

Overview of Mephista-15

M. Barrachin, E. Fischer, B. Piar

December 14, 2016

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
BA1C2 (S)	BA1C2
BA1C1O3 (C)	BA1C1O3
BA1CS2MO2O8 (S)	BA1CS2MO2O8
BA1FE12O19 (S)	BA1FE12O19
BA1FE2O4 (S)	BA1FE2O4
BA2FE2O5 (S)	BA2FE2O5
BA2FE6O11 (S)	BA2FE6O11
BA7FE4O13 (S)	BA7FE4O13
BA1LA2O4 (S)	BA1LA2O4
BA1MO2O7 (S)	BA1MO2O7
BA2MO1O5 (S)	BA2MO1O5
BA3MO1O6 (S)	BA3MO1O6
BA1MO1O4 (S)	BA1MO1O4
BA1O2 (S)	BA1O2
BA1O3SI1 (S)	BA1O3SI1
BA1O5SI2 (S)	BA1O5SI2
BA2O4SI1 (S)	BA2O4SI1
BA2O8SI3 (S)	BA2O8SI3
BA3O13SI5 (S)	BA3O13SI5
BA5O21SI8 (S)	BA5O21SI8
BA1O4U1 (S)	BA1O4U1
BA1SI1 (S)	BA1SI1
BA1SI2 (S)	BA1SI2
C1 (GRA_HEX_A9)	C
C2CE1 (S)	C2CE1
C3CE2 (S)	C3CE2
C1CS2O3 (S)	C1CS2O3
C1FE1O3 (S)	C1FE1O3
C5FE1O5 (L)	C5FE1O5
C2LA1 (LT)	C2LA1
C1MO1 (SHP)	C1MO1

continued on next page

continued from previous page	
LatSubSol name	TDB name
C1M0106 (S)	C1M0106
C6M0106 (S)	C6M0106
C1.7M01U1 (S)	C17M01U1
C2M01U1 (S)	C2M01U1
C1O3SR1 (C)	C1O3SR1
C1O5U1 (S)	C1O5U1
C0.4PU0.6 (S)	C04PU06
C2RU1U2 (S)	C2RU1U2
C1SI1 (S)	C1SI1
C3SI16U20 (T2)	C3SI16U20
C2SI2U3 (T1)	C2SI2U3
C2SR1 (S)	C2SR1
CE2FE17 (S)	CE2FE17
CE1FE2 (S)	CE1FE2
CE3RU1 (S)	CE3RU1
CE7RU3 (S)	CE7RU3
CE16RU9 (S)	CE16RU9
CE4RU3 (S)	CE4RU3
CE1RU2 (S)	CE1RU2
CE5SI3 (S)	CE5SI3
CE3SI2 (S)	CE3SI2
CE5SI4 (S)	CE5SI4
CE1SI1 (S)	CE1SI1
CE3SI5 (S)	CE3SI5
CE1SI2 (S)	CE1SI2
BA1CE103 (S)	BA1CE103
CE1FE103 (S)	CE1FE103
CE1M0208 (S)	CE1M0208
CE2M03013 (S)	CE2M03013
CE205SI1 (S)	CE205SI1
CE14039SI9 (S)	CE14039SI9
CE207SI2 (S)	CE207SI2
CE1O3SR1 (S)	CE1O3SR1
CE207ZR2 (S)	CE207ZR2
CS1 (BCC_A2)	CS
CS2M0207 (S)	CS2M0207
CS2M03010 (S)	CS2M03010
CS2M05016 (S)	CS2M05016
CS2M07022 (S)	CS2M07022
CS2M04013 (S)	CS2M04013
CS102 (S)	CS102
CS201 (S)	CS201
CS202 (S)	CS202
CS701 (S)	CS701
CS204RU1 (S)	CS204RU1
CS203SI1 (C)	CS203SI1
CS205SI2 (C)	CS205SI2
continued on next page	

continued from previous page	
LatSubSol name	TDB name
CS209SI4 (C)	CS209SI4
CS2012U4 (S)	CS2012U4
CS204U1 (S)	CS204U1
CS207U2 (S)	CS207U2
CS4017U5 (S)	CS4017U5
CS2013U4 (S)	CS2013U4
CS2016U5 (S)	CS2016U5
CS2018U6 (S)	CS2018U6
CS203.56U1 (S)	CS20356U1
CS2022U7 (S)	CS2022U7
CS2027U9 (S)	CS2027U9
CS2046U15 (S)	CS2046U15
CS203ZR1 (S)	CS203ZR1
CS404ZR1 (S)	CS404ZR1
CS4016ZR7 (S)	CS4016ZR7
CS6017ZR7 (S)	CS6017ZR7
FE1LA103 (S)	FE1LA103
FE12LA1019.5 (S)	FE12LA10195
FE2MO1 (LAVES)	FE2MO1
FE1MO104 (S)	FE1MO104
FE304 (S)	FE304
FE101.5 (S)	FE1015
FE103SI1 (WOLLASTONITE)	FE103SI1
FE204SI1 (FAYALITE)	FE204SI1
FE10022SR7 (S)	FE10022SR7
FE12019SR1 (S)	FE12019SR1
FE205SR2 (S)	FE205SR2
FE206SR3 (S)	FE206SR3
FE104U1 (S)	FE104U1
FE1SI1 (S)	FE1SI1
FE1SI2 (S)	FE1SI2
FE2SI1 (S)	FE2SI1
FE3SI7 (S)	FE3SI7
FE5SI3 (S)	FE5SI3
FE333U250ZR417 (e)	FE0333U025ZR0417
FE6U71ZR23 (l)	FE006U071ZR023
FE50U18ZR32 (k)	FE05U018ZR032
FE1ZR2 (S)	FE1ZR2
FE1ZR3 (S)	FE1ZR3
FE735ZR265 (S)	FE735ZR265
LA2MO3012 (S)	LA2MO3012
LA205SI1 (S)	LA205SI1
LA207SI2 (S)	LA207SI2
LA4012SI3 (S)	LA4012SI3
LA407SR1 (S)	LA407SR1
LA409SR3 (S)	LA409SR3
LA205ZR1 (S)	LA205ZR1

continued on next page

continued from previous page	
LatSubSol name	TDB name
LA207ZR2 (S)	LA207ZR2
LA1RU2 (S)	LA1RU2
LA3RU1 (S)	LA3RU1
LA5RU2 (S)	LA5RU2
LA5RU3 (S)	LA5RU3
LA7RU3 (S)	LA7RU3
LA1SI1 (S)	LA1SI1
LA1SI2 (S)	LA1SI2
LA3SI2 (S)	LA3SI2
MO1O2 (S)	MO1O2
MO1O2.750 (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
PU19RU1 (S)	PU19RU1
PU3RU1 (S)	PU3RU1
PU5RU3 (S)	PU5RU3
PU1RU1 (S)	PU1RU1
PU1RU2 (S)	PU1RU2
PU1SI1 (S)	PU1SI1
PU1SI2 (S)	PU1SI2
PU3SI2 (S)	PU3SI2
PU3SI5 (S)	PU3SI5
PU5SI3 (S)	PU5SI3
RU1SI1 (S)	RU1SI1
RU2SI1 (S)	RU2SI1
continued on next page	

continued from previous page	
LatSubSol name	TDB name
RU2SI3 (S)	RU2SI3
RU4SI3 (S)	RU4SI3
RU5SI3 (S)	RU5SI3
RU1U2 (S)	RU1U2
RU4U3 (S)	RU4U3
RU474U526 (S)	RU474U526
RU5U3 (S)	RU5U3
RU1ZR1 (S)	RU1ZR1
RU2ZR1 (S)	RU2ZR1
SI1SR1 (S)	SI1SR1
SI1SR2 (S)	SI1SR2
SI2SR1 (S)	SI2SR1
SI1U3 (HIGH_T)	SI1U3_1
SI1U3 (LOW_T)	SI1U3_2
SI1.88U1 (S)	SI188U1
SI3U1 (S)	SI3U1
SI511U489 (S)	SI511U489
SI5U3 (S)	SI5U3
SI1ZR1 (S)	SI1ZR1
SI1ZR2 (S)	SI1ZR2
SI1ZR3 (S)	SI1ZR3
SI2ZR1 (S)	SI2ZR1
SI2ZR3 (S)	SI2ZR3
SI3ZR5 (S)	SI3ZR5
SI4ZR5 (S)	SI4ZR5
BA1H2 (C)	BA1H2
BA1H2O2 (C)	BA1H2O2
C1H2O2 (L)	C1H2O2
C1H4 (L)	C1H4
C1H4O1 (L)	C1H4O1
C2H4O2 (L)	C2H4O2
C2H6 (L)	C2H6
C2H6O1 (L)	C2H6O1
C2H6O2 (L)	C2H6O2
C3H6 (L)	C3H6
C3H6O1 (L)	C3H6O1
C3H6O2 (L)	C3H6O2
C3H8 (L)	C3H8
C3H8O1 (L)	C3H8O1
C3H8O3 (L)	C3H8O3
CS1H1 (S)	CS1H1
CS1H1O1 (C)	CS1H1O1
FE1H1O2 (S)	FE1H1O2
FE1H2O2 (S)	FE1H2O2
FE1H3O3 (S)	FE1H3O3
FE2H2O4 (S)	FE2H2O4
H2LA1 (S)	H2LA1
continued on next page	

continued from previous page	
LatSubSol name	TDB name
H2O1 (L)	H2O1
H2O2SR1 (C)	H2O2SR1
H2O4U1 (S)	H2O4U1
H2PU1 (S)	H2PU1
H2SR1 (C)	H2SR1
H2ZR1 (S)	H2ZR1
H3LA1O3 (S)	H3LA1O3
H3PU1 (S)	H3PU1
H3U1 (S)	H3U1
H4O5U1 (S)	H4O5U1
H6SI2 (S)	H6SI2
C10CS1 (S)	C10CS1
C24CS1 (S)	C24CS1
C36CS1 (S)	C36CS1
C48CS1 (S)	C48CS1
C60CS1 (S)	C60CS1
C8CS1 (S)	C8CS1

1.3 Condensed Solutions

LatSubSol name	mult	atoms	TDB name
LIQUID	3	Ba, O, Mo, C, Ce, Cs, Fe, La, Pu, Si, Sr, U, Zr, Ru	LIQUID
FCC_C1	2	Ba, O, Ce, Fe, La, U, Sr, Pu, Zr	FCCC1
BCC_A2	3	Ba, C, Ce, Fe, La, Mo, Pu, Ru, Si, Sr, U, Zr, O	BCCA2
FCC_A1	2	Ba, C, Ce, Fe, La, Mo, Pu, Ru, Si, Sr, U, Zr	FCCA1
PEROVSKITE	2	Ba, Mo, O, Pu, U, Zr, Sr	PEROVSKITE
HCP_A3	2	C, Fe, Mo, Pu, Ru, U, Zr, O	HCPA3
TET (OXIDE)	1	Ba, O, Ce, Fe, La, Pu, U, Zr	TETOXIDE
MONOCLINIC	1	Ce, O, Pu, Zr	MONOCLINIC
LAVES	2	Fe, Pu, U, Zr	LAVES
FELM6	1	Fe, Pu, U	FELM6
BETA	1	Pu, U, Zr	BETA
GAMMA	1	Pu, U, Zr	GAMMA
DZETA	1	Pu, U, Zr	DZETA
ETA	1	Pu, U, Zr	ETA
TET_A6	1	Pu, U, Zr	TETA6
ALPHA	1	Pu, Zr	ALPHA
TETA	1	Pu, Zr	TETA
DELTA	1	U, Zr	DELTA
CC	1	Ba, O, Ce, La, Sr, Zr	CC
TCHERNOBYLITE	1	O, Si, U, Zr	TCHERNOBYLITE
C2LA (1+x) (HT)	1	C, La	C2LA1xHT
C3LA (2+x)	1	C, La	C3LA2x
DIA_A4	1	Ru, Si	DIAA4
TET (METAL)	1	Fe, Mo, Pu, Ru, Si, U, Zr	TETMETAL
ORT_A20	1	Fe, Pu, Si, U, Zr	ORTA20
MO-ZR (C15)	1	Mo, Zr	MOZRC15
CS2MOO4 (SS)	1	Ba, Mo, O, Cs	CS2MOO4SS
BCC	1	O, Pu	BCC
FCC_B1	2	Ba, O, Fe, Sr	FCCB1
FCC_B1 (4)	2	C, Pu, U, Zr, O	FCCB14
BCT	1	C, U, O	BCT
C-MO (ETA)	1	C, Mo	CMOETA
FE-MO (MU)	1	Fe, Mo	FEMOMU
FE-MO (R)	1	Fe, Mo	FEMOR
FE-MO (SIGMA)	1	Fe, Mo	FEMOSIGMA
MO-RU (SIGMA1)	1	Mo, Ru	MORUSIGMA1
MO-SI (MO5SI3)	1	Mo, Si	MOSIMO5SI3
C-PU-U (M2C3)	1	C, Pu, U	CPUUM2C3
SI2U3 (SS)	1	C, Si, U	SI2U3SS
C-FE-MO (KSI)	1	C, Fe, Mo	CFEMOKSI

continued on next page

continued from previous page			
LatSubSol name	mult	atoms	TDB name
C-FE-MO (M3C1_CEM)	1	C, Fe, Mo	CFEMOM3C1CEM
C-FE-MO (M6C1)	1	C, Fe, Mo	CFEMOM6C1
CE-LA (DHCP)	1	Ce, La	CELADHCP
CxRU3U1 (SS)	1	C, Ru, U	CxRU3U1SS
CE1O1.5 (SS)	1	Ce, O, Zr	CE1O15SS
C-PHASE	1	Ce, O	CPHASE

1.4 Gas

LatSubSol 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
C1H1 (G)	C1H1
C1H1O1 (G)	C1H1O1
C1H1O2 (G)	C1H1O2
C1H2 (G)	C1H2
C1H2O1 (G)	C1H2O1
C1H2O2 (G) C	C1H2O2_1
C1H2O2 (G) T	C1H2O2_2
C1H3 (G)	C1H3
C1H3O1 (G) 1	C1H3O1_1
C1H3O1 (G) 2	C1H3O1_2
C1H4 (G)	C1H4
C1H4O1 (G)	C1H4O1
C1O1 (G)	C1O1
C1O2 (G)	C1O2
C1SI1 (G)	C1SI1
C1SI2 (G)	C1SI2
C1SI3 (G)	C1SI3
C1SI4 (G)	C1SI4
C2 (G)	C2
C2H1 (G)	C2H1
C2H2 (G)	C2H2

continued on next page

continued from previous page	
LatSubSol name	TDB name
C2H201 (G)	C2H201
C2H202 (G)	C2H202
C2H3 (G)	C2H3
C2H4 (G)	C2H4
C2H401 (G) 1	C2H401_1
C2H401 (G) 2	C2H401_2
C2H402 (G) 1	C2H402_1
C2H402 (G) 2	C2H402_2
C2H404 (G)	C2H404
C2H5 (G)	C2H5
C2H6 (G)	C2H6
C2H601 (G) 1	C2H601_1
C2H601 (G) 2	C2H601_2
C2H601SI1 (G)	C2H601SI1
C2H602 (G)	C2H602
C2H8SI1 (G)	C2H8SI1
C2O1 (G)	C2O1
C2SI1 (G)	C2SI1
C2SI2 (G)	C2SI2
C2SI3 (G)	C2SI3
C3 (G)	C3
C3H4 (G) 1	C3H4_1
C3H4 (G) 2	C3H4_2
C3H4 (G) 3	C3H4_3
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
C3H6 (G) 1	C3H6_1
C3H6 (G) 2	C3H6_2
C3H601 (G) 1	C3H601_1
C3H601 (G) 2	C3H601_2
C3H601 (G) 3	C3H601_3
C3H601 (G) 4	C3H601_4
C3H601 (G) 5	C3H601_5
C3H602 (G)	C3H602
C3H603 (G)	C3H603
C3H7 (G) 1	C3H7_1
C3H7 (G) 2	C3H7_2
C3H8 (G)	C3H8
C3H801 (G) 1	C3H801_1
C3H801 (G) 2	C3H801_2
C3H801 (G) 3	C3H801_3
C3O2 (G)	C3O2
C4 (G)	C4
continued on next page	

continued from previous page	
LatSubSol name	TDB name
C5 (G)	C5
C5FE105 (G)	C5FE105
C6MO106 (G)	C6MO106
CE1 (G)	CE
CE101 (G)	CE101
CS1 (G)	CS
CS1H1 (G)	CS1H1
CS1H101 (G)	CS1H101
CS101 (G)	CS101
CS2 (G)	CS2
CS2H202 (G)	CS2H202
CS2MO104 (G)	CS2MO104
CS201 (G)	CS201
CS202 (G)	CS202
CS204RU1 (G)	CS204RU1
FE1 (G)	FE
FE1H202 (G)	FE1H202
FE101 (G)	FE101
FE2 (G)	FE2
H1 (G)	H
H1MO101 (G)	H1MO101
H1MO3 (G)	H1MO3
H101 (G)	H101
H101SR1 (G)	H101SR1
H102 (G)	H102
H1SI1 (G)	H1SI1
H1SR1 (G)	H1SR1
H1ZR1 (G)	H1ZR1
H2 (G)	H2
H2MO102 (G)	H2MO102
H2MO104 (G)	H2MO104
H201 (G)	H201
H202 (G)	H202
H202SR1 (G)	H202SR1
H2SI1 (G)	H2SI1
H3SI1 (G)	H3SI1
H4SI1 (G)	H4SI1
H6SI2 (G)	H6SI2
LA1 (G)	LA
LA101 (G)	LA101
LA201 (G)	LA201
LA202 (G)	LA202
MO1 (G)	MO
MO101 (G)	MO101
MO102 (G)	MO102
MO103 (G)	MO103
MO206 (G)	MO206

continued on next page

continued from previous page	
LatSubSol name	TDB name
MO309 (G)	MO309
MO4012 (G)	MO4012
MO5015 (G)	MO5015
O1 (G)	O
O1PU1 (G)	O1PU1
O1SI1 (G)	O1SI1
O1SR1 (G)	O1SR1
O1U1 (G)	O1U1
O1ZR1 (G)	O1ZR1
O2 (G)	O2
O2PU1 (G)	O2PU1
O2SI1 (G)	O2SI1
O2SI2 (G)	O2SI2
O2U1 (G)	O2U1
O2ZR1 (G)	O2ZR1
O3 (G)	O3
H1O1RU1 (G)	H1O1RU1
H2O2RU1 (G)	H2O2RU1
O1RU1 (G)	O1RU1
O2RU1 (G)	O2RU1
O3RU1 (G)	O3RU1
O3U1 (G)	O3U1
O4RU1 (G)	O4RU1
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 – 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 ₂
Ba – Fe – O	BaO – FeO BaO – Fe ₂ O ₃
Ba – La – O	BaO – La ₂ O 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 – Fe – Mo	full
C – O – U	full
C – O – Zr	full
C – O – Pu	full
C – U – Zr	full
C – U – Pu	full
Ce – O – La	CeO ₂ – La ₂ O ₃
Ce – O – Mo	CeO ₂ – MoO ₃ Ce ₂ O ₃ – MoO ₃
Ce – O – Pu	CeO ₂ – PuO ₂ Ce ₂ O ₃ – PuO ₂

continued on next page

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

3 Major Updates from Mephista-11 to Mephista-15

The description of some binary systems have been improved:

- C – Pu: improved modelling of the liquidus.
- C – U: **C3U2 (S)** made unstable at low temperature.
- O – Pu: melting temperature of **O2PU1 (S)** increased ; improved modelling of **LIQUID**.

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

- Ce – O – Pu: revised modelling of $\text{CeO}_2 - \text{PuO}_2$ and $\text{Ce}_2\text{O}_3 - \text{PuO}_2$.
- Fe – O – Pu: revised modelling of $\text{FeO} - \text{PuO}_2$ and $\text{Fe}_2\text{O}_3 - \text{PuO}_2$.
- La – O – Pu: revised modelling of $\text{La}_2\text{O}_3 - \text{PuO}_2$.
- Mo – O – Pu: revised modelling of $\text{MoO}_3 - \text{PuO}_2$.
- O – Pu – Si: revised modelling of $\text{SiO}_2 - \text{PuO}_2$.
- O – Pu – Sr: revised modelling of $\text{SrO} - \text{PuO}_2$.
- O – Pu – Zr: revised modelling of $\text{PuO}_2 - \text{ZrO}_2$.
- C – O – Pu: revised modelling of the full system.

The description of some ternary systems have been improved:

- O – Pu – U: improved modelling of $\text{PuO}_2 - \text{UO}_2$; improved modelling of the **FCC_C1** miscibility gap.
- Ba – O – Pu: improved modelling of $\text{BaO} - \text{PuO}_2$.
- Ba – Mo – O: improved modelling of **BA1MO1O4 (G)** .
- C – Pu – U: improved modelling of the full system.

Contents

1	General Description	3
2	Assessed Systems	14
3	Major Updates from Mephista-11 to Mephista-15	16