

SGTE Solutions Database (SSOL8)

Technical Information

Available Starting with Thermo-Calc Version 2022a



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About the SGTE Solutions Database (SSOL8)

Database name (acronym):	SGTE Solutions Database (SSOL)
Database owner:	Scientific Group Thermodata Europe (SGTE)
Database version:	8.0

The SSOL8 SGTE Solutions Database is a thermodynamic database which contains critical assessments for many binary and ternary, and some higher order systems.

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.



Go to the [General Alloys and Pure Substances](#) page on our website where you can access PDFs of the SGTE technical information documents and learn about the compatible kinetic database.

Included Elements (79)

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, SSOL8 is based on the critical evaluation of binary, ternary and in some cases higher order systems. A total of 947 critically assessed systems (783 binary, 144 ternary, 19 quaternary and 1 quinary) are included in the SSOL8 database in this 79 element framework. The complete list of all these critically assessed systems is given in the next section of this document. The ASSESSED_SYSTEMS command is in the database for all the assessed systems, which enables you to calculate phase diagrams of these systems using the BINARY and TERNARY modules in Console Mode.

A large number of phases (2023), including various multicomponent solution phases and many important intermetallic compounds, are included in SSOL8. The complete list of the phases and their models are attached at the end of this document. 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, are able to describe a possible 2nd-order transition between the pair of phases and are used in some systems. Examples of this are the BCC_A2/ BCC_B2 transition in the Al-Fe system and the FCC_A1/ FCC_L12 transition in the Al-Ni system.



Some B2-type phases are modeled as stoichiometric phases and a separate phase name (B2_BCC) is created in addition to the BCC_B2 phase in the order-disorder model.

The SSOL8 database enables predictions (such as multicomponent phase equilibria and Scheil solidification simulations of industrial alloys) to be made for multicomponent systems and alloys of industrial importance. This means that the SSOL8 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.

SSOL8 Assessed Binary Systems

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

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

<i>Binary Systems</i>									
Eu-In	Eu-Mg	Eu-Pb	Eu-Pd	Eu-Sn	Eu-Te	Fe-Gd	Fe-In	Fe-La	Fe-Mg
Fe-Mn	Fe-Mo	Fe-N	Fe-Nb	Fe-Nd	Fe-Ni	Fe-Np	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-La	Ga-Li	Ga-Mg	Ga-N	Ga-Na	Ga-Ni	Ga-P	Ga-Pb	Ga-Pt	Ga-Sb
Ga-Sc	Ga-Si	Ga-Sn	Ga-Sr	Ga-Tb	Ga-Ti	Ga-Tl	Ga-V	Ga-Zn	Ga-Zr
Gd-Ge	Gd-Li	Gd-Mg	Gd-Mn	Gd-Mo	Gd-Ni	Gd-Pb	Gd-Sc	Gd-Si	Gd-Y
Gd-Zn	Gd-Zr	Ge-Hf	Ge-In	Ge-K	Ge-Mg	Ge-Mn	Ge-Na	Ge-Nb	Ge-Ni
Ge-Pb	Ge-Pt	Ge-Ru	Ge-Sb	Ge-Sc	Ge-Si	Ge-Sn	Ge-Sr	Ge-Te	Ge-Ti
Ge-Tl	Ge-V	Ge-Yb	Ge-Zn	Ge-Zr	Hf-Mn	Hf-Mo	Hf-Nb	Hf-Ni	Hf-Si
Hf-Sn	Hf-Ta	Hf-Ti	Hf-V	Hf-W	Hf-Zr	Hg-Mg	Hg-Pb	Hg-Sn	Hg-Zn
H-La	H-Li	H-Nd	H-Ni	Ho-Mg	Ho-Mn	Ho-Mo	Ho-Tb	Ho-V	H-Pd
In-La	In-Ni	In-P	In-Pb	In-Pd	In-Pt	In-Sb	In-Se	In-Si	In-Sn
In-Yb	In-Zn	Ir-Ni	Ir-Pd	Ir-Pt	Ir-Rh	Ir-Ru	Ir-Zr	K-Na	K-Rb
K-Zr	La-Mg	La-Ni	La-Sb	La-Sc	La-Sn	La-V	Li-Mg	Li-N	Li-Na
Li-Pb	Li-Sb	Li-Sc	Li-Si	Li-Sn	Li-Sr	Li-Zr	Lu-Sb	Mg-Mn	Mg-Nd
Mg-Ni	Mg-Pb	Mg-Pr	Mg-Ru	Mg-Sc	Mg-Si	Mg-Sm	Mg-Sn	Mg-Sr	Mg-Tb
Mg-Ti	Mg-Tm	Mg-V	Mg-Y	Mg-Yb	Mg-Zn	Mg-Zr	Mn-Mo	Mn-N	Mn-Nb
Mn-P	Mn-Pb	Mn-Pr	Mn-Sc	Mn-Si	Mn-Sm	Mn-Sn	Mn-Sr	Mn-Ti	Mn-V
Mn-W	Mn-Y	Mn-Zn	Mn-Zr	Mo-N	Mo-Nb	Mo-Ni	Mo-P	Mo-Pd	Mo-Sc
Mo-Si	Mo-Ta	Mo-Ti	Mo-V	Mo-W	Mo-Y	Mo-Zr	Na-Rb	Na-Sr	Na-Zn
Na-Zr	Nb-Ni	Nb-Si	Nb-Sn	Nb-Ta	Nb-Ti	Nb-V	Nb-W	Nb-Y	Nb-Zr
Nd-Ni	Nd-Pr	Nd-Sb	Nd-Sc	Nd-Y	Nd-Zn	Ni-P	Ni-Pb	Ni-Pd	Ni-Ru

<i>Binary Systems</i>									
Ni-Sb	Ni-Sc	Ni-Si	Ni-Sm	Ni-Sn	Ni-Sr	Ni-Ta	Ni-Th	Ni-Ti	Ni-V
Ni-W	Ni-Y	Ni-Zn	Ni-Zr	N-Nb	N-Ni	N-Si	N-Ta	N-Ti	N-U
N-V	N-W	N-Zr	Os-Si	Pb-Pd	Pb-Pt	Pb-Sb	Pb-Si	Pb-Sn	Pb-Sr
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	P-Sb	P-Si	P-Sn	Pt-Rh	Pt-Ru	Pt-Sb
Pt-Si	Pt-Sn	Pt-Ta	Pt-Ti	Pt-V	Re-Si	Re-Ti	Ru-Si	Ru-Sn	Ru-Zr
Sb-Si	Sb-Sm	Sb-Sn	Sb-Tb	Sb-Tm	Sb-Y	Sb-Zn	Sc-Si	Sc-Sr	Sc-Th
Sc-V	Sc-W	Sc-Y	Sc-Zr	Se-Te	Si-Sn	Si-Sr	Si-Ta	Si-Te	Si-Ti
Si-U	Si-V	Si-W	Si-Y	Si-YB	Si-Zn	Si-Zr	Sm-Sn	Sm-Zn	Sn-Ti
Sn-V	Sn-Y	Sn-Zn	Sn-Zr	Sr-Zn	Ta-Ti	Ta-V	Ta-W	Ta-Zr	Th-Zn
Ti-V	Ti-W	Ti-Zn	Ti-Zr	Tl-Zn	U-V	U-Zr	V-W	V-Y	V-Zr
W-Zr	Y-Zr	Zn-Zr							

SSOL8 Assessed Ternary Systems

<i>Assessed Ternary Systems</i>				
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-C-V
Al-Ca-Si	Al-Cu-Li	Al-Cu-Mg	Al-Cu-Si	Al-Cu-Zn
Al-Er-Mg	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	As-Cu-Ni	As-Ga-In	Au-Bi-Sb	Au-In-Pb
Au-In-Sb	Au-In-Sn	Au-Ni-Sn	B-Fe-Nd	B-Mo-Ti
Bi-Cu-Ga	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-Nb	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-Si	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

<i>Assessed Ternary Systems</i>				
Cu-Fe-Ni	Cu-Fe-P	Cu-H-Pd	Cu-In-Sn	Cu-Mg-Si
Cu-Mg-Zn	Cu-Ni-Pb	Cu-Ni-Sn	Dy-Fe-Tb	Fe-Mn-N
Fe-Mn-Nb	Fe-Mn-Ni	Fe-Mn-Si	Fe-Mn-V	Fe-Mo-N
Fe-Mo-Ni	Fe-Mo-P	Fe-Mo-V	Fe-Mo-W	Fe-N-Nb
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	H-Nd-Ni	In-Sb-Sn	In-Sn-Zn
Mo-N-Ni	Mo-Ni-W	N-Si-Ti	Pb-Pd-Sn	

SSOL8 Assessed Quaternary and Quinary Systems

<i>Quaternary and Quinary Systems</i>
C-Co-Cr-W
C-Co-Fe-Ni
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-Cr-Mo-V
C-Fe-Mn-V
C-Fe-Mo-V
C-Fe-Mo-W
C-Fe-Ni-W
C-Fe-V-W
Co-Fe-Ni-W
Cr-Fe-Mn-N
Cr-Fe-N-Ni
C-Co-Fe-Ni-W

SSOL8 Phase Models

This information is contained on the following pages.

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
GAS:G	1	1					AL1 AL2 B B2 C C2 C3 C4 C5 C60 CA CA2 CAH CD CU CU2 CUH H2 HLI LA LI LI2 MG MG2 ND NI1 NI2 N1 N2 N3 O2 P1 P2 P3 P4 TE TE2 TE3 TE4 TE5 TE6 TE7				
LIQUID:L	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 AG2TE AL2S3 AL2TE3 AL2U BA4BI3 BABI3 BAPB BICS BICS3 BIL13 BI2MG3 BINA3 BIRB BIRB3 BI2SE3 BI3YB4 CA2SN CDSE CDTE CR3GE1 CU2SE GE3MN5_F GETE IN2SE3 PBTE PTSN LASN LI2C2 LIH LI4PB LI3SB MG2PB MG2SN SI2TE3				
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 ND NI NP O OS P 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	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 ND NI O OS P PB PD PR PT PU RB RE RH RU S SB SC SI SN SR TA TC 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 ND NI O OS P PB PD PR PT PU RB RE RH RU S SB SC SI SN SR TA TC 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_4SL	5	0.25	0.25	0.25	0.25	1	AL AU CU CO IR PT V	AL AU CU CO IR PT V	AL AU CU CO IR PT V	AL AU CU CO IR PT 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	2	1	1				AL CO IN NI PD	VA CO NI PD			
A2_BCC	2	1	3				AL CO HF IR VA	VA			
B2_BCC	3	0.5	0.5	3			AL CO HF IR VA	AL CO HF IR VA	VA		
HCP_A3	2	1	0.5				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 LU MG MN MO NA NB ND NI NP OS PB PD PR PT PU RB RE RH RU SB SC SI SM SN SR TA TB TC TH TI TL TM U V W Y YB ZN ZR	B C N VA			
HCP_4SL	5	0.25	0.25	0.25	0.25	0.5	CD CO MG V	CD CO MG V	CD CO MG V	CD CO MG 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	2	1	2				AG AL AM AU BI CE FE GA IN LA MG MN ND NI NP PR PU SC SN Y ZR	H VA			
DIAMOND_A4	1	1					AL B BI C GA GE NB P PD RU SI SN SR TI ZN				
BCT_A5	1	1					AG AL BI CA 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 NI SI U V ZR				
RHOMBOHEDRAL_A7	1	1					AS BA BI FE GE IN ND P PB PD SB SN TB TM Y ZN				

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
HEXAGONAL_A8	1	1					SE TE				
RHOMBO_A10	1	1					CD HG PB ZN				
ALPHA_RHOMBO_B	1	1					B				
BETA_RHOMB_BCSI	2	93	12				B	B C CU MN MO NB SI ZR			
CHI_A12	3	24	10	24			CR FE	CR MO TI W	CR FE MO W		
CBCC_A12	2	1	1				AL CO CR DY FE HO MG MN MO NB NI SI SM SN TI V ZN ZR	VA C B N			
CUB_A13	2	1	1				AG AL CE CO CR DY FE GE HF HO MG MN MO NB 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 NI SI U ZR				
SIGMA	3	8	4	18			AL CO FE MN NI RE	CR MO TI V W	AL CO CR FE MO MN NI RE 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		
MU_D85	4	1	4	2	6		FE MN NB	NB	FE NB	FE MN NB	
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		
ZINCBLENDE_B3	2	0.5	0.5				AL CD GA IN	AS P SB TE			
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					AM FE NP				
TETRAG_AD	1	1					AM FE NP				
BCT_AA	1	1					PA				
ALPHA_PU	1	1					AL PU				
BETA_PU	1	1					PU				
GAMMA_PU	1	1					AL PU				
RHOMBO_C19	1	1					AL MG MN PD SM ZN				
OMEGA_ZR	1	1					ZR				
LAVES_C14	2	2	1				AL CA CO CR CU DY ER FE HO MG MN MO NB NI SR TA TI V W ZN ZR	AL CA CO CR CU DY ER FE HO MG MN MO NB NI SR TA TI V W ZN ZR			
C14_LAVES	2	2	1				FE MN NB	FE MN NB			
LAVES_C15	2	2	1				AL CO CR CU DY ER FE GD HF HO MG MN MO NB NI SC SI TA TI V W Y ZN ZR	AL CO CR CU DY ER FE GD HF HO MG MN MO NB ND NI SC 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		

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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			
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			
B2M	2	2	1				B	HF			
B4M3	2	4	3				B	HF			
M2B_TETR	2	0.667	0.333				NI	B			
MB2_C32	2	1	2				B,MO,TI,ZR	B,MO,TI,ZR			
MB_B33	2	0.5	0.5				MO,TI,VA	B,TI,VA			
MO2B	2	0.667	0.333				MO,TI,VA	B,VA			
MO2B5	2	0.32	0.68				MO,TI,VA	B,VA			
MOB4	2	0.2	0.8				MO,TI,VA	B,VA			
MOB_A	2	0.5	0.5				MO,TI,VA	B,VA			
NB3B2_D5A	2	3	2				NB	B			
NBB_B33	2	1	1				NB	B NB			
NB5B6	2	5	6				NB	B			
NB3B4_D7B	2	3	4				NB	B			
NB2B3	2	2	3				NB	B			
NBB2_C32	2	1	2				B NB	B NB			
NDB4	1	1					ND1B4				
NDB6	1	1					ND1B6				
NDB66	1	1					ND1B66				
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		
TI3B4	2	3	4				MO,TI	B			
TIB_B27	2	1	1				MO,TI,ZR	B,MO,TI			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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			
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			
AG51DY14	2	0.7846	0.2154				AG	DY			
AG2DY	2	0.6667	0.3333				AG	DY			
AGDY	2	0.5	0.5				AG	DY			
AG51ER14	2	0.7846	0.2154				AG	ER			
AG2ER	2	0.6667	0.3333				AG	ER			
AGER	2	0.5	0.5				AG	ER			
AG2GA	2	2	1				AG	AG GA VA			
AG3GA2_B2	2	3	2				AG	GA			
AG51GD14	2	51	14				AG	GD			
AG2GD_C11B	2	2	1				AG	GD			
AGGD_B2	2	1	1				AG	GD			
AGIN2	2	0.33	0.67				AG	IN			
AG5LA_C14	2	5	1				AG	LA			
AG51LA14	2	51	14				AG	LA			
AG2LA	2	2	1				AG	LA			
AGLA_B2	2	1	1				AG	LA			
AGMG3	2	0.25	0.75				AG	MG			
AG3MG	2	0.75	0.25				AG	MG			
AGND	2	0.5	0.5				AG	ND			
AG2NA_C15	2	2	1				AG	NA			
AG2ND_BETA	2	0.667	0.333				AG	ND			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AG2ND_ALPHA	2	0.667	0.333				AG	ND			
AG51ND14	2	0.785	0.215				AG	ND			
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			
AG655TE345	2	0.655	0.345				AG	TE			
AGTI2	2	1	2				AG	TI			
AGTI	2	1	1				AG TI	AG TI			
AG51Y14	2	51	14				AG	Y			
AG2Y_C11B	2	2	1				AG	Y			
AGY_B2	2	1	1				AG	Y			
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				
AL2AU	1	1					AL2AU				
AL2AU5	1	1					AL2AU5				
AL4BA_D13	2	4	1				AL	BA			
AL13BA7	2	13	7				AL	BA			
AL5BA4	2	5	4				AL	BA			
AL4CA_D13	2	4	1				AL	CA			
AL2CA_C15	2	2	1				AL	CA			
ALCA	2	1	1				AL	CA			
AL3CA8	2	3	8				AL	CA			
AL2CASI2	3	2	1	2			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			
AL45CR7	2	45	7				AL	CR			
AL5CR	2	5	1				AL	CR			
AL4CR	2	4	1				AL VA	CR			
AL8CR5_ALPHA	4	12	5	5	4		AL	CR	AL CR	AL CR	
AL8CR5_BETA	4	2	3	2	6		AL CR	AL CR	CR	AL	
ALCR2_C11B	2	1	2				AL CR	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		

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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			
AL2DY3	2	2	3				AL	DY			
ALDY2	2	1	2				AL	DY			
ALER	2	1	1				AL MG	ER			
ALER2	2	1	2				AL	ER			
AL2ER3	2	2	3				AL	ER			
ALERMG_T	3	0.6667	0.1	0.2333			AL	ER	MG		
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			
AL3HF_D023	2	3	1				AL	HF			
AL3HF_D022	2	3	1				AL	HF			
AL2HF_C14	2	2	1				AL	HF			
AL3HF2	2	3	2				AL	HF			
ALHF_B33	2	1	1				AL	HF			
AL3HF4	2	3	4				AL	HF			
AL2HF3	2	2	3				AL	HF			
ALHF2_C16	2	1	2				AL	HF			
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			
AL9IR2	2	9	2				AL	IR			
AL45IR13	2	45	13				AL	IR			
AL13IR4	2	13	4				AL	IR			
AL28IR9	2	28	9				AL	IR			
AL3IR_D018	2	3	1				AL	IR			
AL5IR2	2	2.7	1				AL	IR			
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			
GAMMA_A12	3	5	12	12			ER 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			
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			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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	3	1				AL	NI			
AL3NI2	3	3	2	1			AL	AL NI	VA NI		
AL3NI5	2	3	5				AL	NI			
AL4PD	2	4	1				AL	PD			
AL3PD	2	3	1				AL	PD			
AL21PD8	2	21	8				AL	PD			
AL3PD2_D513	2	3	2				AL PD	AL PD			
ALPD_B2	2	1	1				AL PD	PD VA			
AL3PD5	2	3	5				AL	PD			
AL2PD5	2	2	5				AL	AL PD			
ALPD2_C37	2	1	2				AL PD	AL PD			
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			
AL4PU_D1B	2	4	1				AL	PU			
AL3PU_9HA	2	3	1				AL	PU			
AL3PU_9HB	2	3	1				AL	PU			
AL3PU_6H	2	3	1				AL	PU			
AL3PU_L12	2	3	1				AL	PU			
AL2PU_C15	2	2	1				AL	PU			
ALPU_A12	2	1	1				AL	PU			
ALPU3	2	1	3				AL	PU			
AL12RE	2	12	1				AL	RE			
AL6RE_D2H	2	6	1				AL	RE			
AL4RE_LT	2	4	1				AL RE	AL RE			
AL4RE_HT	2	4	1				AL RE	RE			
AL3RE	2	3	1				AL	RE			
AL11RE4	2	11	4				AL	RE			
ALRE_B11	2	1	1				AL	RE			
ALRE2_C11B	2	1	2				AL	AL RE			
ALRU	2	1	1				AL	RU			
AL13RU4	2	13	4				AL	RU			
AL2RU	2	2	1				AL	RU			
AL3RU2	2	3	2				AL	RU			
AL6RU	2	6	1				AL	RU			
ALS	2	1	1				AL	S			
AL2S3_ALPHA	2	2	3				AL	S			
AL2S3_D51	2	2	3				AL	S			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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	2	1	1				AL	TA			
ALTA_SIGMA	3	10	4	16			AL CO TA V	TA V	AL CO TA V		
AL3TA	2	3	1				AL	TA			
AL3TA2	2	3	2				AL	TA			
AL7TA5	2	7	5				AL	TA			
AL69TA39	2	69	39				AL	TA			
ALTE	2	1	1				AL	TE			
AL2TE3_ALPHA	2	2	3				AL	TE			
AL2TE3_BETA	2	2	3				AL	TE			
AL2TE5	2	2	5				AL	TE			
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			
AL4U_D1B	2	4	1				AL	U			
AL3U_L12	2	3	1				AL	U			
AL2U_C15	2	2	1				AL	U			
AL45V7	2	45	7				AL	V			
AL8V5	4	6	2	3	2		AL	AL,V	AL,V	V	
AL21V2	2	21	2				AL	V			
AL23V4	2	23	4				AL	V			
AL2W	2	2	1				AL	W			
AL4W	2	4	1				AL	W			
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			
AL3YB_L12	2	3	1				AL	YB			
AL2YB_C15	2	2	1				AL	YB			
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			
AM6FE_D2C	2	6	1				AM	FE			
AMFE2_C15	2	1	2				AM	FE			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
AM3GA_ALPHA	2	3	1				AM	GA			
AM3GA_L12	2	3	1				AM	GA			
AM5GA3	2	5	3				AM	GA			
AMGA_ALPHA	2	1	1				AM	GA			
AMGA_BETA	2	1	1				AM	GA			
AM2GA3	2	2	3				AM	GA			
AMGA2_C32	2	1	2				AM	GA			
AMGA3_ALPHA	2	1	3				AM	GA			
AMGA3_BETA	2	1	3				AM	GA			
AMGA3_GAMMA	2	1	3				AM	GA			
AM2GA7	2	2	7				AM	GA			
AM3GA11	2	3	11				AM	GA			
AMGA4_D1B	2	1	4				AM	GA			
AMGA6	2	1	6				AM	GA			
AM2GA15	2	2	15				AM	GA			
ASCUNI	3	0.334	0.333	0.333			AS	CU	NI		
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			
AU6CE	2	6	1				AU	CE			
AU51CE14	2	51	14				AU	CE			
AU2CE	2	2	1				AU	CE			
AU4CE3	2	4	3				AU	CE			
AUCE_B27	2	1	1				AU	CE			
AUCE_B33	2	1	1				AU	CE			
AUCE2_C37	2	1	2				AU	CE			
AU4ER_D1A	2	4	1				AU	ER			
AU3ER_D0A	2	3	1				AU	ER			
AU2ER_C11B	2	2	1				AU	ER			
AU10ER7	2	10	7				AU	ER			
AUER_B33	2	1	1				AU	ER			
AUER_B2	2	1	1				AU	ER			
AUER2_C37	2	1	2				AU	ER			
AU7GA2_HT	2	0.7895	0.2105				AU	GA			
AU7GA2_LT	2	7	2				AU	GA			
AU7GA3	2	7	3				AU	GA			
AUGA_B31	2	1	1				AU	GA			
AUGA2_C1	2	1	2				AU	GA			
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			
AU6HO	2	6	1				AU	HO			
AU4HO_D1A	2	4	1				AU	HO			
AU51HO14	2	51	14				AU	HO			
AU3HO_D0A	2	3	1				AU	HO			
AU2HO_C11B	2	2	1				AU	HO			
AU10HO7	2	10	7				AU	HO			
AUHO_B33	2	1	1				AU	HO			
AUHO_B2	2	1	1				AU	HO			
AUHO2_C37	2	1	2				AU	HO			
AUIN	2	0.5	0.5				AU	IN, SB, SN			
AUIN2	2	0.3333	0.6667				AU	IN, SB, SN			
AU3IN	2	3	1				AU	IN			
AU7IN3	2	7	3				AU	IN			
AUIN_BETA	2	7.065	1.935				AU	IN			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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	14	4				AU	IN			
AU4IN3SN3	3	0.4	0.3	0.3			AU	IN,SN	IN,SN		
AU6LA	2	6	1				AU	LA			
AU51LA14	2	51	14				AU	LA			
AU2LA	2	2	1				AU	LA			
AULA_B27	2	1	1				AU	LA			
AULA_B33	2	1	1				AU	LA			
AULA2_C37	2	1	2				AU	LA			
AUNI2SN4	3	0.143	0.286	0.571			AU	NI	SN		
AU6ND	2	6	1				AU	ND			
AU51ND14	2	51	14				AU	AU ND			
AU36ND17	2	36	17				AU	ND			
AU4ND3	2	4	3				AU	ND			
AUND_B27	2	1	1				AU	ND			
AUND_B33	2	1	1				AU	ND			
AUND_B2	2	1	1				AU	ND			
AUND2_C37	2	1	2				AU	ND			
AUPB2	2	1	2				AU	PB			
AUPB3	2	1	3				AU	PB			
AU2PB	2	2	1				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			
AU4SC_D1A	2	4	1				AU	SC			
AU3SC_D0A	2	3	1				AU	SC			
AU2SC_C11B	2	2	1				AU	SC			
AUSC_B2	2	1	1				AU	SC			
AUSC2_C37	2	1	2				AU	SC			
AU2SC7	2	2	7				AU	SC			
AUSN	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	2	1	2				AU	TE			
TI3AU	2	3	1				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			
AU4TM_D1A	2	4	1				AU	TM			
AU3TM_D0A	2	3	1				AU	TM			
AU2TM_C11B	2	2	1				AU	TM			
AU10TM7	2	10	7				AU	TM			
AUTM_B33	2	1	1				AU	TM			
AUTM_B2	2	1	1				AU	TM			
AUTM2_C37	2	1	2				AU	TM			
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			
CEB4_D1E	2	1	4				CE	B			
CEB6_D21	2	1	6				CE	B			
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			
RE3B_E1A	2	3	1				RE	B			
RE7B3_D102	2	7	3				RE	B			
REB2	2	1	2				RE B	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			
ZRB_B1	2	1	1				ZR	B			
ZRB12	2	1	12				TI,ZR	B			
BA2BI	2	2	1				BA	BI			
BA5BI3_D88	2	5	3				BA	BI			
BA4BI3_D73	2	4	3				BA	BI			
BA11BI10	2	11	10				BA	BI			
BABI3	2	1	3				BA	BI			
BACU	1	1					BA1CU				
BACU13	1	1					BA1CU13				
BAMG2_C14	2	0.333	0.667				BA	MG			
BA6MG23_D8A	2	0.207	0.793				BA	MG			
BA2MG17	2	0.105	0.895				BA	MG			
BA2PB_C37	2	2	1				BA	PB			
BA5PB3_D8L	2	5	3				BA	PB			
BAPB_B33	2	1	1				BA	PB			
BA17PB23	2	17	23				BA	PB			
BA3PB5_LT	2	3	5				BA	PB			
BA3PB5_HT	2	3	5				BA	PB			
BAPB3	2	1	3				BA	PB			
BE22MO	2	22	1				BE	MO			
BE12MO_D2B	2	12	1				BE	MO			
BE2MO_C14	2	2	1				BE	MO			
BEMO3_A15	2	1	3				BE	MO			
BE13PU_D23	2	13	1				BE	PU			
BE12V_D2B	2	12	1				BE	V			
BE17V2	2	17	2				BE	V			
BE2V_C14	2	2	1				BE	V			
BI2CE	2	2	1				BI	CE			
BICE_B1	2	1	1				BI	CE			
BI3CE4_D73	2	3	4				BI	CE			
BI3CE5_D88	2	3	5				BI	CE			
BICE2	2	1	2				BI	CE			
BI2CS_C15	2	2	1				BI	CS			
BI4CS5	2	4	5				BI	CS			
BI2CS3	2	2	3				BI	CS			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
BICS3_D03	2	1	3				BI	CS			
BIDY_B1	2	1	1				BI	DY			
BI3DY5	2	3	5				BI	DY			
BIER_B1	2	1	1				BI	ER			
BI3ER5	2	3	5				BI	ER			
BI2GD	2	2	1				BI	GD			
BIGD_B1	2	1	1				BI	GD			
BI3GD4_D73	2	3	4				BI	GD			
BI3GD5	2	3	5				BI	GD			
BIHO_B1	2	1	1				BI	HO			
BI3HO5	2	3	5				BI	HO			
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			
BI4K5	2	0.444444	0.555556				BI	K			
BI2LA	2	2	1				BI	LA			
BILA_B1	2	1	1				BI	LA			
BI3LA4_D73	2	3	4				BI	LA			
BI3LA5_D88	2	3	5				BI	LA			
BILA2	2	1	2				BI	LA			
BILI_L10	2	1	1				BI	LI			
BILI_HT	2	1	1				BI	LI			
BILI3_D03	2	1	3				BI	LI			
BI2LU	2	2	1				BI	LU			
BILU_B1	2	1	1				BI	LU			
BI3LU5	2	3	5				BI	LU			
BI2MG3_D52	2	2	3				BI VA	MG			
BI2MG3_BETA	2	2	3				BI VA	MG			
BIMN_B81	2	1	1				BI	MN			
BIMN_B82	2	1	1.08				BI	MN			
BINA_L10	2	1	1				BI	NA			
BINA3_D018	2	1	3				BI	NA			
BI2ND	2	2	1				BI	ND			
BIND_B1	2	1	1				BI	ND			
BI3ND4_D73	2	3	4				BI	ND			
BI3ND5_D88	2	3	5				BI	ND			
BIND2	2	1	2				BI	ND			
BINI	3	1	1	1			NI,VA	VA	BI		
BI3NI	2	0.75	0.25				BI	NI			
BI2PD	2	2	1				BI	PD			
BIPD	2	1	1				BI	PD			
BI3PD5	1	1					BI PD				
BIPD3	2	1	3				BI	PD			
BI2RB_C15	2	2	1				BI	RB			
BI4RB5	2	4	5				BI	RB			
BI2RB3	2	2	3				BI	RB			
BIRB3_D018	2	1	3				BI	RB			
BIRB3_D03	2	1	3				BI	RB			
BI3SE2	2	3	2				BI	SE			
BISE	3	2	1	2			BI	BI SE	SE		
BI2SE3_C33	2	2	3				BI	SE			
BI3SR_L12	2	3	1				BI	SR			
BI10SR11	2	10	11				BI	SR			
BI3SR5_D88	2	3	5				BI	SR			
BI3SR5_HT	2	3	5				BI	SR			
BISR2	2	1	2				BI	SR			
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			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
BI2TE	2	2	1				BI	TE			
BI4TE3	2	4	3				BI	TE			
BITE	2	2	3				BI	BI TE			
BI2TE3_C33	2	2	3				BI	TE			
BI2TI	2	2	1				BI	TI			
BI3TI2	2	3	2				BI	TI			
BI9TI8	2	9	8				BI	TI			
BITI2	2	1	2				BI	TI			
BITI3	2	1	3				BI	TI			
BITL_EPSILON	1	1					BI TL				
BITM	2	1	1				BI	TM			
BI3TM5	2	3	5				BI	TM			
BI2U	2	2	1				BI	U			
BI4U3_D73	2	4	3				BI	U			
BIU_B1	2	1	1				BI	U			
BIY	2	1	1				BI	Y			
BI3Y5	2	3	5				BI	Y			
BI2YB_C49	2	2	1				BI	YB			
BI10YB11	2	10	11				BI	YB			
BI3YB4_D73	2	3	4				BI	YB			
BI3YB5	2	3	5				BI	YB			
BIYB2	2	1	2				BI	YB			
FCC_B1	2	1	1				U	C C2 N VA			
BCT_U	2	1	1				U	C C2 VA			
CE2C3_D5C	2	2	3				CE	C			
CEC2_C11A	2	1	2				CE	C			
CEC2_BETA	2	1	2				CE	C			
LI2C2_ALPHA	2	1	1				LI	C			
LI2C2_C1	2	1	1				LI	C			
LIC6	2	1	6				LI	C			
MG2C3	2	2	3				MG	C			
MGC2	2	1	2				MG	C			
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			
CA3IN	2	3	1				CA	IN			
CAIN	2	1	1				CA	IN			
CAIN2	2	1	2				CA	IN			
CA2SN_C37	2	2	1				CA	SN			
CA5SN3_D8L	2	5	3				CA	SN			
CA36SN23	2	36	23				CA	SN			
CA31SN20	2	31	20				CA	SN			
CA7SN6	2	7	6				CA	SN			
CASN_B33	2	1	1				CA	SN			
CASN3_L12	2	1	3				CA	SN			
CD6GD	2	6	1				CD	GD			
CD58GD13	2	58	13				CD	GD			
CD45GD11	2	45	11				CD	GD			
CD3GD_D019	2	3	1				CD	GD			
CD2GD	2	2	1				CD	GD			
CDGD_B2	2	1	1				CD	GD			
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			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CAMG2	1	1					CA1MG2				
CA2PB_C37	2	2	1				CA	PB			
CA5PB3	2	5	3				CA	PB			
CAPB_L10	2	1	1				CA	PB			
CAPB3_L12	2	1	3				CA	PB			
CASI	2	1	1				CA	SI			
CASI2	2	1	2				CA	SI			
CA2SI	2	2	1				CA	SI			
CA3SI4	2	3	4				CA	SI			
CA5SI3	2	5	3				CA	SI			
CA14SI19	2	14	19				CA	SI			
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				
CD11NA2_D8C	2	11	2				CD	NA			
CD2NA	2	2	1				CD	NA			
CD11PU_D2E	2	11	1				CD	PU			
CD6PU	2	6	1				CD	PU			
CD4PU	2	4	1				CD	PU			
CD2PU	2	2	1				CD	PU			
CDSB_OMEGA	2	1	1				CD ZN	SB			
CDSE_B4	2	1	1				CD	SE			
CD11SR	2	11	1				CD	SR			
CD6SR	2	6	1				CD	SR			
CD58SR13	2	58	13				CD	SR			
CD2SR	2	2	1				CD	SR			
CDSR_B2	2	1	1				CD	SR			
CD3SR5_D8L	2	3	5				CD	SR			
CDTI_B11	2	1	1				CD	TI			
CDTI2	2	1	2				CD	TI			
CD6Y	2	6	1				CD	Y			
CD58Y13	2	58	13				CD	Y			
CD45Y11	2	45	11				CD	Y			
CD3Y	2	3	1				CD	Y			
CD2Y	2	2	1				CD	Y			
CDY_B2	2	1	1				CD	Y			
CEFE2_C15	2	1	2				CE	FE			
CE2FE17	2	2	17				CE	FE			
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			
CE5SI3_D8L	2	5	3				CE	SI			
CE3SI2_D5A	2	3	2				CE	SI			
CE5SI4	2	5	4				CE	SI			
CESI_B27	2	1	1				CE	SI			

Phase Name	Stoichiometry						Occupancy				
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CE3SI5	2	3	5				CE	SI			
CES12_CC	2	1	2				CE	SI			
CE3SN_L12	2	3	1				CE	SN			
CE5SN3	2	5	3				CE	SN			
CE5SN4	2	5	4				CE	SN			
CE11SN10	2	11	10				CE	SN			
CE3SN5	2	3	5				CE	SN			
CE3SN7	2	3	7				CE	SN			
CE2SN5	2	2	5				CE	SN			
CESN3_L12	2	1	3				CE	SN			
CEZN_B2	2	1	1				CE	ZN			
CEZN2	2	1	2				CE	ZN			
CEZN3	2	1	3				CE	ZN			
CE3ZN11	2	3	11				CE	ZN			
CE13ZN58	2	13	58				CE	ZN			
CEZN5_D2D	2	1	5				CE	ZN			
CE3ZN22	2	3	22				CE	ZN			
CE2ZN17	2	2	17				CE	ZN			
CEZN11	2	1	11				CE	ZN			
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			
CO5DY	2	5	1				CO	DY			
CO17DY2	2	17	2				CO	DY			
CO17ER2	2	17	2				CO	ER			
CO5ER_D2D	2	5	1				CO	ER			
CO7ER2	2	7	2				CO	ER			
CO3ER	2	3	1				CO	ER			
CO2ER_C15	2	2	1				CO	ER			
CO7ER12	2	7	12				CO	ER			
COER3_D011	2	1	3				CO	ER			
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			
CO11HF2	2	11	2				CO	HF			
CO23HF6_D8A	2	23	6				CO	HF			
COHF2	2	1	2				CO HF	CO HF			
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				

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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				
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			
CO11U2	2	11	2				CO	U			
CO4U	2	4	1				CO	U			
CO3U	2	3	1				CO	U			
CO2U_C15	2	2	1				CO U	CO U			
COU_BA	2	1	1				CO	U			
COU6_D2C	2	1	6				CO	U			
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			
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			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CRGE	2	0.5	0.5				CR	GE			
CR11GE19	2	0.367	0.633				CR	GE			
CRHF_C14	2	2	1				CR HF	CR HF			
CRHF_C15	2	2	1				CR HF	CR HF			
CR3MN5	2	3	5				CR	MN TI			
CRNI2	2	1	2				CR,MO,NI,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			
CS2IN3	2	2	3				CS	IN			
CSIN3	2	1	3				CS	IN			
CSNA_S	2	1	2				CS	NA			
CU7AS3	2	7	3				CU	AS			
CU3AS	2	3	1.15				CU	CU,AS			
CU7AS	2	7	1				CU	AS			
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			
CUGA_ZETAP	2	0.778	0.222				CU	GA			
CUGA2	2	1	2				CU	GA			
CU9GA4_GAMMA1	4	6	3	3	1		CU	CU,GA	CU,GA	GA	
CU9GA4_GAMMA2	4	3	3	3	4		CU	CU,VA	CU,GA	GA	
CU9GA4_GAMMA3	3	6	3	4			CU,VA	CU,GA	GA		
CU3GE_D018	2	0.765	0.235				CU	GE			
CU3GE_D0A	2	0.75	0.25				CU	GE			
CU3GE_D03	2	0.735	0.265				CU	GE			
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			
CUIN_DELTA	2	0.7	0.3				CU	IN SN			
CUIN_GAMMA	3	0.654	0.115	0.231			AG,CU,IN	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			
CU7HG6_D810	2	7	6				CU	HG			
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			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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			
CUMGSJ_SIGMA	3	16	6	7			CU	MG	SI		
CUMGSJ_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				
CUPT_L11	2	0.5	0.5				CU PT	CU PT			
CUSB_ZETA	2	0.77	0.23				CU	SB			
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			
CUSC_B2	2	1	1				CU	SC			
CU2SE_ALPHA	2	2	1				CU SE	SE			
CU2SE_BETA	2	2	1				CU SE	SE			
CU3SE2	2	3	2				CU	SE			
CUSE_ALPHA	2	1	1				CU	SE			
CUSE_BETA	2	1	1				CU	SE			
CUSE_B18	2	1	1				CU	SE			
CUSE2_C18	2	1	2				CU	SE			
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				
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			
CU5TM_C15B	2	5	1				CU	TM			
CU9TM2	2	9	2				CU	TM			
CU7TM2	2	7	2				CU	TM			
CU2TM	2	2	1				CU	TM			
CUTM_B2	2	1	1				CU	TM			
CUY	1	1					CU1Y				
CU2YR	1	1					CU2Y				
CU7Y2	1	1					CU7Y2				
CU4Y	1	1					CU4Y				

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
CU2YH	1	1					CU2Y				
CU6Y	2	5	1				CU	CU2 Y			
CU5YB_D2D	2	5	1				CU	YB			
CU9YB2	2	9	2				CU	YB			
CU7YB2	2	7	2				CU	YB			
CU2YB	2	2	1				CU	YB			
CUYB_B27	2	1	1				CU	YB			
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			
CU51ZR14	2	51	14				CU	ZR			
D_GAMMA	1	1					AL CU SI ZN				
DYMN2_C15	2	1	2				DY	MN			
DY6MN23_D8A	2	6	23				DY	MN			
DYMN12_D2B	2	1	12				DY	MN			
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			
ER5GE3_D88	2	5	3				ER GE	GE			
ER5GE4	2	5	4				ER	GE			
ER11GE10	2	11	10				ER	GE			
ERGE_B33	2	1	1				ER	GE			
ER3GE4	2	3	4				ER	GE			
ER2GE3_LT	2	2	3				ER	GE			
ER2GE3_C32	2	2	3				ER	GE			
ERGE2_LT	2	1	2				ER	GE			
ERGE2_MT	2	1	2				ER	GE			
ERGE2_HT	2	1	2				ER	GE			
ER2GE5	2	2	5				ER	GE			
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			
ER5SB3	2	5	3				ER	SB			
ERSB_B1	2	1	1				ER	SB			
ERSB_BETA	2	1	1				ER	SB			
ERSB2	2	1	2				ER	SB			
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			
EU2PB_C37	2	2	1				EU	EU PB			
EU5PB3_D8M	2	5	3				EU	PB			
EUPB_L10	2	1	1				EU	EU PB			
EUPB_HT	2	1	1				EU	EU PB			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
EUPB3_L12	2	1	3				EU	PB			
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			
EUSN3	2	1	3				EU	SN			
EUTE_B1	2	1	1				EU TE	TE			
EU4TE7	2	4	7				EU	TE			
EU3TE7	2	3	7				EU	TE			
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				
FE17ND2	2	0.89474	0.10526				FE	ND			
FE17ND5	2	0.77273	0.22727				FE	ND			
FE2NP_C15	2	2	1				FE	NP			
FENP6_D2C	2	1	6				FE	NP			
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			
FEU6	2	1	6				FE U	FE U			
FE2U	2	2	1				FE U	FE U			
FE17Y2	2	17	2				FE	Y			
FE23Y6	2	23	6				FE Y	Y FE			
FE3Y	2	3	1				FE	Y			
FE2Y	2	2	1				FE Y	Y FE			
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		

Phase Name	Stoichiometry						Occupancy				
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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				
GA6LA	2	6	1				GA	LA			
GA4LA	2	4	1				GA	LA			
GA2LA_C32	2	2	1				GA	GA LA			
GALA_B33	2	1	1				GA	LA			
GA3LA5	2	3	5				GA	LA			
GALA3_L12	2	1	3				GA	LA			
GA14LI3	2	14	3				GA	LI			
GA7LI2	2	7	2				GA	LI			
GA9LI5	2	9	5				GA	LI			
GALI_B32	2	1	1				GA LI	LI VA			
GA4LI5	2	4	5				GA	LI			
GA2LI3	2	2	3				GA	LI			
GALI2	2	1	2				GA	LI			
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			
GAN	2	1	1				GA	N			
GA4NA_D13	2	4	1				GA	NA			
GA39NA22	2	39	22				GA	NA			
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			
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			
GAPT3	2	0.25	0.75				GA PT	GA PT			
GA3SC_L12	2	3	1				GA	SC			
GA2SC	2	2	1				GA	SC			
GASC_B33	2	1	1				GA	SC			
GA4SC5	2	4	5				GA	SC			
GA3SC5	2	3	5				GA	SC			
GA4SR_D13	2	4	1				GA	SR			
GA2SR_C32	2	2	1				GA	SR			
GA7SR8	2	7	8				GA	SR			
GA6TB	2	6	1				GA	TB			
GA3TB	2	3	1				GA	TB			
GA2TB_C32	2	2	1				GA	TB			
GATB_B33	2	1	1				GA	TB			
GA3TB5_D8L	2	3	5				GA	TB			
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			
GA41V8	2	41	8				GA	V			
GA5V2	2	5	2				GA	V			
GA7V6_D82	4	2	3	2	6		V	V	GA V	GA V	
GA5V6	2	5	6				GA V	GA V			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
GAV3_A15	2	1	3				GA V	GA V			
GA3ZR_D023	2	3	1				GA	ZR			
GA2ZR	2	2	1				GA	ZR			
GA5ZR3	2	5	3				GA	ZR			
GA3ZR2	2	3	2				GA	ZR			
GAZR_BG	2	1	1				GA	ZR			
GAZR_BETA	2	1	1				GA	ZR			
GA4ZR5	2	4	5				GA	ZR			
GA2ZR3_D5A	2	2	3				GA	ZR			
GA3ZR5_D88	2	3	5				GA	ZR			
GAZR2_C16	2	1	2				GA	ZR			
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			
GD5PB3_D88	2	5	3				GD PB	PB			
GD5PB4_LT	2	5	4				GD	PB			
GD5PB4_HT	2	5	4				GD	PB			
GD11PB10	2	11	10				GD	PB			
GD6PB7	2	6	7				GD	PB			
GDPB2	2	1	2				GD	PB			
GDPB3_L12	2	1	3				GD	PB			
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			
GDZN_B2	2	1	1				GD	ZN			
GDZN2	2	1	2				GD	ZN			
GDZN3	2	1	3				GD	ZN			
GD3ZN11	2	3	11				GD	ZN			
GD13ZN58	2	13	58				GD	ZN			
GD3ZN22	2	3	22				GD	ZN			
GD2ZN17	2	2	17				GD	ZN			
GDZN12_D2B	2	1	12				GD	ZN			
GE2HF_C49	2	2	1				GE	HF			
GE4HF5	2	4	5				GE	HF			
GE2HF3_D5A	2	2	3				GE	HF			
GE3HF5_D88	2	3	5				GE	HF			
GEHF2_C16	2	1	2				GE	HF			
GEHF3	2	1	3				GE	HF			
GE4K	2	4	1				GE	K			
GEK	2	1	1				GE	K			
GEK3	2	1	3				GE	K			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
GEMG2	2	1	2				GE	MG			
GE8MN11	2	11	8				MN	GE			
GE3MN5_D88	2	5	3				MN	GE			
GEMN2_B82	2	2	1				GE MN	GE MN			
GE2MN5_LT	2	5	2				MN	GE			
GE2MN5_HT	2	5	2				GE MN	GE MN			
GEMN3_D022	2	3	1				MN	GE			
GEMN3_D023	2	3	1				MN	GE MN			
B20_GERU	2	1	1				GE SI	RU			
ALPHA_GE3RU2	2	3	2				GE	RU			
BETA_GE3RU2	2	3	2				GE SI SN	RU			
GE4NA	2	4	1				GE	NA			
GENA	2	1	1				GE	NA			
GENA3	2	1	3				GE	NA			
GE2NB_C40	2	2	1				GE NB	GE NB			
GE3NB5_D8M	3	4	1	3			NB	GE NB	GE VA		
GENB3_A15	2	1	3				GE NB	NB			
GENI_B31	2	0.5	0.5				GE	NI			
GE3NI5_B82	3	1	1	1			GE	NI	NI VA		
GE3NI5_PRIME	2	0.375	0.625				GE	NI			
GENI2_C37	2	0.335	0.665				GE	NI			
GE2NI5	2	0.28	0.72				GE	NI			
GENI3_B32	2	0.256	0.744				GE	NI			
GE2PT_C18	2	2	1				GE	PT			
GE3PT2	2	3	2				GE	PT			
GEPT_B31	2	1	1				GE	PT			
GE2PT3	2	2	3				GE	PT			
GEPT2_C22	2	1	2				GE	PT			
GEPT3	2	1	3				GE PT	PT			
GE2SC_C49	2	2	1				GE	SC			
GESC_B33	2	1	1				GE	SC			
GE10SC11	2	10	11				GE	SC			
GE4SC5	2	4	5				GE	SC			
GE3SC5_D88	2	3	5				GE SC	GE SC			
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			
GETE_LOW	2	1	1				GE VA	TE			
GETE_B1	2	1	1				GE VA	TE			
GETE_GAMMA	2	49	51				GE	TE			
GE2TI_C54	2	2	1				GE	TI			
GE5TI6	2	5	6				GE	TI			
GE3TI5_D88	2	3	5				GE	TI			
GEV3	2	1	3				GE	V			
GE31V17	2	31	17				GE	V			
GE3V5	2	3	5				GE	V			
GE8V11	2	8	11				GE	V			
GE8YB3	2	8	3				GE	YB			
GE5YB3	2	5	3				GE	YB			
GE10YB11	2	10	11				GE	YB			
GE4YB5	2	4	5				GE	YB			
GE3YB5_D88	2	3	5				GE	YB			
GEYB2_C37	2	1	2				GE	YB			
GE2ZR_C49	2	2	1				GE	ZR			
GEZR_B27	2	1	1				GE	ZR			
GE4ZR5	2	4	5				GE	ZR			
GE3ZR5_D88	2	3	5				GE	ZR			
GEZR3	2	1	3				GE	ZR			
NDNI5H3	4	1	5	3	6		ND	NI	H	H VA	
NDNI5H6	4	1	5	3	6		ND	NI	H	H VA	
HFMN	2	1	1				HF	MN			
HFMN2_C14	2	1	2				HF MN	HF MN			
HFNIA	2	1	1				HF	NI			
HFNI3A	2	1	3				HF	NI			

Phase Name	Stoichiometry					Occupancy				
	Number of Sublattices	SL1	SL2	SL3	SL4	SL1	SL2	SL3	SL4	SL5
HFNI8	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			
HF5SN3_D88	2	5	3			HF	SN			
HF5SN4	2	5	4			HF	SN			
HFSN2_C40	2	1	2			HF	SN			
HGPB2_L10	2	1	2			HG	PB			
NDH_GAMMA	2	1	2			ND	H VA			
NDH2	3	1	2	1		ND	H VA	H VA		
HG2MG_C11B	2	2	1			HG	MG			
HGMG_B2	2	1	1			HG	MG			
HG3MG5_D88	2	3	5			HG	MG			
HGMG2_C37	2	1	2			HG	MG			
HG2MG5	2	2	5			HG	MG			
HGMG3	2	1	3			HG	MG			
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			
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			
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			
IN7PT3_D8F	2	7	3			IN	PT			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
IN2PT_C1	2	2	1				IN	PT			
IN3PT2_D513	2	3	2				IN	PT			
INPT_HT	2	1	1				IN PT	IN PT			
IN5PT6	2	5	6				IN PT	IN PT			
IN9PT13	2	9	13				IN	IN PT			
IN2PT3_ALPHA	2	2	3				IN	PT			
IN2PT3_B82	2	2	3				IN PT	IN PT			
INPT2	2	1	2				IN	PT			
IN4SE3	2	4	3				IN	SE			
INSE	2	1	1				IN	SE			
IN6SE7	2	6	7				IN	SE			
IN9SE11	2	9	11				IN	SE			
IN5SE7	2	5	7				IN	SE			
IN2SE3_C33	2	2	3				IN	SE			
IN2SE3_BETA	2	2.02	2.98				IN	SE			
IN2SE3_GAMMA	2	2	3				IN	SE			
IN2SE3_DELTA	2	2	3				IN	SE			
INSN_GAMMA	1	1					IN SN				
IN3YB	2	3	1				IN	YB			
IN2YB	2	2	1				IN	YB			
INYB2	2	1	2				IN	YB			
IN2YB5	2	2	5				IN	YB			
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			
KNA2_C14	2	1	2				K	NA			
LAH3	3	1	2	1			LA	H VA	H VA		
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				
LA2SB	2	2	1				LA	SB			
LA3SB2	2	3	2				LA	SB			
LASB_B1	2	1	1				LA	SB			
LASB2	2	1	2				LA	SB			
LA5SN3_D8M	2	0.625	0.375				LA	SN			
LA5SN3_D88	2	0.625	0.375				LA	SN			
LA5SN4	2	0.555	0.445				LA	SN			
LA11SN10	2	0.524	0.476				LA	SN			
LASN_B33	2	0.5	0.5				LA	SN			
LA2SN3	2	0.4	0.6				LA	SN			
LA3SN5	2	0.375	0.625				LA	SN			
LASN3_L12	2	0.25	0.75				LA	SN			
LIH	2	1	1				LI	H			
LI3N	2	3	1				LI	N			
LI4PB	2	4	1				LI	PB			
LI7PB2	2	7	2				LI	LI PB			
LI3PB_D03	2	3	1				LI	PB			
LI5PB2	2	5	2				LI	PB			
LIPB_ALPHA	2	1	1				LI PB	LI PB			
LIPB_B2	2	1	1				LI PB	LI PB			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
LI3SB_D018	2	3	1				LI	SB			
LI2SB	2	2	1				LI	SB			
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			
LI23SR6_D8A	2	23	6				LI	SR			
LI2SR3	2	2	3				LI	SR			
LU3SB	2	3	1				LU	SB			
LU5SB3	2	5	3				LU	SB			
LUSB_B1	2	1	1				LU	SB			
LUSB_BETA	2	1	1				LU	SB			
LUSB2	2	1	2				LU	SB			
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			
MGSC	1	1					MG15C				
MG2SI	2	2	1				MG	SI			
MG41SM5	2	41	5				MG	SM			
MG5SM	2	5	1				MG	SM			
MG3SM_D03	2	3	1				MG	SM			
MG2SM_C15	2	2	1				MG	SM			
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			
MN23PR6_D8A	2	23	6				MN	PR			
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			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
MG2PB_C1	2	2	1				MG	PB			
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			
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			
NAZN13	2	1	13				NA	ZN			
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		
ND3NI_D011	2	3	1				ND	NI			
ND7NI3_D102	2	7	3				ND	NI			
NDNI_B33	2	1	1				ND	NI			
NDNI2_C15	2	1	2				ND	NI			
NDNI3	2	1	3				ND	NI			
ND2NI7	2	2	7				ND	NI			
NDNI5_D2D	3	1	5	3			ND	NI	H VA		
ND2NI17	2	2	17				ND	NI			
NDSB	1	1					ND1SB				
NDSB2	1	1					ND1SB2				
ND2SB	1	1					ND2SB				
ND4SB3	1	1					ND4SB3				
ND5SB3	1	1					ND5SB3				
NDZN_B2	2	1	1				ND	ZN			
NDZN2	2	1	2				ND	ZN			
NDZN3	2	1	3				ND	ZN			
ND3ZN11	2	3	11				ND	ZN			
ND13ZN58	2	13	58				ND	ZN			
ND3ZN22	2	3	22				ND	ZN			
ND2ZN17	2	2	17				ND	ZN			
NDZN11	2	1	11				ND	ZN			
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			

Phase Name	Stoichiometry						Occupancy				
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
NI17SM2	2	17	2				NI	SM			
NI3SB_D0A	2	3	1				NI	NI SB			
NI3SB_D03	3	2	1	1			NI VA	NI VA	SB		
NI5SB2_LT	2	5	2				NI	NI SB			
NISB_B81	3	1	1	1			NI VA	NI VA	SB		
NISB2_C18	2	1	2				NI	SB			
NI5SC_D2D	2	5	1				NI	SC			
NI7SC2	2	7	2				NI	SC			
NISC2	2	7	18				NI	SC			
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		
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			
NI17TH2	2	19	2				NI	TH			
NI5TH_D2D	2	5	1				NI	TH			
NI7TH2_ALPHA	2	7	2				NI	TH			
NI7TH2_BETA	2	7	2				NI	TH			
NI2TH_C32	2	2	1				NI	TH			
NI7TH4	2	7	4				NI	TH			
NITH	2	1	1				NI	TH			
NI3TH7_D102	2	3	7				NI	TH			
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			
SI2SR_ALPHA	2	2	1				SI	SR			
SI2SR_BETA	2	2	1				SI VA	SR			
SISR_B33	2	1	1				SI	SR			
SI3SR5_D8L	2	3	5				SI	SR			
SISR2_C37	2	1	2				SI	SR			
SRPB3	2	1	3				SR	PB			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
SR3PB5	2	3	5				SR	PB			
SR2PB3	2	2	3				SR	PB			
SRPB	2	1	1				SR	PB			
SR5PB4	2	5	4				SR	PB			
SR5PB3	2	5	3				SR	PB			
SR2PB	2	2	1				SR	PB			
SN4P3	2	4	3				SN	P			
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			
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			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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				
PT7SB	2	7	1				PT	SB			
PT5SB_L12	2	5	1				PT SB	PT SB			
PT3SB_D023	2	3	1				PT	SB			
PT3SB2	2	3	2				PT	SB			
PTSB_B81	2	1	1				PT	SB			
PTSB2_C2	2	1	2				PT	SB			
PTSI	2	1	1				PT	SI			
PT782SI218	2	0.782	0.218				PT	SI			
PT5SI2	2	0.714	0.286				PT	SI			
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			
PT3SN_L12	2	3	1				PT	SN			
PTSN_B81	2	1	1				PT	SN			
PT2SN3	2	2	3				PT	SN			
PTSN2_C1	2	1	2				PT	SN			
PTSN4_D1C	2	1	4				PT	SN			
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			
PT3V_D022	2	3	1				PT V	PT V			
PT2V	2	2	1				PT V	PT V			
PTV_B19	2	1	1				PT V	PT V			
PTV3_A15	2	1	3				PT V	PT V			
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			
RE2SI	2	2	1				RE	SI			
RESI_B20	2	1	1				RE	SI			
RESI2	2	1	2				RE	SI VA			
RE24TI5_A12	2	24	5				RE	TI			
RETI_B2	2	1	1				RE	TI			
RU2SI	2	2	1				RU	SI			
RU4SI3	2	4	3				RU	SI			
RU3SN7	2	3	7				RU	GE SN			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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			
SB2TB	2	2	1				SB	TB			
SBTB_B1	2	1	1				SB	TB			
SBTB_BETA	2	1	1				SB	TB			
SB3TB4_D73	2	3	4				SB	TB			
SB3TB4_BETA	2	3	4				SB	TB			
SB3TB5_D88	2	3	5				SB	TB			
SB2TM	2	2	1				SB	TM			
SBTM_B1	2	1	1				SB	TM			
SBTM_BETA	2	1	1				SB	TM			
SB3TM5_ALPHA	2	3	5				SB	TM			
SB3TM5_BETA	2	3	5				SB	TM			
SBY_B1	2	1	1				SB	Y			
SB3Y4_D73	2	3	4				SB	Y			
SB3Y5_D88	2	3	5				SB	Y			
SBY3	2	1	3				SB	Y			
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			
SI3N4	2	3	4				SI	N			
TA2SI	2	0.666667	0.333333				TA	SI			
TA3SI	2	0.75	0.25				TA	SI			
TAS12	2	0.333333	0.666667				TA	SI			
TA5SI3	2	0.625	0.375				TA	SI			
SI2TE3_LT	2	2	3				SI	TE			
SI2TE3_HT	2	2	3				SI	TE			
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			
SM5SN3	2	0.625	0.375				SM	SN			
SM4SN3	2	0.571	0.429				SM	SN			
SM5SN4	2	0.556	0.444				SM	SN			
SM11SN10	2	0.524	0.476				SM	SN			
SM2SN3	2	0.4	0.6				SM	SN			
SMSN2	2	0.333	0.667				SM	SN			
SMSN3	2	0.25	0.75				SM	SN			
SMZN_B2	2	1	1				SM	ZN			
SMZN2	2	1	2				SM	ZN			
SMZN3	2	1	3				SM	ZN			
SM3ZN11	2	3	11				SM	ZN			
SM13ZN58	2	13	58				SM	ZN			
SM3ZN22	2	3	22				SM	ZN			
SM2ZN17	2	2	17				SM	ZN			
SMZN11_D2B	2	1	11				SM	ZN			
V3SI	2	3	1				SI V	SI V			
V5SI3	2	5	3				V	SI			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
V6SI5	2	6	5				V	SI			
VS12	2	1	2				V	SI			
V2ALC	3	2	1	1			V	AL	C		
V3ALC2	3	3	1	2			V	AL	C		
V4ALC3	4	4	1	2	1		V	AL	C	C VA	
WS12	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			
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				
SN12	2	1	2				SN	TI			
SN13	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			
SN3Y	2	3	1				SN	Y			
SN5Y2	2	5	2				SN	Y			
SN2Y	2	2	1				SN	Y			
SN10Y11	2	10	11				SN	Y			
SN4Y5	2	4	5				SN	Y			
SN3Y5	2	3	5				SN	Y			
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			
TA4C3	2	0.62	0.38				TA	C			
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			
T12ZN	2	2	1				TI	ZN			
T1ZN	2	1	1				TI	ZN			
T1ZN2	2	1	2				TI	ZN			
T1ZN3	2	1	3				TI	ZN			
T1ZN5	2	1	5				TI	ZN			
T1ZN10	2	1	10				TI	ZN			

Phase Name	Stoichiometry					Occupancy					
	Number of Sublattices	SL1	SL2	SL3	SL4	SL5	SL1	SL2	SL3	SL4	SL5
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			
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			