

IRSN NUCLEA-20 Nuclear Alloys-Oxides Database (NUCL20)

Technical Information

Available Starting with Thermo-Calc Version 2022b



About the IRSN NUCLEA-20 Nuclear Alloys-Oxides Database (NUCL20)

IRSN NUCLEA-20 Nuclear Alloys-Oxides Database (NUCL20) is a thermodynamic and properties database owned by IRSN that can be applied to study fundamental scientific issues and efficiently investigate practical engineering problems in both the In-Vessel and Ex-Vessel nuclear reactor circumstances. It effectively enables you to calculate the thermochemical equilibrium states at any step of an eventually-severe accident, and to utilize the calculation results for improving the predictions and treatments of thermo-hydraulic or other accidents, enhancing the design and engineering of modern and safety-prioritized nuclear reactors and assisting in the assessment and processing of nuclear fuel and waste managements.

The database contains critically-assessed and internally-consistent thermodynamic data for the entire field from metal to oxide domains within an 18-element framework, +H and +Ar, which are only for the gaseous phase and for hydrides and hydrous oxides/silicates.

 [NUCL: IRSN NUCLEA-Nuclear Alloys-Oxides Database Revision History](#). The current version of the database is NUCL20.

Included Elements (18+2)

Ag	Al	Ar	B	Ba	C	Ca	Cr	Fe	H
In	La	Mg	Ni	O	Ru	Si	Sr	U	Zr

Included Phases and Assessed Systems



See the *Overview of NUCLEA-20* pages at the end of this PDF that have details such as atoms, stoichiometric condensed phases, condensed solutions, gas, and the assessed binary, ternary, and quaternary systems.

Available Solution and Stoichiometric Phases

Condensed solution phases: <i>(solids/liquid phases)</i>	65 phases
Condensed stoichiometric phases: <i>(solid/liquid substances)</i>	510 phases
Gaseous mixture phase: <i>(ideal gaseous mixture)</i>	209 gaseous species



The hydrogen element (H) being as a major component is added into the system, while its dissolution in condensed solid and liquid solution phases has not been taken into account yet. The Ar component is only present in the gaseous mixture phase. Included condensed stoichiometric phases (pure substances) are widely ranged: intermediate metallic compounds, oxides and hydroxides, silicates and hydrous silicates, hydrides, carbides and carbonates, borides and borates, and some simple inorganic/organic substances.

Available Assessments and Evaluations

Binary subsystems: (<i>metallic alloys, carbides, borides, oxides</i>)	153
Ternary subsystems: (<i>metallic alloys, carbides, borides, oxides, silicates</i>)	105
Quaternary subsystems: (<i>oxides, silicates, borates</i>)	18



For many other ternary, quaternary and higher-order subsystems, the analytical descriptions of lower-order constituent subsystems are effectively combined and used (through appropriate extrapolations) to predict multicomponent systems, especially for compositions and temperatures which have not been experimentally evaluated. Depending on the complexity of multicomponent systems, such an analytical prediction is more or less accurate.

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 equilibrium 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.

Additional Resources

This document is available on our website on the [Nuclear Materials Databases](#) page, where you can also link to many other resources. Alternatively, when in Thermo-Calc, press F1 to search the online help for more information.

NUCL: IRSN NUCLEA-Nuclear Alloys-Oxides Database Revision History

Current Database Version

Database name (acronym):	IRSN NUCLEA-20 Nuclear Alloys-Oxides Database (NUCL20)
Database owner:	IRSN
Database version:	20

Changes in the Most Recent Database Release

NUCL19 (NUCLEA-19) to NUCL20 (NUCLEA-20)

Software release version: 2022b (June 2022)

Binary Systems

- Updated binary system: Ag-In as taken from E. Fischer et al., Calphad, 64:292–305, 2019.
- Change to B-Ni: The name of the compound $B_{0.414}Ni_{0.586}$ is changed to $B_{7}Ni_{10}$.

Pseudo-binary Systems

A bug fix for the pseudo binary system, Ba-Ca-O BaO-CaO

Ternary Systems

Change of name for three ternary stoichiometric phases:

- Fe-U-Zr: The name of the ternary stoichiometric phases, $Fe_{333}U_{250}Zr_{417}$ (e), $Fe_{60}U_{71}Zr_{23}$ (l), and $Fe_{503}U_{18}Zr_{32}$ (k) are changed to $Fe_{40}U_{3}Zr_{5}$, $Fe_{60}U_{71}Zr_{23}$, and $Fe_{253}U_{9}Zr_{16}$, respectively.

Pseudo-ternary Systems

Two new systems and one reassessment:

- Al-Ca-O-Zr: Modeling of the $CaO-Al_2O_3-ZrO_2$ pseudo-ternary system
- Al-O-Si-Zr: Reassessment of the $Al_2O_3-SiO_2-ZrO_2$ pseudo-ternary system
- Ca-Mg-O-Zr: Modeling of the $CaO-MgO-ZrO_2$ pseudo-ternary system

Previous Releases

NUCL15 (NUCLEA-15) to NUCL19 (NUCLEA-19)

IRSN NUCLEA-Nuclear Alloys-Oxides Database (NUCL19)

Software release version: 2021a (January 2021)

Binary Systems

- Ag-Mg: The lattice-stability of Mg (FCC_A1) available in the Unary 5.0 SGTE database taken into account.
- Ag-Zr: Change of the decomposition nature of AG1ZR1 and AG1ZR2, to congruent and peritectic respectively
- Al-Fe: Sundman et al., Acta Materialia, 57(10):2896–2908, 2009.
- Al-Mg: Liang et al. Z. Metallkde., 89(8):536–540, 1998.
- B-Cr: Revision of the thermodynamic properties of the stoichiometric phases.
- B-Ni: Sun et al., International Journal of Materials Research, 100:59–67, 2009.
- B-Si: The lattice-stability of metastable B(dia_A4) available in the Unary 5.0 SGTE database taken into account
- Ba-Mg: Error correction
- Ba-Si: Three additional stoichiometric phases, BA2SI1, BA5SI3, BA1SI1, BA3SI4.
- Ca-La: FCC_A1 is not more stable above 1500 K.
- Cr-Ru: The lattice-stability of Ru(BCC_A2) available in the Unary 5.0 SGTE database taken into account
- Cr-Zr: Yang et al. Journal of Nuclear Materials, 441(1-3):190–202, 2013.
- Fe-Ni: Introduction of the FeNi₃ phase as a stoichiometric phase.
- Fe-Ru: The lattice-stability of Ru(BCC_A2) available in the Unary 5.0 SGTE database taken into account
- Fe-Si: Y. Yuan et al. Calphad, 44:54–61, 2014.
- Fe-U: The lattice-stabilities of Fe(ORT_A20) and Fe(TET) available in the Unary 5.0 SGTE database taken into account
- In-Mg: The lattice-stabilities of Mg(FCC_A1) and In(FCC_A1) available in the Unary 5.0 SGTE database taken into account.
- In-O: Improvement of the modeling of solubility of oxygen in indium liquid
- La-Mg: F. Zhang, Journal of Alloys and Compounds, 663:279–288, 2016.
- La-U: Improvement of liquid thermodynamic properties
- La-Zr: N. Mattern et al. Calphad, 52:8–20, 2016.

- Mg-U: The lattice-stability of U (hcp_A3) available in the Unary 5.0 SGTE database taken into account.
- Mg-Zr: R. Arroyave et al., Calphad, 29(3):230–238, 2005.
- Ni-U: The lattice-stability of U (FCC_A2) available in the Unary 5.0 SGTE database taken into account
- Ru-U: The lattice-stability of Ru (BCC_A2) and U (hcp_A3) available in the Unary 5.0 SGTE database taken into account. The Ru3U compound is now modeled as a solution phase, CxRU3U1(SS).
- Si-Sr: Li et al. System. Calphad, 35(4):594–600, 2011.

Pseudo-binary Systems

Al-Ba-O Al₂O₃-BaO

- Introducing two new stoichiometric compounds in the BaO-rich region, AL2BA4O7(S), and AL2BA7O10(S)

Al-La-O Al₂O₃-La₂O₃

- Improvement of AlLaO₃ thermodynamic properties.

Al-O-Sr Al₂O₃-SrO

- Al₁₂SrO₁₉ melts congruently whereas its decomposition was previously considered to be peritectic.

Ba-O-Si BaO-SiO₂

- Additional compound in the BaO-rich part, BA3O5SI1(S).

Ca-O-Sr CaO-SrO

- Improvement with consideration of new experimental data.

Ca-O-Zr CaO-ZrO₂

- Description of the solubility of CaO in the ZrO₂ tetragonal phase, and the solubility of ZrO₂ in the CaO FCC_B1.

In-O-Zr In₂O₃-ZrO₂

- Improvement of the modeling in the zirconia-rich region.

La-O-U La₂O₃-UO₂

- Improvement of the oxygen potential above the solid solution FCC_C1.

La-O-Si La_2O_3 - SiO_2

- Improvement of the thermodynamic properties of $\text{La}_2\text{Si}_2\text{O}_7$

O-Si-Sr SiO_2 -SrO

- Improvement with consideration of new experimental data.

O-Si-Zr SiO_2 - ZrO_2

- Improvement of the description of the ZrSiO_4 compound (thermodynamic properties and decomposition temperature)

Ternary Systems

- C-O-Zr: Improvement with consideration of new experimental data.
- Cr-O-Zr: Modeling of the ternary system in the metallic-oxidic part.
- Reassessment of the Fe-O-U, Fe-O-Zr, and O-U-Zr systems.

Pseudo-ternary Systems

Ca-O-Si-Zr: Modeling of the $\text{CaO-SiO}_2\text{-ZrO}_2$ pseudo-ternary system

NUCL10 (NUCLEA-10) to NUCL15 (NUCLEA-15)

IRSN NUCLEA- Nuclear Alloys-Oxides Database (NUCL15_4)

Software release version: 2017a (March 2017)

Binary Systems

The description of some binary systems are improved:

- Ag-Al: improved limits of the FCC_A1+HCP_A3 biphasic domain.
- Ag-B: added LIQUID miscibility gap.
- Al-In: improved limits of the LIQUID miscibility gap.
- Al-Zr: added $\text{Al}_3\text{Zr}_4(\text{S})$ and improved modeling of the stoichiometric condensed phases.
- B-C: BETA_B decomposition changed to peritectic.
- C-U: $\text{C}_3\text{U}_2(\text{S})$ made unstable at low temperature.

- Cr-La: improved modeling of LIQUID.
- Cr-O: improved modeling of LIQUID.
- In-Zr: added In1Zr1(S), In2Zr1(S), In1Zr2(S); In3Zr1(S) decomposition changed to peritectic.
- La -Ni: added La5Ni19(S).

Ternary Systems

The description of some ternary systems are improved:

- Al-O-Fe: Al_2FeO_4 decomposition changed to peritectic in $\text{AlO}_{1.5}$ -FeO; SPINEL domain extended in $\text{AlO}_{1.5}$ -FeO $_{1.5}$.
- Ca-Cr-O: added assessment of CaO-CrO-Cr $_2$ O $_3$ for oxygen partial pressures ranging from equilibrium with metallic chromium to $P_{\text{O}_2} = 10^{-3}$ atm.
- Cr-O-Si: added assessment of CrO-Cr $_2$ O $_3$ -SiO $_2$ for oxygen partial pressures ranging from equilibrium with metallic chromium to $P_{\text{O}_2} = 0.21$ atm.
- Ni-O-Si: improved limits of the LIQUID miscibility gap in NiO-SiO $_2$; improved modeling of Ni $_2$ O $_4$ Si1(S).

Quaternary Systems

The description of some quaternary systems are improved:

- Al-Ca-Fe-O: added assessments of Al $_2$ O $_3$ -CaO-Fe $_2$ O $_3$ and Al $_2$ O $_3$ -CaO-FeO.
- Al-Fe-O-Si: added assessments of Al $_2$ O $_3$ -Fe $_2$ O $_3$ -SiO $_2$ and Al $_2$ O $_3$ -FeO-SiO $_2$.
- Ca-Cr-O-Si: improved assessment of CaO-CrO-Cr $_2$ O $_3$ for reducing conditions and for oxidizing conditions at low CaO-content; added Ca $_3$ Cr $_2$ O $_{12}$ Si $_3$ (Uvarovite), Ca $_5$ Cr $_5$ O $_{50}$ Si $_20$ (Gillespite).

IRSN NUCLEA-20 Nuclear Alloys-Oxides Database (NUCL20)

Overview Including Phase and System Information

Available Starting with Thermo-Calc Version 2022b



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Overview of NUCLEA-20

January 10, 2022

1 General Description

1.1 Atoms

18 + 2 atoms

U, O, Zr	fuel element
Ag, In, B, C	control rod
Fe, Cr, Ni	vessel and internal structure
Si, Mg, Al, Ca	concrete
Ba, La, Ru, Sr	fission products
Ar, H	gas

1.2 Stoichiometric Condensed Phases

NTB name	TDB name
AG1BA1 (S)	AG1BA1_S
AG2BA1 (S)	AG2BA1_S
AG2BA3 (S)	AG2BA3_S
AG5BA1 (S)	AG5BA1_S
AG2C1O3 (S)	AG2C1O3_S
AG1CA1 (S)	AG1CA1_S
AG1CA3 (S)	AG1CA3_S
AG2CA1 (S)	AG2CA1_S
AG3CA5 (S)	AG3CA5_S
AG7CA2 (S)	AG7CA2_S
AG9CA2 (S)	AG9CA2_S
AG2CR1O4 (S)	AG2CR1O4_S
AG1IN2 (S)	AG1IN2_S
AG2IN1 (S)	AG2IN1_S
AG3IN1 (S)	AG3IN1_S
AG1LA1 (S)	AG1LA1_S
AG2LA1 (S)	AG2LA1_S
AG5LA1 (S)	AG5LA1_S
AG46LA14 (S)	AG46LA14_S
AG1MG3 (S)	AG1MG3_S
AG3MG1 (S)	AG3MG1_S
AG2O1 (S)	AG2O1_S
AG1SR1 (S)	AG1SR1_S
AG2SR1 (S)	AG2SR1_S
AG2SR3 (S)	AG2SR3_S
AG4SR1 (S)	AG4SR1_S
AG5SR1 (S)	AG5SR1_S
AG1ZR1 (S)	AG1ZR1_S
AG1ZR2 (S)	AG1ZR2_S
AL1B2 (S)	AL1B2_S

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NTB name	TDB name
AL1B10 (S)	AL1B10_S
AL1B12 (S)	AL1B12_S
AL4B2O9 (S)	AL4B2O9_S
AL4BA1 (S)	AL4BA1_S
AL5BA4 (S)	AL5BA4_S
AL13BA7 (S)	AL13BA7_S
AL2BA1O4 (S)	AL2BA1O4_S
AL2BA3O6 (S)	AL2BA3O6_S
AL2BA4O7 (S)	AL2BA4O7_S
AL2BA7O10 (S)	AL2BA7O10_S
AL12BA1O19 (S)	AL12BA1O19_S
AL4C3 (S)	AL4C3_S
AL4C4SI1 (S)	AL4C4SI1_S
AL8C7SI1 (S)	AL8C7SI1_S
AL1CA1 (S)	AL1CA1_S
AL2CA1 (S)	AL2CA1_S03
AL3CA8 (S)	AL3CA8_S
AL4CA1 (S)	AL4CA1_S
AL2CA3H12O12 (S)	AL2CA3H12O12_S
AL2CA4H26O20 (S)	AL2CA4H26O20_S
AL2CA1H4O10SI2 (S)	AL2CA1H4O10SI2_S
AL4CA3MG1O10 (S)	AL4CA3MG1O10_S
AL16CA1MG2O27 (S)	AL16CA1MG2O27_S
AL28CA2MG2O46 (S)	AL28CA2MG2O46_S
AL14CA12O33 (S) Mayenite	AL14CA12O33_S
AL2CA1O8SI2 (S) Anorthite	AL2CA1O8SI2_S
AL2CA2O7SI1 (S) Melilite	AL2CA2O7SI1_S
AL12CA13O35ZR2 (S)	AL12CA13O35ZR2_S
AL2CA1SI2 (S)	AL2CA1SI2_S
AL1CR2 (S)	AL1CR2_S
AL4CR1 (S)	AL4CR1_S
AL8CR5 (S)	AL8CR5_S
AL9CR4 (S)	AL9CR4_S
AL13CR2 (S)	AL13CR2_S
AL2FE1 (S)	AL2FE1_S
AL5FE2 (S)	AL5FE2_S
AL1FE1O3 (S)	AL1FE1O3_S
AL2FE3O12SI3 (S) Almandine	AL2FE3O12SI3_S
AL4FE2O18SI5 (S) Ferrocordierite	AL4FE2O18SI5_S
AL1H3 (S)	AL1H3_S01
AL1H1O2 (S) Boehmite	AL1H1O2_S1
AL1H1O2 (S) Diaspore	AL1H1O2_S2
AL1H3O3 (S) Amorphous	AL1H3O3_S1
AL1H3O3 (S) Hydrargillite	AL1H3O3_S2
AL2H4O9SI2 (S) Dickite	AL2H4O9SI2_S1
AL2H4O9SI2 (S) Halloysite	AL2H4O9SI2_S2
AL2H4O9SI2 (S) Kaolinite	AL2H4O9SI2_S3

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NTB name	TDB name
AL1LA1 (S)	AL1LA1_S02
AL1LA3 (S)	AL1LA3_S
AL2LA1 (S)	AL2LA1_S
AL3LA1 (S)	AL3LA1_S
AL11LA3 (S)	AL11LA3_S
AL12LA5 (S)	AL12LA5_S
AL1LA1O3 (S)	AL1LA1O3_S
AL11LA1O18 (S)	AL11LA1O18_S
AL30MG23 (S)	AL30MG23_S
AL140MG89 (S)	AL140MG89_S
AL4MG2O18SI5 (S) Cordierite	AL4MG2O18SI5_S
AL18MG7O40SI3 (S) Saphirine	AL18MG7O40SI3_S
AL1NI3 (S)	AL1NI3_S
AL3NI1 (S)	AL3NI1_S
AL3NI2 (S)	AL3NI2_S
AL2O4SR1 (S) HT	AL2O4SR1_S1
AL2O4SR1 (S) LT	AL2O4SR1_S2
AL2O6SR3 (S)	AL2O6SR3_S
AL4O7SR1 (S)	AL4O7SR1_S
AL6O23SR14 (S) LT	AL6O23SR14_S1
AL6O23SR14 (S) HT	AL6O23SR14_S2
AL12O19SR1 (S)	AL12O19SR1_S
AL1RU1 (S)	AL1RU1_S
AL2RU1 (S)	AL2RU1_S
AL3RU2 (S)	AL3RU2_S
AL6RU1 (S)	AL6RU1_S
AL13RU4 (S)	AL13RU4_S
AL1SR1 (S)	AL1SR1_S
AL2SR1 (S)	AL2SR1_S
AL4SR1 (S)	AL4SR1_S
AL2U1 (S)	AL2U1_S
AL3U1 (S)	AL3U1_S
AL4U0.9 (S)	AL4U0_9_S
AL1ZR1 (S)	AL1ZR1_S
AL1ZR2 (S)	AL1ZR2_S
AL1ZR3 (S)	AL1ZR3_S
AL2ZR1 (S)	AL2ZR1_S
AL2ZR3 (S)	AL2ZR3_S
AL3ZR1 (S)	AL3ZR1_S
AL3ZR2 (S)	AL3ZR2_S
AL3ZR4 (S)	AL3ZR4_S
AL3ZR5 (S)	AL3ZR5_S
AL4ZR5 (S)	AL4ZR5_S
B6BA1 (S)	B6BA1_S
B2BA1O4 (S)	B2BA1O4_S
B2BA3O6 (S)	B2BA3O6_S
B4BA1O7 (S)	B4BA1O7_S

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NTB name	TDB name
B8BA1O13 (S)	B8BA1O13_S
B1C1U1 (S)	B1C1U1_S
B2C1U1 (S)	B2C1U1_S
B2C7U5 (S)	B2C7U5_S
B6CA1 (S)	B6CA1_S
B2CA1O4 (S)	B2CA1O4_S
B2CA2O5 (S)	B2CA2O5_S
B2CA3O6 (S)	B2CA3O6_S
B4CA1O7 (S)	B4CA1O7_S
B2CA1O8SI2 (S)	B2CA1O8SI2_S
B2CA5O10SI1 (S)	B2CA5O10SI1_S
B1CR1 (S)	B1CR1_S
B1CR2 (S)	B1CR2_S
B2CR1 (S)	B2CR1_S
B3CR5 (S)	B3CR5_S
B4CR1 (S)	B4CR1_S
B4CR3 (S)	B4CR3_S
B1FE1 (S)	B1FE1_S05
B1FE2 (S)	B1FE2_S
B1FE1O3 (S)	B1FE1O3_S
B1FE3O6 (S)	B1FE3O6_S
B2FE1O4 (S)	B2FE1O4_S
B2FE2O5 (S)	B2FE2O5_S
B2FE3O6 (S)	B2FE3O6_S
B2FE3U1 (S)	B2FE3U1_S
B4FE1U1 (S)	B4FE1U1_S
B5H9 (L)	B5H9_L
B10H14 (C) Decaborane	B10H14_S
B1H1O2 (C)	B1H1O2_S
B1H3O3 (S)	B1H3O3_S
B2H4O4 (S)	B2H4O4_S
B3H3O3 (S) Boroxine	B3H3O3_S
B1IN1O3 (S)	B1IN1O3_S
B4LA1 (S)	B4LA1_S
B6LA1 (S)	B6LA1_S
B9LA1 (S)	B9LA1_S
B1LA1O3 (S)	B1LA1O3_S
B1LA3O6 (S)	B1LA3O6_S
B3LA1O6 (S)	B3LA1O6_S
B2MG1 (S)	B2MG1_S
B4MG1 (S)	B4MG1_S07
B7MG1 (S)	B7MG1_S
B2MG2O5 (S)	B2MG2O5_S
B2MG3O6 (S)	B2MG3O6_S
B4MG1O7 (S)	B4MG1O7_S
B1NI1 (S)	B1NI1_S
B1NI2 (S)	B1NI2_S

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NTB name	TDB name
B1NI3 (S)	B1NI3_S
B7NI10 (S)	B7NI10_S
B27NI35 (S)	B27NI35_S
B2NI2O5 (S)	B2NI2O5_S
B2NI3O6 (S)	B2NI3O6_S
B1O1.5 (S)	B1O1_5_S
B2O4SR1 (S)	B2O4SR1_S
B2O5SR2 (S)	B2O5SR2_S
B2O6SR3 (S)	B2O6SR3_S
B4O7SR1 (S)	B4O7SR1_S
B6O10SR1 (S)	B6O10SR1_S
B1RU1 (S)	B1RU1_S
B2RU1 (S)	B2RU1_S
B3RU2 (S)	B3RU2_S
B3RU7 (S)	B3RU7_S
B3SI1 (S)	B3SI1_S
B6SI1 (S)	B6SI1_S
B14SI1 (S)	B14SI1_S
B6SR1 (S)	B6SR1_S
B2U1 (S)	B2U1_S
B4U1 (S)	B4U1_S
B12U1 (S)	B12U1_S
B1ZR1 (S)	B1ZR1_S
B2ZR1 (S)	B2ZR1_S
B4ZR3 (S)	B4ZR3_S
B12ZR1 (S)	B12ZR1_S
BA1C2 (S)	BA1C2_S
BA1C1O3 (C)	BA1C1O3_S
BA1CR1O4 (S)	BA1CR1O4_S
BA1CR2O4 (S)	BA1CR2O4_S
BA3CR2O6 (S)	BA3CR2O6_S
BA1FE2O4 (S)	BA1FE2O4_S
BA1FE12O19 (S)	BA1FE12O19_S
BA2FE2O5 (S)	BA2FE2O5_S
BA2FE6O11 (S)	BA2FE6O11_S
BA7FE4O13 (S)	BA7FE4O13_S
BA1H2 (C)	BA1H2_S08
BA1H2O2 (C)	BA1H2O2_S
BA1IN1 (S)	BA1IN1_S
BA1IN2 (S)	BA1IN2_S09
BA1IN4 (S)	BA1IN4_S
BA5IN2 (S)	BA5IN2_S10
BA5IN3 (S)	BA5IN3_S
BA13IN1 (S)	BA13IN1_S
BA1IN2O4 (S)	BA1IN2O4_S
BA2IN2O5 (S)	BA2IN2O5_S
BA3IN2O6 (S)	BA3IN2O6_S

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NTB name	TDB name
BA4IN6O13 (S)	BA4IN6O13_S
BA5IN2O8 (S)	BA5IN2O8_S
BA1LA2O4 (S)	BA1LA2O4_S
BA1MG2 (S)	BA1MG2_S
BA2MG17 (S)	BA2MG17_S
BA6MG23 (S)	BA6MG23_S
BA1NI1O2 (S)	BA1NI1O2_S
BA3NI1O4 (S)	BA3NI1O4_S
BA1O2 (S)	BA1O2_S
BA1O3SI1 (S)	BA1O3SI1_S
BA1O5SI2 (S)	BA1O5SI2_S
BA2O4SI1 (S)	BA2O4SI1_S
BA2O8SI3 (S)	BA2O8SI3_S
BA3O5SI1 (S)	BA3O5SI1_S
BA3O13SI5 (S)	BA3O13SI5_S
BA5O21SI8 (S)	BA5O21SI8_S
BA1O4U1 (S)	BA1O4U1_S
BA1SI1 (S)	BA1SI1_S
BA1SI2 (S)	BA1SI2_S
BA2SI1 (S)	BA2SI1_S
BA3SI4 (S)	BA3SI4_S
BA5SI3 (S)	BA5SI3_S
C1 (S) Graphite	C_S18
C2CA1 (S)	C2CA1_S12
C2CA1MG1O6 (S)	C2CA1MG1O6_S
C1CA1O3 (C)	C1CA1O3_S
C2CR3 (S)	C2CR3_S
C6CR1O6 (S)	C6CR1O6_S
C1FE1O3 (S)	C1FE1O3_S
C5FE1O5 (L)	C5FE1O5_L
C1H4 (L)	C1H4_L11
C2H6 (L)	C2H6_L13
C3H6 (L)	C3H6_L14
C3H8 (L)	C3H8_L15
C1H2O2 (L)	C1H2O2_L
C1H4O1 (L)	C1H4O1_L
C2H4O2 (L)	C2H4O2_L
C2H6O1 (L)	C2H6O1_L
C2H6O2 (L)	C2H6O2_L
C3H6O1 (L)	C3H6O1_L
C3H6O2 (L)	C3H6O2_L
C3H8O1 (L)	C3H8O1_L
C3H8O3 (L)	C3H8O3_L
C2LA1 (S) LT	C2LA1_S
C2MG1 (S)	C2MG1_S
C3MG2 (S)	C3MG2_S
C1MG1O3 (C)	C1MG1O3_S

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NTB name	TDB name
C1NI103 (S)	C1NI103_S
C4NI104 (L)	C4NI104_L
C103SR1 (C)	C103SR1_S
C105U1 (S)	C105U1_S
C2RU1U2 (S)	C2RU1U2_S
C1SI1 (S)	C1SI1_S
C2SI2U3 (S)	C2SI2U3_S
C3SI16U20 (S)	C3SI16U20_S
C2SR1 (S)	C2SR1_S
C3U2 (S)	C3U2_S
CA1CR104 (S)	CA1CR104_S
CA1CR204 (S) HT	CA1CR204_S1
CA1CR204 (S) LT	CA1CR204_S2
CA2CR13020 (S)	CA2CR13020_S
CA1CR1010SI4 (S) Gillespite	CA1CR1010SI4_S
CA3CR2012SI3 (S) Uvarovite	CA3CR2012SI3_S
CA1FE305 (S) (S)	CA1FE305_S
CA1FE407 (S)	CA1FE407_S
CA1FE507 (S)	CA1FE507_S
CA1FE106SI2 (S) Hedenbergite	CA1FE106SI2_S
CA1H2 (C)	CA1H2_S16
CA2H2MG5024SI8 (S) Tremolite	CA2H2MG5024SI8_S
CA1H2O2 (S)	CA1H2O2_S
CA1H407SI2 (S)	CA1H407SI2_S
CA2H5O10.5SI3 (S)	CA2H5O10_5SI3_S
CA3H6O10SI2 (S)	CA3H6O10SI2_S
CA4H3O11.5SI3 (S)	CA4H3O11_5SI3_S
CA5H6O20SI6 (S)	CA5H6O20SI6_S
CA5H11O22.5SI6 (S)	CA5H11O22_5SI6_S
CA5H21O27.5SI6 (S)	CA5H21O27_5SI6_S
CA6H2O19SI6 (S)	CA6H2O19SI6_S
CA12H14O31SI6 (S)	CA12H14O31SI6_S
CA1IN1 (S)	CA1IN1_S
CA1IN2 (S)	CA1IN2_S
CA3IN1 (S)	CA3IN1_S
CA1MG2 (S)	CA1MG2_S
CA2MG107SI2 (S) Akermanite	CA2MG107SI2_S
CA3MG108SI2 (S) Merwinite	CA3MG108SI2_S
CA1NI2 (S)	CA1NI2_S
CA1NI3 (S)	CA1NI3_S
CA1NI5 (S)	CA1NI5_S
CA2NI7 (S)	CA2NI7_S
CA1O2 (S)	CA1O2_S
CA103SI1 (S) Pseudowollastonite	CA103SI1_S
CA204SI1 (S) Larnite	CA204SI1_S
CA305SI1 (S) Hatrurite	CA305SI1_S
CA307SI2 (S) Rankinite	CA307SI2_S

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NTB name	TDB name
CA2012SI4ZR1 (S)	CA2012SI4ZR1_S
CA309SI2ZR1 (S)	CA309SI2ZR1_S
CA104U1 (S)	CA104U1_S
CA103ZR1 (S)	CA103ZR1_S
CA1SI1 (S)	CA1SI1_S
CA1SI2 (S)	CA1SI2_S
CA2SI1 (S)	CA2SI1_S
CR1LA103 (S)	CR1LA103_S
CR102 (S)	CR102_S
CR103 (C)	CR103_S
CR5012 (S)	CR5012_S
CR8021 (S)	CR8021_S
CR301ZR3 (S)	CR301ZR3_S
CR2RU1 (S)	CR2RU1_S
CR3RU1 (S)	CR3RU1_S
CR1SI1 (S)	CR1SI1_S
CR1SI2 (S)	CR1SI2_S
CR3SI1 (S)	CR3SI1_S
CR5SI3 (S)	CR5SI3_S
FE1H102 (S) Goethite	FE1H102_S
FE1H202 (S)	FE1H202_S
FE1H303 (S)	FE1H303_S
FE1LA103 (S)	FE1LA103_S
FE12LA1019.5 (S)	FE12LA1019_5_S
FE1NI3 (S)	FE1NI3_S
FE205SR2 (S)	FE205SR2_S
FE206SR3 (S)	FE206SR3_S
FE10022SR7 (S)	FE10022SR7_S
FE12019SR1 (S)	FE12019SR1_S
FE104U1 (S)	FE104U1_S
FE1SI1 (S)	FE1SI1_S
FE1SI2 (S)	FE1SI2_S
FE2SI1 (S)	FE2SI1_S
FE3SI7 (S)	FE3SI7_S
FE5SI3 (S)	FE5SI3_S
FE1U6 (S)	FE1U6_S
FE4U3ZR5 (S)	FE4U3ZR5_S
FE6U71ZR23 (S)	FE6U71ZR23_S
FE25U9ZR16 (S)	FE25U9ZR16_S
FE1ZR2 (S)	FE1ZR2_S
FE1ZR3 (S)	FE1ZR3_S
FE73ZR27 (S)	FE73ZR27_S
H2LA1 (S)	H2LA1_S
H3LA103 (S)	H3LA103_S
H2MG1 (S)	H2MG1_S19
H2MG102 (S)	H2MG102_S
H2MG3012SI4 (S)	H2MG3012SI4_S

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NTB name	TDB name
H2MG7O24SI8 (S)	H2MG7O24SI8_S
H4MG3O9SI2 (S)	H4MG3O9SI2_S
H2O1 (L)	H2O1_L
H2O2SR1 (C)	H2O2SR1_S
H2O4U1 (S)	H2O4U1_S
H4O5U1 (S)	H4O5U1_S
H6SI2 (S)	H6SI2_S
H2SR1 (C)	H2SR1_S
H3U1 (S)	H3U1_S
H2ZR1 (S)	H2ZR1_S
IN1LA1 (S)	IN1LA1_S
IN1LA2 (S)	IN1LA2_S
IN1LA3 (S)	IN1LA3_S
IN2LA1 (S)	IN2LA1_S
IN3LA1 (S)	IN3LA1_S
IN5LA3 (S)	IN5LA3_S
IN1MG2 (S)	IN1MG2_S
IN1MG3 (S)	IN1MG3_S
IN2MG5 (S)	IN2MG5_S
IN7MG3 (S)	IN7MG3_S
IN1NI1 (S)	IN1NI1_S
IN1NI2 (S)	IN1NI2_S
IN1NI3 (S)	IN1NI3_S
IN3NI2 (S)	IN3NI2_S
IN7NI3 (S)	IN7NI3_S
IN21NI29 (S)	IN21NI29_S
IN2O3 (S)	IN2O3_S
IN2O4SR1 (S)	IN2O4SR1_S
IN1SR1 (S)	IN1SR1_S
IN1SR3 (S)	IN1SR3_S
IN2SR1 (S)	IN2SR1_S
IN2SR3 (S)	IN2SR3_S
IN3SR1 (S)	IN3SR1_S
IN3SR2 (S)	IN3SR2_S
IN5SR1 (S)	IN5SR1_S
IN5SR2 (S)	IN5SR2_S
IN3U1 (S)	IN3U1_S
IN1ZR1 (S)	IN1ZR1_S
IN1ZR2 (S)	IN1ZR2_S
IN1ZR3 (S)	IN1ZR3_S
IN2ZR1 (S)	IN2ZR1_S
IN3ZR1 (S)	IN3ZR1_S
LA1MG1 (S)	LA1MG1_S20
LA1MG2 (S)	LA1MG2_S
LA1MG12 (S)	LA1MG12_S
LA2MG17 (S)	LA2MG17_S
LA5MG41 (S)	LA5MG41_S

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NTB name	TDB name
LA1NI1 (S)	LA1NI1_S
LA1NI3 (S)	LA1NI3_S
LA1NI5 (S)	LA1NI5_S
LA2NI3 (S)	LA2NI3_S
LA2NI7 (S)	LA2NI7_S
LA3NI1 (S)	LA3NI1_S
LA5NI19 (S)	LA5NI19_S
LA7NI3 (S)	LA7NI3_S
LA7NI16 (S)	LA7NI16_S
LA2O5SI1 (S)	LA2O5SI1_S
LA2O7SI2 (S)	LA2O7SI2_S
LA4O12SI3 (S)	LA4O12SI3_S
LA4O7SR1 (S)	LA4O7SR1_S
LA4O9SR3 (S)	LA4O9SR3_S
LA2O5ZR1 (S)	LA2O5ZR1_S
LA2O7ZR2 (S)	LA2O7ZR2_S
LA1RU2 (S)	LA1RU2_S
LA3RU1 (S)	LA3RU1_S
LA5RU2 (S)	LA5RU2_S
LA5RU3 (S)	LA5RU3_S
LA7RU3 (S)	LA7RU3_S
LA1SI1 (S)	LA1SI1_S
LA1SI2 (S)	LA1SI2_S
LA3SI2 (S)	LA3SI2_S
MG1NI2 (S)	MG1NI2_S
MG2NI1 (S)	MG2NI1_S
MG1O3SI1 (S) Clinoenstatite	MG1O3SI1_S1
MG1O3SI1 (S) Enstatite	MG1O3SI1_S2
MG1O3SI1 (S) Proenstatite	MG1O3SI1_S3
MG1O4U1 (S)	MG1O4U1_S
MG2SI1 (S)	MG2SI1_S
MG2SR1 (S)	MG2SR1_S
MG17SR2 (S)	MG17SR2_S
MG23SR6 (S)	MG23SR6_S
MG38SR9 (S)	MG38SR9_S
NI2O4SI1 (S)	NI2O4SI1_S
NI1SI1 (S)	NI1SI1_S
NI2SI1 (S)	NI2SI1_S
NI3SI1 (S) HT	NI3SI1_S1
NI3SI1 (S) MT	NI3SI1_S2
NI3SI2 (S)	NI3SI2_S
NI7SI13 (S)	NI7SI13_S
NI29SI9 (S) LT	NI29SI9_S
NI31SI12 (S)	NI31SI12_S
NI1SR1 (S)	NI1SR1_S
NI1U6 (S)	NI1U6_S
NI2U1 (S)	NI2U1_S

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NTB name	TDB name
NI5U1 (S)	NI5U1_S
NI7U5 (S)	NI7U5_S
NI9U7 (S)	NI9U7_S
NI39U11 (S)	NI39U11_S
NI77U23 (S)	NI77U23_S
NI1ZR1 (S)	NI1ZR1_S
NI1ZR2 (S)	NI1ZR2_S
NI3ZR1 (S)	NI3ZR1_S
NI5ZR1 (S)	NI5ZR1_S
NI7ZR2 (S)	NI7ZR2_S
NI11ZR9 (S)	NI11ZR9_S
NI21ZR8 (S)	NI21ZR8_S
NI23ZR17 (S)	NI23ZR17_S
O2RU1 (S)	O2RU1_S
O2SI1 (S) Cristobalite	O2SI1_S1
O2SI1 (S) Quartz_HT	O2SI1_S2
O2SI1 (S) Quartz_LT	O2SI1_S3
O2SI1 (S) Tridymite	O2SI1_S4
O3SI1SR1 (S)	O3SI1SR1_S
O4SI1SR2 (S)	O4SI1SR2_S
O5SI1SR3 (S)	O5SI1SR3_S
O2SR1 (S)	O2SR1_S
O4SR2ZR1 (S)	O4SR2ZR1_S
O7SR3ZR2 (S)	O7SR3ZR2_S
O3U1 (S)	O3U1_S
O8U3 (S)	O8U3_S
O9U4 (S)	O9U4_S
O2ZR1 (S) Monoclinic	O2ZR1_S
RU1SI1 (S)	RU1SI1_S
RU2SI1 (S)	RU2SI1_S
RU2SI3 (S)	RU2SI3_S
RU4SI3 (S)	RU4SI3_S
RU5SI3 (S)	RU5SI3_S
RU1U2 (S)	RU1U2_S
RU4U3 (S)	RU4U3_S
RU5U3 (S)	RU5U3_S
RU12U13 (S) LT	RU12U13_S1
RU12U13 (S) HT	RU12U13_S2
RU1ZR1 (S)	RU1ZR1_S
RU2ZR1 (S)	RU2ZR1_S
SI1SR1 (S)	SI1SR1_S
SI1SR2 (S)	SI1SR2_S
SI2SR1 (S) LT	SI2SR1_S
SI3SR5 (S)	SI3SR5_S
SI1U3 (S) HT	SI1U3_S1
SI1U3 (S) LT	SI1U3_S2
SI1.88U1 (S)	SI1_88U1_S

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NTB name	TDB name
SI3U1 (S)	SI3U1_S
SI5U3 (S)	SI5U3_S
SI511U489 (S)	SI511U489_S
SI1ZR1 (S)	SI1ZR1_S
SI1ZR2 (S)	SI1ZR2_S
SI1ZR3 (S)	SI1ZR3_S
SI2ZR1 (S)	SI2ZR1_S
SI2ZR3 (S)	SI2ZR3_S
SI3ZR5 (S)	SI3ZR5_S
SI4ZR5 (S)	SI4ZR5_S

1.3 Condensed Solutions

NTB name	mult	atoms	TDB name
ALPHAP_C2S	1	Ca, O, Si, Mg	ALPHAP_C2S
ALPHA_C2S	1	Ca, O, Si, Mg	ALPHA_C2S_SS04
Al12Mg17_SS	1	Al, Mg	Al12Mg17_SS
Al13Fe4_SS	1	Al, Fe	Al13Fe4_SS
Al8Fe5_SS	1	Al, Fe	Al8Fe5_SS
B4C	1	B, C	B4C_SS06
BCC_A2 (1)	2	Al, C, Cr, Fe, In, La, Mg, Ni, Ru, Si, U, Zr	BCC_A2_1
BCC_A2 (2)	2	Ag, C, Al, Cr, Fe, In, Ni, Ru, Si, U, Zr, O	BCC_A2_2
BCC_A2 (3)	1	Ba, Ca, Sr	BCC_A2_3
BCC_A2 (4)	1	Ag, C, Ca, In, La, Mg	BCC_A2_4
BCC_A2 (5)	1	In, Ni	BCC_A2_5
BCC_A2 (6)	1	Ag, Al, In, Mg	BCC_A2_6
BCT_U	1	C, U, O	BCT_U
BETA_B	1	B, C, Si	BETA_B
C2AF	1	Al, Ca, O, Fe	C2AF
C2La_SS	1	C, La	C2La_SS
C3AF	1	Al, Ca, O, Fe	C3AF
C3La2_SS	1	C, La	C3La2_SS
CA2F2	1	Al, Ca, O, Fe	CA2F2
CA6F6	1	Al, Ca, O, Fe	CA6F6
CAF	2	Al, Ca, O, Fe	CAF_SS17
CAF3	1	Al, Ca, O, Fe	CAF3
CC_La2O3	1	Ba, O, Ca, La, Sr, Zr	CC_La2O3
CEMENTITE	1	B, Cr, Fe, Ni, C	CEMENTITE
CORUNDUM	2	Al, O, Cr, Fe, Zr	CORUNDUM
CUB_A13	1	Ag, Al	CUB_A13
DELTA_UZr2	1	U, Zr	DELTA_UZr2
DHCP	1	La, Mg	DHCP
DIA_A4	1	B, Ru, Si, Sr	DIA_A4
DIOPSIDE	1	Ca, Mg, O, Si	DIOPSIDE
FCC_A1 (1)	1	Ag, C, Al, Cr, Fe, In, Ni, Ru, Si, U, Zr	FCC_A1_1

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NTB name	mult	atoms	TDB name
FCC_A1 (2)	1	Ag, Al, In, Mg	FCC_A1_2
FCC_A1 (3)	1	Ba, Ca, La, Sr	FCC_A1_3
FCC_A1 (4)	1	Ag, C, Ba, Ca, In, La, Mg	FCC_A1_4
FCC_B1 (1)	1	Ca, O, Fe, Mg, Ni, Sr	FCC_B1_1
FCC_B1 (2)	1	Al, O, Ca, Cr, Fe, Mg, Ni, Si	FCC_B1_2
FCC_B1 (3)	2	Ba, O, Ca, Fe, Mg, Ni, Sr, Zr	FCC_B1_3
FCC_B1 (4)	2	C, U, Zr, O	FCC_B1_4
FCC_C1	2	Ba, O, Ca, Cr, Fe, In, La, Mg, Sr, U, Zr	FCC_C1
FCC_L10	1	In, Mg	FCC_L10
FCC_L12	1	In, Mg	FCC_L12
HCP_A3 (1)	2	Ag, C, Al, Cr, Fe, In, La, Mg, Ni, Ru, U, Zr, O	HCP_A3_1
HCP_A3 (2)	1	Ag, Al, In	HCP_A3_2
HCP_A3 (3)	1	In, Ni	HCP_A3_3
LAVES_C14	1	Cr, Zr	LAVES_C14
LAVES_C15 (1)	2	Cr, Fe, U, Zr	LAVES_C15_1
LIQUID	3	Ag, Al, O, Si, Ca, B, Ba, La, Sr, C, Cr, Fe, In, Mg, Ni, U, Zr, Ru	LIQUID
LaMg3_SS	1	La, Mg	LaMg3_SS
M23C6_BC	1	B, Fe, C	M23C6_BC
M23C6_CrFeNi	1	C, Cr, Fe, Ni	M23C6_CrFeNi
M7C3	1	C, Cr, Fe, Ni	M7C3
MULLITE	1	Al, B, O, Si	MULLITE
OLIVINE	2	Ca, O, Si, Fe, Mg	OLIVINE
ORT_A20	1	Fe, Si, U, Zr	ORT_A20
PEROVSKITE	1	Ba, O, U, Zr, Sr	PEROVSKITE
Ru3U_SS	1	C, Ru, U	Ru3U_SS
SIGMA	1	Cr, Fe, Ni	SIGMA
SPINEL	1	Al, Fe, O, Mg, Ni, Cr	SPINEL
Si2Sr_SS_HT	1	Si, Sr	Si2Sr_SS_HT
Si2U3_SS	1	C, Si, U	Si2U3_SS
TCHERNOBYLITE	1	O, Si, U, Zr	TCHERNOBYLITE
TET_A6	1	In, Mg	TET_A6
TET_METAL	1	Al, Cr, Fe, Ru, Si, U, Zr	TET_METAL
TET_OXIDE	1	Ba, O, Ca, Cr, Fe, In, La, Mg, U, Zr	TET_OXIDE
WOLLASTONITE	2	Ca, O, Si, Fe, Mg	WOLLASTONITE

1.4 Gas

NTB name	TDB name
AG1 (G)	AG
AG2 (G)	AG2
AG1O1 (G)	AG1O1
AL1 (G)	AL
AL2 (G)	AL2
AL1B1O2 (G)	AL1B1O2
AL1C1 (G)	AL1C1
AL1C2 (G)	AL1C2
AL2C2 (G)	AL2C2
AL1H1 (G)	AL1H1
AL1H2 (G)	AL1H2
AL1H3 (G)	AL1H3
AL1H1O1 (G) 1	AL1H1O1_1
AL1H1O1 (G) 2	AL1H1O1_2
AL1H1O2 (G)	AL1H1O2
AL1H2O2 (G)	AL1H2O2
AL1O1 (G)	AL1O1
AL1O2 (G)	AL1O2
AL2O1 (G)	AL2O1
AL2O2 (G)	AL2O2
AL2O3 (G)	AL2O3
AR1 (G)	AR
B1 (G)	B
B2 (G)	B2
B1BA1O2 (G)	B1BA1O2
B1C1 (G)	B1C1
B1C2 (G)	B1C2
B2C1 (G)	B2C1
B1H1 (G)	B1H1
B1H2 (G)	B1H2
B1H3 (G)	B1H3
B2H6 (G)	B2H6
B5H9 (G)	B5H9
B10H14 (G)	B10H14
B1H1O1 (G) 1	B1H1O1_1
B1H1O1 (G) 2	B1H1O1_2
B1H1O2 (G)	B1H1O2
B1H2O1 (G)	B1H2O1
B1H2O2 (G)	B1H2O2
B1H3O1 (G)	B1H3O1
B1H3O2 (G)	B1H3O2
B1H3O3 (G)	B1H3O3
B2H4O4 (G)	B2H4O4
B3H3O3 (G)	B3H3O3
B3H3O6 (G)	B3H3O6

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NTB name	TDB name
B101 (G)	B101
B102 (G)	B102
B201 (G)	B201
B202 (G)	B202
B203 (G)	B203
B102SR1 (G)	B102SR1
BA1 (G)	BA
BA1H1 (G)	BA1H1
BA1H101 (G)	BA1H101
BA1H202 (G)	BA1H202
BA101 (G)	BA101
BA201 (G)	BA201
C1 (G)	C
C2 (G)	C2
C3 (G)	C3
C4 (G)	C4
C5 (G)	C5
C6CR106 (G)	C6CR106
C5FE105 (G)	C5FE105
C1H1 (G)	C1H1
C1H2 (G)	C1H2
C1H3 (G)	C1H3
C1H4 (G)	C1H4
C2H1 (G)	C2H1
C2H2 (G)	C2H2
C2H3 (G)	C2H3
C2H4 (G)	C2H4
C2H5 (G)	C2H5
C2H6 (G)	C2H6
C3H4 (G) 1	C3H4_1
C3H4 (G) 2	C3H4_2
C3H4 (G) 3	C3H4_3
C3H6 (G) 1	C3H6_1
C3H6 (G) 2	C3H6_2
C3H7 (G) 1	C3H7_1
C3H7 (G) 2	C3H7_2
C3H8 (G)	C3H8
C1H101 (G)	C1H101
C1H102 (G)	C1H102
C1H201 (G)	C1H201
C1H202 (G) C	C1H202_1
C1H202 (G) T	C1H202_2
C1H301 (G) 1	C1H301_1
C1H301 (G) 2	C1H301_2
C1H401 (G)	C1H401
C2H201 (G)	C2H201
C2H202 (G)	C2H202

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NTB name	TDB name
C2H4O1 (G) 1	C2H4O1_1
C2H4O1 (G) 2	C2H4O1_2
C2H4O2 (G) 1	C2H4O2_1
C2H4O2 (G) 2	C2H4O2_2
C2H4O4 (G)	C2H4O4
C2H6O1 (G) 1	C2H6O1_1
C2H6O1 (G) 2	C2H6O1_2
C2H6O2 (G)	C2H6O2
C3H4O1 (G) 1	C3H4O1_1
C3H4O1 (G) 2	C3H4O1_2
C3H4O1 (G) 3	C3H4O1_3
C3H4O2 (G) 1	C3H4O2_1
C3H4O2 (G) 2	C3H4O2_2
C3H4O3 (G)	C3H4O3
C3H6O1 (G) 1	C3H6O1_1
C3H6O1 (G) 2	C3H6O1_2
C3H6O1 (G) 3	C3H6O1_3
C3H6O1 (G) 4	C3H6O1_4
C3H6O1 (G) 5	C3H6O1_5
C3H6O2 (G)	C3H6O2
C3H6O3 (G)	C3H6O3
C3H8O1 (G) 1	C3H8O1_1
C3H8O1 (G) 2	C3H8O1_2
C3H8O1 (G) 3	C3H8O1_3
C2H6O1SI1 (G)	C2H6O1SI1
C2H8SI1 (G)	C2H8SI1
C4NI1O4 (G)	C4NI1O4
C1O1 (G)	C1O1
C1O2 (G)	C1O2
C2O1 (G)	C2O1
C3O2 (G)	C3O2
C1SI1 (G)	C1SI1
C1SI2 (G)	C1SI2
C1SI3 (G)	C1SI3
C1SI4 (G)	C1SI4
C2SI1 (G)	C2SI1
C2SI2 (G)	C2SI2
C2SI3 (G)	C2SI3
CA1 (G)	CA
CA2 (G)	CA2
CA1H1 (G)	CA1H1
CA1H1O1 (G)	CA1H1O1
CA1H2O2 (G)	CA1H2O2
CA1O1 (G)	CA1O1
CR1 (G)	CR
CR2 (G)	CR2
CR1O1 (G)	CR1O1

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NTB name	TDB name
CR102 (G)	CR102
CR103 (G)	CR103
FE1 (G)	FE
FE2 (G)	FE2
FE1H2O2 (G)	FE1H2O2
FE1O1 (G)	FE1O1
H1 (G)	H
H2 (G)	H2
H1IN1 (G)	H1IN1
H1IN1O1 (G)	H1IN1O1
H1MG1 (G)	H1MG1
H1MG1O1 (G)	H1MG1O1
H2MG1O2 (G)	H2MG1O2
H1NI1 (G)	H1NI1
H2NI1O2 (G)	H2NI1O2
H1O1 (G)	H1O1
H1O2 (G)	H1O2
H2O1 (G)	H2O1
H2O2 (G)	H2O2
H1O1RU1 (G)	H1O1RU1
H2O2RU1 (G)	H2O2RU1
H2O3SI1 (G)	H2O3SI1
H4O4SI1 (G)	H4O4SI1
H1O1SR1 (G)	H1O1SR1
H2O2SR1 (G)	H2O2SR1
H1SI1 (G)	H1SI1
H2SI1 (G)	H2SI1
H3SI1 (G)	H3SI1
H4SI1 (G)	H4SI1
H6SI2 (G)	H6SI2
H1SR1 (G)	H1SR1
H1ZR1 (G)	H1ZR1
IN1 (G)	IN
IN2 (G)	IN2
IN1O1 (G)	IN1O1
IN2O1 (G)	IN2O1
LA1 (G)	LA
LA1O1 (G)	LA1O1
LA2O1 (G)	LA2O1
LA2O2 (G)	LA2O2
MG1 (G)	MG
MG2 (G)	MG2
MG1O1 (G)	MG1O1
NI1 (G)	NI
NI1O1 (G)	NI1O1
O1 (G)	O
O2 (G)	O2

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NTB name	TDB name
O3 (G)	O3
O1RU1 (G)	O1RU1
O2RU1 (G)	O2RU1
O3RU1 (G)	O3RU1
O4RU1 (G)	O4RU1
O1SI1 (G)	O1SI1
O2SI1 (G)	O2SI1
O2SI2 (G)	O2SI2
O1SR1 (G)	O1SR1
O1U1 (G)	O1U1
O2U1 (G)	O2U1
O3U1 (G)	O3U1
O1ZR1 (G)	O1ZR1
O2ZR1 (G)	O2ZR1
RU1 (G)	RU
SI1 (G)	SI
SI2 (G)	SI2
SI3 (G)	SI3
SR1 (G)	SR
SR2 (G)	SR2
U1 (G)	U
ZR1 (G)	ZR
ZR2 (G)	ZR2

2 Assessed Systems

2.1 Binary Systems

assessed binary systems								
Ag – Al	Ag – B	Ag – Ba	Ag – C	Ag – Ca	Ag – Cr	Ag – Fe	Ag – In	Ag – La
Ag – Mg	Ag – Ni	Ag – O	Ag – Ru	Ag – Si	Ag – Sr	Ag – U	Ag – Zr	Al – B
Al – Ba	Al – C	Al – Ca	Al – Cr	Al – Fe	Al – In	Al – La	Al – Mg	Al – Ni
Al – O	Al – Ru	Al – Si	Al – Sr	Al – U	Al – Zr	B – Ba	B – C	B – Ca
B – Cr	B – Fe	B – In	B – La	B – Mg	B – Ni	B – O	B – Ru	B – Si
B – Sr	B – U	B – Zr	Ba – C	Ba – Ca	Ba – Cr	Ba – Fe	Ba – In	Ba – La
Ba – Mg	Ba – Ni	Ba – O	Ba – Ru	Ba – Si	Ba – Sr	Ba – U	Ba – Zr	C – Ca
C – Cr	C – Fe	C – In	C – La	C – Mg	C – Ni	C – O	C – Ru	C – Si
C – Sr	C – U	C – Zr	Ca – Cr	Ca – Fe	Ca – In	Ca – La	Ca – Mg	Ca – Ni
Ca – O	Ca – Ru	Ca – Si	Ca – Sr	Ca – U	Ca – Zr	Cr – Fe	Cr – In	Cr – La
Cr – Mg	Cr – Ni	Cr – O	Cr – Si	Cr – Ru	Cr – Sr	Cr – U	Cr – Zr	Fe – In
Fe – La	Fe – Mg	Fe – Ni	Fe – O	Fe – Ru	Fe – Si	Fe – Sr	Fe – U	Fe – Zr
In – La	In – Mg	In – Ni	In – O	In – Ru	In – Si	In – Sr	In – U	In – Zr
La – Mg	La – Ni	La – O	La – Ru	La – Si	La – Sr	La – U	La – Zr	Mg – Ni
Mg – O	Mg – Ru	Mg – Si	Mg – Sr	Mg – U	Mg – Zr	Ni – O	Ni – Ru	Ni – Si
Ni – Sr	Ni – U	Ni – Zr	O – Ru	O – Si	O – Sr	O – U	O – Zr	Ru – Si
Ru – Sr	Ru – U	Ru – Zr	Si – Sr	Si – U	Si – Zr	Sr – U	Sr – Zr	U – Zr

2.2 Ternary Systems

system	assessed sub-systems
Al – B – O	Al ₂ O ₃ – B ₂ O ₃
Al – Ba – O	Al ₂ O ₃ – BaO
Al – Ca – O	Al ₂ O ₃ – CaO
Al – Cr – O	Al ₂ O ₃ – Cr ₂ O ₃
Al – Fe – O	Al ₂ O ₃ – FeO – Fe ₂ O ₃
Al – In – O	Al ₂ O ₃ – In ₂ O ₃
Al – La – O	Al ₂ O ₃ – La ₂ O ₃
Al – Mg – O	Al ₂ O ₃ – MgO
Al – Ni – O	Al ₂ O ₃ – NiO
Al – O – Si	Al ₂ O ₃ – SiO ₂
Al – O – Sr	Al ₂ O ₃ – SrO
Al – O – U	Al ₂ O ₃ – UO ₂
Al – O – Zr	Al ₂ O ₃ – ZrO ₂
B – Ba – O	B ₂ O ₃ – BaO
B – C – Fe	full
B – C – U	full
B – C – Zr	full
B – Ca – O	B ₂ O ₃ – CaO
B – Cr – O	B ₂ O ₃ – Cr ₂ O ₃
B – Fe – O	B ₂ O ₃ – FeO – Fe ₂ O ₃
B – Fe – U	full
B – Fe – Zr	full
B – In – O	B ₂ O ₃ – In ₂ O ₃
B – La – O	B ₂ O ₃ – La ₂ O ₃
B – Mg – O	B ₂ O ₃ – MgO
B – Ni – O	B ₂ O ₃ – NiO
B – O – Si	B ₂ O ₃ – SiO ₂
B – O – Sr	B ₂ O ₃ – SrO
B – O – U	B ₂ O ₃ – UO ₂
B – O – Zr	B ₂ O ₃ – ZrO ₂
Ba – Ca – O	BaO – CaO
Ba – Cr – O	BaO – Cr ₂ O ₃
Ba – Fe – O	BaO – FeO BaO – Fe ₂ O ₃
Ba – In – O	BaO – In ₂ O ₃
Ba – La – O	BaO – La ₂ O ₃
Ba – Mg – O	BaO – MgO
Ba – Ni – O	BaO – NiO
Ba – O – Si	BaO – SiO ₂
Ba – O – Sr	BaO – SrO
Ba – O – U	BaO – UO ₂
Ba – O – Zr	BaO – ZrO ₂
C – Cr – Fe	full
C – Cr – Ni	full
C – Fe – Ni	full
C – O – U	full
C – O – Zr	full
C – U – Zr	full

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system	assessed sub-systems
Ca – Cr – O	CaO – CrO – Cr ₂ O ₃
Ca – Fe – O	CaO – FeO – Fe ₂ O ₃
Ca – In – O	CaO – In ₂ O ₃
Ca – La – O	CaO – La ₂ O ₃
Ca – Mg – O	CaO – MgO
Ca – Ni – O	CaO – NiO
Ca – O – Si	CaO – SiO ₂
Ca – O – Sr	CaO – SrO
Ca – O – U	CaO – UO ₂
Ca – O – Zr	CaO – ZrO ₂
Cr – Fe – O	full
Cr – Fe – Ni	full
Cr – Fe – Zr	full
Cr – In – O	Cr ₂ O ₃ – In ₂ O ₃
Cr – La – O	Cr ₂ O ₃ – La ₂ O ₃
Cr – Mg – O	Cr ₂ O ₃ – MgO
Cr – Ni – O	full
Cr – O – Si	CrO – Cr ₂ O ₃ – SiO ₂
Cr – O – Sr	Cr ₂ O ₃ – SrO
Cr – O – U	Cr ₂ O ₃ – UO ₂
Cr – O – Zr	full
Fe – In – O	FeO – In ₂ O ₃ Fe ₂ O ₃ – In ₂ O ₃
Fe – La – O	FeO – La ₂ O ₃ Fe ₂ O ₃ – La ₂ O ₃
Fe – Mg – O	FeO – MgO Fe ₂ O ₃ – MgO
Fe – Ni – O	full
Fe – O – Si	FeO – Fe ₂ O ₃ – SiO ₂
Fe – O – Sr	FeO – SrO Fe ₂ O ₃ – SrO
Fe – O – U	full
Fe – O – Zr	full
Fe – U – Zr	full
In – La – O	In ₂ O ₃ – La ₂ O ₃
In – Mg – O	In ₂ O ₃ – MgO
In – Ni – O	In ₂ O ₃ – NiO
In – O – Si	In ₂ O ₃ – SiO ₂
In – O – Sr	In ₂ O ₃ – SrO
In – O – U	In ₂ O ₃ – UO ₂
In – O – Zr	In ₂ O ₃ – ZrO ₂
La – Mg – O	La ₂ O ₃ – MgO
La – Ni – O	La ₂ O ₃ – NiO
La – O – Si	La ₂ O ₃ – SiO ₂
La – O – Sr	La ₂ O ₃ – SrO
La – O – U	La ₂ O ₃ – UO ₂
La – O – Zr	La ₂ O ₃ – ZrO ₂
Mg – Ni – O	MgO – NiO
Mg – O – Si	MgO – SiO ₂
Mg – O – Sr	MgO – SrO
Mg – O – U	MgO – UO ₂
Mg – O – Zr	MgO – ZrO ₂

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system	assessed sub-systems
Ni – O – Si	NiO – SiO ₂
Ni – O – Sr	NiO – SrO
Ni – O – U	NiO – UO ₂
Ni – O – Zr	NiO – ZrO ₂
O – Si – Sr	SrO – SiO ₂
O – Si – U	SiO ₂ – UO ₂
O – Si – Zr	SiO ₂ – ZrO ₂
O – Sr – U	SrO – UO ₂
O – Sr – Zr	SrO – ZrO ₂
O – U – Zr	full

2.3 Quaternary Systems

system	assessed sub-systems
Al – B – Ca – O	Al ₂ O ₃ – B ₂ O ₃ – CaO
Al – B – O – Si	Al ₂ O ₃ – B ₂ O ₃ – SiO ₂
Al – B – O – Mg	Al ₂ O ₃ – B ₂ O ₃ – MgO
Al – Ca – Fe – O	Al ₂ O ₃ – CaO – FeO – Fe ₂ O ₃
Al – Ca – O – Si	Al ₂ O ₃ – CaO – SiO ₂
Al – Ca – O – Zr	Al ₂ O ₃ – CaO – ZrO ₂
Al – Fe – O – Si	Al ₂ O ₃ – FeO – Fe ₂ O ₃ – SiO ₂
Al – O – Si – U	Al ₂ O ₃ – SiO ₂ – UO ₂
Al – O – Si – Zr	Al ₂ O ₃ – SiO ₂ – ZrO ₂
Al – O – U – Ar	Al ₂ O ₃ – UO ₂ – ZrO ₂
B – Ca – Mg – O	B ₂ O ₃ – CaO – MgO
B – Ca – O – Si	B ₂ O ₃ – CaO – SiO ₂
B – Mg – O – Si	B ₂ O ₃ – MgO – SiO ₂
Ca – Cr – O – Si	CaO – CrO – Cr ₂ O ₃ – SiO ₂
Ca – Fe – O – Si	CaO – FeO – Fe ₂ O ₃ – SiO ₂
Ca – Mg – O – Zr	CaO – MgO – ZrO ₂
Ca – O – Si – Zr	CaO – SiO ₂ – ZrO ₂
O – Si – U – Zr	SiO ₂ – UO ₂ – ZrO ₂