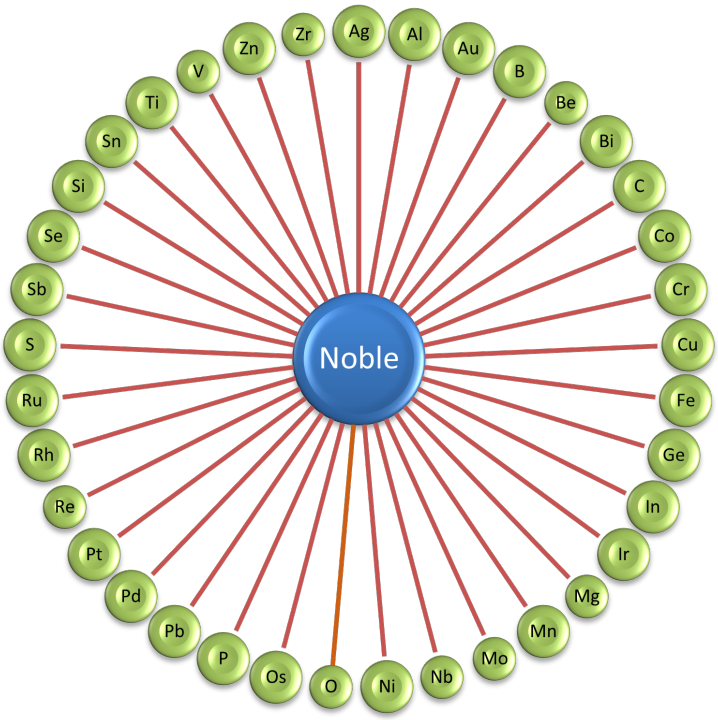
Pandat™ 2024

Database Manual

CompuTherm LLC

PanNoble

Database for multi-component noble metal alloys, copper alloys, and solder alloys



PANDAT™ SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (37)

Total of **37** components are included in the database as listed here:

Ag, Al, Au, B, Be, Bi, C, Co, Cr, Cu, Fe, Ge, In, Ir, Mg, Mn, Mo, Nb, Ni, O, Os, P, Pb, Pd, Pt, Re, Rh, Ru, S, Sb, Se, Si, Sn, Ti, V, Zn and Zr

1.2 Suggested Applicable Alloy Systems

The current PanNoble database can be used for several series of alloys:

(a) Noble metal alloys:

- Silver alloys with major alloying elements of Cu, Ni, Sn, Zn, Sn, and Ge
- Gold alloys with alloying elements of Ag, Cu, Pd, Pt, Al, Fe, Ni, and Zn
- Platinum group metals (Ru, Rh, Pd, Os, Ir, Pt) and their alloys

(b) Wrought (C10100-C79999) and Cast (C80000-C96999) Copper alloys:

- Coppers (C10100-C15999 and C80000-C81399) with majority Cu >99.95% and small amount of trace elements, such as Ni, S, Se, Sn, etc.
- High-copper alloys (C16000-C19999 and C81400-83299) with major alloying elements of Be, Cr, Ni, Si, Sn, and minor elements Ag, Al, Co, Fe, Pb, P, Zr, etc.
- Brasses (C20000-C49999 and C83300-C89999)) with major alloying elements of Pb, Sn, Zn and other minor elements Al, As, Bi, Fe, Ni, P, Sb, Se, Si, etc.
- Bronzes (C50000-C69999 and C90000-C95999) with major alloying elements of Ni, Sn and minor elements Al, Fe, Mn, P, Pb, Sb, Si, etc.
- Copper-Nickel alloys (C70000-C79999 and C96000-C96999) with major alloying elements of Fe, Ni, Zn and minor alloying elements Be, C, Mn, Nb, Pb, Si, Sn, etc.
- Copper-Lead alloys (C98000-C98999) with major alloying elements of Pb and minor elements Ag, Fe, Ni, P, Sn, Sn, Zn, etc.

- Copper- Nickel- Aluminum special alloys (C99000- C99999) with major alloying elements of Al, Fe, Ni and minor elements Co, Mn, Pb, Si, Sn, etc.

(c) Solder alloys:

- Commercial Pb/Sn-base micro-soldering alloy system with major alloying elements of Ag, Al, Au, Bi, Cu, In, Ni, Sb, Zn, etc.

(d) Pd-Sb-based lead-acid battery grid alloys with major alloying elements of Sb and minor elements As, Cu, Se, Sn, etc.

(e) High-entropy alloys of the Al-Co-Cr-Cu-Fe-Mn-Ni system with the addition of other minor elements in this database

The suggested composition range for each element is listed in Table 1.1. It should be noted that this given composition range is rather conservative. It is derived from the chemistries of the multicomponent commercial alloys that have been used to validate the current database. In the subsystems, many of these elements can be applied to a much wider composition range. In fact, some subsystems are valid in the entire composition range as given in Section 1.5 .

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Al, Co, Cr, Cu, Fe, O, Mn, Ni	0 ~ 100
Bi, In, Pb, Se, Sn, Zn	0 ~ 50
Ag, Au, Ir, Pd, Pt, Sb, Ti	0 ~ 30
Ge, Mg, Mo, Nb, Os, Re, Rh, Ru, Si, V, Zr	0 ~ 10
B, Be, C, P, S	0 ~ 3

1.3 What is new in PanNoble2024

- Addition of the component O
- Add the Au-Mo binary description
- Update thermodynamic description of the Ag-Bi-Cu-Sn quaternary system

1.4 Phases

Total of **949** phases are included in the database and a few key phases are listed in Table 1.2. Information on all the other phases may be displayed through TDB viewer of Pandat™

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
Ag3X	(0.75)(0.25)	(Ag,Al,Cu,Sb,Zn)(Ag,Bi,Sb,Sn)
Al7Cu2Fe	(7)(2)(1)	(Al)(Cu)(Fe)
AlPt	(1)(1)	(Al)(Pt)
Au2Pb	(0.667)(0.333)	(Au)(Pb)
Be3Co	(0.75)(0.25)	(Be)(Co)
BiIn	(0.5)(0.5)	(Bi)(In)
Chi	(24)(10)(24)	(Mo,Re)(Mo,Nb,Re)(Nb,Re)
Co5Ge2	(0.714)(0.286)	(Co)(Ge)
Cr2Pd3	(0.4)(0.6)	(Cr)(Pd)
Cu3P	(3)(1)	(Cu)(P)
Cu3Pd	(0.75)(0.25)(1)	(Cu,Pd)(Cu,Pd)(Va)

Name	Lattice Size	Constituent
CuBiSe2	(1)(1)(2)	(Cu)(Bi)(Se)
CuPd	(1)(1)	(Cu,Pd)(Cu,Pd)
CuS	(1)(1)	(Cu)(S)
Fcc	(1)(1)	(Ag,Al,Au,B,Be,Bi,Co,Cr,Cu,Fe,Ge,In, Ir,Mg,Mn,Mo,Nb,Ni,Os,P,Pb,Pd,Pt,Re, Rh,Ru,S,Sb,Si,Sn,Ti,V,Zn,Zr)(C,O,Va)
Gammabrass	(1)	(Ag,Al,Cu,Fe,Ni,Si,Zn)
Ge2Pt3	(0.4)(0.6)	(Ge)(Pt)
Ge2Ti	(2)(1)	(Ge)(Ti)
InPt	(1)(1)	(In,Pt)(In,Pt)
NiIn	(1)(1)	(Ni)(In)
OsSi	(0.5)(0.5)	(Os)(Si)
Pb2Pd	(0.667)(0.333)	(Pb)(Pd)
Pt10Zr7	(10)(7)	(Pt)(Zr)
ReSi2	(1)(2)	(Re)(Si,Va)
ReTi	(1)(1)	(Re)(Ti)
Ru2Si	(0.6667) (0.3333)	(Ru)(Si)
Sb2Se3	(0.4)(0.6)	(Sb)(Se)
Sn5Ti6	(0.455)(0.545)	(Sn)(Cu,Ti)

Name	Lattice Size	Constituent
SnTi2	(0.333)(0.667)	(Sn)(Ti)
SnV3	(0.25)(0.75)	(Sn,V)(V)
SnZr4	(3)(1)	(Sn,Zr)(Sn,Zr)

1.5 Assessed Subsystems

A total of **626** subsystems, including 458 binary and 168 ternary subsystems have been assessed. The modeling status is indicated by numbers. The systems with number 10 are fully assessed in the whole composition range. The higher value shows higher reliability of the system.

Binary Systems (458)

Ag-Al(10)	Ag-Au(10)	Ag-B(10)	Ag-Bi(10)	Ag-C(10)	Ag-Co(10)	Ag-Cr(10)
Ag-Cu(10)	Ag-Fe(10)	Ag-Ge(10)	Ag-In(10)	Ag-Ir(10)	Ag-Mg(10)	Ag-Mn(10)
Ag-Mo(10)	Ag-Ni(10)	Ag-O(5)	Ag-Os(10)	Ag-Pb(10)	Ag-Pd(10)	Ag-Pt(10)
Ag-Re(10)	Ag-Rh(10)	Ag-Ru(10)	Ag-Sb(10)	Ag-Si(10)	Ag-Sn(10)	Ag-Ti(10)
Ag-V(10)	Ag-Zn(10)	Ag-Zr(10)	Al-Au(10)	Al-B(10)	Al-Be(10)	Al-Bi(10)
Al-C(10)	Al-Co(10)	Al-Cr(10)	Al-Cu(10)	Al-Fe(10)	Al-Ge(10)	Al-In(10)
Al-Ir(10)	Al-Mg(10)	Al-Mn(10)	Al-Mo(10)	Al-Nb(10)	Al-Ni(10)	Al-O(10)
Al-Os(10)	Al-P(10)	Al-Pb(10)	Al-Pd(10)	Al-Pt(10)	Al-Re(10)	Al-Ru(10)
Al-Sb(10)	Al-Se(10)	Al-Si(10)	Al-Sn(10)	Al-Ti(10)	Al-V(10)	Al-Zn(10)
Al-Zr(10)	Au-B(10)	Au-Bi(10)	Au-C(10)	Au-Co(10)	Au-Cr(10)	Au-Cu(10)
Au-Fe(10)	Au-Ge(10)	Au-In(10)	Au-Ir(5)	Au-Mn(10)	Au-Ni(10)	Au-O(5)
Au-Os(10)	Au-Pb(10)	Au-Pd(10)	Au-Pt(10)	Au-Re(10)	Au-Rh(10)	Au-Ru(10)
Au-Sb(10)	Au-Se(10)	Au-Si(10)	Au-Sn(10)	Au-Ti(10)	Au-Zn(10)	Au-Zr(10)
B-C(10)	B-Co(10)	B-Cr(10)	B-Cu(10)	B-Fe(10)	B-Ge(10)	B-Ni(10)
B-O(10)	B-P(5)	B-Pb(10)	B-Pt(10)	B-Re(10)	B-Sb(10)	B-Se(10)

B-Si(10) B-Sn(10) B-Ti(10) B-Zn(10) B-Zr(10) Be-Co(10) Be-Cu(10)
Be-Ni(10) Be-O(10) Be-Si(10) Bi-Co(10) Bi-Cr(10) Bi-Cu(10) Bi-Fe(10)
Bi-Ge(10) Bi-In(10) Bi-Mg(10) Bi-Mn(10) Bi-Ni(10) Bi-O(10) Bi-Os(10)
Bi-P(10) Bi-Pb(10) Bi-Pd(10) Bi-S(5) Bi-Sb(10) Bi-Se(10) Bi-Si(10)
Bi-Sn(10) Bi-Ti(10) Bi-Zn(10) C-Co(10) C-Cr(10) C-Cu(5) C-Fe(10)
C-Ge(10) C-Ir(10) C-Mg(10) C-Mn(10) C-Mo(10) C-Nb(10) C-Ni(10)
C-O(10) C-P(10) C-Pd(10) C-Pt(10) C-Re(10) C-Rh(10) C-Ru(10)
C-Si(10) C-Sn(10) C-Ti(10) C-V(10) C-Zn(10) C-Zr(10) Co-Cr(10)
Co-Cu(10) Co-Fe(10) Co-Ge(10) Co-In(10) Co-Ir(10) Co-Mn(10) Co-Mo(10)
Co-Nb(10) Co-Ni(10) Co-O(10) Co-Os(5) Co-P(8) Co-Pb(10) Co-Pd(10)
Co-Pt(10) Co-Re(10) Co-Rh(10) Co-Ru(10) Co-Sb(10) Co-Si(10) Co-Sn(10)
Co-Ti(10) Co-V(10) Co-Zn(10) Co-Zr(10) Cr-Cu(10) Cr-Fe(10) Cr-Ge(10)
Cr-In(10) Cr-Ir(10) Cr-Mn(10) Cr-Mo(10) Cr-Nb(10) Cr-Ni(10) Cr-O(10)
Cr-Os(10) Cr-P(5) Cr-Pb(10) Cr-Pd(10) Cr-Pt(10) Cr-Re(10) Cr-Rh(10)
Cr-Ru(10) Cr-S(5) Cr-Sb(10) Cr-Se(10) Cr-Si(10) Cr-Sn(10) Cr-Ti(10)
Cr-V(10) Cr-Zn(10) Cr-Zr(10) Cu-Fe(10) Cu-Ge(10) Cu-In(10) Cu-Ir(10)
Cu-Mg(10) Cu-Mn(10) Cu-Mo(10) Cu-Nb(10) Cu-Ni(10) Cu-O(10) Cu-Os(10)
Cu-P(5) Cu-Pb(10) Cu-Pd(10) Cu-Pt(10) Cu-Re(10) Cu-Rh(10) Cu-Ru(10)
Cu-S(10) Cu-Sb(10) Cu-Se(10) Cu-Si(10) Cu-Sn(10) Cu-Ti(10) Cu-V(10)
Cu-Zn(10) Cu-Zr(10) Fe-In(10) Fe-Ir(10) Fe-Mg(10) Fe-Mn(10) Fe-Mo(10)
Fe-Nb(10) Fe-Ni(10) Fe-O(10) Fe-Os(10) Fe-P(5) Fe-Pb(10) Fe-Pd(10)
Fe-Pt(10) Fe-Re(10) Fe-Rh(10) Fe-Ru(10) Fe-S(10) Fe-Sb(10) Fe-Se(5)
Fe-Si(10) Fe-Sn(10) Fe-Ti(10) Fe-V(10) Fe-Zn(10) Fe-Zr(10) Ge-In(10)
Ge-Mg(10) Ge-Mn(10) Ge-Mo(10) Ge-Nb(10) Ge-Ni(10) Ge-O(10) Ge-P(10)
Ge-Pb(10) Ge-Pd(10) Ge-Pt(10) Ge-Ru(10) Ge-Sb(10) Ge-Si(10) Ge-Sn(10)
Ge-Ti(10) Ge-V(10) Ge-Zn(10) In-Ir(10) In-Ni(10) In-O(10) In-P(5)
In-Pb(10) In-Pd(10) In-Pt(10) In-Sb(10) In-Si(10) In-Sn(10) In-V(10)
In-Zn(10) Ir-Ni(10) Ir-O(10) Ir-Os(5) Ir-Pd(10) Ir-Pt(10) Ir-Re(10)

Ir-Rh(10) Ir-Ru(10) Ir-Zr(10) Mg-Mn(10) Mg-Ni(10) Mg-O(10) Mg-Ru(10)
Mg-Sb(10) Mg-Si(10) Mg-Sn(10) Mg-Ti(10) Mg-Zn(10) Mg-Zr(10) Mn-Mo(10)
Mn-Nb(10) Mn-Ni(10) Mn-O(10) Mn-Os(10) Mn-P(10) Mn-Pb(10) Mn-Pd(10)
Mn-Pt(10) Mn-Re(10) Mn-Rh(10) Mn-Ru(10) Mn-S(10) Mn-Se(10) Mn-Si(10)
Mn-Sn(10) Mn-Ti(10) Mn-V(10) Mn-Zn(10) Mn-Zr(10) Mo-Nb(10) Mo-Ni(10)
Mo-O(10) Mo-Pd(10) Mo-Pt(10) Mo-Re(10) Mo-Ru(10) Mo-Si(10) Mo-Sn(10)
Mo-Ti(10) Mo-V(10) Mo-Zr(10) Nb-O(10) Nb-Pt(10) Nb-Re(10) Nb-Si(10)
Nb-Sn(10) Nb-Ti(10) Nb-V(10) Nb-Zr(10) Ni-O(10) Ni-Os(10) Ni-P(10)
Ni-Pb(10) Ni-Pd(10) Ni-Pt(10) Ni-Re(10) Ni-Rh(10) Ni-Ru(10) Ni-S(10)
Ni-Sb(5) Ni-Se(10) Ni-Si(10) Ni-Sn(10) Ni-Ti(10) Ni-V(10) Ni-Zn(10)
Ni-Zr(10) O-Os(5) O-P(10) O-Pb(10) O-Pd(5) O-Re(5) O-Rh(5)
O-Ru(5) O-S(10) O-Sb(7) O-Se(5) O-Si(10) O-Sn(10) O-Ti(10)
O-V(10) O-Zn(5) O-Zr(10) Os-Pd(10) Os-Pt(10) Os-Re(10) Os-Rh(10)
Os-Ru(10) Os-Si(10) P-Si(5) P-Sn(5) P-Zn(5) Pb-Pd(10) Pb-Pt(10)
Pb-Re(10) Pb-Rh(10) Pb-Ru(10) Pb-S(10) Pb-Sb(10) Pb-Se(10) Pb-Si(10)
Pb-Sn(10) Pb-Ti(10) Pb-Zn(10) Pd-Pt(10) Pd-S(8) Pd-Sb(5) Pd-Se(10)
Pd-Si(10) Pd-Sn(10) Pd-Zn(10) Pd-Zr(10) Pt-Re(10) Pt-Rh(10) Pt-Ru(10)
Pt-Sb(10) Pt-Si(10) Pt-Sn(10) Pt-Ti(10) Pt-V(10) Pt-Zr(10) Re-Rh(10)
Re-Si(10) Re-Ti(10) Re-Zr(10) Rh-Ru(10) Ru-Si(10) Ru-Ti(10) Ru-Zr(10)
S-Zn(10) Sb-Se(10) Sb-Si(10) Sb-Sn(10) Sb-Ti(10) Sb-Zn(10) Se-Si(10)
Se-Sn(10) Se-Zn(10) Si-Sn(10) Si-Ti(10) Si-V(10) Si-Zn(10) Si-Zr(10)
Sn-Ti(10) Sn-V(10) Sn-Zn(10) Sn-Zr(10) Ti-V(10) Ti-Zn(10) Ti-Zr(10)
V-Zn(10) V-Zr(10) Zn-Zr(10)

Ternary Systems (168)

Ag-Al-Au(10) Ag-Al-Cu(10) Ag-Al-Ge(10) Ag-Al-Si(10) Ag-Al-Sn(10) Ag-Al-Zn(10)
Ag-Au-Bi(10) Ag-Au-Cu(10) Ag-Au-Ge(10) Ag-Au-Pb(10) Ag-Au-Si(10) Ag-Au-Sn(10)
Ag-Bi-Cu(10) Ag-Bi-In(10) Ag-Bi-Pb(10) Ag-Bi-Sb(10) Ag-Bi-Sn(10) Ag-Bi-Zn(10)
Ag-Cu-In(10) Ag-Cu-Ni(10) Ag-Cu-Pb(10) Ag-Cu-Sn(10) Ag-Cu-Zn(10) Ag-In-Pd(10)

Ag-In-Sb(10)	Ag-In-Sn(10)	Ag-Pb-Sb(10)	Ag-Pb-Sn(10)	Ag-Sb-Sn(10)	Ag-Sn-Zn(10)
Al-Bi-Cu(10)	Al-Bi-Zn(10)	Al-C-Co(10)	Al-C-Mn(10)	Al-C-Ni(10)	Al-Co-Cr(10)
Al-Co-Cu(10)	Al-Co-Fe(10)	Al-Co-Mn(10)	Al-Co-Ni(10)	Al-Cr-Cu(10)	Al-Cr-Fe(10)
Al-Cr-Ni(10)	Al-Cu-Fe(10)	Al-Cu-Mn(10)	Al-Cu-Ni(10)	Al-Cu-Sb(10)	Al-Cu-Si(10)
Al-Cu-Sn(10)	Al-Cu-Zn(10)	Al-Fe-Mn(10)	Al-Fe-Ni(10)	Al-Fe-Si(10)	Al-Fe-Zn(10)
Al-In-Sb(10)	Al-In-Sn(10)	Al-Mn-Ni(10)	Al-Pb-Zn(10)	Al-Si-Sn(10)	Al-Si-Zn(10)
Al-Sn-Zn(10)	Au-Ge-Sb(10)	Au-Ge-Sn(10)	Au-In-Sb(10)	Au-In-Sn(10)	Au-Ni-Sn(10)
Au-Pt-Re(10)	Au-Sb-Si(10)	Au-Si-Sn(10)	B-Co-Fe(10)	B-Cu-Fe(10)	B-Fe-Ni(10)
B-Ni-Si(10)	Bi-Cu-Ni(10)	Bi-Cu-Pb(10)	Bi-Cu-Sb(10)	Bi-Cu-Se(10)	Bi-Cu-Sn(10)
Bi-Cu-Zn(10)	Bi-In-Pb(10)	Bi-In-Sb(10)	Bi-In-Sn(10)	Bi-Sb-Sn(10)	Bi-Sb-Zn(10)
Bi-Se-Sn(10)	Bi-Se-Zn(10)	Bi-Sn-Zn(10)	C-Co-Fe(10)	C-Co-Ni(10)	C-Cr-Fe(10)
C-Cu-Fe(10)	C-Fe-Ni(10)	Co-Cr-Cu(10)	Co-Cr-Fe(10)	Co-Cr-Ni(10)	Co-Cu-Fe(10)
Co-Cu-Mn(10)	Co-Cu-Ni(10)	Co-Fe-Pd(10)	Co-Fe-Re(10)	Co-Mn-Ni(10)	Co-Mn-Pd(10)
Co-Ni-P(6)	Co-Ni-Re(10)	Cr-Cu-Fe(10)	Cr-Cu-Mn(10)	Cr-Cu-Ni(10)	Cr-Cu-Si(10)
Cr-Cu-Sn(10)	Cr-Cu-Ti(10)	Cr-Fe-Mn(10)	Cr-Fe-Ni(10)	Cr-Fe-P(10)	Cr-Fe-S(10)
Cr-Fe-Si(10)	Cr-Mn-Ni(10)	Cr-Mn-S(10)	Cr-Ni-Pd(10)	Cr-Ni-S(10)	Cr-Ni-Si(10)
Cu-Fe-Mn(10)	Cu-Fe-Ni(10)	Cu-Fe-P(10)	Cu-Fe-S(10)	Cu-Fe-Sb(10)	Cu-Fe-Si(10)
Cu-Fe-Zn(10)	Cu-In-Sn(10)	Cu-Mn-Ni(10)	Cu-Mn-Zn(10)	Cu-Ni-P(10)	Cu-Ni-Pb(10)
Cu-Ni-Sb(10)	Cu-Ni-Si(10)	Cu-Ni-Sn(10)	Cu-Ni-Ti(10)	Cu-Ni-Zn(10)	Cu-P-Sn(10)
Cu-Pb-S(10)	Cu-Pb-Sb(10)	Cu-Pb-Zn(10)	Cu-Sb-Se(10)	Cu-Sb-Sn(10)	Cu-Sb-Zn(10)
Cu-Se-Zn(10)	Cu-Si-Ti(10)	Cu-Si-Zn(10)	Cu-Sn-Ti(10)	Cu-Sn-Zn(10)	Cu-Ti-Zn(10)
Fe-Mn-Ni(10)	Fe-Mn-S(10)	Fe-Mn-Si(10)	Fe-Ni-Pd(10)	Fe-Ni-Re(10)	Fe-Ni-S(10)
Fe-Ni-Si(10)	Fe-Si-Sn(10)	In-Pb-Zn(10)	In-Sb-Sn(10)	In-Sn-Zn(10)	Mn-Ni-S(10)
Ni-Si-Ti(10)	Ni-Si-Zn(10)	Ni-Sn-Zn(10)	Pb-Sb-Sn(10)	Pb-Sb-Zn(10)	Pd-Rh-Ru(10)

1.6 Database Validation

The current thermodynamic database can be used to calculate the phase diagrams not only for the noble-metal-rich systems (Ag-, Au-, Cu-, Ir-, Pd- and Pt-) but also other common alloying systems, such as Pb and/or Sn-rich solders. Extensive tests and validations have been carried out on the current thermodynamic database using the published experimental data in the literature. A few examples are given below. Figure 1.1 shows the Pt-Sn binary phase diagram with experimental phase boundary data plotted on it. Figure 1.2 shows two isoplethal sections in the of the Ag-Au-Bi ternary system: (a) Ag-Au-85 at.%Bi; (b) Au-Bi-20 at.%Ag. The experimentally measured phase boundary data are also plotted on them for comparison. Figure 1.3 shows comparison between the calculated and measured liquidus temperatures for some Cu-rich alloys.

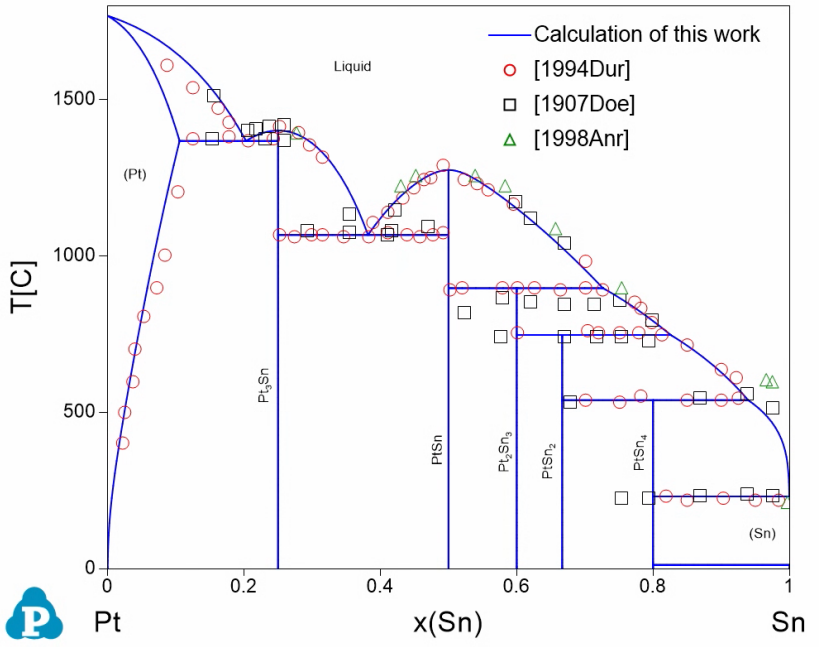


Figure 1.1: Comparison between the calculated Pt-Sn phase diagram with the experimental data

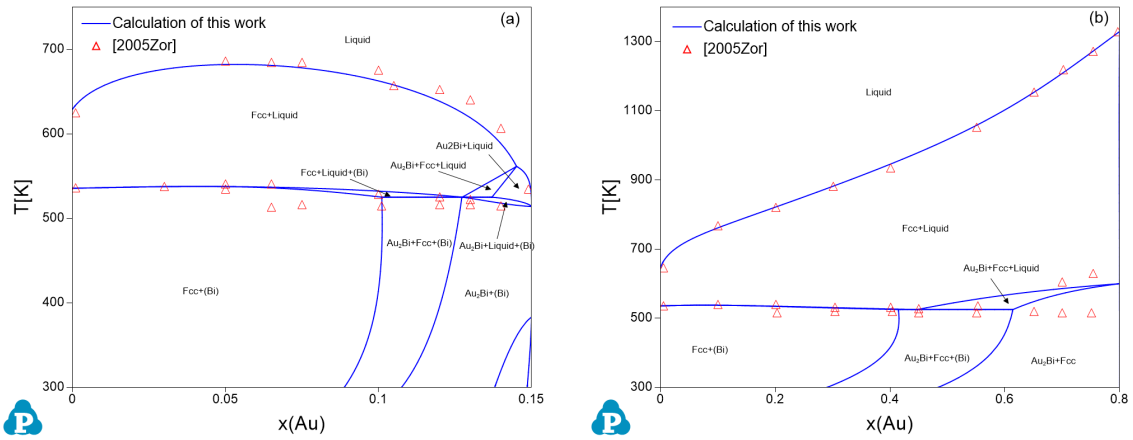


Figure 1.2: Comparison between the calculated isopleths and experimentally measured data of the Ag-Au-Bi ternary system (a) Ag-Au-85 at.%Bi; (b) Au-Bi-20 at.%Ag

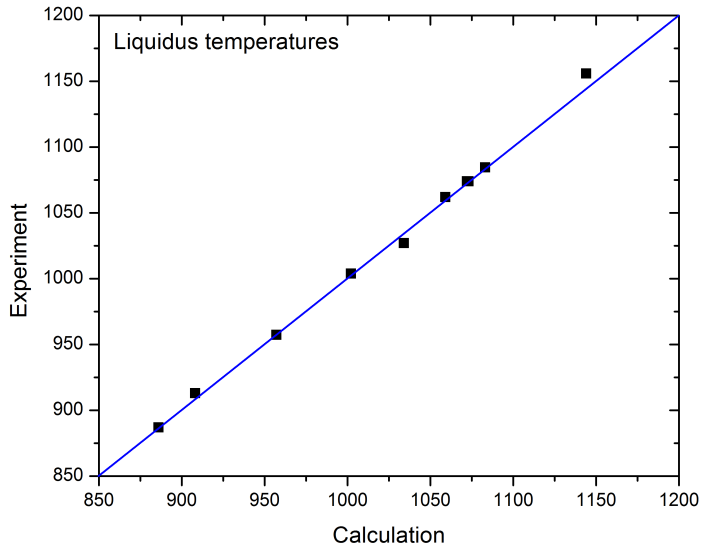


Figure 1.3: Comparison between the calculated and experimentally measured liquidus temperatures of [1982Bac]

Figure 1.4 toFigure 1.8 show the calculated constituent binary phase diagrams, isothermal section and liquidus projection of the Pd-Rh-Ru ternary system.

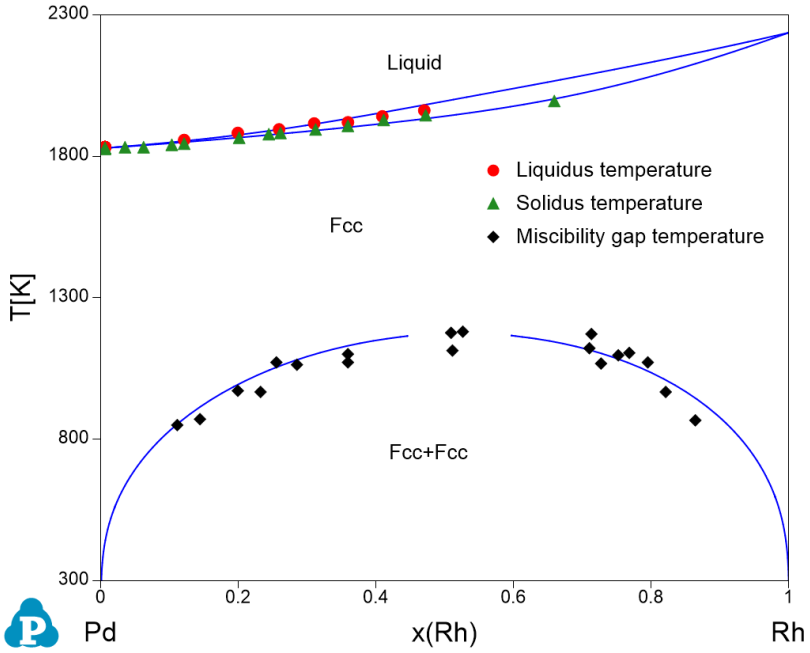


Figure 1.4: Calculated Pd-Rh phase diagram and experimental data from ref. [2016Gos]

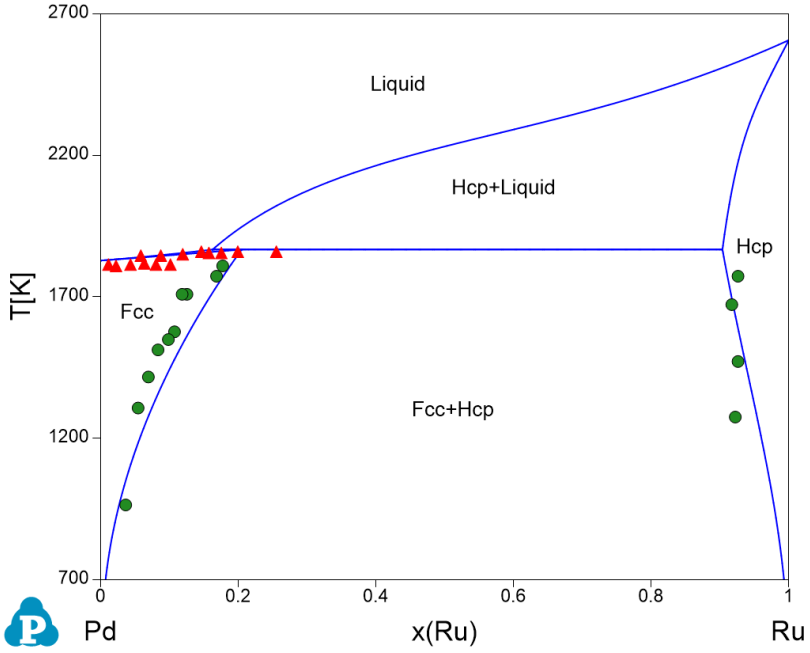


Figure 1.5: Calculated Pd-Ru phase diagram and experimental data from ref. [2016Gos]

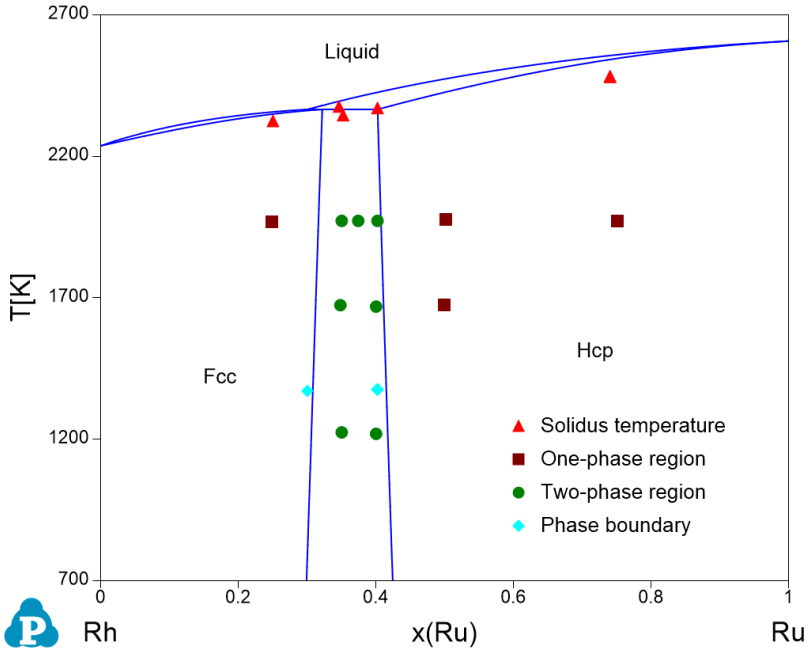


Figure 1.6: Calculated Rh-Ru phase diagram and experimental data from ref. [2016Gos]

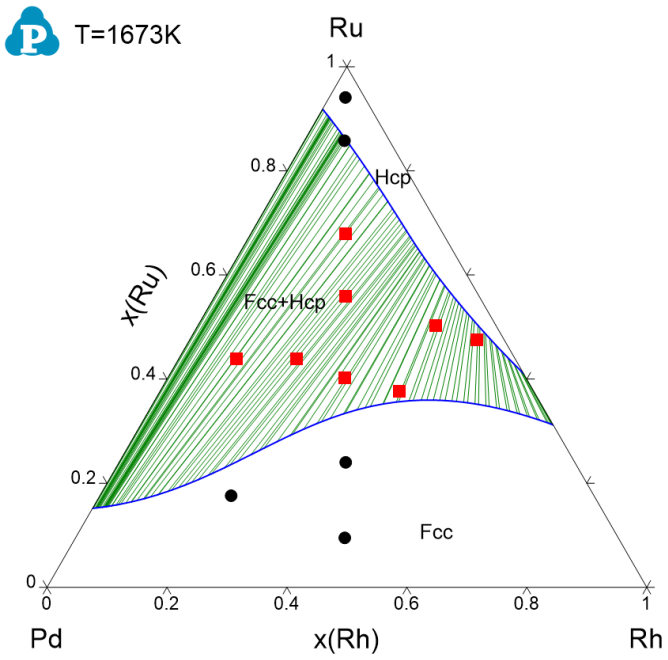


Figure 1.7: Calculated Pd-Rh-Ru isothermal section at 1673K and experimental data from ref. [1984Rae]

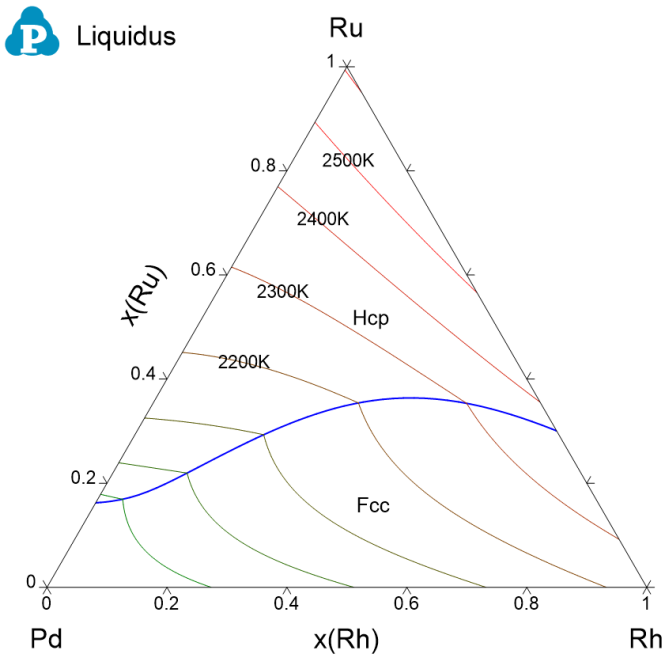


Figure 1.8: Calculated liquidus projection of the Pd-Rh-Ru ternary system

2 Mobility Database

PanNoble2024_MB is an atomic mobility database for noble metal alloys, which is compatible with the `PanNoble2024_TH` thermodynamic database and suitable for the simulation of diffusion- controlled phenomena using the **PanDiffusion** module, **PanEvolution** module, and/or **PanSolidification** module.

2.1 Phases

The atomic mobility within the **Liquid**, **Bcc**, **Fcc**, and **Hcp** solution phases are assessed in this database.

2.2 Self-diffusivity of Pure Elements

The color represents the following meaning:

: Validated

: Estimated

: No data

Table 2.1: Assessed self-diffusivity of pure elements with different crystal structures

	Ag	Al	Au	Be	Bi	Co	Cr	Cu	Fe	Ge	In	Ir	Mg	Mn	Mo	Nb
Bcc																
Fcc																
Hcp																
	Ni	Os	Pb	Pd	Pt	Re	Rh	Ru	Sb	Se	Si	Sn	Ti	V	Zn	Zr
Bcc																
Fcc																
Hcp																

2.3 Assessed Systems

In addition to the assessed self-diffusivities shown above, the impurity diffusion data for all included elements in the current `PanNoble2024_MB` database are also assessed. In the following, the assessed chemical-diffusivity within the binary and ternary systems for the Bcc, Fcc, and Hcp phases are listed, respectively.

Fcc Phase

Ag-Al	Ag-Sn	Ag-Zn	Au-Pt	Al-Cu	Al-Mg	Al-Si	Al-Zn	Co-Al	Co-Cr
Co-Fe	Co-Ni	Co-Cu	Co-Pd	Co-Pt	Cr-Ni	Cu-Ag	Cu-Au	Cu-Fe	Cu-Mg
Cu-Ti	Cu-Si	Cu-Zn	Fe-Si	Fe-Mn	Fe-Cr	Fe-Ni	Ni-Al	Ni-Au	Ni-Re
Ni-Ru	Ni-Mo	Ni-Nb	Ni-Mn	Ni-Ir	Ni-Rh	Ni-Pt	Ni-Ge	Ni-Ti	Ni-V
Ni-Zn	Pt-Al	V-Nb							

Ag-Al-Zn	Al-Cu-Mg	Al-Cu-Zn	Co-Cr-Ni	Cu-Ag-Au	Cu-Al-Si
Cu-Co-Ni	Cu-Cr-Ni	Cu-Fe-Mn	Cu-Fe-Ni	Cu-Mn-Ni	Cu-Ni-Zn
Fe-Mn-Si	Fe-Cr-Ni	Ni-Al-Cr	Ni-Al-Mn	Ni-Al-Nb	Ni-Co-Re
Ni-Co-Ru	Ni-Cr-Nb	Ni-Cu-Mn			

Bcc phase

Fe-Al	Fe-Cr	Ti-Al	Ti-Cr	Ti-Cu	Ti-Mo	Ti-Nb	Ti-V	Ti-Zr	Mo-Nb
Mo-Zr	Nb-Zr								

Fe-Cr-Ni	Ti-Al-Cr	Ti-Al-Fe			

Hcp phase

Mg-Al	Mg-Zn								

Mg-Al-Zn					

2.4 Database Validation

The simulated concentration profiles of a series of noble metal alloys are shown below to validate the current `PanNoble2024_MB` database.

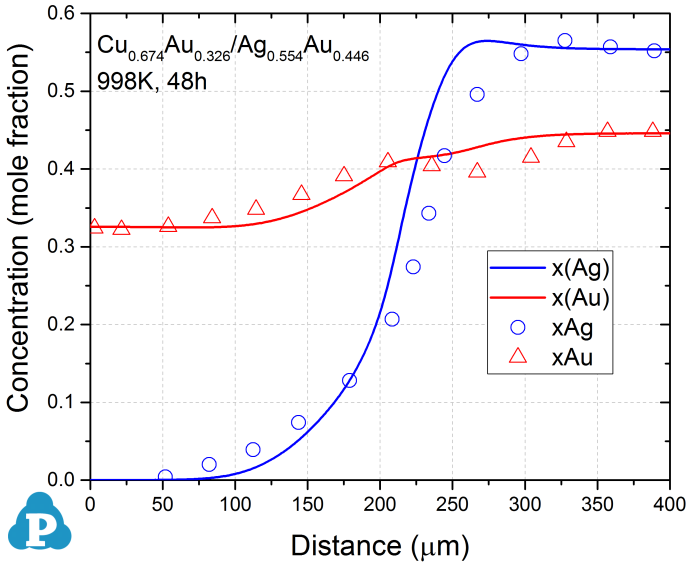


Figure 2.1: Concentration profiles of Cu0.674Au0.326/Ag0.554Au0.446 annealed at 998K for 48h [2011Liu]

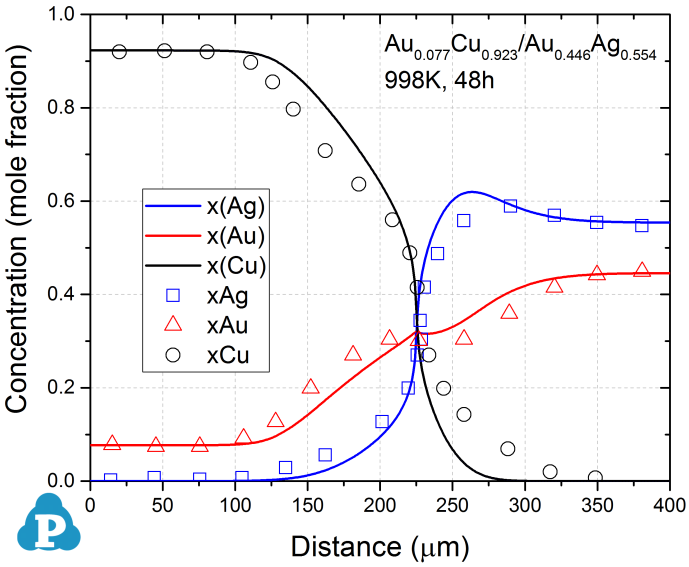


Figure 2.2: Concentration profiles of Au0.077Cu0.923/Au0.446Ag0.554 annealed at 998K for 48h [2011Liu]

3 Thermophysical Property Database

The thermophysical property database **PanNoble2024_ TP** is compatible with the `PanNoble2024_ TH` thermodynamic database and suitable for the simulation of thermophysical properties of noble metal alloys. It includes the molar volume data for all the phases, surface tension and viscosity properties for the liquid phase.

3.1 Molar Volume

The current molar volume database covers all 949 phases assessed in the `PanNoble2024_ TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of the alloys.

The simulated density changes vs. temperature of a series of noble metal alloys are shown below to validate the current `PanNoble2024_MV` database.

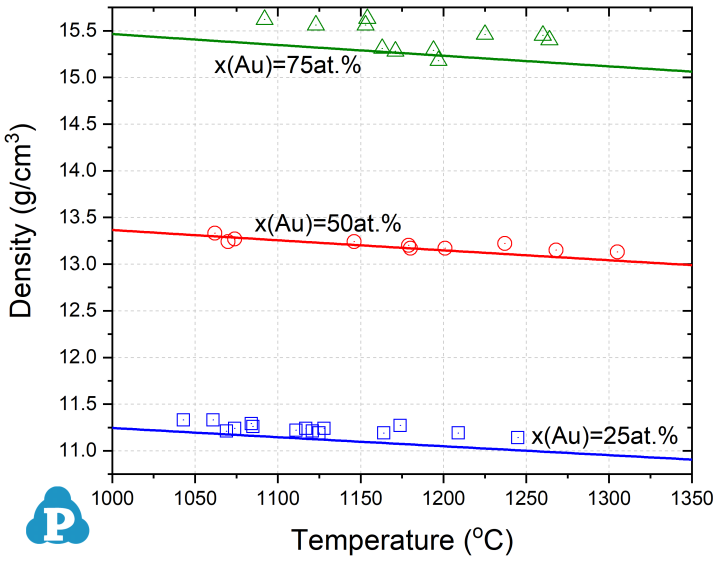


Figure 3.1: Density of Ag-Au binary liquid alloys [2006Bri]

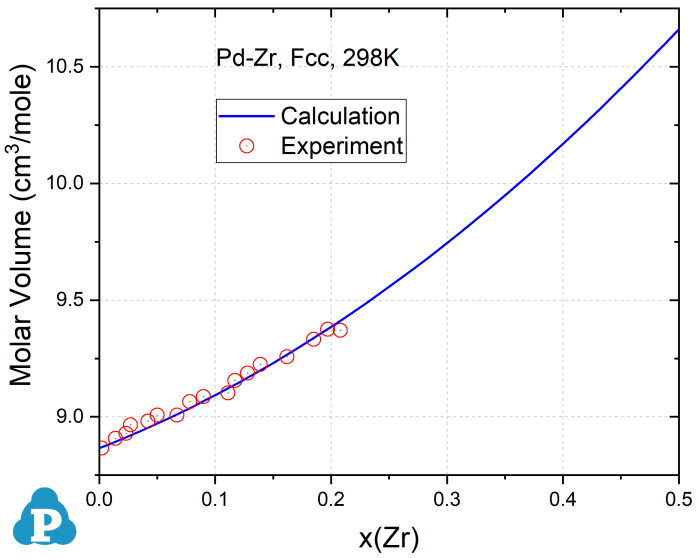


Figure 3.2: Molar volume of Pd-Zr Fcc binary alloys at 298K [2013He]

3.2 Surface Tension

The surface tension of the liquid phase is added into the property database. Figure 3.3 shows the surface tension of a series of Cu-Ni alloys in comparison with experimental data.

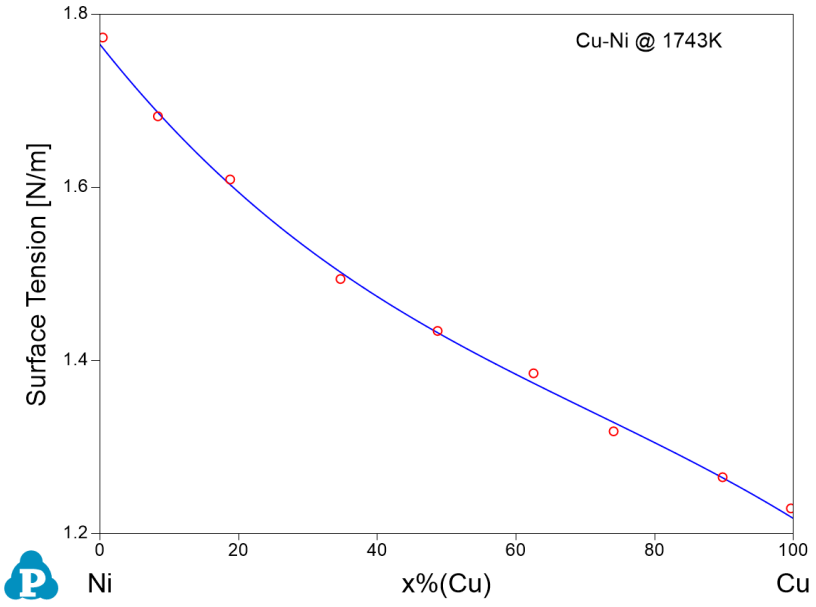


Figure 3.3: Surface tension of Cu-Ni alloys

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.4 shows the viscosity of Cu-Mg alloys in comparison with experimental data.

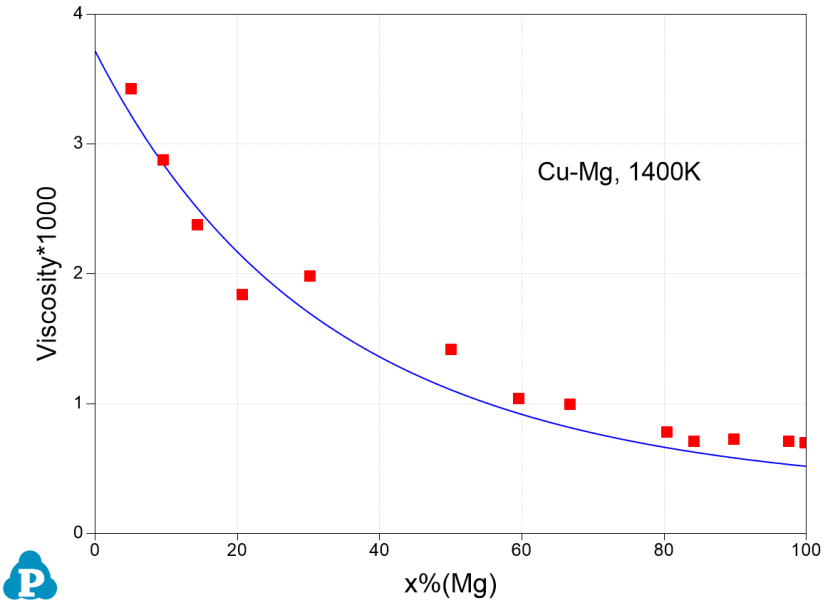


Figure 3.4: Viscosity of the Cu-Mg alloys

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PanNoble2024: List of Phases

Phases (949)

Name	Model	Lattice Size	Constituent
A_BeO	CEF (ST2)	(1)(1)	(Be)(O)
A_Bi2O3	CEF (ST2)	(2)(3)	(Bi)(O)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
A_phase	CEF (SLN)	(0.8)(0.2)	(Au,Cu)(Sn)
Ag15Pt17	CEF (ST2)	(0.46875) (0.53125)	(Ag)(Pt)
Ag2O2	CEF (ST2)	(2)(2)	(Ag)(O)
Ag3X	CEF (SLN)	(0.75)(0.25)	(Ag,Al,Cu,Sb,Zn)(Ag,Bi,Sb,Sn)
Ag9In4	CEF (SLN)	(6)(3)(3)(1)	(Ag)(Ag,Cu,In)(Ag,In)(In)
AgIn2	CEF (SLN)	(1)(2)	(Ag,Cu)(In)
AgInPd_T	CEF (ST3)	(0.156)(0.26) (0.584)	(Ag)(In)(Pd)
AgMg3	CEF (ST2)	(0.23)(0.77)	(Ag)(Mg)
AgMg4	CEF (ST2)	(0.2)(0.8)	(Ag)(Mg)
AgTi2	CEF (ST2)	(1)(2)	(Ag)(Ti)
AgZn_Zeta	CEF (SLN)	(1)	(Ag,Sn,Zn)
AgZr	CEF (ST2)	(0.5)(0.5)	(Ag)(Zr)

Name	Model	Lattice Size	Constituent
AgZr2	CEF (ST2)	(0.333333) (0.666667)	(Ag)(Zr)
Al10Cu10Fe	CEF (ST3)	(10)(10)(1)	(Al)(Cu)(Fe)
Al10Fe3Ni	CEF (ST3)	(10)(3)(1)	(Al)(Fe)(Ni)
Al10FeNi3	CEF (ST3)	(10)(1)(3)	(Al)(Fe)(Ni)
Al10V	CEF (ST2)	(10)(1)	(Al)(V)
Al11Cr2	CEF (ST2)	(10)(1)(2)	(Al)(Al)(Cr)
Al11Mn4_HT	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al11Mn4_LT	CEF (ST2)	(11)(4)	(Al)(Mn)
Al11Re4	CEF (ST2)	(11)(4)	(Al)(Re)
Al12Mn	CEF (ST2)	(12)(1)	(Al)(Mn)
Al12Mo	CEF (ST2)	(12)(1)	(Al)(Mo)
Al12Re	CEF (ST2)	(12)(1)	(Al)(Re)
Al13Co4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Co)(Al,Va)
Al13Cr2	CEF (ST2)	(13)(2)	(Al)(Cr)
Al13Fe4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al,Cu)(Co,Cr,Fe,Mn,Ni) (Al,Cu,Va)
Al13Ir4	CEF (ST2)	(0.765) (0.235)	(Al)(Ir)

Name	Model	Lattice Size	Constituent
Al13Ru4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Ru)(Al,Va)
Al15_FeMn3Si2	CEF (SLN)	(16)(4)(1)(2)	(Al)(Fe,Mn)(Si)(Al,Si)
Al17Mo4	CEF (ST2)	(17)(4)	(Al)(Mo)
Al1Fe1O3	CEF (ST3)	(1)(1)(3)	(Al+3)(Fe+3)(O-2)
Al20Cu2Mn3	CEF (ST3)	(0.8)(0.08) (0.12)	(Al)(Cu)(Mn)
Al21Pd8	CEF (ST2)	(21)(8)	(Al)(Pd)
Al21Pt5	CEF (ST2)	(21)(5)	(Al)(Pt)
Al21Pt8	CEF (ST2)	(21)(8)	(Al)(Pt)
Al22Mo5	CEF (ST2)	(22)(5)	(Al)(Mo)
Al23CuFe4	CEF (ST3)	(23)(1)(4)	(Al)(Cu)(Fe)
Al23V4	CEF (ST2)	(23)(4)	(Al)(V)
Al2Au	CEF (SLN)	(2)(1)	(Al,Au)(Al,Au)
Al2Fe	CEF (ST2)	(2)(1)	(Al)(Fe)
Al2Pd5	CEF (SLN)	(2)(5)	(Al)(Al,Pd)
Al2Pt	CEF (ST2)	(2)(1)	(Al)(Pt)
Al2Ru	CEF (SLN)	(2)(1)(1)	(Al)(Ru)(Al,Ru,Va)
Al2Se3	CEF (ST2)	(0.4)(0.6)	(Al)(Se)
Al2Ti	CEF (ST2)	(2)(1)	(Al)(Ti)

Name	Model	Lattice Size	Constituent
Al2Zr	CEF (ST2)	(2)(1)	(Al)(Zr)
Al2Zr3	CEF (ST2)	(2)(3)	(Al)(Zr)
Al3Au8	CEF (ST2)	(3)(8)	(Al)(Au)
Al3Co	CEF (ST2)	(3)(1)	(Al)(Co)
Al3CoCu	CEF (ST3)	(3)(1)(1)	(Al)(Co)(Cu)
Al3Ir	CEF (ST2)	(0.75)(0.25)	(Al)(Ir)
Al3Mo	CEF (ST2)	(3)(1)	(Al)(Mo)
Al3Nb	CEF (ST2)	(3)(1)	(Al)(Nb)
Al3Ni	CEF (ST2)	(0.75)(0.25)	(Al)(Ni)
Al3Ni2	CEF (SLN)	(3)(2)(1)	(Al)(Al,Ni)(Ni,Va)
Al3Ni5	CEF (ST2)	(0.375) (0.625)	(Al)(Ni)
Al3Pd	CEF (ST2)	(3)(1)	(Al)(Pd)
Al3Pd2	CEF (SLN)	(3)(2)	(Al,Pd)(Al,Pd)
Al3Pd5	CEF (ST2)	(3)(5)	(Al)(Pd)
Al3Pt2	CEF (ST2)	(3)(2)	(Al)(Pt)
Al3Pt5	CEF (ST2)	(3)(5)	(Al)(Pt)
Al3Ru2	CEF (SLN)	(3)(2)(1)	(Al)(Al,Ru)(Ru,Va)
Al3Ti	CEF (SLN)	(0.25)(0.75)	(Al,Ti)(Al,Si,Ti)
Al3V	CEF (ST2)	(3)(1)	(Al)(V)

Name	Model	Lattice Size	Constituent
Al3Zr	CEF (ST2)	(3)(1)	(Al)(Zr)
Al3Zr2	CEF (ST2)	(3)(2)	(Al)(Zr)
Al3Zr4	CEF (ST2)	(3)(4)	(Al)(Zr)
Al3Zr5	CEF (ST2)	(3)(5)	(Al)(Zr)
Al45Ir13	CEF (ST2)	(0.776) (0.224)	(Al)(Ir)
Al4C3	CEF (ST2)	(4)(3)	(Al)(C)
Al4Cr	CEF (ST2)	(4)(1)	(Al)(Cr)
Al4Mo	CEF (ST2)	(4)(1)	(Al)(Mo)
Al4Pd	CEF (ST2)	(4)(1)	(Al)(Pd)
Al4Re	CEF (ST2)	(4)(1)	(Al)(Re)
Al4Zr5	CEF (ST2)	(4)(5)	(Al)(Zr)
Al5Co2	CEF (SLN)	(5)(2)	(Al)(Co,Fe)
Al5CoCu4	CEF (ST3)	(5)(1)(4)	(Al)(Co)(Cu)
Al5Fe2	CEF (ST2)	(5)(2)	(Al)(Fe)
Al5Fe4	CEF (SLN)	(1)	(Al,Fe)
Al5Mo	CEF (ST2)	(5)(1)	(Al)(Mo)
Al5Ti2	CEF (ST2)	(5)(2)	(Al)(Ti)
Al63Mo37	CEF (ST2)	(63)(37)	(Al)(Mo)
Al6CoCu3	CEF (ST3)	(6)(1)(3)	(Al)(Co)(Cu)

Name	Model	Lattice Size	Constituent
Al6Cu2Fe	CEF (ST3)	(6)(2)(1)	(Al)(Cu)(Fe)
Al6Mn	CEF (ST2)	(6)(1)	(Al)(Mn)
Al6Re	CEF (ST2)	(6)(1)	(Al)(Re)
Al6Ru	CEF (ST2)	(6)(1)	(Al)(Ru)
Al73Ir27	CEF (ST2)	(0.73)(0.27)	(Al)(Ir)
Al7CoCu2	CEF (ST3)	(7)(1)(2)	(Al)(Co)(Cu)
Al7Cu2Fe	CEF (ST3)	(7)(2)(1)	(Al)(Cu)(Fe)
Al7Cu4Ni	CEF (ST3)	(7)(4)(1)	(Al)(Cu)(Ni)
Al7V	CEF (ST2)	(7)(1)	(Al)(V)
Al8Cr5_H	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Cr5_L	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Mn5	CEF (SLN)	(12)(5)(9)	(Al)(Mn)(Al,Mn)
Al8Mo3	CEF (ST2)	(8)(3)	(Al)(Mo)
Al8V5	CEF (ST2)	(8)(5)	(Al)(V)
Al9Co2	CEF (ST2)	(9)(2)	(Al)(Co)
Al9Cr4_H	CEF (ST2)	(9)(4)	(Al)(Cr)
Al9Cr4_L	CEF (ST2)	(9)(4)	(Al)(Cr)
Al9FeNi	CEF (ST3)	(9)(1)(1)	(Al)(Fe)(Ni)
Al9Ir2	CEF (ST2)	(0.818) (0.182)	(Al)(Ir)

Name	Model	Lattice Size	Constituent
Al9Mn3Si	CEF (ST3)	(0.6923) (0.2308) (0.0769)	(Al)(Mn)(Si)
AlAu	CEF (ST2)	(1)(1)	(Al)(Au)
AlAu4	CEF (SLN)	(1)(4)	(Al)(Ag,Au)
AlB12H	CEF (ST2)	(1)(12)	(Al)(B)
AlB12L	CEF (ST2)	(1)(12)	(Al)(B)
AlB2	CEF (ST2)	(1)(2)	(Al)(B)
AlCr2	CEF (ST2)	(1)(2)	(Al)(Cr)
AlCuZn_Tau	CEF (SLN)	(0.1)(0.4)(0.4) (0.1)	(Al,Cu)(Al)(Cu)(Zn)
AlCu_Delta	CEF (SLN)	(0.4)(0.6)	(Al)(Ag,Cu)
AlCu_Eps	CEF (SLN)	(0.5)(0.5)	(Ag,Al,Cu)(Ag,Cu)
AlCu_Eta	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Ag,Cu)
AlCu_Gamma	CEF (SLN)	(4)(1)(8)	(Al)(Al,Cu)(Ag,Cu)
AlCu_Gamma_H	CEF (SLN)	(4)(1)(8)	(Al,Zn)(Al,Cu,Zn)(Ag,Cu)
AlCu_Theta	CEF (SLN)	(0.667) (0.333)	(Al)(Ag,Al,Cu)
AlCu_Zeta	CEF (SLN)	(0.45)(0.55)	(Al)(Ag,Cu)
AlMg_Beta	CEF (ST2)	(89)(140)	(Mg)(Al)
AlMg_Eps	CEF (ST2)	(23)(30)	(Mg)(Al)

Name	Model	Lattice Size	Constituent
AlMg_Gamma	CEF (SLN)	(10)(24)(24)	(Mg)(Al,Mg)(Al,Mg)
AlMo3	CEF (SLN)	(1)(3)	(Al,Mo)(Al,Mo)
AlNb3	CEF (SLN)	(3)(1)	(Nb)(Al,Nb)
AlP	CEF (ST2)	(0.5)(0.5)	(Al)(P)
AlPd	CEF (SLN)	(1)(1)	(Al,Pd)(Pd,Va)
AlPd2	CEF (SLN)	(1)(2)	(Al,Pd)(Al,Pd)
AlPt	CEF (ST2)	(1)(1)	(Al)(Pt)
AlPt3	CEF (SLN)	(0.25)(0.75) (1)	(Al,Pt)(Al,Pt)(Va)
AlRe	CEF (ST2)	(1)(1)	(Al)(Re)
AlRe2	CEF (ST2)	(1)(2)	(Al)(Re)
AlSb	CEF (ST2)	(0.5)(0.5)	(Al)(Sb)
AlZr	CEF (ST2)	(1)(1)	(Al)(Zr)
AlZr2	CEF (ST2)	(1)(2)	(Al)(Zr)
AlZr3	CEF (ST2)	(1)(3)	(Al)(Zr)
Alpha-GePd5	CEF (ST2)	(1)(5)	(Ge)(Pd)
Alpha_AlFeSi	CEF (SLN)	(0.66)(0.19) (0.05)(0.1)	(Al)(Fe)(Si)(Al,Si)
Alpha_B	CEF (ST1)	(1)	(B)
Alpha_Bi2Mg3	CEF (SLN)	(2)(3)	(Bi,Va)(Mg)

Name	Model	Lattice Size	Constituent
Alpha_BiMn	CEF (ST2)	(0.5)(0.5)	(Bi)(Mn)
Alpha_Co2Si	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Alpha_Cr5Si3	CEF (ST2)	(5)(3)	(Cr)(Si)
Alpha_Cu2Se	CEF (SLN)	(2)(1)	(Cu,Se)(Se)
Alpha_CuSe	CEF (ST2)	(1)(1)	(Cu)(Se)
Alpha_InPd2	CEF (SLN)	(0.333) (0.667)	(In)(Ag,Pd)
Alpha_InPd3	CEF (SLN)	(0.25)(0.75)	(In)(Ag,Pd)
Alpha_IrZr	CEF (SLN)	(1)(1)	(Ir,Zr)(Zr)
Alpha_Mg3Sb2	CEF (SLN)	(0.6)(0.4)	(Mg)(Mg,Sb)
Alpha_Pd2Si	CEF (SLN)	(2)(1)	(Pd,Si)(Si)
Alpha_Si4Zr5	CEF (ST2)	(4)(5)	(Si)(Zr)
Alpha_SiZr	CEF (ST2)	(1)(1)	(Si)(Zr)
Alpha_TiMn	CEF (ST2)	(1)(1)	(Mn)(Ti)
As2O3	CEF (ST2)	(2)(3)	(Sb)(O)
Au11Mn4	CEF (ST2)	(11)(4)	(Au)(Mn)
Au13Mn4	CEF (ST2)	(13)(4)	(Au)(Mn)
Au2Bi	CEF (SLN)	(0.66667) (0.33333)	(Ag,Au)(Bi)
Au2Mn	CEF (ST2)	(2)(1)	(Au)(Mn)

Name	Model	Lattice Size	Constituent
Au2O3	CEF (SLN)	(2)(3)	(Ag,Au)(O)
Au2Pb	CEF (ST2)	(0.667) (0.333)	(Au)(Pb)
Au2Ti	CEF (ST2)	(0.6667) (0.3333)	(Au)(Ti)
Au33Mn9	CEF (ST2)	(33)(9)	(Au)(Mn)
Au3In	CEF (ST2)	(0.75)(0.25)	(Au)(In)
Au3Mn	CEF (ST2)	(3)(1)	(Au)(Mn)
Au3Sn	CEF (SLN)	(0.75)(0.25)	(Au)(Au,Sn)
Au4Cr	CEF (ST2)	(0.8)(0.2)	(Au)(Cr)
Au4In	CEF (ST2)	(0.77778) (0.22222)	(Au)(In)
Au4In3Sn3	CEF (SLN)	(0.4)(0.3)(0.3)	(Au)(In,Sn)(In,Sn)
Au4Mn	CEF (ST2)	(4)(1)	(Au)(Mn)
Au4Ti	CEF (SLN)	(0.8)(0.2)	(Au)(Au,Ti)
Au5Mn2	CEF (ST2)	(5)(2)	(Au)(Mn)
Au5Sn	CEF (SLN)	(0.84)(0.16)	(Au,Cu)(Sn)
Au5Zn3	CEF (ST2)	(0.625) (0.375)	(Au)(Zn)
Au7In3	CEF (ST2)	(0.7)(0.3)	(Au)(In)
AuB2	CEF (ST2)	(1)(2)	(Au)(B)

Name	Model	Lattice Size	Constituent
AuIn	CEF (SLN)	(0.5)(0.5)	(Au)(In,Sb,Sn)
AuIn2	CEF (SLN)	(0.33333) (0.66667)	(Au)(In,Sb,Sn)
AuIn_ALPHA1	CEF (SLN)	(1)	(Au,In,Sn)
AuIn_BETA	CEF (ST2)	(0.785) (0.215)	(Au)(In)
AuIn_GAMA	CEF (SLN)	(0.69231) (0.23077) (0.07692)	(Au)(Au,In)(In)
AuIn_PHY	CEF (SLN)	(0.5) (0.33333) (0.16667)	(Au)(Au,In)(In)
AuMn2	CEF (ST2)	(1)(2)	(Au)(Mn)
AuNi2Sn4	CEF (ST3)	(0.143) (0.286) (0.571)	(Au)(Ni)(Sn)
AuPb2	CEF (ST2)	(0.333) (0.667)	(Au)(Pb)
AuPb3	CEF (ST2)	(0.25)(0.75)	(Au)(Pb)
AuSb2	CEF (SLN)	(0.33333) (0.66667)	(Au)(In,Sb)
AuSe	CEF (ST2)	(0.5)(0.5)	(Au)(Se)
AuSn2	CEF (ST2)	(0.33333) (0.666667)	(Au)(Sn)

Name	Model	Lattice Size	Constituent
AuSn4	CEF (SLN)	(0.2)(0.8)	(Au,Ni)(In,Sn)
AuTi	CEF (SLN)	(0.5)(0.5)	(Au,Ti)(Ti,Va)
AuTi3	CEF (ST2)	(0.25)(0.75)	(Au)(Ti)
AuZn_ALF1	CEF (SLN)	(0.6)(0.2)(0.2)	(Au)(Au,Zn)(Zn)
AuZn_ALF2	CEF (ST2)	(0.75)(0.25)	(Au)(Zn)
AuZn_ALF3	CEF (SLN)	(0.64286) (0.25) (0.10714)	(Au)(Au,Zn)(Zn)
AuZn_Beta	CEF (SLN)	(0.5)(0.5)	(Au,Zn)(Au,Zn)
AuZn_DELT	CEF (ST2)	(0.44)(0.56)	(Au)(Zn)
AuZn_EPS1	CEF (SLN)	(1)	(Au,Zn)
AuZn_EPS2	CEF (ST2)	(0.15)(0.85)	(Au)(Zn)
AuZn_GAM1	CEF (SLN)	(0.15385) (0.15385) (0.23077) (0.46153)	(Au,Zn)(Au)(Au,Zn)(Zn)
AuZn_GAM2	CEF (ST2)	(0.25)(0.75)	(Au)(Zn)
B11	CEF (SLN)	(0.5)(0.5)	(Ag,Cu,Ni,Ti)(Ag,Cu,Ni,Ti)
B13P2	CEF (ST2)	(0.867) (0.133)	(B)(P)
B14P	CEF (ST2)	(0.933) (0.067)	(B)(P)

Name	Model	Lattice Size	Constituent
B2	CEF (SLN)	(1)(1)	(Ag,Al,Au,Be,Co,Cr,Cu,Fe,In, Ir,Mn,Ni,Pd,Pt,Re,Ru,Rh,Ti,Zn) (Al,Au,Be,Co,Cr,Cu,Fe,Ir,Mn, Ni,Pd,Pt,Re,Ru,Zn,Zr,Va)
B2O3	CEF (ST2)	(2)(3)	(B)(O)
B2Ti	CEF (ST2)	(2)(1)	(B)(Ti)
B4C	CEF (SLN)	(1)(1)	(B12,B11C)(B2,B2C,BC2)
B4Ti3	CEF (ST2)	(4)(3)	(B)(Ti)
BCT_A5	CEF (SLN)	(1)	(Ag,Al,Bi,Cu,Ge,In,Ni, Pb,Pd,Sb,Sn,Ti,Zn)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
BP	CEF (ST2)	(0.5)(0.5)	(B)(P)
BRONZE	CEF (SLN)	(2)(5)(1)	(V+4,V+5)(O-2)(Va)
BTi	CEF (ST2)	(1)(1)	(B)(Ti)
B_BeO	CEF (ST2)	(1)(1)	(Be)(O)
B_phase	CEF (SLN)	(0.11)(0.69) (0.2)	(Au)(Au,Cu)(Sn)
Bcc	CEF (SLN)	(1)(3)	(Ag,Al,Au,B,Be,Bi,Co,Cr,Cu,Fe, Ge,In,Ir,Mg,Mn,Mo,Nb,Ni,Os, P,Pb,Pd,Pt,Re,Rh,Ru,S,Sb, Si,Sn,Ti,V,Zn,Zr)(C,O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Ag,Al,Be,Cu,Fe,Mg,Pd,Pt,Re, Ru,Ti,Zr)(Ag,Al,Be,Cu,Fe,Mg,

Name	Model	Lattice Size	Constituent
			Pd,Pt,Re,Ru,Ti,Zr)(Va)
Be3Co	CEF (ST2)	(0.75)(0.25)	(Be)(Co)
Be7Co	CEF (ST2)	(0.875) (0.125)	(Be)(Co)
Beta	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
Beta1_Ni3Si	CEF (ST2)	(0.763) (0.237)	(Ni)(Si)
Beta2_Ni3Si	CEF (ST2)	(3)(1)	(Ni)(Si)
Beta3_Ni3Si	CEF (ST2)	(3)(1)	(Ni)(Si)
Beta_AlFeSi	CEF (SLN)	(0.598) (0.152)(0.1) (0.15)	(Al)(Fe)(Si)(Al,Si)
Beta_B	CEF (SLN)	(1)(0.129)	(B,Cu,Si,Zr)(C,Va)
Beta_Bi2Mg3	CEF (SLN)	(1)(3)(6)	(Bi)(Bi,Va)(Mg)
Beta_BiMn	CEF (ST2)	(0.481) (0.519)	(Bi)(Mn)
Beta_Co2Si	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Beta_Cu2Se	CEF (SLN)	(2)(1)	(Cu,Se)(Se)
Beta_CuSe	CEF (ST2)	(1)(1)	(Cu)(Se)
Beta_InPd2	CEF (ST2)	(0.34)(0.66)	(In)(Pd)
Beta_InPd3	CEF (ST2)	(0.26)(0.74)	(In)(Pd)

Name	Model	Lattice Size	Constituent
Beta_IrZr	CEF (SLN)	(1)(1)	(Ir,Zr)(Ir,Zr)
Beta_Mg3Sb2	CEF (SLN)	(0.4)(0.5)(0.1)	(Mg,Sb)(Mg,Sb)(Mg)
Beta_Pd2Si	CEF (SLN)	(2)(1)	(Pd,Si)(Si)
Beta_Si4Zr5	CEF (ST2)	(4)(5)	(Si)(Zr)
Beta_SiZr	CEF (ST2)	(1)(1)	(Si)(Zr)
Beta_TiMn	CEF (ST2)	(0.515) (0.485)	(Mn)(Ti)
Bi2S3	CEF (ST2)	(2)(3)	(Bi)(S)
Bi3In5	CEF (ST2)	(0.375) (0.625)	(Bi)(In)
Bi3Ni	CEF (ST2)	(0.75)(0.25)	(Bi)(Ni)
BiIn	CEF (ST2)	(0.5)(0.5)	(Bi)(In)
BiIn2	CEF (ST2)	(0.333333) (0.666667)	(Bi)(In)
BiIn_BEA	CEF (SLN)	(1)	(Bi,In,Pb,Sn)
BiNi	CEF (SLN)	(1)(1)(1)	(Bi)(Ni)(Bi,Cu,Ni,Va)
C11	CEF (SLN)	(2)(1)	(Pd,Ti)(Pd,Ti)
C2V3	CEF (ST2)	(2)(3)	(C)(V)
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Au,Bi,Co,Cr,Cu,Fe,Mn, Mo,Nb,Ni,Pd,Pt,Os,Ru,Si,Sn, Ti,V,Zn)(C,Va)
CUB_A13	CEF (SLN)	(1)(1)	(Ag,Al,Bi,Cr,Cu,Co,Fe,Ge,

Name	Model	Lattice Size	Constituent
			Mn,Mo,Nb,Ni,Pd,Pt,Os,Ru, Si,Sn,Ti,V,Zn)(C,Va)
C_phase	CEF (SLN)	(0.6667) (0.3333)	(Au,Cu)(Sn)
Cementite	CEF (SLN)	(3)(1)	(Co,Cr,Fe,Ni)(B,C)
Chi	CEF (SLN)	(24)(10)(24)	(Mo,Re)(Mo,Nb,Re)(Nb,Re)
Co11Zr2	CEF (ST2)	(11)(2)	(Co)(Zr)
Co23Zr6	CEF (ST2)	(23)(6)	(Co)(Zr)
Co2P	CEF (SLN)	(2)(1)	(Co,Ni)(P)
Co3Ge	CEF (ST2)	(0.75)(0.25)	(Co)(Ge)
Co3Mo	CEF (ST2)	(3)(1)	(Co)(Mo)
Co3Si	CEF (ST2)	(0.75)(0.25)	(Co)(Si)
Co3Sn2	CEF (SLN)	(1)(1)(0.5) (0.5)	(Co)(Sn)(Co,Va)(Co,Va)
Co3V	CEF (ST2)	(3)(1)	(Co)(V)
Co4Zn	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
Co5Ge2	CEF (ST2)	(0.714) (0.286)	(Co)(Ge)
Co5Ge7	CEF (ST2)	(0.417) (0.583)	(Co)(Ge)
Co7Nb2	CEF (ST2)	(7)(2)	(Co)(Nb)

Name	Model	Lattice Size	Constituent
CoFe3Re	CEF (ST3)	(0.2)(0.6)(0.2)	(Co)(Fe)(Re)
CoGe	CEF (SLN)	(0.5)(0.5)	(Co,Ge)(Co,Ge)
CoGe2	CEF (ST2)	(0.333) (0.667)	(Co)(Ge)
CoIn2	CEF (ST2)	(0.3333) (0.6667)	(Co)(In)
CoIn3	CEF (ST2)	(0.25)(0.75)	(Co)(In)
CoP	CEF (ST2)	(0.5)(0.5)	(Co)(P)
CoSb	CEF (SLN)	(0.3333) (0.3333) (0.3333)	(Sb)(Co,Va)(Co,Va)
CoSb2	CEF (ST2)	(0.3333) (0.6667)	(Co)(Sb)
CoSb3	CEF (ST2)	(0.25)(0.75)	(Co)(Sb)
CoSi	CEF (SLN)	(0.5)(0.5)	(Co,Si)(Co,Si)
CoSi2	CEF (ST2)	(1)(2)	(Co)(Si)
CoSn	CEF (ST2)	(0.5)(0.5)	(Co)(Sn)
CoSn2	CEF (ST2)	(0.333) (0.667)	(Co)(Sn)
CoSn3	CEF (ST2)	(0.25)(0.75)	(Co)(Sn)
CoTi2	CEF (ST2)	(1)(2)	(Co)(Ti)
CoV3	CEF (ST2)	(1)(3)	(Co)(V)

Name	Model	Lattice Size	Constituent
CoZn14	CEF (ST2)	(0.0714286) (0.928571)	(Co)(Zn)
CoZn7	CEF (ST2)	(0.125) (0.875)	(Co)(Zn)
CoZr2	CEF (ST2)	(1)(2)	(Co)(Zr)
CoZr3	CEF (ST2)	(1)(3)	(Co)(Zr)
Corundum	CEF (SLN)	(2)(1)(3)	(Al+3,Cr+2,Cr+3,Fe+2,Fe+3, Ti+3,V+3,V+4,Va) (Cr+3,Fe+3,Ni+2,Va)(O-2)
Cr11Ge19	CEF (ST2)	(0.367) (0.633)	(Cr)(Ge)
Cr11Ge8	CEF (ST2)	(0.579) (0.421)	(Cr)(Ge)
Cr2B	CEF (ST2)	(0.667) (0.333)	(Cr)(B)
Cr2Os	CEF (ST2)	(2)(1)	(Cr)(Os)
Cr2Pd3	CEF (ST2)	(0.4)(0.6)	(Cr)(Pd)
Cr3B4	CEF (ST2)	(0.4286) (0.5714)	(Cr)(B)
Cr3C2	CEF (ST2)	(3)(2)	(Cr)(C)
Cr3Ge	CEF (SLN)	(0.75)(0.25)	(Cr,Ge)(Cr,Ge)
Cr3Ir	CEF (SLN)	(3)(1)	(Cr,Ir)(Cr,Ir)

Name	Model	Lattice Size	Constituent
Cr3Mn5	CEF (ST2)	(3)(5)	(Cr)(Mn)
Cr3Os	CEF (ST2)	(3)(1)	(Cr)(Os)
Cr3Pt	CEF (SLN)	(3)(1)	(Cr,Pt)(Cr,Pt)
Cr3Rh	CEF (ST2)	(3)(1)	(Cr)(Rh)
Cr3Ru	CEF (ST2)	(0.685) (0.315)	(Cr)(Ru)
Cr3Si	CEF (SLN)	(3)(1)	(Cr,Ni,Si)(Cr,Si)
Cr5B3	CEF (ST2)	(0.625) (0.375)	(Cr)(B)
Cr5Ge3	CEF (SLN)	(0.625) (0.375)	(Cr,Ge)(Cr,Ge)
Cr5Ge3_LT	CEF (SLN)	(0.625) (0.375)	(Cr,Ge)(Cr,Ge)
CrB4	CEF (ST2)	(0.2)(0.8)	(Cr)(B)
CrGe	CEF (ST2)	(0.5)(0.5)	(Cr)(Ge)
CrPd	CEF (ST2)	(0.5)(0.5)	(Cr)(Pd)
CrSb	CEF (ST2)	(0.5)(0.5)	(Cr)(Sb)
CrSb2	CEF (ST2)	(0.3333) (0.6667)	(Cr)(Sb)
CrSi2	CEF (SLN)	(1)(2)	(Cr,Si)(Cr,Si)
CrZn17	CEF (ST2)	(0.0556) (0.9444)	(Cr)(Zn)

Name	Model	Lattice Size	Constituent
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
Cu1.75S	CEF (ST2)	(1.75)(1)	(Cu)(S)
Cu1.93S	CEF (ST2)	(1.93)(1)	(Cu)(S)
Cu10Sb3	CEF (ST2)	(0.77)(0.23)	(Cu)(Sb)
Cu10Sn3	CEF (SLN)	(1)	(Cu,Sn)
Cu10Zr7	CEF (ST2)	(10)(7)	(Cu)(Zr)
Cu11In9	CEF (SLN)	(0.55)(0.45)	(Ag,Cu)(In)
Cu15Si4	CEF (SLN)	(0.789474) (0.210526)	(Cu,Zn)(Si)
Cu16In9	CEF (ST2)	(0.64)(0.36)	(Cu)(In)
Cu17Sb3	CEF (ST2)	(0.85)(0.15)	(Cu)(Sb)
Cu19Si6	CEF (ST2)	(0.76)(0.24)	(Cu)(Si)
Cu2In3Sn	CEF (ST3)	(0.33333) (0.5) (0.16667)	(Cu)(In)(Sn)
Cu2Mg	CEF (SLN)	(1)(2)	(Cu,Mg)(Cu,Mg)
Cu2O	CEF (SLN)	(2)(1)	(Ag,Cu)(O)
Cu2P7	CEF (ST2)	(2)(7)	(Cu)(P)
Cu2S_H	CEF (ST2)	(2)(1)	(Cu)(S)
Cu2S_L	CEF (ST2)	(2)(1)	(Cu)(S)
Cu2Sb	CEF (ST2)	(0.67)(0.33)	(Cu)(Sb)

Name	Model	Lattice Size	Constituent
Cu2SnTi	CEF (ST3)	(2)(1)(1)	(Cu)(Sn)(Ti)
Cu2Ti	CEF (SLN)	(0.667) (0.333)	(Cu,Ni)(Ti)
Cu33Si7	CEF (ST2)	(0.825) (0.175)	(Cu)(Si)
Cu3BiSe3	CEF (ST3)	(3)(1)(3)	(Cu)(Bi)(Se)
Cu3Ni27Sn10	CEF (ST3)	(0.075) (0.675)(0.26)	(Cu)(Ni)(Sn)
Cu3P	CEF (ST2)	(3)(1)	(Cu)(P)
Cu3Pd	CEF (SLN)	(0.75)(0.25) (1)	(Cu,Pd)(Cu,Pd)(Va)
Cu3Pd_1	CEF (SLN)	(0.75)(0.25) (1)	(Cu,Pd)(Cu,Pd)(Va)
Cu3Pd_2	CEF (SLN)	(0.75)(0.25) (1)	(Cu,Pd)(Cu,Pd)(Va)
Cu3Sb	CEF (ST2)	(0.75)(0.25)	(Cu)(Sb)
Cu3Se2	CEF (ST2)	(3)(2)	(Cu)(Se)
Cu3Sn	CEF (SLN)	(3)(1)	(Ag,Cu,Sn)(Cu,In,Sn,Zn)
Cu3Ti2	CEF (SLN)	(0.6)(0.4)	(Ag,Cu)(Ti)
Cu41Sn11	CEF (SLN)	(41)(11)	(Cu,Sn)(Cu,In,Sn)
Cu4Sb	CEF (ST2)	(0.8)(0.2)	(Cu)(Sb)
Cu4Ti	CEF (SLN)	(0.8)(0.2)	(Ag,Cu,Ni,Ti)(Cu,Ni,Ti)

Name	Model	Lattice Size	Constituent
Cu4Ti3	CEF (SLN)	(0.571) (0.429)	(Ag,Cu)(Ti)
Cu51Zr14	CEF (ST2)	(51)(14)	(Cu)(Zr)
Cu56Si11	CEF (SLN)	(0.835821) (0.164179)	(Cu,Zn)(Si)
Cu5Zr	CEF (ST2)	(5)(1)	(Cu)(Zr)
Cu6Sn5L	CEF (SLN)	(1)(1)(1)	(Ag,Au,Cu)(Cu,Sn,Va)(Sn)
Cu77In23	CEF (SLN)	(0.77)(0.23)	(Cu)(In,Sn)
Cu7In3	CEF (SLN)	(0.7)(0.3)	(Cu)(In,Sn)
Cu8Zr3	CEF (ST2)	(8)(3)	(Cu)(Zr)
Cu9BiSe6	CEF (ST3)	(9)(1)(6)	(Cu)(Bi)(Se)
CuBi3Se5	CEF (ST3)	(1)(3)(5)	(Cu)(Bi)(Se)
CuBiSe2	CEF (ST3)	(1)(1)(2)	(Cu)(Bi)(Se)
CuIn_Eta	CEF (SLN)	(0.545) (0.122) (0.333)	(Cu)(Ag,Cu,In,Sn)(In,Sn)
CuIn_Gamma	CEF (SLN)	(0.654) (0.115) (0.231)	(Ag,Cu)(Ag,Cu,In)(In,Sn)
CuMg2	CEF (ST2)	(0.33333) (0.66667)	(Cu)(Mg)
CuNiTi	CEF (SLN)	(0.666667) (0.333333)	(Cu,Ni)(Ti)

Name	Model	Lattice Size	Constituent
CuNiTi_B19	CEF (SLN)	(0.5)(0.5)	(Cu,Ni,Va)(Cu,Ni,Ti)
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuP2	CEF (ST2)	(1)(2)	(Cu)(P)
CuPd	CEF (SLN)	(1)(1)	(Cu,Pd)(Cu,Pd)
CuS	CEF (ST2)	(1)(1)	(Cu)(S)
CuSbSe2	CEF (ST3)	(0.25)(0.25) (0.5)	(Cu)(Sb)(Se)
CuSe2	CEF (ST2)	(1)(2)	(Cu)(Se)
CuSiTi	CEF (ST3)	(1)(1)(1)	(Cu)(Si)(Ti)
CuSn3Ti5	CEF (ST3)	(5)(3)(1)	(Ti)(Sn)(Cu)
CuSnTi	CEF (ST3)	(1)(1)(1)	(Cu)(Sn)(Ti)
CuSn_Gamma	CEF (SLN)	(1)	(Ag,Cu,Ni,Sn)
CuZn_BETA	CEF (SLN)	(1)	(Cu,Sn,Zn)
CuZn_Eps	CEF (SLN)	(1)	(Ag,Al,Cu,Sn,Zn)
CuZr	CEF (ST2)	(0.5)(0.5)	(Cu)(Zr)
CuZr2	CEF (ST2)	(1)(2)	(Cu)(Zr)
D0_19	CEF (SLN)	(0.75)(0.25)	(Al,Cu,Ni,Sn,Ti) (Al,Ni,Sn,Ti)
D0_24	CEF (SLN)	(0.75)(0.25) (0.5)	(Pd,Pt,Zr)(Pd,Pt,Zr)(Va)
D_Bi2O3	CEF (ST2)	(2)(3)	(Bi)(O)

Name	Model	Lattice Size	Constituent
Delta	CEF (ST2)	(0.117647) (0.882353)	(Co)(Zn)
DeltaP_Sb3Zn4	CEF (ST2)	(3.094) (3.906)	(Sb)(Zn)
Delta_AlFeSi	CEF (SLN)	(5)(1)	(Al,Si)(Fe)
Delta_Ni2Si	CEF (ST2)	(2)(1)	(Ni)(Si)
Delta_Sb3Zn4	CEF (ST2)	(3.087) (3.913)	(Sb)(Zn)
Diamond	CEF (SLN)	(1)	(Ag,Al,Au,B,C,Ge,Nb,Sb,Si, Sn,Ti,Zn)
Digenite	CEF (SLN)	(2)(1)(1)	(Cu,Fe,Pb,Zn,Va)(Cu,Va)(S)
Disorder	CEF (SLN)	(1)(1)	(Mn,Pd)(Va)
Do24	CEF (SLN)	(1)	(Au,Sn)
Eps_CuGe	CEF (ST2)	(0.765) (0.235)	(Cu)(Ge)
Epsilon	CEF (ST2)	(0.375) (0.625)	(Ge)(Ni)
Epsilon_Ni3Si2	CEF (ST2)	(3)(2)	(Ni)(Si)
Eta_CuGe	CEF (ST2)	(0.75)(0.25)	(Cu)(Ge)
Eta_MC	CEF (SLN)	(1)(1)	(Mo)(C,Va)
Eta_Sb2Zn3	CEF (ST2)	(2)(3)	(Sb)(Zn)
Fcc	CEF (SLN)	(1)(1)	(Ag,Al,Au,B,Be,Bi,Co,Cr,Cu,

Name	Model	Lattice Size	Constituent
			Fe,Ge,In,Ir,Mg,Mn,Mo,Nb,Ni,Os,P,Pb,Pd,Pt,Re,Rh,Ru,S,Sb,Si,Sn,Ti,V,Zn,Zr)(C,O,Va)
Fe2Si	CEF (ST2)	(0.666667) (0.333333)	(Fe)(Si)
Fe3Sn2	CEF (ST2)	(3)(2)	(Fe)(Sn)
Fe4Re	CEF (SLN)	(4)(1)	(Fe,Re)(Fe,Re)
Fe5Mn2Pd6	CEF (ST3)	(0.38461) (0.15385) (0.46154)	(Fe)(Mn)(Pd)
Fe5Sn3	CEF (ST2)	(5)(3)	(Fe)(Sn)
FeB	CEF (ST2)	(1)(1)	(Fe)(B)
FeNiSi_Tau	CEF (SLN)	(8)(2)	(Fe,Ni)(Si)
FeP	CEF (SLN)	(1)(1)	(Cr,Fe)(P)
FePd	CEF (SLN)	(0.5)(0.5)	(Fe,Pd)(Fe,Pd)
FeS	CEF (SLN)	(1)(1)	(Cr,Cu,Fe,Mn,Ni,Va)(S)
FeS2	CEF (ST2)	(1)(2)	(Fe)(S)
FeSb	CEF (SLN)	(0.3333) (0.3333) (0.3333)	(Sb)(Fe,Va)(Fe,Va)
FeSb2	CEF (ST2)	(0.3333) (0.6667)	(Fe)(Sb)

Name	Model	Lattice Size	Constituent
FeSi	CEF (ST2)	(1)(1)	(Fe)(Si)
FeSi2_H	CEF (ST2)	(0.3)(0.7)	(Fe)(Si)
FeSi2_L	CEF (ST2)	(0.333333) (0.666667)	(Fe)(Si)
FeSn	CEF (ST2)	(1)(1)	(Fe)(Sn)
FeSn2	CEF (ST2)	(1)(2)	(Fe)(Sn)
FeTi	CEF (ST2)	(1)(1)	(Fe)(Ti)
FeZn13	CEF (SLN)	(0.072) (0.928)	(Fe,Zn)(Fe,Zn)
FeZn3	CEF (SLN)	(0.25)(0.75)	(Fe,Zn)(Fe,Zn)
FeZn7	CEF (SLN)	(0.125) (0.875)	(Fe,Zn)(Fe,Zn)
FeZr2	CEF (SLN)	(1)(2)	(Al,Fe,Zr)(Zr)
FeZr3	CEF (SLN)	(1)(3)	(Al,Fe,Zr)(Fe,Zr)
Gamma	CEF (SLN)	(4)(1)(8)	(Ag,Ni,Si,Zn)(Ag,Cu,Ni,Zn) (Cu,Zn)
Gamma_AlFeSi	CEF (ST3)	(0.635) (0.205)(0.16)	(Al)(Fe)(Si)
Gamma_BeX	CEF (SLN)	(1)	(Be,Co,Ni)
Gamma_BeX'	CEF (SLN)	(1)	(Be,Co,Ni)
Gamma_CuSe	CEF (ST2)	(1)(1)	(Cu)(Se)
Gamma_Ni3Ge	CEF (ST2)	(0.256)	(Ge)(Ni)

Name	Model	Lattice Size	Constituent
		(0.744)	
Gamma_Ni5Si2	CEF (ST2)	(5)(2)	(Ni)(Si)
Gammabrass	CEF (SLN)	(1)	(Ag,Al,Cu,Fe,Ni,Si,Zn)
Gas	GAS	(1)	(Ag,Al,AlO,AlO2,Al2,Al2O, Al2O2,Al2O3,C1O1,C1O2, Fe,FeO,FeO2,Fe2,In,In2, InO,In2O,Ir,IrO2,IrO3,Mg, Mg2,MgO,Mn,O,O2,O3,P, PO,PO2,P4O6,P4O10,Pb, Pb2,PbO,Pb2O2,Pb3O3, Pb4O4,Pb5O5,Pb6O6,S,S2, S3,S4,S5,S6,S7,S8,S2O,SO, SO2,SO3,Se,Se2,Se3,Se4, Se5,Se6,Se7,Se8,SeO,SeO2, Sn,Sn2,SnO,SnO2,Si,Si2,Si3, SiO,SiO2,Ti,TiO,TiO2,Zn,Zr, Zr2,ZrO,ZrO2)
Ge23Mo13	CEF (ST2)	(23)(13)	(Ge)(Mo)
Ge2Mn5	CEF (SLN)	(0.286) (0.714)	(Ge,Mn)(Ge,Mn)
Ge2Mn5_LT	CEF (ST2)	(0.286) (0.714)	(Ge)(Mn)
Ge2Mo	CEF (ST2)	(2)(1)	(Ge)(Mo)
Ge2Pt	CEF (ST2)	(0.667) (0.333)	(Ge)(Pt)

Name	Model	Lattice Size	Constituent
Ge2Pt3	CEF (ST2)	(0.4)(0.6)	(Ge)(Pt)
Ge2Ti	CEF (ST2)	(2)(1)	(Ge)(Ti)
Ge31V17	CEF (ST2)	(0.646) (0.354)	(Ge)(V)
Ge3Mn5	CEF (ST2)	(0.375) (0.625)	(Ge)(Mn)
Ge3Mo5	CEF (ST2)	(3)(5)	(Ge)(Mo)
Ge3Pt2	CEF (ST2)	(0.6)(0.4)	(Ge)(Pt)
Ge3Ru2	CEF (ST2)	(0.6)(0.4)	(Ge)(Ru)
Ge3Ru2_alpha	CEF (ST2)	(0.6)(0.4)	(Ge)(Ru)
Ge3Ti5	CEF (ST2)	(3)(5)	(Ge)(Ti)
Ge3V5	CEF (ST2)	(0.375) (0.625)	(Ge)(V)
Ge5Ti6	CEF (ST2)	(5)(6)	(Ge)(Ti)
Ge8Mn11	CEF (ST2)	(0.421) (0.579)	(Ge)(Mn)
Ge8Pd21	CEF (ST2)	(8)(21)	(Ge)(Pd)
Ge8V11	CEF (ST2)	(0.421) (0.579)	(Ge)(V)
Ge9Pd25	CEF (ST2)	(9)(25)	(Ge)(Pd)
GeMn2	CEF (SLN)	(0.333) (0.667)	(Ge,Mn)(Ge,Mn)

Name	Model	Lattice Size	Constituent
GeMn3	CEF (SLN)	(0.25)(0.75)	(Ge,Mn)(Mn)
GeMn3_LT	CEF (ST2)	(0.25)(0.75)	(Ge)(Mn)
GeMo3	CEF (ST2)	(1)(3)	(Ge)(Mo)
GeNi3	CEF (SLN)	(0.75)(0.25) (1)	(Ge,Ni)(Ge,Ni)(Va)
GeP	CEF (ST2)	(1)(1)	(Ge)(P)
GePd	CEF (ST2)	(1)(1)	(Ge)(Pd)
GePd2	CEF (ST2)	(1)(2)	(Ge)(Pd)
GePd3	CEF (ST2)	(1)(3)	(Ge)(Pd)
GePt	CEF (ST2)	(0.5)(0.5)	(Ge)(Pt)
GePt2	CEF (ST2)	(0.333) (0.667)	(Ge)(Pt)
GePt3	CEF (SLN)	(0.25)(0.75)	(Ge,Pt)(Pt)
GeRu	CEF (ST2)	(0.5)(0.5)	(Ge)(Ru)
GeV3	CEF (ST2)	(0.25)(0.75)	(Ge)(V)
Graphite	CEF (SLN)	(1)	(B,C)
HEXAGONAL_A8	CEF (ST1)	(1)	(Se)
H_Sigma_CrMn	CEF (SLN)	(8)(4)(18)	(Mn)(Cr)(Cr,Mn)
Halite	CEF (SLN)	(1)(1)	(Al+3,Co+2,Cr+3,Fe+2,Fe+3, Mg+2,Mn+2,Mn+3,Ni+2,V, V+2,V+3,Va)(O-2,Va)

Name	Model	Lattice Size	Constituent
Hcp	CEF (SLN)	(1)(0.5)	(Ag,Al,Au,B,Be,Bi,Co,Cr,Cu,Fe,Ge,In,Ir,Mg,Mn,Mo,Nb,Ni,Os,Pb,Pd,Pt,Re,Rh,Ru,Sb,Si,Sn,Ti,V,Zn,Zr)(C,O,Va)
Heusler	CEF (SLN)	(3)(1)	(Cu,Zn)(Ti)
In2Ir	CEF (SLN)	(0.6667) (0.3333)	(In,Ir)(In,Ir)
In2Pt	CEF (ST2)	(2)(1)	(In)(Pt)
In2Pt3_alpha	CEF (ST2)	(2)(3)	(In)(Pt)
In2Pt3_beta	CEF (SLN)	(2)(3)	(In,Pt)(In,Pt)
In3Ir_HT	CEF (SLN)	(0.75)(0.25)	(In)(In,Ir)
In3Ir_LT	CEF (SLN)	(0.75)(0.25)	(In)(In,Ir)
In3Pd2	CEF (SLN)	(0.6)(0.4)	(Ag,In)(Pd)
In3Pd5	CEF (ST2)	(0.375) (0.625)	(In)(Pd)
In3Pt2	CEF (ST2)	(3)(2)	(In)(Pt)
In5Pt6	CEF (SLN)	(5)(6)	(In,Pt)(In,Pt)
In7Pd3	CEF (ST2)	(0.71)(0.29)	(In)(Pd)
In7Pt3	CEF (ST2)	(7)(3)	(In)(Pt)
In9Pt13	CEF (SLN)	(9)(13)	(In)(In,Pt)
InP	CEF (ST2)	(0.5)(0.5)	(In)(P)

Name	Model	Lattice Size	Constituent
InPb_BEA	CEF (SLN)	(1)	(In,Pb)
InPt	CEF (SLN)	(1)(1)	(In,Pt)(In,Pt)
InPt2	CEF (ST2)	(1)(2)	(In)(Pt)
InPt3	CEF (SLN)	(0.25)(0.75) (1)	(In,Pt)(In,Pt)(Va)
InSb	CEF (ST2)	(0.5)(0.5)	(In)(Sb)
InSn_BETA	CEF (SLN)	(1)	(In,Sn)
InSn_GAMMA	CEF (SLN)	(1)	(Bi,In,Sb,Sn)
Ir2Zr	CEF (ST2)	(2)(1)	(Ir)(Zr)
Ir3Zr	CEF (SLN)	(3)(1)	(Ir,Zr)(Ir,Zr)
Ir3Zr5	CEF (ST2)	(3)(5)	(Ir)(Zr)
IrZr2	CEF (ST2)	(1)(2)	(Ir)(Zr)
IrZr3	CEF (ST2)	(1)(3)	(Ir)(Zr)
Kappa	CEF (SLN)	(3)(1)(0.565)	(Co,Fe,Mn)(Al)(C)
L10	CEF (SLN)	(0.5)(0.5)	(Al,Fe,Mn,Ni,Pt,Ti) (Al,Fe,Mn,Ni,Pt,Ti)
L12	CEF (SLN)	(0.75)(0.25)	(Al,Co,Cr,Cu,Fe,Ge,Ir,Mn, Ni,Pd,Pt,Re,Ru,Si,Ti) (Al,Co,Cr,Cu,Fe,Ge,Ir,Mn, Ni,Pd,Pt,Re,Ru,Si,Ti)
L12_S	CEF (SLN)	(0.75)(0.25) (1)	(Mn,Pd)(Mn,Pd)(Va)

Name	Model	Lattice Size	Constituent
LAVES_PHASE_BETA	CEF (SLN)	(6)(4)(2)	(Cr,Ti)(Cr,Ti)(Cr)
LAVES_PHASE_GAMMA	CEF (SLN)	(6)(4)(2)	(Cr,Ti)(Cr,Ti)(Cr)
Laves_C14	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Mg,Mn,Mo,Nb,Re,Ti,Zn,Zr) (Co,Cr,Fe,Mg,Mn,Mo,Nb,Ti,Zn,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Be,Co,Cr,Cu,Fe,Mo,Nb,Ni,Ti,Zr) (Be,Co,Cr,Cu,Fe,Mo,Nb,Ni,Ti,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Co,Cr,Cu,Fe,Ni,Ti,Zr) (Co,Cr,Cu,Fe,Nb,Ni,Ti,Zr)
Liquid	CEF (SLN)	(1)	(Ag,Al,Au,B,Be,Bi,Bi2Mg3,Bi2Se3,C,Co,Co2P,Cr,CrS,Cr3Ge,CrSe,Cu,Cu2S,Cu2Se,Cu3P,Fe,FeS,FeSe,Ge,Ge3Mn5,GePd2,In,Ir,Mg,Mg2Sn,Mn,MnS,MnSe,Mo,Nb,Ni,NiS,Ni2P,O,Os,P,Pb,PbS,PbSe,Pd,Pt,PtSn,Re,Rh,Ru,S,Sb,Se,SeNi,SeSn,Se2Si,SeZn,Si,Sn,Ti,V,Zn,ZnS,Zr,Al2O3,B2O3,BeO,Be2O2,Bi2/5O3/5,CoO,Co2O3,Cr2/3O,CuO,Cu2O,

Name	Model	Lattice Size	Constituent
			Cu2O3,FeO,FeO3/2,Ge1/2O, In2/3O,MgO,MnO,Mn2/3O, MoO2,MoO3,NbO,NbO2, Nb2O5,NiO,P4O10,P4O6, PbO,SO3,Sb4O6,SiO2,SnO, SnO2,TiO,TiO3/2,TiO2,VO, VO2,VO3/2,VO5/2,Zr1/2O)
M23C6	CEF (SLN)	(20)(3)(6)	(Cr,Fe,Mn,Ni)(Cr,Fe,Mn,Ni)(C)
M2B	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Ni)(B)
M2P	CEF (SLN)	(2)(1)	(Co,Cr,Cu,Fe,Mn,Ni)(P)
M2Si	CEF (SLN)	(2)(1)	(Cr,Ni)(Si)
M3P	CEF (SLN)	(3)(1)	(Co,Cr,Cu,Fe,Mn,Ni)(P)
M5C2	CEF (ST2)	(5)(2)	(Mn)(C)
M6Sn5	CEF (SLN)	(1)(1)(1)	(Ag,Au,Cu,Ni)(Cu,Sn,Ni,Zn,Va) (In,Sn,Zn)
M7C3	CEF (SLN)	(7)(3)	(Cr,Fe,Mn,Ni,Re)(C)
MB	CEF (SLN)	(1)(1)	(Co,Fe,Ni)(B)
MB2	CEF (SLN)	(1)(2)	(Al,Cr)(B,Va)
MB_B33	CEF (SLN)	(0.5)(0.5)	(Cr,Fe,Ni)(B,Va)
MONO_S	CEF (ST1)	(1)	(S)
MSi	CEF (SLN)	(1)(1)	(Cr,Fe,Ni)(Si)
MTi2	CEF (SLN)	(1)(2)	(Ag,Al,Cu,Ni,Zn)(Cr,Ti)

Name	Model	Lattice Size	Constituent
M_Ni4B3	CEF (ST2)	(0.564) (0.436)	(Ni)(B)
Mg2C3	CEF (ST2)	(0.4)(0.6)	(Mg)(C)
Mg2Ge	CEF (SLN)	(2)(1)	(Mg)(Ge,Si)
Mg2Ni	CEF (ST2)	(2)(1)	(Mg)(Ni)
Mg2Si	CEF (ST2)	(0.5)(0.25) (0.25)	(Mg)(Si)(Va)
Mg2Sn	CEF (ST2)	(0.5)(0.25) (0.25)	(Mg)(Sn)(Va)
Mg2Zn11	CEF (ST2)	(5)(6)(2)	(Zn)(Zn)(Mg)
Mg2Zn3	CEF (ST2)	(2)(3)	(Mg)(Zn)
Mg7Zn3	CEF (ST2)	(51)(20)	(Mg)(Zn)
MgC2	CEF (ST2)	(0.333333) (0.666667)	(Mg)(C)
MgNi2	CEF (SLN)	(1)(2)	(Mg,Ni)(Mg,Ni)
MgZn	CEF (ST2)	(12)(13)	(Mg)(Zn)
Mn11Si19	CEF (ST2)	(11)(19)	(Mn)(Si)
Mn19Sn6	CEF (ST2)	(19)(6)	(Mn)(Sn)
Mn2Sn	CEF (ST2)	(2)(1)	(Mn)(Sn)
Mn2Ti_C14	CEF (SLN)	(2)(1)	(Mn,Ti)(Mn,Ti)
Mn2Zr	CEF (SLN)	(2)(1)	(Mn)(Zr,Va)

Name	Model	Lattice Size	Constituent
Mn3O4_A	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3O4_B	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3P2	CEF (ST2)	(3)(2)	(Mn)(P)
Mn3Si	CEF (ST2)	(3)(1)	(Mn)(Si)
Mn3Ti	CEF (ST2)	(3)(1)	(Mn)(Ti)
Mn4Ti	CEF (ST2)	(0.815) (0.185)	(Mn)(Ti)
Mn5Si3	CEF (SLN)	(2)(3)(3)	(Cr,Fe,Si,Ti)(Cr,Si,Sn,Ti) (Cr,Fe,Ti)
Mn5Si3_L	CEF (ST2)	(5)(3)	(Mn)(Si)
Mn6Si	CEF (ST2)	(0.85)(0.15)	(Mn)(Si)
Mn9Si2	CEF (ST2)	(0.825) (0.175)	(Mn)(Si)
MnNi2	CEF (SLN)	(1)(2)	(Mn,Ni)(Ni)
MnP	CEF (ST2)	(1)(1)	(Mn)(P)
MnP4	CEF (ST2)	(1)(4)	(Mn)(P)
MnPd2	CEF (ST2)	(1)(2)	(Mn)(Pd)
MnPt7	CEF (ST2)	(1)(7)	(Mn)(Pt)
MnS	CEF (SLN)	(1)(1)	(Cr,Fe,Mn)(S)
MnS2	CEF (ST2)	(1)(2)	(Mn)(S)
MnSi	CEF (ST2)	(1)(1)	(Mn)(Si)

Name	Model	Lattice Size	Constituent
MnSn2	CEF (ST2)	(1)(2)	(Mn)(Sn)
MnX_L10	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Mn,Ni,Pd) (Co,Cr,Fe,Mn,Ni,Pd)
MnZn9	CEF (ST2)	(0.1)(0.9)	(Mn)(Zn)
Mo3C2	CEF (ST2)	(3)(2)	(Mo)(C)
Mo3Pt	CEF (SLN)	(0.75)(0.25)	(Mo,Pt)(Mo,Pt)
Mo3Si	CEF (SLN)	(3)(1)(3)	(Mo)(Mo,Si)(Va)
Mo3Sn	CEF (ST2)	(3)(1)	(Mo)(Sn)
Mo4O11	CEF (ST2)	(0.266667) (0.733333)	(Mo)(O)
Mo5Si3	CEF (SLN)	(0.5)(0.125) (0.375)	(Mo)(Mo,Si)(Mo,Si)
Mo6Pt	CEF (SLN)	(3)(1)	(Mo,Pt)(Mo,Pt)
Mo7C3	CEF (ST2)	(7)(3)	(Mo)(C)
Mo8O23	CEF (ST2)	(0.258064) (0.741935)	(Mo)(O)
Mo9O26	CEF (ST2)	(0.257143) (0.742857)	(Mo)(O)
MoC	CEF (ST2)	(1)(1)	(Mo)(C)
MoNi	CEF (SLN)	(0.428571) (0.357143) (0.214286)	(Ni)(Mo,Ni)(Mo)

Name	Model	Lattice Size	Constituent
MoNi3	CEF (SLN)	(0.75)(0.25)	(Mo,Ni)(Mo,Ni)
MoNi4	CEF (ST2)	(0.2)(0.8)	(Mo)(Ni)
MoO3	CEF (ST2)	(1)(3)	(Mo)(O)
MoPt	CEF (SLN)	(0.5)(0.5)	(Mo,Pt)(Mo,Pt)
MoPt2	CEF (SLN)	(0.3333) (0.6667)	(Mo,Pt)(Mo,Pt)
MoSi2	CEF (ST2)	(1)(2)	(Mo)(Si)
MoSn	CEF (ST2)	(1)(1)	(Mo)(Sn)
MoSn2	CEF (ST2)	(1)(2)	(Mo)(Sn)
Mu	CEF (SLN)	(7)(2)(4)	(Co,Fe,Mo,Mn,Nb)(Mo,Nb) (Co,Fe,Mo,Nb)
Nb2O5	CEF (ST2)	(2)(5)	(Nb)(O)
Nb2Pt	CEF (SLN)	(2)(1)	(Nb,Pt)(Nb,Pt)
Nb3Ge	CEF (SLN)	(0.75)(0.25)	(Nb)(Ge,Nb,Va)
Nb3Pt	CEF (SLN)	(3)(1)	(Nb,Pt)(Nb,Pt)
Nb3Si	CEF (ST2)	(0.75)(0.25)	(Nb)(Si)
Nb3Sn	CEF (SLN)	(3)(1)	(Nb,Sn)(Nb,Sn)
Nb5Ge3	CEF (SLN)	(0.5)(0.125) (0.375)	(Nb)(Ge,Nb)(Ge,Va)
Nb5Si3_alpha	CEF (SLN)	(0.625) (0.375)	(Nb,Si)(Si)

Name	Model	Lattice Size	Constituent
Nb5Si3_beta	CEF (SLN)	(0.5)(0.125) (0.375)	(Nb)(Nb,Si)(Nb,Si)
Nb6Sn5	CEF (SLN)	(24)(16)(4)	(Nb)(Sn)(Nb,Sn)
NbGe2	CEF (SLN)	(0.333) (0.667)	(Ge,Nb)(Ge,Nb)
NbO	CEF (ST2)	(1)(1)	(Nb)(O)
NbO2	CEF (ST2)	(1)(2)	(Nb)(O)
NbPt	CEF (ST2)	(1)(1)	(Nb)(Pt)
NbPt2	CEF (ST2)	(1)(2)	(Nb)(Pt)
NbPt3	CEF (ST2)	(1)(3)	(Nb)(Pt)
NbSi2	CEF (SLN)	(0.333) (0.667)	(Nb,Si)(Si)
NbSn2	CEF (ST2)	(1)(2)	(Nb)(Sn)
Ni10Zr7	CEF (ST2)	(10)(7)	(Ni)(Zr)
Ni11Zr9	CEF (ST2)	(11)(9)	(Ni)(Zr)
Ni12P5_H	CEF (ST2)	(12)(5)	(Ni)(P)
Ni12P5_L	CEF (SLN)	(12)(5)	(Co,Ni)(P)
Ni13In9	CEF (SLN)	(1)(1)(1)	(Ni,Va)(Ni)(In)
Ni21Zr8	CEF (ST2)	(21)(8)	(Ni)(Zr)
Ni2Ge	CEF (ST2)	(0.335) (0.665)	(Ge)(Ni)

Name	Model	Lattice Size	Constituent
Ni2In	CEF (ST2)	(2)(1)	(Ni)(In)
Ni2In3	CEF (ST2)	(2)(3)	(Ni)(In)
Ni2In_ZET	CEF (SLN)	(1)(1)(1)	(Ni,Va)(Ni)(In,Ni)
Ni2V	CEF (ST2)	(0.6667) (0.3333)	(Ni)(V)
Ni3B	CEF (ST2)	(0.75)(0.25)	(Ni)(B)
Ni3In	CEF (ST2)	(3)(1)	(Ni)(In)
Ni3In7	CEF (ST2)	(3)(7)	(Ni)(In)
Ni3S2	CEF (ST2)	(0.6)(0.4)	(Ni)(S)
Ni3Se2_H	CEF (ST2)	(0.6)(0.4)	(Ni)(Se)
Ni3Se2_L	CEF (ST2)	(0.6)(0.4)	(Ni)(Se)
Ni3Sn2	CEF (SLN)	(0.5)(0.25) (0.25)	(Ni,Sn)(Au,Ni)(Au,Ni)
Ni3Sn4	CEF (SLN)	(0.4286) (0.5714)	(Cu,Ni)(Ni,Sn)
Ni3Ti	CEF (SLN)	(0.75)(0.25)	(Ni,Ti)(Ni,Ti)
Ni3V	CEF (SLN)	(3)(1)	(Ni,V)(Ni,V)
Ni3Zr	CEF (ST2)	(3)(1)	(Ni)(Zr)
Ni5Ge2	CEF (ST2)	(0.28)(0.72)	(Ge)(Ni)
Ni5Ge3	CEF (SLN)	(1)(1)(1)	(Ge)(Ni)(Ni,Va)
Ni5P2_H	CEF (ST2)	(5)(2)	(Ni)(P)

Name	Model	Lattice Size	Constituent
Ni5P2_L	CEF (ST2)	(5)(2)	(Ni)(P)
Ni5P4	CEF (ST2)	(5)(4)	(Ni)(P)
Ni5Sb2	CEF (ST2)	(0.714) (0.286)	(Ni)(Sb)
Ni5Si2B	CEF (ST3)	(4.29)(2) (1.43)	(Ni)(Si)(B)
Ni5Zr	CEF (SLN)	(5)(1)	(Ni,Zr)(Zr,Va)
Ni6Si2B	CEF (ST3)	(6)(2)(1)	(Ni)(Si)(B)
Ni7Zr2	CEF (ST2)	(7)(2)	(Ni)(Zr)
NiB	CEF (ST2)	(0.5)(0.5)	(Ni)(B)
NiGe	CEF (ST2)	(0.5)(0.5)	(Ge)(Ni)
NiIn	CEF (ST2)	(1)(1)	(Ni)(In)
NiIn_DEL	CEF (SLN)	(1)(1)	(In,Ni)(Ni,Va)
NiP	CEF (ST2)	(1)(1)	(Ni)(P)
NiP2	CEF (ST2)	(1)(2)	(Ni)(P)
NiP3	CEF (ST2)	(1)(3)	(Ni)(P)
NiSb	CEF (ST2)	(0.5)(0.5)	(Ni)(Sb)
NiSb2	CEF (ST2)	(0.3333) (0.6667)	(Ni)(Sb)
NiSe	CEF (ST2)	(0.5)(0.5)	(Se)(Ni)
NiSe2	CEF (ST2)	(0.6667)	(Se)(Ni)

Name	Model	Lattice Size	Constituent
		(0.3333)	
NiSi	CEF (ST2)	(1)(1)	(Ni)(Si)
NiSi2	CEF (ST2)	(1)(2)	(Ni)(Si)
NiSnZn_T1	CEF (SLN)	(0.36)(0.38) (0.26)	(Ni,Sn,Va)(Ni,Sn)(Zn,Va)
NiSnZn_T2	CEF (SLN)	(0.55)(0.26) (0.19)	(Ni,Va)(Sn)(Sn,Zn,Va)
NiSnZn_T3	CEF (SLN)	(0.482) (0.204) (0.314)	(Ni,Va)(Sn)(Sn,Zn,Va)
NiSnZn_T4	CEF (SLN)	(0.505)(0.39) (0.105)	(Ni,Sn,Va)(Sn,Zn)(Sn,Zn,Va)
NiTi2	CEF (SLN)	(1)(2)	(Cu,Ni)(Ti)
NiV3	CEF (ST2)	(0.25)(0.75)	(Ni)(V)
NiZn8	CEF (ST2)	(1)(8)	(Ni)(Zn)
NiZn_Beta1	CEF (SLN)	(1)(1)	(Cu,Ni,Zn)(Ni,Zn)
NiZr	CEF (ST2)	(1)(1)	(Ni)(Zr)
NiZr2	CEF (ST2)	(1)(2)	(Ni)(Zr)
ORTHORHOMBIC_S	CEF (ST1)	(1)	(S)
O_Ni4B3	CEF (ST2)	(0.586) (0.414)	(Ni)(B)
Os2Si3	CEF (ST2)	(0.4)(0.6)	(Os)(Si)

Name	Model	Lattice Size	Constituent
OsSi	CEF (ST2)	(0.5)(0.5)	(Os)(Si)
OsSi2	CEF (ST2)	(0.333) (0.667)	(Os)(Si)
P3Sn4	CEF (ST2)	(3)(4)	(P)(Sn)
P4O10	CEF (ST2)	(4)(10)	(P)(O)
PSi	CEF (ST2)	(1)(1)	(P)(Si)
Pb12O17	CEF (ST2)	(12)(17)	(Pb)(O)
Pb12O19	CEF (ST2)	(12)(19)	(Pb)(O)
Pb2Pd	CEF (ST2)	(0.667) (0.333)	(Pb)(Pd)
Pb3O4	CEF (ST2)	(3)(4)	(Pb)(O)
Pb3Pd5_alpha	CEF (ST2)	(0.375) (0.625)	(Pb)(Pd)
Pb3Pd5_beta	CEF (SLN)	(1)(1)(1)	(Pd)(Pb)(Pd,Va)
Pb3Pd5_gamma	CEF (SLN)	(1)(1)(1)	(Pd)(Pb)(Pd,Va)
Pb9Pd13	CEF (ST2)	(0.41)(0.59)	(Pb)(Pd)
PbO_alpha	CEF (ST2)	(1)(1)	(Pb)(O)
PbO_beta	CEF (ST2)	(1)(1)	(Pb)(O)
PbPd	CEF (ST2)	(0.5)(0.5)	(Pb)(Pd)
PbPd3	CEF (SLN)	(0.75)(0.25)	(Pd)(Pb,Pd)
PbS	CEF (ST2)	(1)(1)	(Pb)(S)

Name	Model	Lattice Size	Constituent
Pd11Zr9	CEF (ST2)	(11)(9)	(Pd)(Zr)
Pd14Si3	CEF (ST2)	(14)(3)	(Pd)(Si)
Pd15Si4	CEF (ST2)	(15)(4)	(Pd)(Si)
Pd16S7	CEF (ST2)	(0.696) (0.304)	(Pd)(S)
Pd17Se15	CEF (ST2)	(17)(15)	(Pd)(Se)
Pd19Si10	CEF (ST2)	(19)(10)	(Pd)(Si)
Pd20Sb7	CEF (ST2)	(20)(7)	(Pd)(Sb)
Pd20Sn13	CEF (SLN)	(0.6)(0.4)	(Pd,Sn)(Pd,Sn)
Pd21Si4	CEF (SLN)	(21)(4)	(Pd,Si)(Si)
Pd2Sb	CEF (ST2)	(2)(1)	(Pd)(Sb)
Pd2Sn	CEF (ST2)	(0.667) (0.333)	(Pd)(Sn)
Pd2Sn_gamma	CEF (SLN)	(1)(1)(1)	(Pd)(Sn)(Pd,Va)
Pd2Zn	CEF (ST2)	(2)(1)	(Pd)(Zn)
Pd2Zn9	CEF (SLN)	(2)(9)	(Pd,Zn)(Pd,Zn)
Pd34Se11	CEF (ST2)	(34)(11)	(Pd)(Se)
Pd39Si20	CEF (ST2)	(39)(20)	(Pd)(Si)
Pd3Bi	CEF (ST2)	(0.75)(0.25)	(Pd)(Bi)
Pd3S	CEF (ST2)	(0.75)(0.25)	(Pd)(S)

Name	Model	Lattice Size	Constituent
Pd3Sb	CEF (SLN)	(3)(1)	(Pd,Sb)(Sb)
Pd3Si	CEF (ST2)	(3)(1)	(Pd)(Si)
Pd3Sn	CEF (SLN)	(0.75)(0.25)	(Pd,Sn)(Pd,Sn)
Pd3Sn2_alpha	CEF (ST2)	(0.6)(0.4)	(Pd)(Sn)
Pd3Sn2_beta	CEF (ST2)	(0.6)(0.4)	(Pd)(Sn)
Pd3Sn2_delta	CEF (ST2)	(0.59)(0.41)	(Pd)(Sn)
Pd3Ti	CEF (ST2)	(3)(1)	(Pd)(Ti)
Pd3Ti2	CEF (ST2)	(3)(2)	(Pd)(Ti)
Pd4S	CEF (ST2)	(0.8)(0.2)	(Pd)(S)
Pd4Se_HT	CEF (ST2)	(4)(1)	(Pd)(Se)
Pd4Se_LT	CEF (ST2)	(4)(1)	(Pd)(Se)
Pd4Zr3	CEF (ST2)	(4)(3)	(Pd)(Zr)
Pd5Bi3	CEF (SLN)	(1)(1)	(Bi,Pd)(Va)
Pd5Sb2	CEF (ST2)	(5)(2)	(Pd)(Sb)
Pd5Sb3	CEF (SLN)	(5)(3)	(Pd,Sb)(Pd,Sb)
Pd5Si	CEF (ST2)	(5)(1)	(Pd)(Si)
Pd7Se2	CEF (ST2)	(7)(2)	(Pd)(Se)
Pd7Se4	CEF (ST2)	(7)(4)	(Pd)(Se)
Pd8Sb3	CEF (ST2)	(8)(3)	(Pd)(Sb)
Pd9Se2	CEF (ST2)	(9)(2)	(Pd)(Se)

Name	Model	Lattice Size	Constituent
Pd9Si2	CEF (ST2)	(9)(2)	(Pd)(Si)
PdBi	CEF (ST2)	(0.5)(0.5)	(Pd)(Bi)
PdBi2	CEF (ST2)	(0.334) (0.666)	(Pd)(Bi)
PdO	CEF (ST2)	(1)(1)	(Pd)(O)
PdS	CEF (ST2)	(0.5)(0.5)	(Pd)(S)
PdSb	CEF (ST2)	(1)(1)	(Pd)(Sb)
PdSb2	CEF (ST2)	(1)(2)	(Pd)(Sb)
PdSe	CEF (ST2)	(1)(1)	(Pd)(Se)
PdSe2	CEF (ST2)	(1)(2)	(Pd)(Se)
PdSi	CEF (ST2)	(1)(1)	(Pd)(Si)
PdSn	CEF (SLN)	(0.5)(0.5)	(Pd,Va)(Pd,Sn)
PdSn2	CEF (SLN)	(0.333) (0.667)	(Pd,Sn)(Sn)
PdSn3	CEF (SLN)	(0.25)(0.75)	(Pd)(Pd,Sn)
PdSn4	CEF (SLN)	(0.2)(0.8)	(Pd)(Pd,Sn)
PdTi	CEF (SLN)	(1)(1)	(Pd,Ti)(Pd,Ti)
PdTi3	CEF (ST2)	(1)(3)	(Pd)(Ti)
PdZn2	CEF (ST2)	(1)(2)	(Pd)(Zn)
PdZn_Beta	CEF (SLN)	(1)(1)	(Pd,Zn)(Pd,Zn)

Name	Model	Lattice Size	Constituent
PdZn_Beta1	CEF (SLN)	(1)(1)	(Pd,Zn)(Pd,Zn)
PdZn_Eta	CEF (ST2)	(0.09)(0.91)	(Pd)(Zn)
PdZr2	CEF (SLN)	(1)(1)(1)	(Pd)(Zr)(Pd,Zr)
PdZr_alpha	CEF (ST2)	(1)(1)	(Pd)(Zr)
PdZr_beta	CEF (ST2)	(1)(1)	(Pd)(Zr)
Pt10Zr7	CEF (ST2)	(10)(7)	(Pt)(Zr)
Pt17Si8_alpha	CEF (ST2)	(0.68)(0.32)	(Pt)(Si)
Pt17Si8_beta	CEF (ST2)	(0.68)(0.32)	(Pt)(Si)
Pt25Si7	CEF (ST2)	(0.782) (0.218)	(Pt)(Si)
Pt2B	CEF (ST2)	(2)(1)	(Pt)(B)
Pt2Si_alpha	CEF (ST2)	(0.667) (0.333)	(Pt)(Si)
Pt2Si_beta	CEF (ST2)	(0.667) (0.333)	(Pt)(Si)
Pt2Sn3	CEF (ST2)	(0.4)(0.6)	(Pt)(Sn)
Pt2V	CEF (SLN)	(0.667) (0.333)	(Pt,V)(Pt,V)
Pt3B	CEF (ST2)	(3)(1)	(Pt)(B)
Pt3B2	CEF (ST2)	(3)(2)	(Pt)(B)
Pt3Pb	CEF (ST2)	(1)(3)	(Pb)(Pt)

Name	Model	Lattice Size	Constituent
Pt3Sb	CEF (ST2)	(0.75)(0.25)	(Pt)(Sb)
Pt3Sb2	CEF (ST2)	(0.6)(0.4)	(Pt)(Sb)
Pt3Si_alpha	CEF (ST2)	(0.75)(0.25)	(Pt)(Si)
Pt3Si_beta	CEF (ST2)	(0.75)(0.25)	(Pt)(Si)
Pt3Sn	CEF (ST2)	(0.75)(0.25)	(Pt)(Sn)
Pt3V	CEF (SLN)	(0.75)(0.25)	(Pt,V)(Pt,V)
Pt3Zr5	CEF (SLN)	(3)(5)	(Pt,Zr)(Pt,Zr)
Pt4Zr	CEF (SLN)	(4)(1)	(Pt,Zr)(Pt,Zr)
Pt4Zr3	CEF (SLN)	(4)(3)	(Pt,Zr)(Pt,Zr)
Pt5Sb	CEF (SLN)	(0.833) (0.167)	(Pt,Sb)(Pt,Sb)
Pt5Si2	CEF (ST2)	(0.714) (0.286)	(Pt)(Si)
Pt6Si5	CEF (ST2)	(0.545) (0.455)	(Pt)(Si)
Pt7Sb	CEF (ST2)	(0.875) (0.125)	(Pt)(Sb)
PtPb	CEF (ST2)	(1)(1)	(Pb)(Pt)
PtPb4	CEF (ST2)	(4)(1)	(Pb)(Pt)
PtSb	CEF (ST2)	(0.5)(0.5)	(Pt)(Sb)
PtSb2	CEF (ST2)	(0.333) (0.667)	(Pt)(Sb)

Name	Model	Lattice Size	Constituent
PtSi	CEF (ST2)	(0.5)(0.5)	(Pt)(Si)
PtSn	CEF (ST2)	(0.5)(0.5)	(Pt)(Sn)
PtSn2	CEF (ST2)	(0.33333) (0.66667)	(Pt)(Sn)
PtSn4	CEF (ST2)	(0.2)(0.8)	(Pt)(Sn)
PtV	CEF (SLN)	(0.5)(0.5)	(Pt,V)(Pt,V)
PtV3	CEF (SLN)	(0.25)(0.75)	(Pt,V)(Pt,V)
PtZr_alpha	CEF (SLN)	(1)(1)	(Pt,Zr)(Pt,Zr)
Quartz	CEF (SLN)	(1)(2)	(Ge,Si)(O)
RED_P	CEF (ST1)	(1)	(P)
RHOMBOHEDRAL_A7	CEF (SLN)	(1)	(Ag,Al,Bi,Ge,In,Mn,Pb,Pd,Sb,Sn,Zn)
R_Al4Mn	CEF (ST2)	(461)(107)	(Al)(Mn)
R_Phase	CEF (SLN)	(27)(14)(12)	(Fe)(Mo)(Fe,Mo)
Re24Ti5	CEF (ST2)	(24)(5)	(Re)(Ti)
Re24Zr5	CEF (ST2)	(0.8276) (0.1724)	(Re)(Zr)
Re25Zr21	CEF (ST2)	(0.5435) (0.4565)	(Re)(Zr)
Re2O7	CEF (ST2)	(2)(7)	(Re)(O)
Re2Si	CEF (ST2)	(2)(1)	(Re)(Si)

Name	Model	Lattice Size	Constituent
Re3B	CEF (ST2)	(0.75)(0.25)	(Re)(B)
Re7B3	CEF (ST2)	(0.7)(0.3)	(Re)(B)
ReB2	CEF (SLN)	(1)(2)	(B,Re)(B)
ReO2	CEF (ST2)	(1)(2)	(Re)(O)
ReO3	CEF (ST2)	(1)(3)	(Re)(O)
ReSi	CEF (ST2)	(0.5)(0.5)	(Re)(Si)
ReSi2	CEF (SLN)	(1)(2)	(Re)(Si,Va)
ReTi	CEF (ST2)	(1)(1)	(Re)(Ti)
Rh2O3	CEF (ST2)	(2)(3)	(Rh)(O)
Ru2Si	CEF (ST2)	(0.6667) (0.3333)	(Ru)(Si)
Ru2Si3	CEF (ST2)	(0.4)(0.6)	(Ru)(Si)
Ru2Zr_C14	CEF (SLN)	(2)(1)	(Ru,Zr)(Ru,Zr)
Ru4Si3	CEF (ST2)	(0.5714) (0.4286)	(Ru)(Si)
RuSi	CEF (ST2)	(0.5)(0.5)	(Ru)(Si)
Rutile	CEF (SLN)	(1)(2)	(Ge+4,Ir+4,Mn+4,Os+4, Rh+4,Ru+4,Pb+4,Sn+4, Ti+3,Ti+4,V+4)(O-2,Va)
Sb2O3_B	CEF (ST2)	(2)(3)	(Sb)(O)
Sb2O4	CEF (ST2)	(2)(4)	(Sb)(O)

Name	Model	Lattice Size	Constituent
Sb2O5	CEF (ST2)	(2)(5)	(Sb)(O)
Sb2Se3	CEF (ST2)	(0.4)(0.6)	(Sb)(Se)
Sb2Sn3	CEF (ST2)	(2)(3)	(Sb)(Sn)
Sb3Zn4	CEF (SLN)	(3)(4)	(Sb)(Zn,Va)
SbSn	CEF (SLN)	(1)	(Pb,Sb,Sn)
SbZn	CEF (SLN)	(1)(1)	(Sb)(Zn,Va)
Se2Bi3	CEF (ST2)	(0.6)(0.4)	(Bi)(Se)
Se2Mn	CEF (ST2)	(1)(2)	(Mn)(Se)
Se2O5	CEF (ST2)	(2)(5)	(Se)(O)
Se3Bi2	CEF (ST2)	(1)	(Bi2Se3)
SeBi	CEF (ST2)	(0.5)(0.5)	(Bi)(Se)
SeCr	CEF (ST2)	(1)	(CrSe)
SeFe	CEF (ST2)	(1)	(FeSe)
SeMn	CEF (ST2)	(1)	(MnSe)
SeO2	CEF (ST2)	(1)(2)	(Se)(O)
SeO3	CEF (ST2)	(1)(3)	(Se)(O)
SePb	CEF (ST2)	(1)	(PbSe)
SeZn	CEF (ST2)	(1)	(SeZn)
Si2Ti	CEF (ST2)	(0.666667) (0.333333)	(Si)(Ti)

Name	Model	Lattice Size	Constituent
Si2V	CEF (ST2)	(0.666667) (0.333333)	(Si)(V)
Si2Zr	CEF (ST2)	(2)(1)	(Si)(Zr)
Si2Zr3	CEF (ST2)	(2)(3)	(Si)(Zr)
Si3V5	CEF (ST2)	(0.375) (0.625)	(Si)(V)
Si3Zr5	CEF (ST2)	(3)(5)	(Si)(Zr)
Si4Ti5	CEF (ST2)	(0.444444) (0.555556)	(Si)(Ti)
Si5V6	CEF (ST2)	(0.454545) (0.545455)	(Si)(V)
SiB3	CEF (ST2)	(0.25)(0.75)	(Si)(B)
SiB6	CEF (ST2)	(0.143) (0.857)	(Si)(B)
SiBN	CEF (SLN)	(61)(1)(8)	(B)(Si)(B,Si)
SiC	CEF (ST2)	(1)(1)	(Si)(C)
SiO_AM	CEF (ST2)	(1)(1)	(Si)(O)
SiSe	CEF (ST2)	(0.5)(0.5)	(Se)(Si)
SiSe2	CEF (ST2)	(1)	(Se2Si)
SiTi	CEF (ST2)	(0.5)(0.5)	(Si)(Ti)
SiTi3	CEF (ST2)	(0.25)(0.75)	(Si)(Ti)

Name	Model	Lattice Size	Constituent
SiV3	CEF (SLN)	(0.75)(0.25)	(Si,V)(Si,V)
SiZr2	CEF (ST2)	(1)(2)	(Si)(Zr)
SiZr3	CEF (ST2)	(1)(3)	(Si)(Zr)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Co,Fe,Mn,Ni,Re,Ru) (Cr,Fe,Mo,Nb,Re,V) (Al,Co,Cr,Fe,Mn,Mo,Nb, Ni,Re,Ru,V)
Sigma_MnMo	CEF (SLN)	(8)(4)(18)	(Mn)(Mo)(Mn,Mo)
Sigma_NbRe	CEF (SLN)	(10)(4)(16)	(Re)(Nb)(Nb,Re)
Sn2V	CEF (ST2)	(1)(2)	(V)(Sn)
Sn2Zr	CEF (ST2)	(2)(1)	(Sn)(Zr)
Sn3Ti2	CEF (ST2)	(0.6)(0.4)	(Sn)(Ti)
Sn3Zr5	CEF (SLN)	(5)(3)(1)	(Zr)(Sn)(Sn,Va)
Sn5Ti6	CEF (SLN)	(0.455) (0.545)	(Sn)(Cu,Ti)
SnSe	CEF (ST2)	(1)	(SeSn)
SnSe2	CEF (ST2)	(0.6667) (0.3333)	(Se)(Sn)
SnTi2	CEF (ST2)	(0.333) (0.667)	(Sn)(Ti)
SnV3	CEF (SLN)	(0.25)(0.75)	(Sn,V)(V)
SnZr4	CEF (SLN)	(3)(1)	(Sn,Zr)(Sn,Zr)

Name	Model	Lattice Size	Constituent
Spinel	CEF (SLN)	(1)(2)(2)(4)	(Al+3,Co+2,Cr+2,Cr+3,Fe+2, Fe+3,Ni+2)(Al+3,Co+3,Cr+3, Fe+2,Fe+3,Va)(Fe+2,Va)(O-2)
T1_CrNiSi	CEF (ST3)	(5)(5)(3)	(Cr)(Ni)(Si)
T2_CrNiSi	CEF (SLN)	(4)(3)	(Cr,Ni)(Si)
T3_CrNiSi	CEF (ST3)	(0.3)(0.5)(0.2)	(Cr)(Ni)(Si)
T4_CrNiSi	CEF (SLN)	(0.133) (0.533) (0.334)	(Cr)(Cr,Si)(Cr,Ni)
TETRAGONAL_A6	CEF (SLN)	(1)	(Bi,In,Pb,Pt,Sn,Zn)
Tau10_AlFeSi	CEF (ST3)	(0.6)(0.25) (0.15)	(Al)(Fe)(Si)
Tau11_AlFeSi	CEF (ST3)	(0.6538) (0.2308) (0.1154)	(Al)(Fe)(Si)
Tau1_AlFeSi	CEF (SLN)	(5)(3)	(Al,Si)(Fe)
Tau3_AlFeSi	CEF (ST3)	(0.55)(0.25) (0.2)	(Al)(Fe)(Si)
Tau7_AlFeSi	CEF (SLN)	(0.75)(0.25)	(Al,Si)(Fe)
Tau8_AlFeSi	CEF (SLN)	(0.66667) (0.33333)	(Al,Si)(Fe)
Theta_CuGe	CEF (ST2)	(0.735) (0.265)	(Cu)(Ge)

Name	Model	Lattice Size	Constituent
Theta_Ni2Si	CEF (SLN)	(1)(1)(1)	(Ni)(Ni,Va)(Si)
Ti10O19	CEF (ST2)	(10)(19)	(Ti)(O)
Ti20O39	CEF (ST2)	(20)(39)	(Ti)(O)
Ti2Bi	CEF (ST2)	(0.3333) (0.6667)	(Bi)(Ti)
Ti2Bi3	CEF (ST2)	(0.6)(0.4)	(Bi)(Ti)
Ti3Bi	CEF (ST2)	(0.25)(0.75)	(Bi)(Ti)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti3Pt	CEF (SLN)	(3)(1)	(Pt,Ti)(Pt,Ti)
Ti3Sb	CEF (ST2)	(3)(1)	(Ti)(Sb)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti4Pt3	CEF (ST2)	(3)(4)	(Pt)(Ti)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti7O13	CEF (ST2)	(7)(13)	(Ti)(O)
Ti8Bi9	CEF (ST2)	(0.5294) (0.4706)	(Bi)(Ti)
Ti8O15	CEF (ST2)	(8)(15)	(Ti)(O)
Ti9O17	CEF (ST2)	(9)(17)	(Ti)(O)
TiBi2	CEF (ST2)	(0.6667)	(Bi)(Ti)

Name	Model	Lattice Size	Constituent
		(0.3333)	
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)
TiPt3	CEF (SLN)	(1)(3)	(Pt,Ti)(Pt)
TiPt8	CEF (ST2)	(8)(1)	(Pt)(Ti)
TiPt_alpha	CEF (SLN)	(1)(1)	(Pt,Ti)(Pt,Ti)
TiPt_beta	CEF (SLN)	(1)(1)	(Pt,Ti)(Pt,Ti)
TiSb	CEF (ST2)	(1)(1)	(Ti)(Sb)
TiSb2	CEF (ST2)	(1)(2)	(Ti)(Sb)
Tridymite	CEF (ST2)	(1)(2)	(Si)(O)
U_Al4Mn	CEF (ST2)	(4)(1)	(Al)(Mn)
V2O5	CEF (ST2)	(2)(5)	(V)(O)
V2O_SS	CEF (SLN)	(1)(0.5)	(V)(O,Va)
V2Zr	CEF (ST2)	(2)(1)	(V)(Zr)
V3O5_HT	CEF (ST2)	(2)(1)(5)	(V+3)(V+4)(O-2)
V3O5_LT	CEF (ST2)	(2)(1)(5)	(V+3)(V+4)(O-2)
V3O7	CEF (ST2)	(2)(1)(7)	(V+5)(V+4)(O-2)
V4O7	CEF (ST2)	(2)(2)(7)	(V+3)(V+4)(O-2)
V4Zn5	CEF (ST2)	(4)(5)	(V)(Zn)
V52O64	CEF (ST2)	(52)(64)	(V)(O)
V5O9	CEF (ST2)	(2)(3)(9)	(V+3)(V+4)(O-2)

Name	Model	Lattice Size	Constituent
V6O11	CEF (ST2)	(2)(4)(11)	(V+3)(V+4)(O-2)
V6O13	CEF (ST2)	(2)(4)(13)	(V+5)(V+4)(O-2)
V7O13	CEF (ST2)	(2)(5)(13)	(V+3)(V+4)(O-2)
V8O15	CEF (ST2)	(2)(6)(15)	(V+3)(V+4)(O-2)
VO2	CEF (SLN)	(1)(2)	(Mo,V,Zr)(O)
VZn16	CEF (ST2)	(1)(16)	(V)(Zn)
VZn3	CEF (ST2)	(1)(3)	(V)(Zn)
WHITE_P	CEF (ST1)	(1)	(P)
Y2O3_cub	CEF (SLN)	(2)(3)(1)	(In+3,Mn+3,Va)(O-2)(O-2,Va)
Y2O3_hex	CEF (SLN)	(2)(3)(1)	(Zr+4)(O-2)(O-2,Va)
Zeta_Sb2Zn3	CEF (ST2)	(2.025) (2.975)	(Sb)(Zn)
Zn10Ti	CEF (ST2)	(10)(1)	(Zn)(Ti)
Zn15Ti	CEF (ST2)	(15)(1)	(Zn)(Ti)
Zn22Zr	CEF (ST2)	(0.956522) (0.0434783)	(Zn)(Zr)
Zn2Ti	CEF (ST2)	(2)(1)	(Zn)(Ti)
Zn2Zr	CEF (ST2)	(0.666667) (0.333333)	(Zn)(Zr)
Zn2Zr3	CEF (ST2)	(0.4)(0.6)	(Zn)(Zr)
Zn39Zr5	CEF (ST2)	(0.886364)	(Zn)(Zr)

Name	Model	Lattice Size	Constituent
		(0.113636)	
Zn3P2	CEF (ST2)	(3)(2)	(Zn)(P)
Zn3Ti	CEF (ST2)	(3)(1)	(Zn)(Ti)
Zn3Zr_h	CEF (ST2)	(0.75)(0.25)	(Zn)(Zr)
Zn3Zr_l	CEF (ST2)	(0.75)(0.25)	(Zn)(Zr)
Zn5Ti	CEF (ST2)	(5)(1)	(Zn)(Ti)
ZnO	CEF (ST2)	(1)(1)	(Zn)(O)
ZnP2	CEF (ST2)	(1)(2)	(Zn)(P)
ZnTi	CEF (ST2)	(1)(1)	(Zn)(Ti)
ZnZr	CEF (ST2)	(0.5)(0.5)	(Zn)(Zr)
ZnZr2	CEF (ST2)	(0.333333) (0.666667)	(Zn)(Zr)
Zr2Au	CEF (ST2)	(2)(1)	(Zr)(Au)
Zr2O	CEF (ST2)	(2)(1)	(Zr)(O)
Zr3Au	CEF (ST2)	(3)(1)	(Zr)(Au)
Zr3Au2	CEF (ST2)	(3)(2)	(Zr)(Au)
Zr3O	CEF (ST2)	(3)(1)	(Zr)(O)
Zr6O	CEF (ST2)	(6)(1)	(Zr)(O)
Zr7Au10	CEF (ST2)	(7)(10)	(Zr)(Au)
ZrAu	CEF (SLN)	(1)(1)	(Au,Zr)(Au,Zr)

Name	Model	Lattice Size	Constituent
ZrAu2	CEF (ST2)	(1)(2)	(Zr)(Au)
ZrAu3	CEF (ST2)	(1)(3)	(Zr)(Au)
ZrAu4	CEF (ST2)	(1)(4)	(Zr)(Au)
ZrB	CEF (ST2)	(1)(1)	(Zr)(B)
ZrB12	CEF (ST2)	(1)(12)	(Zr)(B)
ZrB2	CEF (ST2)	(1)(2)	(Zr)(B)
ZrO2_Cubic	CEF (SLN)	(1)(2)	(Zr)(O,Va)
ZrO2_Tetragonal	CEF (SLN)	(1)(2)	(Zr)(O,Va)
a_Co5Ge3	CEF (ST2)	(0.625) (0.375)	(Co)(Ge)
a_ZnS	CEF (ST2)	(1)(1)	(Zn)(S)
alpha-NbPt	CEF (ST2)	(43)(57)	(Nb)(Pt)
alpha_AlAu2	CEF (SLN)	(1)(2)	(Al)(Al,Au)
b_Co5Ge3	CEF (SLN)	(0.125)(0.5) (0.375)	(Co,Va)(Co)(Co,Ge)
b_ZnS	CEF (ST2)	(1)(1)	(Zn)(S)
beta_AlAu2	CEF (SLN)	(1)(2)	(Al)(Al,Au)
beta_AlAu4	CEF (SLN)	(1)(4)	(Al,Au)(Au)
gamma_AlAu2	CEF (SLN)	(1)(2)	(Al,Au)(Al,Au)