IRSN Mephista-20 Nuclear Fuels Database (MEPH20)

Technical Information

Available Starting with Thermo-Calc Version 2022b

Document created 3/4/2022

About the IRSN Mephista-20 Nuclear Fuels Database (MEPH20)

IRSN Mephista-20 Nuclear Fuels Database (MEPH20) is a thermodynamic and properties database, owned by IRSN, which can be applied to successfully study fundamental scientific issues and efficiently investigate practical engineering problems in new generation nuclear fuels. It effectively allows you to calculate the thermochemical equilibrium states in nuclear fuels and to utilize the calculation results for enhancing the design and engineering of modern and safety-prioritized nuclear reactors, improving the predictions and treatments of operational accidents and assisting 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 a 15-element framework, +H and +Ar, which are only for the gaseous phase and for hydrides and hydrous oxides/silicates.

MEPH: IRSN Mephista Nuclear Fuels Database Revision History. The current version of the database is MEPH20.

Elements (15+2)

Ar	Ba	C	Ce	Cr	Cs	Fe	H	La	Mo
O	Pu	Ru	Si	Sr	U	Zr			

Phases and Assessed Subsystems

See the *Overview of Mephista-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: *(solid/liquid phases)*	51 phases
Condensed stoichiometric phases: *(solid/liquid substances)*	263 phases
Gaseous mixture phase: *(ideal gaseous mixture)*	165 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, and some simple inorganic/organic substances.

Available Assessments and Evaluations

Binary subsystems: *(metallic alloys, carbides, oxides)*	105
Ternary subsystems: *(metallic alloys, carbides, oxides, silicates)*	61
Quaternary subsystems: *(oxides, silicates)*	2

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 will be 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.

MEPH: IRSN Mephista Nuclear Fuels Database Revision History

Current Database Version

Database name (acronym):	**IRSN Mephista-20 Nuclear Fuels Database (MEPH20)**
Database owner:	**IRSN**
Database version:	**20**

Changes in the Most Recent Database Release

MEPH19 (Mephista-19) to MEPH20 (Mephista-20)

Software release version: 2022b (June 2022)

New Element

- Added element Cr

New Binary Systems

- Added 14 binary systems related to the addition of Cr.

  All X-Cr (with X=Ba, C, Ce, Cs, Fe, La, Mo, O, Pu, Ru, U, Si, Sr, Zr) are modeled.

New Ternary Systems

- Added 6 fully modeled ternary systems related to the addition of Cr.

  Cr-Fe-O, Cr-Fe-Zr, C-Cr-Fe, Ce-Cr-O, Cr-Mo-O, and Cr-O-Zr.

New Pseudo-binary Sections

For the following 5 ternary systems where there is not enough experimental data, only pseudo-binary sections are modeled:

- Ba-Cr-O modeled as BaO − Cr_2O_3
- Cr-La-O modeled as Cr_2O_3 − La_2O
- Cr-O-Si modeled as CrO − SiO_2 and Cr_2O_3-SiO_2
- Cr-O-Sr modeled as Cr_2O_3 − SrO
- Cr-O-U modeled as Cr_2O_3 − UO_2

Previous Releases

MEPH15 (Mephista-15-1) to MEPH19 (Mephista-19)

IRSN Mephista Nuclear Fuels Database (MEPH19)

Software release version: 2021a (January 2021)

Binary Systems

- Cr-Ru and 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
- La-U: Improvement of liquid thermodynamic properties
- La-Zr: N. Mattern et al. Calphad, 52:8–20, 2016.
- 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., Calphad, 35(4):594–600, 2011.
- Si-Zr: Revised to suppress the appearance of a miscibility gap at the liquid state.
- U-Zr: The lattice-stability of U(hcp_A3) available in the Unary 5.0 SGTE database taken into account. Improvement of the modeling of liquid and DELTA_UZr_2 thermodynamic properties

Pseudo-binary Systems

- Ba-O-Si BaO-SiO_2: Additional compound in the BaO-rich part, BA3O5SI1(S).
- La-O-U La_2O_3-UO_2: 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 $La_2Si_2O_7$
- 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.
- Reassessment of the Fe-O-U, Fe-O-Zr, and O-U-Zr systems

MEPH11 (Mephista-11) to MEPH15 (Mephista-15)

IRSN Mephista Nuclear Fuels Database (MEPH15_1)

Software release version: 2017a (March 2017)

Binary Systems

The description of some binary systems are improved:

- C-Pu: improved modeling of the liquidus.
- C-U: C3U2(S) made unstable at low temperature.
- O-Pu: melting temperature of O2Pu1(S) increased and the improved modeling of LIQUID.

Ternary Systems

The description of the following ternary systems are re-assessed by taking into account the previous improvements:

- Ce-O-Pu: revised modeling of CeO_2-PuO_2 and Ce_2O_3-PuO_2.
- Fe-O-Pu: revised modeling of FeO-PuO_2 and Fe_2O_3-PuO_2.
- La-O-Pu: revised modeling of La_2O_3-PuO_2.
- Mo-O -Pu: revised modeling of MoO_3-PuO_2.
- O-Pu -Si: revised modeling of SiO_2-PuO_2.
- O-Pu-Sr: revised modeling of SrO-PuO_2.
- O-Pu-Zr: revised modeling of PuO_2-ZrO_2.
- C-O-Pu: revised modeling of the full system.

The description of some ternary systems are improved:

- O-Pu-U: improved modeling of PuO_2-UO_2; improved modeling of the FCC_C1 miscibility gap.
- Ba-O-Pu: improved modeling of BaO-PuO_2.
- Ba-Mo-O: improved modeling of Ba1Mo1O4 (G).
- C-Pu-U: improved modeling of the full system.

IRSN Mephista-20 Nuclear Fuels Database (MEPH20)

Overview Including Phase and System Information

Available Starting with Thermo-Calc Version 2022b

Document created 2/23/2022

Contents

Overview of Mephista-20

January 10, 2022

1 General Description

1.1 Atoms

15 + 2 atoms

U, Pu, O	fuel
Fe, Si, C, Zr, Cr	cladding
Ba, La, Ru, Sr, Cs, Mo, Ce	fission products
Ar, H	gas

1.2 Stoichiometric Condensed Phases

NTB name	TDB name
BA1C2(S)	**BA1C2_S**
BA1C1O3(C)	**BA1C1O3_S**
BA1CE1O3(S)	**BA1CE1O3_S**
BA1CR1O4(S)	**BA1CR1O4_S**
BA1CR2O4(S)	**BA1CR2O4_S**
BA3CR2O6(S)	**BA3CR2O6_S**
BA1CS2MO2O8(S)	**BA1CS2MO2O8_S**
BA1FE2O4(S)	**BA1FE2O4_S**
BA1FE12O19(S)	**BA1FE12O19_S**
BA2FE2O5(S)	**BA2FE2O5_S**
BA2FE6O11(S)	**BA2FE6O11_S**
BA7FE4O13(S)	**BA7FE4O13_S**
BA1H2(C)	**BA1H2_S01**
BA1H2O2(C)	**BA1H2O2_S**
BA1LA2O4(S)	**BA1LA2O4_S**
BA1MO1O4(S)	**BA1MO1O4_S**
BA1MO2O7(S)	**BA1MO2O7_S**
BA2MO1O5(S)	**BA2MO1O5_S**
BA3MO1O6(S)	**BA3MO1O6_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**

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NTB name	TDB name
BA2SI1(S)	BA2SI1_S
BA3SI4(S)	BA3SI4_S
BA5SI3(S)	BA5SI3_S
C1(GRA_HEX_A9)	C_S11
C2CE1(S)	C2CE1_S
C3CE2(S)	C3CE2_S
C2CR3(M3C2)(C-CR-FE-NI)	C2CR3_S
C6CR1O6(S)	C6CR1O6_S
C8CS1(S)	C8CS1_S
C10CS1(S)	C10CS1_S
C24CS1(S)	C24CS1_S
C36CS1(S)	C36CS1_S
C48CS1(S)	C48CS1_S
C60CS1(S)	C60CS1_S
C1CS2O3(S)	C1CS2O3_S
C1FE1O3(S)	C1FE1O3_S
C5FE1O5(L)	C5FE1O5_L
C1H4(L)	C1H4_L02
C2H6(L)	C2H6_L04
C3H6(L)	C3H6_L05
C3H8(L)	C3H8_L06
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
C1MO1(S)	C1MO1_S03
C1MO1O6(S)	C1MO1O6_S
C6MO1O6(S)	C6MO1O6_S
C1.7MO1U1(S)	C1_7MO1U1_S
C2MO1U1(S)	C2MO1U1_S
C1O3SR1(C)	C1O3SR1_S
C1O5U1(S)	C1O5U1_S
C0.4PU0.6(S)	C0_4PU0_6_S
C2RU1U2(S)	C2RU1U2_S
C1SI1(S)	C1SI1_S
C2SI2U3(S)	C2SI2U3_S
C3SI16U20(S)	C3SI16U20_S
C2SR1(S)	C2SR1_S
CE1CR1O3(S)	CE1CR1O3_S
CE1FE2(S)	CE1FE2_S
CE2FE17(S)	CE2FE17_S

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NTB name	TDB name
CE1FE1O3(S)	CE1FE1O3_S
CE1MO2O8(S)	CE1MO2O8_S
CE2MO3O13(S)	CE2MO3O13_S
CE5O9(S)	CE5O9_S
CE7O12(S	CE7O12_S
CE11O20(S)	CE11O20_S
CE19O34(S)	CE19O34_S
CE26O47(S)	CE26O47_S
CE2O5SI1(S)	CE2O5SI1_S
CE2O7SI2(S)	CE2O7SI2_S
CE14O39SI9(S)	CE14O39SI9_S
CE1O3SR1(S)	CE1O3SR1_S
CE2O7ZR2(S)	CE2O7ZR2_S
CE1RU2(S)	CE1RU2_S
CE3RU1(S)	CE3RU1_S
CE4RU3(S)	CE4RU3_S
CE7RU3(S)	CE7RU3_S
CE16RU9(S)	CE16RU9_S
CE1SI1(S)	CE1SI1_S
CE1SI2(S)	CE1SI2_S
CE3SI2(S)	CE3SI2_S
CE3SI5(S)	CE3SI5_S
CE5SI3(S)	CE5SI3_S
CE5SI4(S)	CE5SI4_S
CR1LA1O3(S)	CR1LA1O3_S
CR1O2(S)	CR1O2_S
CR1O3(C)	CR1O3_S
CR5O12(S)	CR5O12_S
CR8O21(S)	CR8O21_S
CR3O1ZR3(S)	CR3O1ZR3_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
CS1(BCC_A2)	CS_S10
CS1H1(S)	CS1H1_S07
CS1H1O1(C)	CS1H1O1_S
CS2MO2O7(S)	CS2MO2O7_S
CS2MO3O10(S)	CS2MO3O10_S
CS2MO4O13(S)	CS2MO4O13_S
CS2MO5O16(S)	CS2MO5O16_S
CS2MO7O22(S)	CS2MO7O22_S
CS1O2(S)	CS1O2_S
CS2O1(S)	CS2O1_S08
CS2O2(S)	CS2O2_S09

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NTB name	TDB name
CS7O1(S)	CS7O1_S
CS2O4RU1(S)	CS2O4RU1_S
CS2O3SI1(C)	CS2O3SI1_S
CS2O5SI2(C)	CS2O5SI2_S
CS2O9SI4(C)	CS2O9SI4_S
CS2O3.56U1(S)	CS2O3_56U1_S
CS2O4U1(S)	CS2O4U1_S
CS2O7U2(S)	CS2O7U2_S
CS2O12U4(S)	CS2O12U4_S
CS2O13U4(S)	CS2O13U4_S
CS2O16U5(S)	CS2O16U5_S
CS2O18U6(S)	CS2O18U6_S
CS2O22U7(S)	CS2O22U7_S
CS2O27U9(S)	CS2O27U9_S
CS2O46U15(S)	CS2O46U15_S
CS4O17U5(S)	CS4O17U5_S
CS2O3ZR1(S)	CS2O3ZR1_S
CS4O4ZR1(S)	CS4O4ZR1_S
CS4O16ZR7(S)	CS4O16ZR7_S
CS6O17ZR7(S)	CS6O17ZR7_S
FE1H1O2(S)	FE1H1O2_S
FE1H2O2(S)	FE1H2O2_S
FE1H3O3(S)	FE1H3O3_S
FE1LA1O3(S)	FE1LA1O3_S
FE12LA1O19.5(S)	FE12LA1O19_5_S
FE2MO1(S)Laves_C14	FE2MO1_S
FE1MO1O4(S)	FE1MO1O4_S
FE1O3SI1(S)Wollastonite	FE1O3SI1_S
FE2O4SI1(S)Fayalite	FE2O4SI1_S
FE2O5SR2(S)	FE2O5SR2_S
FE2O6SR3(S)	FE2O6SR3_S
FE10O22SR7(S)	FE10O22SR7_S
FE12O19SR1(S)	FE12O19SR1_S
FE1O4U1(S)	FE1O4U1_S
FE1SI1(S)	FE1SI1_S
FE1SI2(S)	FE1SI2_S
FE2SI1(S)	FE2SI1_S
FE3SI7(S)	FE3SI7_S
FE5SI3(S)	FE5SI3_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
H3LA1O3(S)	H3LA1O3_S

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NTB name	TDB name
H2O1(L)	H2O1_L
H2O2SR1(C)	H2O2SR1_S
H2O4U1(S)	H2O4U1_S
H4O5U1(S)	H4O5U1_S
H2PU1(S)	H2PU1_S
H3PU1(S)	H3PU1_S
H6SI2(S)	H6SI2_S
H2SR1(C)	H2SR1_S
H3U1(S)	H3U1_S
H2ZR1(S)	H2ZR1_S
LA2MO3O12(S)	LA2MO3O12_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
MO1O2(S)	MO1O2_S
MO1O2.75(S)	MO1O2_75_S
MO1O2.875(S)	MO1O2_875_S
MO1O2.889(S)	MO1O2_889_S
MO1O3(S)	MO1O3_S
MO1O4SR1(S)	MO1O4SR1_S
MO2O8ZR1(S)	MO2O8ZR1_S
MO5RU3(S)	MO5RU3_S
MO1SI2(S)	MO1SI2_S
MO3SI1(S)	MO3SI1_S
MO1U2(S)	MO1U2_S
O3PU2(S)	O3PU2_S
O3.04PU2(S)	O3_04PU2_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

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NTB name	TDB name
O2SR1(S)	O2SR1_S
O4SR2ZR1(S)	O4SR2ZR1_S
O7SR3ZR2(S)	O7SR3ZR2_S
O3U1(S)	O3U1_S
O8U3(S)	O8U3_S
O9U4(S)	O9U4_S
PU1RU1(S)	PU1RU1_S
PU1RU2(S)	PU1RU2_S
PU3RU1(S)	PU3RU1_S
PU5RU3(S)	PU5RU3_S
PU19RU1(S)	PU19RU1_S
PU1SI1(S)	PU1SI1_S
PU1SI2(S)	PU1SI2_S
PU3SI2(S)	PU3SI2_S
PU3SI5(S)	PU3SI5_S
PU5SI3(S)	PU5SI3_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
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
ALPHA_Ce2O3	1	Ce, O	**ALPHA_Ce2O3**
ALPHA_Pu	1	Pu, Zr	**ALPHA_Pu**
BCC_A2	3	Ba, C, Ce, Cr, Fe, La, Mo, Pu, Ru, Si, Sr, U, Zr, O	**BCC_A2**
BCT_U	1	C, U, O	**BCT_U**
BETA_Pu	1	Pu, U, Zr	**BETA_Pu**
C2La_SS	1	C, La	**C2La_SS**
C3La2_SS	1	C, La	**C3La2_SS**
CC_La2O3	1	Ba, O, Ce, La, Sr, Zr	**CC_La2O3**
CEMENTITE	1	C, Cr, Fe, Mo	**CEMENTITE**
CORUNDUM	2	Cr, O, Fe, Zr	**CORUNDUM**
Ce2O3_SS	1	Ce, O, Zr	**Ce2O3_SS**
Cs2MoO4_SS	1	Ba, Mo, O, Cs	**Cs2MoO4_SS**
DELTA_UZr2	1	U, Zr	**DELTA_UZr2**
DHCP	1	Ce, La	**DHCP**
DIA_A4	1	Ru, Si, Sr	**DIA_A4**
DZETA_Pu	1	Pu, U, Zr	**DZETA_Pu**
ETA_CMo	1	C, Mo	**ETA_CMo**
ETA_Pu	1	Pu, U, Zr	**ETA_Pu**
FCC_A1	2	Ba, C, Ce, Cr, Fe, La, Mo, Pu, Ru, Si, Sr, U, Zr	**FCC_A1**
FCC_B1	2	Ba, O, Fe, Sr	**FCC_B1_SS12**
FCC_B1(4)	2	C, Pu, U, Zr, O	**FCC_B1_4**
FCC_C1	2	Ba, O, Ce, Cr, Fe, La, U, Sr, Pu, Zr	**FCC_C1**
FEM6_PuU	1	Fe, Pu, U	**FEM6_PuU**
GAMMA_Pu	1	Pu, U, Zr	**GAMMA_Pu**
HCP_A3	2	C, Ce, Cr, Fe, La, Mo, Pu, Ru, U, Zr, O	**HCP_A3**
KSI_CARBIDE	1	C, Fe, Mo	**KSI_CARBIDE**
LAVES_C14	1	Cr, Zr	**LAVES_C14**
LAVES_C15(1)	2	Cr, Fe, Pu, U, Zr	**LAVES_C15_1**
LAVES_C15(2)	1	Mo, Zr	**LAVES_C15_2**
LIQUID	3	Ba, O, Mo, C, Ce, Cr, Cs, Fe, La, Pu, Si, Sr, U, Zr, Ru	**LIQUID**
M23C6_CrFeMo	1	C, Cr, Fe, Mo	**M23C6_CrFeMo**
M2C3_PuU	1	C, Pu, U	**M2C3_PuU**
M6C	1	C, Cr, Fe, Mo	**M6C**
M7C3	1	C, Cr, Fe, Mo	**M7C3**
MONOCLINIC	1	Ce, O, Pu, Zr	**MONOCLINIC**
MU_FeMo	1	Fe, Mo	**MU_FeMo**
Mo5Si3_SS	1	Mo, Si	**Mo5Si3_SS**
ORT_A20	1	Fe, Pu, Si, U, Zr	**ORT_A20**
PEROVSKITE	2	Ba, Mo, O, Pu, U, Zr, Sr	**PEROVSKITE**
PuO1.61_SS	1	O, Pu	**PuO1_61_SS**
R_FeMo	1	Fe, Mo	**R_FeMo**
Ru3U_SS	1	C, Ru, U	**Ru3U_SS**

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NTB name	mult	atoms	TDB name
SIGMA	1	Cr, Fe, Mo	**SIGMA**
SPINEL	1	Cr, O, Fe	**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	Pu, U, Zr	**TET_A6**
TET_METAL	1	Cr, Fe, Mo, Pu, Ru, Si, U, Zr	**TET_METAL**
TET_OXIDE	1	Ba, O, Ce, Cr, Fe, La, Pu, U, Zr	**TET_OXIDE**
THETA_PuZr	1	Pu, Zr	**THETA_PuZr**

1.4 Gas

NTB name	TDB name
AR1(G)	**AR**
BA1(G)	**BA**
BA1H1(G)	**BA1H1**
BA1H1O1(G)	**BA1H1O1**
BA1H2O2(G)	**BA1H2O2**
BA1MO1O4(G)	**BA1MO1O4**
BA1O1(G)	**BA1O1**
BA2O1(G)	**BA2O1**
C1(G)	**C**
C2(G)	**C2**
C3(G)	**C3**
C4(G)	**C4**
C5(G)	**C5**
C6CR1O6(G)	**C6CR1O6**
C5FE1O5(G)	**C5FE1O5**
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**

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NTB name	TDB name
C1H1O1(G)	C1H1O1
C1H1O2(G)	C1H1O2
C1H2O1(G)	C1H2O1
C1H2O2(G)C	C1H2O2_1
C1H2O2(G)T	C1H2O2_2
C1H3O1(G)1	C1H3O1_1
C1H3O1(G)2	C1H3O1_2
C1H4O1(G)	C1H4O1
C2H2O1(G)	C2H2O1
C2H2O2(G)	C2H2O2
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
C6MO1O6(G)	C6MO1O6
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

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NTB name	TDB name
C2SI3(G)	C2SI3
CE1(G)	CE
CE1O1(G)	CE1O1
CR1(G)	CR
CR2(G)	CR2
CR1O1(G)	CR1O1
CR1O2(G)	CR1O2
CR1O3(G)	CR1O3
CS1(G)	CS
CS2(G)	CS2
CS1H1(G)	CS1H1
CS1H1O1(G)	CS1H1O1
CS2H2O2(G)	CS2H2O2
CS2MO1O4(G)	CS2MO1O4
CS1O1(G)	CS1O1
CS2O1(G)	CS2O1
CS2O2(G)	CS2O2
CS2O4RU1(G)	CS2O4RU1
FE1(G)	FE
FE2(G)	FE2
FE1H2O2(G)	FE1H2O2
FE1O1(G)	FE1O1
H1(G)	H
H2(G)	H2
H1MO3(G)	H1MO3
H1MO1O1(G)	H1MO1O1
H2MO1O2(G)	H2MO1O2
H2MO1O4(G)	H2MO1O4
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
LA1(G)	LA
LA1O1(G)	LA1O1

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NTB name	TDB name
LA2O1 (G)	**LA2O1**
LA2O2 (G)	**LA2O2**
MO1 (G)	**MO**
MO1O1 (G)	**MO1O1**
MO1O2 (G)	**MO1O2**
MO1O3 (G)	**MO1O3**
MO2O6 (G)	**MO2O6**
MO3O9 (G)	**MO3O9**
MO4O12 (G)	**MO4O12**
MO5O15 (G)	**MO5O15**
O1 (G)	**O**
O2 (G)	**O2**
O3 (G)	**O3**
O1PU1 (G)	**O1PU1**
O2PU1 (G)	**O2PU1**
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**
PU1 (G)	**PU**
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						
Ba – C	Ba – Ce	Ba – Cr	Ba – Cs	Ba – Fe	Ba – La	Ba – Mo
Ba – O	Ba – Pu	Ba – Ru	Ba – Si	Ba – Sr	Ba – U	Ba – Zr
C – Ce	C – Cr	C – Cs	C – Fe	C – La	C – Mo	C – O
C – Pu	C – Ru	C – Si	C – Sr	C – U	C – Zr	Ce – Cr
Ce – Cs	Ce – Fe	Ce – La	Ce – Mo	Ce – O	Ce – Pu	Ce – Ru
Ce – Si	Ce – Sr	Ce – U	Ce – Zr	Cr – Cs	Cr – Fe	Cr – La
Cr – Mo	Cr – O	Cr – Pu	Cr – Ru	Cr – Si	Cr – Sr	Cr – U
Cr – Zr	Cs – Fe	Cs – La	Cs – Mo	Cs – O	Cs – Pu	Cs – Ru
Cs – Si	Cs – Sr	Cs – U	Cs – Zr	Fe – La	Fe – Mo	Fe – O
Fe – Pu	Fe – Ru	Fe – Si	Fe – Sr	Fe – U	Fe – Zr	La – Mo
La – O	La – Pu	La – Ru	La – Si	La – Sr	La – U	La – Zr
Mo – O	Mo – Pu	Mo – Ru	Mo – Si	Mo – Sr	Mo – U	Mo – Zr
O – Pu	O – Ru	O – Si	O – Sr	O – U	O – Zr	Pu – Ru
Pu – Si	Pu – Sr	Pu – U	Pu – 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
Ba – Ce – O	$BaO - CeO_2$
Ba – Cr – O	$BaO - Cr_2O_3$
Ba – Fe – O	$BaO - FeO$ $BaO - Fe_2O_3$
Ba – La – O	$BaO - La_2O_3$
Ba – Mo – O	$BaO - MoO_3$
Ba – O – Si	$BaO - SiO_2$
Ba – O – Sr	$BaO - SrO$
Ba – O – U	$BaO - UO_2$
Ba – O – Zr	$BaO - ZrO_2$
Ba – O – Pu	$BaO - PuO_2$
C – Cr – Fe	full
C – Fe – Mo	full
C – O – U	full
C – O – Zr	full
C – O – Pu	full
C – U – Zr	full
C – U – Pu	full
Ce – Cr – O	full
Ce – O – La	$CeO_2 - La_2O_3$
Ce – O – Mo	$CeO_2 - MoO_3$ $Ce_2O_3 - MoO_3$
Ce – O – Pu	$CeO_2 - PuO_2$ $Ce_2O_3 - PuO_2$
Ce – O – Si	$Ce_2O_3 - SiO_2$
Ce – O – Sr	$CeO_2 - SrO$

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system	assessed sub-systems
Ce – O – U	$CeO_2 - UO_2$ $Ce_2O_3 - UO_2$
Ce – O – Zr	$CeO_2 - ZrO_2$ $Ce_2O_3 - ZrO_2$
Cr – Fe – O	full
Cr – Fe – Zr	full
Cr – La – O	$Cr_2O_3 - La_2O_3$
Cr – Mo – O	full
Cr – O – Si	$CrO - Cr_2O_3 - SiO_2$
Cr – O – Sr	$Cr_2O_3 - SrO$
Cr – O – U	$Cr_2O_3 - UO_2$
Cr – O – Zr	full
Cs – Mo – O	$Cs_2MoO_4 - MoO_3$
Fe – La – O	$FeO - La_2O_3$ $Fe_2O_3 - La_2O_3$
Fe – O – Pu	full
Fe – O – Si	$FeO - Fe_2O_3 - SiO_2$
Fe – O – Sr	$FeO - SrO$ $Fe_2O_3 - SrO$
Fe – O – U	full
Fe – O – Zr	full
Fe – Pu – U	full
Fe – Pu – Zr	full
Fe – U – Zr	full
La – O – Pu	$La_2O_3 - PuO_2$
La – O – Si	$La_2O_3 - SiO_2$
La – O – Sr	$La_2O_3 - SrO$
La – O – U	$La_2O_3 - UO_2$
La – O – Zr	$La_2O_3 - ZrO_2$
Mo – O – Pu	$MoO_3 - PuO_2$
Mo – O – Zr	$MoO_3 - ZrO_2$
O – Pu – Si	$SiO_2 - PuO_2$
O – Pu – Sr	$SrO - PuO_2$
O – Pu – U	full
O – Pu – Zr	full
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
Pu – U – Zr	full

2.3 Quaternary Systems

system	assessed sub-systems
Ba – Cs – Mo – O	$BaMoO_4 - Cs_2MoO_4$
O – Si – U – Zr	$SiO_2 - UO_2 - ZrO_2$