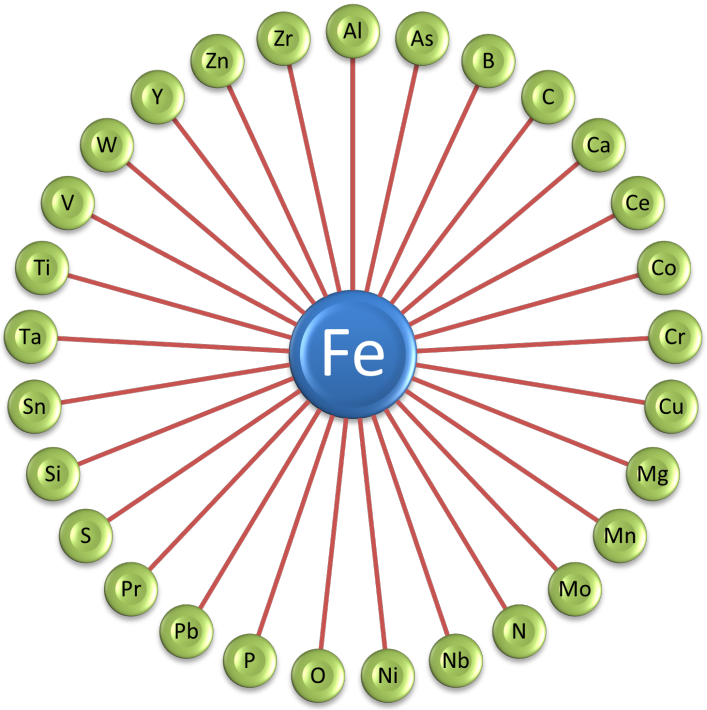
Pandat™ 2024

Database Manual

CompuTherm LLC

PanIron

Database for multi-component Fe-rich alloys



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (30)

Total of **30** components are included in the database as listed here:

Major alloying elements: Co, Cr, **Fe**, Mo, Ni, V and W.

Minor alloying elements: Al, As, B, C, Ca, Ce, Cu, Mg, Mn, N, Nb, O, P, Pb, Pr, S, Si, Sn, Ta, Ti, Y, Zn 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 subsystems are valid in the entire composition range as given in Section 1.4 .

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Fe	50 ~ 100
Cr, Ni	0 ~ 34
Mn	0 ~ 15
Al, Co, Mo	0 ~ 10
Pb, V, W	0 ~ 7
B, C, Cu, Nb, Si, Ti	0 ~ 5
As, Ca, Ce, Mg, N, O, Pr	0 ~ 0.5
P, S, Sn, Ta, Y, Zn, Zr	0 ~ 0.1

1.3 Phases

Total of **704** 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 PanCo2024:List of All Phases. Users can also view it through TDB viewer of Pandat™ .

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
Bcc(ferrite)	(1)(3)	(Al,As,Ca,Ce,Co,Cr,Cu,Fe,Mg,Mn,Mo,Nb,Ni,P, Pb,Pr,S,Si,Sn,Ta,Ti,V,W,Y,Zn,Zr)(B,C,N,O,Va)
Cementite	(3)(1)	(Co,Cr,Fe,Mn,Mo,Nb,Ni,V,W)(B,C,N)
Fcc(austenite)	(1)(1)	(Al,As,Ca,Ce,Co,Cr,Cu,Fe,Mg,Mn,Mo,Nb,Ni,P, Pb,Pr,S,Si,Sn,Ta,Ti,V,W,Y,Zn,Zr)(B,C,N,O,Va)
Graphite	(1)	(B,C)
Laves_C14	(2)(1)	(Al,Co,Cr,Fe,Mg,Mn,Mo,Nb,Ni,Ti,W,Zn,Zr) (Al,Co,Cr,Fe,Mg,Mn,Mo,Nb,Ni,Ti,W,Zn,Zr)
M23C6	(20)(3)(6)	(Co,Cr,Fe,Mn,Ni,V)(Co,Cr,Fe,Mn,Mo,Ni,V,W)(B,C)
M6C	(2)(2)(2)(1)	(Co,Fe,Ni)(Cr,Mo,Nb,W)(Co,Cr,Fe,Mo,Nb,Ni,Si,V,W)(C)
M7C3	(7)(3)	(Co,Cr,Fe,Mn,Mo,Ni,V,W)(C)
Mu_PHASE	(7)(2)(4)	(Al,Co,Cr,Fe,Mo,Mn,Nb,Ni,Ta)(Mo,Nb,Ta,W) (Al,Co,Cr,Fe,Mo,Nb,Ni,Ta,W)
Sigma	(8)(4)(18)	(Al,Co,Cr,Fe,Mn,Ni,Si,Ta)(Cr,Fe,Mo,Nb,Ta,Ti,V,W) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,W)

1.4 Assessed Subsystems

A total of **351** subsystems, including 317 binary, 32 ternary and **2** quaternary 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 (317)

Al-As(10)	Al-B(10)	Al-C(10)	Al-Ca(10)	Al-Ce(10)	Al-Co(10)
Al-Cr(10)	Al-Cu(10)	Al-Fe(10)	Al-Mg(10)	Al-Mn(10)	Al-Mo(10)
Al-N(10)	Al-Nb(10)	Al-Ni(10)	Al-P(10)	Al-Pb(10)	Al-S(10)
Al-Si(10)	Al-Sn(10)	Al-Ta(10)	Al-Ti(10)	Al-V(10)	Al-W(10)
Al-Y(10)	Al-Zn(10)	Al-Zr(10)	As-Co(10)	As-Cu(10)	As-Fe(10)
As-Mn(10)	As-Ni(10)	As-Pb(10)	B-C(10)	B-Ca(10)	B-Ce(10)
B-Co(10)	B-Cr(10)	B-Fe(10)	B-Mg(10)	B-Mn(10)	B-Mo(10)
B-Nb(10)	B-Ni(10)	B-Pr(10)	B-Si(10)	B-Ta(10)	B-Ti(10)
B-V(10)	B-W(10)	B-Zr(10)	C-Ce(10)	C-Co(10)	C-Cr(10)
C-Fe(10)	C-Mg(10)	C-Mn(10)	C-Mo(10)	C-Nb(10)	C-Ni(10)
C-Pr(10)	C-Si(10)	C-Ta(10)	C-Ti(10)	C-V(10)	C-W(10)
C-Zr(10)	Ca-Ce(10)	Ca-Cu(10)	Ca-Fe(10)	Ca-Mg(10)	Ca-Mn(10)
Ca-Mo(10)	Ca-Ni(10)	Ca-Pb(10)	Ca-S(10)	Ca-Si(10)	Ca-Sn(10)
Ca-Ti(10)	Ca-V(10)	Ca-Zn(10)	Ce-Co(10)	Ce-Cr(10)	Ce-Cu(10)
Ce-Fe(10)	Ce-Mg(10)	Ce-Mn(10)	Ce-Mo(10)	Ce-Ni(10)	Ce-Si(10)
Ce-Sn(10)	Ce-Ti(10)	Ce-V(10)	Ce-Y(10)	Ce-Zn(10)	Ce-Zr(10)
Co-Cr(10)	Co-Cu(10)	Co-Fe(10)	Co-Mg(10)	Co-Mn(10)	Co-Mo(10)
Co-N(10)	Co-Nb(10)	Co-Ni(10)	Co-P(10)	Co-Pb(10)	Co-Si(10)
Co-Sn(10)	Co-Ta(10)	Co-Ti(10)	Co-V(10)	Co-W(10)	Co-Y(10)
Co-Zn(10)	Co-Zr(10)	Cr-Cu(10)	Cr-Fe(10)	Cr-Mg(10)	Cr-Mn(10)
Cr-Mo(10)	Cr-N(10)	Cr-Nb(10)	Cr-Ni(10)	Cr-P(10)	Cr-Pb(10)

Cr-S(10)	Cr-Si(10)	Cr-Sn(10)	Cr-Ta(10)	Cr-Ti(10)	Cr-V(10)
Cr-W(10)	Cr-Y(10)	Cr-Zn(10)	Cr-Zr(10)	Cu-Fe(10)	Cu-Mg(10)
Cu-Mn(10)	Cu-Mo(10)	Cu-N(10)	Cu-Nb(10)	Cu-Ni(10)	Cu-P(10)
Cu-Pb(10)	Cu-Pr(10)	Cu-S(10)	Cu-Si(10)	Cu-Sn(10)	Cu-Ta(10)
Cu-Ti(10)	Cu-V(10)	Cu-W(10)	Cu-Y(10)	Cu-Zn(10)	Cu-Zr(10)
Fe-Mg(10)	Fe-Mn(10)	Fe-Mo(10)	Fe-N(10)	Fe-Nb(10)	Fe-Ni(10)
Fe-P(10)	Fe-Pb(10)	Fe-S(10)	Fe-Si(10)	Fe-Sn(10)	Fe-Ta(10)
Fe-Ti(10)	Fe-V(10)	Fe-W(10)	Fe-Y(10)	Fe-Zn(10)	Fe-Zr(10)
Mg-Mn(10)	Mg-Mo(10)	Mg-N(10)	Mg-Nb(10)	Mg-Ni(10)	Mg-Pb(10)
Mg-Pr(10)	Mg-S(10)	Mg-Si(10)	Mg-Sn(10)	Mg-Ti(10)	Mg-V(10)
Mg-Y(10)	Mg-Zn(10)	Mg-Zr(10)	Mn-Mo(10)	Mn-N(10)	Mn-Nb(10)
Mn-Ni(10)	Mn-P(10)	Mn-Pb(10)	Mn-Pr(10)	Mn-S(10)	Mn-Si(10)
Mn-Sn(10)	Mn-Ta(10)	Mn-Ti(10)	Mn-V(10)	Mn-W(10)	Mn-Y(10)
Mn-Zn(10)	Mn-Zr(10)	Mo-N(10)	Mo-Nb(10)	Mo-Ni(10)	Mo-P(10)
Mo-Pb(10)	Mo-S(10)	Mo-Si(10)	Mo-Sn(10)	Mo-Ta(10)	Mo-Ti(10)
Mo-V(10)	Mo-Y(10)	Mo-Zr(10)	N-Nb(10)	N-Ni(10)	N-Si(10)
N-Ta(10)	N-Ti(10)	N-V(10)	N-W(10)	N-Zr(10)	Nb-Ni(10)
Nb-P(10)	Nb-Si(10)	Nb-Sn(10)	Nb-Ta(10)	Nb-Ti(10)	Nb-V(10)
Nb-W(10)	Nb-Y(10)	Nb-Zr(10)	Ni-P(10)	Ni-Pb(10)	Ni-Pr(10)
Ni-S(10)	Ni-Si(10)	Ni-Sn(10)	Ni-Ta(10)	Ni-Ti(10)	Ni-V(10)
Ni-W(10)	Ni-Y(10)	Ni-Zn(10)	Ni-Zr(10)	P-Si(10)	P-Ti(10)
Pb-Si(10)	Pb-Sn(10)	Pb-Zn(10)	Pb-Zr(10)	Pr-Y(10)	Pr-Zn(10)
S-Ti(10)	Si-Sn(10)	Si-Ta(10)	Si-Ti(10)	Si-V(10)	Si-W(10)
Si-Y(10)	Si-Zn(10)	Si-Zr(10)	Sn-Ti(10)	Sn-V(10)	Sn-Y(10)
Sn-Zn(10)	Sn-Zr(10)	Ta-Ti(10)	Ta-V(10)	Ta-W(10)	Ta-Zr(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)
Al-O(10)	B-O(10)	C-O(10)	Ca-O(10)	Ce-O(10)	Co-O(10)

Cr-O(10)	Cu-O(10)	Fe-O(10)	Mg-O(10)	Mn-O(10)	Mo-O(10)
Nb-O(10)	Ni-O(10)	O-P(10)	O-Pb(10)	O-S(10)	O-Si(10)
O-Sn(10)	O-Ta(10)	O-Ti(10)	O-V(10)	O-W(10)	O-Y(10)
O-Zr(10)	O-Pr(9)	B-Cu(8)	B-N(5)	O-Zn(5)	

Ternary Systems (32)

Al-C-Fe(10)	B-Co-Fe(10)	B-Cr-Fe(10)	B-Fe-Mo(10)	B-Fe-Ni(10)	B-Fe-Si(10)
C-Co-Fe(10)	C-Cr-Fe(10)	C-Cr-Mn(10)	C-Fe-Mn(10)	C-Fe-Mo(10)	C-Fe-Ni(10)
C-Fe-Si(10)	C-Fe-W(10)	Co-Fe-Ni(10)	Co-Fe-W(10)	Cr-Fe-Mn(10)	Cr-Fe-Mo(10)
Cr-Fe-Ni(10)	Cr-Fe-W(10)	Cr-Fe-N(10)	Cr-Fe-P(10)	Fe-Mn-Ni(10)	Fe-Mn-W(10)
Fe-Mn-P(10)	Fe-Mo-Ni(10)	Fe-Mo-W(10)	Fe-Mo-P(10)	Fe-Ni-P(10)	Fe-Ni-S(10)
Co-Cr-Fe(8)	Co-Fe-Mo(8)				

Quaternary Systems (**2**)

C-Cr-Fe-Mn(10)	Al-C-Fe-Mn(10)

1.5 Database Validation

The current thermodynamic database for iron-based alloy systems has been extensively tested and validated using the published experimental data. This database can be used to calculate phase equilibria for multi-component iron alloys, such as the equilibrium between Bcc (ferrite) and Fcc (austenite). It can be used to predict phase transformation temperatures, such as liquidus, solidus, and so on. The fraction of each phase as a function of temperature, partitioning of components in different phases can also be calculated. In addition to equilibrium calculations, Scheil simulations can also be carried out using this database.

Some validation results are presented below.

Figure 1.1 and Figure 1.2 show comparison between the calculated and experimentally measured liquidus and solidus temperatures for variety of steels. Figure 1.3 shows comparison between the calculated and experimentally observed amounts of austenite in duplex stainless steels. Figure 1.4 is a comparison between the calculated and experimentally measured partitioning of Fe, Cr, Mo, and Ni in ferrite and austenite. Figure

1.5 ~ Figure 1.9 are comparisons between the calculated and experimentally observed equilibrium compositions for Fe, C, Co, Cr, Mo, Si, V and W in austenite, ferrite, M_6C, MC and M_2C at 1200 °C, respectively. These figures show reasonable agreement between the calculated values using the current PanFe database and the experimental determined ones.

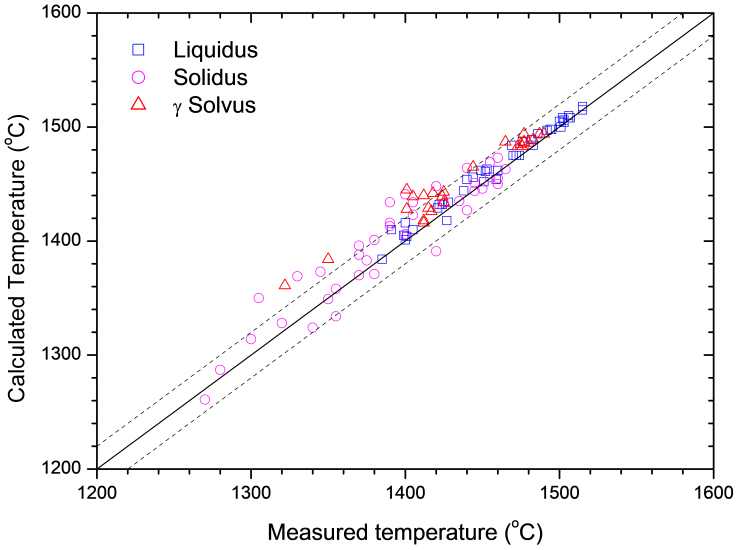


Figure 1.1: Comparison between the calculated liquidus and solidus temperatures for iron-based alloys with experimental data from [1977Jer]

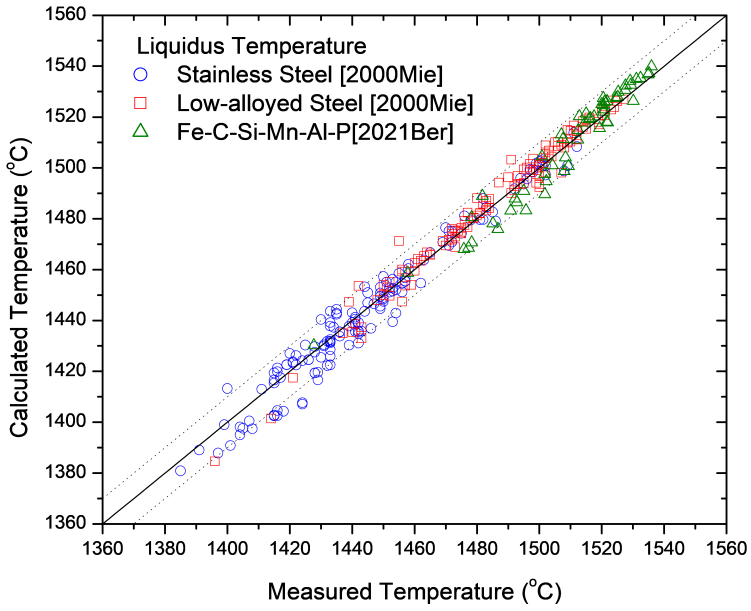


Figure 1.2: Comparison between the calculated liquidus temperatures for iron-based alloys with experimental data from [2000Mie,2021Ber]

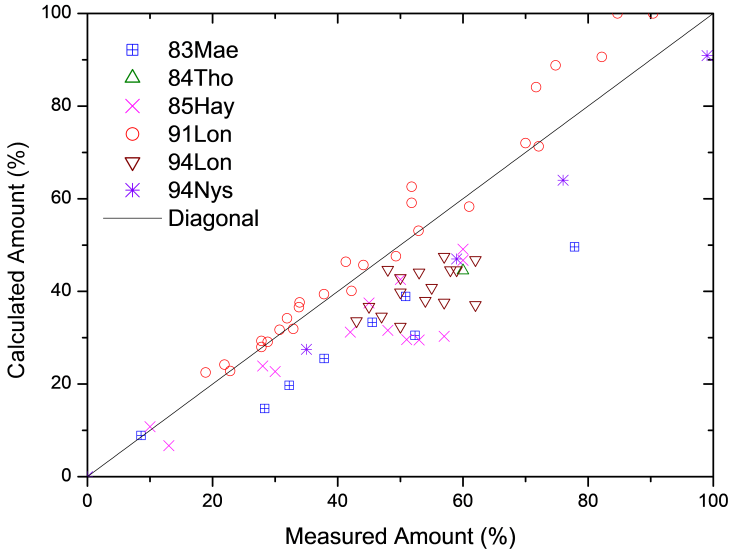


Figure 1.3: Comparison between the calculated and experimentally measured amounts of austenite in duplex stainless steels of austenite (Fcc)

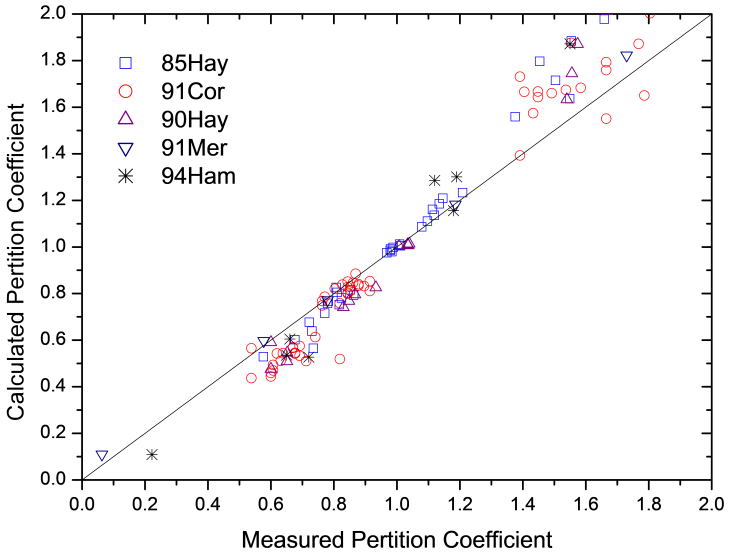


Figure 1.4: Comparison between the calculated and experimentally measured partitioning of Fe, Cr, Mo and Ni in ferrite and austenite

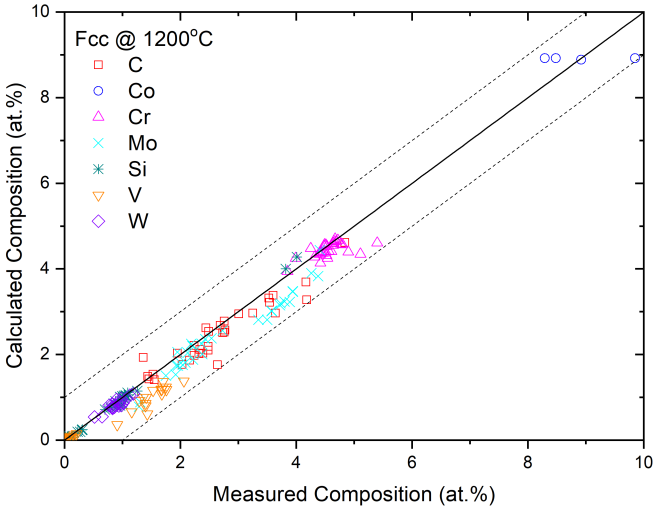


Figure 1.5: Comparison between the calculated and measured equilibrium compositions of C, Co, Cr, Mo, Si, V and W in the Fcc phase at 1200 °C

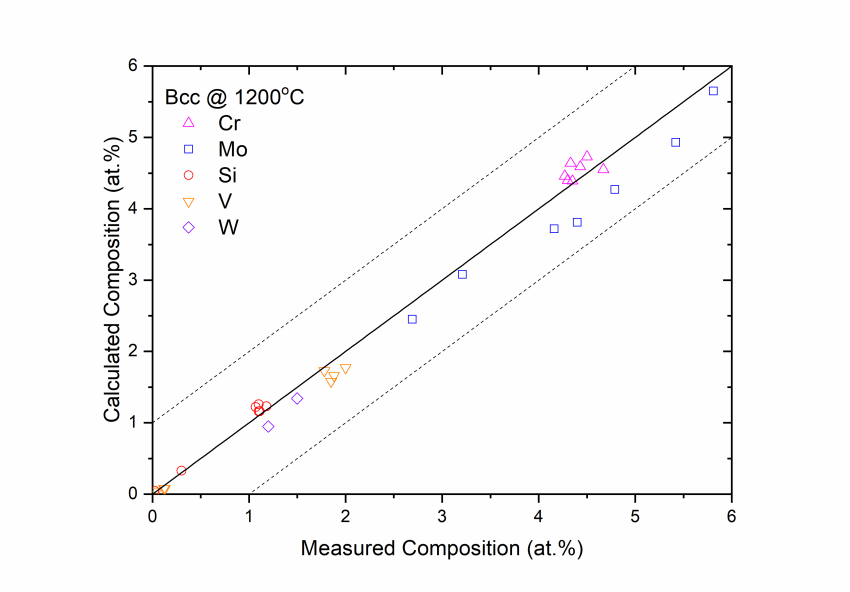


Figure 1.6: Comparison between the calculated and measured equilibrium compositions of Cr, Mo, Si, V and W in the Bcc (ferrite) phase at 1200 °C

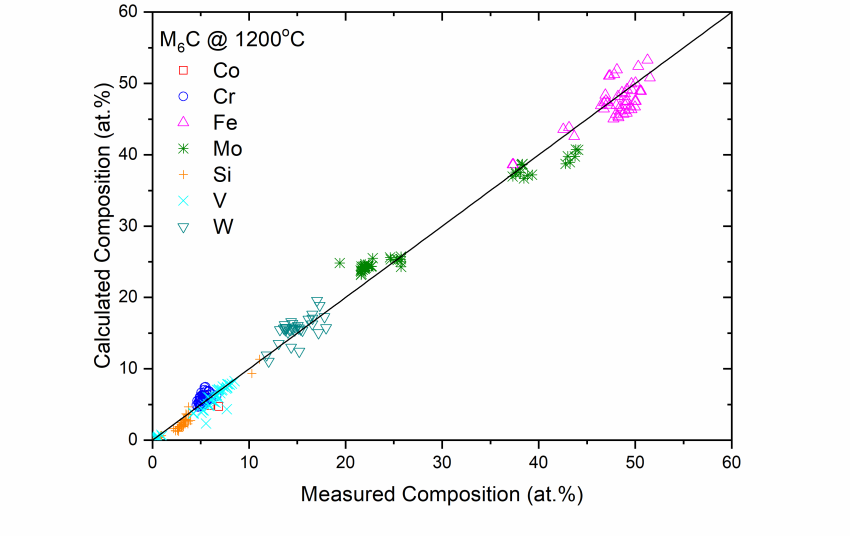


Figure 1.7: Comparison between the calculated and measured equilibrium compositions of Cr, Mo, Fe, V and W in the M_6C phase at 1200 °C

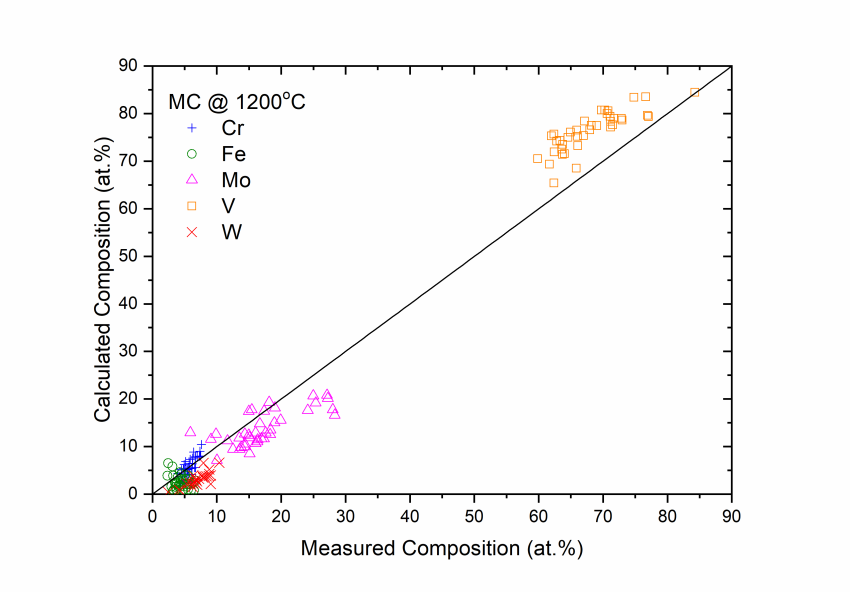


Figure 1.8: Comparison between the calculated and measured equilibrium compositions of Cr, Fe, Mo, V and W in the MC phase at 1200 °C

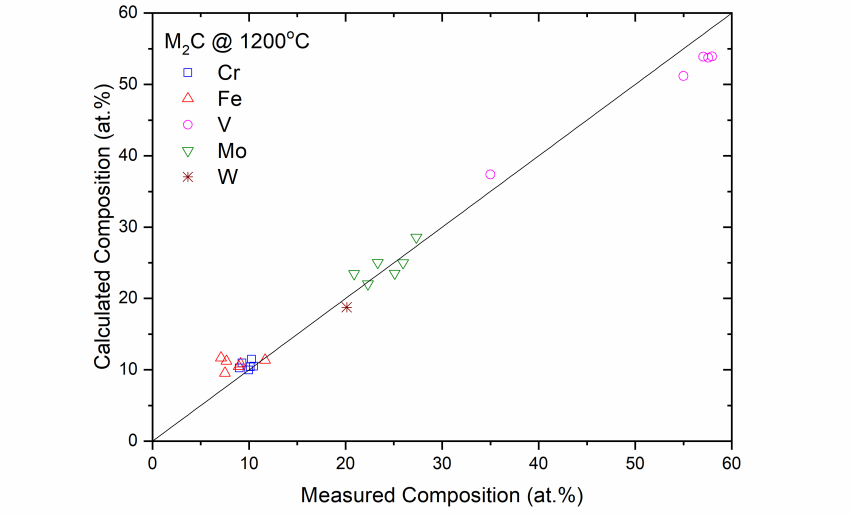


Figure 1.9: Comparison between the calculated and measured equilibrium compositions of Cr, Fe, Mo, V and W in the M_2C (Hcp) phase at 1200 °C

2 Mobility Database

PanFe2024_MB is an atomic mobility database for Fe-based alloys, which is compatible with the `PanFe2024_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

	Al	As	Ca	Ce	Co	Cr	Cu	Fe	Mg	Mn	Mo	Nb	Ni	Pb	Pr	Si	Sn	Ta	Ti	V
Bcc																				
Fcc																				
Hcp																				

	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

Al-Co	Al-Cu	Al-Mg	Al-Ni	Al-Si	Al-W	Al-Zn	Co-Cr	Co-Cu	Co-Fe
Co-Ni	Cr-Fe	Cr-Ni	Cu-Fe	Cu-Mg	Cu-Si	Cu-Sn	Cu-Ti	Cu-Zn	Fe-Mn
Fe-Ni	Fe-Si	Mn-Ni	Mo-Ni	Nb-Ni	Ni-Ta	Ni-Ti	Ni-V	Ni-W	Ni-Zn

Al-Co-W	Al-Cr-Ni	Al-Cu-Mg	Al-Cu-Si	Al-Cu-Zn	Al-Mg-Zn
Al-Mn-Ni	Al-Nb-Ni	Co-Cr-Ni	Co-Cr-W	Co-Cu-Fe	Co-Cu-Ni
Co-Fe-Ni	Co-Mo-W	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	Mo-Nb	Mo-Ta	Mo-Ti	Mo-W
Mo-Zr	Nb-Ta	Nb-Ti	Nb-V	Nb-W	Nb-Zr	Ta-Ti	Ta-W	Ti-V	Ti-Zr
V-Zr									

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

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 Fe-based alloys. A few examples of such simulation are shown below.

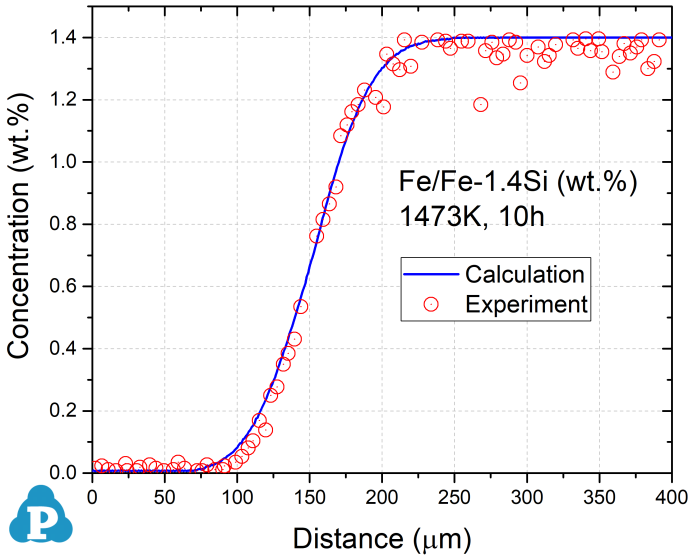


Figure 2.1: Concentration profile of Fe/Fe-1.4Si (wt.%) annealed at 1473K for 10h [2015Zhe]

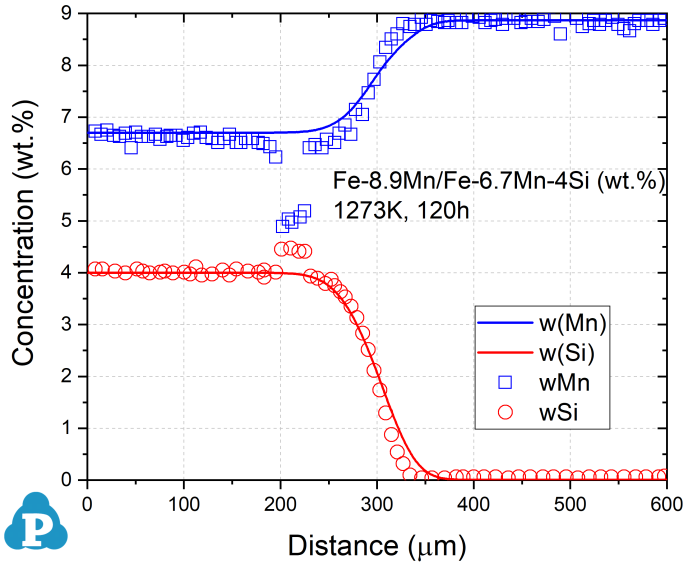


Figure 2.2: Concentration profile of Fe-8.9Mn/Fe-6.7Mn-4Si (wt.%) at 1273K for 120h [2015Zhe]

3 Thermophysical Property Database

The thermophysical property database **PanFe2024_TP** is compatible with the `PanFe2024_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Fe-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 **704** phases assessed in the `PanFe2024_TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of Fe-based alloys.

The simulated density changes vs. temperature of a series of Fe-based alloys are shown below to validate the current `PanFe2024_MV` database.

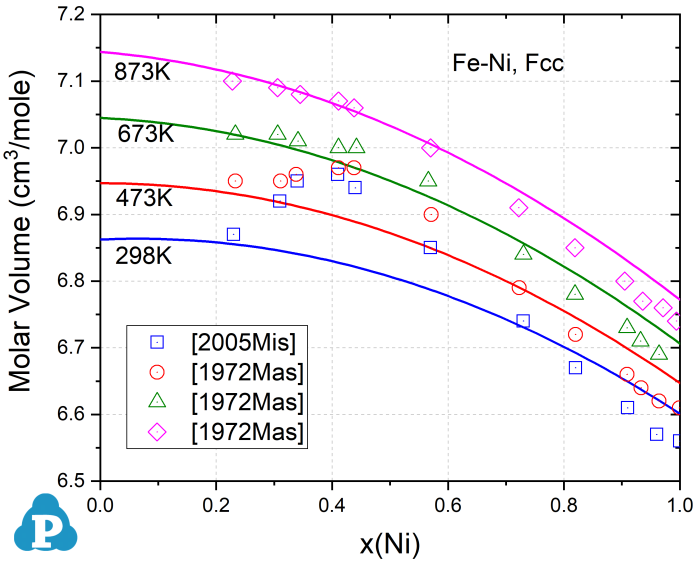


Figure 3.1: Molar volume of Fe-Ni Fcc alloys [1972Shi, 2005Mis]

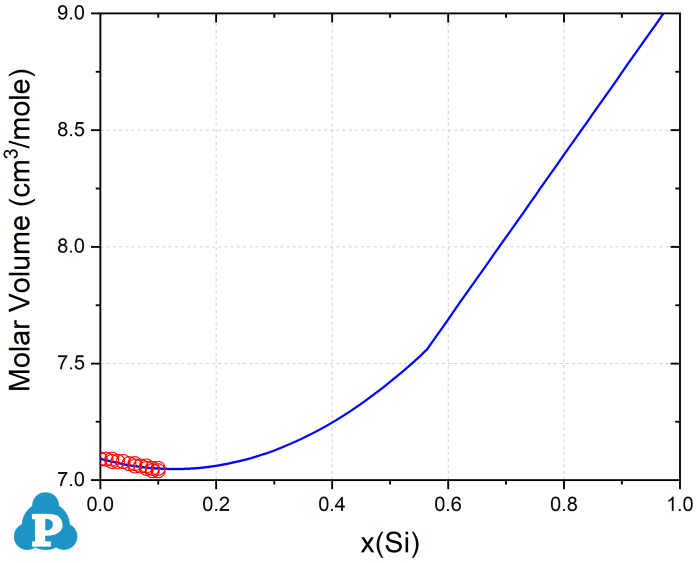


Figure 3.2: Molar volume of Fe-Si Bcc binary alloys at 298K [2006Hal]

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 Fe-Mn alloys in comparison with experimental data.

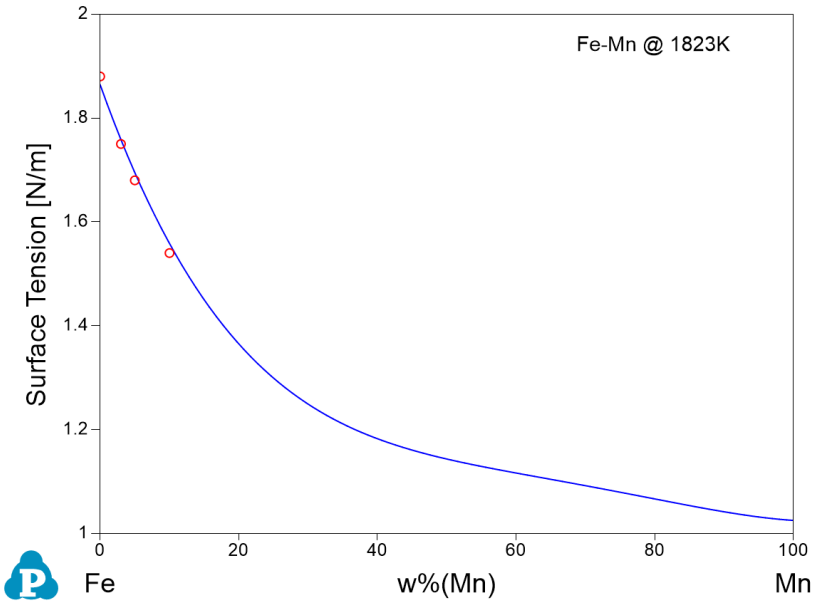


Figure 3.3: Surface tension of Fe-Mn alloy

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.4 shows the viscosity of a Fe-Cr-Ni alloy in comparison with experimental data.

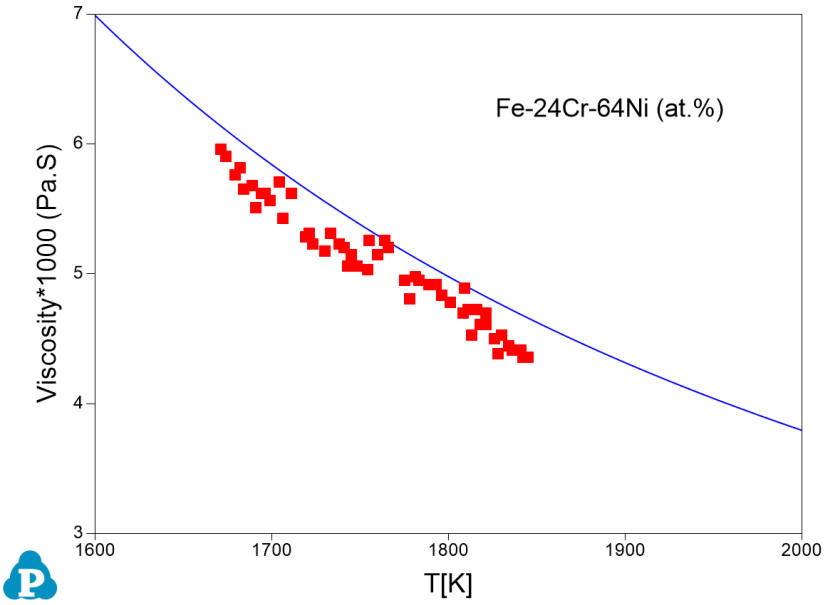


Figure 3.4: Viscosity of the Fe-24Cr-64Ni alloy

4 References

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PanFe 2024: List of Phases

Phases (**704**)

Name	Model	Lattice Size	Constituent
A3B	CEF (SLN)	(3)(1)	(Co,Cr,Fe,Mo,Nb)(Al,Cr,Mo,Nb,W)
AL12MN	CEF (ST2)	(12)(1)	(Al)(Mn)
AL6MN	CEF (ST2)	(6)(1)	(Al)(Mn)
AL8MN5	CEF (SLN)	(12)(5)(9)	(Al)(Mn)(Al,Mn)
ALPHA_B	CEF (ST1)	(1)	(B)
A_RE2O3	CEF (SLN)	(2)(2)(1)	(Ce+3,Ce+2,Pr+3) (O-2)(O-2,Va)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
Al10CeFe2	CEF (ST3)	(10)(1)(2)	(Al)(Ce)(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)
Al11Ce3_H	CEF (ST2)	(11)(3)	(Al)(Ce)
Al11Ce3_L	CEF (ST2)	(11)(3)	(Al)(Ce)
Al11Cr2	CEF (ST2)	(10)(1)(2)	(Al)(Al)(Cr)
Al11Ti5	CEF (ST2)	(17)(8)	(Al)(Ti)
Al12M	CEF (ST2)	(12)(1)	(Al)(Mo)
Al12W	CEF (ST2)	(12)(1)	(Al)(W)
Al13Cr2	CEF (ST2)	(13)(2)	(Al)(Cr)
Al13M4	CEF (SLN)	(0.6275) (0.235)	(Al)(Co,Cr,Fe,Mo)(Al,Va)

Name	Model	Lattice Size	Constituent
		(0.1375)	
Al17Mo4	CEF (ST2)	(17)(4)	(Al)(Mo)
Al22Mo5	CEF (ST2)	(22)(5)	(Al)(Mo)
Al23CuFe4	CEF (ST3)	(23)(1)(4)	(Al)(Cu)(Fe)
Al23V4	CEF (ST2)	(23)(4)	(Al)(V)
Al2CaSi2	CEF (ST3)	(2)(1)(2)	(Al)(Ca)(Si)
Al2Cu	CEF (SLN)	(0.667)(0.333)	(Al)(Al,Cu)
Al2Fe	CEF (SLN)	(2)(1)	(Al)(Co,Cr,Fe,Mo)
Al2S3	CEF (ST2)	(2)(3)	(Al)(S)
Al2Ti	CEF (ST2)	(2)(1)	(Al)(Ti)
Al2W	CEF (ST2)	(2)(1)	(Al)(W)
Al2Y3	CEF (ST2)	(0.4)(0.6)	(Al)(Y)
Al2Zr3	CEF (ST2)	(0.4)(0.6)	(Al)(Zr)
Al3Ca8	CEF (ST2)	(0.272727) (0.727272)	(Al)(Ca)
Al3Ce	CEF (ST2)	(0.75)(0.25)	(Al)(Ce)
Al3Co	CEF (ST2)	(3)(1)	(Al)(Co)
Al3M	CEF (SLN)	(3)(1)	(Al,Ti)(Nb,Ti,V,W)
Al3Mo	CEF (ST2)	(3)(1)	(Al)(Mo)
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)
Al3Zr	CEF (ST2)	(0.75)(0.25)	(Al)(Zr)
Al3Zr2	CEF (ST2)	(0.6)(0.4)	(Al)(Zr)
Al3Zr4	CEF (ST2)	(0.42857) (0.57143)	(Al)(Zr)

Name	Model	Lattice Size	Constituent
Al3Zr5	CEF (ST2)	(0.375)(0.625)	(Al)(Zr)
Al4C3	CEF (SLN)	(4)(3)	(Al,Si)(C)
Al4Ca	CEF (ST2)	(0.8)(0.2)	(Al)(Ca)
Al4Cr	CEF (ST2)	(4)(1)	(Al)(Cr)
Al4Mo	CEF (ST2)	(4)(1)	(Al)(Mo)
Al4W	CEF (ST2)	(4)(1)	(Al)(W)
Al4Zr5	CEF (ST2)	(0.444444) (0.555556)	(Al)(Zr)
Al5Co2	CEF (ST2)	(5)(2)	(Al)(Co)
Al5Fe2	CEF (SLN)	(5)(2)	(Al)(Co,Cr,Fe,Mo)
Al5Mo	CEF (ST2)	(5)(1)	(Al)(Mo)
Al5W	CEF (ST2)	(5)(1)	(Al)(W)
Al63Mo37	CEF (ST2)	(63)(37)	(Al)(Mo)
Al69Ta39	CEF (SLN)	(0.6389) (0.3611)	(Al,Ta)(Al,Ta)
Al77W23	CEF (ST2)	(77)(23)	(Al)(W)
Al7Cu2Fe	CEF (ST3)	(7)(2)(1)	(Al)(Cu)(Fe)
Al7V	CEF (ST2)	(7)(1)	(Al)(V)
Al7W3	CEF (ST2)	(7)(3)	(Al)(W)
Al8CeFe2	CEF (ST3)	(8)(1)(2)	(Al)(Ce)(Fe)
Al8CeM4	CEF (SLN)	(8)(1)(4)	(Al)(Ce)(Fe,Mn)
Al8Cr5_H	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Cr5_L	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Fe5	CEF (SLN)	(8)(5)	(Al,Fe)(Al,Fe)
Al8FeTi3	CEF (ST3)	(8)(1)(3)	(Al)(Fe)(Ti)

Name	Model	Lattice Size	Constituent
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)
AlAs	CEF (ST2)	(0.5)(0.5)	(Al)(As)
AlB12	CEF (ST2)	(1)(12)	(Al)(B)
AlCa	CEF (ST2)	(0.5)(0.5)	(Al)(Ca)
AlCe	CEF (ST2)	(1)(1)	(Al)(Ce)
AlCe3_H	CEF (ST2)	(1)(3)	(Al)(Ce)
AlCe3_L	CEF (ST2)	(1)(3)	(Al)(Ce)
AlCr2	CEF (ST2)	(1)(2)	(Al)(Cr)
AlCu_Delta	CEF (ST2)	(0.4)(0.6)	(Al)(Cu)
AlCu_Eps1	CEF (SLN)	(0.4)(0.6)	(Al,Cu)(Al,Cu)
AlCu_Eps2	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Cu)
AlCu_Eta	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Cu)
AlCu_Zeta	CEF (ST2)	(0.45)(0.55)	(Al)(Cu)
AlMg_Beta	CEF (ST2)	(89)(140)	(Mg)(Al)
AlMg_Eps	CEF (ST2)	(23)(30)	(Mg)(Al)
AlMg_Gamma	CEF (SLN)	(10)(24)(24)	(Mg)(Al,Mg)(Al,Mg)
AlMo3	CEF (SLN)	(1)(3)	(Al,Mo)(Al,Mo)
AlN	CEF (ST2)	(1)(1)	(Al)(N)
AlP	CEF (ST2)	(0.5)(0.5)	(Al)(P)
AlS	CEF (ST2)	(1)(1)	(Al)(S)

Name	Model	Lattice Size	Constituent
AlTi	CEF (SLN)	(1)(1)	(Al,Ti,V)(Al,Ti,V)
AlTi3	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Sn,Ti,V)(Al,Sn,Ti,V)(Va)
AlY	CEF (ST2)	(0.5)(0.5)	(Al)(Y)
AlY2	CEF (ST2)	(0.333333) (0.666667)	(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_CeC2	CEF (ST2)	(0.333333) (0.666667)	(Ce)(C)
Alpha_Co2Si	CEF (SLN)	(2)(1)	(Co,Fe,Ni,Si)(Co,Si)
Alpha_PrC2	CEF (ST2)	(0.333333) (0.666667)	(Pr)(C)
Alpha_Ta5Si3	CEF (ST2)	(5)(3)	(Ta)(Si)
Alpha_YZn2	CEF (ST2)	(1)(2)	(Y)(Zn)
As2O3	CEF (ST2)	(2)(3)	(As)(O)
As2O5	CEF (ST2)	(2)(5)	(As)(O)
As5CoFe	CEF (SLN)	(5)(3)	(As)(Co,Fe)
B2	CEF (SLN)	(1)(1)	(Al,Co,Fe,Mo,Ni,Ti) (Co,Cu,Fe,Mn,Mo,Ni,Ti,Zr,Va)
B2O3	CEF (ST2)	(2)(3)	(B)(O)
B3Si	CEF (SLN)	(6)(2)(6)	(B)(Si)(B,Si)
B4C	CEF (SLN)	(1)(1)	(B11C1,B12) (B2,C1B2,C2B1,B1C2,B2C1)

Name	Model	Lattice Size	Constituent
B4Ce	CEF (ST2)	(0.8)(0.2)	(B)(Ce)
B4Mo	CEF (ST2)	(0.8)(0.2)	(B)(Mo)
B4Pr	CEF (ST2)	(0.8)(0.2)	(B)(Pr)
B5Mo2	CEF (SLN)	(2)(5)	(Mo)(B,Va)
B5Pr2	CEF (ST2)	(0.714)(0.286)	(B)(Pr)
B6Si	CEF (SLN)	(210)(23)(48)	(B)(Si)(B,Si)
BCC_A12	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Mg,Mn,Ni,Si,Sn,Ta,Ti,V,Zn)(C,N,Va)
BCT_A5	CEF (SLN)	(1)	(Al,Pb,Sn)
BETA_RHOMB_B	CEF (SLN)	(93)(12)	(B)(B,C,Cu,Si,Zr)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
BN_HP4	CEF (ST2)	(1)(1)	(B)(N)
B_NSi	CEF (SLN)	(61)(1)(8)	(B)(Si)(B,Si)
Bcc	CEF (SLN)	(1)(3)	(Al,As,Ca,Ce,Co,Cr,Cu,Fe,Mg,Mn,Mo,Nb,Ni,P,Pb,Pr,S,Si,Sn,Ta,Ti,V,W,Y,Zn,Zr)(B,C,N,O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Al,Co,Cr,Fe,Mg,Ni,Pr,Si,Ti)(Al,Co,Cr,Fe,Mg,Ni,Pr,Si,Ti)(Va)
Beta2_Ni3Si	CEF (ST2)	(3)(1)	(Ni)(Si)
Beta3_Ni3Si	CEF (ST2)	(3)(1)	(Ni)(Si)
Beta_CeC2	CEF (ST2)	(0.333333)(0.666667)	(Ce)(C)
Beta_Co2Si	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Beta_PrC2	CEF (SLN)	(0.333333)(0.666667)	(Pr)(C,Va)

Name	Model	Lattice Size	Constituent
Beta_YZn2	CEF (ST2)	(1)(2)	(Y)(Zn)
CHI_A12	CEF (SLN)	(24)(10)(24)	(Cr,Fe,Ni)(Cr,Mo,Ta,W) (Cr,Fe,Mo,Ni,Ta,W)
CUB_A13	CEF (SLN)	(1)(1)	(Al,Ce,Co,Cr,Cu,Fe,Mg,Mn,Ni, P,Si,Sn,Ta,Ti,V,Zn)(C,N,Va)
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)
Ca5Zn3	CEF (ST2)	(5)(3)	(Ca)(Zn)
Ca7Sn6	CEF (ST2)	(7)(6)	(Ca)(Sn)

Name	Model	Lattice Size	Constituent
CaCu	CEF (ST2)	(0.5)(0.5)	(Ca)(Cu)
CaCu5	CEF (ST2)	(0.166667) (0.833333)	(Ca)(Cu)
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)
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)
Ce11O20	CEF (ST2)	(11)(20)	(Ce)(O)
Ce11Sn10	CEF (ST2)	(0.5238) (0.4762)	(Ce)(Sn)
Ce13Zn58	CEF (ST2)	(0.183)(0.817)	(Ce)(Zn)
Ce19O34	CEF (ST2)	(19)(34)	(Ce)(O)
Ce2C3	CEF (ST2)	(0.4)(0.6)	(Ce)(C)
Ce2Mg17	CEF (ST2)	(2)(17)	(Ce)(Mg)
Ce2Sn5	CEF (ST2)	(0.2857) (0.7143)	(Ce)(Sn)

Name	Model	Lattice Size	Constituent
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)
Ce3Sn	CEF (ST2)	(0.75)(0.25)	(Ce)(Sn)
Ce3Sn5	CEF (ST2)	(0.375)(0.625)	(Ce)(Sn)
Ce3Sn7	CEF (ST2)	(0.3)(0.7)	(Ce)(Sn)
Ce3Zn11	CEF (ST2)	(0.214)(0.786)	(Ce)(Zn)
Ce3Zn22	CEF (ST2)	(0.12)(0.88)	(Ce)(Zn)
Ce40O72	CEF (ST2)	(40)(72)	(Ce)(O)
Ce4Fe4C7	CEF (ST3)	(4)(4)(7)	(Ce)(Fe)(C)
Ce5Mg41	CEF (ST2)	(5)(41)	(Ce)(Mg)
Ce5Si4	CEF (ST2)	(0.555556) (0.444444)	(Ce)(Si)
Ce5Sn3	CEF (ST2)	(0.625)(0.375)	(Ce)(Sn)
Ce5Sn4	CEF (ST2)	(0.5556) (0.4444)	(Ce)(Sn)
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)
CeCrFe	CEF (ST3)	(0.12)(0.23) (0.65)	(Ce)(Cr)(Fe)
CeFe2Si2	CEF (ST3)	(1)(2)(2)	(Ce)(Fe)(Si)
CeFeSi	CEF (ST3)	(1)(1)(1)	(Ce)(Fe)(Si)
CeMg	CEF (ST2)	(0.5)(0.5)	(Ce)(Mg)

Name	Model	Lattice Size	Constituent
CeMg12	CEF (ST2)	(1)(12)	(Ce)(Mg)
CeMg3	CEF (ST2)	(1)(3)	(Ce)(Mg)
CeNi	CEF (ST2)	(0.5)(0.5)	(Ce)(Ni)
CeNi3	CEF (ST2)	(0.25)(0.75)	(Ce)(Ni)
CeNi5	CEF (ST2)	(0.1667) (0.8333)	(Ce)(Ni)
CeSi	CEF (ST2)	(0.5)(0.5)	(Ce)(Si)
CeSn3	CEF (ST2)	(0.25)(0.75)	(Ce)(Sn)
CeZn	CEF (ST2)	(0.5)(0.5)	(Ce)(Zn)
CeZn11	CEF (ST2)	(0.083)(0.917)	(Ce)(Zn)
CeZn2	CEF (ST2)	(0.333)(0.667)	(Ce)(Zn)
CeZn3	CEF (ST2)	(0.25)(0.75)	(Ce)(Zn)
CeZn5	CEF (ST2)	(0.167)(0.833)	(Ce)(Zn)
Cementite	CEF (SLN)	(3)(1)	(Co,Cr,Fe,Mn,Mo,Nb,Ni,V,W) (B,C,N)
Co11Ce24	CEF (ST2)	(11)(24)	(Co)(Ce)
Co11Zr2	CEF (ST2)	(11)(2)	(Co)(Zr)
Co17Y2	CEF (ST2)	(17)(2)	(Co)(Y)
Co19R5	CEF (SLN)	(19)(5)	(Co,Fe)(Ce,Pr)
Co23Zr6	CEF (ST2)	(23)(6)	(Co)(Zr)
Co2P	CEF (ST2)	(2)(1)	(Co)(P)
Co2Pr5	CEF (ST2)	(0.286)(0.714)	(Co)(Pr)
Co2Ta_C36	CEF (SLN)	(2)(1)	(Co,Ta)(Co,Ta)
Co2Y	CEF (ST2)	(2)(1)	(Co)(Y)
Co2Zn15	CEF (ST2)	(0.117647) (0.882353)	(Co)(Zn)

Name	Model	Lattice Size	Constituent
Co3B	CEF (SLN)	(3)(1)	(Co,Fe)(B)
Co3Pr4	CEF (ST2)	(0.459)(0.541)	(Co)(Pr)
Co3R	CEF (SLN)	(3)(1)	(Co,Fe)(Ce,Pr)
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)
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)
Co5R	CEF (SLN)	(5)(1)	(Co,Fe)(Ce,Pr)
Co5Y	CEF (ST2)	(5)(1)	(Co)(Y)
Co5Y8	CEF (ST2)	(5)(8)	(Co)(Y)
Co7R2	CEF (SLN)	(7)(2)	(Co,Fe)(Ce,Pr)
Co7Ta2	CEF (ST2)	(7)(2)	(Co)(Ta)
Co7Y2	CEF (ST2)	(7)(2)	(Co)(Y)
Co7Y6	CEF (ST2)	(7)(6)	(Co)(Y)
CoAs3	CEF (ST2)	(1)(3)	(Co)(As)
CoP	CEF (ST2)	(0.5)(0.5)	(Co)(P)
CoPr3	CEF (ST2)	(0.25)(0.75)	(Co)(Pr)
CoSi	CEF (SLN)	(0.5)(0.5)	(Co,Si)(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)
CoTa2	CEF (SLN)	(1)(2)	(Co,Ta)(Ta)

Name	Model	Lattice Size	Constituent
CoTi2	CEF (ST2)	(1)(2)	(Co)(Ti)
CoV3	CEF (ST2)	(1)(3)	(Co)(V)
CoY	CEF (ST2)	(1)(1)	(Co)(Y)
CoY3	CEF (ST2)	(1)(3)	(Co)(Y)
CoZn14	CEF (ST2)	(0.0714286) (0.928571)	(Co)(Zn)
CoZn7	CEF (ST2)	(0.125)(0.875)	(Co)(Zn)
CoZn_Beta	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
CoZr2	CEF (ST2)	(1)(2)	(Co)(Zr)
CoZr3	CEF (ST2)	(1)(3)	(Co)(Zr)
Co_Ni3W	CEF (SLN)	(3)(1)	(Co,Ni)(W)
Corundum	CEF (SLN)	(2)(1)(3)	(Al+3,Cr+2,Cr+3,Fe+2,Fe+3, Mn+3,Ti+3,V+3,V+4) (Cr+3,Fe+3,Ni+2,Va)(O-2)
Cr2B_Orth	CEF (SLN)	(2)(1)	(Cr,Fe,Mo)(B)
Cr2S2	CEF (ST2)	(0.512)(0.488)	(Cr)(S)
Cr2S3	CEF (SLN)	(2)(3)	(Cr,Fe)(S)
Cr3Mn5	CEF (SLN)	(3)(5)	(Cr)(Mn,Ti)
Cr3S4	CEF (SLN)	(3)(4)	(Cr,Fe)(S)
Cr5B3	CEF (SLN)	(0.625)(0.375)	(Cr,Fe,Mo)(B)
Cr8Fe16Ti5	CEF (SLN)	(0.86)(0.14)	(Cr,Fe)(Ti)
CrB4	CEF (SLN)	(0.2)(0.8)	(Cr,Fe)(B)
CrZn17	CEF (ST2)	(0.05556) (0.94444)	(Cr)(Zn)
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
Cu10Sn3	CEF (SLN)	(1)	(Cu,Sn)

Name	Model	Lattice Size	Constituent
Cu10Zr7	CEF (ST2)	(10)(7)	(Cu)(Zr)
Cu15Si4	CEF (ST2)	(0.789474) (0.210526)	(Cu)(Si)
Cu19Si6	CEF (ST2)	(0.76)(0.24)	(Cu)(Si)
Cu2Ce	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Ce)
Cu2O	CEF (ST2)	(2)(1)	(Cu)(O)
Cu2Pr	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Pr)
Cu2S	CEF (ST2)	(2)(1)	(Cu)(S)
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)
Cu33Si7	CEF (ST2)	(0.825)(0.175)	(Cu)(Si)
Cu3As	CEF (ST2)	(0.75)(0.25)	(Cu)(As)
Cu3P	CEF (SLN)	(3)(1)	(Cu,Fe)(P)
Cu3Sn	CEF (SLN)	(3)(1)	(Cu,Sn)(Cu,Sn)
Cu3Ti2	CEF (ST2)	(0.6)(0.4)	(Cu)(Ti)
Cu41Sn11	CEF (SLN)	(41)(11)	(Cu,Sn)(Cu,Sn)
Cu4Ce	CEF (ST2)	(0.8)(0.2)	(Cu)(Ce)
Cu4Pr	CEF (ST2)	(0.8)(0.2)	(Cu)(Pr)
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)

Name	Model	Lattice Size	Constituent
Cu51Zr14	CEF (ST2)	(51)(14)	(Cu)(Zr)
Cu5As2	CEF (ST2)	(5)(2)	(Cu)(As)
Cu5Ce	CEF (ST2)	(0.833333) (0.166667)	(Cu)(Ce)
Cu5Pr	CEF (ST2)	(0.833333) (0.166667)	(Cu)(Pr)
Cu5Zr	CEF (ST2)	(5)(1)	(Cu)(Zr)
Cu6Ce	CEF (ST2)	(0.857143) (0.142857)	(Cu)(Ce)
Cu6Pr	CEF (ST2)	(0.857143) (0.142857)	(Cu)(Pr)
Cu6Sn5H	CEF (SLN)	(1)(1)(1)	(Cu)(Cu,Sn)(Sn)
Cu6Sn5L	CEF (SLN)	(1)(1)(1)	(Cu)(Cu,Sn)(Sn)
Cu6Y	CEF (SLN)	(5)(1)	(Cu)(Cu2,Y)
Cu7Y2	CEF (ST2)	(7)(2)	(Cu)(Y)
Cu8As	CEF (ST2)	(8)(1)	(Cu)(As)
Cu8Zr3	CEF (ST2)	(8)(3)	(Cu)(Zr)
CuCe	CEF (ST2)	(0.5)(0.5)	(Ce)(Cu)
CuMg2	CEF (ST2)	(1)(2)	(Cu)(Mg)
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuPr	CEF (ST2)	(0.5)(0.5)	(Cu)(Pr)
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)
CuZn_BETA	CEF (SLN)	(1)(1)	(Cu,Zn)(Zn)

Name	Model	Lattice Size	Constituent
CuZn_EPS	CEF (SLN)	(1)	(Cu,Zn)
CuZn_GAMMA	CEF (SLN)	(0.15385) (0.15385) (0.23077) (0.46154)	(Cu,Zn)(Cu,Zn)(Cu)(Zn)
CuZr	CEF (ST2)	(1)(1)	(Cu)(Zr)
CuZr2	CEF (ST2)	(1)(2)	(Cu)(Zr)
D0_22_Al3Ta	CEF (SLN)	(0.75)(0.25)	(Al)(Al,Ta)
DHCP	CEF (SLN)	(1)(1)	(Ce,Mg,Mn,Pr,Y,Zn)(C,Va)
Delta	CEF (SLN)	(3)(1)	(Cr,Nb,Ni)(Cr,Nb,Ni)
Diamond	CEF (SLN)	(1)	(Al,B,C,P,Si,Sn,Ti)
EPS	CEF (SLN)	(1)	(Al,Cu)
Epsilon_Ni3Si2	CEF (SLN)	(3)(2)	(Fe,Ni)(Si)
Eta	CEF (SLN)	(0.75)(0.25)	(Fe,Ni,Ti)(Al,Mo,Ni,Ti)
Eta_MC	CEF (SLN)	(1)(1)	(Mo,W)(C,Va)
F_Ce2O4	CEF (SLN)	(2)(4)	(Ce+3,Ce+4)(O-2,Va)
Fcc	CEF (SLN)	(1)(1)	(Al,As,Ca,Ce,Co,Cr,Cu,Fe,Mg, Mn,Mo,Nb,Ni,P,Pb,Pr,S,Si,Sn, Ta,Ti,V,W,Y,Zn,Zr)(B,C,N,O,Va)
Fe10Si2B3	CEF (ST3)	(10)(2)(3)	(Fe)(Si)(B)
Fe17Y2	CEF (ST2)	(17)(2)	(Fe)(Y)
Fe23Y6	CEF (ST2)	(23)(6)	(Fe)(Y)
Fe2As	CEF (SLN)	(2)(1)	(Co,Cu,Fe,Mn,Ni)(As)
Fe2Si	CEF (SLN)	(0.666667) (0.333333)	(Fe)(Si,Sn)
Fe2Ta3	CEF (SLN)	(2)(3)	(Fe,Ta)(Fe,Ta)

Name	Model	Lattice Size	Constituent
Fe3As2	CEF (SLN)	(1)(0.75)	(Co,Fe)(As,Va)
Fe3Sn2	CEF (ST2)	(3)(2)	(Fe)(Sn)
Fe3Y	CEF (ST2)	(3)(1)	(Fe)(Y)
Fe4N	CEF (SLN)	(4)(1)	(Co,Cr,Fe,Mn,Ni)(C,N,Va)
Fe5Ni3Si2	CEF (SLN)	(3)(1)(1)	(Fe,Ni)(Ni)(Si)
Fe5Si2B	CEF (ST3)	(4.7)(2)(1)	(Fe)(Si)(B)
Fe5SiB2	CEF (ST3)	(5)(1)(2)	(Fe)(Si)(B)
Fe5Sn3	CEF (ST2)	(5)(3)	(Fe)(Sn)
Fe7Al67Zr26	CEF (ST3)	(7)(67)(26)	(Fe)(Al)(Zr)
Fe8Si2C	CEF (ST3)	(8)(2)(1)	(Fe)(Si)(C)
FeAl2Zr6	CEF (SLN)	(1)(2)(6)	(Fe)(Al,Zr)(Zr)
FeAs	CEF (SLN)	(1)(1)	(Co,Fe,Mn,Ni)(As)
FeAs2	CEF (SLN)	(1)(2)	(Co,Fe,Ni)(As)
FeCN_CHI	CEF (SLN)	(5)(2)	(Fe)(C,N)
FeCr2S4	CEF (SLN)	(1)(2)(4)	(Cr,Fe)(Cr,Fe)(S)
FeMnP	CEF (ST3)	(1)(1)(1)	(Fe)(Mn)(P)
FeMo4Zr9	CEF (ST3)	(1)(4)(9)	(Fe)(Mo)(Zr)
FeNb2P	CEF (ST3)	(1)(2)(1)	(Fe)(Nb)(P)
FeNb4P	CEF (ST3)	(1)(4)(1)	(Fe)(Nb)(P)
FeNbP	CEF (SLN)	(2)(1)	(Fe,Nb)(P)
FeP	CEF (SLN)	(1)(1)	(Cr,Fe,Mn)(P)
FeS	CEF (SLN)	(1)(1)	(Cr,Fe,Mg,Mn,Ni,Ti,Va)(S)
FeSi2_H	CEF (ST2)	(3)(7)	(Fe)(Si)
FeSi2_L	CEF (ST2)	(1)(2)	(Fe)(Si)
FeSn	CEF (SLN)	(0.5)(0.5)	(Fe)(Sn,Si)

Name	Model	Lattice Size	Constituent
FeSn2	CEF (ST2)	(1)(2)	(Fe)(Sn)
FeTiP	CEF (ST3)	(1)(1)(1)	(Fe)(Ti)(P)
FeZn13	CEF (SLN)	(0.072)(0.856)(0.072)	(Fe,Va)(Zn)(Zn,Va)
FeZn3	CEF (SLN)	(0.137)(0.118)(0.745)	(Fe)(Fe,Si,Zn)(Zn)
FeZn7	CEF (SLN)	(0.058)(0.18)(0.525)(0.237)	(Fe)(Fe,Si,Zn)(Zn)(Zn)
FeZn_Gamma	CEF (SLN)	(0.154)(0.154)(0.231)(0.461)	(Fe,Si,Zn)(Fe,Zn)(Fe,Mn,Zn)(Zn)
FeZr2	CEF (SLN)	(1)(2)	(Al,Fe,Zr)(Zr)
FeZr3	CEF (SLN)	(1)(3)	(Al,Fe,Zr)(Fe,Zr)
GAS	GAS	(1)	(N,N2,O,O2,O3,C,C2,C3,C4,C5,Al,AlO,AlO2,Al2,Al2O,Al2O2,Al2O3,C1O1,C1O2,Fe,FeO,FeO2,Fe2,Ca,CaO,Mg,Mg2,MgO,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,Sn,Sn2,SnO,SnO2,Si,Si2,Si3,SiO,SiO2,Ti,TiO,TiO2,Y,YO,Zr,Zr2,ZrO,ZrO2)
Gamma	CEF (SLN)	(1)(1)	(Al,Cu,Si)(Va)
Gamma_H	CEF (SLN)	(4)(1)(8)	(Al)(Al,Cu)(Cu)
Gamma_Ni5Si2	CEF (SLN)	(5)(2)	(Fe,Ni)(Si)
Graphite	CEF (SLN)	(1)	(B,C)

Name	Model	Lattice Size	Constituent
HT_AL11MN4	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
H_L21	CEF (SLN)	(0.5)(0.5)(1)	(Al,Fe,Ni,Ti)(Al,Fe,Ni,Ti) (Fe,Ni,Va)
H_RE2O3	CEF (SLN)	(2)(2)(1)	(Ce+3,Ce+2,Pr+3)(O-2)(O-2,Va)
Halite	CEF (SLN)	(1)(1)	(Al+3,Ca+2,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)
Hcp	CEF (SLN)	(1)(0.5)	(Al,As,Ca,Ce,Co,Cr,Cu,Fe,Mg,Mn, Mo,Nb,Ni,Pb,Pr,Si,Sn,Ta,Ti,V,W, Y,Zn,Zr)(B,C,N,O,Va)
Kappa	CEF (SLN)	(3)(1)(1)	(Fe,Mn)(Al,Fe,Mn)(C,Va)
Ksi_Carbide	CEF (SLN)	(3)(1)	(Cr,Fe,Mo,W)(C)
L12_FCC	CEF (SLN)	(0.75)(0.25)	(Al,Co,Cu,Mo,Ni,Ti) (Al,Co,Cu,Mo,Ni,Ti)
LT_AL11MN4	CEF (ST2)	(11)(4)	(Al)(Mn)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Co,Cr,Fe,Mg,Mn,Mo,Nb,Ni,Ti, W,Zn,Zr)(Al,Ca,Co,Cr,Fe,Mg,Mn, Mo,Nb,Ni,Ti,W,Y,Zn,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Co,Cr,Cu,Fe,Mg,Mn,Mo,Nb, Ni,Ti,V,W,Zr)(Ca,Ce,Co,Cr,Cu, Fe,Mg,Mn,Mo,Nb,Ni,Pr,Ti,Y,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Cr,Fe,Mn,Ti,Zr)(Cr,Fe,Mn,Ti,Zr)
Liquid	CEF (SLN)	(1)	(Al,AlN,Al2S3,As,B,C,Ca,Ca2Pb, Ca1S1,Ca2Sn,Ce,Co,Co2P,Cr, Cr1S1,Cu,Fe,Fe1S1,Mg,Mg1S1, Mg2Sn,Mn,Mn1S1,Mo,Mo2S3, N,Nb,Ni,Ni1S1,O,P,Pb,Pr,S,Si,

Name	Model	Lattice Size	Constituent
			Sn,Ta,Ti,V,W,Y,Zn,Zr,Si3N4, Al2O3,As2O3,As2O5,B2O3,CaO, CeO3/2,CeO2,CoO,Co2O3, Cr2/3O,CuO,Cu2O,Cu2O3,FeO, FeO3/2,MgO,MnO,MnO3/2,MoO2, MoO3,NbO,NbO2,Nb2O5,NiO, P4O6,P4O10,PbO,Pr2/3O,SO3, SiO2,SnO,SnO2,Ta2O5,TiO, TiO3/2,TiO2,VO,VO2,VO3/2, VO5/2,WO2,WO3,Y2O3,Zr1/2O)
M12C	CEF (ST3)	(6)(6)(1)	(Co)(W)(C)
M12Zr	CEF (SLN)	(12)(1)	(Al,Fe)(Zr)
M17R2_hR57	CEF (SLN)	(17)(2)	(Al,Co,Fe,Si)(Ce,Pr)
M23C6	CEF (SLN)	(20)(3)(6)	(Co,Cr,Fe,Mn,Ni,V) (Co,Cr,Fe,Mn,Mo,Ni,V,W)(B,C)
M23Fe6	CEF (SLN)	(23)(6)	(Al,Ti)(Fe)
M2B	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Mo,Mn,Ni,Ta,W)(B)
M2P	CEF (SLN)	(2)(1)	(Cr,Cu,Fe,Mn,Mo,Nb,Ni,Ti)(P)
M2SiO4	CEF (SLN)	(2)(1)	(FeO,MnO,NiO)(SiO2)
M2Si_tI12	CEF (SLN)	(2)(1)	(Ta,Zr)(Si)
M2Ta_C14	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Mn,Ta)(Co,Cr,Fe,Ta)
M2Ta_C15	CEF (SLN)	(2)(1)	(Co,Cr,Ta)(Co,Ta)
M3B2	CEF (SLN)	(0.6)(0.4)	(Cr,Fe,Mo,Nb,Ta,V)(B)
M3B4	CEF (SLN)	(0.429)(0.571)	(Cr,Mn,Nb,Ta,Ti,V)(B)
M3C2	CEF (SLN)	(3)(2)	(Co,Cr,Mo,V,W)(C)
M3P	CEF (SLN)	(3)(1)	(Cr,Fe,Mn,Mo,Ni,Ti)(P)

Name	Model	Lattice Size	Constituent
M3Si_cF16	CEF (SLN)	(3)(1)	(Fe,Mn)(Si)
M3Si_cP8	CEF (SLN)	(3)(1)	(Cr,Mo,Nb,Si,V)(Cr,Mo,Si,V)
M3Si_tP32	CEF (SLN)	(3)(1)	(Mo,Ta,Ti,Zr)(Si)
M5As2	CEF (SLN)	(5)(2)	(Co,Fe,Ni)(As)
M5C2	CEF (SLN)	(5)(2)	(Fe,Mn,V)(C)
M5Si3_hP16	CEF (SLN)	(5)(3)	(Fe,Mn,Nb,Ti,Y,Zr)(Si)
M5Si3_tI32	CEF (SLN)	(0.625)(0.375)	(Ce,Cr,Fe,Mn,Mo,Nb,Ni,Si, Ta,Ti,V,W)(Mo,Nb,Si)
M6C	CEF (SLN)	(2)(2)(2)(1)	(Co,Fe,Ni)(Cr,Mo,W) (Co,Cr,Fe,Mo,Ni,Si,V,W)(C)
M7C3	CEF (SLN)	(7)(3)	(Co,Cr,Fe,Mn,Mo,Ni,V,W)(C)
MB2	CEF (SLN)	(0.333)(0.667)	(Al,Cr,Fe,Mn,Mo,Nb,Ti,V)(B,Va)
MB6	CEF (SLN)	(1)(6)	(B,Ca,Ce,Pr)(B)
MB_OC8	CEF (SLN)	(0.5)(0.5)	(Cr,Fe,Mo,Nb,Ni,Ta,V,W)(B,Va)
MB_OP8	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Mn,Ti)(B)
MO2	CEF (SLN)	(1)(2)	(Mo,V,W,Zr)(O)
MSi	CEF (SLN)	(0.5)(0.5)	(Cr,Fe,Mn,Ni)(Si,Sn)
MSi2_cF12	CEF (SLN)	(1)(2)	(Co,Fe,Mn,Ni)(Al,Si)
MSi2_hP9	CEF (SLN)	(1)(2)	(Cr,Fe,Nb,Ni,Ta,V)(Si)
MSi2_tI12	CEF (SLN)	(1)(2)	(Ca,Ce)(Si)
MSi2_tI6	CEF (SLN)	(1)(2)	(Mo,Nb,W)(Si,Va)
Mg12Pr	CEF (ST2)	(12)(1)	(Mg)(Pr)
Mg24Y5	CEF (SLN)	(24)(5)	(Mg)(Mg,Y)
Mg2C3	CEF (ST2)	(0.4)(0.6)	(Mg)(C)
Mg2Ni	CEF (ST2)	(2)(1)	(Mg)(Ni)

Name	Model	Lattice Size	Constituent
Mg2Pb	CEF (ST2)	(2)(1)	(Mg)(Pb)
Mg2Pr	CEF (ST2)	(2)(1)	(Mg)(Pr)
Mg2Si	CEF (ST2)	(2)(1)	(Mg)(Si)
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)
Mg3N2	CEF (ST2)	(3)(2)	(Mg)(N)
Mg3Pr	CEF (SLN)	(3)(1)	(Mg)(Mg,Pr)
Mg41Pr5	CEF (ST2)	(41)(5)	(Mg)(Pr)
Mg5Pr	CEF (ST2)	(5)(1)	(Mg)(Pr)
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)	(1)(2)	(Mg)(C)
MgNi2	CEF (SLN)	(1)(2)	(Mg,Ni)(Mg,Ni)
MgY	CEF (SLN)	(0.5)(0.5)	(Mg,Y)(Mg)
MgZn	CEF (ST2)	(12)(13)	(Mg)(Zn)
Mn11Si19	CEF (ST2)	(11)(19)	(Mn)(Si)
Mn12Y	CEF (ST2)	(12)(1)	(Mn)(Y)
Mn19Sn6	CEF (ST2)	(19)(6)	(Mn)(Sn)
Mn23Pr6	CEF (ST2)	(23)(6)	(Mn)(Pr)
Mn23Y6	CEF (ST2)	(23)(6)	(Mn)(Y)
Mn2Sn	CEF (ST2)	(2)(1)	(Mn)(Sn)

Name	Model	Lattice Size	Constituent
Mn3As	CEF (ST2)	(3)(1)	(Mn)(As)
Mn3P2	CEF (ST2)	(3)(2)	(Mn)(P)
Mn6N4	CEF (ST2)	(6)(4)	(Mn)(N)
Mn6N5	CEF (ST2)	(6)(5)	(Mn)(N)
Mn6Si	CEF (ST2)	(17)(3)	(Mn)(Si)
Mn9Si2	CEF (ST2)	(33)(7)	(Mn)(Si)
MnB4	CEF (ST2)	(0.2)(0.8)	(Mn)(B)
MnNi2	CEF (SLN)	(1)(2)	(Mn,Ni)(Ni)
MnNi3	CEF (SLN)	(1)(3)	(Mn,Ni)(Mn,Ni)
MnP4	CEF (ST2)	(1)(4)	(Mn)(P)
MnS	CEF (SLN)	(1)(1)	(Ca,Cr,Fe,Mg,Mn)(S)
MnS2	CEF (SLN)	(1)(2)	(Fe,Mn)(S)
MnSn2	CEF (ST2)	(1)(2)	(Mn)(Sn)
MnZn9	CEF (ST2)	(0.1)(0.9)	(Mn)(Zn)
Mo2S3	CEF (ST2)	(2)(3)	(Mo)(S)
Mo3P	CEF (ST2)	(3)(1)	(Mo)(P)
Mo4O11	CEF (ST2)	(0.266667) (0.733333)	(Mo)(O)
Mo8O23	CEF (ST2)	(0.258064) (0.741935)	(Mo)(O)
Mo9O26	CEF (ST2)	(0.257143) (0.742857)	(Mo)(O)
MoNi3	CEF (SLN)	(1)(3)	(Mo,Ti)(Ni)
MoNi4	CEF (ST2)	(1)(4)	(Mo)(Ni)
MoNi_Delta	CEF (SLN)	(24)(20)(12)	(Cr,Fe,Ni)(Cr,Fe,Mo,Ni)(Mo)

Name	Model	Lattice Size	Constituent
MoO2	CEF (ST2)	(1)(2)	(Mo)(O)
MoO3	CEF (ST2)	(1)(3)	(Mo)(O)
MoP	CEF (ST2)	(1)(1)	(Mo)(P)
MoS2	CEF (ST2)	(1)(2)	(Mo)(S)
MoSn	CEF (ST2)	(1)(1)	(Mo)(Sn)
MoSn2	CEF (ST2)	(1)(2)	(Mo)(Sn)
Mu_PHASE	CEF (SLN)	(7)(2)(4)	(Al,Co,Cr,Fe,Mo,Mn,Nb,Ni,Ta) (Mo,Nb,Ta,W) (Al,Co,Cr,Fe,Mo,Nb,Ni,Ta,W)
Nb2O5	CEF (ST2)	(2)(5)	(Nb)(O)
Nb3P	CEF (ST2)	(3)(1)	(Nb)(P)
Nb3Sn	CEF (SLN)	(3)(1)	(Nb,Sn)(Nb,Sn)
Nb5B6	CEF (ST2)	(5)(6)	(Nb)(B)
Nb6Sn5	CEF (SLN)	(24)(16)(4)	(Nb)(Sn)(Nb,Sn)
Nb7P4	CEF (ST2)	(7)(4)	(Nb)(P)
NbNi8	CEF (ST2)	(1)(8)	(Nb)(Ni)
NbO	CEF (ST2)	(1)(1)	(Nb)(O)
NbO2	CEF (ST2)	(1)(2)	(Nb)(O)
NbP	CEF (ST2)	(1)(1)	(Nb)(P)
NbP2	CEF (ST2)	(1)(2)	(Nb)(P)
NbSn2	CEF (ST2)	(1)(2)	(Nb)(Sn)
Ni10Zr7	CEF (ST2)	(10)(7)	(Ni)(Zr)
Ni11Zr9	CEF (ST2)	(11)(9)	(Ni)(Zr)
Ni12P5	CEF (ST2)	(12)(5)	(Ni)(P)
Ni12P5_L	CEF (ST2)	(12)(5)	(Ni)(P)

Name	Model	Lattice Size	Constituent
Ni17Y2	CEF (ST2)	(17)(2)	(Ni)(Y)
Ni21Zr8	CEF (ST2)	(21)(8)	(Ni)(Zr)
Ni2SiO4	CEF (ST3)	(2)(1)	(NiO)(SiO2)
Ni2Ta	CEF (SLN)	(2)(1)	(Ni,Ta)(Ni,Ta)
Ni2V	CEF (ST2)	(2)(1)	(Ni)(V)
Ni2V7	CEF (ST2)	(2)(7)	(Ni)(V)
Ni2Y	CEF (ST2)	(2)(1)	(Ni)(Y)
Ni2Y3	CEF (ST2)	(2)(3)	(Ni)(Y)
Ni3B	CEF (SLN)	(0.75)(0.25)	(Fe,Ni)(B)
Ni3S2	CEF (ST2)	(0.6)(0.4)	(Ni)(S)
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)
Ni3Ta	CEF (SLN)	(3)(1)	(Ni,Ta)(Ni,Ta)
Ni3Ta_L	CEF (ST2)	(0.75)(0.25)	(Ni)(Ta)
Ni3V	CEF (ST2)	(3)(1)	(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)
Ni5P2	CEF (ST2)	(5)(2)	(Ni)(P)
Ni5P2_L	CEF (ST2)	(5)(2)	(Ni)(P)

Name	Model	Lattice Size	Constituent
Ni5Y	CEF (ST2)	(5)(1)	(Ni)(Y)
Ni5Zr	CEF (SLN)	(5)(1)	(Ni,Zr)(Zr,Va)
Ni7Y2	CEF (ST2)	(7)(2)	(Ni)(Y)
Ni7Zr2	CEF (ST2)	(7)(2)	(Ni)(Zr)
Ni8Ta	CEF (ST2)	(8)(1)	(Ni)(Ta)
NiMo	CEF (SLN)	(24)(20)(12)	(Ni)(Al,Mo,Ni)(Mo)
NiS2	CEF (ST2)	(1)(2)	(Ni)(S)
NiSi	CEF (SLN)	(1)(1)	(Fe,Ni)(Si)
NiTa2	CEF (SLN)	(1)(2)	(Ni,Ta)(Ni,Ta)
NiTi2	CEF (ST2)	(0.333333) (0.666667)	(Ni)(Ti)
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)
NiZn8	CEF (ST2)	(0.111)(0.889)	(Ni)(Zn)
NiZn_Beta1	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)
Orthorhombic	CEF (ST1)	(1)	(S)
P2O5	CEF (ST2)	(2)(5)	(P)(O)
PI	CEF (SLN)	(12.8)(7.2)(4)	(Cr)(Fe,Ni)(N)
P_PHASE	CEF (SLN)	(24)(20)(12)	(Cr,Fe,Ni)(Cr,Fe,Mo,Ni)(Mo)
P_Red	CEF (ST1)	(1)	(P)

Name	Model	Lattice Size	Constituent
P_White	CEF (ST1)	(1)	(P)
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	CEF (SLN)	(0.8837) (1.1163)	(Al,Ta)(Al,Ta)
Pr11O20	CEF (ST2)	(11)(20)	(Pr)(O)
Pr13Zn58	CEF (ST2)	(0.183)(0.817)	(Pr)(Zn)
Pr2C3	CEF (SLN)	(0.4)(0.6)	(Pr)(C,Va)
Pr2Ni7	CEF (ST2)	(0.2222) (0.7778)	(Pr)(Ni)
Pr2Y	CEF (SLN)	(2)(1)	(Pr,Y)(Pr,Y)
Pr2Zn17_alpha	CEF (ST2)	(0.105)(0.895)	(Pr)(Zn)
Pr2Zn17_beta	CEF (ST2)	(0.105)(0.895)	(Pr)(Zn)
Pr3Ni	CEF (ST2)	(0.75)(0.25)	(Pr)(Ni)
Pr3O5	CEF (SLN)	(2)(3)(1)	(Pr+3,Pr+4)(O-2)(O-2,Va)
Pr3Zn11	CEF (ST2)	(0.214)(0.786)	(Pr)(Zn)
Pr3Zn22	CEF (ST2)	(0.12)(0.88)	(Pr)(Zn)
Pr40O72	CEF (ST2)	(40)(72)	(Pr)(O)
Pr6O11	CEF (ST2)	(6)(11)	(Pr)(O)

Name	Model	Lattice Size	Constituent
Pr7Ni3	CEF (ST2)	(0.7)(0.3)	(Pr)(Ni)
Pr7O12	CEF (ST2)	(7)(12)	(Pr)(O)
Pr9O16	CEF (ST2)	(9)(16)	(Pr)(O)
PrNi	CEF (ST2)	(0.5)(0.5)	(Pr)(Ni)
PrNi3	CEF (ST2)	(0.25)(0.75)	(Pr)(Ni)
PrNi5	CEF (ST2)	(0.1667) (0.8333)	(Pr)(Ni)
PrO2	CEF (SLN)	(1)(2)(1)	(Pr+3,Pr+4)(O-2,Va)(O-2,Va)
PrZn	CEF (ST2)	(0.5)(0.5)	(Pr)(Zn)
PrZn11	CEF (ST2)	(0.083)(0.917)	(Pr)(Zn)
PrZn2_alpha	CEF (ST2)	(0.333)(0.667)	(Pr)(Zn)
PrZn2_beta	CEF (ST2)	(0.333)(0.667)	(Pr)(Zn)
PrZn3	CEF (ST2)	(0.25)(0.75)	(Pr)(Zn)
Quartz	CEF (ST2)	(1)(2)	(Si)(O)
Rhombohedral_ A7	CEF (ST1)	(1)	(As)
R_AL4MN	CEF (ST2)	(461)(107)	(Al)(Mn)
R_PHASE	CEF (SLN)	(27)(14)(12)	(Co,Cr,Fe,Mn,Ni)(Mo,W) (Co,Cr,Fe,Mn,Mo,Ni,W)
Rutile	CEF (SLN)	(1)(2)	(Mn+4,Sn+4,Ti+3,Ti+4,V+4) (O-2,Va)
Shp_MC	CEF (SLN)	(1)(1)	(Mo,W)(C,N)
Si2Ti	CEF (ST2)	(2)(1)	(Si)(Ti)
Si2Y_H	CEF (ST2)	(2)(1)	(Si)(Y)
Si2Y_R	CEF (ST2)	(2)(1)	(Si)(Y)
Si2Zr3	CEF (ST2)	(2)(3)	(Si)(Zr)

Name	Model	Lattice Size	Constituent
Si3N4	CEF (ST2)	(3)(4)	(Si)(N)
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)	(Si)(C)
SiP	CEF (ST2)	(1)(1)	(P)(Si)
SiTi	CEF (ST2)	(0.5)(0.5)	(Si)(Ti)
SiY	CEF (ST2)	(1)(1)	(Si)(Y)
SiZr	CEF (ST2)	(1)(1)	(Si)(Zr)
SiZr2	CEF (ST2)	(1)(2)	(Si)(Zr)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Co,Cr,Fe,Mn,Ni,Si,Ta) (Cr,Fe,Mo,Nb,Ta,Ti,V,W)(Al,Co,Cr, Fe,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,W)
SigmaH	CEF (SLN)	(8)(4)(18)	(Mn)(Cr)(Cr,Mn,Ti)
Sn10Y11	CEF (ST2)	(10)(11)	(Sn)(Y)
Sn2S3	CEF (ST2)	(2)(3)	(Sn)(S)
Sn2V	CEF (ST2)	(2)(1)	(Sn)(V)
Sn2Y	CEF (ST2)	(2)(1)	(Sn)(Y)
Sn2Zr	CEF (ST2)	(2)(1)	(Sn)(Zr)
Sn3Ti2	CEF (ST2)	(0.6)(0.4)	(Sn)(Ti)
Sn3Ti5	CEF (ST2)	(3)(5)	(Sn)(Ti)

Name	Model	Lattice Size	Constituent
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)
Sn4Y5	CEF (ST2)	(4)(5)	(Sn)(Y)
Sn5Ti6	CEF (ST2)	(5)(6)	(Sn)(Ti)
Sn5Y2	CEF (ST2)	(5)(2)	(Sn)(Y)
SnS	CEF (ST2)	(1)(1)	(Sn)(S)
SnS2	CEF (ST2)	(1)(2)	(Sn)(S)
SnTi2	CEF (ST2)	(1)(2)	(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)	(Co+2,Cr+2,Cr+3,Fe+2,Fe+3, Mg+2,Mn+2,Ni+2) (Al+3,Co+3,Cr+3,Fe+2, Fe+3,Mg+2,Mn+2,Mn+3,Mn+4, Ni+2,Va)(Fe+2,Va)(O-2)
Spinel_T	CEF (SLN)	(1)(2)(2)(4)	(Cr+2,Cr+3,Fe+2,Fe+3,Mn+2, Mn+3)(Cr+3,Fe+2,Fe+3,Mn+2, Mn+3,Va)(Fe+2,Va)(O-2)
Ta2O5_S	CEF (SLN)	(1)	(Ta,Ta2O5)
Ta2O5_S2	CEF (SLN)	(1)	(Ta,Ta2O5)
Ta2Si	CEF (ST2)	(2)(1)	(Ta)(Si)
TaB2	CEF (SLN)	(1)(2)	(Ta,Va)(B,Va)
TaV2_C14	CEF (SLN)	(2)(1)	(Ta,V)(Ta,V)
TaV2_C15	CEF (SLN)	(2)(1)	(Ta,V)(Ta,V)
TaW_B2	CEF (SLN)	(1)(1)	(Ta,W)(Ta,W)

Name	Model	Lattice Size	Constituent
Theta_Ni2Si	CEF (SLN)	(1)(1)(1)	(Fe,Ni)(Fe,Ni,Va)(Si)
Ti10O19	CEF (ST2)	(10)(19)	(Ti)(O)
Ti17P10	CEF (ST2)	(0.63)(0.37)	(Ti)(P)
Ti20O39	CEF (ST2)	(20)(39)	(Ti)(O)
Ti2C_N	CEF (SLN)	(2)(1)	(Ti)(C,N)
Ti2S	CEF (SLN)	(2)(1)	(Ti)(S,Va)
Ti3N2	CEF (ST2)	(0.71)(0.29)	(Ti)(N)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti3P	CEF (ST2)	(3)(1)	(Ti)(P)
Ti4N3	CEF (ST2)	(0.685)(0.315)	(Ti)(N)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti4P3	CEF (ST2)	(4)(3)	(Ti)(P)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti5P3	CEF (ST2)	(0.61)(0.39)	(Ti)(P)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti7O13	CEF (ST2)	(7)(13)	(Ti)(O)
Ti8O15	CEF (ST2)	(8)(15)	(Ti)(O)
Ti8S3	CEF (ST2)	(8)(3)	(Ti)(S)
Ti8S9	CEF (ST2)	(8)(9)	(Ti)(S)
Ti9O17	CEF (ST2)	(9)(17)	(Ti)(O)
TiMn3	CEF (SLN)	(3)(1)	(Cr,Mn)(Ti)
TiMn4	CEF (SLN)	(0.815)(0.185)	(Cr,Mn)(Ti)
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)
TiP	CEF (ST2)	(1)(1)	(Ti)(P)

Name	Model	Lattice Size	Constituent
TiP2	CEF (ST2)	(1)(2)	(Ti)(P)
Tridymite	CEF (ST2)	(1)(2)	(Si)(O)
U_AL4MN	CEF (ST2)	(4)(1)	(Al)(Mn)
V2B3	CEF (ST2)	(0.4)(0.6)	(V)(B)
V2O5	CEF (ST2)	(2)(5)	(V)(O)
V2O_SS	CEF (SLN)	(1)(0.5)	(V)(O,Va)
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)
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)
VZn16	CEF (ST2)	(1)(16)	(V)(Zn)
VZn3	CEF (ST2)	(1)(3)	(V)(Zn)
W2B5	CEF (SLN)	(2)(5)	(W)(B,Va)
WB3	CEF (ST2)	(2)(9)	(W)(B)
WB_ALPHA	CEF (SLN)	(1)(1)	(W)(B,Va)
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	Constituent
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,Pr+3)(O-2)(O-2,Va)
Y13Zn58	CEF (ST2)	(0.183)(0.817)	(Y)(Zn)
Y2O3_cub	CEF (SLN)	(2)(3)(1)	(Fe+3,Mn+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)
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)
ZnZr2	CEF (ST2)	(0.333333) (0.666667)	(Zn)(Zr)

Name	Model	Lattice Size	Constituent
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_Beta	CEF (SLN)	(1)(2)	(Zr)(O,Va)
ZrO2_Gamma	CEF (SLN)	(1)(2)	(Zr)(O,Va)
a_Ce2Ni7	CEF (ST2)	(0.2222) (0.7778)	(Ce)(Ni)
a_MnNi	CEF (SLN)	(1)(1)	(Mn,Va)(Mn,Ni)
alpha_Al3Y	CEF (ST2)	(0.75)(0.25)	(Al)(Y)
alpha_TiMn	CEF (SLN)	(1)(1)	(Cr,Mn)(Ti)
b_MnNi	CEF (SLN)	(1)(1)	(Mn,Ni)(Mn,Ni)
beta_Al3Y	CEF (ST2)	(0.75)(0.25)	(Al)(Y)
beta_TiMn	CEF (SLN)	(0.515)(0.485)	(Cr,Mn)(Ti)
m_Ni4B3	CEF (ST2)	(0.564)(0.436)	(Ni)(B)
o_Ni4B3	CEF (ST2)	(0.586)(0.414)	(Ni)(B)