

SSOL6 – SGTE Solutions Database

<i>Database name:</i>	SGTE Solutions Database	<i>Database acronym:</i>	SSOL
<i>Database owner:</i>	Scientific Group Thermodata Europe (SGTE)	<i>Database version:</i>	6.1

The SSOL6 Solutions Database is a thermodynamic database which contains critical assessments for many binary and ternary, and some higher order systems. SSOL6 can be used with Thermo-Calc, the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA, and the TC Programming Interfaces.

This general alloy solutions database is designed for various applications related to alloy design, coatings, joining, heat treatment and inorganic materials. As many as 79 elements have been included in this database now:

Ag	Al	Am	As	Au	B	Ba	Be	Bi	C	Ca	Cd	Ce	Co	Cr	Cs	Cu
Dy	Er	Eu	Fe	Ga	Gd	Ge	H	Hf	Hg	Ho	In	Ir	K	La	Li	Lu
Mg	Mn	Mo	N	Na	Nb	Nd	Ni	Np	O	Os	P	Pa	Pb	Pd	Pr	Pt
Pu	Rb	Re	Rh	Ru	S	Sb	Sc	Se	Si	Sm	Sn	Sr	Ta	Tb	Tc	Te
Th	Ti	Tl	Tm	U	V	W	Y	Yb	Zn	Zr						

Developed using the CALPHAD approach, SSOL6 is based on the critical evaluation of binary, ternary and in some cases higher order systems. In total, 575 binary systems and 133 ternary systems, as well as 20 higher-order systems, which had been critically assessed, are included in the SSOL6 database in this 79 elements framework. The complete list of all these critically assessed systems is given in the next section of this document. The command “ASSESSSED_SYSTEMS” had been added in the database for all the assessed systems, which enables the users to calculate phase diagrams of these systems using the BINARY and TERNARY modules.

A huge number of (1331) phases, including various multicomponent solution phases and many important intermetallic compounds, have been included in SSOL6. The complete list of the phases and their models are attached at the end of this documents. It should be noted that the GAS phase is rejected by default in the database and one should restore it if it is relevant to a calculation.

Order-disorder models, which describe a pair of ordered and disordered phases with a single Gibbs energy function and thus is able to describe a possible 2nd-order transition between the pair of phases, had been employed to some systems, such as BCC_A2/ BCC_B2 in the Al-Fe system and FCC_A1/ FCC_L12 in the Al-Ni system. It should be noted that some B2-type phases had been modeled as stoichiometric phases and thus a separate phase named as “B2_BCC” was created in addition to the BCC_B2 phase in the order-disorder model.

The SSOL6 database enables predictions (such as multi-component phase equilibria and Scheil solidification simulations of industrial alloys) to be made for multicomponent systems and alloys of industrial importance. This means that the SSOL6 database may be utilized to extrapolate to higher-order systems by combining several critically assessed systems. However, such extrapolations require experiences in CALPHAD and a good understanding of the involved systems. And the producer or vendor should be contacted if problems occur.

List of Assessed Binary Systems

Ag-Al	Ag-Au	Ag-B	Ag-Ba
Ag-Be	Ag-Bi	Ag-C	Ag-Ca
Ag-Cd	Ag-Ce	Ag-Cr	Ag-Cu
Ag-Fe	Ag-Ge	Ag-In	Ag-Ir
Ag-Mg	Ag-Mo	Ag-Mn	Ag-Nb

Ag-Ni	Ag-Os	Ag-Pb	Ag-Pd
Ag-Pt	Ag-Rh	Ag-Ru	Ag-Sb
Ag-Sc	Ag-Si	Ag-Sn	Ag-Sr
Ag-Te	Ag-Ti	Ag-Tl	Ag-V
Ag-W	Ag-Zn	Ag-Zr	Al-As
Al-Au	Al-B	Al-Be	Al-Bi
Al-C	Al-Ca	Al-Ce	Al-Co
Al-Cr	Al-Cu	Al-Dy	Al-Er
Al-Fe	Al-Ga	Al-Gd	Al-Ge
Al-Hg	Al-Ho	Al-In	Al-La
Al-Li	Al-Mg	Al-Mn	Al-Mo
Al-N	Al-Nb	Al-Nd	Al-Ni
Al-P	Al-Pb	Al-Pr	Al-Pt
Al-Ru	Al-Sb	Al-Sc	Al-Si
Al-Sm	Al-Sn	Al-Sr	Al-Ta
Al-Th	Al-Ti	Al-V	Al-W
Al-Y	Al-Zn	Al-Zr	As-Au
As-Ga	As-Ge	As-In	As-Ni
As-P	As-Pb	As-Pt	As-Sb
Au-B	Au-Bi	Au-C	Au-Co
Au-Cr	Au-Cu	Au-Ge	Au-Hf
Au-In	Au-Ni	Au-Pb	Au-Pd
Au-Pr	Au-Rh	Au-Ru	Au-Sb
Au-Si	Au-Sn	Au-Te	Au-Ti
Au-Tl	Au-Zr	Au-Zn	B-Ba
B-C	B-Ca	B-Co	B-Cr
B-Cu	B-Fe	B-Hf	B-Mg
B-Mn	B-Mo	B-N	B-Nd
B-Ni	B-Sc	B-Si	B-Sr
B-Ti	B-U	B-V	B-W
B-Zr	Ba-Cu	Ba-Eu	Ba-Ru
Ba-Sr	Ba-Y	Bi-Cu	Bi-Ga
Bi-Ge	Bi-Hg	Bi-In	Bi-K
Bi-Tm	Bi-Ni	Bi-Pb	Bi-Pd
Bi-Sb	Bi-Si	Bi-Sn	Bi-Tb
Bi-Tl	Bi-Y	Bi-Zn	C-Co
C-Cr	C-Cu	C-Fe	C-Hf
C-Ir	C-Mn	C-Mo	C-N
C-Nb	C-Ni	C-Os	C-P
C-Pb	C-Pd	C-Pt	C-Pu
C-Rh	C-Ru	C-Si	C-Ta
C-Ti	C-U	C-V	C-W
C-Zn	C-Zr	Ca-Cu	Ca-Ga
Ca-H	Ca-Li	Ca-Mg	Ca-Ru
Ca-Si	Ca-Sr	Ca-Zn	Cd-Ga
Cd-Ge	Cd-Hg	Cd-In	Cd-Pb
Cd-Sb	Cd-Zn	Ce-Co	Ce-Cr
Ce-Cu	Ce-Mg	Ce-Mn	Ce-Mo

Ce-Ni	Ce-Sb	Ce-V	Ce-Y
Co-Cr	Co-Cu	Co-Dy	Co-Fe
Co-Ga	Co-Gd	Co-Ge	Co-In
Co-Mn	Co-Mo	Co-N	Co-Nb
Co-Ni	Co-Pd	Co-Pt	Co-Sb
Co-Si	Co-Sm	Co-Sn	Co-Ta
Co-Ti	Co-V	Co-W	Co-Y
Co-Zn	Co-Zr	Cr-Cu	Cr-Fe
Cr-Ga	Cr-Ge	Cr-La	Cr-Mg
Cr-Mn	Cr-Mo	Cr-N	Cr-Nb
Cr-Ni	Cr-P	Cr-Pd	Cr-Pt
Cr-Ru	Cr-Si	Cr-Sn	Cr-Ta
Cr-Ti	Cr-V	Cr-W	Cr-Zn
Cr-Y	Cr-Zr	Cs-K	Cs-Na
Cs-Rb	Cu-Er	Cu-Eu	Cu-Fe
Cu-Ge	Cu-H	Cu-Hf	Cu-Ho
Cu-In	Cu-Ir	Cu-La	Cu-Li
Cu-Mg	Cu-Mn	Cu-Mo	Cu-Nb
Cu-Nd	Cu-Ni	Cu-P	Cu-Pb
Cu-Pd	Cu-Pr	Cu-Rh	Cu-Sb
Cu-Sc	Cu-Si	Cu-Sm	Cu-Sn
Cu-Sr	Cu-Ti	Cu-Tl	Cu-V
Cu-Y	Cu-Zn	Cu-Zr	Dy-Er
Dy-Fe	Dy-Ho	Dy-Mg	Dy-Ni
Dy-Tb	Er-Ho	Er-Ni	Er-Tb
Eu-In	Eu-Mg	Eu-Pd	Eu-Sn
Fe-Gd	Fe-La	Fe-Mg	Fe-Mn
Fe-Mo	Fe-N	Fe-Nb	Fe-Nd
Fe-Ni	Fe-P	Fe-Pb	Fe-Pd
Fe-Pr	Fe-Ru	Fe-Sb	Fe-Sc
Fe-Si	Fe-Sm	Fe-Sn	Fe-Sr
Fe-Ta	Fe-Tb	Fe-Ti	Fe-U
Fe-V	Fe-W	Fe-Y	Fe-Zn
Fe-Zr	Ga-Ge	Ga-Hg	Ga-In
Ga-Mg	Ga-N	Ga-Ni	Ga-P
Ga-Pb	Ga-Pt	Ga-Sb	Ga-Si
Ga-Sn	Ga-Ti	Ga-Zn	Gd-Ge
Gd-Li	Gd-Mg	Gd-Mn	Gd-Mo
Gd-Ni	Gd-Sc	Gd-Si	Gd-Zr
Ge-In	Ge-Mg	Ge-Pb	Ge-Ru
Ge-Sb	Ge-Si	Ge-Sn	Ge-Sr
Ge-Te	Ge-Tl	Ge-V	Ge-Zn
H-Li	H-Pd	Hf-Mo	Hf-Nb
Hf-Ni	Hf-Si	Hf-Ta	Hf-Ti
Hf-W	Hf-Zr	Hg-Pb	Hg-Sn
Hg-Zn	Ho-Mg	Ho-Mn	Ho-Mo
Ho-Tb	Ho-V	In-La	In-Ni
In-P	In-Pb	In-Pd	In-Sb

In-Si	In-Sn	In-Yb	In-Zn
Ir-Ni	Ir-Pd	Ir-Pt	Ir-Rh
Ir-Ru	Ir-Zr	K-Rb	Sn-V
Sn-Zn	Sn-Zr	Sr-Zn	Ta-Ti
Ta-V	La-Mg	La-Ni	La-V
Li-Mg	Li-N	Li-Na	Li-Si
Li-Sn	Li-Zr	Mg-Mn	Mg-Nd
Mg-Ni	Mg-Pr	Mg-Ru	Mg-Sc
Mg-Si	Mg-Sn	Mg-Sr	Mg-Tb
Mg-Tm	Mg-V	Mg-Y	Mg-Yb
Mg-Zn	Mg-Zr	Mn-Mo	Mn-N
Mn-Ni <i>Temporarily Removed</i>	Mn-P	Mn-Pb	Mn-Sc
Mn-Si	Mn-Sm	Mn-Sn	Mn-Ti
Mn-V	Mn-W	Mn-Y	Mn-Zn
Mn-Zr	Mo-N	Mo-Nb	Mo-Ni
Mo-P	Mo-Pd	Ta-W	Ta-Zr
Th-Zn	Ti-V	Ti-W	Ti-Zn
Mo-Si	Mo-Ta	Mo-Ti	Mo-V
Mo-W	Mo-Y	Mo-Zr	N-Nb
N-Ni	N-Si	N-Ta	N-Ti
N-U	N-V	N-W	N-Zr
Na-Rb	Nb-Ni	Nb-Si	Nb-Sn
Nb-Ta	Nb-Ti	Nb-V	Nb-W
Nb-Zr	Nd-Pr	Nd-Sb	Nd-Sc
Nd-Y	Ni-P	Ni-Pb	Ni-Ru
Ni-Pd	Ni-Si	Ni-Sm	Ni-Sn
Ni-Sr	Ni-Ta	Ni-Ti	Ni-V
Ni-W	Ni-Y	Ni-Zn	Ni-Zr
Os-Si	P-Sb	P-Si	Ti-Zr
Tl-Zn	U-V	U-Zr	V-W
V-Y	Pb-Pd	Pb-Pt	Pb-Sb
Pb-Si	Pb-Sn	Pb-Te	Pb-Tl
Pb-Zn	Pb-Zr	Pd-Rh	Pd-Ru
Pd-Sc	Pd-Si	Pd-Sm	Pd-Sn
Pd-Tb	Pd-Zn	Pd-Zr	Pr-Sb
Pt-Rh	Pt-Ru	Pt-Si	Pt-Ta
Pt-Ti	Ru-Si	Ru-Sn	Ru-Zr
Sb-Si	Sb-Sm	Sb-Sn	Sb-Zn
Sc-Si	Sc-V	Sc-Y	Sc-Zr
Se-Te	Si-Sn	Si-Ta	Si-Ti
Si-U	Si-V	Si-W	Si-Y
Si-Yb	Si-Zn	Si-Zr	Sn-Ti
V-Zr	W-Zr	Y-Zr	Zn-Zr

List of Assessed Ternary Systems

Ag-Au-Bi	Ag-Au-Sb	Ag-Bi-Sn	Ag-Cu-Ni
Ag-Cu-Pb	Ag-Cu-Sn	Ag-In-Sn	Ag-Ni-Sn
Al-C-Si	Al-Ca-Si	Al-Cu-Li	Al-Cu-Mg
Al-Cu-Si	Al-Cu-Zn	Al-Fe-Mn	Al-Fe-Si
Al-Ga-In	Al-Ga-Sn	Al-Mg-Mn	Al-Mg-Si
Al-Mg-Zn	Al-Mn-Si	Al-Si-Zn	Al-Sn-Zn
Au-Bi-Sb	Au-In-Pb	Au-In-Sb	Au-In-Sn
Au-Ni-Sn	B-Fe-Nd	Bi-Ga-Zn	Bi-In-Pb
Bi-In-Sn	Bi-Sb-Sn	Bi-Sn-Zn	C-Co-Cr
C-Co-Fe	C-Co-Ni	C-Co-W	C-Cr-Fe
C-Cr-Mn	C-Cr-Mo	C-Cr-N	C-Cr-Ni
C-Cr-Si	C-Cr-Ti	C-Cr-V	C-Cr-W
C-Cu-Fe	C-Fe-Mn	C-Fe-Mo	C-Fe-N
C-Fe-Nb	C-Fe-Ni	C-Fe-Si	C-Fe-Ti
C-Fe-V	C-Fe-W	C-Mn-Si	C-Mn-V
C-Mo-N	C-Mo-Ti	C-Mo-V	C-Mo-W
C-N-Ti	C-Ni-Si	C-Ni-Ti	C-Ni-W
C-Si-Ti	C-Ti-W	C-V-W	Cd-Ga-In
Co-Cr-W	Co-Fe-N	Co-Fe-W	Co-Ni-W
Cr-Fe-Mn	Cr-Fe-Mo	Cr-Fe-N	Cr-Fe-Ni
Cr-Fe-P	Cr-Fe-Ti	Cr-Fe-V	Cr-Fe-W
Cr-Mn-N	Cr-Mn-Ti	Cr-Mo-N	Cr-Mo-Ni
Cr-Mo-W	Cr-N-Ni	Cr-N-Ti	Cr-N-V
Cr-N-W	Cr-Ni-Ta	Cr-Ni-W	Cr-Si-Ti
Cr-Ti-V	Cu-Fe-Ni	Cu-In-Sn	Cu-Fe-P
Cu-H-Pd	Cu-Mg-Si	Cu-Mg-Zn	Cu-Ni-Pb
Cu-Ni-Sn	Dy-Fe-Tb	Fe-Mn-N	Fe-Mn-Ni - Temporarily Removed
Fe-Mn-Si	Fe-Mn-V	Fe-Mo-N	Fe-Mo-Ni
Fe-Mo-P	Fe-Mo-V	Fe-Mo-W	Fe-N-Ni
Fe-N-Ti	Fe-N-V	Fe-N-W	Fe-Ni-P
Fe-Ni-W	Fe-Si-Zn	Fe-Ti-W	Fe-U-Zr
Ga-In-Sb	Ge-Ru-Si	Ge-Ru-Sn	In-Sb-Sn
In-Sn-Zn	Mo-N-Ni	Mo-Ni-W	N-Si-Ti
Pb-Pd-Sn			

List of Assessed Quaternary Systems

C-Co-Cr-W	C-Co-Fe-Ni	C-Co-Fe-Ni-W	C-Co-Fe-W
C-Co-Ni-W	C-Cr-Fe-Mn	C-Cr-Fe-Mo	C-Cr-Fe-Ni
C-Cr-Fe-Si	C-Cr-Fe-V	C-Cr-Fe-W	C-Fe-Mn-V
C-Fe-Mo-V	C-Fe-Mo-W	C-Fe-Ni-W	C-Fe-V-W
C-Cr-Mo-V	Co-Fe-Ni-W	Cr-Fe-Mn-N	Cr-Fe-N-Ni

List of All Phases Models

Phase Name	Stoichiometry						Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5	
GAS	1	1					AL1 AL2 CA CA2 CAH CU CU2 CUH H H2 HLI LI LI2 N1 N2 N3 O2					
LIQUID	1	1					AG AL AM AS AU B BA BE BI C CA CD CE CO CR CS CU DY ER EU FE GA GD GE H HF HG HO IN IR K LA LI LU MG MN MO N N1U NA NB ND NI NP O OS P PA PB PD PR PT PU RB RE RH RU S SB SC SE SI SM SN SR TA TB TC TE TH TI TL TM U V W Y YB ZN ZR MG2SN GETE CR3GE1 AG2TE PBTE LIH					
FCC_A1	2	1	1				AG AL AM AS AU BA BE BI CA CD CE CO CR CS CU DY ER EU FE GA GD GE HF HG HO IN IR K LA LI MG MN MO NA NB N NI O OS P PB PD PR PT PU RB RE RH RU S SB SC SI SM SN SR TA TB C TH TI TL U V W Y YB ZN ZR	VA C H N B				
FCC_L12	3	0.75	0.25	1			AG AL AM AS AU BA BE BI CA CD CE CO CR CS CU DY ER FE GA GD GE HF HG HO IN IR K LA LI MG MN MO NA NB N NI O OS P PB PD PR PT PU RB RE RH RU S SB SC SI SN SR TA T TH TI TL U V W Y YB ZN ZR	AG AL AM AS AU BA BE BI CA CD CE CO CR CS CU DY ER FE GA GD GE HF HG HO IN IR K LA LI MG MN MO NA NB N NI O OS P PB PD PR PT PU RB RE RH RU S SB SC SI SN SR TA T TH TI TL U V W Y YB ZN ZR	B C N VA			
FCC_L10	2	0.5	0.5				MN NI	MN NI				
FCC_AUCU	5	0.25	0.25	0.25	0.25	1	AU CU	AU CU	AU CU	AU CU	VA	
FCC_COV	5	0.25	0.25	0.25	0.25	1	CO V	CO V	CO V	CO V	VA	
BCC_A2	2	1	3				AG AL AM AS AU BA BE BI CA CD CE CO CR CS CU DY ER EU FE GA GD GE HF HO IN IR K LA LI MG MN MO NA NB ND NI NP O OS P PA PB PD PR PT PU RB RE RH RU S SB SC SI SM SN SR TA TB TC TH TI TL TM U V W Y YB ZN ZR	B C H N VA				
BCC_B2	3	0.5	0.5	3			AG AL AM AS AU BA BE BI CA CD CE CO CR CS CU DY ER EU FE GA GD GE HF HO IN IR K LA LI MG MN MO NA NB ND NI NP O OS P PA PB PD PR PT PU RB RE RH RU S SB SC SI SM SN SR TA TB TC TH TI TL TM U V W Y YB ZN ZR	AG AL AM AS AU BA BE BI CA CD CE CO CR CS CU DY ER EU FE GA GD GE HF HO IN IR K LA LI MG MN MO NA NB ND NI NP O OS P PA PB PD PR PT PU RB RE RH RU S SB SC SI SM SN SR TA TB TC TH TI TL TM U V W Y YB ZN ZR	B C H N VA			
B2_BCC	2	1	1				AL CO IN NI PD	VA CO NI PD				
HCP_A3	2	1	0.5				AG AL AS AU BA BE BI CA CD CE CO CR CS	B C N VA				

Phase Name	Stoichiometry					Occupancy						
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5	
							CU DY ER EU FE GA GD GE HF HG HO IN IR K LA LI LU MG MN MO NA NB ND NI OS PB PD PR PT RB RE RH RU SB SC SI SM SN SR TA TB TC TI TL TM U V W Y YB ZN ZR					
HCP_ORD	5	0.25	0.25	0.25	0.25	0.5	CO V	CO V	CO V	CO V	VA	
HCP_ZN	2	1	0.5				AG AL AU BI CD CR CU FE GA HG IN MG PB PD SI SN ZN	VA				
DHCP	1	1					AL AM AU CE IN LA MG ND PR SC SN Y					
DIAMOND_A4	1	1					AL B BI C GA GE P PD RU SI SN TI ZN					
BCT_A5	1	1					AG AL BI CD GA GE IN NI PB PD SB SN TI ZN					
TETRAGONAL_A6	1	1					BI CD EU GA HG IN PB PU SN YB ZN					
TET_ALPHA1	1	1					BI IN PB SN					
TETRAGONAL_U	1	1					FE SI U V ZR					
RHOMBOHEDRAL_A7	1	1					AS BI GE IN P PB PD SB SN TB TM Y ZN					
HEXAGONAL_A8	1	1					SE TE					
RHOMBO_A10	1	1					CD HG PB ZN					
BETA_RHOMBO_B	1	1					B MN					
ALPHA_RHOMBO_B	1	1					B					
BETA_RHOMB_BCSI	2	93	12				B	B C CU SI				
CHI_A12	3	24	10	24			CR FE	CR MO TI W	CR FE MO W			
CBCC_A12	2	1	1				AL CO CR FE HO MG MN MO NI SI SM SN TI V ZN ZR	VA C B N				
CUB_A13	2	1	1				AG AL CE CO CR FE HO MG MN MO NI SI SM SN TI V ZN ZR	VA B C N				
CUB_A15	2	3	1				MO TI	AL				
ORTHORHOMBIC_A20	1	1					FE SI U ZR					
SIGMA	3	8	4	18			AL CO FE MN NI	CR MO TI V W	AL CO CR FE MO MN NI SI TI V W			
HIGH_SIGMA	3	8	4	18			FE MN	CR MO	CR FE MN MO TI			
MU_PHASE	3	7	2	4			CO CR FE MN MO NI TA	MN MO NB TA TI W	CO CR FE NI MN MO NB TA TI W			
P_PHASE	3	24	20	12			CR NI FE	CR MO NI FE	MO			
R_PHASE	3	27	14	12			CO CR FE MN NI	MO W	CO CR FE MN MO NI W			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
ZINCBLLENDE_B3	2	0.5	0.5				AL GA IN	AS P SB			
GRAPHITE	1	1					B C				
RED_P	1	1					AS P				
WHITE_P	1	1					P				
MONOCLINIC	1	1					S				
ORTHORHOMBIC_S	1	1					S				
ORTHORHOMBIC_GA	1	1					GA				
ORTHORHOMBIC_AC	1	1					NP				
TETRAG_AD	1	1					NP				
BCT_AA	1	1					PA				
ALPHA_PU	1	1					PU				
BETA_PU	1	1					PU				
GAMMA_PU	1	1					PU				
RHOMBO_C19	1	1					AL MN PD SM				
OMEGA_ZR	1	1					ZR				
LAVES_C14	2	2	1				AL CA CO CR CU DY FE HO MG MN MO NB NI SR TA TI V W ZN ZR	AL CA CO CR CU DY FE HO MG MN MO NB NI SR TA TI V W ZN ZR			
LAVES_C15	2	2	1				AL CO CR CU DY ER FE GD HF HO MG MN MO NB NI SI TA TI V W Y ZN ZR	AL CO CR CU DY ER FE GD HF HO MG MN MO NB ND NI SI TA TI V W Y ZN ZR			
LAVES_C36	2	2	1				AL CO CR CU HF MG MN MO NI SI TA TI V ZN ZR	AL CO CR CU HF MG MN MO NI TA TI V ZN ZR			
CEMENTITE	2	3	1				CO CR FE MN MO NB NI V W	C N			
KSI_CARBIDE	2	3	1				CR FE MO W	C			
M23C6	3	20	3	6			CO CR FE MN NI V	CO CR FE MN MO NI V W	C		
M7C3	2	7	3				CO CR FE MN MO NI V W	C			
M6C	4	2	2	2	1		CO FE NI	MO W	CO CR FE MO NI V W	C	
M3C2	2	3	2				CR FE MN MO V W	C			
V3C2	2	3	2				FE MN V	C			
M5C2	2	5	2				FE MN V	C			
M12C	3	6	6	1			CO	W	C		
MC_SHP	2	1	1				MO W	C N			
MC_ETA	2	1	1				MO V W	VA C			
AL4C3	2	4	3				AL SI	C			
AL8SIC7	3	8	1	7			AL	SI	C		
AL4SIC4	3	4	1	4			AL	SI	C		
CR2VC2	3	2	1	2			CR	V	C		
FE8S12C	3	8	2	1			FE	SI	C		
SIC	2	1	1				SI	C			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
ALN	2	1	1				AL	N			
M4N	2	4	1				CR CO FE MN NI	VA C N			
FECN_CHI	2	5	2				FE	C N			
PI_PHASE	3	12.8	7.2	4			CR	FE NI	N		
TI2N	2	2	1				TI	C N			
B4C	2	1	1				B11C1 B12	B2 C1B2 C2B B1C2 B2C1			
BN_HP4	2	1	1				B	N			
MN6N4	2	6	4				MN	N			
MN6N5	2	6	5				MN	N			
EPSILON_TAN	1	1					TA1N				
TI3N2	1	1					TI.71N.29				
TI4N3	1	1					TI.685N.315				
ALB2	2	1	2				AL	B			
ALB12_ALPHA	2	1	12				AL	B			
BAB6	2	1	6				BA	B			
CAB6	2	1	6				CA	B			
SRB6	2	1	6				SR	B			
CR2B_ORTH	2	0.667	0.333				CR	B			
CR3B4	2	0.429	0.571				CR	B			
CR5B3	2	0.625	0.375				CR	B			
CRB	2	0.5	0.5				CR	B			
CRB2	2	0.333	0.667				CR	B			
CRB4	2	0.2	0.8				CR	B			
FE2B	1	1					FE2B				
FEB	1	1					FE1B				
FENDB_T1	1	1					FE14ND2B1				
FENDB_T2	1	1					ND1.11FE4B4				
FENDB_T3	1	1					FE2ND5B6				
BM	2	1	1				B	HF TI			
B2M	2	2	1				B	HF TI			
M2B_TETR	2	0.667	0.333				MO NI	B			
B4M3	2	4	3				B	HF TI			
MOB	2	0.5	0.5				MO	B			
MOB4	2	0.2	0.8				MO	B			
MOB2	2	0.38	0.62				MO	B			
MO2B5	2	0.32	0.68				MO	B			
NDB4	1	1					ND1B4				
NDB6	1	1					ND1B6				
NDB66	1	1					ND1B66				

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
ND2B5	1	1					ND2B5				
ND2Y_C19	2	2	1				ND Y	ND Y			
NI3B	2	0.75	0.25				NI	B			
NI4B3_O	2	0.586	0.414				NI	B			
NI4B3_M	2	0.564	0.436				NI	B			
NIB	2	0.5	0.5				NI	B			
SIB3	3	6	2	6			B	SI	B SI		
SIB6	3	210	23	48			B	SI	B SI		
B_NSI	3	61	1	8			B	SI	B SI		
VB	2	0.5	0.5				V	B			
VB2	2	0.333	0.667				V	B			
V2B3	2	0.4	0.6				V	B			
V3B2	2	0.6	0.4				V	B			
V3B4	2	0.4286	0.5714				V	B			
WB_ALPHA	2	1	1				W	B VA			
WB_BETA	2	1	1				W	B VA			
WB3	1	1					W2B9				
W2B	1	1					W2B1				
W2B5	2	2	5				W	B VA			
ASP	1	1					AS P				
CU3P	2	3	1				CU FE	P			
FEP	2	1	1				FE	P			
M2P	2	2	1				CR FE MO NI	P			
M3P	2	3	1				CR FE CU MO NI	P			
MNP	1	1					MN1P				
MNP3	1	1					MN1P3				
MN3P	1	1					MN3P				
MN2P	1	1					MN2P				
MOP	2	1	1				MO	P			
NI5P2_H	2	5	2				NI	P			
NI5P2_L	2	5	2				CU NI	P			
NI6P5	2	6	5				NI	P			
NI12P5	2	12	5				NI	P			
PSI	2	1	1				P	SI			
AGBA	2	1	1				AG	BA			
AG2BA	2	2	1				AG	BA			
AG2BA3	2	2	3				AG	BA			
AG5BA	2	5	1				AG	BA			
AG3BE8	2	2.97	8.03				AG	BE			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AGCA	2	1	1				AG	CA			
AGCA3	2	1	3				AG	CA			
AG2CA	2	2	1				AG	CA			
AG3CA5	2	3	5				AG	CA			
AG7CA2	2	7	2				AG	CA			
AG9CA2	2	9	2				AG	CA			
AGCD	2	1	1				AG	CD			
AG2CD3	2	2	3				AG	CD			
AGCD_ETA	1	1					AG CD				
AGCE	2	1	1				AG	CE			
AG2CE	2	2	1				AG	CE			
AG4CE	2	4	1				AG	CE			
AG51CE14	2	51	14				AG	CE			
AGIN2	2	0.33	0.67				AG	IN			
AGMG3	2	0.25	0.75				AG	MG			
AG3MG	2	0.75	0.25				AG	MG			
AGSB_ORTHO	2	0.75	0.25				AG AU SB	AG AU BI SB SN			
AGSC	2	1	1				AG	SC			
AG2SC	2	2	1				AG	SC			
AG4SC	2	4	1				AG	SC			
AGSR	2	1	1				AG	SR			
AG2SR	2	2	1				AG	SR			
AG2SR3	2	2	3				AG	SR			
AG4SR	2	4	1				AG	SR			
AG5SR	2	5	1				AG	SR			
AG2TE	2	2	1				AG,PB	TE			
AG5TE3	2	31	19				AG	TE			
AG65TE345	2	0.655	0.345				AG	TE			
AGTI2	2	1	2				AG	TI			
AGTI	2	1	1				AG TI	AG TI			
AGZN_GAMMA	4	2	2	3	6		AG ZN	AG ZN	AG	ZN	
AGZN_ZETA	2	1	2				ZN	AG ZN			
AGZR2	2	0.33333	0.66667				AG	ZR			
AGZR	2	0.5	0.5				AG	ZR			
ALM_D019	2	3	1				AL MO NB TA TI V W	AL MO NB TA TI V W			
AL3M_D022	2	3	1				AL MO TI	MO NB TA TI V			
ALAU	1	1					AL1AU				
ALAU2	1	1					AL1AU2				
ALAU4	1	1					AL1AU4				

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AL2AU	1	1					AL2AU				
AL2AU5	1	1					AL2AU5				
AL2CA	1	1					AL2CA				
AL4CA	1	1					AL4CA				
AL2CASI2	3	0.4	0.2	0.4			AL	CA	SI		
ALCE_AMORPHOUS	1	1					AL CE				
AL_CEND	2	1	1				AL	CE ND			
AL_CEND3_H	2	1	3				AL	CE			
AL_CEND3_L	2	1	3				AL	CE ND			
AL2_CEND	2	2	1				AL	CE			
AL3_CEND	2	3	1				AL	CE ND			
AL11_CEND3_H	2	11	3				AL	CE ND			
AL11_CEND3_L	2	11	3				AL	CE ND			
AL5CO2	2	5	2				AL	CO			
AL3CO	2	3	1				AL	CO			
AL13CO4	2	13	4				AL	CO			
AL9CO2	2	9	2				AL	CO			
ALCR2	2	1	2				AL,CR	AL,CR			
AL4CR	2	4	1				AL	AL,CR			
AL8CR5_BETA	2	8	5				AL,CR	AL,CR			
AL8CR5_ALPHA	2	8	5				AL,CR	AL,CR			
AL11CR2	2	11	2				AL	AL,CR			
AL7CR	2	7	1				AL	AL CR			
ALCU_ETA	2	1	1				CU AL	CU ZN			
ALCU_EPSILON	2	1	1				AL CU ZN	CU			
ALCU_THETA	2	2	1				AL	AL CU			
ALCU_DELTA	2	2	3				AL ZN	CU			
ALCU_ZETA	2	9	11				AL ZN	CU			
ALCULI_R	3	0.55	0.117	0.333			AL	CU	LI		
ALCULI_T1	3	0.5	0.25	0.25			AL	CU	LI		
ALCULI_T2	3	0.57	0.11	0.32			AL	CU	LI		
ALCULI_TB	3	0.6	0.32	0.08			AL	CU	LI		
ALCUMG_QPHASE	3	7	3	6			AL	CU	MG		
ALCUMG_SPHASE	3	2	1	1			AL	CU	MG		
ALCUMG_VPHASE	3	5	6	2			AL	CU	MG		
ALCUZN_GAMMA_H	4	2	2	3	6		CU	AL,CU	CU	AL,CU	
ALCUZN_TAU	4	1	4	4	1		AL,CU	AL	CU	ZN	
AL3DY_D024	2	3	1				AL	DY			
ALDY	2	1	1				AL	DY			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AL2DY3	2	2	3				AL	DY			
ALDY2	2	1	2				AL	DY			
ALER	2	1	1				AL	ER			
ALER2	2	1	2				AL	ER			
AL2ER3	2	2	3				AL	ER			
AL3ER	2	3	1				AL	ER			
AL2FE	2	2	1				AL	FE MN			
AL5FE2	2	5	2				AL	FE MN			
AL5FE4	1	1					AL FE MN				
AL13FE4	3	0.6275	0.235	0.1375			AL	FE MN	AL VA SI		
ALFESI_ALPHA	4	0.6612	0.19	0.0496	0.0992		AL	FE	SI	AL SI	
ALFESI_BETA	3	14	3	3			AL	FE	SI		
ALFESI_GAMMA	3	3	1	1			AL	FE	SI		
ALFESI_DELTA	3	0.55	0.15	0.3			AL	FE	SI		
ALFESI_TAU1	3	2	2	1			AL	FE	SI		
ALFESI_TAU3	3	2	1	1			AL	FE	SI		
AL3GD	2	3	1				AL	GD			
ALGD	2	1	1				AL	GD			
AL2GD3	2	2	3				AL	GD			
ALGD2	2	1	2				AL	GD			
HOAL3	2	3	1				AL	DY HO			
ALHO	2	1	1				AL	HO			
AL2HO3	2	2	3				AL	HO			
ALHO2	2	1	2				AL	HO			
ALLA	1	1					AL1LA				
ALLA3	1	1					AL1LA3				
AL2LA	1	1					AL2LA				
AL3LA	1	1					AL3LA				
AL11LA3D	1	1					AL11LA3				
AL11LA3F	1	1					AL11LA3				
AL53LA22	1	1					AL53LA22				
ALLI	2	1	1				AL LI MG	LI MG VA			
AL2LI3	2	2	3				AL	LI			
AL4LI9	2	4	9				AL	LI			
ALMG_BETA	2	89	140				MG	AL ZN			
ALMG_GAMMA	3	5	12	12			MG	AL MG ZN	AL MG ZN		
ALMG_GAMMA1	3	5	12	12			DY HO MG	MG	MG		
ALMG_EPSILON	2	23	30				MG	AL ZN			
ALMG_DZETA	2	21	19				AL	MG			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AL12MG17	3	24	10	24			LI MG	AL LI MG	AL MG		
ALMGMN_T	3	18	3	2			AL	MG	MN		
ALMGZN_PHI	2	6	5				MG	AL ZN			
ALMGZN_TAU	4	26	6	48	1		MG	AL MG	AL CU MG ZN	AL	
AL4MN	2	4	1				AL	FE MN			
AL6MN	2	6	1				AL	FE MN			
AL8MN5_D810	3	12	4	10			AL SI	MN	AL FE MN		
AL11MN4	2	11	4				AL	FE MN			
AL12MN	2	12	1				AL	FE MN			
ALMNSI_ALPHA	4	16	4	1	2		AL	MN	SI	AL SI	
ALMNSI_DELTA	3	2	1	3			AL	MN	SI		
ALMNSI_BETA	4	15	1	4	6		AL	SI	AL SI	MN	
AL4MO	2	4	1				AL	MO			
AL5MO	2	5	1				AL	MO			
AL8MO3	2	8	3				AL	MO			
AL12MO	2	12	1				AL	MO			
AL63MO37	2	63	37				AL	MO			
ALNB2	3	0.533	0.333	0.134			AL NB	AL NB	NB		
ALNB3	2	0.75	0.25				AL NB	AL NB			
AL3NB	2	0.25	0.75				AL NB	AL NB			
ALND2	2	1	2				AL	ND			
AL3NI	2	0.75	0.25				AL	NI			
AL3NI2	3	3	2	1			AL	AL NI	VA NI		
AL3NI5	2	0.375	0.625				AL	NI			
ALPR	2	1	1				AL	PR			
AL11PR3	2	11	3				AL	PR			
ALPR2	2	1	2				AL	PR			
ALPR3	2	1	3				AL	PR			
AL2PR	2	2	1				AL	PR			
AL3PR	2	3	1				AL	PR			
ALPT3	2	0.25	0.75				AL PT	AL PT			
AL21PT5	2	21	5				AL	PT			
AL21PT8	2	21	8				AL	PT			
AL2PT	2	2	1				AL	PT			
AL3PT2	2	3	2				AL	PT			
ALPT	2	1	1				AL	PT			
AL3PT5	2	3	5				AL	PT			
ALRU	2	1	1				AL	RU			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AL13RU4	2	13	4				AL	RU			
AL2RU	2	2	1				AL	RU			
AL3RU2	2	3	2				AL	RU			
AL6RU	2	6	1				AL	RU			
AL3SC	2	3	1				AL	SC			
AL2SC	2	2	1				AL	SC			
ALSC	2	1	1				AL	SC			
ALSC2	2	1	2				AL	SC			
AL11SM3_HT	2	11	3				AL	SM			
AL11SM3_LT	2	11	3				AL	SM			
ALSM	2	1	1				AL	SM			
ALSM2	2	1	2				AL	SM			
AL2SM	2	2	1				AL	SM			
AL3SM	2	3	1				AL	SM			
AL7SR8	2	7	8				AL	SR			
AL2SR	2	2	1				AL	SR			
AL4SR	2	4	1				AL	SR			
ALTA	1	1					AL1TA				
ALTA_SIGMA	3	10	4	16			AL CO TA V	TA V	AL CO TA V		
AL3TA	1	1					AL3TA				
AL3TA2	1	1					AL3TA2				
AL7TA5	1	1					AL7TA5				
AL69TA39	1	1					AL69TA39				
AL7TH2	2	7	2				AL	TH			
AL3TH_D019	2	3	1				AL	TH			
AL2TH_C32	2	2	1				AL	TH			
AL3TH2	2	3	2				AL	TH			
ALTH_BF	2	1	1				AL	TH			
AL2TH3_D5A	2	2	3				AL	TH			
ALTH2_C16	2	1	2				AL	TH			
ALTI	2	1	1				AL MO NB TA TI V W	AL MO NB TA TI V W			
AL2TI	2	2	1				AL	TI			
AL11TI5	2	17	8				AL	TI			
AL7V	2	7	1				AL	V			
AL8V5	2	8	5				AL	V			
AL10V	2	10	1				AL	V			
AL23V4	2	23	4				AL	V			
AL2W	2	2	1				AL	W			
AL4W	2	4	1				AL	W			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AL5W	2	5	1				AL	W			
AL7W3	2	7	3				AL	W			
AL12W	2	12	1				AL	W			
AL77W23	2	77	23				AL	W			
ALY_BF	2	1	1				AL	Y			
ALY2_C23	2	1	2				AL	Y			
AL2Y3	2	2	3				AL	Y			
AL3Y_BETA	2	3	1				AL	Y			
AL3Y_D019	2	3	1				AL	Y			
AL3Y5	2	3	5				AL	Y			
ALZR	2	1	1				AL	ZR			
ALZR2	2	1	2				AL	ZR			
ALZR3	2	1	3				AL	ZR			
AL2ZR	2	2	1				AL	ZR			
AL2ZR3	2	2	3				AL	ZR			
AL3ZR	2	3	1				AL	ZR			
AL3ZR2	2	3	2				AL	ZR			
AL3ZR5	2	3	5				AL	ZR			
AL4ZR5	2	4	5				AL	ZR			
AS2GE	2	0.6666	0.3333				AS	GE			
ASGE	2	0.5	0.5				AS	GE			
ASNI	2	1	1				AS	NI			
AS2NI	2	2	1				AS	NI			
AS2NI5	2	2	5				AS	NI			
AS8NI11	2	8	11				AS	NI			
AS2PT	2	2	1				AS	PT			
AU2BI_C15	2	2	1				AG, AU	BI			
AU5HF	2	5	1				AU	AU HF			
AU4HF	2	4	1				AU	HF			
AU3HF	2	3	1				AU	HF			
AU2HF	2	2	1				AU	AU HF			
AU10HF7	2	10	7				AU	HF			
AUHF_ALPHA	2	1	1				AU	AU HF			
AUHF_BETA	2	1	1				AU	AU HF			
AUHF2	2	1	2				AU	HF			
AUIN	2	0.5	0.5				AU	IN, SB, SN			
AUIN2	2	0.3333	0.6667				AU	IN, SB, SN			
AU3IN	2	0.75	0.25				AU	IN			
AU7IN3	2	0.7	0.3				AU	IN			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AUIN_BETA	2	0.785	0.215				AU	IN			
AUIN_GAMMA	3	0.69231	0.23077	0.07692			AU	AU,IN	IN		
AUIN_PSI	3	0.5	0.33333	0.16667			AU	AU,IN	IN		
AUIN_BETAP	2	0.77778	0.22222				AU	IN			
AU4IN3SN3	3	0.4	0.3	0.3			AU	IN,SN	IN,SN		
AUNI2SN4	3	0.143	0.286	0.571			AU	NI	SN		
AUPB2	2	0.3333	0.6667				AU	PB			
AUPB3	2	0.25	0.75				AU	PB			
AU2PB	2	0.6667	0.3333				AU	PB			
AU6PR	2	6	1				AU	PR			
AU51PR14	2	51	14				AU	PR			
AU36PR17	2	36	17				AU	PR			
AU2PR	2	2	1				AU	PR			
AU4PR3	2	4	3				AU	PR			
AUPR_ALPHA	2	1	1				AU	PR			
AUPR_BETA	2	1	1				AU	PR			
AUPR_GAMMA	2	1	1				AU	PR			
AUPR2	2	1	2				AU	PR			
AUSB2	2	0.333333	0.666667				AG AU	BI IN SB			
AU1SN	2	0.5	0.5				AU NI	IN SN			
AUSN2	2	0.333333	0.666667				AU	SN			
AUSN4	2	0.2	0.8				AU NI	IN SN			
AU5SN	2	0.84	0.16				AU	SN			
AUTE2	1	1					AU1TE2				
TI3AU	2	0.75	0.25				TI	AU			
TIAU	2	0.5	0.5				TI VA	AU TI			
TIAU2	2	1	2				TI	AU			
TIAU4	2	0.2	0.8				AU TI	AU			
AU10ZR7	2	10	7				AU	ZR			
AUZR	2	1	1				AU	ZR			
AUZR2	2	1	2				AU	ZR			
AUZR3	2	1	3				AU	ZR			
AU2ZR	2	2	1				AU	ZR			
AU2ZR3	2	2	3				AU	ZR			
AU3ZR	2	3	1				AU	ZR			
AU4ZR	2	4	1				AU	ZR			
AUZN_A3	3	0.64286	0.25	0.10714			AU	AU,ZN	ZN		
AUZN_A1	3	0.6	0.2	0.2			AU	AU,ZN	ZN		
AUZN_A2	2	0.75	0.25				AU	ZN			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AUZN_BETA	2	0.5	0.5				AU,ZN	AU,ZN			
AUZN_DELTA	2	0.44	0.56				AU	ZN			
AUZN_G2	2	0.25	0.75				AU	ZN			
AUZN_G3	3	0.12	0.16	0.72			AU	AU,ZN	ZN		
AUZN_E1	2	0.15	0.85				AU	ZN			
AU5ZN3	2	0.625	0.375				AU	ZN			
AUZN_BRASS	4	2	2	3	6		AU,ZN	AU	AU,ZN	ZN	
B2_INYB	2	0.5	0.5				IN,YB	IN,YB			
B27_COB	2	1	1				CO	B			
CO3B	2	3	1				CO	B			
C16_CO2B	2	2	1				CO	B			
B2MG	2	2	1				B	MG			
B4MG	2	4	1				B	MG			
B7MG	2	7	1				B	MG			
D2B_B12SC1	2	12	1				B	SC			
C32_B2SC1	2	2	1				B	SC			
MNB4	2	1	4				MN	B			
MNB2	2	1	2				MN	B			
MN3B4	2	3	4				MN	B			
MNB	2	1	1				MN	B			
MN2B_TET	2	2	1				MN	B			
MN2B_ORTHO	2	0.670691	0.329309				MN	B			
B12U	2	0.923	0.077				B	U			
B4U	2	0.8	0.2				B	U			
B2U	2	0.667	0.333				B	U			
BZR	2	1	1				B	ZR			
B12ZR	2	12	1				B	ZR			
B2ZR	2	2	1				B	ZR			
B4ZR3	2	4	3				B	ZR			
BACU	1	1					BA1CU				
BACU13	1	1					BA1CU13				
BIIN	2	0.5	0.5				BI	IN			
BIIN_EPSILON	1	1					BI IN				
BIIN_BRASS	2	0.333333	0.666667				BI	IN			
BI3IN5	2	0.375	0.625				BI	IN			
BIK3A	2	0.25	0.75				BI	K			
BIK3B	2	0.25	0.75				BI	K			
BI2K	2	0.666667	0.333333				BI	K			
BI2K3	2	0.4	0.6				BI	K			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
BI4K5	2	0.444444	0.555556				BI	K			
BINI	3	1	1	1			NI,VA	VA	BI		
BI3NI	2	0.75	0.25				BI	NI			
BITB	2	1	1				BI	TB			
BI3TB4	2	3	4				BI	TB			
BI3TB5_ALPHA	2	3	5				BI	TB			
BI3TB5_BETA	2	3	5				BI	TB			
BI2PD	2	2	1				BI	PD			
BIPD	2	1	1				BI	PD			
BI3PD5	1	1					BI PD				
BIPD3	2	1	3				BI	PD			
BITL_EPSILON	1	1					BI TL				
BITM	2	1	1				BI	TM			
BI3TM5	2	3	5				BI	TM			
BIY	2	1	1				BI	Y			
BI3Y5	2	3	5				BI	Y			
FCC_B1	2	1	1				U	C C2 N VA			
BCT_U	2	1	1				U	C C2 VA			
C3U2	2	2	3				U	C			
CACU	1	1					CA1CU				
CACU5	1	1					CA1CU5				
CA2CU	1	1					CA2CU				
CAGA	2	1	1				CA	GA			
CA11GA7	2	11	7				CA	GA			
CAGA2	2	1	2				CA	GA			
CAGA4	2	1	4				CA	GA			
CA25GA59	2	25	59				CA	GA			
CA28GA11	2	28	11				CA	GA			
CA3GA5	2	3	5				CA	GA			
CA3GA8	2	3	8				CA	GA			
CA5GA3	2	5	3				CA	GA			
CAH_GAMMA	2	1	0.5				CA	H,VA			
CAH2_ALPHA	2	1	2				CA	H			
CAH2_BETA	2	1	2				CA	H			
CALI2	2	1	2				CA	LI			
CAMG2	1	1					CA1MG2				
CASI	1	1					CA1SI				
CASI2	1	1					CA1SI2				
CA2SI	1	1					CA2SI				

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
D23_CAZN13	2	1	13				CA	ZN			
D2D_CAZN5	2	1	5				CA	ZN			
CA3ZN	2	3	1				CA	ZN			
CA5ZN3	2	5	3				CA	ZN			
CAZN	2	1	1				CA	ZN			
CAZN11	2	1	11				CA	ZN			
CAZN2	2	1	2				CA	ZN			
CAZN3	2	1	3				CA	ZN			
CD3IN	2	3	1				CD	IN			
CDIN_ALPHA	1	1					CD IN				
CDSB_OMEGA	2	1	1				CD ZN	SB			
CEMG	2	1	1				CE	MG			
CEMG2	2	1	2				CE	MG			
CEMG3	2	1	3				CE	MG			
CEMG12	2	1	12				CE	MG			
CE2MG17	2	2	17				CE	MG			
CE5MG41	2	5	41				CE	MG			
CE7NI3	2	7	3				CE	NI			
CENI	2	1	1				CE	NI			
CENI2	2	1	2				CE	NI			
CENI3	2	1	3				CE	NI			
CE2NI7	2	2	7				CE	NI			
CENI5	2	1	5				CE	NI			
CE2SB	2	2	1				CE	SB			
CE4SB3_D73	2	4	3				CE	SB			
CESB_B1	2	1	1				CE	SB			
CESB2	2	1	2				CE	SB			
CO2CE	1	1					CO2CE				
CO3CE	1	1					CO3CE				
CO5CE	1	1					CO5CE				
CO7CE2	1	1					CO7CE2				
CO11CE24	1	1					CO11CE24				
CO17CE2	1	1					CO17CE2				
CO19CE5	1	1					CO19CE5				
CODY3	2	1	3				CO	DY			
CO7DY12	2	7	12				CO	DY			
CO2DY	2	2	1				CO	DY			
CO3DY	2	3	1				CO	DY			
CO7DY2	2	7	2				CO	DY			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CO5DY	2	5	1				CO	DY			
CO17DY2	2	17	2				CO	DY			
COGA	2	0.5	0.5				CO VA	CO GA			
COGA3	2	1	3				CO	GA			
CO17GD2	2	17	2				CO	GD			
CO5GD	2	5	1				CO	GD			
CO7GD2	2	7	2				CO	GD			
CO3GD	2	3	1				CO	GD			
CO2GD	2	2	1				CO	GD			
CO3GD4	2	3	4				CO	GD			
COGD3	2	1	3				CO	GD			
CO23GD6	2	23	6				CO	GD			
COGE	2	1	1				CO	GE			
CO3GE	2	3	1				CO	GE			
COGE2	2	1	2				CO	GE			
CO5GE2	2	5	2				CO	GE			
CO5GE3	2	5	3				CO	GE			
CO5GE7	2	5	7				CO	GE			
COIN2	2	1	2				CO	IN			
COIN3	2	1	3				CO	IN			
CO3MO	2	3	1				CO	MO			
CONB_MU	4	1	2	4	6		CO NB	NB CO	NB	CO	
CONB_LAMBDA	2	2	1				CO NB	NB CO			
CO3NB	1	1					CO3NB				
CO7NB2	1	1					CO7NB2				
CO16NB9	1	1					CO16NB9				
COPT	1	1					CO PT				
COPT3	1	1					CO PT				
COSB_B81	3	0.3333	0.3333	0.3333			CO VA	CO VA	SB		
COSB2_C18	2	0.3333	0.6667				CO	SB			
COSB3_D02	2	0.25	0.75				CO	SB			
COSI2	2	1	2				CO	SI			
COSI	2	0.5	0.5				CO,SI	CO,SI			
CO2SI_ALPHA	2	2	1				CO,SI	CO,SI			
CO2SI_BETA	2	2	1				CO,SI	CO,SI			
CO3SI	2	3	1				CO	SI			
COSM3	1	1					CO1SM3				
CO2SM	1	1					CO2SM				
CO3SM	1	1					CO3SM				

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CO4SM9	1	1					CO4SM9				
CO5SM	1	1					CO5SM				
CO7SM2	1	1					CO7SM2				
CO17SM2	1	1					CO17SM2				
CO19SM5	1	1					CO19SM5				
COSN	2	1	1				CO	SN			
COSN2	2	1	2				CO	SN			
CO3SN2_A	2	3	2				CO	SN			
CO3SN2_B	2	3	2				CO	SN			
COTA2	1	1					CO1TA2				
CO7TA2	1	1					CO7TA2				
COTI2	2	1	2				CO	TI			
COV3_A15	2	1	3				CO	V			
COZN	1	1					CO ZN				
CO4ZN	1	1					CO ZN				
CO2ZN15	2	0.117647	0.882353				CO	ZN			
COZN7	2	0.125	0.875				CO	ZN			
COZN14	2	0.071429	0.928571				CO	ZN			
CO3W	2	3	1				CO NI	W			
CO7Y2	2	7	2				CO	Y			
CO3Y	2	3	1				CO	Y			
CO2Y	2	2	1				CO	Y			
CO3Y2	2	3	2				CO	Y			
CO7Y6	2	7	6				CO	Y			
COY	2	1	1				CO	Y			
CO3Y4	2	3	4				CO	Y			
CO5Y8	2	5	8				CO	Y			
COY3	2	1	3				CO	Y			
CO17Y2	3	1	2	15			CO2 Y	CO2 Y	CO		
CO5Y	3	1	4	1			CO2 Y	CO	CO VA		
CO11ZR2	2	0.846	0.154				CO	ZR			
CO4ZR	2	0.8	0.2				CO	ZR			
CO2ZR	2	0.68	0.32				CO	ZR			
COZR	2	0.5	0.5				CO	ZR			
COZR2	2	0.333	0.667				CO	ZR			
COZR3	2	0.25	0.75				CO	ZR			
CR3GA	2	3	1				CR	GA			
CRGA	2	1	1				CR	GA			
CR5GA6	2	5	6				CR	GA			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CRGA4	2	1	4				CR	GA			
CR3GE	2	0.75	0.25				CR,GE	CR,GE			
CR5GE3	2	0.625	0.375				CR,GE	CR,GE			
LCR5GE3	2	0.625	0.375				CR,GE	CR,GE			
CR11GE8	2	0.579	0.421				CR	GE			
CRGE	2	0.5	0.5				CR	GE			
CR11GE19	2	0.367	0.633				CR	GE			
CR3MN5	2	3	5				CR	MN TI			
CRNI2	2	1	2				CR,MO,W	MO,NI,W			
CRPD	2	0.5	0.5				CR	PD			
CR2PD3	2	0.4	0.6				CR	PD			
A15_CR3PT	2	0.8	0.2				CR	PT			
L12_CRPT2	1	1					CR,PT				
CR2RU	2	2	1				CR	RU			
CR3RU	2	3	1				CR	RU			
CRSI2	2	1	2				CR TI SI	CR SI			
CR3SI_A15	3	3	1	3			CR FE SI TI	CR SI AL NB	C VA		
CR5SI3	2	5	3				CR FE TI	SI			
CRZN13	2	1	13				CR	ZN			
CRZN17	2	1	17				CR	ZN			
CSNA_S	2	1	2				CS	NA			
CUCE	1	1					CU1CE				
CU2CE	1	1					CU2CE				
CU4CE	1	1					CU4CE				
CU5CE	1	1					CU5CE				
CU6CE	1	1					CU6CE				
CUER	2	1	1				CU	ER			
CU2ER	2	2	1				CU	ER			
CU5ER	2	5	1				CU	ER			
CU7ER2	2	7	2				CU	ER			
CU9ER2	2	9	2				CU	ER			
CU5EU	2	5	1				CU	EU			
CU2EU	2	2	1				CU	EU			
CUEU	2	1	1				CU	EU			
CUEU2	2	1	2				CU	EU			
CU3GE	1	1					CU3GE				
CUIN_BETA	2	4	1				CU	IN			
CUIN_ETA	3	0.545	0.122	0.333			CU, NI	CU, IN, SN	IN, SN		
CUIN_ETAP	2		0.64	0.36			CU	IN			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CUIN_DELTA	2	0.7	0.3				CU	IN SN			
CUIN_GAMMA	3	0.654	0.115	0.231			AG,CU	AG,CU,IN	IN,SN		
CUIN_THETA	2	0.55	0.45				CU	IN			
CU2IN3SN	3	0.333	0.5	0.167			CU	IN	SN		
CU77INSN23	2	0.77	0.23				CU	IN, SN			
CU3NI27SN10	3	0.075	0.675	0.25			CU	NI	SN		
CU10HF7	2	10	7				CU	HF			
CUHF2	2	1	2				CU	HF			
CU5HF1	2	5	1				CU	HF			
CU51HF14	2	51	14				CU	HF			
CU8HF3	2	8	3				CU	HF			
CU5HO_C15B	2	5	1				CU	HO			
CU5HO_D2D	2	5	1				CU	HO			
CU9HO2	2	9	2				CU	HO			
CU7HO2	2	7	2				CU	HO			
CU2HO	2	2	1				CU	HO			
CUHO_B2	2	1	1				CU	HO			
CU37LA3	2	37	3				CU	LA			
CU6LA_ALPHA	2	6	1				CU	LA			
CU6LA_BETA	2	6	1				CU	LA			
CU5LA	2	5	1				CU	LA			
CU4LA	2	4	1				CU	LA			
CU2LA	2	2	1				CU	LA			
CULA	2	1	1				CU	LA			
CUMG2	2	1	2				CU	MG			
CUMGSI_SIGMA	3	16	6	7			CU	MG	SI		
CUMGSI_TAU	2	2	1				CU,SI	MG			
CUND	1	1					CU1ND				
CU2ND	1	1					CU2ND				
CU4ND	1	1					CU4ND				
CU5ND	1	1					CU5ND				
CU6ND	1	1					CU6ND				
CUPD_B2	3	0.5	0.5	1			CU PD	CU PD	H VA		
CUPR	1	1					CU1PR				
CU2PR	1	1					CU2PR				
CU4PR	1	1					CU4PR				
CU5PR	1	1					CU5PR				
CU6PR	1	1					CU6PR				
CUSB_ZETA	2	0.77	0.23				CU	SB			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CUSB_GAMMA	2	0.85	0.15				CU	SB			
CUSB_ETA	2	0.67	0.33				CU	SB			
CUSB_EPSILON	2	0.75	0.25				CU	SB			
CUSB_DELTA	2	0.8	0.2				CU	SB			
CU4SC_D1A	2	4	1				CU	SC			
CU2SC_C11B	2	2	1				CU	SC			
CU5C_B2	2	1	1				CU	SC			
CU15SI4_EPSILON	2	15	4				CU	SI			
CU19SI6_ETA	2	19	6				CU	SI			
CU33SI7_GAMMA	2	33	7				CU	SI			
CU9SI2_DELTA	2	9	2				CU	SI			
CUSM	1	1					CU1SM				
CU2SM	1	1					CU2SM				
CU4SM	1	1					CU4SM				
CU5SM	1	1					CU5SM				
CU6SM	1	1					CU6SM				
CUSN_GAMMA_DO3	2	0.75	0.25				CU SN	CU SN			
CU3SN	2	0.75	0.25				CU, NI	IN, SN			
CU6SN5_P	2	0.545	0.455				CU	SN			
CU41SN11	2	0.788	0.212				CU	IN, SN			
CU10SN3	2	0.769	0.231				CU	SN			
CUTI	2	1	1				CU TI	CU TI			
CUTI2	2	1	2				CU	TI			
CU2TI	2	2	1				CU	TI			
CU3TI2	2	3	2				CU	TI			
CU4TI	2	4	1				CU TI	CU TI			
CU4TI3	2	4	3				CU	TI			
CUY	1	1					CU1Y				
CU2YR	1	1					CU2Y				
CU7Y2	1	1					CU7Y2				
CU4Y	1	1					CU4Y				
CU2YH	1	1					CU2Y				
CU6Y	2	5	1				CU	CU2 Y			
CUZN_GAMMA	4	2	2	3	6		CU,ZN	AL,CU,SI,ZN	CU,ZN	AL,CU,MG,SI,ZN	
CUZR	2	1	1				CU	ZR			
CUZR2	2	1	2				CU	ZR			
CU5ZR	2	5	1				CU	ZR			
CU8ZR3	2	8	3				CU	ZR			
CU10ZR7	2	10	7				CU	ZR			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CU51ZR14	2	51	14				CU	ZR			
D_GAMMA	1	1					AL CU SI ZN				
DY3NI_D011	2	3	1				DY	NI			
DY3NI2	2	3	2				DY	NI			
DYNI_B27	2	1	1				DY	NI			
DYNI2_C15	2	1	2				DY	NI			
DYNI3	2	1	3				DY	NI			
DY2NI7	2	2	7				DY	NI			
DYNI4	2	1	4				DY	NI			
DY4NI17	2	4	17				DY	NI			
DYNI5_D2D	2	1	5				DY	NI			
DY2NI17	2	2	17				DY	NI			
ER3NI	2	3	1				ER	NI			
ER3NI2	2	3	2				ER	NI			
ERNI	2	1	1				ER	NI			
ERNI2	2	1	2				ER	NI			
ERNI3	2	1	3				ER	NI			
ER2NI7	2	2	7				ER	NI			
ER4NI17	2	4	17				ER	NI			
ERNI4	2	1	4				ER	NI			
ER5NI22	2	5	22				ER	NI			
ERNI5	2	1	5				ER	NI			
ER2NI17	2	2	17				ER	NI			
EUMG_B2	2	1	1				EU	MG			
EUMG2_C14	2	1	2				EU	MG			
EUMG4	2	1	4				EU	MG			
EUMG5	2	1	5				EU	MG			
EU2MG17	2	2	17				EU	MG			
EU5PD2	2	5	2				EU	PD			
EU3PD2	2	3	2				EU	PD			
EUPD	2	1	1				EU	PD			
EUPD2	2	1	2				EU	PD			
EUPD3	2	1	3				EU	PD			
EUPD5	2	1	5				EU	PD			
EUPD7	2	1	7				EU	PD			
EU2SN	2	2	1				EU	SN			
EU5SN3	2	5	3				EU	SN			
EUSN	2	1	1				EU	SN			
EU3SN5	2	3	5				EU	SN			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
EUSN3	2	1	3				EU	SN			
FE2R	2	2	1				FE	DY TB			
FE3R	2	3	1				FE	DY TB			
FE17R2	2	17	2				FE	DY TB			
FE23R6	2	23	6				FE	DY TB			
FE2GD	1	1					FE2GD				
FE3GD	1	1					FE3GD				
FE17GD2	1	1					FE17GD2				
FE23GD6	1	1					FE23GD6				
FE2NB_LAVES_C14	2	2	1				FE	NB			
FE17ND2	2	0.89474	0.10526				FE	ND			
FE17ND5	2	0.77273	0.22727				FE	ND			
FEPD	2	0.5	0.5				FE PD	FE PD			
FEPD3	2	0.25	0.75				FE PD	FE PD			
FE17PR2	2	17	2				FE	PR			
FE2PR	2	2	1				FE	PR			
FESB	2	1	1				FE	FE SB			
FESB2	1	1					FE1SB2				
FE2SC	2	2	1				FE	SC			
FESC7	2	1	7				FE	SC			
MSI	2	1	1				CR FE MN NI	SI			
FESI2_H	2	3	7				FE	SI			
FESI2_L	2	1	2				FE	SI			
FE2SI	2	2	1				FE	SI			
M3SI	2	3	1				FE MN	SI			
M5SI3	2	5	3				CR FE MN	SI			
FE17SM2	2	17	2				FE	SM			
FE3SM	2	3	1				FE	SM			
FE2SM	2	2	1				FE	SM			
FESN	1	1					FE1SN				
FESN2	1	1					FE1SN2				
FE3SN2	1	1					FE3SN2				
FE5SN3	1	1					FE5SN3				
FE7TA6_MU	2	7	6				FE	TA			
FE2TA_LAVES_C14	2	2	1				FE	TA			
FETI	2	1	1				FE	TI			
FEU6	2	1	6				FE U	FE U			
FE2U	2	2	1				FE U	FE U			
FE17Y2	2	17	2				FE	Y			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
FE23Y6	2	23	6				FE	Y			
FE3Y	2	3	1				FE	Y			
FE2Y	2	2	1				FE	Y			
FEZN_GAMMA_D82	4	0.154	0.154	0.231	0.461		FE,ZN	FE,ZN	FE,SI,ZN	ZN	
FEZN_GAMMA_D81	3	0.137	0.118	0.745			FE	FE,SI,ZN	ZN		
FEZN_DELTA	4	0.058	0.18	0.525	0.237		FE	FE,SI,ZN	ZN	ZN	
FEZN_ZETA	3	0.072	0.856	0.072			FE,VA	ZN	SI,VA,ZN		
FEUZR_EPSILON	3	30	30	40			FE	U	ZR		
FEUZR_DELTA	2	1	2				FE U ZR	FE U ZR			
FEUZR_LAMBDA	3	6	71	23			FE	U	ZR		
FEUZR_KAPPA	3	48	20	32			FE	U	ZR		
FE6W6C	3	6	6	1			FE	W	C		
FEW3C	3	1	3	1			FE	W	C		
FEZR2	2	1	2				FE ZR	FE ZR			
FEZR3	2	1	3				FE ZR	FE ZR			
FE23ZR6	1	1					FE23ZR6				
GAN	2	1	1				GA	N			
GE2SR	2	2	1				GE	SR			
GESR_BF	2	1	1				GE	SR			
GE3SR5_D8L	2	3	5				GE	SR			
GESR2_C23	2	1	2				GE	SR			
NI5GA3	2	0.63	0.37				NI	GA			
NI3GA2	2	0.6	0.4				NI	GA			
NI3GA4	2	0.43	0.57				NI	GA			
NI2GA3	2	0.4	0.6				NI	GA			
NIGA4	2	0.2	0.8				NI	GA			
MG5GA2	2	5	2				MG	GA			
MG2GA	2	2	1				MG	GA			
MGGA	2	1	1				MG	GA			
MGGA2	2	1	2				MG	GA			
MG2GA5	2	2	5				MG	GA			
GANI_B2	2	0.5	0.5				GA NI	NI VA			
GA6PT	2	0.857	0.143				GA	PT			
GA7PT3	2	0.7	0.3				GA	PT			
GA2PT	2	0.667	0.333				GA	PT			
GA3PT2	2	0.6	0.4				GA	PT			
GAPT	2	0.5	0.5				GA	PT			
GA3PT5	2	0.375	0.625				GA	PT			
GAPT2	2	0.333	0.667				GA	PT			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
GAPT3	2	0.25	0.75				GA PT	GA PT			
GATI3	2	1	3				GA TI	GA TI			
GATI2	2	1	2				GA	TI			
GA3TI5	2	3	5				GA	TI			
GA4TI5	2	4	5				GA TI	GA TI			
GATI	2	1	1				GA TI	GA TI			
GA3TI2	2	3	2				GA	TI			
GA2TI	2	2	1				GA	TI			
GA3TI	2	3	1				GA	TI			
GDGE	2	1	1				GD	GE			
GD5GE3	2	5	3				GD	GE			
GD5GE4	2	5	4				GD	GE			
GD3GE5_A	2	3	5				GD	GE			
GD41GE59_A	2	41	59				GD	GE			
GD14GE36	2	1	2.57				GD	GE			
GD3GE5_B	2	3	5				GD	GE			
GD41GE59_B	2	41	59				GD	GE			
GD2GE3	2	2	3				GD	GE			
GDMG	1	1					GD1MG				
GDMG2	1	1					GD1MG2				
GDMG3	1	1					GD1MG3				
GDMG5	1	1					GD1MG5				
M12R	2	12	1				MN	GD			
M23R6	2	23	6				MN	GD			
M2R	2	2	1				MN	GD			
GD3NI	2	3	1				GD	NI			
GD3NI2	2	3	2				GD	NI			
GDNI	2	1	1				GD	NI			
GDNI2	2	1	2				GD	NI			
GDNI3	2	1	3				GD	NI			
GD2NI7	2	2	7				GD	NI			
GDNI4	2	1	4				GD	NI			
GDNI5	2	1	5				GD	NI			
GD2NI17	2	2	17				GD	NI			
GDSI	2	1	1				GD	SI			
GDSI2	2	1	2				GD	SI			
GD3SI5	2	3	5				GD	SI			
GD5SI3	2	5	3				GD	SI			
GD5SI4	2	5	4				GD	SI			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
GEMG2	2	1	2				GE	MG			
B20_GERU	2	1	1				GE SI	RU			
ALPHA_GE3RU2	2	3	2				GE	RU			
BETA_GE3RU2	2	3	2				GE SI SN	RU			
GETE_LOW	2	1	1				GE VA	TE			
GETE_B1	2	1	1				GE VA	TE			
GETE_GAMMA	2	49	51				GE	TE			
GEV3	2	1	3				GE	V			
GE31V17	2	31	17				GE	V			
GE3V5	2	3	5				GE	V			
GE8V11	2	8	11				GE	V			
HFNIA	2	1	1				HF	NI			
HFNI3A	2	1	3				HF	NI			
HFNIB	2	1	1				HF	NI			
HFNI3B	2	1	3				HF	NI			
HFNI5	2	1	5				HF	NI			
HF2NI7	2	2	7				HF	NI			
HF3NI7	2	3	7				HF	NI			
HF7NI10	2	7	10				HF	NI			
HF9NI11	2	9	11				HF	NI			
HF8NI21	2	8	21				HF	NI			
NIHF2	2	2	1				HF	NI VA			
HF2SI	2	2	1				HF	SI			
HF5SI3	2	5	3				HF	SI			
HF3SI2	2	3	2				HF	SI			
HF5SI4	2	5	4				HF	SI			
HFSI	2	1	1				HF	SI			
HFSI2	2	1	2				HF	SI			
HGPB2_L10	2	1	2				HG	PB			
HGSN38_B	2	1	38				HG	SN			
HGSN12_G	2	1	6				HG VA	SN			
HGSN4	2	1	4				HG	SN			
HGSN7_D	2	1	7				HG	SN			
HG3ZN	2	0.75	0.25				HG	ZN			
HGZN2	2	1	2				HG	ZN			
HGZN3	2	1	3				HG	ZN			
HOMN2	2	2	1				MN	HO			
MN23M6_D8A	2	0.793	0.207				MN	HO SM			
HOMN12_D2B	2	12	1				MN	HO			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
ALPHA_INEU2	2	1	2				IN	EU			
BETA_INEU2	2	1	2				IN	EU			
INEU	2	1	1				IN	EU			
IN2EU	2	2	1				IN	EU			
IN4EU	2	4	1				IN	EU			
IN3LA	2	3	1				IN	LA			
IN2LA	2	2	1				IN	LA			
IN5LA3	2	5	3				IN	LA			
IN57LA43	2	57	43				IN	LA			
INLA	2	1	1				IN	LA			
INLA2	2	1	2				IN	LA			
INLA3	2	1	3				IN	LA			
IN3YB	2	3	1				IN	YB			
IN2YB	2	2	1				IN	YB			
INYB2	2	1	2				IN	YB			
IN2YB5	2	2	5				IN	YB			
NI2IN3	2	2	3				NI	IN			
NIIN	2	1	1				NI	IN			
NI3IN7	2	3	7				NI	IN			
NI3IN	2	3	1				NI	IN			
NI2IN	2	2	1				NI	IN			
INNI_ZETA	3	1	1	1			NI,VA	NI	IN,NI		
INNI_ZETA_PRIME	3	1	1	1			NI,VA	NI	IN		
INNI_DELTA	2	1	1				NI,VA	IN,NI			
INPD2_BETA	2	0.34	0.66				IN	PD			
INPD3_BETA	2	0.26	0.74				IN	PD			
INPD2_ALPHA	2	0.333	0.667				IN	PD			
INPD3_ALPHA	2	0.25	0.75				IN	PD			
IN7PD3	2	0.71	0.29				IN	PD			
IN3PD2	2	0.6	0.4				IN	AG,PD			
IN3PD5	2	0.375	0.625				IN	PD			
INSN_GAMMA	1	1					IN SN				
IR3ZR5	2	3	5				IR	ZR			
IR2ZR	2	2	1				IR	ZR			
IRZR2	2	1	2				IR	ZR			
IRZR3	2	1	3				IR	ZR			
IR3ZR	2	3	1				IR ZR	IR ZR			
IRZR_ALPHA	2	1	1				IR ZR	ZR			
IRZR_BETA	2	1	1				IR ZR	IR ZR			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
LAMG3	2	1	3				LA, MG	MG			
LAMG12	2	1	12				LA, MG	LA, MG			
LAMG	2	1	1				LA	MG			
LAMG2	2	1	2				LA	MG			
LA2MG17	2	2	17				LA	MG			
LANI	1	1					LA1NI				
LANI3	1	1					LA1NI3				
LANI5	1	1					LA1NI5				
LA2NI3	1	1					LA2NI3				
LA2NI7_ALPHA	1	1					LA2NI7				
LA2NI7_BETA	1	1					LA2NI7				
LA3NI	1	1					LA3NI				
LA7NI3	1	1					LA7NI3				
LA7NI16	1	1					LA7NI16				
LIH	2	1	1				LI	H			
LI3N	2	3	1				LI	N			
LI7SI3	1	1					LI7SI3				
LI12SI7	1	1					LI12SI7				
LI13SI4	1	1					LI13SI4				
LI22SI5	1	1					LI22SI5				
LI22SN5	2	22	5				LI	SN			
LI7SN2	2	7	2				LI	SN			
LI13SN5	2	13	5				LI	SN			
LI5SN2	2	5	2				LI	SN			
LI7SN3	2	7	3				LI	SN			
LISN	2	1	1				LI	SN			
LI2SN5	2	2	5				LI	SN			
MG2NI	2	2	1				MG	NI			
M6SI5	2	6	5				CR, TI	SI			
MG3LN	2	3	1				MG	DY			
MG12PR	2	12	1				MG	PR			
MG41PR5	2	41	5				MG, PR	MG, PR			
MGPR_B2	2	1	1				MG, PR	MG, PR			
MG2PR	2	2	1				MG	PR			
MG3PR	2	3	1				MG	MG, PR			
MG2RE	2	2	1				MG	ND			
MG41RE5	2	41	5				MG	ND			
MG3RE	2	3	1				MG	MG ND			
MG5RE	2	5	1				MG	ND			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
MGSC	1	1					MG1SC				
MG2SI	2	2	1				MG	SI			
MG2SN	1	1					MG2SN				
MG17SR2	2	17	2				MG	SR			
MG38SR9	2	38	9				MG	SR			
MG23SR6	2	23	6				MG	SR			
MG2TB	2	2	1				MG	MG TB			
MG3TB	2	3	1				MG	MG TB			
MG24TB5	2	24	5				MG	TB			
MG5TB	2	5	1				MG	TB			
MG24TM5	2	24	5				MG	TM			
MG2TM	2	2	1				MG	TM			
MGTM_B2	2	1	1				MG VA	MG TM			
MG2Y	2	2	1				MG Y	MG ND Y			
MG24Y5	3	24	4	1			MG	MG Y	Y		
MGYB_LAVES_C14	2	2	1				MG YB	MG YB			
MGZN	2	12	13				MG	AL CU ZN			
MG2ZN3	2	2	3				MG	AL CU ZN			
MG2ZN11	3	2	6	5			MG	CU ZN	AL ZN		
MG7ZN3	2	51	20				MG	ZN			
MNMO_LAVES_PHASE	2	2	1				MN	MO			
MN23SC6	2	23	6				MN	SC			
MN2SC	2	2	1				MN	SC			
MNSC4	2	1	4				MN	SC			
MN6SI	2	0.857143	0.142857				MN	SI			
MN9SI2		2	0.818182	0.181818			MN	SI			
MN5SI2	2	0.714286	0.285714				MN	SI			
MN11SI19	2	0.366667	0.633333				MN	SI			
MN2SM_LAVES_C14	2	2	1				MN	SM			
MN19SN6	2	19	6				MN	SN			
MN2SN	2	2	1				MN	SN			
MNSN2	2	1	2				MN	SN			
MN3TI	2	3	1				CR MN	TI			
MN4TI	2	0.815	0.185				CR MN	TI			
TIMN_ALPHA	2	1	1				CR MN	TI			
TIMN_BETA	2	0.515	0.485				CR MN	TI			
MN12Y	2	12	1				MN	Y			
MN23Y6	2	23	6				MN	Y			
MN2Y	2	2	1				MN	Y			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
MNZN9	2	1	9				MN	ZN			
MN2ZR	2	2	1				MN ZR	MN ZR			
MONI4_BETA	2	1	4				MO	NI			
MONI3_GAMMA	2	1	3				MO	NI			
MONI_DELTA	3	24	20	12			CR NI FE	CR MO NI FE	MO		
MO3SI	2	0.75	0.25				MO	SI			
MO5SI3	2	0.625	0.375				MO	SI			
MOSI2	2	0.333333	0.666667				MO	SI			
NBNI_MU	2	7	6				NI NB	NB			
NI3NB	2	3	1				NI NB	NB NI			
NB3SI	2	0.75	0.25				NB	SI			
NB5SI3	2	0.625	0.375				NB	SI			
NBSI2	2	1	2				NB	SI			
NBSN2	1	1					NB1SN2				
NB3SN_C15	2	3	1				NB SN	NB SN			
NB6SN5	3	24	16	4			NB	SN	NB SN		
NDSB	1	1					ND1SB				
NDSB2	1	1					ND1SB2				
ND2SB	1	1					ND2SB				
ND4SB3	1	1					ND4SB3				
ND5SB3	1	1					ND5SB3				
NISI2_C1	2	1	2				NI	SI			
NI3SI_MONOCL	2	3	1				NI	SI			
NI3SI_ORTHO	2	3	1				NI	SI			
NI2SI_C37	2	2	1				CR NI	SI			
NI3SI2	2	3	2				NI	SI			
NI5SI2	2	5	2				CR NI	SI			
NISI_B31	2	1	1				NI	SI			
NI2SI_HEX	3	1	1	1			NI	NI VA	SI		
NISM3	2	1	3				NI	SM			
NISM	2	1	1				NI	SM			
NI2SM	2	2	1				NI	SM			
NI3SM	2	3	1				NI	SM			
NI7SM2	2	7	2				NI	SM			
NI19SM5	2	19	5				NI	SM			
NI5SM	2	5	1				NI	SM			
NI17SM2	2	17	2				NI	SM			
NI3SN2	3	0.5	0.25	0.25			NI,SN	AU,CU,NI	AU,CU,NI		
NI3SN4	3	0.25	0.25	0.5			CU,NI	NI,SN	SN		

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
NI3SN_LT	2	0.75	0.25				CU,NI	IN,SN			
NISR	2	1	1				NI	SR			
NI2TA	2	0.666667	0.333333				NI	TA			
NI3MOTA	2	0.75	0.25				NI TA	NI TA			
NI8TA	2	0.888889	0.111111				NI	TA			
NITA	4	0.076923	0.307692	0.153846	0.461538		NI TA	TA	NI TA	NI	
NITA2	2	0.333333	0.666667				NI TA	TA			
NITi2	3	1	2	0.5			NI	TI	C VA		
NI3Ti	2	0.75	0.25				NI Ti	NI Si Ti			
Ti3SiC2	3	3	1	2			Ti	Si	C		
NI2V	2	2	1				NI	V			
NI3V	2	3	1				NI	V			
NI2V7	2	2	7				NI	V			
NIW	2	1	1				NI	W			
NIW2	2	1	2				NI	W			
NI4W	2	4	1				NI	W			
NI17Y2	2	17	2				NI	Y			
NI5Y	2	5	1				NI	Y			
NI4Y	2	4	1				NI	Y			
NI7Y2	2	7	2				NI	Y			
NI3Y	2	3	1				NI	Y			
NI2Y	2	2	1				NI	Y			
NIY	2	1	1				NI	Y			
NI2Y3	2	2	3				NI	Y			
NIY3	2	1	3				NI	Y			
NIZN_BETA1	1	1					NI ZN				
NIZN_DELTA	2	0.111	0.889				NI	ZN			
NIZN_GAMMA	1	1					NI ZN				
NI10ZR7	2	0.575	0.425				NI ZR	VA ZR			
NI11ZR9	2	0.55	0.45				NI	ZR			
NI21ZR8	2	0.725	0.275				NI	ZR			
NI3ZR	2	0.75	0.25				NI ZR	VA ZR			
NI5ZR	2	0.833	0.167				NI ZR	VA ZR			
NI7ZR2	2	0.78	0.22				CR NI	ZR			
NIZR	2	0.5	0.5				NI	ZR			
NIZR2	2	0.333	0.667				CR NI	ZR			
OSSI	2	0.5	0.5				OS	SI			
OS2Si3	2	0.4	0.6				OS	SI			
OSSI2	2	0.333333	0.666667				OS	SI			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
PT3PB	2	3	1				PT	PB			
PTPB	2	1	1				PT	PB			
PTPB4	2	1	4				PT	PB			
PBTE	2	1	1				PB	TE			
PDPB	1	1					PD1PB				
PDPB2	1	1					PD1PB2				
PD3PB	2	0.75	0.25				PD	PB PD			
PD5PB3_ALPHA	1	1					PD5PB3				
PD5PB3_BETA	3	1	1	1			PD	PB	VA PD		
PD5PB3_GAMMA	3	1	1	1			PD	PB	VA PD		
PD13PB9	1	1					PD0.59PB0.41				
PD3SC	2	3	1				PD	SC			
PD2SC	2	2	1				PD	SC			
PDSC2	2	1	2				PD	SC			
PDSC4	2	1	4				PD	SC			
PDSC	2	1	1				PD VA	SC			
PDSI	2	1	1				PD	SI			
PD19SI10	2	19	10				PD	SI			
PD39SI20	2	39	20				PD	SI			
PD2SI_BETA	2	2	1				PD,SI	SI			
PD2SI_ALPHA	2	2	1				PD,SI	SI			
PD3SI	2	3	1				PD	SI			
PD15SI4	2	15	4				PD	SI			
PD9SI2	2	9	2				PD	SI			
PD14SI3	2	14	3				PD	SI			
PD5SI	2	5	1				PD	SI			
PD21SI4	2	21	4				PD,SI	SI			
MPD3	2	1	3				PD,SM	PD			
MSM_A	2	1	1				PD,SM	SM			
MSM_B	2	1	1				PD,SM	SM			
PD7SM	2	7	1				PD	SM			
PD5SM	2	5	1				PD	SM			
PD21SM10	2	21	10				PD	SM			
PD4SM3	2	4	3				PD	SM			
PD2SM3	2	2	3				PD	SM			
PD3SM7	2	3	7				PD	SM			
PD2SN_GAMMA	3	1	1	1			PD	SN	PD,VA		
PDSN	2	0.5	0.5				PD,VA	PD,SN			
PDSN2	2	0.333	0.667				PD,SN	SN			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
PDSN3	2	0.25	0.75				PB,PD	PD,SN			
PDSN4	2	0.2	0.8				PD	PB,PD,SN			
PD3SN	2	0.75	0.25				PD,SN	SN,PD			
PD3SN2_ALPHA	2	0.6	0.4				PD	SN			
PD3SN2_BETA	2	0.6	0.4				PD	SN			
PD3SN2_DELTA	2	0.59	0.41				PD	SN			
PD2SN	2	0.667	0.333				PD	SN			
PD20SN13	2	0.6	0.4				PD,SN	PD,SN			
PD3TB	2	3	1				PD	PD,TB			
PD7TB	2	7	1				PD	TB			
PDTB_A	2	1	1				PD,TB	TB			
PDTB_B	2	1	1				PD,TB	TB			
PD21TB10	2	21	10				PD	TB			
PD3TB2_A	2	3	2				PD	TB			
PD3TB2_B	2	3	2				PD	TB			
PD4TB3	2	4	3				PD	TB			
PD2TB3	2	2	3				PD	TB			
PD2TB5	2	2	5				PD	TB			
PDZN_GAMMA	2	2	9				PD,ZN	PD,ZN			
PDZN_BETA	2	1	1				PD,ZN	PD,ZN			
PDZN_1BETA	2	1	1				PD,ZN	PD,ZN			
PDZN2	2	1	2				PD	ZN			
PD2ZN	2	2	1				PD	ZN			
PDZN_ETA	2	0.09	0.91				PD	ZN			
PD3ZR	2	3	1				PD ZR	PD ZR			
PDZRM	3	1	1	1			PD	ZR	PD ZR		
PD4ZR3	2	4	3				PD	ZR			
PD11ZR9	2	11	9				PD	ZR			
PDZR_ALPHA	2	1	1				PD	ZR			
PDZR_BETA	2	1	1				PD	ZR			
PDZR_GAMMA	2	1	1				PD VA	PD ZR			
PRSB	1	1					PR1SB				
PRSB2	1	1					PR1SB2				
PR2SB	1	1					PR2SB				
PR4SB3	1	1					PR4SB3				
PR5SB3	1	1					PR5SB3				
PTSI	2	1	1				PT	SI			
PT782SI218	2	0.782	0.218				PT	SI			
PT5SI2	2	0.714	0.286				PT	SI			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
PT6SI5	2	6	5				PT	SI			
PT17SI8_ALPHA	2	17	8				PT	SI			
PT2SI_ALPHA	2	2	1				PT	SI			
PT3SI_ALPHA	2	3	1				PT	SI			
PT17SI8_BETA	2	17	8				PT	SI			
PT2SI_BETA	2	2	1				PT	SI			
PT3SI_BETA	2	3	1				PT	SI			
PTTA_SIGMA	1	1					PT TA				
PT2TA	2	0.667	0.333				PT	TA			
PT3TA	2	0.75	0.25				PT	TA			
PTTA	2	0.5	0.5				PT	TA			
PTTA6	2	0.143	0.857				PT	TA			
PT8TI	2	8	1				PT	TI			
PT3TI	2	1	3				PT, TI	PT			
PTTI_ALPHA	2	1	1				PT, TI	PT, TI			
PTTI_BETA	2	1	1				PT, TI	PT, TI			
PT3TI4	2	3	4				PT	TI			
PTTI3	2	3	1				PT, TI	PT, TI			
PUC_B1	2	1	1				PU	C VA			
PU3C2	2	0.6	0.4				PU	C			
PU2C3_D5C	2	0.4	0.6				PU	C			
PUC2_C11A	2	1	2				PU	C			
RU2SI	2	2	1				RU	SI			
RU4SI3	2	4	3				RU	SI			
RU3SN7	2	3	7				RU	GE SN			
RU2SN3	2	2	3				RU	GE SN			
RUZR	2	1	1				RU	ZR			
RU2ZR	2	2	1				RU	ZR			
SBSN	2	1	1				BI, IN, PB, SB, SN	BI, IN, SB, SN			
SB2SN3	2	2	3				SB	SN			
SBZN_BETA	2	0.5	0.5				SB	ZN			
SBZN_DELTA	2	0.425	0.575				SB	ZN			
SBZN_ZETA	2	0.4	0.6				SB	ZN			
SBZN_EPSILON	2	0.425	0.575				SB	ZN			
SBZN_ETA	2	0.38	0.62				SB	ZN			
SBZN_GAMMA	2	0.45	0.55				SB	ZN			
SCSI	2	1	1				SC	SI			
SC2SI3	2	2	3				SC	SI			
SC5SI3	2	5	3				SC	SI			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
SI3N4	2	3	4				SI	N			
TA2SI	2	0.666667	0.333333				TA	SI			
TA3SI	2	0.75	0.25				TA	SI			
TASI2	2	0.333333	0.666667				TA	SI			
TA5SI3	2	0.625	0.375				TA	SI			
TISI	2	1	1				TI	SI			
TI3SI	2	3	1				TI	SI			
TISI2	2	1	2				CR TI	SI			
D88_M5SI3	4	2	3	3	1		CR SI TI	CR SI TI	CR NI TI	C N VA	
TI5SI4	2	5	4				TI	SI			
B27_SIU	2	0.511	0.489				SI	U			
C32_S15U3	2	0.625	0.375				SI	U			
L12_S13U	2	0.75	0.25				SI	U			
L12_SIU3_H	2	0.25	0.75				SI	U			
SIU3_L	2	0.25	0.75				SI	U			
CC_S12U	2	0.652778	0.347222				SI	U			
SI2U3	2	0.4	0.6				SI	U			
V3SI	2	3	1				SI V	SI V			
V5SI3	2	5	3				V	SI			
V6SI5	2	6	5				V	SI			
VS12	2	1	2				V	SI			
WSI2	2	0.666667	0.333333				SI	W			
W5SI3	2	0.375	0.625				SI	W			
YSI	2	1	1				SI	Y			
YSI2_H	2	2	1				SI	Y			
YSI2_R	2	2	1				SI	Y			
Y5SI3	2	3	5				SI	Y			
Y5SI4	2	4	5				SI	Y			
Y3SI5_R	2	5	3				SI	Y			
Y3SI5_H	2	5	3				SI	Y			
YBSI174	2	1.74	1				SI	YB			
YB3SI5	2	5	3				SI	YB			
YB8SI11	2	11	8				SI	YB			
YBSI	2	1	1				SI	YB			
YB5SI4	2	4	5				SI	YB			
YB5SI3	2	3	5				SI	YB			
ZRSI	2	1	1				SI	ZR			
ZR2SI	2	1	2				SI	ZR			
ZR3SI	2	1	3				SI	ZR			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
ZRSI2	2	2	1				SI	ZR			
ZR3SI2	2	2	3				SI	ZR			
ZR5SI3	2	3	5				SI	ZR			
ZR5SI4	2	4	5				SI	ZR			
SMSB	1	1					SM1SB				
SMSB2	1	1					SM1SB2				
SM2SB	1	1					SM2SB				
SM4SB3	1	1					SM4SB3				
SM5SB3	1	1					SM5SB3				
SNTI2	2	1	2				SN	TI			
SNTI3	2	1	3				SN TI	SN TI			
SN3TI5	2	3	5				SN	TI			
SN5TI6	2	5	6				SN	TI			
SN3V2	2	3	2				SN	V			
SNV3	2	0.205	0.795				SN	V			
SNZR4	2	1	4				SN	ZR			
SN2ZR	2	2	1				SN	ZR			
SN3ZR5	2	3	5				SN	ZR			
SRCU	1	1					SR1CU				
SRCU5	1	1					SR1CU5				
SRZN	2	1	1				SR	ZN			
SRZN13	2	1	13				SR	ZN			
SRZN2	2	1	2				SR	ZN			
SRZN5_ALPHA	2	1	5				SR	ZN			
SRZN5_BETA	2	1	5				SR	ZN			
TH2ZN_C16	2	2	1				TH	ZN			
THZN2	2	1	2				TH	ZN			
THZN4_D13	2	1	4				TH	ZN			
TH2ZN17	2	2	17				TH	ZN			
TI2ZN	2	2	1				TI	ZN			
TIZN	2	1	1				TI	ZN			
TIZN2	2	1	2				TI	ZN			
TIZN3	2	1	3				TI	ZN			
TIZN5	2	1	5				TI	ZN			
TIZN10	2	1	10				TI	ZN			
TIZN15	2	1	15				TI	ZN			
U2N3_ALPHA	2	2	3				U VA	N			
U2N3_BETA	2	0.413	0.587				U	N			
V2ZR	2	2	1				V	ZR			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
W2ZR	2	2	1				W	ZR			
ZRPB2	1	1					ZR1PB2				
ZR4PB	1	1					ZR4PB				
ZR5PB3	1	1					ZR5PB3				
ZN22ZR	2	22	1				ZN	ZR			
ZN39ZR5	2	39	5				ZN	ZR			
ZN3ZR_LT	2	3	1				ZN	ZR			
ZN3ZR	2	3	1				ZN	ZR			
ZN2ZR	2	2	1				ZN	ZR			
ZNZR	2	1	1				ZN	ZR			
ZN2ZR3	2	2	3				ZN	ZR			
ZNZR2	2	1	2				ZN	ZR			