TCOX8: TCS Metal Oxide Solutions Database

<table>
<thead>
<tr>
<th>Database name</th>
<th>TCS Metal Oxide Solutions Database</th>
<th>Database acronym:</th>
<th>TCOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>Database owner:</td>
<td>Thermo-Calc Software AB</td>
<td>Database version:</td>
<td>8.0</td>
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</tbody>
</table>

TCOX8 is a thermodynamic database for slags and oxides for use with Thermo-Calc and the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA). Developed using the CALPHAD approach, TCOX is based on the critical evaluation of binary, ternary and important higher order systems which enables predictions to be made for multicomponent systems. The database is the result of a long-term collaboration with academia. The first release of the database was in August 1992.

Included Elements (24)

<table>
<thead>
<tr>
<th></th>
<th>Al</th>
<th>Ar</th>
<th>C</th>
<th>Ca</th>
<th>Co</th>
<th>Cr</th>
<th>Cu</th>
<th>F</th>
<th>Fe</th>
<th>Gd</th>
<th>La</th>
<th>Mg</th>
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<tbody>
<tr>
<td>Mn</td>
<td>Mo</td>
<td>Nb</td>
<td>Ni</td>
<td>O</td>
<td>P</td>
<td>S</td>
<td>Si</td>
<td>V</td>
<td>W</td>
<td>Y</td>
<td>Zr</td>
<td></td>
</tr>
</tbody>
</table>

Ar is only included in the gas phase.

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, but the database is of course not limited to this. Despite the name of the database, it can be used even 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.

TCOX has been developed in a CALPHAD spirit in order to give an accurate thermodynamic description of the multi-component systems of interest. In total, 241 binary systems and 218 ternary systems in this 24-element framework have been assessed to their full range of composition and temperature. In addition, TCOX also contains assessments of 88 pseudo-ternary oxide systems, 28 oxy-fluoride and oxy-sulfide systems, and some higher order systems as well. The systems and composition ranges which have been assessed are described below. The most accurate calculations will be obtained in or near these sub-systems and composition ranges.

However, intermetallic compounds and carbides are not included in the database. For solid phases, the TCOX database is compatible with TCFE Steels/Fe-Alloys Database, TCNI Ni-based Superalloys Database and SSOL Solutions Database. Thus, if needed, more metallic phases can be obtained by appending from TCFE, TCNI, SSOL and/or other appropriate databases. However, one must keep in mind that the LIQUID phase

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from other databases and the IONIC_LIQ phase from TCOX should never be simultaneously considered in the same defined system/calculation, as they both represent the liquid phase using two different models. The binary O- and S-systems can be calculated with the BINARY module in Thermo-Calc.

TCOX contains 352 phases in total. The liquid metal and slag (IONIC_LIQ) is described with the ionic two-sublattice liquid model [1985, Hillert; 1991, Sundman] using a single Gibbs energy curve. 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.

TCOX 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]. The complete list of phases is given in Phases Included in TCOX.

**Limits**

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

**Database Revision History**

If you are interested in the revision history for this database, the information is available in the online help (from Thermo-Calc go to Help>Online Help) or in the release notes on our website.
Assessed Systems

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

Assessed Metallic Systems

All metal-metal binaries except Ca-W, Ca-Zr, Gd-La, Gd-P, La-Nb, La-P, La-Si, Mg-P, P-V, P-W and P-Zr are assessed. Many ternary metallic systems are also assessed. No intermetallic phases are included in the database. If needed, more solid phases can be appended from TCFE, TCNI, TCAL or other appropriate databases.

Assessed Binary Oxide Systems

<table>
<thead>
<tr>
<th></th>
<th>Al-O</th>
<th>Ca-O</th>
<th>Co-O</th>
<th>Cr-O</th>
<th>Cu-O</th>
<th>Fe-O</th>
<th>Gd-O</th>
<th>La-O</th>
<th>Mg-O</th>
<th>Mn-O</th>
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</thead>
<tbody>
<tr>
<td>Mo-O</td>
<td>Nb-O</td>
<td>Ni-O</td>
<td>P-O</td>
<td>Si-O</td>
<td>V-O</td>
<td>W-O</td>
<td>Y-O</td>
<td>Zr-O</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Assessed Ternary Oxide Systems, Me1-Me2-O

[Diagram of ternary oxide systems]

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

<p>|          | Al-Ca-Co-O | Al-Ca-Cr-O | Al-Ca-Fe-O | Al-Ca-Mg-O | Al-Ca-Mn-O | Al-Ca-Nb-O | Al-Ca-Ni-O | Al-Ca-Si-O | Al-Ca-O-Si | Al-Ca-O-Y | Al-Cr-O-Zr | Al-Co-O-Si | Al-Cr-Fe-O | Al-Cr-Mg-O | Al-Cr-Ni-O | 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-Y | Al-Mg-O-Zr | Al-Mn-O-Si | Al-O-P-Si | Al-O-Si-Y | Al-O-Si-Zr | Al-O-Y-Zr | Ca-Co-O-Si | 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-Gd-O-Si | Ca-Mg-Mn-O | Ca-Mg-O-P | Ca-Mg-O-Si | Ca-Mg-O-Zr | Ca-Mn-O-P | Ca-Mn-O-Si | Ca-Mn-O-Y | Ca-Nb-O-Si | Ca-Ni-O-Si | Ca-O-P-Si | Ca-O-Si-Y | Ca-O-Si-Zr | Ca-O-Y-Zr | Co-Cr-O-Si | Co-Cu-La-O | 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-Y | Cr-La-Mn-O | Cr-Mg-O-Si | Cr-Mn-Ni-O | Cu-Fe-O-Si | Cu-Mg-O-Si | Fe-Mg-O-Si | Fe-Mn-O-Si | Fe-Ni-O-Si-O | Gd-La-O-Si | Gd-O-Si-Y-O | Gd-O-Si-Zr-O |</p>
<table>
<thead>
<tr>
<th>Assessed Higher Order Oxide Systems</th>
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<tbody>
<tr>
<td>Al-Ca-Co-O-Si</td>
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<tr>
<td>Al-Ca-O-Si-Y</td>
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<tr>
<td>Al-La-O-Y-Zr</td>
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<td>Gd-La-O-Y-Zr</td>
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<table>
<thead>
<tr>
<th>Assessed Binary Sulfide Systems</th>
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</thead>
<tbody>
<tr>
<td>Al-S</td>
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<tr>
<td>Mn-S</td>
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<table>
<thead>
<tr>
<th>Assessed Ternary Sulfide Systems, Me1-Me2-S</th>
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<tbody>
<tr>
<td>Al</td>
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<tr>
<td>Mo</td>
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### Assessed Oxy-sulfide Systems

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<tr>
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<th>Al-\text{O-S}</th>
<th>Ca-\text{O-S}</th>
<th>Co-\text{O-S}</th>
<th>Cr-\text{O-S}</th>
<th>Cu-\text{O-S}</th>
<th>Fe-\text{O-S}</th>
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<tr>
<td>Mg-\text{O-S}</td>
<td>Mg-\text{O-S}</td>
<td>\text{O-SSi}</td>
<td>Al-Ca-\text{O-S}</td>
<td>Al-Mg-\text{O-S}</td>
<td>Al-Mn-\text{O-S}</td>
<td></td>
</tr>
<tr>
<td>Ca-Fe-\text{O-S}</td>
<td>Ca-Mg-\text{O-S}</td>
<td>Ca-\text{O-SSi}</td>
<td>Cu-Fe-\text{O-S}</td>
<td>Fe-O-S\text{Si}</td>
<td>Mg-O-S\text{Si}</td>
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<tr>
<td>Mn-O-S-Si</td>
<td>Al-Ca-Mn-\text{O-S}</td>
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### Assessed Binary Fluoride Systems

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<tr>
<th></th>
<th>AlF\text{3}</th>
<th>Ca-F</th>
<th>CoF\text{2}</th>
<th>CoF\text{3}</th>
<th>CrF\text{2}</th>
<th>CrF\text{3}</th>
<th>CuF</th>
<th>CuF\text{2}</th>
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<tr>
<td>FeF\text{2}</td>
<td>FeF\text{3}</td>
<td>GdF\text{3}</td>
<td>LaF\text{3}</td>
<td>MgF\text{2}</td>
<td>MnF\text{2}</td>
<td>MoF\text{4}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NbF\text{2}</td>
<td>NbF\text{5}</td>
<td>NiF\text{2}</td>
<td>SiF\text{4}</td>
<td>VF\text{2}</td>
<td>YF\text{3}</td>
<td>ZrF\text{4}</td>
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</table>

### Assessed Ternary Fluoride Systems

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<thead>
<tr>
<th></th>
<th>Al-Ca-F</th>
<th>Al-F-Mg</th>
<th>Al-F-Zr</th>
<th>Ca-Co-F</th>
<th>Ca-Cr-F</th>
<th>Ca-Fe-F</th>
<th>Ca-F-Gd</th>
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<tbody>
<tr>
<td>Ca-F-La</td>
<td>Ca-F-Mg</td>
<td>Ca-F-Mn</td>
<td>Co-F-Gd</td>
<td>Co-F-Mg</td>
<td>Co-F-Ni</td>
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<tr>
<td>F-Gd-Mg</td>
<td>F-Gd-Y</td>
<td>F-La-Zr</td>
<td>F-Mg-La</td>
<td>F-Mg-Y</td>
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</table>
## Assessed Oxy-fluoride Systems

<table>
<thead>
<tr>
<th>Al-F-O</th>
<th>Ca-F-O</th>
<th>Co-F-O</th>
<th>F-Mg-O</th>
<th>Al-Ca-F-O</th>
<th>Ca-F-Mg-F-O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca-Fe-F-O</td>
<td>Ca-F-O-P</td>
<td>Ca-F-O-Si</td>
<td>F-Mg-O-Si</td>
<td>Al-Ca-F-Mg-O</td>
<td>Al-Ca-F-O-Si</td>
</tr>
</tbody>
</table>
TCOX Calculation Examples

Figure 1: Calculated phase diagram of the CaO-Al₂O₃-SiO₂ system [2006, Mao]. Ano: anorthite, C1A1: CaAl₂O₄, C1A2: CaAl₂O₇, C1A6: CaAl₁₂O₁₉, C3A1: Ca₃Al₂O₈, Cor: corundum, Cri: cristobalite, Geh: gehlenite, Hat: hatrurite, Mul: mullite, Pse-Wol: pseudo-wollastonite, Ran: rankinite, Tri: tridymite.
Figure 2: Calculated \( \text{CaMgSi}_2\text{O}_6 \) (diopside)-\( \text{FeO}_x \) section in air.

![Diagram of CaMgSi2O6 (diopside)-FeOx section in air.]

Figure 3: Calculated Fe-O phase diagram [1991, Sundman].

![Diagram of Fe-O phase diagram.]

Figure 4: Calculated [2008, Kjellqvist] and experimental phase diagram of Cr-Fe-O in air [1960, Muan].

![Diagram of Cr-Fe-O phase diagram.]

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Figure 5: Calculated [2010, Kjellqvist] and experimental phase diagram of Fe-Mn-O at 1000 °C [1967, Schwerdt; 1990, Franke; 1956, Foster; 1971, Ono; 1975, Duquesnoy; 1987, Falke; 1964, Bergstein; 1965, Tretjakov].

Figure 6: Calculated and experimental [1966, Greskovich] isothermal section of Al₂O₃-Cr₂O₃-MgO at 1700 °C and P_{O_2}=1.
Figure 7: Isothermal section of CaO-Cr$_2$O$_3$-Mn$_2$O$_3$ calculated at 1600 °C in air.

Figure 8: Calculated isothermal sections of CaO-SiO$_2$-YO$_{1.5}$ (left) and CaO-SiO$_2$-GdO$_{1.5}$ (right) at 1600 °C, compared to data on 3-phase corners and tie-lines from Poerschke [2017, 2016a, 2016b].
Figure 9: Calculated and experimental phase diagrams for CaO-ZrO₂ (top) and MgO-ZrO₂ (bottom) [see Figure 9 References].
Figure 10: Isothermal sections of CaO-MgO-ZrO$_2$ calculated at 1300 °C and 1500 °C with experimental data [1993, Yin].

Figure 11: Calculated effect of CaF$_2$ on the Al$_2$O$_3$-CaO-SiO$_2$ system at 1600 °C.
Figure 12: Sulfur in ladle slag. An impressive amount of sulfide capacity measurements have been made for a variety of slag systems over the years, but the results are very scattered. Allertz [2016] used a different method with equilibrium between copper and slag. Sulfur was added as Cu$_2$S. Different CMAS slags were then equilibrated with Cu and Cu$_2$S under controlled oxygen partial pressures. The equilibrium sulfur contents in the copper and slag were then analyzed.
Figure 13: Isothermal section of the Al$_2$O$_3$-CaO-CaS system at 1600 °C with experimental data [1984, Ozturk; 2013, Piao].

Figure 14: Calculated effect of inclusion composition of 18-8 stainless steel. The stability and composition of sulfides have been investigated [1980, Ono] at 1100 °C by varying the Mn concentration of the steel: Fe - 0.06% C - 0.6% Si - 0.2% S - 8.4% Ni - 18.2% Cr.
Figure 15: Comparison of experimental and calculated phosphorus solubility in liquid iron in equilibrium with slag in the Ca-Fe-Mg-O-P-Si system [see Figure 15 References].

Acknowledgement

Professor Malin Selleby, Dr. Bengt Hallstedt and David Dilner are acknowledged for many valuable discussions and important contributions.
TCOX References


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**Figure 9 References**


**Figure 15 References**


Phases Included in TCOX

In total there are 352 phases in the databases. Phases and constituents can be listed in the DATABASE module and the 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 Database module.

The Liquid Solution

The liquid phase contains all elements in the TCOX database. 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:

\[
(\text{Al}^{+3}, \text{Ca}^{+2}, \text{Co}^{+2}, \text{Cr}^{+2}, \text{Cu}^{+1}, \text{Fe}^{+2}, \text{Gd}^{+3}, \text{La}^{+3}, \text{Mg}^{+2}, \text{Mn}^{+2}, \text{Mo}^{+4}, \text{Nb}^{+2}, \text{Ni}^{+2}, \text{P}^{+5}, \text{Si}^{+4}, \text{V}^{+2}, \text{W}^{+6}, \text{Y}^{+3}, \\
\text{Zr}^{+4})_p (\text{AlO}_2^{-1}, \text{F}^{-1}, \text{O}^{-2}, \text{PO}_4^{-3}, \text{S}^{-2}, \text{SiO}_4^{-4}, \text{SO}_4^{2-}, \text{Va}, \text{C}, \text{C}_3\text{S}_2\text{Z}_1/6, \text{CoF}_3, \text{CoO}_3/2, \text{CrF}_3, \text{CrO}_3/2, \text{CuF}_2, \text{CuO}, \text{FeF}_3, \text{FeO}_3/2, \text{M}_3\text{S}_2\text{Z}_1/6, \text{MnO}_3/2, \text{NbF}_5, \text{NbO}_2, \text{NbO}_5/2, \text{PO}_5/2, \text{S}, \text{SiO}_2, \text{VO}_2, \text{VO}_3/2, \text{VO}_5/2)_q
\]

Alloy Phases

**BCC_A2**

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

**FCC_A1**

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

**HCP_A3**

Containing Al, Ca, Co, Cr, Cu, Fe, Gd, La, Mg, Mn, Mo, Nb, Ni, P, S, Si, 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, V and Zr with C modeled interstitially.

**CBCC_A12**

α-Mn, containing Al, Co, Cr, Fe, Mg, Mo, Nb, Ni, Si, V and Zr with C modeled interstitially.
**DIAMOND_FCC_A4**

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

**GRAPHITE**

This is pure carbon.

**RED_P, WHITE_P**

This is pure phosphor. Phosphor 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).

**Gas Phase**

A reduced gas phase containing Al1F3, AR, C1O1, C1O2, CA1F2, F, F2, O, O10P4, O1P1, O2P1, O1S1, O2, O2S1, O3S1, O5P2, P2, P4 and S2.

**Solid Solutions**

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. 135 solutions are modeled in the database.

**Alabandite**

This is CaS (oldhamite), MnS (alabandite), MgS, GdS, LaS and ZrS solid solution.

**AIPO₄**

There are three modifications (S1, S2 and S3) of AIPO₄ with solubility of SiO₂.

**α-Spinel**

This is low-temperature tetragonal Mn₃O₄ 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.

**Anhydrite**

This is (Ca,Cu,Fe,Mg,Mn,Ni)SO₄.
Apatite
This is (Ca,Mg)$_2$(Gd,Y)$_8$(SiO$_4$)$_6$O$_2$ solid solution dissolving Zr.

β-V-O
This is β-V-O.

Bronze
This is (Ca,Fe)$_x$V$_2$O$_5$ bronze.

Calcium ferro-aluminates
C3A1: This is Ca$_3$Al$_2$O$_6$ dissolving ferric Fe.

C12A7: This is Ca$_{12}$Al$_{14}$O$_{32}$ dissolving ferric Fe. C12A7 is not stable in the anhydrous CaO-Al$_2$O$_3$ 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$_2$O$_4$ dissolving ferric Fe.

C1A2: This is CaAl$_4$O$_7$ dissolving ferric Fe.

C1A6: This is CaAl$_{12}$O$_{19}$ dissolving ferric Fe.

C1A1F2: This is Al$_2$CaFe$_4$O$_{10}$ with a variation in Al/Fe: CaAlFe$_2$(Al,Fe)$_3$O$_{10}$.

C2F: This is Ca$_2$Fe$_2$O$_5$ dissolving Al.

Ca$_3$P$_2$O$_8$ (α and β)
α-Ca$_3$P$_2$O$_8$ dissolving Mg and Si and β-Ca$_3$P$_2$O$_8$ dissolving Mg.

Ca$_2$P$_2$O$_7$ (α, β and γ)
α, β and γ-Ca$_2$P$_2$O$_7$ dissolving Mg.

Ca$_2$SiO$_4$ (α and α’)
α-Ca$_2$SiO$_4$- α’-Ca$_3$P$_2$O$_8$ dissolving Gd, Mg, Mn, Y and α’-Ca$_2$SiO$_4$ dissolving Fe, Gd, Mg, Mn, P and Y.

Ca$_3$S$_3$Fe$_4$O$_x$
This is the oxy-sulfide 3CaS.4FeO-3CaS.4Fe$_2$O$_3$.
\[ \text{Ca}_3\text{Y}_2\text{Si}_3\text{O}_{12} \]  
This is \( \text{Ca}_3(\text{Gd,Y})_2(\text{SiO}_4)_3 \).

\[ \text{Ca}_3\text{Y}_2\text{Si}_6\text{O}_{18} \]  
This is \( \text{Ca}_3(\text{Gd,Y})_2(\text{SiO}_4)_6 \).

\[ \text{Ca}_4\text{Nb}_2\text{O}_{9-\text{HT11}} \]  
This is the high-temperature \( \text{Ca}_4\text{Nb}_2\text{O}_9 \) phase with excess CaO.

\[ \text{Ca}_4\text{Nb}_2\text{O}_{9-\text{LT21}} \]  
This is the low-temperature \( \text{Ca}_4\text{Nb}_2\text{O}_9 \) phase with excess CaO.

\[ \text{Ca}_3\text{Co}_2\text{O}_6 \]  
This is \( \text{Ca}_3\text{Co}_2\text{O}_6 \) dissolving Cu.

\[ \text{Ca}_3\text{Co}_4\text{O}_9 \]  
This is \( \text{Ca}_3\text{Co}_4\text{O}_9 \) dissolving Cu.

\[ \text{CaCr}_2\text{O}_4-\text{A} \]  
This is the high-temperature \( \text{CaCr}_2\text{O}_4 \) dissolving Al and Fe.

\[ \text{CaF}_2-\text{S1} \]  
This is low-temperature \( \text{CaF}_2 \) dissolving CaO and MgF\(_2\).

\[ \text{CaF}_2-\text{S2} \]  
This is high-temperature \( \text{CaF}_2 \) and CuF\(_2\) dissolving CaO and MgF\(_2\).

\[ \text{Ca}_3\text{Mg}_3\text{P}_4\text{O}_{16} \]  
This is \( \text{Ca}_3\text{Mg}_3\text{P}_4\text{O}_{16} \).

\[ \text{CaMnO}_3 \]  
This is \( \text{CaMnO}_3 \) and low-temperature \( \text{CaZrO}_3 \) dissolving Y.

\[ \text{Ca}_5\text{P}_2\text{SiO}_{12} \]  
This is \( \text{Ca}_5\text{P}_2\text{SiO}_{12} \).
CaSFeO
This is the oxy-sulfide CaS. FeO-CaS. Fe₂O₃.

CaSO₄-HT
This is (Ca, Co, Mg)SO₄.

CaV₂O₄
This is CaFe₂O₄, β-CaCr₂O₄, CaV₂O₄, and CaY₂O₄ solid solution dissolving Al. Prototype phase is CaV₂O₄.

CaV₂O₆
This is (Ca, Mg, Mn)₆V₂O₆.

CaY₄O₇
This is Ca(Gd, Y)₄O₇.

CaYAl₃O₇
This is Ca(Gd, Y)₃AlO₇.

CaYAlO₄
This is Ca(Gd, Y)AlO₄.

CaZrO₃-C
This is the cubic high-temperature CaZrO₃ phase dissolving Y.

Chalcopyrite
This is an intermediate solid solution phase in the Cu-Fe-S system around the composition CuFeS₂.

Co₉S₈
This is Co₉S₈ dissolving Fe and Ni.

Columbite
This is (Ca, Co, Fe, Mg, Mn)₂Nb₂O₆ with excess FeO and MgO.

Cordierite
This is Al₄(Fe, Mg, Mn)₂Si₅O₈.
**Corundum**
This is Corundum (Al₂O₃), Eskolaite (Cr₂O₃), Hematite (Fe₂O₃) and Karelianite (V₂O₃) solid solution dissolving Mn and Ni.

**Cr₂S₃**
This is Cr₂S₃ dissolving Fe.

**Cr₃S₄**
This is Cr₃S₄ dissolving Fe, Mn and Ni.

**CrNbO₄**
This is CrNbO₄ solid solution with excess Cr₂O₃ and Nb₂O₅.

**Cr₂P₄O₁₃**
This is Cr₂P₄O₁₃ and (Cr,Fe)₂V₄O₁₃.

**CuF₂**
This is CrF₂ and low temperature CuF₂.

**CuLa₂O₄**
This is CuLa₂O₄ with solubility of Co.

**CuP₂O₆**
This is (Co,Cu,Ni)P₂O₆.

**CuO**
This is CuO with solubility of Co.

**Cristobalite**
This is SiO₂ with solubility of AlPO₄.

**Delafossite**
This is Cu(Al,Cr,Fe,La,Mn,Y)O₂.

**Digenite**
This is Cu₂S solid solution with excess S and solubility of Fe, Mg and Mn.
DyMn$_2$O$_5$
This is Mn$_2$(Gd,Y)O$_5$ solid solution. Prototype phase is DyMn$_2$O$_5$.

FeF$_3$
This is (Al,Co,Cr,Fe)F$_3$.

Fe$_2$O$_{12}$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 and Y.

Garnet
This is grossular (Ca$_3$Al$_2$Si$_3$O$_{12}$), uvarovite (Ca$_3$Cr$_2$Si$_3$O$_{12}$) and spessartine (Mn$_3$Al$_2$Si$_3$O$_{12}$).

GdF$_3$
This is high temperature (Gd,Y)F$_3$.

Gd$_2$Si$_2$O$_7$
This is (Gd,La)$_2$Si$_2$O$_7$. 
$\text{Gd}_2\text{SiO}_5$

This is (Gd,La)$_2$SiO$_5$.

**Halite**

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

**Hatruite**

This is Ca$_3$SiO$_5$ dissolving Gd and Y.

**β1-Heazlewoodite**

This is non-stoichiometric high-temperature Ni$_3$S$_2$ dissolving Co and Fe.

**β2-Heazlewoodite**

This is non-stoichiometric high-temperature Ni$_4$S$_3$ dissolving Fe.

**LaF$_3$**

This is low temperature (Gd,La,Y)F$_3$.

**La$_2$S$_3$**

This is (Gd,La)$_2$S$_3$.

**La$_2$MnO$_4$**

This is La$_2$(Mn,Ni)O$_4$ solid solution dissolving Co.

**La$_3$Ni$_2$O$_7$**

This is La$_3$Ni$_2$O$_7$ dissolving Co.

**La$_4$Ni$_3$O$_{10}$**

This is La$_4$Ni$_3$O$_{10}$ 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.
\(\alpha\)-\(M_2O_3\)

This is hexagonal \(\alpha\)-La\(_2\)O\(_3\) and Gd\(_2\)O\(_3\) solid solution dissolving Ca, Mg, Y and Zr.

\(\beta\)-\(M_2O_3\)

This is monoclinic \(\beta\)-Gd\(_2\)O\(_3\) dissolving Al, Ca, Co, La, Mg, Y and Zr.

\(c\)-\(M_2O_3\)

This is Mn\(_2\)O\(_3\), cubic Gd\(_2\)O\(_3\) and Y\(_2\)O\(_3\) solid solution dissolving Al, Ca, Co, Cr, Fe, La, Mg, Ni, Y and Zr.

\(h\)-\(M_2O_3\)

This is hexagonal La\(_2\)O\(_3\), Gd\(_2\)O\(_3\) and Y\(_2\)O\(_3\) solid solution dissolving Ca, Mg, Mn and Zr.

\(x\)-\(M_2O_3\)

This is \(x\)-La\(_2\)O\(_3\) and high-temperature cubic Gd\(_2\)O\(_3\) solid solution dissolving Ca, Mg, Y and Zr.

**Melilite**

This is Gehlenite (Ca\(_2\)Al\(_2\)SiO\(_7\)), Fe-Gehlenite (Ca\(_2\)Fe\(_2\)SiO\(_7\)), Åkermanite (Ca\(_2\)MgSiO\(_7\)), Fe-Åkermanite (Ca\(_2\)FeSiO\(_7\)) and Ca\(_2\)CoSi\(_2\)O\(_7\).

**MgF\(_2\)**

This is (Co,Fe,Mg,Mn,Ni,V)F\(_2\).

**Mg\(_2\)P\(_2\)O\(_7\) (\(\alpha\) and \(\beta\))**

This is \(\alpha\) and \(\beta\)-Mg\(_2\)P\(_2\)O\(_7\) dissolving Ca.

**Mg\(_2\)V\(_2\)O\(_7\)**

This is (Co,Mg,Ni)\(_2\)V\(_2\)O\(_7\).

**Mg\(_3\)P\(_2\)O\(_8\)**

This is Mg\(_3\)P\(_2\)O\(_8\) dissolving Ca.

**Mg\(_3\)V\(_2\)O\(_8\)**

This is (Co,Mg,Ni)\(_3\)V\(_2\)O\(_8\).
**MgWO$_4$-type**
This is (Al,Fe)NbO$_4$ and (Co,Fe,Mg,Mn,Ni)WO$_4$ solid solution. Prototype MgWO$_4$.

**Mn$_4$Nb$_2$O$_9$**
This is (Co,Fe,Mg,Mn)$_4$Nb$_2$O$_9$.

**MoS$_2$**
This is (Mo,W)$_2$S$_2$ solid solution.

**Mullite**
Mullite (around $\text{Al}_6\text{Si}_2\text{O}_{13}$) solid solution dissolving Fe.

**Nb$_2$O$_5$**
This is Nb$_2$O$_5$ dissolving Mg and V.

**Ni$_6$MnO$_8$-type**
This is (Mg,Ni)$_6$MnO$_8$.

**Ni$_7$S$_6$**
This is Ni$_7$S$_6$ dissolving Fe.

**Ni$_9$S$_8$**
This is Ni$_9$S$_8$ dissolving Fe.

**NiMnO$_3$**
This is NiMnO$_3$ with Ilmenite structure.

**NiNb$_2$O$_6$**
This is NiNb$_2$O$_6$. This phase has the same structure as the Nb$_2$FeO$_6$ phase, but is modeled separately.

**NiV$_2$O$_6$**
This is (Co,Ni)V$_2$O$_6$. 
Olivine
This is Calcio-olivine (Ca$_2$SiO$_4$) – Co$_2$SiO$_4$ – Fayalite (Fe$_2$SiO$_4$) – Forsterite (Mg$_2$SiO$_4$) – Tephroite (Mn$_2$SiO$_4$) – Ni$_2$SiO$_4$ – Kirschsteinite (CaFeSiO$_4$) – Monticellite (CaMgSiO$_4$) solid solution dissolving Cr and Cu.

Pentlandite
This is ternary (Fe,Ni)$_3$S$_8$.

Perovskite
This is (Cr,Fe,Mn)LaO$_3$.

Pyrite
This is Cattierite (CoS$_2$), Pyrite (FeS$_2$) – Hauerite (MnS$_2$) – Vaesite (NiS$_2$).

Pyrochlore
This is (Gd,La)$_2$Zr$_2$O$_7$ solid solution dissolving Y.

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$_2$O$_6$).

Clino-pyroxene: This is clino-enstatite (MgSiO$_3$), clino-ferrosilit (FeSiO$_3$), diopside (CaMgSi$_2$O$_6$), niopside (CaNiSi$_2$O$_6$), pigeonite ((Mg,Fe,Ca)Si$_2$O$_6$), hedenbergite (CaFeSi$_2$O$_6$) dissolving Co.

Ortho-pyroxene: This is enstatite (MgSiO$_3$) and ortho-diopside (CaMgSi$_2$O$_6$) with Fe solubility.

Proto-pyroxene: This is proto-enstatite (MgSiO$_3$) and proto-diopside (CaMgSi$_2$O$_6$) dissolving Co, Cr and Fe.

Pyrrhotite
This is Pyrrhotite (FeS) – CoS – CrS– NbS – NiS – 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 MnO₂ – NbO₂ – high temperature VO₂ solid solution dissolving Fe.

Spiral
This is the cubic AB₂O₄-type spinel solid solution containing Al-Ca-Co-Cr-Cu-Fe-Mg-Mn-Ni-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 (MgAl₂O₄), Magnetite (Fe₃O₄), Cuprospinel (CrFe₂O₄), Hercynite (FeAl₂O₄) 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)Cr₂S₄ – Co₃S₄ – FeNi₂S₄ – Ni₃S₄.

Tridymite
This is SiO₂ with solubility of AlPO₄.

V₃O₅-HT
This is high temperature V₃O₅ dissolving Al, Cr and Mn.

V₄O₇
This is V₄O₇ dissolving Al and Mn.

VO₂-LT
This is low temperature VO₂, MoO₂ and WO₂.

Wollastonite
This is CaSiO₃ dissolving Fe, Mg and Mn.

YAG
This is (Gd,Y)₃(Al,Fe)₅O₁₂ solid solution dissolving Cr and La.

YAM
This is (Gd,Y)₄Al₂O₉ and Cuspidine (Ca₂Y₂Si₂O₉) solid solution dissolving La.
YAP
This is \((\text{Gd,Y})(\text{Al,Co,Cr,Fe})\text{O}_3\) solid solution dissolving Ca, Mn and La.

\(\text{Y}_3\text{NbO}_7\)
This is \(\text{Y}_3\text{NbO}_7\) solid solution with excess \(\text{Nb}_2\text{O}_5\) and \(\text{Y}_2\text{O}_3\).

\(\text{YNbO}_4\)
This is \(\text{YNbO}_4\) solid solution with excess \(\text{Y}_2\text{O}_3\).

Zircon
This is Zircon \((\text{ZrSiO}_4)\) and \((\text{Gd,Y})\text{PO}_4\) solid solution.

\(\text{m-ZrO}_2\)
This is monoclinic \(\text{ZrO}_2\) solid solution dissolving Al, Ca, Cr, Gd, La and Y.

\(\text{t-ZrO}_2\)
This is tetragonal \(\text{ZrO}_2\) solid solution dissolving Al, Ca, Cr, Fe, Gd, La, Mg, Mn, Ni and Y.
# Stoichiometric Compounds

203 stoichiometric compounds are modeled in the database.

<table>
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<th>Formula</th>
<th>Symbol</th>
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