low-temperature $NaAlO_2$ and mid-temperature $NaFeO_2$ with solubility of Si.

γ-$NaFeO_2$

This is mid-temperature $NaAlO_2$ and high-temperature $NaFeO_2$ with solubility of Si.

δ-$NaAlO_2$

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

$Na_2CaAl_4O_8$

This is $Na_2CaAl_4O_8$ solid solution.

NbO_2

This is NbO_2 dissolving Fe.

Nb_2O_5

This is Nb_2O_5 dissolving Mg and V.

Nepheline (α and β)

This is $NaAlSiO_4$ with solubility of Si.

γ-Nepheline

This is $NaAlSiO_4$ 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_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.

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.

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.

$YNbO_4$

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.

TCOX10 Stoichiometric Compounds

276 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 Molar Volume Assessed Systems and Phases.

Stoichiometric Compound	*Molar Volume Status*
ALBITE_LOW	Assessed
ALBITE_MONO	Assessed
AF	Assessed
AL2P6SI4O26	Unassessed
AL2S3	Assessed
AL2SIO4F	Assessed
AL3PO7	Estimated
ALF3_S2	Assessed
ALNB11O29	Estimated
ALNB49O124	Estimated
ALP3O9	Assessed
ANDALUSITE	Assessed
ANILITE	Assessed
C11A7F	Unassessed
C13A6Z2	Unassessed
C1A8M2	Unassessed
C2A14M2	Unassessed
C3A2M1	Unassessed
C3A3F	Unassessed
C4WF4	Assessed

Stoichiometric Compound	*Molar Volume Status*
C4WF8	Estimated
CA10P6O25	Estimated
CA10SI3O15F2	Unassessed
CA10V6O19	Estimated
CA15CU18O35	Estimated
CA2ALNBO6	Assessed
CA2CUO3	Assessed
CA2NB2O7	Assessed
CA2P6O17	Estimated
CA2V2O7	Assessed
CA2ZRSI4O12	Estimated
CA3COAL4O10	Assessed
CA3NB2O8	Estimated
CA3TI2O7	Assessed
CA3TI8AL12O37	Unassessed
CA3V2O8	Assessed
CA3WO6	Estimated
CA3ZRSI2O9	Assessed
CA4MG2P6O21	Unassessed
CA4P2O9_A	Assessed
CA4P2O9_B	Assessed
CA4P6O19	Estimated
CA4TI3O10	Assessed

Stoichiometric Compound	*Molar Volume Status*
CA4V2O9	Estimated
CA5SI2O8F2	Unassessed
CA6ZR19O44	Estimated
CA7P2SI2O16	Unassessed
CA9V6O18	Estimated
CACO3	Assessed
CACRSI4O10	Unassessed
CACU2O3	Assessed
CAMG3O16S4	Unassessed
CAMN2O4	Assessed
CANA2SIO4	Assessed
CANA2SI5O12	Estimated
CANA4SI3O9	Estimated
CA2NA2SI2O7	Estimated
CA2NA2SI3O9	Estimated
CA3NA2SI6O16	Assessed
CAP2O6_A	Assessed
CAP2O6_B	Assessed
CAP2O6_G	Assessed
CAP4O11_A	Assessed
CAP4O11_B	Assessed
CAV2O5	Assessed
CAV3O7	Assessed

Stoichiometric Compound	*Molar Volume Status*
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

Stoichiometric Compound	*Molar Volume Status*
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
CUPRITE	Assessed
CUSPIDINE	Assessed
CW3F	Assessed
CWF	Assessed
DJURLEITE	Assessed
FE18P2O24	Estimated
FE2P2O7	Assessed
FE2PO5	Assessed

Stoichiometric Compound	*Molar Volume Status*
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
KYANITE	Assessed
LA1S2	Assessed
LA2CR3O12	Estimated
LA2CRO6	Assessed
LA2NB12O33	Estimated
LA2TI3O9	Estimated
LA3NBO7	Assessed
LA4SI3O12	Estimated
LA4TI3O12	Estimated

Stoichiometric Compound	*Molar Volume Status*
LA4TI9O24	Estimated
LAAL11O18	Estimated
LAFE12O19	Estimated
LANB3O9	Estimated
LANBO4	Assessed
LANIO3	Assessed
LARNITE	Assessed
MERWINITE	Assessed
MGCO3	Assessed
MGNA2SI4O10	Estimated
MG2NA2SI6O15	Estimated
MG2NB34O87	Estimated
MG5NB4O15	Estimated
MGP2O6	Assessed
MGP4O11	Assessed
MN2P2O7	Assessed
MN2V2O7	Assessed
MN3P2O8	Assessed
MN9SI3O14S1	Unassessed
MNF2_S1	Assessed
MNF3	Assessed
MNP2O6	Assessed
MNYO3_HEX	Assessed

Stoichiometric Compound	*Molar Volume Status*
MO2S3	Estimated
MO4O11	Estimated
MO8O23	Estimated
MO9O26	Assessed
MOF4	Estimated
MOO3	Estimated
NA2CO3_S1	Assessed
NA2CO3_S2	Assessed
NA2CA3AL16O28	Unassessed
NA2CAAL4O8	Unassessed
NA2CA8AL6O18	Unassessed
NAF1	Assessed
NAFE2O3	Assessed
NA2FEO2	Estimated
NA3FEO3	Assessed
NA3FE5O9	Assessed
NA4FEO3	Assessed
NA4FE6O11	Estimated
NA5FEO4	Assessed
NA8FE2O7	Estimated
NAFESI2O6	Assessed
NA2FESIO4	Estimated
NA5FESI4O12	Estimated

Stoichiometric Compound	*Molar Volume Status*
NA8FE6SI15O40	Estimated
NA2O1_S1	Assessed
NA2O1_S2	Assessed
NA2O1_S3	Assessed
NAPO3	Assessed
NA3PO4	Estimated
NA4P2O7	Assessed
NAS2	Assessed
NA2S1	Assessed
NA2SIO3	Assessed
NA2SI2O5_ALPHA	Assessed
NA2SI2O5_BETA	Assessed
NA2SI2O5_GAMMA	Assessed
NA4SIO4	Assessed
NA6SI2O7	Assessed
NA6SI8O19	Assessed
NA10SIO7	Estimated
NA2TIO3_S1	Assessed
NA2TIO3_S2	Assessed
NA2TI3O7	Assessed
NA2TI6O13	Assessed
NA4TIO4	Assessed
NA8TI5O14	Assessed

Stoichiometric Compound	*Molar Volume Status*
NA2V2O6	Assessed
NA4V2O7	Assessed
NA6V2O8	Estimated
NBF5	Assessed
NBO	Assessed
NI2P2O7	Assessed
NI3P2O8	Assessed
NI3S2_LT	Assessed
NI4NB2O9	Estimated
NINB14O36	Estimated
NINB36O91	Estimated
NINB68O171	Estimated
NIOCALITE_C10NS6	Unassessed
NIS_LT	Estimated
P2O5_H	Assessed
P2O5_O	Assessed
P2O5_OP	Assessed
P2S5	Assessed
PSEUDO_WOLLASTONITE	Assessed
Q_ALMGZRO	Unassessed
RANKINITE	Assessed
SAPPHIRINE	Unassessed
SI3P4O16	Estimated

Stoichiometric Compound	*Molar Volume Status*
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
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

Stoichiometric Compound	*Molar Volume Status*
V3O5_LT	Assessed
V3O7	Assessed
V52O64	Assessed
V6O13	Assessed
WO2_72	Assessed
WO2_90	Assessed
WO2_96	Assessed
WO3_HT	Assessed
WO3_LT	Assessed
Y2S2A_Y2SI2O7	Assessed
Y2S2B_Y2SI2O7	Assessed
Y2S2D_Y2SI2O7	Assessed
Y2S2G_Y2SI2O7	Assessed
Y2SIO5	Assessed
ZR11NB4O32	Estimated
ZR13NB4O36	Estimated
ZR15NB4O40	Estimated
ZR3Y4O12	Assessed
ZR5NB2O15	Estimated
ZR6NB2O17	Estimated
ZR7NB2O19	Estimated
ZR8NB2O21	Estimated
ZRF4	Assessed

Stoichiometric Compound	*Molar Volume Status*
ZRO8S2	Assessed
ZRS2	Assessed
ZRTI2O6	Assessed
ZRTIO4_ALPHA	Estimated

TCOX10 Properties Data

In this section:

TCOX10 Viscosity for Ionic Liquids

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 TCOX10, 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.

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

Model Description

The model for TCS Metal Oxide Solutions Database (TCOX) viscosity of slag:

$$RTln\eta = RTln\eta_0 + E$$

where η is viscosity, $\eta_0 = \frac{hN_A}{V_m}$ and E is activation energy.

The excess parameters are expanded via R-K. An example of viscosity of A-B liquid oxide:

$$RTln\eta_{A-B} = y_A(RTln\eta_0^A + E_A) + y_B(RTln\eta_0^B + E_B) + \sum_i y_A \cdot y_B(y_A - y_B)^i \cdot VISC^i$$

The parameter of *VISC* stands for *R · T · ln(viscosity)*. In Thermo-Calc software, VISC is implemented as *VISC(ionic)*. In order to quickly acquire the actual viscosity, the parameter of *DVIS(ionic)* should be used. By coupling to the database, it makes use of the site fractions of each species, which reflects the structural change in the oxide melt.

Units for the viscosity of oxide slag:

- Pa·s (pascal-second) is the SI unit, mostly used for oxide slag
- CGS unit is poise (P), 1 poise=0.1 Pa·s
- Centipoise is also common (cP) because it is equivalent to mPa·s.

Unary Assessed Systems

Al_2O_3

CaF_2, CaO , CaS, Cr_2O_3, CuO_x

CaO and CaS are estimated based on other predictions and data of ternaries.

Fe-O

MgO, MnO

Na_2O, NiO

P_2O_5

SiO_2

TiO_2

V_2O_5

ZrO_2

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

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

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

TCOX10 Molar Volume Model

Molar volume can be used to establish a connection with some significant physical properties, for example, viscosity, electrical conductivity and surface tension. It is the reciprocal of density multiplied by molar mass.

Model Description

The model used to describe the molar volume at ambient pressures is:

$$V_m(T) = V_0 exp(\int_{T_0}^{T} 3\alpha dT)$$

A simple polynomial is used to model non-magnetic volumetric expansivity above 298K:

$$3\alpha = a + bT + cT^2 + dT^3 + eT^{-2}$$

The model described above is implemented in Thermo-Calc software with two parameters, V0 and VA, and α is the linear thermal expansivity at 1 bar and 3α is the volumetric thermal expansivity.

Molar Volume Descriptions

Parameter	Unit	Description
V0 (phase, constituent array)	m^3/mol	Volume at 1 bar and reference temperature T0
VA (phase, constituent array)	None	$\int_{T_0}^{T} 3\alpha dT$

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 TCOX10 Stoichiometric Compounds.

Liquid Solution Phases

Unary Systems

CaO, MgO, Al_2O_3, SiO_2, MnO ^{E}, FeO, Fe_2O_3, CaF_2, MgF_2, TiO_2, 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, 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, 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

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:	**10.0**

Changes in the Most Recent Database Release

Changes from TCOX9 to TCOX10

Software release version 2020b (June 2020)

- Addition of 3 new elements: N, Na, H (Hydrogen only in gas).
- H: Added H, H2, C1H4 and H2O to the gas phase.
- 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 8 binary metallic systems. Added Na-O from literature and assessed the Na-S system. Assessed 8 ternary Me-Na-O and 11 higher order oxide systems as indicated in the TCOX information sheet.
- The following systems have been assessed for version 10: C-Ca-O and C-Mg-O.
- The following systems have been reassessed for version 10: Cr-O, Ca-Cr-O, Cr-Si-O, Ca-Cr-Si-O.
- Reassessed the vacancy fraction on the FCC metallic sublattice to get a Va-fraction of 1e-5 at liquidus (this was earlier 1e-4).
- 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.
- Added/Assessed molar volumes to the database, both for solid and liquid oxides and metals.
- Assessed viscosity for the liquid metal and oxide. 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.

Previous Releases

TCOX1 was originally released in 1992.

TCOX8 TO TCOX9

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 to TCOX8

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 to TCOX7

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.
- Modelled Fe_2O_3 solubility in MULLITE.
- Modelled ZrO_2 solubility in APATITE.
- Modelled 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

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.
- Modelled 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 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.