

# **IRSN Mephista-19 Nuclear Fuels Database (MEPH19)**

## **Technical Information**

*Available Starting with Thermo-Calc Version 2021a*



## About the IRSN Mephista-19 Nuclear Fuels Database (MEPH19)

### ▶ [MEPH: IRSN Mephista Nuclear Fuels Database Revision History](#)

MEPH19 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 14-element framework, +H and +Ar, which are only for the gaseous phase and for hydrides and hydrous oxides/silicates.

### Elements (14+2)

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

### Phases and Assessed Subsystems



See the *Overview of Mephista-19* 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>	47 phases
Condensed stoichiometric phases: <i>(solid/liquid substances)</i>	242 phases
Gaseous mixture phase: <i>(ideal gaseous mixture)</i>	159 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: ( <i>metallic alloys, carbides, oxides</i> )	91
Ternary subsystems: ( <i>metallic alloys, carbides, oxides, silicates</i> )	50
Quaternary subsystems: ( <i>oxides, silicates</i> )	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 Mephisto Nuclear Fuels Database Revision History

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## Current Database Version

Database name (acronym):	<b>IRSN Mephisto-19 Nuclear Fuels Database (MEPH19)</b>
Database owner:	<b>IRSN</b>
Database version:	<b>19</b>

## Changes in the Most Recent Database Release

### MEPH15 (Mephisto-15-1) to MEPH19 (Mephisto-19)

IRSN Mephisto 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 Ru<sub>3</sub>U compound is now modeled as a solution phase, CxRU<sub>3</sub>U<sub>1</sub> (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<sub>2</sub> thermodynamic properties

#### Pseudo-binary Systems

- Ba-O-Si BaO-SiO<sub>2</sub>: Additional compound in the BaO-rich part, BA3O5Si1(S).
- La-O-U La<sub>2</sub>O<sub>3</sub>-UO<sub>2</sub>: Improvement of the oxygen potential above the solid solution FCC\_C1.
- La-O-Si La<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>: Improvement of the thermodynamic properties of La<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>

- O-Si-Sr  $\text{SiO}_2$ -SrO: Improvement with consideration of new experimental data.
- O-Si-Zr  $\text{SiO}_2$ -ZrO<sub>2</sub>: Improvement of the description of the ZrSiO<sub>4</sub> 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

## Previous Releases

### 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<sub>2</sub>-PuO<sub>2</sub> and Ce<sub>2</sub>O<sub>3</sub>-PuO<sub>2</sub>.
- Fe-O-Pu: revised modeling of FeO-PuO<sub>2</sub> and Fe<sub>2</sub>O<sub>3</sub>-PuO<sub>2</sub>.
- La-O-Pu: revised modeling of La<sub>2</sub>O<sub>3</sub>-PuO<sub>2</sub>.
- Mo-O -Pu: revised modeling of MoO<sub>3</sub>-PuO<sub>2</sub>.
- O-Pu -Si: revised modeling of SiO<sub>2</sub>-PuO<sub>2</sub>.
- O-Pu-Sr: revised modeling of SrO-PuO<sub>2</sub>.
- O-Pu-Zr: revised modeling of PuO<sub>2</sub>-ZrO<sub>2</sub>.
- C-O-Pu: revised modeling of the full system.

The description of some ternary systems are improved:

- O-Pu-U: improved modeling of  $\text{PuO}_2\text{-UO}_2$ ; improved modeling of the FCC\_C1 miscibility gap.
- Ba-O-Pu: improved modeling of BaO-PuO<sub>2</sub>.
- Ba-Mo-O: improved modeling of Ba<sub>1</sub>Mo<sub>10</sub>O<sub>4</sub> (G).
- C-Pu-U: improved modeling of the full system.

## **IRSN Mephista-19 Nuclear Fuels Database (MEPH19)**

### **Overview Including Phase and System Information**

*Available Starting with Thermo-Calc Version 2021a*



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# Overview of Mephisto-19

November 12, 2020

## 1 General Description

### 1.1 Atoms

14 + 2 atoms

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

### 1.2 Stoichiometric Condensed Phases

LatSubSol name	TDB name
<b>BA1C2 (S)</b>	<b>BA1C2</b>
<b>BA1C1O3 (C)</b>	<b>BA1C1O3</b>
<b>BA1CE1O3 (S)</b>	<b>BA1CE1O3</b>
<b>BA1CS2MO2O8 (S)</b>	<b>BA1CS2MO2O8</b>
<b>BA1FE2O4 (S)</b>	<b>BA1FE2O4</b>
<b>BA1FE12O19 (S)</b>	<b>BA1FE12O19</b>
<b>BA2FE2O5 (S)</b>	<b>BA2FE2O5</b>
<b>BA2FE6O11 (S)</b>	<b>BA2FE6O11</b>
<b>BA7FE4O13 (S)</b>	<b>BA7FE4O13</b>
<b>BA1H2 (C)</b>	<b>BA1H2</b>
<b>BA1H2O2 (C)</b>	<b>BA1H2O2</b>
<b>BA1LA2O4 (S)</b>	<b>BA1LA2O4</b>
<b>BA1MO1O4 (S)</b>	<b>BA1MO1O4</b>
<b>BA1MO2O7 (S)</b>	<b>BA1MO2O7</b>
<b>BA2MO1O5 (S)</b>	<b>BA2MO1O5</b>
<b>BA3MO1O6 (S)</b>	<b>BA3MO1O6</b>
<b>BA1O2 (S)</b>	<b>BA1O2</b>
<b>BA1O3SI1 (S)</b>	<b>BA1O3SI1</b>
<b>BA1O5SI2 (S)</b>	<b>BA1O5SI2</b>
<b>BA2O4SI1 (S)</b>	<b>BA2O4SI1</b>
<b>BA2O8SI3 (S)</b>	<b>BA2O8SI3</b>
<b>BA3O5SI1 (S)</b>	<b>BA3O5SI1</b>
<b>BA3O13SI5 (S)</b>	<b>BA3O13SI5</b>
<b>BA5O21SI8 (S)</b>	<b>BA5O21SI8</b>
<b>BA1O4U1 (S)</b>	<b>BA1O4U1</b>
<b>BA1SI1 (S)</b>	<b>BA1SI1</b>
<b>BA1SI2 (S)</b>	<b>BA1SI2</b>
<b>BA2SI1 (S)</b>	<b>BA2SI1</b>
<b>BA3SI4 (S)</b>	<b>BA3SI4</b>
<b>BA5SI3 (S)</b>	<b>BA5SI3</b>

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LatSubSol name	TDB name
C1 (GRA_HEX_A9)	C
C2CE1 (S)	C2CE1
C3CE2 (S)	C3CE2
C8CS1 (S)	C8CS1
C10CS1 (S)	C10CS1
C24CS1 (S)	C24CS1
C36CS1 (S)	C36CS1
C48CS1 (S)	C48CS1
C60CS1 (S)	C60CS1
C1CS2O3 (S)	C1CS2O3
C1FE1O3 (S)	C1FE1O3
C5FE1O5 (L)	C5FE1O5
C1H4 (L)	C1H4
C2H6 (L)	C2H6
C3H6 (L)	C3H6
C3H8 (L)	C3H8
C1H2O2 (L)	C1H2O2
C1H4O1 (L)	C1H4O1
C2H4O2 (L)	C2H4O2
C2H6O1 (L)	C2H6O1
C2H6O2 (L)	C2H6O2
C3H6O1 (L)	C3H6O1
C3H6O2 (L)	C3H6O2
C3H8O1 (L)	C3H8O1
C3H8O3 (L)	C3H8O3
C2LA1 (LT)	C2LA1
C1MO1 (SHP)	C1MO1
C1MO1O6 (S)	C1MO1O6
C6MO1O6 (S)	C6MO1O6
C1.7MO1U1 (S)	C17MO1U1
C2MO1U1 (S)	C2MO1U1
C1O3SR1 (C)	C1O3SR1
C1O5U1 (S)	C1O5U1
C0.4PU0.6 (S)	C04PU06
C2RU1U2 (S)	C2RU1U2
C1SI1 (S)	C1SI1
C2SI2U3 (T1)	C2SI2U3
C3SI16U20 (T2)	C3SI16U20
C2SR1 (S)	C2SR1
CE1FE2 (S)	CE1FE2
CE2FE17 (S)	CE2FE17
CE1FE1O3 (S)	CE1FE1O3
CE1MO2O8 (S)	CE1MO2O8
CE2MO3O13 (S)	CE2MO3O13
CE2O5SI1 (S)	CE2O5SI1
CE2O7SI2 (S)	CE2O7SI2
CE14O39SI9 (S)	CE14O39SI9

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LatSubSol name	TDB name
<b>CE1O3SR1 (S)</b>	<b>CE1O3SR1</b>
<b>CE2O7ZR2 (S)</b>	<b>CE2O7ZR2</b>
<b>CE1RU2 (S)</b>	<b>CE1RU2</b>
<b>CE3RU1 (S)</b>	<b>CE3RU1</b>
<b>CE4RU3 (S)</b>	<b>CE4RU3</b>
<b>CE7RU3 (S)</b>	<b>CE7RU3</b>
<b>CE16RU9 (S)</b>	<b>CE16RU9</b>
<b>CE1SI1 (S)</b>	<b>CE1SI1</b>
<b>CE1SI2 (S)</b>	<b>CE1SI2</b>
<b>CE3SI2 (S)</b>	<b>CE3SI2</b>
<b>CE3SI5 (S)</b>	<b>CE3SI5</b>
<b>CE5SI3 (S)</b>	<b>CE5SI3</b>
<b>CE5SI4 (S)</b>	<b>CE5SI4</b>
<b>CS1 (BCC_A2)</b>	<b>CS</b>
<b>CS1H1 (S)</b>	<b>CS1H1</b>
<b>CS1H1O1 (C)</b>	<b>CS1H1O1</b>
<b>CS2MO2O7 (S)</b>	<b>CS2MO2O7</b>
<b>CS2MO3O10 (S)</b>	<b>CS2MO3O10</b>
<b>CS2MO4O13 (S)</b>	<b>CS2MO4O13</b>
<b>CS2MO5O16 (S)</b>	<b>CS2MO5O16</b>
<b>CS2MO7O22 (S)</b>	<b>CS2MO7O22</b>
<b>CS1O2 (S)</b>	<b>CS1O2</b>
<b>CS2O1 (S)</b>	<b>CS2O1</b>
<b>CS2O2 (S)</b>	<b>CS2O2</b>
<b>CS7O1 (S)</b>	<b>CS7O1</b>
<b>CS2O4RU1 (S)</b>	<b>CS2O4RU1</b>
<b>CS2O3SI1 (C)</b>	<b>CS2O3SI1</b>
<b>CS2O5SI2 (C)</b>	<b>CS2O5SI2</b>
<b>CS2O9SI4 (C)</b>	<b>CS2O9SI4</b>
<b>CS2O3.56U1 (S)</b>	<b>CS2O356U1</b>
<b>CS2O4U1 (S)</b>	<b>CS2O4U1</b>
<b>CS2O7U2 (S)</b>	<b>CS2O7U2</b>
<b>CS2O12U4 (S)</b>	<b>CS2O12U4</b>
<b>CS2O13U4 (S)</b>	<b>CS2O13U4</b>
<b>CS2O16U5 (S)</b>	<b>CS2O16U5</b>
<b>CS2O18U6 (S)</b>	<b>CS2O18U6</b>
<b>CS2O22U7 (S)</b>	<b>CS2O22U7</b>
<b>CS2O27U9 (S)</b>	<b>CS2O27U9</b>
<b>CS2O46U15 (S)</b>	<b>CS2O46U15</b>
<b>CS4O17U5 (S)</b>	<b>CS4O17U5</b>
<b>CS2O3ZR1 (S)</b>	<b>CS2O3ZR1</b>
<b>CS4O4ZR1 (S)</b>	<b>CS4O4ZR1</b>
<b>CS4O16ZR7 (S)</b>	<b>CS4O16ZR7</b>
<b>CS6O17ZR7 (S)</b>	<b>CS6O17ZR7</b>
<b>FE1H1O2 (S)</b>	<b>FE1H1O2</b>
<b>FE1H2O2 (S)</b>	<b>FE1H2O2</b>
<b>FE1H3O3 (S)</b>	<b>FE1H3O3</b>

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LatSubSol name	TDB name
<b>FE2H2O4 (S)</b>	<b>FE2H2O4</b>
<b>FE1LA1O3 (S)</b>	<b>FE1LA1O3</b>
<b>FE12LA1O19.5 (S)</b>	<b>FE12LA1O195</b>
<b>FE2MO1 (LAVES)</b>	<b>FE2MO1</b>
<b>FE1MO1O4 (S)</b>	<b>FE1MO1O4</b>
<b>FE1O1.5 (S)</b>	<b>FE1O15</b>
<b>FE3O4 (S)</b>	<b>FE3O4</b>
<b>FE1O3SI1 (WOLLASTONITE)</b>	<b>FE1O3SI1</b>
<b>FE2O4SI1 (FAYALITE)</b>	<b>FE2O4SI1</b>
<b>FE2O5SR2 (S)</b>	<b>FE2O5SR2</b>
<b>FE2O6SR3 (S)</b>	<b>FE2O6SR3</b>
<b>FE10O22SR7 (S)</b>	<b>FE10O22SR7</b>
<b>FE12O19SR1 (S)</b>	<b>FE12O19SR1</b>
<b>FE1O4U1 (S)</b>	<b>FE1O4U1</b>
<b>FE1SI1 (S)</b>	<b>FE1SI1</b>
<b>FE1SI2 (S)</b>	<b>FE1SI2</b>
<b>FE2SI1 (S)</b>	<b>FE2SI1</b>
<b>FE3SI7 (S)</b>	<b>FE3SI7</b>
<b>FE5SI3 (S)</b>	<b>FE5SI3</b>
<b>FE4U3ZR5 (e)</b>	<b>FE4U3ZR5</b>
<b>FE6U71ZR23 (l)</b>	<b>FE6U71ZR23</b>
<b>FE25U9ZR16 (k)</b>	<b>FE25U9ZR16</b>
<b>FE1ZR2 (S)</b>	<b>FE1ZR2</b>
<b>FE1ZR3 (S)</b>	<b>FE1ZR3</b>
<b>FE73ZR27 (S)</b>	<b>FE73ZR27</b>
<b>H2LA1 (S)</b>	<b>H2LA1</b>
<b>H3LA1O3 (S)</b>	<b>H3LA1O3</b>
<b>H2O1 (L)</b>	<b>H2O1</b>
<b>H2O2SR1 (C)</b>	<b>H2O2SR1</b>
<b>H2O4U1 (S)</b>	<b>H2O4U1</b>
<b>H4O5U1 (S)</b>	<b>H4O5U1</b>
<b>H2PU1 (S)</b>	<b>H2PU1</b>
<b>H3PU1 (S)</b>	<b>H3PU1</b>
<b>H6SI2 (S)</b>	<b>H6SI2</b>
<b>H2SR1 (C)</b>	<b>H2SR1</b>
<b>H3U1 (S)</b>	<b>H3U1</b>
<b>H2ZR1 (S)</b>	<b>H2ZR1</b>
<b>LA2MO3O12 (S)</b>	<b>LA2MO3O12</b>
<b>LA2O5SI1 (S)</b>	<b>LA2O5SI1</b>
<b>LA2O7SI2 (S)</b>	<b>LA2O7SI2</b>
<b>LA4O12SI3 (S)</b>	<b>LA4O12SI3</b>
<b>LA4O7SR1 (S)</b>	<b>LA4O7SR1</b>
<b>LA4O9SR3 (S)</b>	<b>LA4O9SR3</b>
<b>LA2O5ZR1 (S)</b>	<b>LA2O5ZR1</b>
<b>LA2O7ZR2 (S)</b>	<b>LA2O7ZR2</b>
<b>LA1RU2 (S)</b>	<b>LA1RU2</b>
<b>LA3RU1 (S)</b>	<b>LA3RU1</b>

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LatSubSol name	TDB name
LA5RU2 (S)	LA5RU2
LA5RU3 (S)	LA5RU3
LA7RU3 (S)	LA7RU3
LA1SI1 (S)	LA1SI1
LA1SI2 (S)	LA1SI2
LA3SI2 (S)	LA3SI2
MO1O2 (S)	MO1O2
MO1O2.75 (S)	MO1O275
MO1O2.875 (S)	MO1O2875
MO1O2.889 (S)	MO1O2889
MO1O3 (S)	MO1O3
MO1O4SR1 (S)	MO1O4SR1
MO2O8ZR1 (S)	MO2O8ZR1
MO0.333SI0.667 (C11)	MO0333SI0667
MO0.75SI0.25 (M1MO3)	MO075SI025
MO1U2 (S)	MO1U2
O3PU2 (HEXAGONAL)	O3PU2
O3.04PU2 (S)	O304PU2
O2RU1 (S)	O2RU1
O2SI1 (CRISTOBALITE)	O2SI1_1
O2SI1 (H_T_QUARTZ)	O2SI1_2
O2SI1 (L_T_QUARTZ)	O2SI1_3
O2SI1 (TRIDYMITE)	O2SI1_4
O3SI1SR1 (S)	O3SI1SR1
O4SI1SR2 (S)	O4SI1SR2
O5SI1SR3 (S)	O5SI1SR3
O2SR1 (S)	O2SR1
O4SR2ZR1 (S)	O4SR2ZR1
O7SR3ZR2 (S)	O7SR3ZR2
O3U1 (S)	O3U1
O8U3 (S)	O8U3
O9U4 (S)	O9U4
PU1RU1 (S)	PU1RU1
PU1RU2 (S)	PU1RU2
PU3RU1 (S)	PU3RU1
PU5RU3 (S)	PU5RU3
PU19RU1 (S)	PU19RU1
PU1SI1 (S)	PU1SI1
PU1SI2 (S)	PU1SI2
PU3SI2 (S)	PU3SI2
PU3SI5 (S)	PU3SI5
PU5SI3 (S)	PU5SI3
RU1SI1 (S)	RU1SI1
RU2SI1 (S)	RU2SI1
RU2SI3 (S)	RU2SI3
RU4SI3 (S)	RU4SI3
RU5SI3 (S)	RU5SI3

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LatSubSol name	TDB name
<b>RU1U2 (S)</b>	<b>RU1U2</b>
<b>RU4U3 (S)</b>	<b>RU4U3</b>
<b>RU5U3 (S)</b>	<b>RU5U3</b>
<b>RU12U13 (S-L)</b>	<b>RU12U13_1</b>
<b>RU12U13 (S-H)</b>	<b>RU12U13_2</b>
<b>RU1ZR1 (S)</b>	<b>RU1ZR1</b>
<b>RU2ZR1 (S)</b>	<b>RU2ZR1</b>
<b>SI1SR1 (S)</b>	<b>SI1SR1</b>
<b>SI1SR2 (S)</b>	<b>SI1SR2</b>
<b>SI2SR1 (S-A)</b>	<b>SI2SR1</b>
<b>SI3SR5 (S)</b>	<b>SI3SR5</b>
<b>SI1U3 (HIGH_T)</b>	<b>SI1U3_1</b>
<b>SI1U3 (LOW_T)</b>	<b>SI1U3_2</b>
<b>SI1.88U1 (S)</b>	<b>SI188U1</b>
<b>SI3U1 (S)</b>	<b>SI3U1</b>
<b>SI5U3 (S)</b>	<b>SI5U3</b>
<b>SI511U489 (S)</b>	<b>SI511U489</b>
<b>SI1ZR1 (S)</b>	<b>SI1ZR1</b>
<b>SI1ZR2 (S)</b>	<b>SI1ZR2</b>
<b>SI1ZR3 (S)</b>	<b>SI1ZR3</b>
<b>SI2ZR1 (S)</b>	<b>SI2ZR1</b>
<b>SI2ZR3 (S)</b>	<b>SI2ZR3</b>
<b>SI3ZR5 (S)</b>	<b>SI3ZR5</b>
<b>SI4ZR5 (S)</b>	<b>SI4ZR5</b>

### 1.3 Condensed Solutions

LatSubSol name	mult	atoms	TDB name
<b>ALPHA</b>	1	Pu, Zr	<b>ALPHA</b>
<b>BCC</b>	1	O, Pu	<b>BCC</b>
<b>BCC_A2</b>	3	Ba, C, Ce, Fe, La, Mo, Pu, Ru, Si, Sr, U, Zr, O	<b>BCCA2</b>
<b>BCT</b>	1	C, U, O	<b>BCT</b>
<b>BETA</b>	1	Pu, U, Zr	<b>BETA</b>
<b>C-FE-MO (KSI)</b>	1	C, Fe, Mo	<b>CFEMOKSI</b>
<b>C-FE-MO (M3C1_CEM)</b>	1	C, Fe, Mo	<b>CFEMOM3C1CEM</b>
<b>C-FE-MO (M6C1)</b>	1	C, Fe, Mo	<b>CFEMOM6C1</b>
<b>C-MO (ETA)</b>	1	C, Mo	<b>CMOETA</b>
<b>C-PHASE</b>	1	Ce, O	<b>CPHASE</b>
<b>C-PU-U (M2C3)</b>	1	C, Pu, U	<b>CPUUM2C3</b>
<b>C2LA (1+x) (HT)</b>	1	C, La	<b>C2LA1xHT</b>
<b>C3LA (2+x)</b>	1	C, La	<b>C3LA2x</b>
<b>CC</b>	1	Ba, O, Ce, La, Sr, Zr	<b>CC</b>
<b>CE-LA (DHCP)</b>	1	Ce, La	<b>CELADHCP</b>
<b>CE1O1.5 (SS)</b>	1	Ce, O, Zr	<b>CE1O15SS</b>
<b>CS2MOO4 (SS)</b>	1	Ba, Mo, O, Cs	<b>CS2MOO4SS</b>
<b>CxRU3U1 (SS)</b>	1	C, Ru, U	<b>CxRU3U1SS</b>

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LatSubSol name	mult	atoms	TDB name
<b>DELTA</b>	1	U, Zr	<b>DELTA</b>
<b>DIA_A4</b>	1	Ru, Si, Sr	<b>DIAA4</b>
<b>DZETA</b>	1	Pu, U, Zr	<b>DZETA</b>
<b>ETA</b>	1	Pu, U, Zr	<b>ETA</b>
<b>FCC_A1</b>	2	Ba, C, Ce, Fe, La, Mo, Pu, Ru, Si, Sr, U, Zr	<b>FCCA1</b>
<b>FCC_B1</b>	2	Ba, O, Fe, Sr	<b>FCCB1</b>
<b>FCC_B1 (4)</b>	2	C, Pu, U, Zr, O	<b>FCCB14</b>
<b>FCC_C1</b>	2	Ba, O, Ce, Fe, La, U, Sr, Pu, Zr	<b>FCCC1</b>
<b>FE-MO (MU)</b>	1	Fe, Mo	<b>FEMOMU</b>
<b>FE-MO (R)</b>	1	Fe, Mo	<b>FEMOR</b>
<b>FE-MO (SIGMA)</b>	1	Fe, Mo	<b>FEMOSIGMA</b>
<b>FE1M6</b>	1	Fe, Pu, U	<b>FE1M6</b>
<b>GAMMA</b>	1	Pu, U, Zr	<b>GAMMA</b>
<b>HCP_A3</b>	2	C, Fe, La, Mo, Pu, Ru, U, Zr, O	<b>HCPA3</b>
<b>LAVES</b>	2	Fe, Pu, U, Zr	<b>LAVES</b>
<b>LIQUID</b>	3	Ba, O, Mo, C, Ce, Cs, Fe, La, Pu, Si, Sr, U, Zr, Ru	<b>LIQUID</b>
<b>MO-RU (SIGMA1)</b>	1	Mo, Ru	<b>MORUSIGMA1</b>
<b>MO-SI (MO5SI3)</b>	1	Mo, Si	<b>MOSIMO5SI3</b>
<b>MO-ZR (C15)</b>	1	Mo, Zr	<b>MOZRC15</b>
<b>MONOCLINIC</b>	1	Ce, O, Pu, Zr	<b>MONOCLINIC</b>
<b>ORT_A20</b>	1	Fe, Pu, Si, U, Zr	<b>ORTA20</b>
<b>PEROVSKITE</b>	2	Ba, Mo, O, Pu, U, Zr, Sr	<b>PEROVSKITE</b>
<b>SI2SR-B</b>	1	Si, Sr	<b>SI2SRB</b>
<b>SI2U3 (SS)</b>	1	C, Si, U	<b>SI2U3SS</b>
<b>TCHERNOBYLITE</b>	1	O, Si, U, Zr	<b>TCHERNOBYLITE</b>
<b>TET (METAL)</b>	1	Fe, Mo, Pu, Ru, Si, U, Zr	<b>TETMETAL</b>
<b>TET (OXIDE)</b>	1	Ba, O, Ce, Fe, La, Pu, U, Zr	<b>TETOXIDE</b>
<b>TETA</b>	1	Pu, Zr	<b>TETA</b>
<b>TET_A6</b>	1	Pu, U, Zr	<b>TETA6</b>

## 1.4 Gas

LatSubSol name	TDB name
<b>AR1 (G)</b>	<b>AR</b>
<b>BA1 (G)</b>	<b>BA</b>
<b>BA1H1 (G)</b>	<b>BA1H1</b>
<b>BA1H1O1 (G)</b>	<b>BA1H1O1</b>
<b>BA1H2O2 (G)</b>	<b>BA1H2O2</b>
<b>BA1MO1O4 (G)</b>	<b>BA1MO1O4</b>
<b>BA1O1 (G)</b>	<b>BA1O1</b>
<b>BA2O1 (G)</b>	<b>BA2O1</b>
<b>C1 (G)</b>	<b>C</b>
<b>C2 (G)</b>	<b>C2</b>
<b>C3 (G)</b>	<b>C3</b>
<b>C4 (G)</b>	<b>C4</b>
<b>C5 (G)</b>	<b>C5</b>

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LatSubSol name	TDB name
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
C2H401 (G) 1	C2H401_1
C2H401 (G) 2	C2H401_2
C2H402 (G) 1	C2H402_1
C2H402 (G) 2	C2H402_2
C2H404 (G)	C2H404
C2H601 (G) 1	C2H601_1
C2H601 (G) 2	C2H601_2
C2H602 (G)	C2H602
C3H401 (G) 1	C3H401_1
C3H401 (G) 2	C3H401_2
C3H401 (G) 3	C3H401_3
C3H402 (G) 1	C3H402_1
C3H402 (G) 2	C3H402_2
C3H403 (G)	C3H403
C3H601 (G) 1	C3H601_1
C3H601 (G) 2	C3H601_2
C3H601 (G) 3	C3H601_3
C3H601 (G) 4	C3H601_4

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LatSubSol name	TDB name
C3H601 (G) 5	C3H601_5
C3H602 (G)	C3H602
C3H603 (G)	C3H603
C3H801 (G) 1	C3H801_1
C3H801 (G) 2	C3H801_2
C3H801 (G) 3	C3H801_3
C2H601SI1 (G)	C2H601SI1
C2H8SI1 (G)	C2H8SI1
C6M0106 (G)	C6M0106
C101 (G)	C101
C102 (G)	C102
C201 (G)	C201
C302 (G)	C302
C1SI1 (G)	C1SI1
C1SI2 (G)	C1SI2
C1SI3 (G)	C1SI3
C1SI4 (G)	C1SI4
C2SI1 (G)	C2SI1
C2SI2 (G)	C2SI2
C2SI3 (G)	C2SI3
CE1 (G)	CE
CE101 (G)	CE101
CS1 (G)	CS
CS2 (G)	CS2
CS1H1 (G)	CS1H1
CS1H101 (G)	CS1H101
CS2H202 (G)	CS2H202
CS2M0104 (G)	CS2M0104
CS101 (G)	CS101
CS201 (G)	CS201
CS202 (G)	CS202
CS204RU1 (G)	CS204RU1
FE1 (G)	FE
FE2 (G)	FE2
FE1H202 (G)	FE1H202
FE101 (G)	FE101
H1 (G)	H
H2 (G)	H2
H1M03 (G)	H1M03
H1M0101 (G)	H1M0101
H2M0102 (G)	H2M0102
H2M0104 (G)	H2M0104
H101 (G)	H101
H102 (G)	H102
H201 (G)	H201
H202 (G)	H202
H101RU1 (G)	H101RU1

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LatSubSol name	TDB name
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
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

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LatSubSol name	TDB name
<b>SR1 (G)</b>	<b>SR</b>
<b>SR2 (G)</b>	<b>SR2</b>
<b>U1 (G)</b>	<b>U</b>
<b>ZR1 (G)</b>	<b>ZR</b>
<b>ZR2 (G)</b>	<b>ZR2</b>

## 2 Assessed Systems

### 2.1 Binary Systems

assessed binary systems						
Ba – C	Ba – Ce	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 – Cs	C – Fe	C – La	C – Mo	C – O	C – Pu	C – Ru
C – Si	C – Sr	C – U	C – Zr	Ce – Cs	Ce – Fe	Ce – La
Ce – Mo	Ce – O	Ce – Pu	Ce – Ru	Ce – Si	Ce – Sr	Ce – U
Ce – 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 <sub>2</sub>
Ba – Fe – O	BaO – FeO BaO – Fe <sub>2</sub> O <sub>3</sub>
Ba – La – O	BaO – La <sub>2</sub> O <sub>3</sub>
Ba – Mo – O	BaO – MoO <sub>3</sub>
Ba – O – Si	BaO – SiO <sub>2</sub>
Ba – O – Sr	BaO – SrO
Ba – O – U	BaO – UO <sub>2</sub>
Ba – O – Zr	BaO – ZrO <sub>2</sub>
Ba – O – Pu	BaO – PuO <sub>2</sub>
C – Fe – Mo	full
C – O – U	full
C – O – Zr	full
C – O – Pu	full
C – U – Zr	full
C – U – Pu	full

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system	assessed sub-systems
Ce – O – La	CeO <sub>2</sub> – La <sub>2</sub> O <sub>3</sub>
Ce – O – Mo	CeO <sub>2</sub> – MoO <sub>3</sub> Ce <sub>2</sub> O <sub>3</sub> – MoO <sub>3</sub>
Ce – O – Pu	CeO <sub>2</sub> – PuO <sub>2</sub> Ce <sub>2</sub> O <sub>3</sub> – PuO <sub>2</sub>
Ce – O – Si	Ce <sub>2</sub> O <sub>3</sub> – SiO <sub>2</sub>
Ce – O – Sr	CeO <sub>2</sub> – SrO
Ce – O – U	CeO <sub>2</sub> – UO <sub>2</sub> Ce <sub>2</sub> O <sub>3</sub> – UO <sub>2</sub>
Ce – O – Zr	CeO <sub>2</sub> – ZrO <sub>2</sub> Ce <sub>2</sub> O <sub>3</sub> – ZrO <sub>2</sub>
Cs – Mo – O	Cs <sub>2</sub> MoO <sub>4</sub> – MoO <sub>3</sub>
Fe – La – O	FeO – La <sub>2</sub> O <sub>3</sub> Fe <sub>2</sub> O <sub>3</sub> – La <sub>2</sub> O <sub>3</sub>
Fe – O – Pu	full
Fe – O – Si	FeO – Fe <sub>2</sub> O <sub>3</sub> – SiO <sub>2</sub>
Fe – O – Sr	FeO – SrO    Fe <sub>2</sub> O <sub>3</sub> – 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 <sub>2</sub> O <sub>3</sub> – PuO <sub>2</sub>
La – O – Si	La <sub>2</sub> O <sub>3</sub> – SiO <sub>2</sub>
La – O – Sr	La <sub>2</sub> O <sub>3</sub> – SrO
La – O – U	La <sub>2</sub> O <sub>3</sub> – UO <sub>2</sub>
La – O – Zr	La <sub>2</sub> O <sub>3</sub> – ZrO <sub>2</sub>
Mo – O – Pu	MoO <sub>3</sub> – PuO <sub>2</sub>
Mo – O – Zr	MoO <sub>3</sub> – ZrO <sub>2</sub>
O – Pu – Si	SiO <sub>2</sub> – PuO <sub>2</sub>
O – Pu – Sr	SrO – PuO <sub>2</sub>
O – Pu – U	full
O – Pu – Zr	full
O – Si – Sr	SrO – SiO <sub>2</sub>
O – Si – U	SiO <sub>2</sub> – UO <sub>2</sub>
O – Si – Zr	SiO <sub>2</sub> – ZrO <sub>2</sub>
O – Sr – U	SrO – UO <sub>2</sub>
O – Sr – Zr	SrO – ZrO <sub>2</sub>
O – U – Zr	full
Pu – U – Zr	full

### 2.3 Quaternary Systems

system	assessed sub-systems
Ba – Cs – Mo – O	BaMoO <sub>4</sub> – Cs <sub>2</sub> MoO <sub>4</sub>
O – Si – U – Zr	SiO <sub>2</sub> – UO <sub>2</sub> – ZrO <sub>2</sub>