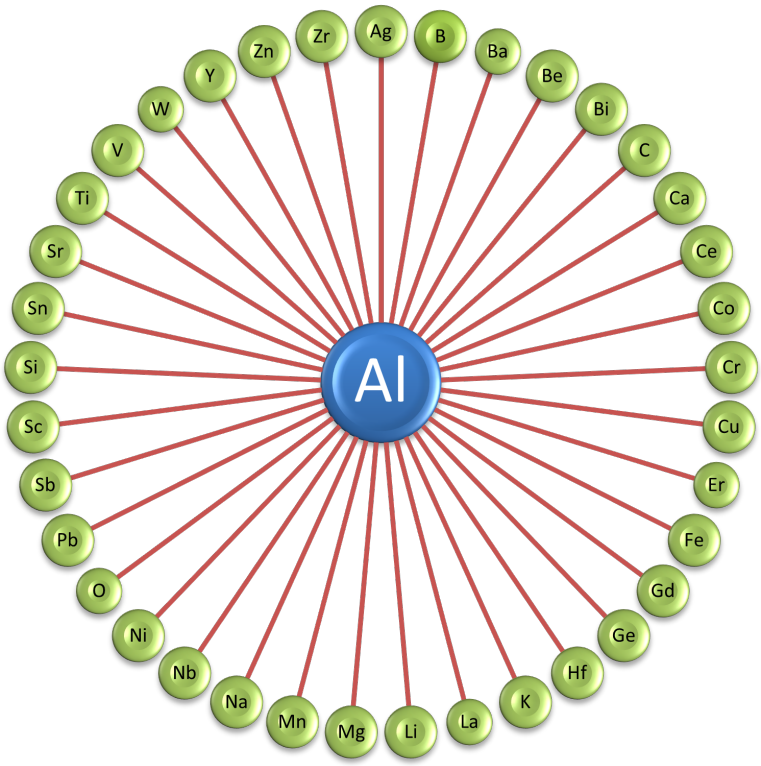
Pandat™ 2024

Database Manual

CompuTherm LLC

PanAluminum

Database for multi-component Aluminum-rich casting and wrought alloys



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (38)

Total of **38** components are included in the database as listed here:

Major alloying elements: **Al**, Cu, Fe, Mg, Mn, Si and Zn

Minor alloying elements: Ag, B, Ba, Be, Bi, C, Ca, Ce, Co, Cr, Er, Gd, Ge, Hf, K, La, Li, Na, Nb, Ni, O, Pb, Sb, Sc, Sn, Sr, Ti, V, W, Y, and Zr

1.2 Suggested Composition Range

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 binary and ternary systems have been fully assessed and they are covered in the full range from 0-100% as given in Section 1.5 .

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Al	80 ~ 100
Cu	0 ~ 5.5
Fe	0 ~ 2.0
Mg	0 ~ 7.6
Mn	0 ~ 1.2
Si	0 ~ 17.5
Zn	0 ~ 8.1
Others	0 ~ 1

1.3 What is new in PanAl2024

- Addition of the component O and the O-X binary systems
- Update the stability of the Al15_FeMn3Si2 phase
- Improved the La-B, and Al-Sc-Si systems

1.4 Phases

Total of **1150** phases are included in the current database. The names and thermodynamic models of some phases are given in Table 1.2. Information on all the other phases is listed in PanAl2024: List of Phases. Users can also view it through TDB viewer of Pandat™ .

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
Ag5Zn8	(2)(2)(3)(6)	(Ag,Zn)(Ag)(Ag,Zn)(Ag,Zn)
AgMg3	(0.23)(0.77)	(Ag,Cu)(Al,Mg)
AgMg4	(0.2)(0.8)	(Ag,Cu)(Al,Mg)
Al18Mg3V2	(18)(3)(2)	(Al)(Mg)(V)
Al2Fe	(2)(1)	(Al)(Cr,Fe,Mn)
Al2LiMg	(0.53)(0.33) (0.14)	(Al)(Li)(Mg)
Al2W	(2)(1)	(Al)(W)
Al5Fe2	(5)(2)	(Al)(Cr,Fe,Mn)
Al5Fe4	(1)	(Al,Fe,Mn)
Al8FeMg3Si6	(8)(3)(1)(6)	(Al)(Mg)(Fe)(Si)

Name	Lattice Size	Constituent
Al8FeMnSi2	(16)(2)(2)(3)	(Al)(Fe)(Mn)(Si)
AlCu_Theta	(0.667)(0.333)	(Al)(Ag,Al,Cu)
AlMg_Gamma	(10)(24)(24)	(Ca,Mg)(Al,Cu,Li,Mg,Zn)(Al,Cu,Mg,Zn)
Alpha_AlFeSi	(0.66)(0.19) (0.05)(0.1)	(Al)(Fe)(Si)(Al,Si)
Cu3Mg2Si	(3)(2)(1)	(Cu)(Mg)(Si)
Delta_AlFeSi	(5)(1)	(Al,Si)(Fe)
Fcc	(1)(1)	(Ag,Al,Ba,Be,Bi,Ca,Ce,Co,Cr,Cu,Er,Fe, Gd,Ge,Hf,K,La,Li,Mg,Mn,Na,Nb,Ni,Pb, Sb,Sc,Si,Sn,Sr,Ti,V,W,Y,Zn,Zr)(B,C,O,Va)
Gamma_AlFeSi	(0.635)(0.205) (0.16)	(Al)(Fe)(Si)
Li2MgSi	(0.5)(0.25) (0.25)	(Li)(Mg)(Si)
LiMg2Si	(0.5)(0.25) (0.25)	(Mg)(Si)(Li,Va)
Mu	(7)(2)(4)	(Co,Fe,Mn,Nb,W)(Nb,W)(Co,Fe,Nb,W)
NbSn2	(1)(2)	(Nb)(Sn)
Q_Al5Cu2Mg8Si6	(0.2381) (0.0952)(0.381) (0.2857)	(Al)(Cu)(Mg)(Si)
T10_AlFeSi	(0.6)(0.25)	(Al)(Fe)(Si)

Name	Lattice Size	Constituent
	(0.15)	
T11_AlFeSi	(0.6538) (0.2308) (0.1154)	(Al)(Fe)(Si)

1.5 Assessed Subsystems

A total of 537 subsystems, including 455 binary and 82 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 (455)

Ag-Al(10)	Ag-B(10)	Ag-Bi(10)	Ag-C(10)	Ag-Ca(10)	Ag-Ce(10)	Ag-Co(10)
Ag-Cr(10)	Ag-Cu(10)	Ag-Er(10)	Ag-Fe(10)	Ag-Gd(10)	Ag-Ge(10)	Ag-La(10)
Ag-Mg(10)	Ag-Na(10)	Ag-Ni(10)	Ag-O(5)	Ag-Pb(10)	Ag-Sb(10)	Ag-Sc(10)
Ag-Si(10)	Ag-Sn(10)	Ag-Sr(10)	Ag-Ti(10)	Ag-V(10)	Ag-W(10)	Ag-Y(10)
Ag-Zn(10)	Ag-Zr(10)	Al-B(10)	Al-Ba(10)	Al-Be(10)	Al-Bi(10)	Al-C(10)
Al-Ca(10)	Al-Ce(10)	Al-Co(10)	Al-Cr(10)	Al-Cu(10)	Al-Er(10)	Al-Fe(10)
Al-Gd(10)	Al-Ge(10)	Al-Hf(10)	Al-K(10)	Al-La(10)	Al-Li(10)	Al-Mg(10)
Al-Mn(10)	Al-Na(10)	Al-Nb(10)	Al-Ni(10)	Al-O(10)	Al-Pb(10)	Al-Sb(10)
Al-Sc(10)	Al-Si(10)	Al-Sn(10)	Al-Sr(10)	Al-Ti(10)	Al-V(10)	Al-W(10)
Al-Y(10)	Al-Zn(10)	Al-Zr(10)	B-C(10)	B-Ca(10)	B-Co(10)	B-Cr(10)
B-Cu(10)	B-Er(10)	B-Fe(10)	B-Hf(10)	B-La(10)	B-Mg(10)	B-Mn(10)
B-Nb(10)	B-Ni(10)	B-O(10)	B-Sc(10)	B-Si(10)	B-Sn(10)	B-Sr(10)
B-Ti(10)	B-V(10)	B-W(10)	B-Zr(10)	Ba-Be(10)	Ba-Bi(10)	Ba-Ca(10)
Ba-Cr(10)	Ba-Cu(10)	Ba-Fe(10)	Ba-Gd(10)	Ba-Ge(10)	Ba-La(10)	Ba-Li(10)
Ba-Mg(10)	Ba-Mn(10)	Ba-Ni(10)	Ba-O(10)	Ba-Pb(10)	Ba-Sc(10)	Ba-Si(10)

Ba-Sr(10) Ba-Ti(10) Ba-V(10) Ba-Y(10) Ba-Zn(10) Be-O(10) Be-Si(10)
Bi-Cr(10) Bi-Cu(10) Bi-Er(10) Bi-Fe(10) Bi-Gd(10) Bi-Ge(10) Bi-La(10)
Bi-Mg(10) Bi-Mn(10) Bi-Ni(10) Bi-O(10) Bi-Pb(10) Bi-Sb(10) Bi-Si(10)
Bi-Sn(10) Bi-Ti(10) Bi-Zn(10) C-Ce(10) C-Co(10) C-Cr(10) C-Fe(10)
C-Ge(10) C-Li(10) C-Mg(10) C-Mn(10) C-Nb(10) C-Ni(10) C-O(10)
C-Si(10) C-V(10) C-W(10) C-Zr(10) Ca-Ce(10) Ca-Cu(10) Ca-Er(10)
Ca-Fe(10) Ca-Gd(10) Ca-La(10) Ca-Li(10) Ca-Mg(10) Ca-Mn(10) Ca-Na(10)
Ca-Ni(10) Ca-O(10) Ca-Pb(10) Ca-Sc(10) Ca-Si(10) Ca-Sn(10) Ca-Sr(10)
Ca-Zn(10) Ce-Co(10) Ce-Cu(10) Ce-Er(10) Ce-Fe(10) Ce-La(10) Ce-Li(10)
Ce-Mg(10) Ce-Mn(10) Ce-Ni(10) Ce-O(10) Ce-Sb(10) Ce-Sc(10) Ce-Si(10)
Ce-Ti(10) Ce-V(10) Ce-Y(10) Ce-Zn(10) Co-Cr(10) Co-Cu(10) Co-Er(10)
Co-Fe(10) Co-Ge(10) Co-La(10) Co-Mn(10) Co-Nb(10) Co-Ni(10) Co-O(10)
Co-Sb(10) Co-Sc(10) Co-Si(10) Co-Sn(10) Co-W(10) Co-Y(10) Co-Zn(10)
Cr-Cu(10) Cr-Fe(10) Cr-Ge(10) Cr-Hf(10) Cr-La(10) Cr-Mg(10) Cr-Mn(10)
Cr-Na(10) Cr-Nb(10) Cr-Ni(10) Cr-O(10) Cr-Sc(10) Cr-Si(10) Cr-Sn(10)
Cr-Ti(10) Cr-V(10) Cr-W(10) Cr-Y(10) Cr-Zn(10) Cr-Zr(10) Cu-Er(10)
Cu-Fe(10) Cu-Gd(10) Cu-Ge(10) Cu-Hf(10) Cu-La(10) Cu-Li(10) Cu-Mg(10)
Cu-Mn(10) Cu-Na(10) Cu-Nb(10) Cu-Ni(10) Cu-O(10) Cu-Pb(10) Cu-Sb(10)
Cu-Sc(10) Cu-Si(10) Cu-Sn(10) Cu-Sr(10) Cu-Ti(10) Cu-V(10) Cu-W(10)
Cu-Y(10) Cu-Zn(10) Cu-Zr(10) Er-Fe(10) Er-Gd(10) Er-Ge(10) Er-Hf(10)
Er-La(10) Er-Li(10) Er-Mg(10) Er-Mn(10) Er-Nb(10) Er-O(5) Er-Sc(10)
Er-Si(10) Er-Ti(10) Er-V(10) Er-W(10) Er-Y(10) Er-Zn(10) Er-Zr(10)
Fe-Gd(10) Fe-Hf(10) Fe-La(10) Fe-Mg(10) Fe-Mn(10) Fe-Nb(10) Fe-Ni(10)
Fe-O(10) Fe-Pb(10) Fe-Sb(10) Fe-Sc(10) Fe-Si(10) Fe-Sn(10) Fe-Sr(10)
Fe-Ti(10) Fe-V(10) Fe-W(10) Fe-Y(10) Fe-Zn(10) Fe-Zr(10) Gd-Mg(10)
Gd-Mn(10) Gd-Ni(10) Gd-O(5) Gd-Sb(10) Gd-Sc(10) Gd-Si(10) Gd-Ti(10)
Gd-Zn(10) Gd-Zr(10) Ge-Hf(10) Ge-K(10) Ge-Mg(10) Ge-Mn(10) Ge-Na(10)
Ge-Nb(10) Ge-Ni(10) Ge-O(10) Ge-Pb(10) Ge-Sb(10) Ge-Sc(10) Ge-Si(10)

Ge-Sn(10) Ge-Sr(10) Ge-Ti(10) Ge-V(10) Ge-W(8) Ge-Zn(10) Hf-Mn(10)
Hf-Nb(10) Hf-Ni(10) Hf-O(10) Hf-Si(10) Hf-Sn(10) Hf-Ti(10) Hf-W(10)
Hf-Zr(10) K-Na(10) K-O(5) La-Mg(10) La-Mn(10) La-Nb(10) La-Ni(10)
La-O(5) La-Pb(10) La-Sb(10) La-Sc(10) La-Si(10) La-Sn(10) La-Ti(10)
La-V(10) La-W(10) La-Zn(10) La-Zr(10) Li-Mg(10) Li-Mn(10) Li-Na(10)
Li-O(10) Li-Sc(10) Li-Si(10) Li-Sn(10) Li-Sr(10) Li-Zn(10) Li-Zr(10)
Mg-Mn(10) Mg-Na(10) Mg-Ni(10) Mg-O(10) Mg-Sb(10) Mg-Sc(10) Mg-Si(10)
Mg-Sn(10) Mg-Sr(10) Mg-Ti(10) Mg-Y(10) Mg-Zn(10) Mg-Zr(10) Mn-Nb(10)
Mn-Ni(10) Mn-O(10) Mn-Pb(10) Mn-Sc(10) Mn-Si(10) Mn-Sn(10) Mn-Sr(10)
Mn-Ti(10) Mn-V(10) Mn-W(10) Mn-Y(10) Mn-Zn(10) Mn-Zr(10) Na-O(7)
Na-Si(10) Na-Sr(10) Na-Zn(10) Nb-Ni(10) Nb-O(10) Nb-Si(10) Nb-Sn(10)
Nb-Sr(10) Nb-Ti(10) Nb-V(10) Nb-W(10) Nb-Y(10) Nb-Zr(10) Ni-O(10)
Ni-Pb(10) Ni-Sb(10) Ni-Si(10) Ni-Sn(10) Ni-Sr(10) Ni-Ti(10) Ni-V(10)
Ni-W(10) Ni-Y(10) Ni-Zn(10) Ni-Zr(10) O-Pb(10) O-Sb(7) O-Sc(5)
O-Si(10) O-Sn(10) O-Sr(5) O-Ti(10) O-V(10) O-W(10) O-Y(10)
O-Zn(5) O-Zr(10) Pb-Sb(10) Pb-Si(10) Pb-Sn(10) Pb-Zn(10) Pb-Zr(10)
Sb-Si(10) Sb-Sn(10) Sb-Zn(10) Sc-Si(10) Sc-Sn(10) Sc-Sr(10) Sc-Ti(10)
Sc-W(10) Sc-Y(10) Sc-Zn(10) Sc-Zr(10) Si-Sn(10) Si-Sr(10) Si-Ti(10)
Si-V(10) Si-W(10) Si-Y(10) Si-Zn(10) Si-Zr(10) Sn-Sr(10) Sn-Ti(10)
Sn-V(10) Sn-W(10) Sn-Y(10) Sn-Zn(10) Sn-Zr(10) Sr-Ti(10) Sr-V(10)
Sr-Y(10) Sr-Zn(10) Ti-V(10) Ti-W(10) Ti-Zr(10) V-W(10) V-Y(10)
V-Zn(10) V-Zr(10) W-Y(10) W-Zr(10) Y-Zn(10) Y-Zr(10) Zn-Zr(10)

Ternary Systems (82)

Ag-Al-Cu(10) Ag-Al-Ge(5) Ag-Al-Mg(10) Ag-Al-Si(10) Ag-Al-Zn(5) Ag-Cu-Mg(10)
Al-B-Fe(8) Al-Ba-Ce(8) Al-Ba-Fe(8) Al-Ba-La(5) Al-Ba-Mn(5) Al-Ba-Si(10)
Al-Ba-Y(5) Al-Be-Si(5) Al-C-Zr(10) Al-Ca-Mg(10) Al-Ca-Mn(5) Al-Ce-Co(5)
Al-Ce-Cu(5) Al-Ce-Fe(10) Al-Ce-Mg(10) Al-Ce-Mn(8) Al-Ce-Si(8) Al-Co-Cu(10)
Al-Co-Fe(10) Al-Co-Mn(5) Al-Co-Si(10) Al-Cr-Fe(10) Al-Cr-Mn(5) Al-Cr-Ni(10)

Al-Cr-Si(10)	Al-Cu-Er(5)	Al-Cu-Fe(10)	Al-Cu-Li(10)	Al-Cu-Mg(10)	Al-Cu-Mn(5)
Al-Cu-Sb(5)	Al-Cu-Sc(5)	Al-Cu-Si(10)	Al-Cu-Zn(10)	Al-Er-Fe(5)	Al-Er-Mg(10)
Al-Er-Mn(5)	Al-Fe-La(8)	Al-Fe-Mg(10)	Al-Fe-Mn(10)	Al-Fe-Ni(10)	Al-Fe-Si(10)
Al-Fe-Y(8)	Al-Fe-Zn(10)	Al-Gd-Mn(8)	Al-Gd-Ni(5)	Al-Ge-Si(5)	Al-La-Mg(5)
Al-La-Mn(5)	Al-La-Si(10)	Al-La-Y(5)	Al-Li-Mg(10)	Al-Li-Si(10)	Al-Li-Zn(10)
Al-Mg-Mn(5)	Al-Mg-Na(5)	Al-Mg-Sb(5)	Al-Mg-Sc(5)	Al-Mg-Si(10)	Al-Mg-V(10)
Al-Mg-Y(5)	Al-Mg-Zn(10)	Al-Mn-Si(10)	Al-Mn-Y(5)	Al-Si-Sn(5)	Al-Si-Sr(10)
Al-Si-Ti(10)	Al-Si-Y(5)	Al-Si-Zn(10)	Al-Si-Zr(10)	Bi-Sn-Zn(10)	Cu-Mg-Si(10)
Cu-Mg-Zn(10)	Fe-Mn-Si(5)	Li-Mg-Si(10)	Mg-Si-Zn(5)		

1.6 Database Validation

The PanAl database is validated by a large amount of phase equilibrium data. Two examples are shown here. Figure 1.1 shows the calculated isotherm of Al-Cu-Mg-Si at 500ºC with Si content of 1.8wt%. The experimental data of D.P. Smith [1962Smi] are plotted on it for comparison. Figure 1.2 shows the calculated isopleth of Al-Fe-Mg-Si at 4wt.%Mg and 0.5wt.%Fe with experimental data from Phillips [1961Phi].

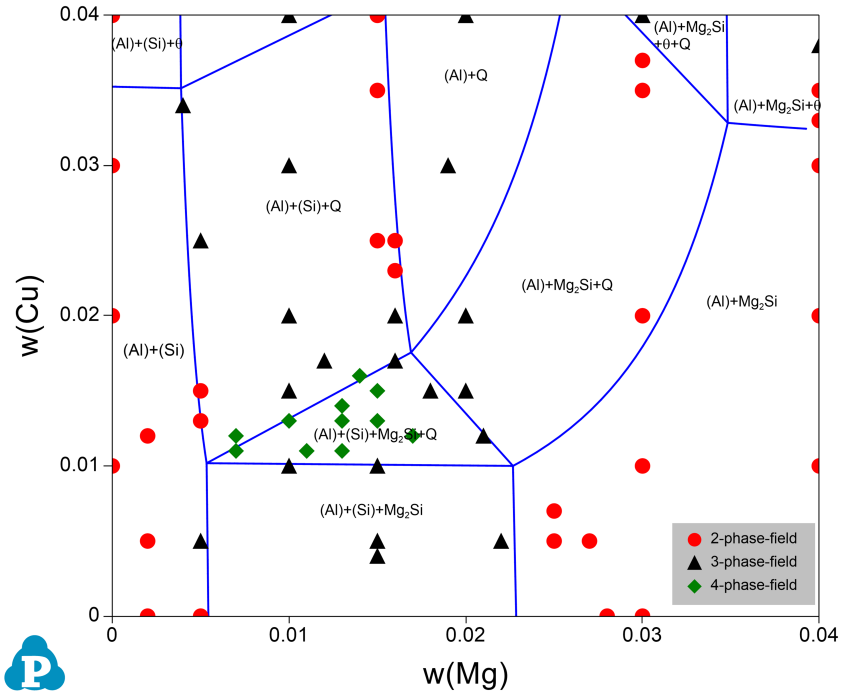


Figure 1.1: Comparison of a calculated isothermal section of Al-Cu-Mg-Si at 1.8wt%Si and at T=500 °C with the experimental data [1962Smi]

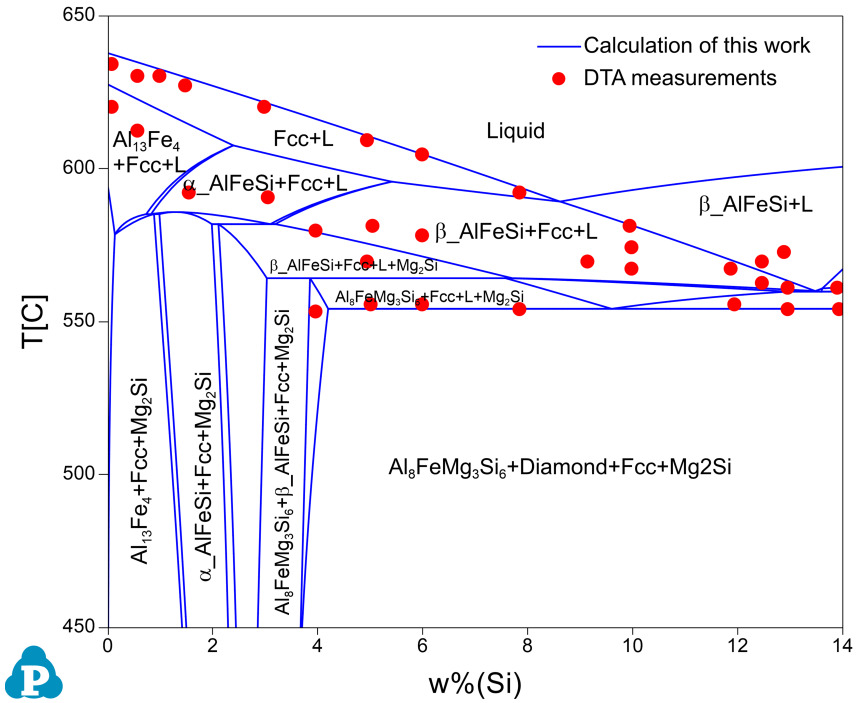


Figure 1.2: Comparison of a calculated isopleth of Al-Fe-Mg-Si at 4wt.%Mg and 0.5wt.%Fe with the experimental data [1961Phi]

In addition to the validation of phase equilibria, the current database has also been subjected to extensive validation by the solidification data of commercial aluminum alloys. The predicted liquidus and solidus temperatures of cast and wrought are shown in Figure 1.3 ~ Figure 1.6 with experimental data, respectively.

Cast aluminum alloys: 201, 206, 208, 242, 295, 296, 308, 319, 356, 357, 359, 360, 380, 383, 384, 390, 771, 850

Wrought aluminum alloys: 2014, 2017, 2024, 2036, 2124, 2218, 2219, 2319, 3003, 3004, 3105, 4032, 5052, 5056, 5083, 5086, 5154, 5182, 5356, 5454, 5456, 5457, 6005, 6009, 6010, 6061, 6063, 6066, 6070, 6101, 6151, 6201, 6205, 6351, 6463, 7005, 7039, 7049, 7075, 7178, 7475

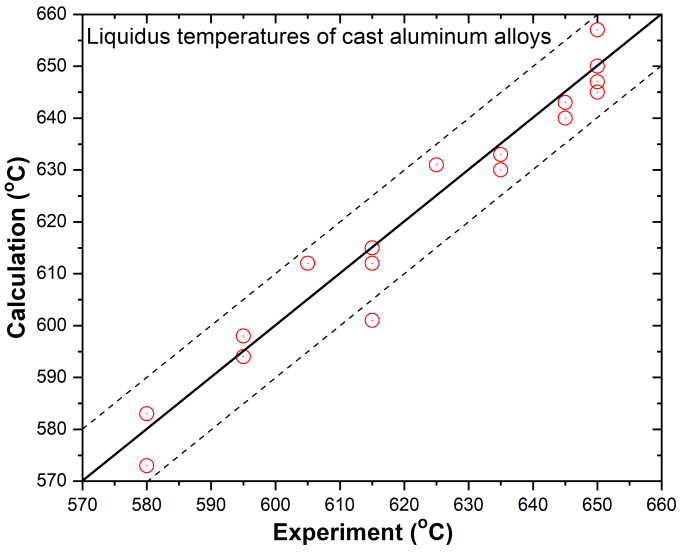


Figure 1.3: Comparison between calculated and experimentally measured liquidus temperatures of cast aluminum alloys

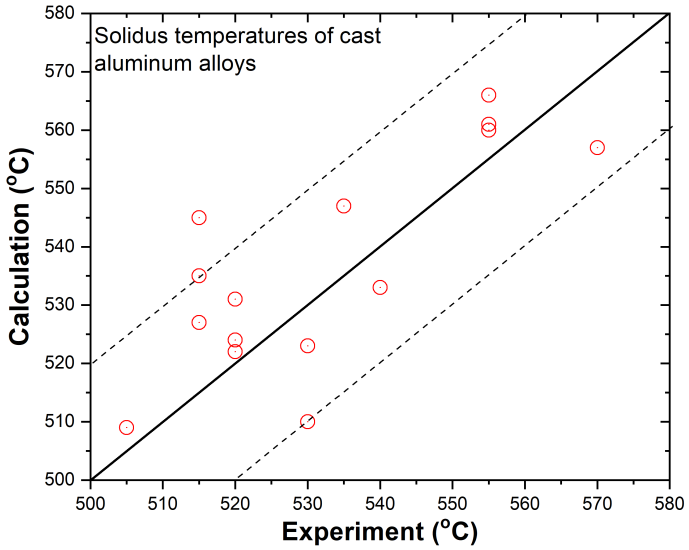


Figure 1.4: Comparison between calculated and experimentally measured solidus temperatures of cast aluminum alloys

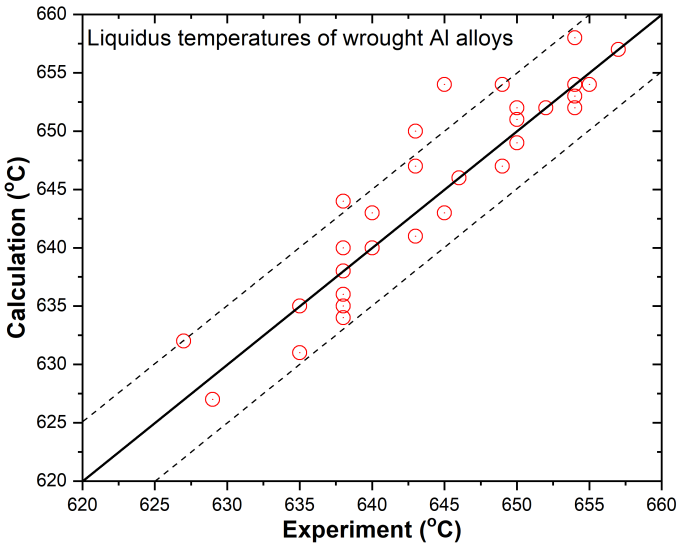


Figure 1.5: Comparison between calculated and experimentally measured liquidus temperatures of wrought aluminum alloys

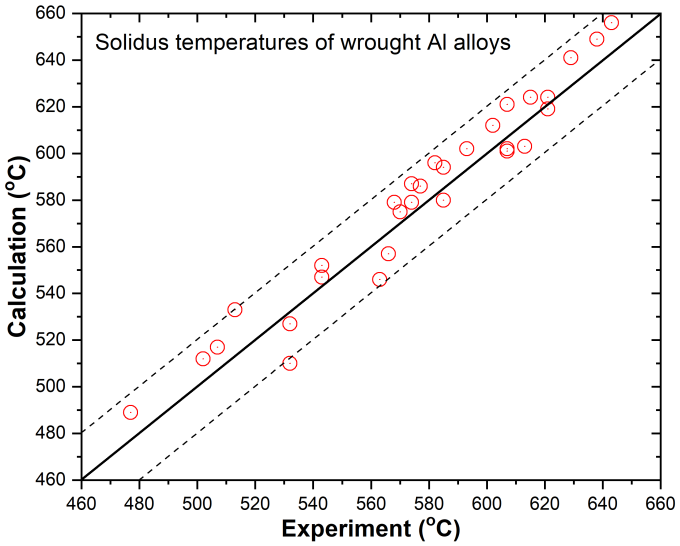


Figure 1.6: Comparison between calculated and experimentally measured solidus temperatures of wrought aluminum alloys

The solidification paths of several commercial aluminum alloys were experimentally investigated by Backerud et al [1986Bac]. The simulated solidification paths using both Scheil model and lever rule for four of these alloys (319.1, A357.2, A6351, A7075) are shown in Figure 1.7 ~ Figure 1.10 with the experimental data of Backerud et al [1986Bac].

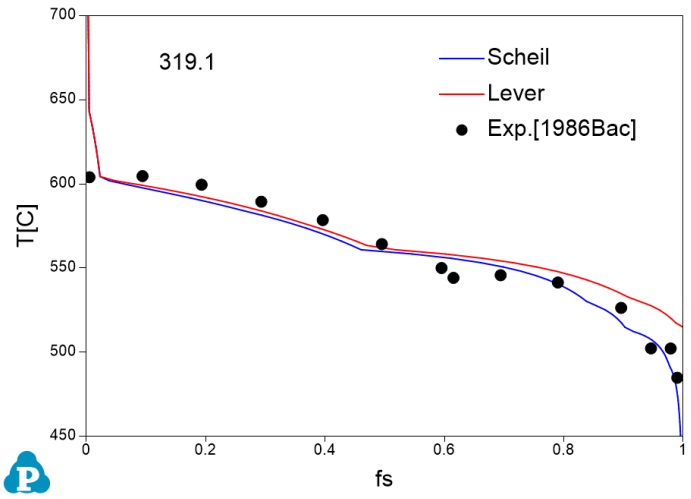


Figure 1.7: Comparison between calculated and experimentally measured solidification paths of 319.1 aluminum alloy

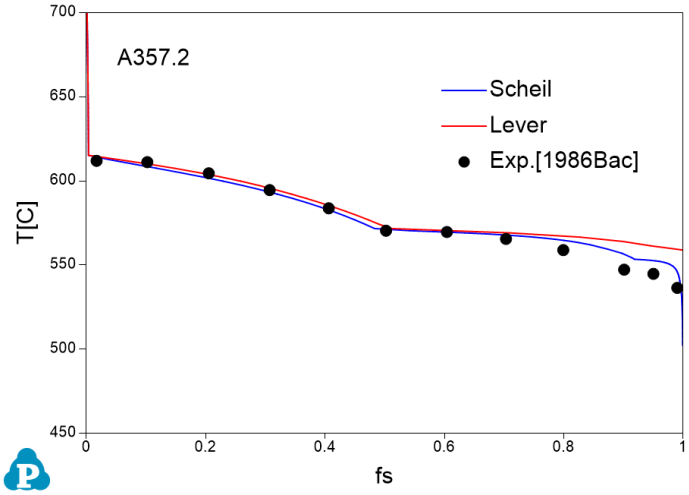


Figure 1.8: Comparison between calculated and experimentally measured solidification paths of A357.2 aluminum alloy

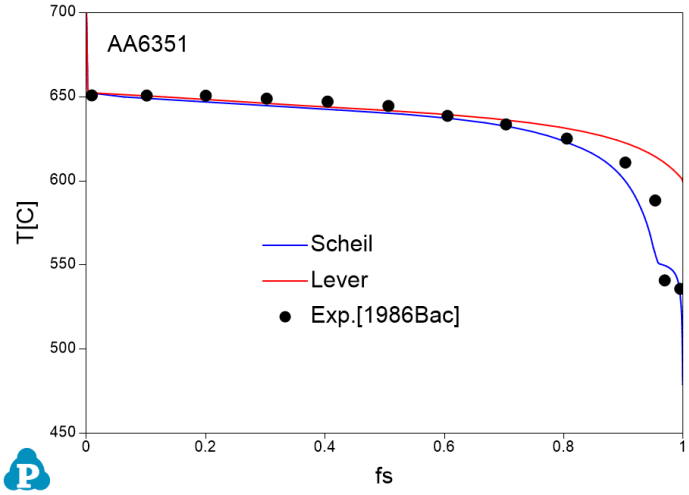


Figure 1.9: Comparison between calculated and experimentally measured solidification paths of AA6351 aluminum alloy

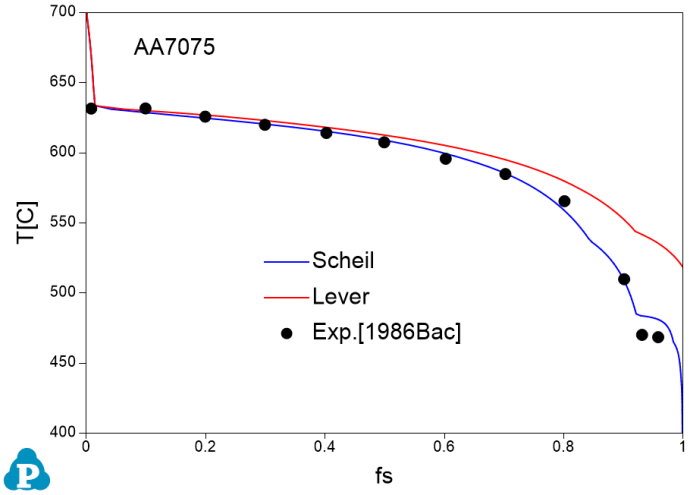


Figure 1.10: Comparison between calculated and experimentally measured solidification paths of AA7075 aluminum alloy

This database can also supply important parameters for processing simulation. One of these parameters is partition coefficient. The calculated partition coefficients have also been extensively validated. Examples for two Al-Cu-Mg-Zn quaternary alloys are given below. Figure 1.11 and Figure 1.12 show comparisons between calculated and measured partition coefficient for Al-4Cu-0.9Mg-2.6Zn (wt%) and Al-2.5Cu-1.3Mg-2.63Zn (wt%), respectively. The good agreement between the experimental and calculated results, as shown in these figures, indicates the reliability of the current PanAl thermodynamic database in providing thermodynamic input for processing simulation.

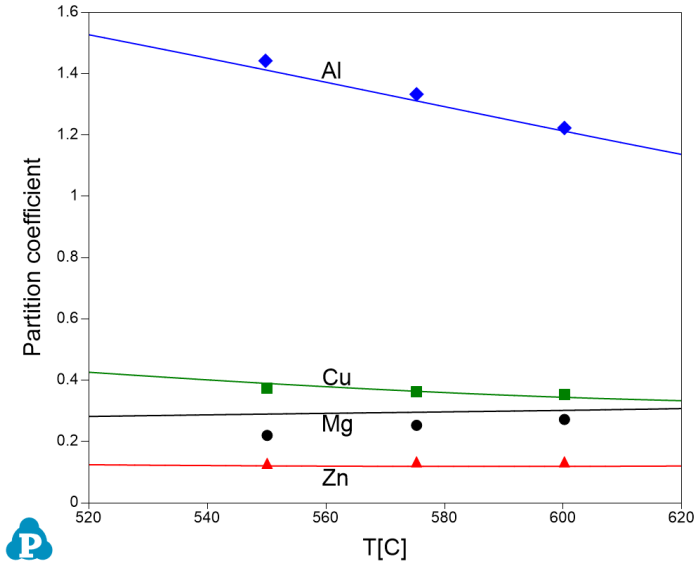


Figure 1.11: Calculated and experimentally determined [1998Lia] partition coefficients of Al-4Cu-0.9Mg-2.6Zn (wt%) alloy

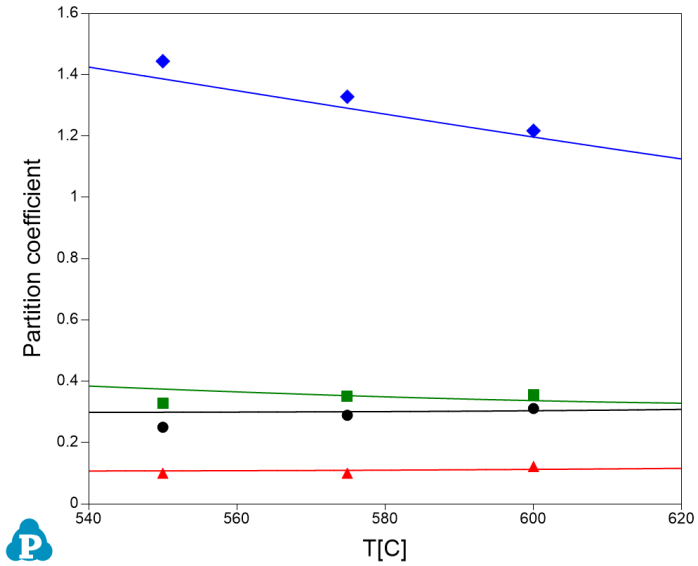


Figure 1.12: Calculated and experimentally determined [1998Lia] partition coefficients of Al-2.5Cu-1.3Mg-2.63Zn (wt%) alloy

2 Mobility Database

PanAl2024_MB is an atomic mobility database for Al-based alloys, which is compatible with the `PanAl2024_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 self-diffusivity of an element is usually described by an analytical expression. For the stable crystal structures, these expressions can be obtained using the available experimental data, while those for the metastable/unstable states are usually estimated from those of the stable states. In the following tables, we use different color to represent different status:

: Validated

: Estimated

: No data

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

	Ag	Al	Ba	Be	Bi	Ca	Ce	Co	Cr	Cu	Er	Fe	Gd	Ge	Hf	K	La	Li	Mg
Bcc																			
Fcc																			
Hcp																			

	Mn	Na	Nb	Ni	Pb	Sb	Sc	Si	Sn	Sr	Ti	V	W	Y	Zn	Zr
Bcc																
Fcc																
Hcp																

2.3 Assessed Systems

In addition to the assessed self-diffusivities shown above, the impurity diffusion data for all elements included in the current mobility database are also assessed. Moreover, chemical-diffusivities available in some binary and ternary systems are also used to assess the interaction parameters. These binary and ternary systems are listed below for the Bcc, Fcc, and Hcp phases, respectively.

Fcc Phase

Ag-Al	Ag-Cu	Ag-Sn	Ag-Zn	Al-Cu	Al-Mg	Al-Ni	Al-Si	Al-W	Al-Zn
Cr-Fe	Cr-Ni	Cu-Fe	Cu-Mg	Cu-Si	Cu-Sn	Cu-Ti	Cu-Zn	Fe-Mn	Fe-Ni
Fe-Si	Ge-Ni	Mn-Ni	Nb-Ni	Ni-Ti	Ni-V	Ni-W	Ni-Zn		

Ag-Al-Zn	Al-Cr-Ni	Al-Cu-Mg	Al-Cu-Si	Al-Cu-Zn	Al-Mg-Zn
Al-Mn-Ni	Al-Nb-Ni	Cr-Cu-Ni	Cr-Fe-Ni	Cr-Nb-Ni	Cu-Fe-Mn
Cu-Fe-Ni	Cu-Mn-Ni	Cu-Ni-Zn	Fe-Mn-Si		

Bcc phase

Al-Fe	Al-Ti	Cr-Fe	Cr-Ti	Cu-Ti	Fe-Ti	Hf-Zr	Nb-Ti	Nb-V	Nb-W
Nb-Zr	Ti-V	Ti-Zr	V-Zr						

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

Hcp phase

Al-Mg	Mg-Zn	Al-Mg-Zn

2.4 Database Validation

The simulated concentration profiles of a series of aluminum alloys are used to validate the current mobility database for Al-based alloys. A few examples of such simulation are shown below.

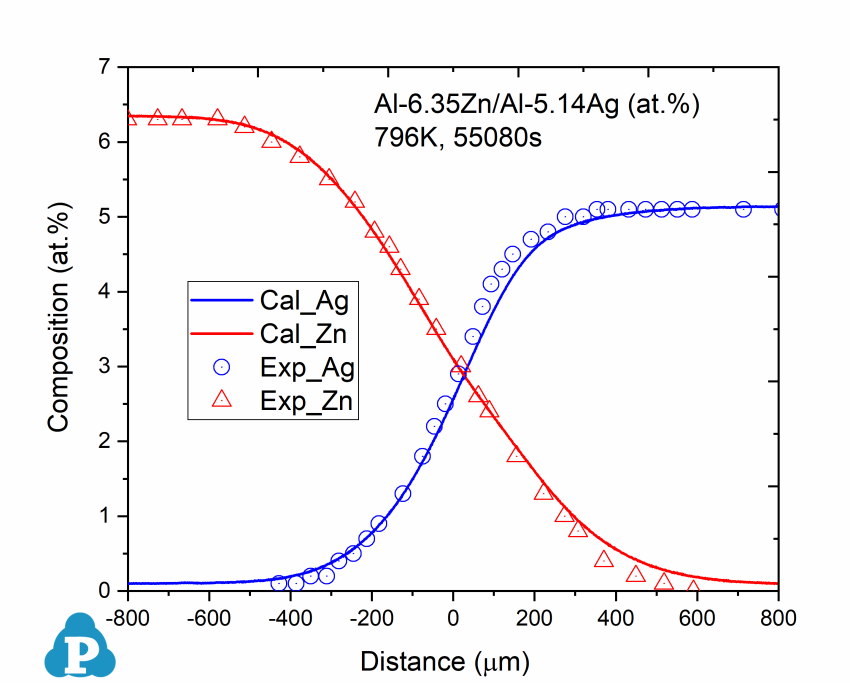


Figure 2.1: Concentration profiles of Al-6.35Zn/Al-5.14Ag (at.%) aged at 796K for 55080s [2011Cui]

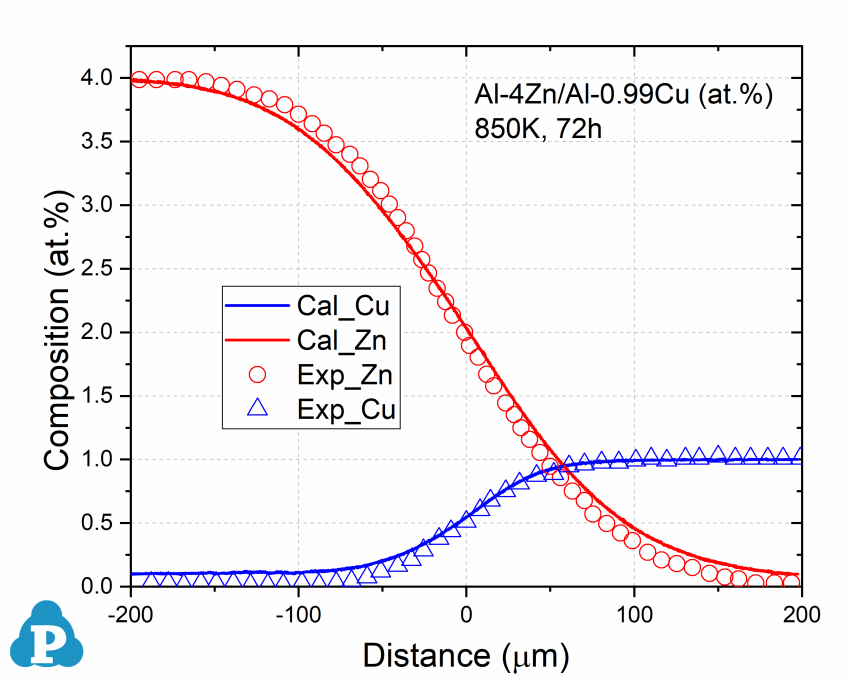


Figure 2.2: Concentration profile of Al-4Zn/Al-0.99Cu (at.%) annealed at 850K for 72h [2010Cha]

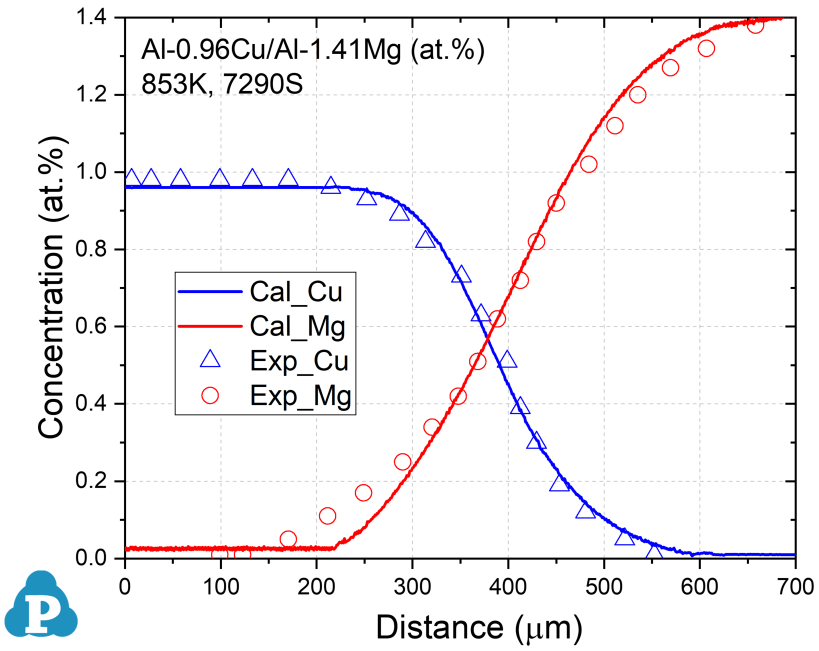


Figure 2.3: Concentration profiles of Al-0.96Cu/Al-1.41Mg (at.%) aged at 853K for 7290s [2010Zha, 2014Xin]

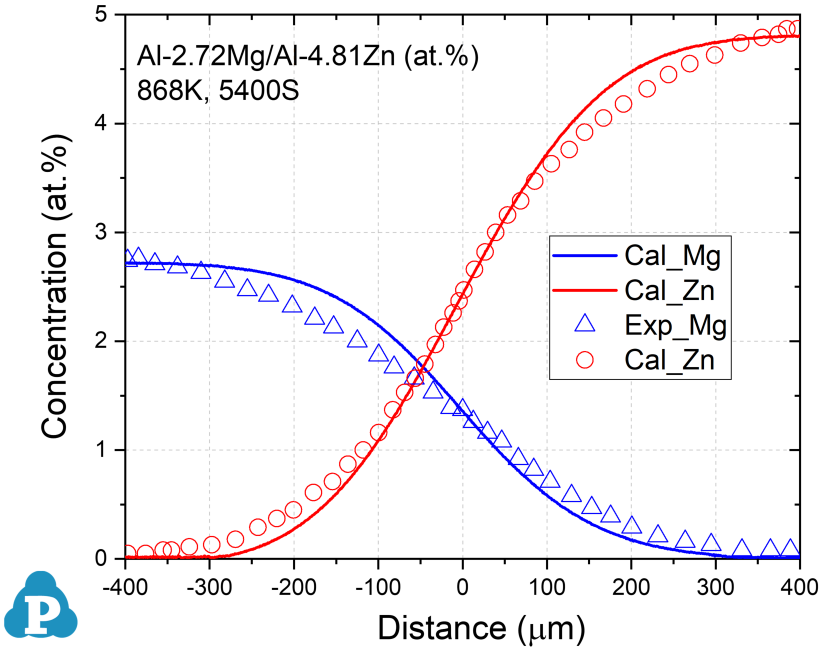


Figure 2.4: Concentration profiles of Al-2.72Mg/Al-4.81Zn (at.%) aged at 868K for 5400s [2008Yao]

2.5 Applications

This mobility database is combined with the thermodynamic database for Al-based alloys, `PanAl_TH`, to simulate the diffusion-controlled phenomena of Al-based alloys. A few examples are given below.

2.5.1 Precipitation kinetics of aluminum alloys

The PanEvolution module was developed for the simulation of precipitation kinetics of multi-component alloys. It has been seamlessly integrated with the thermodynamic calculation engine of Pandat™ software, and has been used to simulate the evolution of microstructure and the corresponding mechanical property responses to heat treatment of 2xxx, 6xxx and 7xxx series of aluminum alloys [2011Cao]. Below shows an example simulation performed for the Al-2.3Mg-6.1Zn (wt%) alloy aged at 160 °C for 1000 hours. The simulated particle size and yield strength evolution with time are compared with experimental data as shown in Figure 2.5

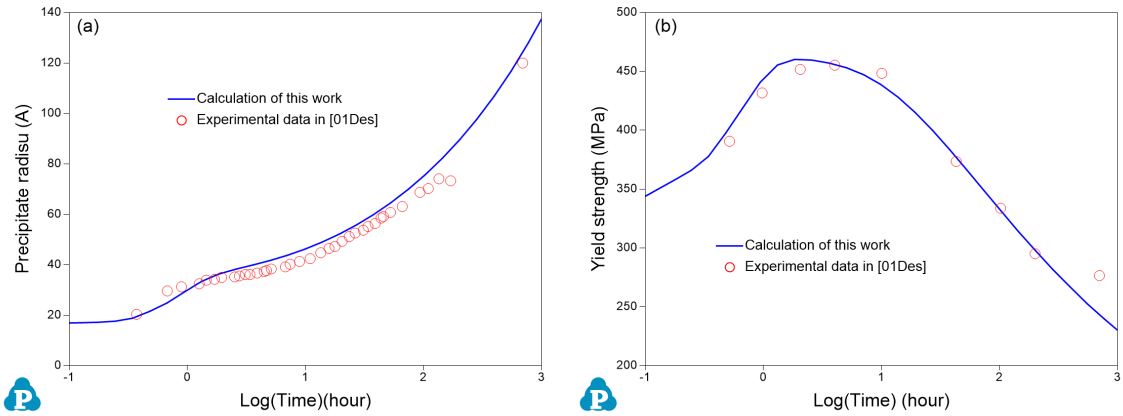


Figure 2.5: Simulated and measured particle size and yield strength evolution with time for Al-2.3Mg-6.1Zn (wt%) alloy aged at 160 °C for 1000 hours

As is seen, the particles grow and coarsen with ageing time, while the yield strength reaches peak between 1 to 10 hours. The yield strength decreases quickly after 10 hours of ageing at 160 °C. The database used to do this simulation is the combined thermodynamic and mobility database of Al-based alloys: `PanAl_TH+MB`. More information regarding to precipitation simulation can be found in PanEvolution module under the Software section.

2.5.2 Dissolution of aluminum alloys

The PanDiffusion module was developed for the simulation of diffusion kinetics of multi-component alloys. In Figure 2.6, dissolution of Si particle in Al-Si binary system was simulated and compared with the experimentally determined data [1992Tun]. In this simulation, the combined thermodynamic and mobility database of Al-based alloys, `PanAl_TH+MB`, is used. More information regarding to diffusion simulation can be found in PanDiffusion module under the Software section.

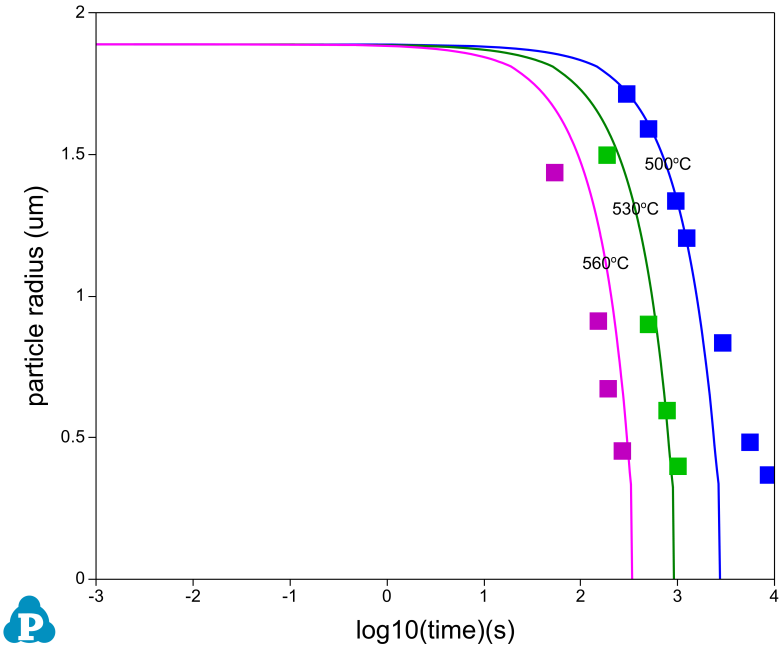


Figure 2.6: Comparison of simulated and experimentally determined dissolution of Si particle in Al-Si binary system

2.5.3 Solidification of aluminum alloys

The PanSolidification module was developed for the simulation of solidification behavior of multi-component alloys considering the effects of back-diffusion in the solid matrix phase, cooling rate, and dendrite arm coarsening. As shown in Figure 2.7, the solidification of the Al-4.5wt.%Cu alloy at the cooling rate of 0.25K/s is simulated and compared with the experimentally determined data [2001Yan].

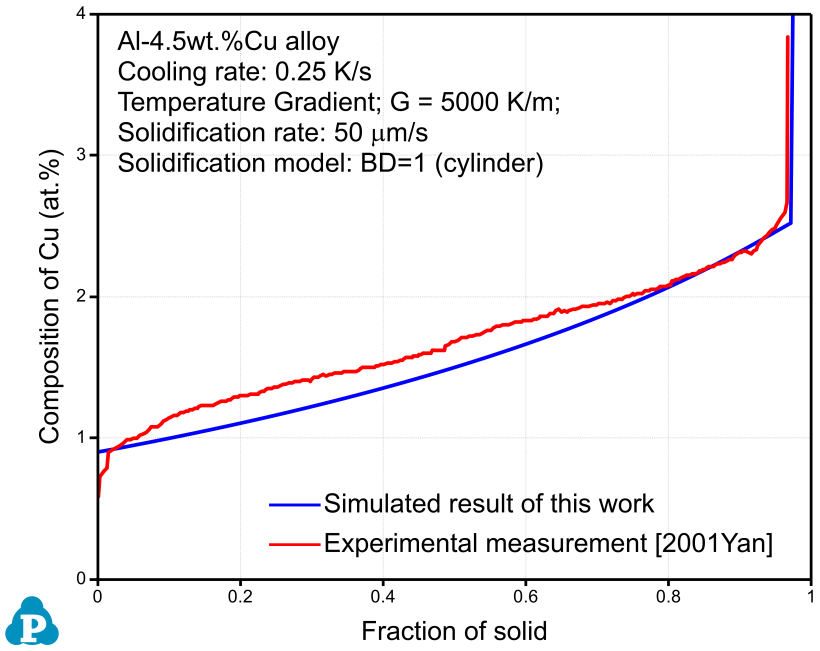


Figure 2.7: Comparison of simulated and experimentally determined Cu composition profile within the Fcc matrix for the Al-4.5wt.%Cu alloy at the cooling rate of 0.25K/s

In this simulation, the combined thermodynamic and mobility database of Al-based alloys, `PanAl_TH+MB`, is used. More information regading to solidification can be found in PanSolidification module under the Software section.

3 Thermophysical Property Database

The thermophysical property database **PanAl2024_TP** is compatible with the `PanAl2024_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Al-based 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 **1150** phases assessed in the `PanAl2024_TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of Al alloys.

Database Validation

The simulated density changes vs. temperature of a series of Al-based alloys are shown below to validate the current `PanAl2024_MV` database.

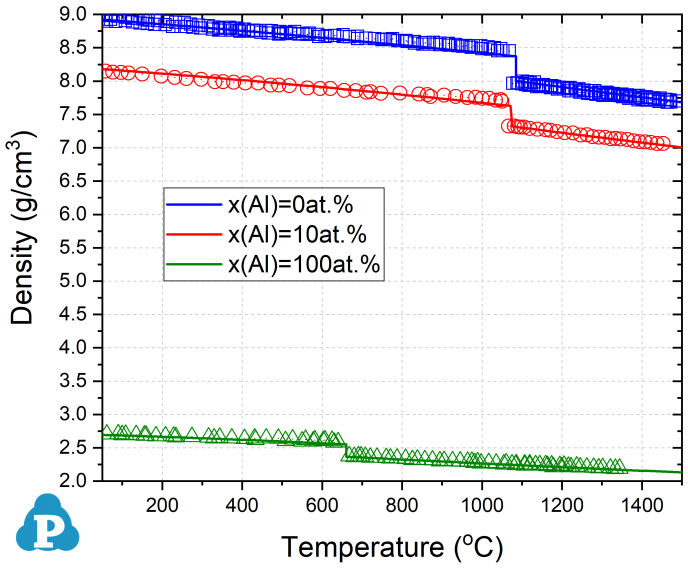


Figure 3.1: Density of Al-Cu binary alloys [2013Kur]

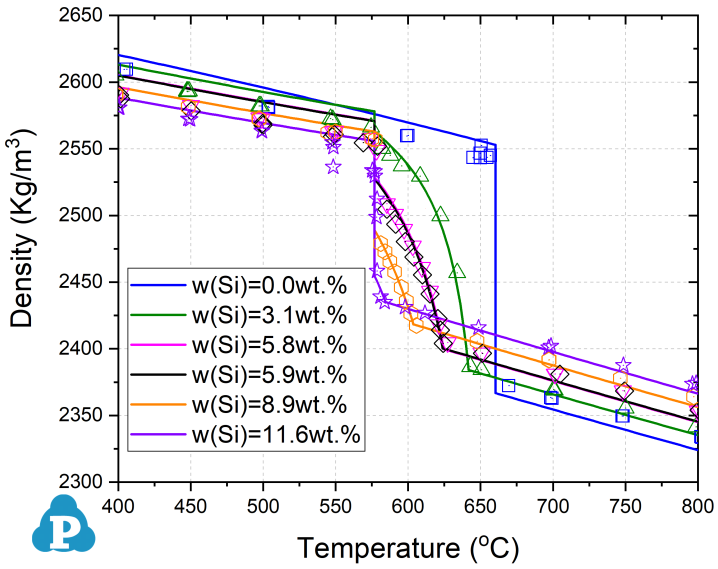


Figure 3.2: Density of Al-Si binary alloys [2001Mag]

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 Al-Cu alloys in comparison with experimental data.

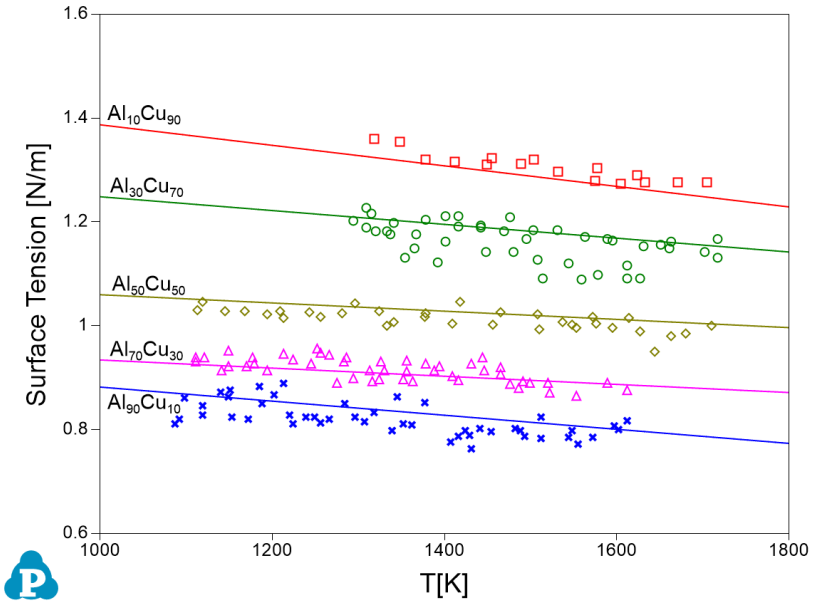


Figure 3.3: Surface tension of Al-Cu alloys

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.4 shows the viscosity of A356 alloy in comparison with experimental data.

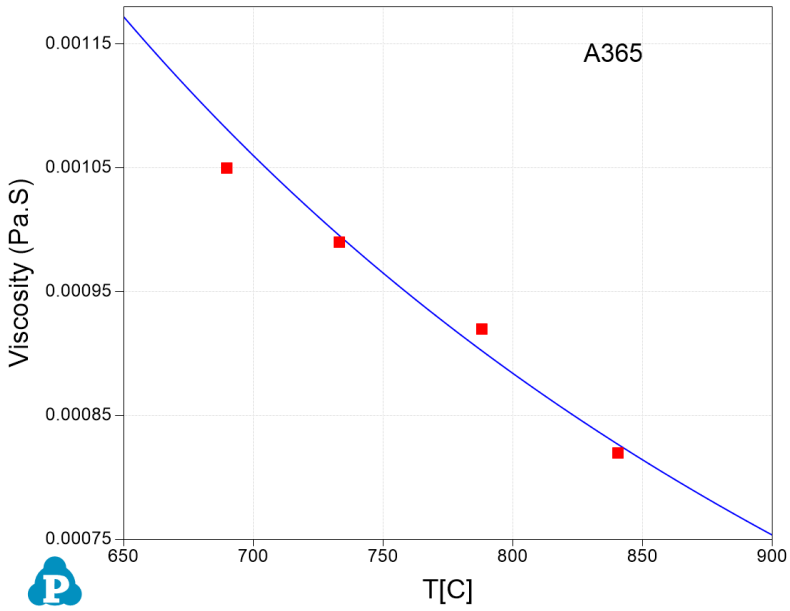


Figure 3.4: Viscosity of the A356 alloy

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PanAl2024: List of Phases

Phases (**1150**)

Name	Model	Lattice Size	Constitue
A_BeO	CEF (ST2)	(1)(1)	(Be)(O)
A_Bi2O3	CEF (ST2)	(2)(3)	(Bi)(O)
A_Li2M3	CEF (SLN)	(2)(3)	(Li)(Li,Zn)
A_Li2M5	CEF (SLN)	(2)(5)	(Li,Zn)(Zn)
A_LiM4	CEF (SLN)	(1)(4)	(Li,Zn)(Li,Zn)
A_RE2O3	CEF (SLN)	(2)(2)(1)	(Ce+3,Ce+2)(O-2)(O-2,Va)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
Ag2Ca	CEF (ST2)	(0.666667) (0.333333)	(Ag)(Ca)
Ag2Na	CEF (ST2)	(2)(1)	(Ag)(Na)
Ag2O2	CEF (ST2)	(2)(2)	(Ag)(O)
Ag2R_oI12	CEF (SLN)	(2)(1)	(Ag)(Ce,La,Sr)
Ag2R_tI6	CEF (SLN)	(0.667)(0.333)	(Ag)(Er,Gd,Sc,Y)
Ag2Sr3	CEF (ST2)	(2)(3)	(Ag)(Sr)
Ag3Ca5	CEF (ST2)	(0.375)(0.625)	(Ag)(Ca)
Ag3Mg	CEF (SLN)	(0.25)(0.25) (0.25)(0.25) (1)	(Ag,Mg)(Ag,Mg)(Ag,Mg)(Ag,Mg)(Va)
Ag3Sb	CEF (SLN)	(0.75)(0.25)	(Ag,Sb)(Ag,Sb)
Ag3Sn	CEF (SLN)	(0.75)(0.25)	(Ag)(Ag,Sn)
Ag4R_tI10	CEF (SLN)	(4)(1)	(Ag)(Ce,Sc,Sr)

Name	Model	Lattice Size	Constitue
Ag51R14	CEF (SLN)	(0.785)(0.215)	(Ag,Er)(Ce,Er,Gd,La,Y)
Ag5R_hP6	CEF (SLN)	(5)(1)	(Ag)(La,Sr)
Ag5Zn8	CEF (SLN)	(2)(2)(3)(6)	(Ag,Zn)(Ag)(Ag,Zn)(Ag,Zn)
Ag7Ca2	CEF (ST2)	(0.777778) (0.222222)	(Ag)(Ca)
Ag9Ca2	CEF (ST2)	(0.818182) (0.181818)	(Ag)(Ca)
AgAlMg	CEF (ST3)	(0.33333) (0.33333) (0.33333)	(Ag)(Al)(Mg)
AgCa	CEF (ST2)	(0.5)(0.5)	(Ag)(Ca)
AgCa3	CEF (ST2)	(0.25)(0.75)	(Ag)(Ca)
AgMg3	CEF (SLN)	(0.23)(0.77)	(Ag,Cu)(Al,Mg)
AgMg4	CEF (SLN)	(0.2)(0.8)	(Ag,Cu)(Al,Mg)
AgSr	CEF (ST2)	(1)(1)	(Ag)(Sr)
AgTi	CEF (SLN)	(1)(1)	(Ag,Ti)(Ag,Ti)
AgTi2	CEF (ST2)	(1)(2)	(Ag)(Ti)
AgZn2	CEF (SLN)	(1)(2)	(Zn)(Ag,Zn)
AgZn3	CEF (SLN)	(1)	(Ag,Zn)
AgZr	CEF (ST2)	(0.5)(0.5)	(Ag)(Zr)
Al10ErFe2	CEF (ST3)	(10)(1)(2)	(Al)(Er)(Fe)
Al10Mn7Ce2	CEF (ST3)	(10)(7)(2)	(Al)(Mn)(Ce)
Al10RM2	CEF (SLN)	(10)(1)(2)	(Al)(Ce,Er,La,Y)(Cu,Fe,Mn)
Al10V	CEF (ST2)	(10)(1)	(Al)(V)
Al11Cr2	CEF (SLN)	(10)(1)(2)	(Al)(Al)(Cr,Mn)
Al11Mn4	CEF (SLN)	(11)(4)	(Al)(Cr,Fe,Mn)

Name	Model	Lattice Size	Constitue
Al11Mn4_H	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al12Mn	CEF (SLN)	(12)(1)	(Al)(Fe,Mn)
Al12W	CEF (ST2)	(12)(1)	(Al)(W)
Al13CeCu13	CEF (ST3)	(13)(1)(13)	(Al)(Ce)(Cu)
Al13CeMg6	CEF (ST3)	(13)(1)(6)	(Al)(Ce)(Mg)
Al13Cr2	CEF (SLN)	(13)(2)	(Al)(Cr,Mg,Mn)
Al13M4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al,Cu)(Co,Cr,Fe,Mn,Ni,Zn) (Al,Si,Zn,Va)
Al14Mn4Si5	CEF (SLN)	(14)(4)(5)	(Al)(Mn)(Al,Si)
Al15_FeMn3Si2	CEF (SLN)	(16)(4)(1)(2)	(Al)(Cr,Fe,Mn)(Si)(Al,Si)
Al16Ce10Si4	CEF (ST3)	(0.533333) (0.333333) (0.133333)	(Al)(Ce)(Si)
Al18Mg3Mn2	CEF (ST3)	(18)(3)(2)	(Al)(Mg)(Mn)
Al18Mg3V2	CEF (ST3)	(18)(3)(2)	(Al)(Mg)(V)
Al1Fe1O3	CEF (ST3)	(1)(1)(3)	(Al+3)(Fe+3)(O-2)
Al23V4	CEF (ST2)	(23)(4)	(Al)(V)
Al2Ba	CEF (ST2)	(2)(1)	(Al)(Ba)
Al2Ba3Si2	CEF (ST3)	(2)(3)(2)	(Al)(Ba)(Si)
Al2BaSi2	CEF (ST3)	(2)(1)(2)	(Al)(Ba)(Si)
Al2CeZn2	CEF (ST3)	(2)(1)(2)	(Al)(Ce)(Zn)
Al2Er3	CEF (ST2)	(0.4)(0.6)	(Al)(Er)
Al2ErMg	CEF (ST3)	(0.66667)(0.1) (0.23333)	(Al)(Er)(Mg)
Al2Fe	CEF (SLN)	(2)(1)	(Al,Cu)(Cr,Fe,Mn,Ni)

Name	Model	Lattice Size	Constitue
Al2Gd3	CEF (ST2)	(0.4)(0.6)	(Al)(Gd)
Al2Hf	CEF (ST2)	(0.666667) (0.333333)	(Al)(Hf)
Al2Hf3	CEF (ST2)	(0.4)(0.6)	(Al)(Hf)
Al2Li3	CEF (SLN)	(2)(3)	(Al,Zn)(Li)
Al2LiMg	CEF (ST3)	(0.53)(0.33) (0.14)	(Al)(Li)(Mg)
Al2Sc_X	CEF (SLN)	(0.666667) (0.333333)	(Al,Mg)(Sc)
Al2Si2Sr	CEF (ST3)	(2)(2)(1)	(Al)(Si)(Sr)
Al2Si2Y	CEF (ST3)	(2)(2)(1)	(Al)(Si)(Y)
Al2Sr	CEF (ST2)	(0.666667) (0.333333)	(Al)(Sr)
Al2Ti	CEF (ST2)	(2)(1)	(Al)(Ti)
Al2W	CEF (ST2)	(2)(1)	(Al)(W)
Al2Y3	CEF (SLN)	(2)(3)	(Al,Mg)(Y)
Al2Zr	CEF (ST2)	(0.666667) (0.333333)	(Al)(Zr)
Al2Zr3	CEF (ST2)	(0.4)(0.6)	(Al)(Zr)
Al3C5Zr2	CEF (ST3)	(3)(5)(2)	(Al)(C)(Zr)
Al3C5Zr3	CEF (ST3)	(3)(5)(3)	(Al)(C)(Zr)
Al3CZr5	CEF (ST3)	(3)(1)(5)	(Al)(C)(Zr)
Al3Ca8	CEF (SLN)	(0.272727) (0.727272)	(Al)(Ca,Mg)
Al3Co	CEF (SLN)	(3)(1)	(Al,Si)(Co)
Al3CoCu	CEF (ST3)	(3)(1)(1)	(Al)(Co)(Cu)

Name	Model	Lattice Size	Constitue
Al3Cu5Zn2	CEF (SLN)	(1)(4)(4)(1)	(Al,Cu)(Al)(Cu)(Zn)
Al3CuLa	CEF (ST3)	(0.6)(0.2)(0.2)	(Al)(Cu)(La)
Al3Hf	CEF (ST2)	(0.75)(0.25)	(Al)(Hf)
Al3Hf2	CEF (ST2)	(0.6)(0.4)	(Al)(Hf)
Al3Hf4	CEF (ST2)	(0.428571) (0.571429)	(Al)(Hf)
Al3Li8Si5	CEF (ST3)	(8)(3)(5)	(Li)(Al)(Si)
Al3Nb	CEF (ST2)	(3)(1)	(Al)(Nb)
Al3Ni	CEF (SLN)	(0.75)(0.25)	(Al,Si)(Fe,Ni)
Al3Ni2	CEF (SLN)	(3)(2)(1)	(Al,Si)(Al,Co,Cu,Fe,Ni,V,Zr) (Co,Cu,Ni,Va)
Al3Ni5	CEF (ST2)	(0.375)(0.625)	(Al)(Ni)
Al3Si2Y2	CEF (ST3)	(3)(2)(2)	(Al)(Si)(Y)
Al3SiZr	CEF (ST3)	(0.65)(0.1) (0.25)	(Al)(Si)(Zr)
Al3Ti	CEF (SLN)	(0.25)(0.75)	(Al,Ti)(Al,Si,Ti)
Al3V	CEF (SLN)	(3)(1)	(Al,V)(V)
Al3Zr	CEF (SLN)	(0.75)(0.25)	(Al)(Sc,Zr)
Al3Zr2	CEF (ST2)	(0.6)(0.4)	(Al)(Zr)
Al3Zr4	CEF (ST2)	(0.42857) (0.57143)	(Al)(Zr)
Al3Zr5	CEF (ST2)	(0.375)(0.625)	(Al)(Zr)
Al3Zr_L12	CEF (ST2)	(0.75)(0.25)	(Al)(Zr)
Al3Zr_Si	CEF (ST3)	(0.75)(0.1) (0.15)	(Al)(Si)(Zr)
Al40Mg17La3	CEF (ST3)	(40)(17)(3)	(Al)(Mg)(La)

Name	Model	Lattice Size	Constitue
Al4C3	CEF (ST2)	(4)(3)	(Al)(C)
Al4Ca	CEF (SLN)	(0.8)(0.2)	(Al,Mg)(Ca)
Al4Ce	CEF (ST2)	(0.8)(0.2)	(Al)(Ce)
Al4CeCo	CEF (ST3)	(4)(1)(1)	(Al)(Ce)(Co)
Al4CeMg4	CEF (ST3)	(4)(1)(4)	(Al)(Ce)(Mg)
Al4La3Si6	CEF (ST3)	(4)(6)(3)	(Al)(Si)(La)
Al4Li9	CEF (SLN)	(4)(9)	(Al,Zn)(Li)
Al4M	CEF (SLN)	(4)(1)	(Al,Si)(Cr,Fe,Mn)
Al4MgY	CEF (ST3)	(4)(1)(1)	(Al)(Mg)(Y)
Al4Mn_U	CEF (SLN)	(0.2)(0.8)	(Fe,Mn)(Al)
Al4Sr	CEF (ST2)	(0.8)(0.2)	(Al)(Sr)
Al4W	CEF (ST2)	(4)(1)	(Al)(W)
Al4Zr5	CEF (ST2)	(0.444444) (0.555556)	(Al)(Zr)
Al53La22	CEF (ST2)	(0.707)(0.293)	(Al)(La)
Al5Co2	CEF (SLN)	(5)(2)	(Al,Si)(Co,Fe)
Al5CoCu4	CEF (ST3)	(5)(1)(4)	(Al)(Co)(Cu)
Al5Fe2	CEF (SLN)	(5)(2)(3)	(Al,Cu)(Cr,Fe,Mn,Ni)(Zn,Va)
Al5Fe4	CEF (SLN)	(1)	(Al,Fe,Mn)
Al5Ti2	CEF (ST2)	(5)(2)	(Al)(Ti)
Al5W	CEF (ST2)	(5)(1)	(Al)(W)
Al60Cu4Mn11	CEF (ST3)	(0.8)(0.05) (0.15)	(Al)(Cu)(Mn)
Al6CoCu3	CEF (ST3)	(6)(1)(3)	(Al)(Co)(Cu)
Al6Cu2Fe	CEF (SLN)	(0.62)(0.255) (0.125)	(Al)(Cu)(Cu,Fe)

Name	Model	Lattice Size	Constitue
Al6_FeMn	CEF (SLN)	(6)(1)	(Al)(Cr,Fe,Mn)
Al71Fe5Ni24	CEF (ST3)	(0.71)(0.05) (0.24)	(Al)(Fe)(Ni)
Al77W23	CEF (ST2)	(77)(23)	(Al)(W)
Al78Fe12La10	CEF (ST3)	(78)(12)(10)	(Al)(Fe)(La)
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)
Al7FeNi	CEF (SLN)	(0.714286) (0.285714)	(Al)(Fe,Ni)
Al7Sr8	CEF (ST2)	(0.466667) (0.533333)	(Al)(Sr)
Al7V	CEF (ST2)	(7)(1)	(Al)(V)
Al7W3	CEF (ST2)	(7)(3)	(Al)(W)
Al8CeCo2	CEF (ST3)	(8)(1)(2)	(Al)(Ce)(Co)
Al8CeFe2	CEF (ST3)	(8)(1)(2)	(Al)(Ce)(Fe)
Al8Cr5_H	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Cr5_L	CEF (SLN)	(8)(5)	(Al)(Cr,Fe)
Al8FeMg3Si6	CEF (ST4)	(8)(3)(1)(6)	(Al)(Mg)(Fe)(Si)
Al8FeMnSi2	CEF (ST4)	(16)(2)(2)(3)	(Al)(Fe)(Mn)(Si)
Al8LaMn	CEF (ST3)	(8)(1)(1)	(Al)(La)(Mn)
Al8Mn4RE	CEF (SLN)	(8)(4)(1)	(Al)(Mn)(Ce,Gd)
Al8Mn5	CEF (SLN)	(0.4615) (0.1923) (0.3462)	(Al)(Fe,Mn)(Al,Fe,Mn,Si)
Al8RM4	CEF (SLN)	(8)(1)(4)	(Al)(Ca,Ce,Er,Gd,La,Y)(Cu,Fe,Mn)

Name	Model	Lattice Size	Constitue
Al8Si15Sr4	CEF (ST3)	(8)(15)(4)	(Al)(Si)(Sr)
Al8V5	CEF (ST2)	(8)(5)	(Al)(V)
Al9BaFe2	CEF (ST3)	(9)(1)(2)	(Al)(Ba)(Fe)
Al9Co2	CEF (SLN)	(9)(2)	(Al,Si)(Co)
Al9Cr4_H	CEF (ST2)	(9)(4)	(Al)(Cr)
Al9Cr4_L	CEF (SLN)	(9)(4)	(Al)(Cr,Fe)
Al9Cu2Y3	CEF (ST3)	(8.5)(2.5)(3)	(Al)(Cu)(Y)
Al9FeNi	CEF (SLN)	(0.818182) (0.181818)	(Al,Si)(Fe,Ni)
Al9Mn3Si	CEF (ST3)	(0.6923) (0.2308) (0.0769)	(Al)(Mn)(Si)
AlB12_Alpha	CEF (ST2)	(1)(12)	(Al)(B)
AlB2	CEF (ST2)	(1)(2)	(Al)(B)
AlB2Fe2	CEF (ST3)	(1)(2)(2)	(Al)(B)(Fe)
AlBa	CEF (ST2)	(1)(1)	(Al)(Ba)
AlBaSi	CEF (SLN)	(2)(1)	(Al,Si)(Ba)
AlCa	CEF (ST2)	(0.5)(0.5)	(Al)(Ca)
AlCaMg	CEF (SLN)	(0.5) (0.166667) (0.333333)	(Al)(Al,Mg)(Ca,Mg)
AlCe2	CEF (ST2)	(1)(2)	(Al)(Ce)
AlCeCu_T2	CEF (SLN)	(0.8947) (0.1053)	(Al,Cu)(Ce)
AlCeCu_T3	CEF (SLN)	(0.8)(0.2)	(Al,Cu)(Ce)
AlCeCu_T4	CEF (ST3)	(0.3333)	(Al)(Ce)(Cu)

Name	Model	Lattice Size	Constitue
		(0.3333) (0.3334)	
AlCeCu_T5	CEF (ST3)	(0.2)(0.4)(0.4)	(Al)(Ce)(Cu)
AlCeSi	CEF (SLN)	(0.666667) (0.333333)	(Al,Si)(Ce)
AlCeSi2	CEF (ST3)	(0.25)(0.25) (0.5)	(Al)(Ce)(Si)
AlCr2	CEF (ST2)	(1)(2)	(Al)(Cr)
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_Prime	CEF (SLN)	(0.667)(0.333)	(Al)(Al,Cu)
AlCu_Theta	CEF (SLN)	(0.667)(0.333)	(Al)(Ag,Al,Cu)
AlCu_Zeta	CEF (ST2)	(0.45)(0.55)	(Al)(Cu)
AlEr	CEF (ST2)	(0.5)(0.5)	(Al)(Er)
AlEr2	CEF (ST2)	(0.333)(0.667)	(Al)(Er)
AlGd	CEF (ST2)	(0.5)(0.5)	(Al)(Gd)
AlGd2	CEF (ST2)	(0.333333) (0.666667)	(Al)(Gd)
AlHf	CEF (ST2)	(0.5)(0.5)	(Al)(Hf)
AlHf2	CEF (ST2)	(0.333333) (0.666667)	(Al)(Hf)
AlLaSi2	CEF (ST3)	(1)(2)(1)	(Al)(Si)(La)
AlLi5Si2	CEF (ST3)	(5.3)(0.7)(2)	(Li)(Al)(Si)
AlLiSi	CEF (ST3)	(1)(1)(1)	(Li)(Al)(Si)
AlMg_Beta	CEF (SLN)	(89)(140)	(Mg,Li)(Al,Cu,Zn)

Name	Model	Lattice Size	Constitue
AlMg_Eps	CEF (SLN)	(23)(30)	(Mg)(Al,Cu,Zn)
AlMg_Gamma	CEF (SLN)	(10)(24)(24)	(Ca,Mg)(Al,Cu,Li,Mg,Zn) (Al,Cu,Mg,Zn)
AlNb3	CEF (SLN)	(3)(1)	(Nb)(Al,Nb)
AlSb	CEF (ST2)	(0.5)(0.5)	(Al)(Sb)
AlSc2	CEF (ST2)	(0.333333) (0.666667)	(Al)(Sc)
AlSc2Si2	CEF (ST3)	(1)(2)(2)	(Al)(Sc)(Si)
AlSc_X	CEF (SLN)	(0.5)(0.5)	(Al,Mg)(Sc)
AlSiSr	CEF (ST3)	(1)(1)(1)	(Al)(Si)(Sr)
AlTi	CEF (SLN)	(0.5)(0.5)	(Al,Ti)(Al,Ti)
AlTi3	CEF (SLN)	(0.75)(0.25)	(Al,Ti)(Al,Ti)
AlY	CEF (ST2)	(1)(1)	(Al)(Y)
AlY2	CEF (ST2)	(1)(2)	(Al)(Y)
AlZr	CEF (ST2)	(0.5)(0.5)	(Al)(Zr)
AlZr2	CEF (ST2)	(0.333333) (0.666667)	(Al)(Zr)
AlZr3	CEF (ST2)	(0.25)(0.75)	(Al)(Zr)
Alpha_AlFeSi	CEF (SLN)	(0.66)(0.19) (0.05)(0.1)	(Al)(Fe)(Si)(Al,Si)
Alpha_Bi2Mg3	CEF (SLN)	(2)(3)	(Bi,Va)(Mg)
Alpha_BiMn	CEF (ST2)	(0.5)(0.5)	(Bi)(Mn)
Alpha_CeC2	CEF (ST2)	(0.333333) (0.666667)	(Ce)(C)
Alpha_Co2Si	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Alpha_Co5Ge3	CEF (ST2)	(0.625)(0.375)	(Co)(Ge)

Name	Model	Lattice Size	Constitue
Alpha_Cr5Ge3	CEF (SLN)	(0.625)(0.375)	(Cr,Ge)(Cr,Ge)
Alpha_Fe2Sc	CEF (ST2)	(0.67)(0.33)	(Fe)(Sc)
Alpha_Mg3Sb2	CEF (SLN)	(0.6)(0.4)	(Mg)(Mg,Sb)
Alpha_Mn2B	CEF (ST2)	(0.670691) (0.329309)	(Mn)(B)
Alpha_Sc5Sn3	CEF (ST2)	(0.625)(0.375)	(Sc)(Sn)
Alpha_TiMn	CEF (ST2)	(1)(1)	(Mn)(Ti)
Alpha_WB	CEF (SLN)	(1)(1)	(W)(B,Va)
Alpha_YZn2	CEF (ST2)	(1)(2)	(Y)(Zn)
B12Er	CEF (ST2)	(0.9231) (0.0769)	(B)(Er)
B2	CEF (SLN)	(1)(1)	(Ag,Al,Bi,Co,Cr,Cu,Fe,Ni,Zn) (Ce,Co,Cr,Cu,Er,Fe,Gd,La,Ni, Sc,Y,Va)
B2Er	CEF (ST2)	(0.667)(0.333)	(B)(Er)
B2Hf	CEF (ST2)	(2)(1)	(B)(Hf)
B2O3	CEF (ST2)	(2)(3)	(B)(O)
B2Ti	CEF (ST2)	(1)(2)	(Ti)(B)
B32	CEF (SLN)	(0.5)(0.5)(3)	(Al,Li,Mg,Zn)(Al,Li,Mg,Zn)(Va)
B3Si	CEF (SLN)	(6)(2)(6)	(B)(Si)(B,Si)
B4C	CEF (SLN)	(1)(1)	(B12,B11C)(B2,B2C,BC2)
B4Er	CEF (ST2)	(0.8)(0.2)	(B)(Er)
B4Hf3	CEF (ST2)	(4)(3)	(B)(Hf)
B4Ti3	CEF (ST2)	(4)(3)	(B)(Ti)
B66Er	CEF (ST2)	(0.985)(0.015)	(B)(Er)
B6Si	CEF (SLN)	(210)(23)(48)	(B)(Si)(B,Si)

Name	Model	Lattice Size	Constitue
BCT_A5	CEF (SLN)	(1)	(Al,Bi,Cu,Pb,Sb,Sn,Zn)
BETA_ RHOMBO_B	CEF (SLN)	(93)(12)	(B)(B,Cu,Mn,Sc,Si,Zr)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
BHf	CEF (ST2)	(1)(1)	(B)(Hf)
BRONZE	CEF (SLN)	(2)(5)(1)	(V+4,V+5)(O-2)(Ca+2,Va)
BTi	CEF (ST2)	(1)(1)	(B)(Ti)
B_BeO	CEF (ST2)	(1)(1)	(Be)(O)
B_Li2M3	CEF (SLN)	(2)(3)	(Li,Zn)(Li,Zn)
B_Li2M5	CEF (SLN)	(2)(5)	(Li,Zn)(Zn)
B_LiM4	CEF (SLN)	(0.2)(0.8)(0.5)	(Al,Li,Zn)(Al,Li,Zn)(Va)
B_NSi	CEF (SLN)	(61)(1)(8)	(B)(Si)(B,Si)
Ba11Bi10	CEF (ST2)	(0.5238) (0.4762)	(Ba)(Bi)
Ba17Pb21	CEF (ST2)	(0.425)(0.575)	(Ba)(Pb)
Ba19Li44	CEF (ST2)	(44)(19)	(Li)(Ba)
Ba2Bi	CEF (ST2)	(0.666667) (0.333333)	(Ba)(Bi)
Ba2Ge	CEF (ST2)	(0.667)(0.333)	(Ba)(Ge)
Ba2Mg17	CEF (ST2)	(0.105)(0.895)	(Ba)(Mg)
Ba2Pb	CEF (ST2)	(0.667)(0.333)	(Ba)(Pb)
Ba2Si	CEF (ST2)	(2)(1)	(Ba)(Si)
Ba2Zn	CEF (ST2)	(2)(1)	(Ba)(Zn)
Ba3Si4	CEF (ST2)	(3)(4)	(Ba)(Si)
Ba4Bi3	CEF (ST2)	(0.5714) (0.4286)	(Ba)(Bi)

Name	Model	Lattice Size	Constitue
Ba5Bi3	CEF (ST2)	(0.625)(0.375)	(Ba)(Bi)
Ba5Ge3	CEF (ST2)	(0.625)(0.375)	(Ba)(Ge)
Ba5Pb3	CEF (ST2)	(0.625)(0.375)	(Ba)(Pb)
Ba5Si3	CEF (ST2)	(5)(3)	(Ba)(Si)
Ba6Ge25	CEF (ST2)	(0.194)(0.806)	(Ba)(Ge)
Ba6Mg23	CEF (ST2)	(0.207)(0.793)	(Ba)(Mg)
Ba8Ge43	CEF (ST2)	(0.157)(0.843)	(Ba)(Ge)
BaBi3	CEF (ST2)	(0.25)(0.75)	(Ba)(Bi)
BaCu	CEF (ST2)	(1)(1)	(Ba)(Cu)
BaGe	CEF (ST2)	(0.5)(0.5)	(Ba)(Ge)
BaGe2	CEF (ST2)	(0.333)(0.667)	(Ba)(Ge)
BaLi4	CEF (ST2)	(4)(1)	(Li)(Ba)
BaM13	CEF (SLN)	(1)(13)	(Ba)(Be,Cu,Zn)
BaMg2	CEF (ST2)	(0.333)(0.667)	(Ba)(Mg)
BaO2	CEF (ST2)	(1)(2)	(Ba)(O)
BaPb	CEF (ST2)	(0.5)(0.5)	(Ba)(Pb)
BaPb3	CEF (ST2)	(0.25)(0.75)	(Ba)(Pb)
BaSi	CEF (ST2)	(1)(1)	(Ba)(Si)
BaSi2	CEF (ST2)	(1)(2)	(Ba)(Si)
BaZn	CEF (ST2)	(1)(1)	(Ba)(Zn)
BaZn2	CEF (ST2)	(1)(2)	(Ba)(Zn)
BaZn5	CEF (ST2)	(1)(5)	(Ba)(Zn)
Bcc	CEF (SLN)	(1)(3)	(Ag,Al,Ba,Be,Bi,Ca,Ce,Co,Cr,Cu, Er,Fe,Gd,Ge,Hf,K,La,Li,Mg,Mn, Na,Nb,Ni,Pb,Sb,Sc,Si,Sn,Sr,Ti, V,W,Y,Zn,Zr)(B,C,O,Va)

Name	Model	Lattice Size	Constitue
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Ag,Al,Cu,Er,Fe,Mg,Si) (Ag,Al,Cu,Er,Fe,Mg,Si)(Va)
Beta_AlFeSi	CEF (SLN)	(0.598)(0.152) (0.1)(0.15)	(Al)(Fe,Mn,Ni)(Si)(Al,Si)
Beta_Bi2Mg3	CEF (SLN)	(1)(3)(6)	(Bi)(Bi,Va)(Mg)
Beta_BiMn	CEF (ST2)	(0.481)(0.519)	(Bi)(Mn)
Beta_CeC2	CEF (ST2)	(0.333333) (0.666667)	(Ce)(C)
Beta_Co2Si	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Beta_Co5Ge3	CEF (SLN)	(0.125)(0.5) (0.375)	(Co,Va)(Co)(Co,Ge)
Beta_Cr5Ge3	CEF (SLN)	(0.625)(0.375)	(Cr,Ge)(Cr,Ge)
Beta_Cr5Si3	CEF (SLN)	(0.625)(0.375)	(Cr)(Cr,Si)
Beta_Fe2Sc	CEF (ST2)	(0.67)(0.33)	(Fe)(Sc)
Beta_Mg3Sb2	CEF (SLN)	(0.4)(0.5)(0.1)	(Mg,Sb)(Mg,Sb)(Mg)
Beta_Mn2B	CEF (ST2)	(0.666667) (0.333333)	(Mn)(B)
Beta_Ni3Ge	CEF (SLN)	(0.75)(0.25) (1)	(Ge,Ni)(Ge,Ni)(Va)
Beta_Sc5Sn3	CEF (ST2)	(0.625)(0.375)	(Sc)(Sn)
Beta_SrZn5	CEF (ST2)	(1)(5)	(Sr)(Zn)
Beta_TiMn	CEF (ST2)	(0.515)(0.485)	(Mn)(Ti)
Beta_WB	CEF (SLN)	(1)(1)	(W)(B,Va)
Beta_YZn2	CEF (ST2)	(1)(2)	(Y)(Zn)
Bi2La	CEF (ST2)	(2)(1)	(Bi)(La)
Bi3La4	CEF (ST2)	(3)(4)	(Bi)(La)

Name	Model	Lattice Size	Constitue
Bi3La5	CEF (ST2)	(3)(5)	(Bi)(La)
Bi3Ni	CEF (ST2)	(0.75)(0.25)	(Bi)(Ni)
Bi3R5_oP32	CEF (SLN)	(0.625)(0.375)	(Er,Gd)(Bi)
BiLa	CEF (ST2)	(1)(1)	(Bi)(La)
BiLa2	CEF (ST2)	(1)(2)	(Bi)(La)
BiNi	CEF (SLN)	(0.3334) (0.3333) (0.3333)	(Bi)(Ni,Va)(Ni,Va)
C14	CEF (SLN)	(1)(2)	(Al,Ca,Co,Cr,Cu,Er,Fe,Mg,Mn,Nb, Ni,Si,Ti,Zn,Zr)(Al,Co,Cr,Cu,Er,Fe, Li,Mg,Mn,Nb,Ni,Si,Ti,W,Zn,Zr)
C15	CEF (SLN)	(1)(2)	(Al,Ca,Ce,Co,Cr,Cu,Er,Fe,Hf,Gd, La,Li,Mg,Nb,Ni,Si,Ti,Y,Zn,Zr) (Al,Co,Cr,Cu,Er,Fe,Li,Mg,Nb,Ni, Si,Ti,W,Zn,Zr)
C2V3	CEF (ST2)	(2)(3)	(C)(V)
C2V_5	CEF (ST3)	(2)(2)(7)	(Ca+2)(V+5)(O-2)
C36	CEF (SLN)	(1)(2)	(Al,Co,Cr,Cu,Fe,Mg,Nb,Ni,Si,Ti,Zn,Zr) (Al,Co,Cr,Cu,Fe,Mg,Ni,Si,Ti,Zn,Zr)
C3V_5	CEF (ST3)	(3)(2)(8)	(Ca+2)(V+5)(O-2)
C4V_5	CEF (ST3)	(4)(2)(9)	(Ca+2)(V+5)(O-2)
C5	CEF (ST3)	(5)(3)(9.5)	(Ca+2)(V+3)(O-2)
C9	CEF (ST3)	(9)(6)(18)	(Ca+2)(V+3)(O-2)
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Ce,Co,Cr,Cu,Fe,Mg,Mn,Nb,Si, Sn,Sr,Ni,Ti,V,Zn,Zr)(C,Va)
CL_MgSi	CEF (SLN)	(1)	(Mg,Si)
CUB_A13	CEF (SLN)	(1)(1)	(Ag,Al,Ce,Co,Cr,Cu,Fe,Ge,Hf,Mg,Mn,

Name	Model	Lattice Size	Constitue
			Nb,Ni,Si,Sn,Sr,Ti,V,Zn,Zr)(C,Va)
CV2_4	CEF (ST3)	(1)(2)(5)	(Ca+2)(V+4)(O-2)
CV3_4	CEF (ST3)	(1)(3)(7)	(Ca+2)(V+4)(O-2)
CV4_4	CEF (ST3)	(1)(4)(9)	(Ca+2)(V+4)(O-2)
CV_3	CEF (ST3)	(1)(2)(4)	(Ca+2)(V+3)(O-2)
CV_4	CEF (ST3)	(1)(1)(3)	(Ca+2)(V+4)(O-2)
CV_5	CEF (ST3)	(1)(2)(6)	(Ca+2)(V+5)(O-2)
C_Ce2O3	CEF (SLN)	(2)(3)(1)	(Ce+3,Ce+4)(O-2)(O-2,Va)
Ca14Si19	CEF (ST2)	(0.424242) (0.575757)	(Ca)(Si)
Ca2Cu	CEF (ST2)	(0.666667) (0.333333)	(Ca)(Cu)
Ca2Ni7	CEF (ST2)	(0.222222) (0.777778)	(Ca)(Ni)
Ca2Pb	CEF (ST2)	(0.667)(0.333)	(Ca)(Pb)
Ca2Si	CEF (ST2)	(0.666667) (0.333333)	(Ca)(Si)
Ca2Sn	CEF (ST2)	(1)(1)(1)	(Ca)(Ca)(Sn)
Ca31Sn20	CEF (ST2)	(31)(20)	(Ca)(Sn)
Ca36Sn23	CEF (ST2)	(36)(23)	(Ca)(Sn)
Ca3Si4	CEF (ST2)	(0.428571) (0.571428)	(Ca)(Si)
Ca3Zn	CEF (ST2)	(3)(1)	(Ca)(Zn)
Ca5Pb3	CEF (ST2)	(0.625)(0.375)	(Ca)(Pb)
Ca5Si3	CEF (ST2)	(0.625)(0.375)	(Ca)(Si)
Ca5Sn3	CEF (ST2)	(5)(3)	(Ca)(Sn)

Name	Model	Lattice Size	Constitue
Ca5Zn3	CEF (ST2)	(5)(3)	(Ca)(Zn)
Ca7Sn6	CEF (ST2)	(7)(6)	(Ca)(Sn)
CaB6	CEF (ST2)	(1)(6)	(Ca)(B)
CaCu	CEF (ST2)	(0.5)(0.5)	(Ca)(Cu)
CaCu5	CEF (ST2)	(0.166667) (0.833333)	(Ca)(Cu)
CaLi2	CEF (ST2)	(0.333333) (0.666667)	(Ca)(Li)
CaNi2	CEF (ST2)	(0.333333) (0.666667)	(Ca)(Ni)
CaNi3	CEF (ST2)	(0.25)(0.75)	(Ca)(Ni)
CaNi5	CEF (ST2)	(0.166667) (0.833333)	(Ca)(Ni)
CaPb	CEF (ST2)	(0.5)(0.5)	(Ca)(Pb)
CaPb3	CEF (ST2)	(0.25)(0.75)	(Ca)(Pb)
CaSi	CEF (ST2)	(0.5)(0.5)	(Ca)(Si)
CaSi2	CEF (ST2)	(0.333333) (0.666667)	(Ca)(Si)
CaSn	CEF (ST2)	(1)(1)	(Ca)(Sn)
CaSn3	CEF (ST2)	(1)(3)	(Ca)(Sn)
CaZn	CEF (ST2)	(1)(1)	(Ca)(Zn)
CaZn11	CEF (ST2)	(1)(11)	(Ca)(Zn)
CaZn13	CEF (ST2)	(1)(13)	(Ca)(Zn)
CaZn2	CEF (ST2)	(1)(2)	(Ca)(Zn)
CaZn3	CEF (ST2)	(1)(3)	(Ca)(Zn)
CaZn5	CEF (ST2)	(1)(5)	(Ca)(Zn)

Name	Model	Lattice Size	Constitue
Ce11O20	CEF (ST2)	(11)(20)	(Ce)(O)
Ce19O34	CEF (ST2)	(19)(34)	(Ce)(O)
Ce2C3	CEF (ST2)	(0.4)(0.6)	(Ce)(C)
Ce2Fe17	CEF (SLN)	(2)(17)	(Ce)(Al,Fe)
Ce2Mg17	CEF (ST2)	(2)(17)	(Ce)(Mg)
Ce2Sb	CEF (ST2)	(2)(1)	(Ce)(Sb)
Ce2Zn17	CEF (ST2)	(0.105)(0.895)	(Ce)(Zn)
Ce3Si2	CEF (ST2)	(0.6)(0.4)	(Ce)(Si)
Ce3Si5	CEF (ST2)	(0.375)(0.625)	(Ce)(Si)
Ce40O72	CEF (ST2)	(40)(72)	(Ce)(O)
Ce4Sb3	CEF (ST2)	(4)(3)	(Ce)(Sb)
Ce5Mg41	CEF (ST2)	(5)(41)	(Ce)(Mg)
Ce5Si3	CEF (ST2)	(0.625)(0.375)	(Ce)(Si)
Ce5Si4	CEF (ST2)	(0.555556) (0.444444)	(Ce)(Si)
Ce62O112	CEF (ST2)	(62)(112)	(Ce)(O)
Ce7Ni3	CEF (ST2)	(0.7)(0.3)	(Ce)(Ni)
Ce7O12	CEF (ST2)	(7)(12)	(Ce)(O)
Ce9O16	CEF (ST2)	(9)(16)	(Ce)(O)
CeFe2	CEF (ST2)	(1)(2)	(Ce)(Fe)
CeMg	CEF (SLN)	(0.5)(0.5)	(Ce)(Al,Mg)
CeMg12	CEF (SLN)	(1)(12)	(Ce)(Al,Mg)
CeMg2	CEF (ST2)	(0.333333) (0.666667)	(Ce)(Mg)
CeMg3	CEF (ST2)	(1)(3)	(Ce)(Mg)

Name	Model	Lattice Size	Constitue
CeNi	CEF (ST2)	(0.5)(0.5)	(Ce)(Ni)
CeNi2	CEF (ST2)	(0.3333) (0.6667)	(Ce)(Ni)
CeNi3	CEF (ST2)	(0.25)(0.75)	(Ce)(Ni)
CeNi5	CEF (ST2)	(0.1667) (0.8333)	(Ce)(Ni)
CeSb	CEF (ST2)	(1)(1)	(Ce)(Sb)
CeSb2	CEF (ST2)	(1)(2)	(Ce)(Sb)
CeSi	CEF (ST2)	(0.5)(0.5)	(Ce)(Si)
CeSi2	CEF (ST2)	(0.333333) (0.666667)	(Ce)(Si)
CeZn	CEF (ST2)	(0.5)(0.5)	(Ce)(Zn)
CeZn11	CEF (ST2)	(0.083)(0.917)	(Ce)(Zn)
Cementite	CEF (ST2)	(3)(1)	(Fe)(C)
Co11Ce24	CEF (ST2)	(11)(24)	(Co)(Ce)
Co13La	CEF (ST2)	(0.929)(0.071)	(Co)(La)
Co17Ce2	CEF (ST2)	(17)(2)	(Co)(Ce)
Co17Er2	CEF (ST2)	(17)(2)	(Co)(Er)
Co17Y2	CEF (ST2)	(17)(2)	(Co)(Y)
Co19Ce5	CEF (ST2)	(19)(5)	(Co)(Ce)
Co19La5	CEF (ST2)	(0.792)(0.208)	(Co)(La)
Co23La27	CEF (ST2)	(0.46)(0.54)	(Co)(La)
Co2B	CEF (ST2)	(2)(1)	(Co)(B)
Co2Ce	CEF (ST2)	(2)(1)	(Co)(Ce)
Co2Er	CEF (ST2)	(2)(1)	(Co)(Er)

Name	Model	Lattice Size	Constitue
Co2Sc	CEF (SLN)	(0.67)(0.33)	(Co,Sc)(Co,Sc)
Co2Y	CEF (ST2)	(2)(1)	(Co)(Y)
Co2Zn15	CEF (ST2)	(0.117647) (0.882353)	(Co)(Zn)
Co3B	CEF (SLN)	(3)(1)	(Co,Fe)(B)
Co3Ce	CEF (ST2)	(3)(1)	(Co)(Ce)
Co3Er	CEF (ST2)	(3)(1)	(Co)(Er)
Co3Ge	CEF (ST2)	(0.75)(0.25)	(Co)(Ge)
Co3La2	CEF (ST2)	(0.6)(0.4)	(Co)(La)
Co3Si	CEF (ST2)	(0.75)(0.25)	(Co)(Si)
Co3Sn2	CEF (SLN)	(1)(1)(0.5) (0.5)	(Co)(Sn)(Co,Va)(Co,Va)
Co3W	CEF (SLN)	(0.75)(0.25)	(Co)(Co,W)
Co3Y	CEF (ST2)	(3)(1)	(Co)(Y)
Co3Y2	CEF (ST2)	(3)(2)	(Co)(Y)
Co3Y4	CEF (ST2)	(3)(4)	(Co)(Y)
Co4Zn	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
Co5Ce	CEF (ST2)	(5)(1)	(Co)(Ce)
Co5Er	CEF (ST2)	(5)(1)	(Co)(Er)
Co5Ge2	CEF (ST2)	(0.714)(0.286)	(Co)(Ge)
Co5Ge7	CEF (ST2)	(0.417)(0.583)	(Co)(Ge)
Co5La	CEF (ST2)	(0.833)(0.167)	(Co)(La)
Co5Y	CEF (ST2)	(5)(1)	(Co)(Y)
Co5Y8	CEF (ST2)	(5)(8)	(Co)(Y)
Co7Ce2	CEF (ST2)	(7)(2)	(Co)(Ce)

Name	Model	Lattice Size	Constitue
Co7Er12	CEF (ST2)	(7)(12)	(Co)(Er)
Co7Er2	CEF (ST2)	(7)(2)	(Co)(Er)
Co7La2	CEF (ST2)	(0.777)(0.223)	(Co)(La)
Co7Nb2	CEF (ST2)	(7)(2)	(Co)(Nb)
Co7Y2	CEF (SLN)	(7)(2)	(Co)(Ce,Y)
Co7Y6	CEF (ST2)	(7)(6)	(Co)(Y)
CoB	CEF (ST2)	(1)(1)	(Co)(B)
CoEr3	CEF (ST2)	(1)(3)	(Co)(Er)
CoGe	CEF (SLN)	(0.5)(0.5)	(Co,Ge)(Co,Ge)
CoGe2	CEF (ST2)	(0.333)(0.667)	(Co)(Ge)
CoLa3	CEF (ST2)	(0.25)(0.75)	(Co)(La)
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)
CoSc	CEF (ST2)	(0.52)(0.48)	(Co)(Sc)
CoSc2	CEF (ST2)	(0.33)(0.67)	(Co)(Sc)
CoSc3	CEF (ST2)	(0.23)(0.77)	(Co)(Sc)
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)

Name	Model	Lattice Size	Constitue
CoY	CEF (ST2)	(1)(1)	(Co)(Y)
CoY3	CEF (ST2)	(1)(3)	(Co)(Y)
CoZn	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
CoZn14	CEF (ST2)	(0.0714286) (0.928571)	(Co)(Zn)
CoZn7	CEF (ST2)	(0.125)(0.875)	(Co)(Zn)
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)
Cr2Hf_C14	CEF (SLN)	(2)(1)	(Cr,Hf)(Cr,Hf)
Cr2Hf_C15	CEF (SLN)	(2)(1)	(Cr,Hf)(Cr,Hf)
Cr2Hf_C36	CEF (SLN)	(2)(4)(6)	(Cr)(Cr,Hf)(Cr,Hf)
Cr3B4	CEF (ST2)	(0.429)(0.571)	(Cr)(B)
Cr3Ge	CEF (SLN)	(0.75)(0.25)	(Cr,Ge)(Cr,Ge)
Cr3Mn5	CEF (ST2)	(3)(5)	(Cr)(Mn)
Cr5B3	CEF (ST2)	(0.625)(0.375)	(Cr)(B)
CrB	CEF (ST2)	(0.5)(0.5)	(Cr)(B)
CrB2	CEF (SLN)	(0.333)(0.667)	(Cr)(B,Va)
CrB4	CEF (ST2)	(0.2)(0.8)	(Cr)(B)
CrGe	CEF (ST2)	(0.5)(0.5)	(Cr)(Ge)
CrZn17	CEF (ST2)	(0.05556) (0.94444)	(Cr)(Zn)
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
Cu10Hf7	CEF (ST2)	(10)(7)	(Cu)(Hf)

Name	Model	Lattice Size	Constitue
Cu10Sb3	CEF (ST2)	(0.77)(0.23)	(Cu)(Sb)
Cu10Sn3	CEF (ST2)	(0.769)(0.231)	(Cu)(Sn)
Cu10Zr7	CEF (ST2)	(10)(7)	(Cu)(Zr)
Cu16Mg6Si7	CEF (ST3)	(0.551724) (0.206897) (0.241379)	(Cu)(Mg)(Si)
Cu17Sb3	CEF (ST2)	(0.85)(0.15)	(Cu)(Sb)
Cu2Ce	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Ce)
Cu2Er	CEF (SLN)	(0.6667) (0.3333)	(Al,Cu)(Er)
Cu2Gd	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Gd)
Cu2La	CEF (ST2)	(0.666667) (0.333333)	(Cu)(La)
Cu2O	CEF (ST2)	(2)(1)	(Cu)(O)
Cu2Sb	CEF (ST2)	(0.67)(0.33)	(Cu)(Sb)
Cu2Sc	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Sc)
Cu2Ti	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Ti)
Cu2Y_H	CEF (ST2)	(2)(1)	(Cu)(Y)
Cu2Y_R	CEF (ST2)	(2)(1)	(Cu)(Y)
Cu37La3	CEF (ST2)	(37)(3)	(Cu)(La)
Cu3Mg2Si	CEF (ST3)	(3)(2)(1)	(Cu)(Mg)(Si)
Cu3Sb	CEF (ST2)	(0.75)(0.25)	(Cu)(Sb)

Name	Model	Lattice Size	Constitue
Cu3Sn	CEF (ST2)	(0.75)(0.25)	(Cu)(Sn)
Cu3Ti2	CEF (ST2)	(0.6)(0.4)	(Cu)(Ti)
Cu41Sn11	CEF (ST2)	(0.788)(0.212)	(Cu)(Sn)
Cu4Ce	CEF (SLN)	(0.8)(0.2)	(Al,Cu)(Ce)
Cu4La	CEF (ST2)	(0.8)(0.2)	(Cu)(La)
Cu4Sb	CEF (ST2)	(0.8)(0.2)	(Cu)(Sb)
Cu4Sc	CEF (ST2)	(0.8)(0.2)	(Cu)(Sc)
Cu4Ti	CEF (SLN)	(0.8)(0.2)	(Cu,Ti)(Cu,Ti)
Cu4Ti3	CEF (ST2)	(0.57143) (0.42857)	(Cu)(Ti)
Cu4Y	CEF (ST2)	(4)(1)	(Cu)(Y)
Cu51Hf14	CEF (ST2)	(51)(14)	(Cu)(Hf)
Cu51Zr14	CEF (ST2)	(51)(14)	(Cu)(Zr)
Cu5Ce	CEF (SLN)	(0.833333) (0.166667)	(Al,Cu)(Ce)
Cu5Er	CEF (ST2)	(0.8333) (0.1667)	(Cu)(Er)
Cu5Gd_H	CEF (ST2)	(0.833333) (0.166667)	(Cu)(Gd)
Cu5Gd_L	CEF (ST2)	(0.833333) (0.166667)	(Cu)(Gd)
Cu5Hf	CEF (ST2)	(5)(1)	(Cu)(Hf)
Cu5La	CEF (ST2)	(0.833333) (0.166667)	(Cu)(La)
Cu5Sr	CEF (ST2)	(5)(1)	(Cu)(Sr)
Cu5Zr	CEF (ST2)	(5)(1)	(Cu)(Zr)

Name	Model	Lattice Size	Constitue
Cu6Ce	CEF (ST2)	(0.857143) (0.142857)	(Cu)(Ce)
Cu6Gd	CEF (ST2)	(0.857143) (0.142857)	(Cu)(Gd)
Cu6La	CEF (ST2)	(0.857143) (0.142857)	(Cu)(La)
Cu6La_L	CEF (ST2)	(0.857143) (0.142857)	(Cu)(La)
Cu6Sn5	CEF (ST2)	(0.545)(0.455)	(Cu)(Sn)
Cu6Sn5_L	CEF (ST2)	(0.545)(0.455)	(Cu)(Sn)
Cu6Y	CEF (SLN)	(5)(1)	(Cu)(Cu2,Y)
Cu7Er2	CEF (ST2)	(0.7778) (0.2222)	(Cu)(Er)
Cu7Gd2	CEF (ST2)	(0.777778) (0.222222)	(Cu)(Gd)
Cu7Y2	CEF (ST2)	(7)(2)	(Cu)(Y)
Cu8Hf3	CEF (ST2)	(8)(3)	(Cu)(Hf)
Cu8Zr3	CEF (ST2)	(8)(3)	(Cu)(Zr)
Cu9Er2	CEF (ST2)	(0.8182) (0.1818)	(Cu)(Er)
Cu9Gd2	CEF (ST2)	(0.818182) (0.181818)	(Cu)(Gd)
CuCe	CEF (ST2)	(0.5)(0.5)	(Ce)(Cu)
CuEr	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Er)
CuGd_H	CEF (ST2)	(0.5)(0.5)	(Cu)(Gd)
CuHf2	CEF (ST2)	(1)(2)	(Cu)(Hf)

Name	Model	Lattice Size	Constitue
CuLa	CEF (ST2)	(0.5)(0.5)	(Cu)(La)
CuMg2	CEF (ST2)	(0.33333) (0.66667)	(Cu)(Mg)
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuSc	CEF (ST2)	(0.5)(0.5)	(Cu)(Sc)
CuSr	CEF (ST2)	(0.5)(0.5)	(Cu)(Sr)
CuTi	CEF (SLN)	(0.5)(0.5)	(Cu,Ti)(Cu,Ti)
CuTi2	CEF (ST2)	(0.333333) (0.666667)	(Cu)(Ti)
CuY	CEF (ST2)	(1)(1)	(Cu)(Y)
CuZr	CEF (ST2)	(0.5)(0.5)	(Cu)(Zr)
DHCP	CEF (SLN)	(1)	(Ag,Al,Bi,Ca,Ce,La,Mg,Mn, Ni,Sc,Y,Zn)
DISORDER	CEF (SLN)	(1)(1)	(Ag,Al,Cr,Er,Mg,Ni,Sc,Si)(Va)
DO3	CEF (SLN)	(0.75)(0.25)	(Cu,Sn)(Cu,Sn)
D_Bi2O3	CEF (ST2)	(2)(3)	(Bi)(O)
DeltaP_Sb3Zn4	CEF (ST2)	(3.094)(3.906)	(Sb)(Zn)
Delta_AlFeSi	CEF (SLN)	(5)(1)	(Al,Si)(Fe)
Delta_Cu33Si7	CEF (ST2)	(0.825)(0.175)	(Cu)(Si)
Delta_Ni3Sb	CEF (SLN)	(0.75)(0.25)	(Ni)(Ni,Sb)
Delta_Sb3Zn4	CEF (ST2)	(3.087)(3.913)	(Sb)(Zn)
Delta_hR9	CEF (SLN)	(0.55)(0.45)	(Ce,La)(Er)
Diamond	CEF (SLN)	(1)	(Ag,Al,B,C,Gd,Ge,Nb,Sb,Si, Sn,Sr,Ti,Zn)
ETA_PRIME	CEF (SLN)	(1)(2)	(Al,Cu,Mg,Zn)(Al,Cu,Mg,Zn)
Eps	CEF (SLN)	(1)(1)	(Al,Cu,Zn)(Va)

Name	Model	Lattice Size	Constitue
Eps_CuGe	CEF (ST2)	(0.765)(0.235)	(Cu)(Ge)
Epsilon	CEF (ST2)	(0.375)(0.625)	(Ge)(Ni)
Epsilon_Cu15Si4	CEF (SLN)	(0.789474) (0.210526)	(Cu,Mg)(Si)
Er11Ge10	CEF (ST2)	(0.523)(0.477)	(Er)(Ge)
Er12Zn17_HT	CEF (ST2)	(2)(17)	(Er)(Zn)
Er12Zn17_LT	CEF (ST2)	(2)(17)	(Er)(Zn)
Er13Zn58	CEF (ST2)	(13)(58)	(Er)(Zn)
Er2Fe17	CEF (ST2)	(2)(17)	(Er)(Fe)
Er2Ge3_HT	CEF (ST2)	(0.4)(0.6)	(Er)(Ge)
Er2Ge3_LT	CEF (ST2)	(0.4)(0.6)	(Er)(Ge)
Er2Ge5	CEF (ST2)	(0.2847) (0.7143)	(Er)(Ge)
Er3Ge4	CEF (ST2)	(0.428)(0.571)	(Er)(Ge)
Er5Ge3	CEF (SLN)	(0.625)(0.375)	(Er,Ge)(Ge)
Er5Ge4	CEF (ST2)	(0.556)(0.444)	(Er)(Ge)
Er5Si3	CEF (ST2)	(5)(3)	(Er)(Si)
Er5Si4	CEF (ST2)	(5)(4)	(Er)(Si)
Er6Fe23	CEF (ST2)	(6)(23)	(Er)(Fe)
ErFe2	CEF (ST2)	(1)(2)	(Er)(Fe)
ErFe3	CEF (ST2)	(1)(3)	(Er)(Fe)
ErGe	CEF (ST2)	(0.5)(0.5)	(Er)(Ge)
ErGe2_HT	CEF (ST2)	(0.333)(0.667)	(Er)(Ge)
ErGe2_LT	CEF (ST2)	(0.333)(0.667)	(Er)(Ge)
ErGe2_MT	CEF (ST2)	(0.333)(0.667)	(Er)(Ge)

Name	Model	Lattice Size	Constitue
ErSix	CEF (ST2)	(1)(0.96)	(Er)(Si)
ErZn12	CEF (ST2)	(1)(12)	(Er)(Zn)
ErZn2	CEF (ST2)	(1)(2)	(Er)(Zn)
ErZn3	CEF (ST2)	(1)(3)	(Er)(Zn)
ErZn5	CEF (ST2)	(1)(5)	(Er)(Zn)
Eta_Cu19Si6	CEF (SLN)	(0.76)(0.24)	(Cu,Mg)(Si)
Eta_CuGe	CEF (ST2)	(0.75)(0.25)	(Cu)(Ge)
Eta_Sb2Zn3	CEF (ST2)	(2)(3)	(Sb)(Zn)
F_Ce2O4	CEF (SLN)	(2)(4)	(Ce+3,Ce+4)(O-2,Va)
Fcc	CEF (SLN)	(1)(1)	(Ag,Al,Ba,Be,Bi,Ca,Ce,Co,Cr, Cu,Er,Fe,Gd,Ge,Hf,K,La,Li,Mg, Mn,Na,Nb,Ni,Pb,Sb,Sc,Si,Sn, Sr,Ti,V,W,Y,Zn,Zr)(B,C,O,Va)
Fe17Gd2_H	CEF (ST2)	(17)(2)	(Fe)(Gd)
Fe17Gd2_L	CEF (ST2)	(17)(2)	(Fe)(Gd)
Fe17Y2	CEF (ST2)	(17)(2)	(Fe)(Y)
Fe23Gd6	CEF (ST2)	(23)(6)	(Fe)(Gd)
Fe23Y6	CEF (ST2)	(23)(6)	(Fe)(Y)
Fe2B	CEF (ST2)	(2)(1)	(Fe)(B)
Fe2Gd	CEF (ST2)	(2)(1)	(Fe)(Gd)
Fe2Hf_C14	CEF (SLN)	(0.6667) (0.3333)	(Fe)(Fe,Hf)
Fe2Hf_C15	CEF (ST2)	(0.6667) (0.3333)	(Fe)(Hf)
Fe2Hf_C36	CEF (ST2)	(0.6667) (0.3333)	(Fe)(Hf)

Name	Model	Lattice Size	Constitue
Fe2Si	CEF (SLN)	(0.666667) (0.333333)	(Fe)(Si,Sn)
Fe2Y	CEF (ST2)	(2)(1)	(Fe)(Y)
Fe3Gd	CEF (ST2)	(3)(1)	(Fe)(Gd)
Fe3Sn2	CEF (ST2)	(3)(2)	(Fe)(Sn)
Fe3Y	CEF (ST2)	(3)(1)	(Fe)(Y)
Fe5Si3	CEF (SLN)	(0.625)(0.375)	(Fe,Ni)(Si)
Fe5Sn3	CEF (ST2)	(5)(3)	(Fe)(Sn)
Fe6Sc29	CEF (ST2)	(0.17)(0.83)	(Fe)(Sc)
FeB	CEF (ST2)	(1)(1)	(Fe)(B)
FeHf2	CEF (ST2)	(0.3333) (0.6667)	(Fe)(Hf)
FeSb	CEF (SLN)	(0.3333) (0.3333) (0.3333)	(Sb)(Fe,Va)(Fe,Va)
FeSb2	CEF (ST2)	(0.3333) (0.6667)	(Fe)(Sb)
FeSi2_H	CEF (ST2)	(3)(7)	(Fe)(Si)
FeSi2_L	CEF (ST2)	(1)(2)	(Fe)(Si)
FeSn	CEF (ST2)	(1)(1)	(Fe)(Sn)
FeSn2	CEF (ST2)	(1)(2)	(Fe)(Sn)
FeTi	CEF (ST2)	(1)(1)	(Fe)(Ti)
FeZn_Delta	CEF (SLN)	(0.058)(0.18) (0.525)(0.237)	(Fe)(Al,Fe,Zn)(Zn)(Zn)
FeZn_Gamma	CEF (SLN)	(0.154)(0.154) (0.231)(0.461)	(Fe,Zn)(Fe,Zn)(Al,Fe,Zn)(Zn)

Name	Model	Lattice Size	Constitue
FeZn_Gamma1	CEF (SLN)	(0.137)(0.118) (0.745)	(Fe)(Al,Fe,Zn)(Zn)
FeZn_Zeta	CEF (SLN)	(0.072)(0.856) (0.072)	(Fe,Va)(Al,Zn)(Al,Zn,Va)
FeZr2	CEF (SLN)	(1)(2)	(Al,Fe,Zr)(Zr)
FeZr3	CEF (SLN)	(1)(3)	(Al,Fe,Zr)(Fe,Zr)
GP_MgSi	CEF (ST2)	(1)(1)	(Mg)(Si)
G_Al12CrMn	CEF (SLN)	(12)(1)	(Al)(Cr,Mn)
Gamma	CEF (SLN)	(1)(1)	(Al,Cu,Si,Zn)(Va)
Gamma2	CEF (SLN)	(0.255)(0.745)	(Al,Fe,Zn)(Zn)
Gamma_AlFeSi	CEF (ST3)	(0.635)(0.205) (0.16)	(Al)(Fe)(Si)
Gamma_ Cu56Si11	CEF (SLN)	(0.835821) (0.164179)	(Cu,Mg)(Si)
Gamma_H	CEF (SLN)	(4)(1)(8)	(Al,Zn)(Al,Cu,Zn)(Ag,Cu)
Gamma_Ni3Ge	CEF (ST2)	(0.256)(0.744)	(Ge)(Ni)
Gas	GAS	(1)	(Ag,Al,AlO,AlO2,Al2,Al2O,Al2O2, Al2O3,C1O1,C1O2,Ca,CaO,Fe, FeO,FeO2,Fe2,Gd,Hf,HfO,HfO2, La,La2O,La2O2,LaO,Li,Li2,Li2O, Li2O2,Mg,Mg2,MgO,Mn,Na,O,O2, O3,Pb,Pb2,PbO,Pb2O2,Pb3O3, Pb4O4,Pb5O5,Pb6O6,Sc,Sc2,ScO, Sn,Sn2,SnO,SnO2,Si,Si2,Si3,SiO, SiO2,Sr,Sr2O,SrO,Ti,TiO,TiO2,Y, YO,Zn,Zr,Zr2,ZrO,ZrO2)
Gd13Zn58	CEF (ST2)	(0.183)(0.817)	(Gd)(Zn)

Name	Model	Lattice Size	Constitue
Gd16Sb39	CEF (ST2)	(16)(39)	(Gd)(Sb)
Gd2Ni17	CEF (ST2)	(2)(17)	(Gd)(Ni)
Gd2Ni7	CEF (ST2)	(2)(7)	(Gd)(Ni)
Gd2Zn17	CEF (ST2)	(2)(17)	(Gd)(Zn)
Gd3Ni	CEF (ST2)	(3)(1)	(Gd)(Ni)
Gd3Ni2	CEF (ST2)	(3)(2)	(Gd)(Ni)
Gd3Si5	CEF (ST2)	(0.375)(0.625)	(Gd)(Si)
Gd3Zn11	CEF (ST2)	(0.214)(0.786)	(Gd)(Zn)
Gd3Zn22	CEF (ST2)	(0.12)(0.88)	(Gd)(Zn)
Gd4Bi3	CEF (ST2)	(0.5714) (0.4286)	(Gd)(Bi)
Gd4Sb3	CEF (ST2)	(4)(3)	(Gd)(Sb)
Gd5Sb3	CEF (ST2)	(0.625)(0.375)	(Gd)(Sb)
Gd5Si3	CEF (SLN)	(0.625)(0.375)	(Gd)(Sb,Si)
Gd5Si4	CEF (ST2)	(0.5556) (0.4444)	(Gd)(Si)
GdBi2	CEF (ST2)	(0.333)(0.667)	(Gd)(Bi)
GdMg2_X	CEF (ST2)	(0.333333) (0.666667)	(Gd)(Mg)
GdMg3_X	CEF (ST2)	(0.25)(0.75)	(Gd)(Mg)
GdMg5	CEF (ST2)	(0.166667) (0.833333)	(Gd)(Mg)
GdNi	CEF (ST2)	(1)(1)	(Gd)(Ni)
GdNi4	CEF (ST2)	(1)(4)	(Gd)(Ni)
GdSi	CEF (ST2)	(0.5)(0.5)	(Gd)(Si)
GdSi2	CEF (ST2)	(0.3333)	(Gd)(Si)

Name	Model	Lattice Size	Constitue
		(0.6667)	
GdZn	CEF (ST2)	(0.5)(0.5)	(Gd)(Zn)
GdZn12	CEF (ST2)	(1)(12)	(Gd)(Zn)
GdZn2	CEF (ST2)	(0.333333) (0.666667)	(Gd)(Zn)
GdZn3	CEF (ST2)	(1)(3)	(Gd)(Zn)
Ge10Sc11	CEF (ST2)	(0.47619) (0.52381)	(Ge)(Sc)
Ge2Sc	CEF (ST2)	(0.666667) (0.333333)	(Ge)(Sc)
Ge2Sr	CEF (ST2)	(0.666667) (0.333333)	(Ge)(Sr)
Ge2Ti	CEF (ST2)	(2)(1)	(Ge)(Ti)
Ge31V17	CEF (ST2)	(0.646)(0.354)	(Ge)(V)
Ge3Sc5	CEF (SLN)	(0.375)(0.625)	(Ge,Sc)(Ge,Sc)
Ge3Sr5	CEF (ST2)	(0.375)(0.625)	(Ge)(Sr)
Ge3Ti5	CEF (ST2)	(3)(5)	(Ge)(Ti)
Ge3V5	CEF (ST2)	(0.375)(0.625)	(Ge)(V)
Ge4K	CEF (ST2)	(0.8)(0.2)	(Ge)(K)
Ge4Na	CEF (ST2)	(0.8)(0.2)	(Ge)(Na)
Ge4Sc5	CEF (ST2)	(0.444444) (0.555556)	(Ge)(Sc)
Ge5Ti6	CEF (ST2)	(5)(6)	(Ge)(Ti)
Ge8V11	CEF (ST2)	(0.421)(0.579)	(Ge)(V)
GeK	CEF (ST2)	(0.5)(0.5)	(Ge)(K)
GeK3	CEF (ST2)	(0.25)(0.75)	(Ge)(K)

Name	Model	Lattice Size	Constitue
GeNa	CEF (ST2)	(0.5)(0.5)	(Ge)(Na)
GeNa3	CEF (ST2)	(0.25)(0.75)	(Ge)(Na)
GeSc	CEF (ST2)	(0.5)(0.5)	(Ge)(Sc)
GeSr	CEF (ST2)	(0.5)(0.5)	(Ge)(Sr)
GeSr2	CEF (ST2)	(0.333333) (0.666667)	(Ge)(Sr)
GeV3	CEF (ST2)	(0.25)(0.75)	(Ge)(V)
Graphite	CEF (SLN)	(1)	(B,C)
H_RE2O3	CEF (SLN)	(2)(2)(1)	(Ce+3,Ce+2,La+3)(O-2)(O-2,Va)
H_Sigma	CEF (SLN)	(8)(4)(18)	(Al,Fe)(Cr)(Al,Cr,Fe)
H_Sigma_CrMn	CEF (SLN)	(8)(4)(18)	(Mn)(Cr)(Cr,Mn)
Halite	CEF (SLN)	(1)(1)	(Al+3,Ba+2,Ca+2,Co+2,Cr+3, Fe+2,Fe+3,Mg+2,Mn+2,Mn+3, Ni+2,Sr+2,V,V+2,V+3,Va) (O-2,Va)
Hcp	CEF (SLN)	(1)(0.5)	(Ag,Al,Ba,Be,Bi,Ca,Ce,Co,Cr, Cu,Er,Fe,Gd,Ge,Hf,K,La,Li,Mg, Mn,Na,Nb,Ni,Pb,Sb,Sc,Si,Sn, Sr,Ti,V,W,Y,Zn,Zr)(B,C,O,Va)
Hf2Ge	CEF (ST2)	(2)(1)	(Hf)(Ge)
Hf2Si	CEF (ST2)	(0.667)(0.333)	(Hf)(Si)
Hf3Ge	CEF (ST2)	(3)(1)	(Hf)(Ge)
Hf3Ge2	CEF (ST2)	(3)(2)	(Hf)(Ge)
Hf3Si2	CEF (ST2)	(0.6)(0.4)	(Hf)(Si)
Hf5Ge3	CEF (ST2)	(5)(3)	(Hf)(Ge)
Hf5Ge4	CEF (ST2)	(5)(4)	(Hf)(Ge)

Name	Model	Lattice Size	Constitue
Hf5Si3	CEF (ST2)	(0.625)(0.375)	(Hf)(Si)
Hf5Si4	CEF (ST2)	(0.556)(0.444)	(Hf)(Si)
Hf5Sn3	CEF (ST2)	(5)(3)	(Hf)(Sn)
Hf5Sn4	CEF (ST2)	(5)(4)	(Hf)(Sn)
HfGe	CEF (ST2)	(1)(1)	(Hf)(Ge)
HfGe2	CEF (ST2)	(1)(2)	(Hf)(Ge)
HfMn	CEF (ST2)	(0.5)(0.5)	(Hf)(Mn)
HfMn2	CEF (SLN)	(1)(2)	(Hf,Mn)(Hf,Mn)
HfSi	CEF (ST2)	(0.5)(0.5)	(Hf)(Si)
HfSi2	CEF (ST2)	(0.333)(0.667)	(Hf)(Si)
HfSiO4	CEF (ST3)	(1)(1)(4)	(Hf)(Si)(O)
HfSn2	CEF (ST2)	(1)(2)	(Hf)(Sn)
KNa2	CEF (ST2)	(1)(2)	(K)(Na)
L12_FCC	CEF (SLN)	(0.75)(0.25) (1)	(Ag,Al,Cr,Er,Mg,Ni,Sc,Si) (Ag,Al,Cr,Er,Mg,Ni,Sc,Si)(Va)
La11Sn10	CEF (ST2)	(0.524)(0.476)	(La)(Sn)
La2Ni3	CEF (ST2)	(2)(3)	(La)(Ni)
La2Ni7	CEF (ST2)	(2)(7)	(La)(Ni)
La2Sb	CEF (ST2)	(2)(1)	(La)(Sb)
La2Sn3	CEF (ST2)	(0.4)(0.6)	(La)(Sn)
La36Si64	CEF (SLN)	(0.36)(0.64)	(La)(Al,Si)
La3Ni	CEF (ST2)	(3)(1)	(La)(Ni)
La3Sb2	CEF (ST2)	(3)(2)	(La)(Sb)
La3Sn5	CEF (ST2)	(0.375)(0.625)	(La)(Sn)
La4Pb3	CEF (ST2)	(0.571)(0.429)	(La)(Pb)

Name	Model	Lattice Size	Constitue
La5Ni19	CEF (ST2)	(5)(19)	(La)(Ni)
La5Pb3	CEF (ST2)	(0.625)(0.375)	(La)(Pb)
La5Pb4	CEF (ST2)	(0.555)(0.445)	(La)(Pb)
La5Sn3_T1	CEF (ST2)	(0.625)(0.375)	(La)(Sn)
La5Sn3_T2	CEF (ST2)	(0.625)(0.375)	(La)(Sn)
La5Sn4	CEF (ST2)	(0.555)(0.445)	(La)(Sn)
La7Ni16	CEF (ST2)	(7)(16)	(La)(Ni)
La7Ni3	CEF (ST2)	(7)(3)	(La)(Ni)
LaB4	CEF (ST2)	(0.2)(0.8)	(La)(B)
LaB6	CEF (ST2)	(0.14286) (0.85714)	(La)(B)
LaB9	CEF (ST2)	(0.1)(0.9)	(La)(B)
LaNi	CEF (ST2)	(1)(1)	(La)(Ni)
LaNi3	CEF (ST2)	(1)(3)	(La)(Ni)
LaPb2	CEF (ST2)	(0.333)(0.667)	(La)(Pb)
LaPb3	CEF (ST2)	(0.25)(0.75)	(La)(Pb)
LaSb	CEF (ST2)	(1)(1)	(La)(Sb)
LaSb2	CEF (ST2)	(1)(2)	(La)(Sb)
LaSn	CEF (ST2)	(0.5)(0.5)	(La)(Sn)
LaSn3	CEF (ST2)	(0.25)(0.75)	(La)(Sn)
LaZn13	CEF (ST2)	(0.071)(0.929)	(La)(Zn)
LaZn4	CEF (ST2)	(0.2)(0.8)	(La)(Zn)
Lambda_Fe2Sc	CEF (ST2)	(0.64)(0.36)	(Fe)(Sc)
Li12Mg3Si4	CEF (ST3)	(0.631579) (0.157895) (0.210526)	(Li)(Mg)(Si)

Name	Model	Lattice Size	Constitue
Li12Si7	CEF (ST2)	(12)(7)	(Li)(Si)
Li13Si4	CEF (ST2)	(13)(4)	(Li)(Si)
Li13Sn5	CEF (ST2)	(13)(5)	(Li)(Sn)
Li22Si5	CEF (ST2)	(22)(5)	(Li)(Si)
Li22Sn5	CEF (ST2)	(22)(5)	(Li)(Sn)
Li23Sr6	CEF (ST2)	(23)(6)	(Li)(Sr)
Li2C2_T1	CEF (ST2)	(0.5)(0.5)	(C)(Li)
Li2C2_T2	CEF (ST2)	(0.5)(0.5)	(C)(Li)
Li2MgSi	CEF (ST3)	(0.5)(0.25) (0.25)	(Li)(Mg)(Si)
Li2O2	CEF (ST2)	(2)(1)	(Li+1)(O2-2)
Li2Sn5	CEF (ST2)	(2)(5)	(Li)(Sn)
Li2Sr3	CEF (ST2)	(2)(3)	(Li)(Sr)
Li5Sn2	CEF (ST2)	(5)(2)	(Li)(Sn)
Li7Si3	CEF (ST2)	(7)(3)	(Li)(Si)
Li7Sn2	CEF (ST2)	(7)(2)	(Li)(Sn)
Li7Sn3	CEF (ST2)	(7)(3)	(Li)(Sn)
Li8MgSi6	CEF (ST3)	(0.533333) (0.066667) (0.4)	(Li)(Mg)(Si)
LiC6	CEF (ST2)	(6)(1)	(C)(Li)
LiMg2Si	CEF (SLN)	(0.5)(0.25) (0.25)	(Mg)(Si)(Li,Va)
LiSn	CEF (ST2)	(1)(1)	(Li)(Sn)
LiZn2	CEF (ST2)	(1)(2)	(Li)(Zn)

Name	Model	Lattice Size	Constitue
Liquid	CEF (SLN)	(1)	(Ag,Al,B,Ba,Ba4Bi3,BaBi3, BaPb,Be,Bi,Bi2Mg3,C,Ca, Ca2Sn,Ca2Pb,Ce,Co,Cr, Cr3Ge,Cu,Er,Fe,Gd,Ge, Ge3Mn5,Hf,K,La,LaSn,Li,Mg, Mg2Sn,Mn,Na,Nb,Ni,O,Pb,Sb, Sc,Si,Sn,Sr,Ti,V,W,Y,Zn,Zr, Al2O3,B2O3,BaO,BeO,Be2O2, Bi2/5O3/5,CaO,CeO3/2,CeO2, CoO,Co2O3,Cr2/3O,CuO,Cu2O, Cu2O3,FeO,FeO3/2,Ge1/2O,HfO2, K2O,Li2O,MgO,MnO,Mn2/3O,Na2O, NbO,NbO2,Nb2O5,NiO,PbO,Sb4O6, SiO2,SnO,SnO2,TiO,TiO3/2,TiO2, VO,VO2,VO3/2,VO5/2,WO2,WO3, Y2O3,Zr1/2O)
M23C6	CEF (SLN)	(20)(3)(6)	(Co,Cr,Fe,Mn,Ni)(Co,Cr,Fe,Mn,Ni)(C)
M2O	CEF (SLN)	(2)(1)	(K+1,Li+1,Na+1)(O-2)
M3C2	CEF (SLN)	(3)(2)	(Cr,W)(C)
M3Si	CEF (SLN)	(3)(1)	(Fe,Mn,Ni)(Si)
M3X	CEF (SLN)	(0.75)(0.25)	(Al,Ni)(Gd,Y)
M5Si3	CEF (SLN)	(0.625)(0.375)	(Cr,Fe,Mn)(Si)
M5X	CEF (SLN)	(0.833)(0.167)	(Al,Ni)(Gd)
M7C3	CEF (SLN)	(7)(3)	(Co,Cr,Fe,Mn,Ni,W)(C)
MG5SI6	CEF (ST2)	(5)(6)	(Mg)(Si)
MSi	CEF (SLN)	(0.5)(0.5)	(Cr,Fe,Mn,Ni)(Al,Si,Sn)
MSi2	CEF (SLN)	(1)(2)	(Cr,Fe,Ni,Si)(Al,Cr,Si)
MZr2_tI6	CEF (SLN)	(1)(2)	(Ag,Cu)(Zr)

Name	Model	Lattice Size	Constitue
Mg17Sr2	CEF (ST2)	(17)(2)	(Mg)(Sr)
Mg23Sr6	CEF (ST2)	(23)(6)	(Mg)(Sr)
Mg24R5	CEF (SLN)	(24)(5)	(Mg)(Er,Mg,Y)
Mg2C3	CEF (ST2)	(0.4)(0.6)	(Mg)(C)
Mg2Si	CEF (SLN)	(2)(1)	(Mg)(Ge,Si)
Mg2Sn	CEF (ST2)	(0.5)(0.25) (0.25)	(Mg)(Sn)(Va)
Mg2Sr	CEF (ST2)	(0.666667) (0.333333)	(Mg)(Sr)
Mg2Y	CEF (ST2)	(2)(1)	(Mg)(Y)
Mg2Zn11	CEF (SLN)	(5)(6)(2)	(Al,Zn)(Zn)(Mg)
Mg2Zn3	CEF (SLN)	(2)(3)	(Mg)(Al,Zn)
Mg38Sr9	CEF (ST2)	(38)(9)	(Mg)(Sr)
Mg7Zn3	CEF (ST2)	(51)(20)	(Mg)(Zn)
MgB2	CEF (ST2)	(1)(2)	(Mg)(B)
MgB4	CEF (ST2)	(1)(4)	(Mg)(B)
MgB7	CEF (ST2)	(1)(7)	(Mg)(B)
MgC2	CEF (ST2)	(0.333333) (0.666667)	(Mg)(C)
MgSc	CEF (ST2)	(0.5)(0.5)	(Mg)(Sc)
MgX	CEF (SLN)	(0.5)(0.5)	(Gd,Mg,Y,Zn)(Mg,Mn,Zn)
MgZn	CEF (SLN)	(12)(13)	(Mg)(Al,Zn)
Mn11Ge8	CEF (ST2)	(0.579)(0.421)	(Mn)(Ge)
Mn11Si19	CEF (ST2)	(11)(19)	(Mn)(Si)
Mn12Er	CEF (ST2)	(1)(12)	(Er)(Mn)

Name	Model	Lattice Size	Constitue
Mn12Gd	CEF (ST2)	(12)(1)	(Mn)(Gd)
Mn12Y	CEF (ST2)	(12)(1)	(Mn)(Y)
Mn19Sn6	CEF (ST2)	(19)(6)	(Mn)(Sn)
Mn23Er6	CEF (ST2)	(6)(23)	(Er)(Mn)
Mn23Gd6	CEF (SLN)	(23)(6)	(Mg,Mn)(Gd)
Mn23Sc6	CEF (ST2)	(0.7931) (0.2069)	(Mn)(Sc)
Mn23Y6	CEF (ST2)	(23)(6)	(Mn)(Y)
Mn2Er	CEF (ST2)	(1)(2)	(Er)(Mn)
Mn2Ge	CEF (SLN)	(0.667)(0.333)	(Ge,Mn)(Ge,Mn)
Mn2Sc	CEF (ST2)	(0.666667) (0.333333)	(Mn)(Sc)
Mn2Sn	CEF (ST2)	(2)(1)	(Mn)(Sn)
Mn2Y	CEF (ST2)	(2)(1)	(Mn)(Y)
Mn2Zr	CEF (SLN)	(2)(1)	(Mn)(Zr,Va)
Mn3B4	CEF (ST2)	(0.428571) (0.571429)	(Mn)(B)
Mn3C	CEF (ST2)	(3)(1)	(Mn)(C)
Mn3Ge	CEF (SLN)	(0.75)(0.25)	(Mn)(Ge,Mn)
Mn3Ge_LT	CEF (ST2)	(0.75)(0.25)	(Mn)(Ge)
Mn3O4_A	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3O4_B	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3Ti	CEF (ST2)	(3)(1)	(Mn)(Ti)
Mn4Ti	CEF (ST2)	(0.815)(0.185)	(Mn)(Ti)
Mn5C2	CEF (ST2)	(5)(2)	(Mn)(C)

Name	Model	Lattice Size	Constitue
Mn5Ge2	CEF (SLN)	(0.714)(0.286)	(Mn,Ge)(Mn,Ge)
Mn5Ge2_LT	CEF (ST2)	(0.714)(0.286)	(Mn)(Ge)
Mn5Ge3	CEF (ST2)	(0.625)(0.375)	(Mn)(Ge)
Mn6Si	CEF (ST2)	(17)(3)	(Mn)(Si)
Mn7Ge	CEF (SLN)	(0.875)(0.125)	(Mn)(Ge,Mn)
Mn9Ge	CEF (SLN)	(0.9)(0.1)	(Mn)(Ge,Mn)
Mn9Si2	CEF (ST2)	(33)(7)	(Mn)(Si)
MnB	CEF (ST2)	(1)(1)	(Mn)(B)
MnB2	CEF (ST2)	(0.333333) (0.666667)	(Mn)(B)
MnB4	CEF (ST2)	(0.2)(0.8)	(Mn)(B)
MnSc4	CEF (ST2)	(0.2)(0.8)	(Mn)(Sc)
MnSn2	CEF (ST2)	(1)(2)	(Mn)(Sn)
Mu	CEF (SLN)	(7)(2)(4)	(Co,Fe,Mn,Nb,W)(Nb,W) (Co,Fe,Nb,W)
Na2O_Beta	CEF (ST2)	(1)	(Na2O)
Na2O_gamma	CEF (ST2)	(1)	(Na2O)
NaSi_HT	CEF (ST2)	(1)(1)	(Na)(Si)
NaSi_LT	CEF (ST2)	(1)(1)	(Na)(Si)
NaZn13	CEF (ST2)	(1)(13)	(Na)(Zn)
Nb2O5	CEF (ST2)	(2)(5)	(Nb)(O)
Nb3B2	CEF (ST2)	(0.6)(0.4)	(Nb)(B)
Nb3B4	CEF (ST2)	(0.429)(0.571)	(Nb)(B)
Nb3Ge	CEF (SLN)	(0.75)(0.25)	(Nb)(Ge,Nb,Va)
Nb3Si	CEF (ST2)	(0.75)(0.25)	(Nb)(Si)

Name	Model	Lattice Size	Constitue
Nb3Sn	CEF (SLN)	(3)(1)	(Nb,Sn)(Nb,Sn)
Nb5B6	CEF (ST2)	(5)(6)	(Nb)(B)
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)
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)
Nb7Ni6	CEF (SLN)	(1)(4)(2)(6)	(Nb,Ni)(Nb)(Nb,Ni)(Nb,Ni)
NbB	CEF (SLN)	(0.5)(0.5)	(Nb)(B,Va)
NbB2	CEF (SLN)	(0.333)(0.667)	(Nb)(B,Va)
NbGe2	CEF (SLN)	(0.333)(0.667)	(Ge,Nb)(Ge,Nb)
NbNi3	CEF (SLN)	(3)(1)	(Nb,Ni)(Nb,Ni)
NbNi8	CEF (ST2)	(8)(1)	(Ni)(Nb)
NbO	CEF (ST2)	(1)(1)	(Nb)(O)
NbO2	CEF (ST2)	(1)(2)	(Nb)(O)
NbSi2	CEF (SLN)	(0.333)(0.667)	(Nb,Si)(Si)
NbSn2	CEF (ST2)	(1)(2)	(Nb)(Sn)
Ni10Hf7	CEF (ST2)	(10)(7)	(Ni)(Hf)
Ni10Zr7	CEF (ST2)	(10)(7)	(Ni)(Zr)
Ni11Hf9	CEF (ST2)	(11)(9)	(Ni)(Hf)
Ni11Zr9	CEF (ST2)	(11)(9)	(Ni)(Zr)
Ni17Y2	CEF (ST2)	(17)(2)	(Ni)(Y)
Ni21Hf8	CEF (ST2)	(21)(8)	(Ni)(Hf)
Ni21Zr8	CEF (ST2)	(21)(8)	(Ni)(Zr)

Name	Model	Lattice Size	Constitue
Ni2B	CEF (ST2)	(0.667)(0.333)	(Ni)(B)
Ni2Ge	CEF (ST2)	(0.335)(0.665)	(Ge)(Ni)
Ni2V	CEF (ST2)	(0.6667) (0.3333)	(Ni)(V)
Ni2Y	CEF (ST2)	(2)(1)	(Ni)(Y)
Ni2Y3	CEF (ST2)	(2)(3)	(Ni)(Y)
Ni3B	CEF (ST2)	(3)(1)	(Ni)(B)
Ni3Hf_Alpha	CEF (ST2)	(3)(1)	(Ni)(Hf)
Ni3Hf_Beta	CEF (ST2)	(3)(1)	(Ni)(Hf)
Ni3Sb	CEF (SLN)	(0.25)(0.5) (0.25)	(Sb)(Ni,Va)(Ni,Va)
Ni3Sn2	CEF (SLN)	(0.5)(0.25) (0.25)	(Ni,Sn)(Ni)(Ni)
Ni3Sn4	CEF (SLN)	(0.4286) (0.5714)	(Ni)(Ni,Sn)
Ni3Sn_H	CEF (SLN)	(0.75)(0.25)	(Ni,Sn)(Ni,Sn)
Ni3Sn_L	CEF (SLN)	(0.75)(0.25)	(Ni,Sn)(Ni,Sn)
Ni3Ti	CEF (SLN)	(0.75)(0.25)	(Ni,Ti)(Ni,Ti)
Ni3V	CEF (SLN)	(3)(1)	(Ni,V)(Ni,V)
Ni3Y	CEF (ST2)	(3)(1)	(Ni)(Y)
Ni3Zr	CEF (ST2)	(3)(1)	(Ni)(Zr)
Ni4W	CEF (ST2)	(4)(1)	(Ni)(W)
Ni4Y	CEF (ST2)	(4)(1)	(Ni)(Y)
Ni5Ge2	CEF (ST2)	(0.28)(0.72)	(Ge)(Ni)
Ni5Ge3	CEF (SLN)	(1)(1)(1)	(Ge)(Ni)(Ni,Va)
Ni5Hf	CEF (ST2)	(5)(1)	(Ni)(Hf)

Name	Model	Lattice Size	Constitue
Ni5Sb2	CEF (SLN)	(0.7143) (0.2857)	(Ni)(Ni,Sb)
Ni5Y	CEF (ST2)	(5)(1)	(Ni)(Y)
Ni5Zr	CEF (SLN)	(5)(1)	(Ni,Zr)(Zr,Va)
Ni7Hf2	CEF (SLN)	(7)(2)	(Ni)(Hf,Ni)
Ni7Hf3	CEF (ST2)	(7)(3)	(Ni)(Hf)
Ni7Y2	CEF (ST2)	(7)(2)	(Ni)(Y)
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)
NiHf	CEF (ST2)	(1)(1)	(Ni)(Hf)
NiHf2	CEF (SLN)	(1)(2)	(Ni,Va)(Hf)
NiHf_Beta	CEF (ST2)	(1)(1)	(Ni)(Hf)
NiSb	CEF (SLN)	(0.3333) (0.3333) (0.3333)	(Sb)(Ni,Va)(Ni,Va)
NiSb2	CEF (ST2)	(0.3333) (0.6667)	(Ni)(Sb)
NiSr	CEF (ST2)	(0.5)(0.5)	(Ni)(Sr)
NiTi	CEF (SLN)	(1)(1)	(Ni,Ti)(Ni,Va)
NiTi2	CEF (ST2)	(1)(2)	(Ni)(Ti)
NiV3	CEF (ST2)	(0.25)(0.75)	(Ni)(V)
NiW	CEF (ST2)	(1)(1)	(Ni)(W)
NiW2	CEF (ST2)	(1)(2)	(Ni)(W)
NiY	CEF (ST2)	(1)(1)	(Ni)(Y)
NiY3	CEF (ST2)	(1)(3)	(Ni)(Y)

Name	Model	Lattice Size	Constitue
NiZn8	CEF (ST2)	(0.111)(0.889)	(Ni)(Zn)
NiZn_Beta	CEF (SLN)	(1)(1)	(Cu,Ni,Zn)(Ni,Zn)
NiZn_Gamma	CEF (SLN)	(1)	(Ni,Zn)
NiZr	CEF (ST2)	(1)(1)	(Ni)(Zr)
NiZr2	CEF (ST2)	(1)(2)	(Ni)(Zr)
PRIME_S	CEF (ST3)	(0.5)(0.25) (0.25)	(Al)(Mg)(Cu)
Pb12O17	CEF (ST2)	(12)(17)	(Pb)(O)
Pb12O19	CEF (ST2)	(12)(19)	(Pb)(O)
Pb2Zr	CEF (ST2)	(2)(1)	(Pb)(Zr)
Pb3O4	CEF (ST2)	(3)(4)	(Pb)(O)
Pb3Zr5	CEF (ST2)	(3)(5)	(Pb)(Zr)
PbO_alpha	CEF (ST2)	(1)(1)	(Pb)(O)
PbO_beta	CEF (ST2)	(1)(1)	(Pb)(O)
PbZr4	CEF (ST2)	(1)(4)	(Pb)(Zr)
Phi_Al2Mg5Zn2	CEF (SLN)	(6)(5)	(Mg)(Al,Cu,Zn)
Q_Al5Cu2Mg8Si6	CEF (ST4)	(0.2381) (0.0952) (0.381) (0.2857)	(Al)(Cu)(Mg)(Si)
Q_Al7Cu3Mg6	CEF (ST3)	(0.4375) (0.375) (0.1875)	(Al)(Mg)(Cu)
Quartz	CEF (SLN)	(1)(2)	(Ge,Si)(O)
R13Zn58	CEF (SLN)	(0.183)(0.817)	(Ce,Gd,Y)(Zn)
R2Mg17	CEF (SLN)	(2)(17)	(Ce,La,Gd,Y)(Mg,Zn)

Name	Model	Lattice Size	Constitue
R3Al11_HT	CEF (SLN)	(11)(3)	(Al)(Ba,Ce,La)
R3Al11_LT	CEF (SLN)	(11)(3)	(Al)(Ba,Ce,La)
R3Al_HT	CEF (ST2)	(1)(3)	(Al)(Ce)
R3Al_LT	CEF (SLN)	(1)(3)	(Al)(Ce,La)
R3Si2	CEF (SLN)	(0.6)(0.4)	(Ce,La,Mg)(Si)
R3Si5	CEF (SLN)	(0.375)(0.625)	(Ce,Gd)(Si)
R3Zn11	CEF (SLN)	(0.214)(0.786)	(Ce,Gd,Y)(Zn)
R3Zn22	CEF (SLN)	(0.12)(0.88)	(Ce,Gd,La)(Zn)
R5Si3_T2	CEF (SLN)	(0.625)(0.375)	(Ce,La)(Si)
R5Si4	CEF (SLN)	(0.555556) (0.444444)	(Ce,La,Mg)(Si)
RAl	CEF (SLN)	(1)(1)	(Al)(Ce,La)
RAl3	CEF (SLN)	(0.75)(0.25)	(Al)(Ce,La,Gd,Y)
RAl3_HT	CEF (ST2)	(0.75)(0.25)	(Al)(Ce)
RMg	CEF (SLN)	(0.5)(0.5)	(Ce,Gd,La,Mg,Y,Zn)(Al,Mg,Mn,Li,Zn)
RMg12	CEF (SLN)	(1)(12)	(Ce,La,Y)(Al,Mg,Zn)
RMg3	CEF (SLN)	(1)(3)	(Ce,Gd,La,Y)(Li,Mg,Zn)
RSi	CEF (SLN)	(0.5)(0.5)	(Ce,Gd,La)(Al,Si)
RSi2_T2	CEF (SLN)	(0.333333) (0.666667)	(Ce,La,Y)(Al,Si)
RZn2	CEF (SLN)	(0.333333) (0.666667)	(Ce,Gd,La)(Zn)
RZn3	CEF (SLN)	(1)(3)	(Ce,Gd,Y)(Zn)
RZn5	CEF (SLN)	(0.167)(0.833)	(Ce,La)(Zn)
R_Al5CuLi3	CEF (ST3)	(0.55)(0.117) (0.333)	(Al)(Cu)(Li)

Name	Model	Lattice Size	Constitue
Rhombohedral_A7	CEF (SLN)	(1)	(Ba,Bi,Ge,Pb,Sb,Sn)
Rutile	CEF (SLN)	(1)(2)	(Ge+4,Mn+4,Pb+4,Sn+4, Ti+3,Ti+4,V+4)(O-2,Va)
S_Al2CuMg	CEF (ST3)	(0.5)(0.25) (0.25)	(Al)(Mg)(Cu)
Sb2O3_B	CEF (ST2)	(2)(3)	(Sb)(O)
Sb2O4	CEF (ST2)	(2)(4)	(Sb)(O)
Sb2O5	CEF (ST2)	(2)(5)	(Sb)(O)
Sb2Sn3	CEF (ST2)	(2)(3)	(Sb)(Sn)
Sb3Zn4	CEF (SLN)	(3)(4)	(Sb)(Zn,Va)
SbSn	CEF (SLN)	(1)	(Sb,Sn)
SbZn	CEF (SLN)	(1)(1)	(Sb)(Zn,Va)
Sc11Sn10	CEF (ST2)	(0.523)(0.477)	(Sc)(Sn)
Sc13Zn58	CEF (ST2)	(0.183099) (0.816901)	(Sc)(Zn)
Sc3Zn17	CEF (ST2)	(0.15)(0.85)	(Sc)(Zn)
Sc5Si3	CEF (ST2)	(0.625)(0.375)	(Sc)(Si)
Sc6Sn5	CEF (ST2)	(0.545)(0.455)	(Sc)(Sn)
ScB12	CEF (ST2)	(0.9231) (0.0769)	(B)(Sc)
ScB2	CEF (ST2)	(0.667)(0.333)	(B)(Sc)
ScSi	CEF (ST2)	(0.5)(0.5)	(Sc)(Si)
ScSn2	CEF (ST2)	(0.333)(0.667)	(Sc)(Sn)
ScZn	CEF (ST2)	(0.5)(0.5)	(Sc)(Zn)
ScZn12	CEF (ST2)	(0.076923)	(Sc)(Zn)

Name	Model	Lattice Size	Constitue
		(0.923077)	
ScZn2	CEF (ST2)	(0.333333) (0.666667)	(Sc)(Zn)
Shp_MC	CEF (ST2)	(1)(1)	(W)(C)
Si2Ti	CEF (ST2)	(0.666667) (0.333333)	(Si)(Ti)
Si2V	CEF (ST2)	(0.666667) (0.333333)	(Si)(V)
Si2Y_H	CEF (ST2)	(2)(1)	(Si)(Y)
Si2Y_R	CEF (ST2)	(2)(1)	(Si)(Y)
Si2Zr	CEF (SLN)	(2)(1)	(Al,Si)(Zr)
Si2Zr3	CEF (ST2)	(2)(3)	(Si)(Zr)
Si3Sr5	CEF (ST2)	(0.625)(0.375)	(Sr)(Si)
Si3Ti5	CEF (SLN)	(2)(3)(3)	(Si,Ti)(Si,Ti)(Ti)
Si3V5	CEF (ST2)	(0.375)(0.625)	(Si)(V)
Si3Y5	CEF (ST2)	(3)(5)	(Si)(Y)
Si3Zr5	CEF (SLN)	(3)(5)	(Al,Si)(Zr)
Si4Ti5	CEF (ST2)	(0.444444) (0.555556)	(Si)(Ti)
Si4Y5	CEF (ST2)	(4)(5)	(Si)(Y)
Si4Zr5	CEF (ST2)	(4)(5)	(Si)(Zr)
Si5V6	CEF (ST2)	(0.454545) (0.545455)	(Si)(V)
Si5Y3_H	CEF (ST2)	(5)(3)	(Si)(Y)
Si5Y3_R	CEF (ST2)	(5)(3)	(Si)(Y)
SiC	CEF (ST2)	(1)(1)	(C)(Si)

Name	Model	Lattice Size	Constitue
SiO_AM	CEF (ST2)	(1)(1)	(Si)(O)
SiSr	CEF (ST2)	(0.5)(0.5)	(Sr)(Si)
SiSr2	CEF (ST2)	(0.666667) (0.333333)	(Sr)(Si)
SiTi	CEF (SLN)	(0.5)(0.5)	(Al,Si)(Ti)
SiTi3	CEF (ST2)	(0.25)(0.75)	(Si)(Ti)
SiV3	CEF (SLN)	(0.75)(0.25)	(Si,V)(Si,V)
SiY	CEF (ST2)	(1)(1)	(Si)(Y)
SiZr	CEF (SLN)	(1)(1)	(Al,Si)(Zr)
SiZr2	CEF (SLN)	(1)(2)	(Al,Si)(Zr)
SiZr3	CEF (ST2)	(1)(3)	(Si)(Zr)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Co,Fe,Mn,Ni)(Cr,Nb,V) (Al,Co,Cr,Fe,Mn,Nb,Ni,V)
Sn10Y11	CEF (ST2)	(10)(11)	(Sn)(Y)
Sn2V	CEF (ST2)	(0.333)(0.333) (0.334)	(V)(Sn)(Sn)
Sn2Y	CEF (ST2)	(2)(1)	(Sn)(Y)
Sn2Zr	CEF (ST2)	(2)(1)	(Sn)(Zr)
Sn3Sr	CEF (ST2)	(0.25)(0.75)	(Sr)(Sn)
Sn3Sr5	CEF (ST2)	(0.625)(0.375)	(Sr)(Sn)
Sn3Ti2	CEF (ST2)	(0.6)(0.4)	(Sn)(Ti)
Sn3Ti5	CEF (ST2)	(3)(5)	(Sn)(Ti)
Sn3Y	CEF (ST2)	(0.75)(0.25)	(Sn)(Y)
Sn3Y5	CEF (ST2)	(0.375)(0.625)	(Sn)(Y)
Sn3Zr5	CEF (SLN)	(5)(3)(1)	(Zr)(Sn)(Sn,Va)

Name	Model	Lattice Size	Constitue
Sn4Sr	CEF (ST2)	(0.2)(0.8)	(Sr)(Sn)
Sn4Y5	CEF (ST2)	(4)(5)	(Sn)(Y)
Sn5Sr3	CEF (ST2)	(0.375)(0.625)	(Sr)(Sn)
Sn5Ti6	CEF (ST2)	(5)(6)	(Sn)(Ti)
Sn5Y2	CEF (ST2)	(5)(2)	(Sn)(Y)
SnSr	CEF (ST2)	(0.5)(0.5)	(Sr)(Sn)
SnSr2	CEF (ST2)	(0.666667) (0.333333)	(Sr)(Sn)
SnTi2	CEF (ST2)	(1)(2)	(Sn)(Ti)
SnTi3	CEF (SLN)	(0.75)(0.25)	(Ti)(Sn,Ti)
SnV3	CEF (SLN)	(0.25)(0.75)	(Sn,V)(V)
SnZr4	CEF (SLN)	(3)(1)	(Sn,Zr)(Sn,Zr)
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)
SrB6	CEF (ST2)	(1)(6)	(Sr)(B)
SrO2	CEF (ST2)	(1)(2)	(Sr)(O)
SrZn	CEF (ST2)	(1)(1)	(Sr)(Zn)
SrZn13	CEF (ST2)	(1)(13)	(Sr)(Zn)
SrZn2	CEF (ST2)	(1)(2)	(Sr)(Zn)
SrZn5	CEF (ST2)	(1)(5)	(Sr)(Zn)
T10_AlFeSi	CEF (ST3)	(0.6)(0.25) (0.15)	(Al)(Fe)(Si)
T11_AlFeSi	CEF (ST3)	(0.6538) (0.2308) (0.1154)	(Al)(Fe)(Si)

Name	Model	Lattice Size	Constitue
T1_Al2CuLi	CEF (ST3)	(0.5)(0.25) (0.25)	(Al)(Cu)(Li)
T1_AlCrSi	CEF (SLN)	(13)(4)(4)	(Al)(Cr,Fe)(Si)
T1_AlFeSi	CEF (SLN)	(5)(3)	(Al,Si)(Fe)
T1_AlGdNi	CEF (ST3)	(0.75)(0.15) (0.1)	(Al)(Ni)(Gd)
T2_Al6CuLi3	CEF (ST3)	(0.57)(0.11) (0.32)	(Al)(Cu)(Li)
T2_AlCrSi	CEF (ST3)	(9)(3)(1)	(Al)(Cr)(Si)
T2_AlCuEr	CEF (SLN)	(0.894737) (0.105263)	(Al,Cu)(Er)
T2_AlGdNi	CEF (ST3)	(0.666)(0.167) (0.167)	(Al)(Ni)(Gd)
T3_AlCrSi	CEF (SLN)	(11)(4)	(Al,Si)(Cr)
T3_AlCuEr	CEF (SLN)	(0.833333) (0.166667)	(Al,Cu)(Er)
T3_AlFeSi	CEF (ST3)	(0.55)(0.25) (0.2)	(Al)(Fe)(Si)
T3_AlGdNi	CEF (ST3)	(0.583)(0.25) (0.167)	(Al)(Ni)(Gd)
T4_AlCuEr	CEF (ST3)	(0.6)(0.2)(0.2)	(Al)(Cu)(Er)
T4_AlGdNi	CEF (ST3)	(0.5)(0.333) (0.167)	(Al)(Ni)(Gd)
T5_AlCuEr	CEF (ST3)	(0.5)(0.3)(0.2)	(Al)(Cu)(Er)
T5_AlGdNi	CEF (ST3)	(0.5)(0.25) (0.25)	(Al)(Ni)(Gd)
T6_AlCuEr	CEF (ST3)	(0.45)(0.3)	(Al)(Cu)(Er)

Name	Model	Lattice Size	Constitue
		(0.25)	
T6_AlGdNi	CEF (ST3)	(0.333)(0.333) (0.333)	(Al)(Ni)(Gd)
T7_AlCuEr	CEF (ST3)	(0.333333) (0.333333) (0.333334)	(Al)(Cu)(Er)
T7_AlFeSi	CEF (SLN)	(0.75)(0.25)	(Al,Si)(Fe)
T8_AlFeSi	CEF (SLN)	(0.66667) (0.33333)	(Al,Si)(Fe)
T_AlLiZn2	CEF (SLN)	(1)(2)	(Li)(Al,Zn)
T_AlLiZn3	CEF (SLN)	(1)(3)	(AlLi,Zn)(Zn)
T_AlMgZn	CEF (SLN)	(26)(6)(48)(1)	(Mg)(Al,Mg)(Al,Cu,Mg,Zn)(Al)
T_CuMgZn	CEF (ST3)	(0.3)(1)(1.7)	(Cu)(Mg)(Zn)
T_FeNiSi	CEF (SLN)	(8)(2)	(Fe,Ni)(Si)
Tao_AlCuSc	CEF (SLN)	(0.6154) (0.3077) (0.0769)	(Al,Cu)(Al,Cu)(Sc)
Tb_Al7Cu4Li	CEF (ST3)	(0.6)(0.32) (0.08)	(Al)(Cu)(Li)
Theta_CuGe	CEF (ST2)	(0.735)(0.265)	(Cu)(Ge)
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)
Ti3Al2Si5	CEF (ST3)	(1)(0.6)(1.4)	(Ti)(Al)(Si)

Name	Model	Lattice Size	Constitue
Ti3Bi	CEF (ST2)	(0.25)(0.75)	(Bi)(Ti)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti7Al5Si14	CEF (ST3)	(7)(5)(14)	(Ti)(Al)(Si)
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) (0.3333)	(Bi)(Ti)
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)
Tridymite	CEF (ST2)	(1)(2)	(Si)(O)
V2B3	CEF (ST2)	(2)(3)	(V)(B)
V2O5	CEF (ST2)	(2)(5)	(V)(O)
V2O_SS	CEF (SLN)	(1)(0.5)	(V)(O,Va)
V2Zr	CEF (ST2)	(2)(1)	(V)(Zr)
V3B2	CEF (ST2)	(3)(2)	(V)(B)
V3B4	CEF (ST2)	(3)(4)	(V)(B)
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)

Name	Model	Lattice Size	Constitue
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)
V5B6	CEF (ST2)	(5)(6)	(V)(B)
V5O9	CEF (ST2)	(2)(3)(9)	(V+3)(V+4)(O-2)
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)
VB	CEF (ST2)	(1)(1)	(V)(B)
VB2	CEF (ST2)	(1)(2)	(V)(B)
VO2	CEF (SLN)	(1)(2)	(Hf,V,W,Zr)(O)
VZn16	CEF (ST2)	(1)(16)	(V)(Zn)
VZn3	CEF (ST2)	(1)(3)	(V)(Zn)
V_Al5Cu6Mg2	CEF (ST3)	(0.38461) (0.15385) (0.46154)	(Al)(Mg)(Cu)
W2B	CEF (ST2)	(2)(1)	(W)(B)
W2B5	CEF (SLN)	(2)(5)	(W)(B,Va)
W2B9	CEF (ST2)	(2)(9)	(W)(B)
W2Ge3	CEF (ST2)	(2)(3)	(W)(Ge)
W5Si3	CEF (ST2)	(5)(3)	(W)(Si)
WO272	CEF (ST2)	(1)(2.72)	(W)(O)
WO290	CEF (ST2)	(1)(2.9)	(W)(O)
WO296	CEF (ST2)	(1)(2.96)	(W)(O)

Name	Model	Lattice Size	Constitue
WO3_A	CEF (ST2)	(1)(3)	(W)(O)
WO3_B	CEF (ST2)	(1)(3)	(W)(O)
WSi2	CEF (ST2)	(1)(2)	(W)(Si)
X_RE2O3	CEF (SLN)	(2)(2)(1)	(Ce+3,Ce+2)(O-2)(O-2,Va)
Y13Zn58	CEF (ST2)	(0.183)(0.817)	(Y)(Zn)
Y2O3_cub	CEF (SLN)	(2)(3)(1)	(Er+3,Gd+3,Mn+3,Sc+3,Y+3,Va) (O-2)(O-2,Va)
Y2O3_hex	CEF (SLN)	(2)(3)(1)	(Y+3,Zr+4)(O-2)(O-2,Va)
Y2Zn17	CEF (ST2)	(2)(17)	(Y)(Zn)
Y3Zn11	CEF (ST2)	(0.214)(0.786)	(Y)(Zn)
YZn	CEF (SLN)	(0.5)(0.5)	(Zn,Y)(Zn)
YZn12	CEF (ST2)	(1)(12)	(Y)(Zn)
YZn3	CEF (ST2)	(1)(3)	(Y)(Zn)
YZn5	CEF (ST2)	(1)(1.5)(3.5)	(Y)(Zn)(Zn)
Zeta_Sb2Zn3	CEF (ST2)	(2.025)(2.975)	(Sb)(Zn)
Zn22Zr	CEF (ST2)	(0.956522) (0.0434783)	(Zn)(Zr)
Zn2Zr	CEF (ST2)	(0.666667) (0.333333)	(Zn)(Zr)
Zn2Zr3	CEF (ST2)	(0.4)(0.6)	(Zn)(Zr)
Zn39Zr5	CEF (ST2)	(0.886364) (0.113636)	(Zn)(Zr)
Zn3Zr_h	CEF (ST2)	(0.75)(0.25)	(Zn)(Zr)
Zn3Zr_l	CEF (ST2)	(0.75)(0.25)	(Zn)(Zr)
ZnO	CEF (ST2)	(1)(1)	(Zn)(O)
ZnZr	CEF (ST2)	(0.5)(0.5)	(Zn)(Zr)

Name	Model	Lattice Size	Constitue
ZnZr2	CEF (ST2)	(0.333333) (0.666667)	(Zn)(Zr)
Zr2O	CEF (ST2)	(2)(1)	(Zr)(O)
Zr3O	CEF (ST2)	(3)(1)	(Zr)(O)
Zr6O	CEF (ST2)	(6)(1)	(Zr)(O)
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)	(Hf,Zr)(O,Va)
ZrO2_Tetragonal	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)
a_Ba3Ge4	CEF (ST2)	(0.429)(0.571)	(Ba)(Ge)
a_Ba3Pb5	CEF (ST2)	(0.375)(0.625)	(Ba)(Pb)
a_Ce2Ni7	CEF (ST2)	(0.2222) (0.7778)	(Ce)(Ni)
a_ErSi	CEF (ST2)	(1)(1)	(Er)(Si)
a_ErSi2	CEF (ST2)	(1)(1.67)	(Er)(Si)
a_Sc3Si5	CEF (ST2)	(0.375)(0.625)	(Sc)(Si)
a_Si2Sr	CEF (ST2)	(0.333333) (0.666667)	(Sr)(Si)
alpha_GdSb	CEF (ST2)	(1)(1)	(Gd)(Sb)
alpha_La3Pb4	CEF (ST2)	(0.429)(0.571)	(La)(Pb)
b_Ba3Ge4	CEF (ST2)	(0.429)(0.571)	(Ba)(Ge)
b_Ba3Pb5	CEF (ST2)	(0.375)(0.625)	(Ba)(Pb)
b_ErSi	CEF (ST2)	(1)(1)	(Er)(Si)
b_ErSi2	CEF (ST2)	(1)(1.67)	(Er)(Si)

Name	Model	Lattice Size	Constitue
b_Sc3Si5	CEF (ST2)	(0.375)(0.625)	(Sc)(Si)
b_Si2Sr	CEF (SLN)	(0.333333) (0.666667)	(Sr)(Si,Va)
beta_GdSb	CEF (ST2)	(1)(1)	(Gd)(Sb)
beta_La3Pb4	CEF (ST2)	(0.429)(0.571)	(La)(Pb)
m_Ni4B3	CEF (ST2)	(0.564)(0.436)	(Ni)(B)
o_Ni4B3	CEF (ST2)	(0.586)(0.414)	(Ni)(B)