

Pandat 2026

Database Manual



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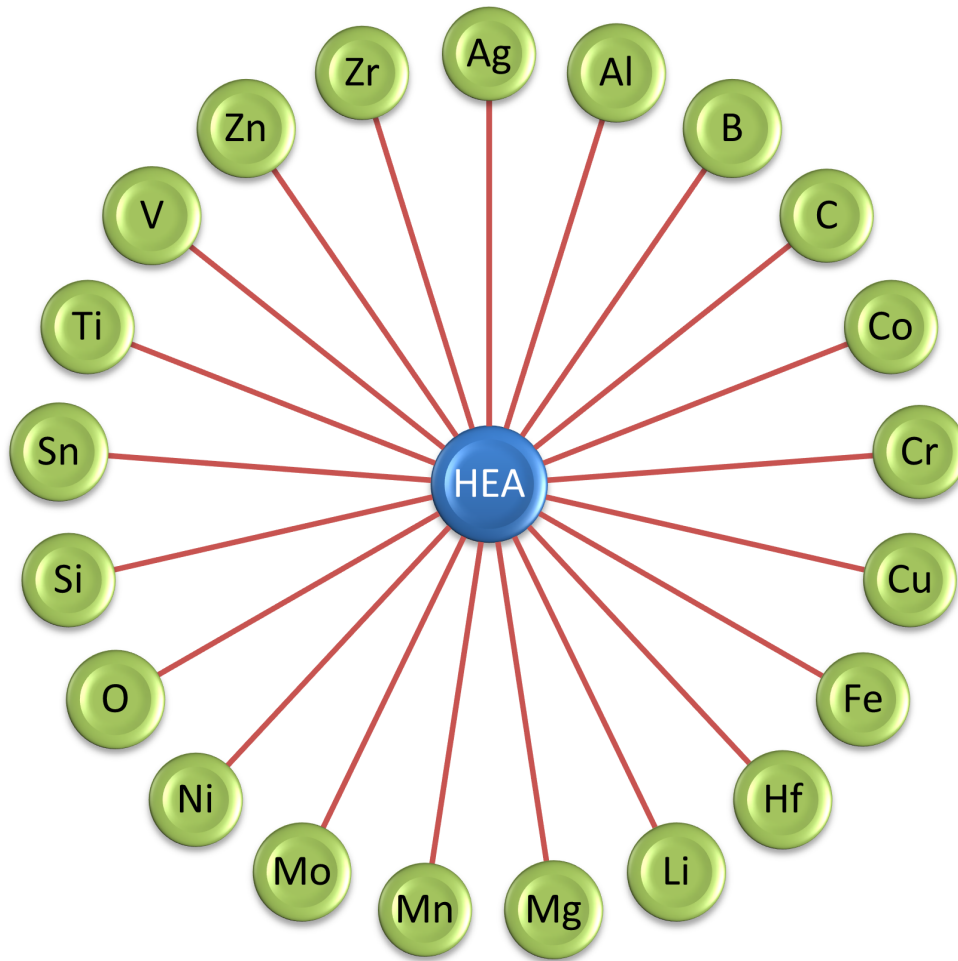
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Database Manuals

PanHEA

Database for multi-component high entropy alloys (HEA)



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Thermodynamic Database

Components (21)

Total of **21** components are included in the database as listed here:

Major alloying elements: Ag, Al, Co, Cr, Cu, Fe, Hf, Li, Mg, Mn, Mo, Ni, O, Si, Sn, Ti, V, Zn and Zr

Minor alloying element: B, C

Suggested Composition Range

The suggested composition range for each element is listed in [Table 1.1](#).

Table 1.1: Suggested composition range

| Elements | Composition Range (wt.%) |
|---|--------------------------|
| Ag, Al, Co, Cr, Cu, Fe, Hf, Li, Mg, Mn, Mo, Ni, Si, Sn, Ti, V, Zn, Zr | 0 ~ 100 |
| B, C, O | 0 ~ 10 |

What is new in PanHEA

- Improve the sub-system descriptions for the Co-Cr-Fe-Mn-Ni-V system
- new ternary system descriptions of Co-Mn-V and Mn-Ni-V

Phases

Total of 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 [PanHEA2026: List of Phases](#). Users can also view it through TDB viewer of Pandat.

Table 2: Phase name and related information

| Name | Lattice Size | Constituent |
|------------|-----------------------|-----------------|
| Al10Cu10Fe | (10)(10)(1) | (Al)(Cu)(Fe) |
| Al10Fe3Ni | (10)(3)(1) | (Al)(Fe)(Ni) |
| Al11Co6Si6 | (11)(6)(6) | (Al)(Co)(Si) |
| Al14Mn4Si5 | (14)(4)(5) | (Al)(Mn)(Al,Si) |
| Al16Co7Zr6 | (16)(7)(6) | (Al)(Co)(Zr) |
| Al17Cr2Mg4 | (21)(2) | (Al,Mg)(Cr) |
| Al20Cu2Mn3 | (0.8)(0.08) (0.12) | (Al)(Cu)(Mn) |
| Al23CuFe4 | (23)(1)(4) | (Al)(Cu)(Fe) |
| Al2Mn2Si3 | (2)(2)(3) | (Al)(Mn)(Si) |
| Al3Co3Si4 | (3)(3)(4) | (Al)(Co)(Si) |
| Al3CoCu | (3)(1)(1) | (Al)(Co)(Cu) |
| Al3Mn4Si2 | (3)(4)(2) | (Al)(Mn)(Si) |
| Al6Cu2Fe | (6)(2)(1) | (Al)(Cu)(Fe) |
| Al6Cu3Ni | (0.6)(0.3)(0.1) | (Al)(Cu)(Ni) |
| Al7Cu2Fe | (7)(2)(1) | (Al)(Cu)(Fe) |
| Al7Cu4Ni | (7)(4)(1) | (Al)(Cu)(Ni) |

| | | |
|---|---------------------------|--------------------------------|
| AlCu ₂ Ti | (0.75)(0.25) | (Al,Cu)(Ti) |
| AlCuTi | (0.6667) (0.3333) | (Al,Cu)(Ti) |
| AlLi ₂ Zr | (0.25)(0.5) (0.25) | (Al)(Li)(Zr) |
| Co ₁₆ Si ₇ Ti ₆ | (16)(7)(6) | (Co)(Si)(Ti) |
| Cr ₈ Fe ₁₆ Ti ₅ | (0.828)(0.172) | (Cr,Fe)(Ti) |
| Cu ₂ MgZr | (2)(1)(1) | (Cu)(Mg)(Zr) |
| Fe ₄ V ₅ Si ₄ | (4)(5)(4) | (Fe)(V)(Si) |
| Fe ₅ Ni ₃ Si ₂ | (0.8)(0.2) | (Fe,Ni)(Si) |
| Fe ₅ V ₃ Si ₂ | (5)(3)(2) | (Fe)(V)(Si) |
| Mg ₂ CrNi | (0.12)(0.33) (0.55) | (Cr,Ni)(Mg,Ni)(Cr,Mg) |
| Mg ₂ SiNi ₃ | (2)(1)(3) | (Mg)(Si)(Ni) |
| Ni ₁₁ Si ₃₁ Zr ₈ | (0.22)(0.62) (0.16) | (Ni)(Si)(Zr) |
| Ni ₂ Si ₉ Zr ₁₄ | (0.08)(0.36) (0.56) | (Ni)(Si)(Zr) |
| NiSnTi | (0.333)(0.333) (0.333) | (Ti)(Ni)(Sn) |
| NiT ₂ Zr | (1)(1)(1) | (Ni,Ti,Zr)(Ni,Ti,Zr)(Ni,Ti,Zr) |

Assessed Subsystems

A total of systems, including binary and 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 (203)

| | | | | | | |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Ag-Al(10) | Ag-B(10) | Ag-C(10) | Ag-Co(10) | Ag-Cr(10) | Ag-Cu(10) | Ag-Fe(10) |
| Ag-Mg(10) | Ag-Mn(10) | Ag-Mo(10) | Ag-Ni(10) | Ag-O(5) | Ag-Si(10) | Ag-Sn(10) |
| Ag-Ti(10) | Ag-V(10) | Ag-Zn(10) | Ag-Zr(10) | Al-B(10) | Al-C(10) | Al-Co(10) |
| Al-Cr(10) | Al-Cu(10) | Al-Fe(10) | Al-Hf(10) | Al-Li(10) | Al-Mg(10) | Al-Mn(10) |
| Al-Mo(10) | Al-Ni(10) | Al-O(10) | Al-Si(10) | Al-Sn(10) | Al-Ti(10) | Al-V(10) |
| Al-Zn(10) | Al-Zr(10) | B-C(10) | B-Co(10) | B-Cr(10) | B-Cu(10) | B-Fe(10) |
| B-Hf(10) | B-Mg(10) | B-Mn(10) | B-Mo(10) | B-Ni(10) | B-O(10) | B-Si(10) |
| B-Sn(10) | B-Ti(10) | B-V(10) | B-Zn(10) | B-Zr(10) | C-Co(10) | C-Cr(10) |
| C-Fe(10) | C-Hf(10) | C-Li(10) | C-Mg(10) | C-Mn(10) | C-Mo(10) | C-Ni(10) |
| C-O(10) | C-Si(10) | C-Sn(10) | C-Ti(10) | C-V(10) | C-Zn(10) | C-Zr(10) |
| Co-Cr(10) | Co-Cu(10) | Co-Fe(10) | Co-Hf(10) | Co-Li(10) | Co-Mg(10) | Co-Mn(10) |
| Co-Mo(10) | Co-Ni(10) | Co-O(10) | Co-Si(10) | Co-Sn(10) | Co-Ti(10) | Co-V(10) |
| Co-Zn(10) | Co-Zr(10) | Cr-Cu(10) | Cr-Fe(10) | Cr-Hf(10) | Cr-Li(10) | Cr-Mg(10) |
| Cr-Mn(10) | Cr-Mo(10) | Cr-Ni(10) | Cr-O(10) | Cr-Si(10) | Cr-Sn(10) | Cr-Ti(10) |
| Cr-V(10) | Cr-Zn(10) | Cr-Zr(10) | Cu-Fe(10) | Cu-Hf(10) | Cu-Li(10) | Cu-Mg(10) |
| Cu-Mn(10) | Cu-Mo(10) | Cu-Ni(10) | Cu-O(10) | Cu-Si(10) | Cu-Sn(10) | Cu-Ti(10) |
| Cu-V(10) | Cu-Zn(10) | Cu-Zr(10) | Fe-Hf(10) | Fe-Li(10) | Fe-Mg(10) | Fe-Mn(10) |
| Fe-Mo(10) | Fe-Ni(10) | Fe-O(10) | Fe-Si(10) | Fe-Sn(10) | Fe-Ti(10) | Fe-V(10) |
| Fe-Zn(10) | Fe-Zr(10) | Hf-Li(10) | Hf-Mg(10) | Hf-Mn(10) | Hf-Mo(10) | Hf-Ni(10) |
| Hf-O(10) | Hf-Si(10) | Hf-Sn(10) | Hf-Ti(10) | Hf-V(10) | Hf-Zr(10) | Li-Mg(10) |
| Li-Mn(10) | Li-Ni(10) | Li-O(10) | Li-Si(10) | Li-Sn(10) | Li-Ti(10) | Li-V(10) |
| Li-Zn(10) | Li-Zr(10) | Mg-Mn(10) | Mg-Mo(10) | Mg-Ni(10) | Mg-O(10) | Mg-Si(10) |
| Mg-Sn(10) | Mg-Ti(10) | Mg-V(10) | Mg-Zn(10) | Mg-Zr(10) | Mn-Mo(10) | Mn-Ni(10) |

| | | | | | | |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Mn-O(10) | Mn-Si(10) | Mn-Sn(10) | Mn-Ti(10) | Mn-V(10) | Mn-Zn(10) | Mn-Zr(10) |
| Mo-Ni(10) | Mo-O(10) | Mo-Si(10) | Mo-Sn(10) | Mo-Ti(10) | Mo-V(10) | Mo-Zr(10) |
| Ni-O(10) | Ni-Si(10) | Ni-Sn(10) | Ni-Ti(10) | Ni-V(10) | Ni-Zn(10) | Ni-Zr(10) |
| O-Si(10) | O-Sn(10) | O-Ti(10) | O-V(10) | O-Zn(5) | O-Zr(10) | Si-Sn(10) |
| Si-Ti(10) | Si-V(10) | Si-Zn(10) | Si-Zr(10) | Sn-Ti(10) | Sn-V(10) | Sn-Zn(10) |
| Sn-Zr(10) | Ti-V(10) | Ti-Zn(10) | Ti-Zr(10) | V-Zn(10) | V-Zr(10) | Zn-Zr(10) |

Ternary Systems (275)

| | | | | | |
|--------------|--------------|--------------|--------------|--------------|--------------|
| Ag-Al-Co(5) | Ag-Al-Cu(10) | Ag-Al-Fe(10) | Ag-Al-Mg(10) | Ag-Al-Si(10) | Ag-Al-Sn(10) |
| Ag-Al-Zn(10) | Ag-Co-Sn(5) | Ag-Cr-Cu(10) | Ag-Cu-Mg(10) | Ag-Cu-Ni(10) | Ag-Cu-Si(10) |
| Ag-Cu-Sn(10) | Ag-Cu-Ti(10) | Ag-Cu-Zr(10) | Ag-Ni-Sn(10) | Ag-Sn-Ti(5) | Al-Co-Cr(10) |
| Al-Co-Cu(10) | Al-Co-Fe(10) | Al-Co-Mg(10) | Al-Co-Mn(10) | Al-Co-Mo(10) | Al-Co-Ni(10) |
| Al-Co-Si(10) | Al-Co-Ti(10) | Al-Co-Zr(10) | Al-Cr-Cu(10) | Al-Cr-Fe(10) | Al-Cr-Mg(10) |
| Al-Cr-Mn(10) | Al-Cr-Mo(10) | Al-Cr-Ni(10) | Al-Cr-Si(10) | Al-Cr-Ti(10) | Al-Cr-Zr(10) |
| Al-Cu-Fe(10) | Al-Cu-Li(10) | Al-Cu-Mg(10) | Al-Cu-Mn(10) | Al-Cu-Mo(10) | Al-Cu-Ni(10) |
| Al-Cu-Si(10) | Al-Cu-Sn(10) | Al-Cu-Ti(10) | Al-Cu-V(10) | Al-Cu-Zn(10) | Al-Cu-Zr(10) |
| Al-Fe-Mg(8) | Al-Fe-Mn(10) | Al-Fe-Mo(8) | Al-Fe-Ni(10) | Al-Fe-Si(10) | Al-Fe-Ti(10) |
| Al-Fe-V(10) | Al-Fe-Zn(10) | Al-Fe-Zr(10) | Al-Li-Mg(10) | Al-Li-Mn(10) | Al-Li-Si(10) |
| Al-Li-Zr(10) | Al-Mg-Mn(10) | Al-Mg-Mo(8) | Al-Mg-Si(10) | Al-Mg-Sn(10) | Al-Mg-Ti(10) |
| Al-Mg-Zn(10) | Al-Mn-Ni(5) | Al-Mn-Si(10) | Al-Mn-Ti(10) | Al-Mn-Zn(10) | Al-Mo-Ni(10) |
| Al-Mo-Si(10) | Al-Mo-Ti(10) | Al-Mo-V(10) | Al-Mo-Zr(10) | Al-Ni-Si(10) | Al-Ni-Ti(10) |
| Al-Ni-V(10) | Al-Ni-Zn(10) | Al-Ni-Zr(10) | Al-Si-Sn(10) | Al-Si-Ti(10) | Al-Si-V(10) |
| Al-Si-Zn(10) | Al-Si-Zr(10) | Al-Sn-Ti(10) | Al-Ti-V(10) | Al-Ti-Zn(10) | Al-Ti-Zr(10) |
| Al-V-Zr(10) | C-Mo-Zr(10) | Co-Cr-Cu(10) | Co-Cr-Fe(10) | Co-Cr-Mn(10) | Co-Cr-Mo(10) |
| Co-Cr-Ni(10) | Co-Cr-Si(10) | Co-Cr-Ti(10) | Co-Cr-V(10) | Co-Cr-Zr(10) | Co-Cu-Fe(10) |
| Co-Cu-Hf(10) | Co-Cu-Mn(10) | Co-Cu-Mo(10) | Co-Cu-Ni(10) | Co-Cu-Ti(10) | Co-Fe-Mn(10) |
| Co-Fe-Mo(10) | Co-Fe-Ni(10) | Co-Fe-Si(10) | Co-Fe-Ti(10) | Co-Fe-V(10) | Co-Fe-Zr(10) |
| Co-Hf-Zr(10) | Co-Mn-Mo(10) | Co-Mn-Ni(10) | Co-Mn-Si(10) | Co-Mn-Ti(10) | Co-Mn-Zr(10) |
| Co-Mo-Ni(10) | Co-Mo-Ti(10) | Co-Mo-Zr(10) | Co-Ni-Si(10) | Co-Ni-Ti(10) | Co-Ni-V(10) |
| Co-Si-Ti(10) | Co-Si-V(10) | Co-Si-Zr(10) | Co-Sn-Ti(10) | Co-V-Zr(10) | Cr-Cu-Fe(10) |

| | | | | | |
|--------------|--------------|--------------|--------------|--------------|--------------|
| Cr-Cu-Mn(10) | Cr-Cu-Mo(5) | Cr-Cu-Ni(10) | Cr-Cu-Sn(10) | Cr-Cu-Ti(10) | Cr-Cu-Zr(10) |
| Cr-Fe-Mg(10) | Cr-Fe-Mn(10) | Cr-Fe-Mo(10) | Cr-Fe-Ni(10) | Cr-Fe-Si(10) | Cr-Fe-Sn(10) |
| Cr-Fe-Ti(10) | Cr-Fe-V(10) | Cr-Fe-Zr(10) | Cr-Mg-Ni(10) | Cr-Mn-Ni(10) | Cr-Mn-Si(10) |
| Cr-Mn-Ti(10) | Cr-Mn-V(10) | Cr-Mn-Zr(10) | Cr-Mo-Ni(10) | Cr-Mo-Si(10) | Cr-Mo-Ti(10) |
| Cr-Mo-V(10) | Cr-Mo-Zr(10) | Cr-Ni-Si(10) | Cr-Ni-Ti(10) | Cr-Ni-V(10) | Cr-Ni-Zr(10) |
| Cr-Si-Ti(10) | Cr-Sn-Ti(10) | Cr-Sn-Zr(5) | Cr-Ti-V(10) | Cr-Ti-Zr(10) | Cr-V-Zr(10) |
| Cu-Fe-Mg(8) | Cu-Fe-Mn(10) | Cu-Fe-Mo(10) | Cu-Fe-Ni(10) | Cu-Fe-Si(10) | Cu-Fe-Sn(10) |
| Cu-Fe-Ti(10) | Cu-Fe-V(10) | Cu-Fe-Zn(8) | Cu-Fe-Zr(10) | Cu-Hf-Ni(10) | Cu-Mg-Mn(8) |
| Cu-Mg-Ni(10) | Cu-Mg-Si(10) | Cu-Mg-Sn(10) | Cu-Mg-Ti(10) | Cu-Mg-Zn(10) | Cu-Mg-Zr(10) |
| Cu-Mn-Ni(10) | Cu-Mn-Si(10) | Cu-Mn-Sn(10) | Cu-Mn-Ti(10) | Cu-Mn-Zn(10) | Cu-Ni-Si(10) |
| Cu-Ni-Sn(10) | Cu-Ni-Ti(10) | Cu-Ni-V(10) | Cu-Ni-Zr(10) | Cu-Si-Sn(10) | Cu-Si-Ti(10) |
| Cu-Si-Zn(10) | Cu-Sn-Ti(10) | Cu-Ti-Zr(10) | Fe-Mg-Mn(5) | Fe-Mg-Si(10) | Fe-Mg-Zn(5) |
| Fe-Mg-Zr(10) | Fe-Mn-Mo(10) | Fe-Mn-Ni(10) | Fe-Mn-Si(10) | Fe-Mn-Ti(10) | Fe-Mn-V(10) |
| Fe-Mn-Zn(5) | Fe-Mn-Zr(10) | Fe-Mo-Ni(10) | Fe-Mo-Si(5) | Fe-Mo-Ti(10) | Fe-Mo-V(10) |
| Fe-Mo-Zr(10) | Fe-Ni-Si(10) | Fe-Ni-Ti(10) | Fe-Ni-V(10) | Fe-Ni-Zn(10) | Fe-Ni-Zr(10) |
| Fe-Si-Sn(10) | Fe-Si-Ti(10) | Fe-Si-V(10) | Fe-Si-Zn(10) | Fe-Si-Zr(10) | Fe-Sn-Zr(10) |
| Fe-Ti-V(10) | Fe-Ti-Zn(10) | Fe-Ti-Zr(10) | Hf-Ni-Ti(10) | Hf-Ni-Zr(5) | Hf-Ti-Zr(10) |
| Li-Mg-Si(10) | Li-Mg-Zr(10) | Mg-Mn-Ni(10) | Mg-Mn-Si(10) | Mg-Mn-Zn(8) | Mg-Ni-Si(10) |
| Mg-Ni-Zn(10) | Mg-Si-Sn(10) | Mg-Si-Zn(10) | Mg-Si-Zr(10) | Mn-Mo-Ni(10) | Mn-Mo-Ti(10) |
| Mn-Ni-Si(10) | Mn-Ni-Ti(10) | Mn-Si-Sn(10) | Mn-Si-Ti(10) | Mn-Si-Zn(5) | Mn-Ti-V(10) |
| Mn-Ti-Zr(10) | Mo-Ni-Si(10) | Mo-Ni-Ti(10) | Mo-Ni-V(10) | Mo-Ni-Zr(10) | Mo-Si-Ti(10) |
| Mo-Si-V(10) | Mo-Si-Zr(10) | Mo-Ti-V(10) | Mo-Ti-Zr(10) | Mo-V-Zr(10) | Ni-Si-Ti(10) |
| Ni-Si-V(10) | Ni-Si-Zn(10) | Ni-Si-Zr(10) | Ni-Sn-Ti(10) | Ni-Sn-Zr(10) | Ni-Ti-V(10) |
| Ni-Ti-Zr(10) | Ni-V-Zr(10) | Si-Ti-V(10) | Sn-Ti-Zr(10) | Ti-V-Zr(10) | |

Database Applications

The PanHEA database is validated by a large amount of experimental data. It is by far the most comprehensive database for alloy design and processing optimization of high entropy alloys for 3rd-transition metals. A few example calculations using the current PanHEA database are given below:

[Figure 1.1](#) shows the calculated isopleth of the $Al_xCoCrFeNi$ system with x varies between 0~2. x is the Al ratio and other elements are in the equal atomic percent. It indicates that Al is a strong stabilizer for both the disorder Bcc and ordered B2 structure, and the later is favored. In addition to the phase equilibrium information with the changing of Al ratio at different temperatures, one can also predict the as-cast microstructures of the HEAs based on the calculated mushy-zone (Liquid + Solid) phase regions (as indicated on top of this figure). It shows that pure Fcc structure will be developed with lower Al ratio, while Bcc structure (Bcc and/or B2) will be developed with higher Al ratio, and a mixture of Fcc+Bcc should be seen in between. Our predictions are exactly what were observed by many researchers who have carried our experimental studies of $Al_xCoCrFeNi$ alloys [[2006Ke](#), [2008Wan](#), [2011Kao](#)].

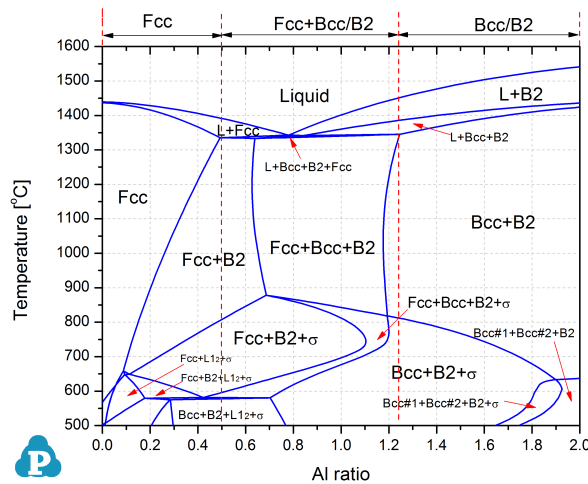


Figure 1.1: Calculated isopleth of the $Al_xCoCrFeNi$ with $x=0\sim 2$

For quantitative analysis on the phase transformations of an alloy at the given composition, the equilibrium calculation is needed. [Figure 1.2](#) shows equilibrium calculation of the $Al_{0.3}CoCrFeNi$ alloy at the temperature range from 600 to 1450 °C. It indicates that this alloy contains single Fcc phase at higher temperatures (>1000 °C). The B2 phase precipitates out at around 1000 °C. At lower temperatures (<700 °C), other phases will form as well, such as σ and L12_Fcc. The alloy with Fcc structure shows good ductility but low strength, while the B2-type intermetallic compounds generally show excellent strength but low ductility. Usually, an HEA with dispersed B2 precipitates within the Fcc matrix has balanced properties and good performance. On the basis of thermodynamic calculations (as shown in [Figure 1.2](#)), the $Al_{0.3}CoCrFeNi$ HEA may meet the requirements. As shown in [Figure 1.2](#), the solvus temperature of B2 is about 1060 °C. When annealing below this temperature, the B2 precipitates will

form. Shu et al. [2009Shu] investigated the microstructure and tensile behaviors of the $\text{Al}_{0.3}\text{CoCrFeNi}$ HEA, and they found that the as-cast structure of this alloy is Fcc and the B2 phase formed when aged at 900 °C for 72h. The tensile strength of this alloy after heat treatment was significantly improved. Prediction from our database agrees with their experimental observation very well.

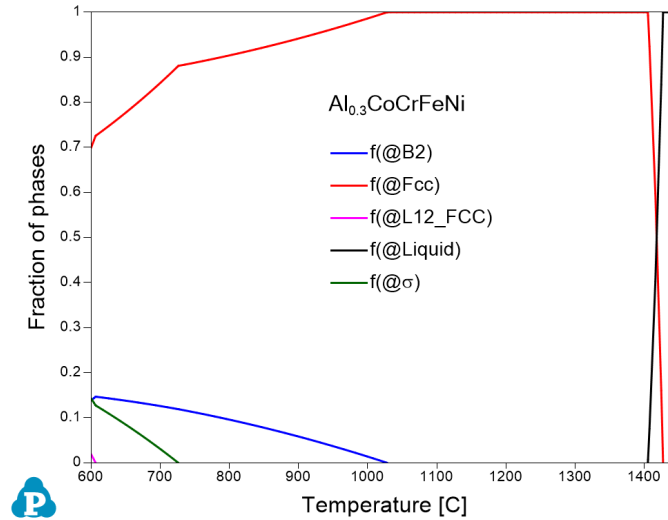


Figure 1.2: Equilibrium calculation of $\text{Al}_{0.3}\text{CoCrFeNi}$ HEA

Mobility Database

PanHEA2026_MB is an atomic mobility database for high entropy alloys (HEA), which is compatible with the PanHEA_TH thermodynamic database and suitable for the simulation of diffusion-controlled phenomena using the **PanDiffusion** module, **PanEvolution** module, and/or **PanSolidification** module.

Phases

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

Self-diffusivity of Pure Elements

The color represents the following meaning:




| | |
|---|-------------|
|  | : Validated |
|  | : Estimated |
|  | : No data |

Table 1: Assessed self-diffusivity of pure elements with different crystal structures

| | Ag | Al | Co | Cr | Cu | Fe | Hf | Li | Mg | Mn | Mo | Ni | Si | Sn | Ti | V | Zr |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| Bcc | Yellow | Yellow | Yellow | Green | Yellow | Green | Green | Green | Yellow | Yellow | Green | Yellow | Yellow | Yellow | Green | Green | Green |
| Fcc | Green | Green | Green | Yellow | Green | Green | Yellow | Yellow | Yellow | Yellow | Yellow | Green | Yellow | Yellow | Yellow | Yellow | Yellow |
| Hcp | Yellow | Yellow | Yellow | Yellow | Yellow | Yellow | Green | Yellow | Green | Yellow | Yellow | Yellow | Yellow | Yellow | Green | Yellow | Green |

Assessed Systems

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

Fcc Phase

| | | | | | | | | | | |
|----------|-------|----------|-------|----------|-------|----------|-------|----------|-------|----------|
| Ag-Al | Ag-Cu | Ag-Sn | Al-Co | Al-Cu | Al-Mg | Al-Ni | Al-Si | Co-Cr | Co-Cu | |
| Co-Fe | Co-Ni | Cr-Fe | Cr-Ni | Cu-Fe | Cu-Mg | Cu-Si | Cu-Sn | Cu-Ti | Fe-Mn | |
| Fe-Ni | Fe-Si | Mn-Ni | Ni-Ti | Ni-V | | | | | | |
| Al-Co-W | | Al-Cr-Ni | | Al-Cu-Mg | | Al-Cu-Si | | Al-Mn-Ni | | Co-Cr-Ni |
| Co-Cu-Fe | | Co-Cu-Ni | | Co-Fe-Ni | | Cr-Cu-Ni | | Cr-Fe-Ni | | Cu-Fe-Mn |
| Cu-Fe-Ni | | Cu-Mn-Ni | | Fe-Mn-Si | | | | | | |

Bcc Phase

| | | | | | | | | | |
|----------|-------|----------|-------|----------|-------|------|-------|--|--|
| Al-Fe | Al-Ti | Cr-Fe | Cr-Ti | Cu-Ti | Fe-Ti | Ti-V | Ti-Zr | | |
| Al-Cr-Ti | | Al-Fe-Ti | | Cr-Fe-Ni | | | | | |

Hcp Phase

| | | |
|-------|--|--|
| Al-Mg | | |
|-------|--|--|

Database Validation

The simulated concentration profiles of a series of high entropy alloys are shown below to validate the current PanHEA_MB database.

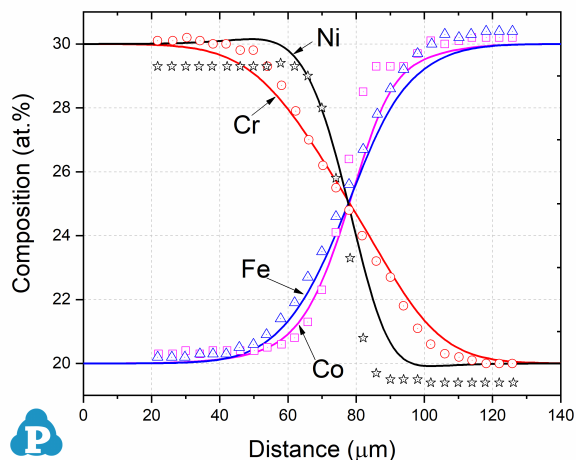


Figure 2.1: Simulated concentration profiles of Co-30Cr-20Fe-30Ni/Co-20Cr-30Fe-20Ni (at.%) diffusion couple annealed at 1000 °C for 100h with experimental data (symbols) of ref. [2015Kul]

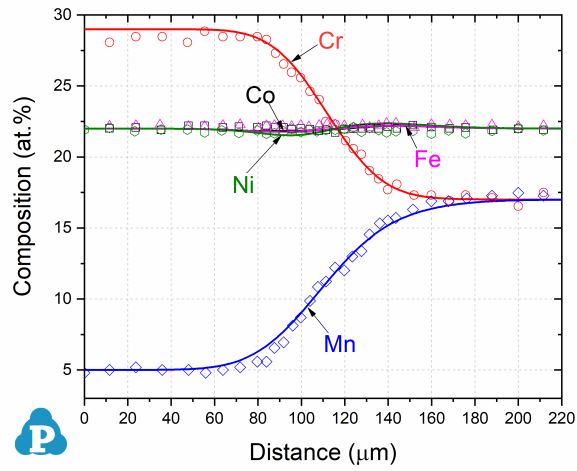


Figure 2.2: Simulated concentration profiles of $\text{Co}_{22}\text{Cr}_{29}\text{Fe}_{22}\text{Mn}_5\text{Ni}_{22}/\text{Co}_{22}\text{Cr}_{17}\text{Fe}_{22}\text{Mn}_{17}\text{Ni}_{22}$ (at.%) diffusion couple annealed at 1000 °C for 100h with experimental data (symbols) from ref. [2013Tsa]

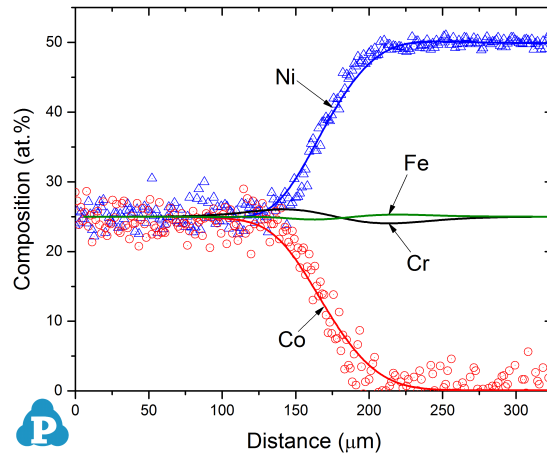


Figure 2.3: Simulated concentration profiles of $\text{Co}_{25}\text{Cr}_{25}\text{Fe}_{25}\text{Ni}_{25}/\text{Ni}_{50}\text{Cr}_{25}\text{Fe}_{25}$ (at.%) diffusion couple annealed at 1120 °C for 48h with experimental data (symbols) of ref. [2017Zha]

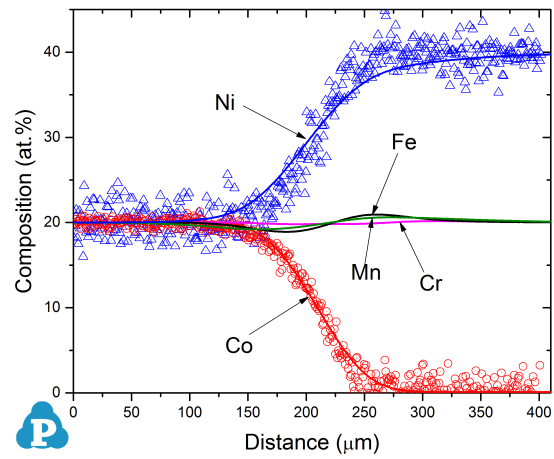


Figure 2.4: Simulated concentration profiles of Co₂₀Cr₂₀Fe₂₀Mn₂₀Ni₂₀/Cr₂₀Fe₂₀Mn₂₀Ni₄₀ (at.%) diffusion couple annealed at 1070 °C for 94.5 h with experimental data (symbols) of ref. [2017Zha]

Thermophysical Property Database

The thermophysical property database **PanHEA2026_TP** is compatible with the PanHEA_TH thermodynamic database and suitable for the simulation of thermophysical properties of high entropy alloys. It includes the molar volume data for all the phases, surface tension and viscosity properties for the liquid phase.

Molar Volume

The current molar volume database covers all **687** phases assessed in the PanHEA_TH database. It is used to calculate the density, thermal expansion, solidification shrinkage of high entropy alloys (HEA).

[Figure 3.1](#) shows the calculated linear thermal expansion coefficients (CTE) for alloys with equiatomic ratio in the Co-Cr-Fe-Ni system (binary CoNi, ternary CoCrNi, CoFeNi, CrFeNi, and quaternary CoCrFeNi), which are in good agreement with the experimental measurements in the literature [\[2018Lap\]](#). [Figure 3.2](#) shows calculated density contour mapping of the Co-Cr-Fe-20Mn-20Ni (at.%) at 1000 °C. One can see that the stable phase regions include Fcc single phase field and Bcc+Fcc two-phase field in this isothermal section. The density of these HEAs at 1000 °C will vary between 7.2~7.9 g/cm³.

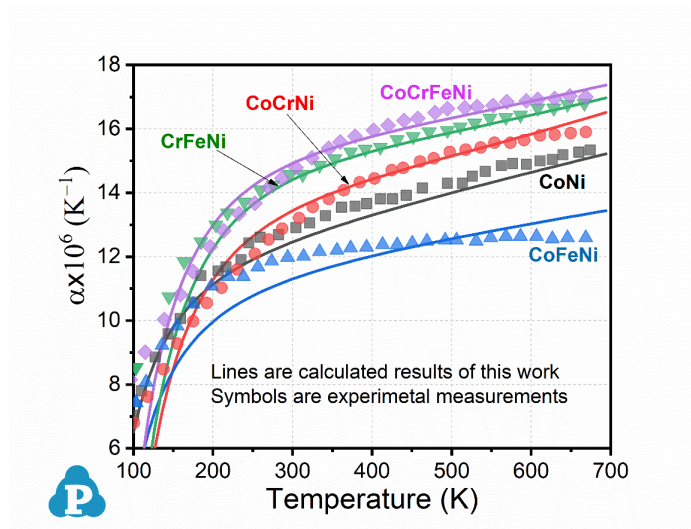


Figure 3.1: Calculated linear thermal expansion coefficient of the HEAs within the Co-Cr-Fe-Mn-Ni system with experimental data from ref. [\[2018Lap\]](#)

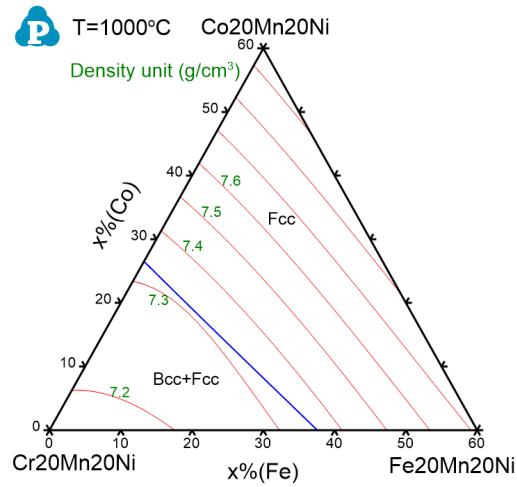


Figure 3.2: Density contour mapping of Co-Cr-Fe-20Mn-20Ni (at.%) at 1000 °C

Surface Tension

The surface tension of the liquid phase is added into the property database. [Figure 3.3](#) shows the surface tension of CoCrFeMnNi high entropy alloy.

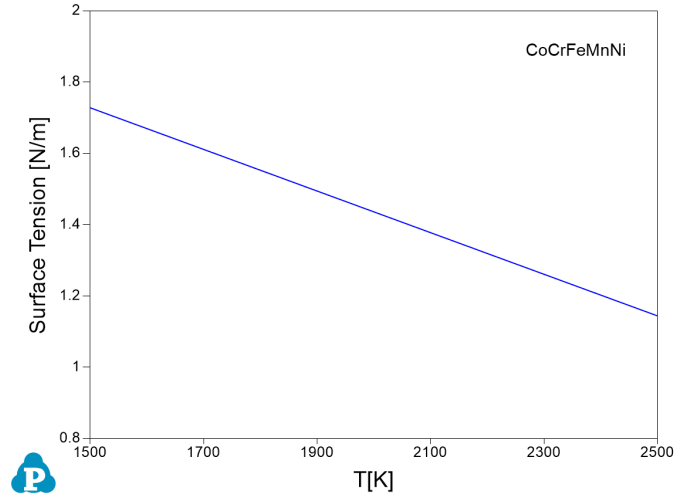


Figure 3.3: Surface tension of CoCrFeMnNi high entropy alloy

Viscosity

The viscosity of the liquid phase is added into the property database. [Figure 3.4](#) shows the viscosity of CoCrFeMnNi high entropy alloy.

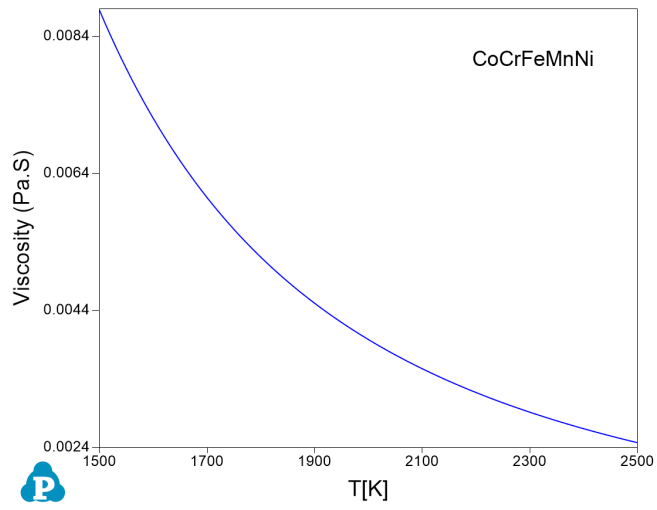


Figure 3.4: Viscosity of the CoCrFeMnNi high entropy alloy

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PanHEA: List of Phases

Phases (687)

| Name | Model | Lattice Size | Constituent |
|--------------------|-----------|------------------------|---|
| A15 | CEF (SLN) | (0.75)(0.25) (0.05) | (Cr,Fe,Mo,Si,Ti,V,Zr) (Al,Cr,Ni,Si,Ti,V)(Va) |
| A3B | CEF (SLN) | (3)(1) | (Co,Cr,Fe,Mo,Si,V)(Al,Cr,Mo,Si,V) |
| ALPHA_RHOMBO _B | CEF (ST1) | (1) | (B) |
| A_Co59Si26V15 | CEF (ST3) | (0.59)(0.26) (0.15) | (Co)(Si)(V) |
| A_Li2Zn3 | CEF (SLN) | (2)(3) | (Li)(Li,Zn) |
| A_Li2Zn5 | CEF (SLN) | (2)(5) | (Li,Zn)(Zn) |
| A_LiZn4 | CEF (SLN) | (1)(4) | (Li,Zn)(Li,Zn) |
| A_TiO | CEF (ST2) | (1)(1) | (Ti)(O) |
| Ag14Cu70Zr16 | CEF (ST3) | (0.14)(0.7)(0.16) | (Ag)(Cu)(Zr) |
| Ag2O2 | CEF (ST2) | (2)(2) | (Ag)(O) |
| Ag3Sn | CEF (SLN) | (0.75)(0.25) | (Ag)(Ag,Sn) |
| Ag5Zn8 | CEF (SLN) | (2)(2)(3)(6) | (Ag,Zn)(Ag)(Ag,Zn)(Ag,Zn) |
| AgMg3 | CEF (SLN) | (0.23)(0.77) | (Ag,Cu)(Al,Mg) |
| AgMg4 | CEF (SLN) | (0.2)(0.8) | (Ag,Cu)(Al,Mg) |
| AgZn2 | CEF (SLN) | (1)(2) | (Zn)(Ag,Zn) |
| AgZn3 | CEF (SLN) | (1) | (Ag,Zn) |
| AgZr | CEF (SLN) | (0.5)(0.5) | (Ag,Cu)(Zr) |
| Al10Cu10Fe | CEF (ST3) | (10)(10)(1) | (Al)(Cu)(Fe) |
| Al10Fe3Ni | CEF (ST3) | (10)(3)(1) | (Al)(Fe)(Ni) |
| Al10FeNi3 | CEF (ST3) | (10)(1)(3) | (Al)(Fe)(Ni) |
| Al10V | CEF (SLN) | (10)(1) | (Al)(Fe,Mo,V) |
| Al114Cu65Mn21 | CEF (ST3) | (114)(65)(21) | (Al)(Cu)(Mn) |
| Al11Co6Si6 | CEF (ST3) | (11)(6)(6) | (Al)(Co)(Si) |

| | | | |
|---------------|-----------|-----------------------------|--|
| Al11Cr2 | CEF (SLN) | (10)(1)(2) | (Al)(Al)(Cr,Mn) |
| Al11Mn4_H | CEF (SLN) | (29)(10) | (Al,Cu,Mn)(Cu,Mn) |
| Al11Mn4_L | CEF (SLN) | (11)(4) | (Al,Zn)(Cr,Mn) |
| Al12Fe7Mo | CEF (ST3) | (0.45)(0.4)(0.15) | (Al)(Fe)(Mo) |
| Al12Mn | CEF (ST2) | (12)(1) | (Al)(Mn) |
| Al12Mo | CEF (SLN) | (12)(1) | (Al)(Mo,V) |
| Al12_Fe3V3Si | CEF (SLN) | (12)(3)(1) | (Al)(Fe,V)(Si) |
| Al13Cr2 | CEF (ST2) | (13)(2) | (Al)(Cr) |
| Al13Cu4Mn3 | CEF (ST3) | (13)(4)(3) | (Al)(Cu)(Mn) |
| Al13M4 | CEF (SLN) | (0.6275)(0.235) (0.1375) | (Al,Cu)(Co,Cr,Fe,Mn,Ni,Si,V,Zn) (Al,Si,Zn,Va) |
| Al14Mn4Si5 | CEF (SLN) | (14)(4)(5) | (Al)(Mn)(Al,Si) |
| Al15_FeMn3Si2 | CEF (SLN) | (16)(4)(1)(2) | (Al)(Fe,Mn)(Si)(Al,Si) |
| Al16Co7Zr6 | CEF (ST3) | (16)(7)(6) | (Al)(Co)(Zr) |
| Al17Cr2Mg4 | CEF (SLN) | (21)(2) | (Al,Mg)(Cr) |
| Al17Mo4 | CEF (SLN) | (17)(4) | (Al)(Mo,V) |
| Al18Mg3Mo2 | CEF (ST3) | (18)(3)(2) | (Al)(Mg)(Mo) |
| Al18Mg3X2 | CEF (SLN) | (18)(3)(2) | (Al)(Mg)(Mn,Ti,V) |
| Al1Fe1O3 | CEF (ST3) | (1)(1)(3) | (Al+3)(Fe+3)(O-2) |
| Al22Mo5 | CEF (SLN) | (22)(5) | (Al)(Mo,V) |
| Al23V4 | CEF (SLN) | (23)(4) | (Al,Cu,Si)(Fe,Mo,V) |
| Al25Co10Si7 | CEF (ST3) | (25)(10)(7) | (Al)(Co)(Si) |
| Al2CoTi | CEF (SLN) | (3)(1) | (Al,Ti)(Co) |
| Al2CoZr6 | CEF (ST3) | (2)(1)(6) | (Al)(Co)(Zr) |
| Al2Fe | CEF (SLN) | (2)(1) | (Al,Cu,Si,Zn)(Co,Cr,Fe,Mn) |
| Al2Hf | CEF (SLN) | (0.66667) (0.33333) | (Al,Si,Ti)(Hf) |
| Al2Hf3 | CEF (SLN) | (0.4)(0.6) | (Al,Si)(Hf) |
| Al2Li3 | CEF (ST2) | (2)(3) | (Al)(Li) |
| Al2LiMg | CEF (ST3) | (0.53)(0.33) (0.14) | (Al)(Li)(Mg) |

| | | | |
|--|-----------|------------------------|--|
| Al ₂ Mn ₂ Si ₃ | CEF (ST3) | (2)(2)(3) | (Al)(Mn)(Si) |
| Al ₂ MnSi ₃ | CEF (ST3) | (2)(1)(3) | (Al)(Mn)(Si) |
| Al ₂ Ti | CEF (SLN) | (2)(1) | (Al,Cr,Ti)(Al,Ti,Zr) |
| Al ₂ Zr | CEF (ST2) | (2)(1) | (Al)(Zr) |
| Al ₂ Zr ₃ | CEF (SLN) | (2)(3) | (Al)(Ti,V,Zr) |
| Al ₃ 1Mn ₈ Zn ₁ 1 | CEF (ST3) | (0.62)(0.16) (0.22) | (Al)(Mn)(Zn) |
| Al ₃ Co | CEF (SLN) | (3)(1) | (Al,Si)(Co) |
| Al ₃ Co ₃ Si ₄ | CEF (ST3) | (3)(3)(4) | (Al)(Co)(Si) |
| Al ₃ CoCu | CEF (ST3) | (3)(1)(1) | (Al)(Co)(Cu) |
| Al ₃ Cu ₅ Zn ₂ | CEF (SLN) | (1)(4)(4)(1) | (Al,Cu)(Al)(Cu)(Zn) |
| Al ₃ Hf ₂ | CEF (SLN) | (0.6)(0.4) | (Al,Si)(Hf) |
| Al ₃ Hf ₄ | CEF (SLN) | (0.42857) (0.57143) | (Al,Si)(Hf) |
| Al ₃ Hf_alpha | CEF (SLN) | (0.75)(0.25) | (Al,Si)(Hf) |
| Al ₃ Hf_beta | CEF (SLN) | (0.75)(0.25) | (Al,Si)(Hf) |
| Al ₃ Li ₈ Si ₅ | CEF (ST3) | (8)(3)(5) | (Li)(Al)(Si) |
| Al ₃ Mn ₄ Si ₂ | CEF (ST3) | (3)(4)(2) | (Al)(Mn)(Si) |
| Al ₃ MnSi ₂ | CEF (ST3) | (3)(1)(2) | (Al)(Mn)(Si) |
| Al ₃ Mo | CEF (SLN) | (3)(1) | (Al)(Mo,V) |
| Al ₃ Ni | CEF (SLN) | (0.75)(0.25) | (Al)(Ni,V) |
| Al ₃ Ni ₅ | CEF (ST2) | (0.375)(0.625) | (Al)(Ni) |
| Al ₃ Ni ₈ Zn ₉ | CEF (ST3) | (3)(8)(9) | (Al)(Ni)(Zn) |
| Al ₃ NiM ₂ | CEF (SLN) | (3)(2)(1) | (Al,Si)(Al,Co,Cu,Ni,V,Zr) (Co,Cu,Ni,Va) |
| Al ₃ V | CEF (SLN) | (3)(1) | (Al,Cu,Ni,Si)(Fe,Mo,V,Zr) |
| Al ₃ Zr | CEF (SLN) | (3)(1) | (Al,Li,Si)(Ti,V,Zr) |
| Al ₃ Zr ₂ | CEF (SLN) | (3)(2) | (Al,Li)(Zr) |
| Al ₃ Zr ₄ | CEF (SLN) | (3)(4) | (Al,Cu,Li)(Zr) |
| Al ₃ Zr ₅ | CEF (SLN) | (3)(5) | (Al)(Li,V,Zr) |
| Al ₄ 1Co ₃₃ Si ₂₃ | CEF (ST3) | (41)(33)(23) | (Al)(Co)(Si) |

| | | | |
|--------------|-----------|--------------------------|---|
| Al43Co19Si12 | CEF (ST3) | (43)(19)(12) | (Al)(Co)(Si) |
| Al4C3 | CEF (SLN) | (4)(3) | (Al,Si)(C) |
| Al4CoZr | CEF (ST3) | (4)(1)(1) | (Al)(Co)(Zr) |
| Al4Cr | CEF (SLN) | (4)(1) | (Al,Si)(Cr) |
| Al4Li9 | CEF (ST2) | (4)(9) | (Al)(Li) |
| Al4Mn4Si2 | CEF (SLN) | (0.8)(0.2) | (Al,Mn)(Si) |
| Al4Mn_R | CEF (ST2) | (461)(107) | (Al)(Mn) |
| Al4Mn_U | CEF (SLN) | (0.2)(0.8) | (Cr,Fe,Mn)(Al,Li,Zn,Va) |
| Al4Mo | CEF (SLN) | (4)(1) | (Al)(Mo,V) |
| Al4Zr5 | CEF (ST2) | (4)(5) | (Al)(Zr) |
| Al5Co2 | CEF (SLN) | (5)(2) | (Al,Si)(Co,Fe) |
| Al5CoCu4 | CEF (ST3) | (5)(1)(4) | (Al)(Co)(Cu) |
| Al5CuTi2 | CEF (SLN) | (0.75)(0.25) | (Al,Cu)(Ti) |
| Al5Fe2 | CEF (SLN) | (5)(2)(3) | (Al,Cu,Si)(Co,Cr,Fe,Mn,Ni,V) (Zn,Va) |
| Al5Fe4 | CEF (SLN) | (1) | (Al,Fe,Mn) |
| Al5Mn2Si5 | CEF (ST3) | (0.7)(0.2)(0.1) | (Al)(Mn)(Si) |
| Al5Mn6Si7 | CEF (ST3) | (5)(6)(7) | (Al)(Mn)(Si) |
| Al5Mo | CEF (SLN) | (5)(1) | (Al)(Mo,V) |
| Al5Ti2 | CEF (SLN) | (5)(2) | (Al,Ti)(Al,Mo,Ti) |
| Al5Ti3 | CEF (ST2) | (5)(3) | (Al)(Ti) |
| Al60Cu4Mn11 | CEF (ST3) | (0.8)(0.05)(0.15) | (Al)(Cu)(Mn) |
| Al63Mo37 | CEF (SLN) | (63)(37) | (Al)(Mo,Ti) |
| Al67Cr8Ti25 | CEF (SLN) | (0.25)(0.08) (0.67) | (Al,Cr,Ti)(Al,Cr)(Al,Cr,Ti) |
| Al6CoCu3 | CEF (ST3) | (6)(1)(3) | (Al)(Co)(Cu) |
| Al6Cu2Fe | CEF (SLN) | (0.62)(0.255) (0.125) | (Al)(Al,Cu)(Fe) |
| Al6Cu3Ni | CEF (ST3) | (0.6)(0.3)(0.1) | (Al)(Cu)(Ni) |
| Al6Mn | CEF (SLN) | (6)(1) | (Al,Li)(Mn) |
| Al6MoZr | CEF (ST3) | (6)(1)(1) | (Al)(Mo)(Zr) |

| | | | |
|--------------|-----------|------------------------------|--|
| Al6Ni3Si | CEF (ST3) | (6)(3)(1) | (Al)(Ni)(Si) |
| Al71Mn16Zn13 | CEF (ST3) | (0.71)(0.16) (0.13) | (Al)(Mn)(Zn) |
| Al7Co4Si2 | CEF (ST3) | (7)(4)(2) | (Al)(Co)(Si) |
| Al7CoCu2 | CEF (ST3) | (7)(1)(2) | (Al)(Co)(Cu) |
| Al7Cu2Fe | CEF (ST3) | (7)(2)(1) | (Al)(Cu)(Fe) |
| Al7Cu4Ni | CEF (ST3) | (7)(4)(1) | (Al)(Cu)(Ni) |
| Al7V | CEF (SLN) | (7)(1) | (Al,Cu,Si)(Fe,Mo,V) |
| Al7VZr2 | CEF (ST3) | (7)(1)(2) | (Al)(V)(Zr) |
| Al8Cr5_H | CEF (SLN) | (8)(5) | (Al)(Cr,Ti) |
| Al8Cr5_L | CEF (SLN) | (8)(5) | (Al,Si)(Cr,Fe,Ti) |
| Al8FeMg3Si6 | CEF (ST4) | (8)(3)(1)(6) | (Al)(Mg)(Fe)(Si) |
| Al8FeMnSi2 | CEF (ST4) | (16)(2)(2)(3) | (Al)(Fe)(Mn)(Si) |
| Al8Mn5 | CEF (SLN) | (0.4615)(0.1923) (0.3462) | (Al)(Cu,Fe,Mn) (Al,Cu,Fe,Mn,Si,Ti,Zn) |
| Al8Mo3 | CEF (SLN) | (8)(3) | (Al,Ti)(Mo,V) |
| Al8V5 | CEF (SLN) | (8)(5) | (Al,Cu,Si)(Fe,Mo,Ni,Ti,V,Zr) |
| Al9Co2 | CEF (SLN) | (9)(2) | (Al,Si)(Co) |
| Al9Cr4_H | CEF (SLN) | (9)(4) | (Al,Si)(Cr) |
| Al9Cr4_L | CEF (SLN) | (9)(4) | (Al,Si)(Cr,Fe) |
| Al9FeNi | CEF (ST3) | (9)(1)(1) | (Al)(Fe)(Ni) |
| AlB12 | CEF (ST2) | (1)(12) | (Al)(B) |
| AlCo2Zr | CEF (ST3) | (1)(2)(1) | (Al)(Co)(Zr) |
| AlCr2 | CEF (SLN) | (1)(2) | (Al,Si)(Cr) |
| AlCu2Ti | CEF (SLN) | (0.75)(0.25) | (Al,Cu)(Ti) |
| AlCuTi | CEF (SLN) | (0.6667)(0.3333) | (Al,Cu)(Ti) |
| AlCu_Delta | CEF (ST2) | (0.4)(0.6) | (Al)(Cu) |
| AlCu_Eps | CEF (SLN) | (0.5)(0.5) | (Al,Cu)(Cu,V) |
| AlCu_Eta | CEF (SLN) | (0.5)(0.5) | (Al,Cu)(Cu,V) |
| AlCu_Gamma | CEF (SLN) | (1)(1) | (Al,Cu,Mn,Si)(Va) |
| AlCu_Theta | CEF (SLN) | (0.667)(0.333) | (Al)(Al,Cu,Ti,V,Zr) |

| | | | |
|--------------|-----------|------------------------------------|-----------------------------------|
| AlCu_Zeta | CEF (ST2) | (0.45)(0.55) | (Al)(Cu) |
| AlFeTi_T1 | CEF (ST3) | (0.25)(0.5)(0.25) | (Al)(Fe)(Ti) |
| AlFeTi_T2 | CEF (ST3) | (0.53448) (0.25172) (0.2138) | (Al)(Fe)(Ti) |
| AlFeTi_T3 | CEF (ST3) | (0.65)(0.075) (0.275) | (Al)(Fe)(Ti) |
| AlFeTi_T4 | CEF (ST3) | (0.35)(0.23) (0.42) | (Al)(Fe)(Ti) |
| AlHf | CEF (SLN) | (0.5)(0.5) | (Al,Si)(Hf) |
| AlLi2Zr | CEF (ST3) | (0.25)(0.5)(0.25) | (Al)(Li)(Zr) |
| 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) |
| AlMg_Eps | CEF (SLN) | (23)(30) | (Mg)(Al,Cu,Zn) |
| AlMg_Gamma | CEF (SLN) | (10)(24)(24) | (Mg)(Al,Cu,Li,Mg,Zn)(Al,Cu,Mg,Zn) |
| AlMnSi | CEF (ST3) | (1)(1)(1) | (Al)(Mn)(Si) |
| AlMoSi_C40 | CEF (SLN) | (2)(1) | (Al,Si)(Mo) |
| AlMoSi_C54 | CEF (ST3) | (0.434)(0.333) (0.233) | (Al)(Mo)(Si) |
| AlNi16Si9 | CEF (ST3) | (1)(16)(9) | (Al)(Ni)(Si) |
| AlNi2Si | CEF (SLN) | (1)(1) | (Ni)(Al,Si,Va) |
| AlNi2Zn | CEF (ST3) | (1)(2)(1) | (Al)(Ni)(Zn) |
| AlNiTi_T1 | CEF (ST3) | (0.65)(0.1)(0.25) | (Al)(Ni)(Ti) |
| AlNiTi_T2 | CEF (SLN) | (0.5517)(0.2069) (0.2414) | (Al,Ti)(Ti)(Ni) |
| AlZr | CEF (SLN) | (1)(1) | (Al,Li)(Zr) |
| AlZr2 | CEF (SLN) | (1)(2) | (Al)(V,Zr) |
| AlZr3 | CEF (ST2) | (1)(3) | (Al)(Zr) |
| Alpha-Mn2B | CEF (ST2) | (0.670691) (0.329309) | (Mn)(B) |
| Alpha_AlFeSi | CEF (SLN) | (0.66)(0.19) (0.05)(0.1) | (Al)(Fe,V)(Si)(Al,Si) |

| | | | |
|----------------|-----------|-------------------------------|--|
| Alpha_Co2Si | CEF (SLN) | (2)(1) | (Co,Cr,Fe,Mn,Si,Ti,Zr)(Co,Si) |
| Alpha_Cr5Si3 | CEF (SLN) | (5)(3) | (Cr,Fe)(Si) |
| Alpha_TiMn | CEF (SLN) | (1)(1) | (Cr,Mn)(Ti) |
| B11 | CEF (SLN) | (0.5)(0.5) | (Ag,Cu,Ni,Ti)(Ag,Cu,Ni,Ti) |
| B2 | CEF (SLN) | (1)(1) | (Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Ni,Si,Ti, V, Zn,Zr) (Co,Cr,Cu,Fe,Hf,Mn,Mo,Ni,Si, Sn,Ti,V,Zr,Va) |
| B2O3 | CEF (ST2) | (2)(3) | (B)(O) |
| B32 | CEF (SLN) | (0.5)(0.5)(3) | (Al,Cu,Li,Mg,Mn,Zn) (Al,Cu,Li,Mg,Mn,Zn)(Va) |
| B4C | CEF (SLN) | (1)(1) | (B12,B11C)(B2,B2C,BC2) |
| B4Hf3 | CEF (ST2) | (4)(3) | (B)(Hf) |
| BCT_A5 | CEF (SLN) | (1) | (Ag,Al,Cu,Ni,Sn,Ti,Zn) |
| BETA_RHOMBO_ B | CEF (SLN) | (93)(12) | (B)(B,Cu,Mn,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)(Va) |
| B_Co27Si27V46 | CEF (ST3) | (0.27)(0.27) (0.46) | (Co)(Si)(V) |
| B_Li2Zn3 | CEF (SLN) | (2)(3) | (Li,Zn)(Li,Zn) |
| B_Li2Zn5 | CEF (SLN) | (2)(5) | (Li,Zn)(Zn) |
| B_LiZn4 | CEF (SLN) | (0.2)(0.8)(0.5) | (Li,Zn)(Li,Zn)(Va) |
| Bcc | CEF (SLN) | (1)(3) | (Ag,Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo, , Ni,Si,Sn,Ti,V,Zn,Zr)(B,C,O,Va) |
| Bcc_B2 | CEF (SLN) | (0.5)(0.5)(3) | (Ag,Al,Co,Cr,Cu,Fe,Mg,Mn,Ni,Si,Ti, V) (Ag,Al,Co,Cr,Cu,Fe,Mg,Mn,Ni,Si,Ti, V) (Va) |
| Beta_AlFeSi | CEF (SLN) | (0.598)(0.152) (0.1)(0.15) | (Al)(Fe,Mn,V)(Si)(Al,Si) |

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| Beta_Co2Si | CEF (SLN) | (2)(1) | (Co,Si)(Co,Si) |
| Beta_TiMn | CEF (SLN) | (0.515)(0.485) | (Cr,Mn,V)(Ti,Zr) |
| CBCC_A12 | CEF (SLN) | (1)(1) | (Al,Co,Cr,Cu,Fe,Mn,Mo,Ni,Si,Sn,Ti,V,Zn,Zr)(C,Va) |
| CHI_A12 | CEF (SLN) | (24)(10)(24) | (Co,Cr,Fe,Ni)(Cr,Mo,Ti,Zr) (Co,Cr,Fe,Mo,Ni) |
| CUB_A13 | CEF (SLN) | (1)(1) | (Ag,Al,Co,Cr,Cu,Fe,Hf,Mg,Mo,Mn,Ni, Si,Sn,Ti,V,Zn,Zr)(C,Va) |
| C_Co34Si27V39 | CEF (ST3) | (0.34)(0.27) (0.39) | (Co)(Si)(V) |
| Cementite | CEF (SLN) | (3)(1) | (Co,Cr,Fe,Mn,Mo,Ni,V)(C) |
| Co10Cu57Ti33 | CEF (ST3) | (0.57)(0.1)(0.33) | (Cu)(Co)(Ti) |
| Co16Si7Ti6 | CEF (ST3) | (16)(7)(6) | (Co)(Si)(Ti) |
| Co2Mg | CEF (ST2) | (2)(1) | (Co)(Mg) |
| Co2Si13Ti5 | CEF (ST3) | (2)(13)(5) | (Co)(Si)(Ti) |
| Co2SiTi | CEF (ST3) | (2)(1)(1) | (Co)(Si)(Ti) |
| Co2SnTi | CEF (SLN) | (1)(1)(1)(1) | (Co,Va)(Co)(Sn)(Ti) |
| Co3B | CEF (SLN) | (3)(1) | (Co,Fe)(B) |
| Co3Cr2Si | CEF (ST3) | (3)(2)(1) | (Co)(Cr)(Si) |
| Co3Cr3Si2 | CEF (ST3) | (3)(3)(2) | (Co)(Cr)(Si) |
| Co3Mn3Mo4 | CEF (ST3) | (0.3)(0.3)(0.4) | (Co)(Mn)(Mo) |
| Co3Si | CEF (ST2) | (0.75)(0.25) | (Co)(Si) |
| Co3Si2Ti | CEF (ST3) | (3)(2)(1) | (Co)(Si)(Ti) |
| Co3Sn2 | CEF (SLN) | (1)(1)(0.5)(0.5) | (Co)(Sn)(Co,Va)(Co,Va) |
| Co3V | CEF (SLN) | (0.75)(0.25) | (Co,Cr,Fe,V)(Co,Cr,Fe,V) |
| Co4Zn | CEF (SLN) | (1)(1) | (Co,Zn)(Va) |
| Co5Cr5Si6 | CEF (ST3) | (5)(5)(6) | (Co)(Cr)(Si) |
| CoMo3Si | CEF (ST3) | (1)(3)(1) | (Co)(Mo)(Si) |
| CoMoZr4 | CEF (ST3) | (1)(1)(4) | (Co)(Mo)(Zr) |
| CoNiTi | CEF (SLN) | (3)(1) | (Co,Ni,Ti)(Co,Ni,Ti) |
| CoSi2Ti | CEF (ST3) | (1)(2)(1) | (Co)(Si)(Ti) |

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| CoSiTi | CEF (ST3) | (1)(1)(1) | (Co)(Si)(Ti) |
| 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) |
| CoSnTi | CEF (ST3) | (1)(1)(1) | (Co)(Sn)(Ti) |
| CoV3 | CEF (SLN) | (1)(3) | (Co,Fe)(Cr,V) |
| 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) |
| CoZn_Delta | CEF (ST2) | (0.117647) (0.882353) | (Co)(Zn) |
| CoZr3 | CEF (ST2) | (1)(3) | (Co)(Zr) |
| Corundum | CEF (SLN) | (2)(1)(3) | (Al+3,Cr+2,Cr+3,Fe+2,Fe+3,Mn+3, Ti+3,V+3,V+4,Va) (Cr+3,Fe+3,Ni+2,Va)(O-2) |
| Cr3B4 | CEF (ST2) | (0.429)(0.571) | (Cr)(B) |
| Cr3Mn5 | CEF (ST2) | (3)(5) | (Cr)(Mn) |
| Cr3Si | CEF (SLN) | (3)(1) | (Co,Cr,Mn,Ni,Si)(Al,Co,Cr,Si) |
| Cr5B3 | CEF (ST2) | (0.625)(0.375) | (Cr)(B) |
| CrB4 | CEF (ST2) | (0.2)(0.8) | (Cr)(B) |
| CrSi2 | CEF (SLN) | (1)(2) | (Cr,Si,Mo)(Al,Cr,Si) |
| CrZn17 | CEF (ST2) | (0.05556) (0.94444) | (Cr)(Zn) |
| Cristobalite | CEF (ST2) | (1)(2) | (Si)(O) |
| Cu10Sn3 | CEF (SLN) | (1) | (Cu,Sn) |
| Cu28Mn61Si11 | CEF (ST3) | (0.28)(0.61) (0.11) | (Cu)(Mn)(Si) |
| Cu2MgZr | CEF (ST3) | (2)(1)(1) | (Cu)(Mg)(Zr) |
| Cu2O | CEF (SLN) | (2)(1) | (Ag,Cu)(O) |
| Cu2SnTi | CEF (ST3) | (2)(1)(1) | (Cu)(Sn)(Ti) |
| Cu2Ti | CEF (SLN) | (0.666667) (0.333333) | (Co,Cu,Fe,Ni)(Ti) |

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| Cu ₂ TiZr | CEF (ST3) | (0.5)(0.25)(0.25) | (Cu)(Ti)(Zr) |
| Cu ₃₃ Mn ₅₀ Si ₁₇ | CEF (ST3) | (0.33)(0.5)(0.17) | (Cu)(Mn)(Si) |
| Cu ₃ Mg ₂ Si | CEF (ST3) | (0.5)(0.3333) (0.1667) | (Cu)(Mg)(Si) |
| Cu ₃ Ni ₂₇ Sn ₁₀ | CEF (ST3) | (0.075)(0.675) (0.26) | (Cu)(Ni)(Sn) |
| Cu ₃ Si ₄ Zr ₂ | CEF (ST3) | (0.3334)(0.4444) (0.2222) | (Cu)(Si)(Zr) |
| Cu ₃ Sn | CEF (SLN) | (3)(1) | (Cu,Sn)(Cu,Sn) |
| Cu ₃ Ti ₂ | CEF (SLN) | (0.6)(0.4) | (Cu,Fe,Ni)(Co,Ti) |
| Cu ₄₁ Sn ₁₁ | CEF (SLN) | (41)(11) | (Cu,Sn)(Cu,Sn) |
| Cu ₄ MgSn | CEF (ST3) | (0.666)(0.167) (0.167) | (Cu)(Mg)(Sn) |
| Cu ₄ MnSn | CEF (ST3) | (0.666)(0.167) (0.167) | (Cu)(Mn)(Sn) |
| Cu ₄ Si ₂ Zr ₃ | CEF (ST3) | (0.4444)(0.2222) (0.3334) | (Cu)(Si)(Zr) |
| Cu ₄ Si ₄ Zr ₃ | CEF (ST3) | (0.3636)(0.3636) (0.2728) | (Cu)(Si)(Zr) |
| Cu ₄ Ti | CEF (SLN) | (0.8)(0.2) | (Cu,Ni,Ti)(Cu,Ni,Ti) |
| Cu ₄ Ti ₃ | CEF (SLN) | (0.57143) (0.42857) | (Co,Cu,Fe,Ni)(Ti) |
| Cu ₅₅ Mg ₂₂ Si ₂₃ | CEF (ST3) | (0.55)(0.22) (0.23) | (Cu)(Mg)(Si) |
| Cu ₆ Sn ₅ L | CEF (SLN) | (1)(1)(1) | (Cu)(Cu,Sn,Va)(Sn) |
| CuMg ₂ | CEF (SLN) | (0.33333) (0.66667) | (Cu,Ni)(Mg) |
| CuMgSn | CEF (ST3) | (0.334)(0.333) (0.333) | (Cu)(Mg)(Sn) |
| CuMnZn | CEF (ST3) | (1)(1)(1) | (Cu)(Mn)(Zn) |
| CuNiTi_T1 | CEF (SLN) | (0.6667)(0.3333) | (Cu,Ni)(Ti) |
| CuNiTi_T2 | CEF (ST3) | (0.035)(0.565) (0.4) | (Cu)(Ni)(Ti) |
| CuNiTi_T3 | CEF (ST3) | (0.035)(0.565) (0.4) | (Cu)(Ni)(Ti) |

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| CuNiTi_T4 | CEF (ST3) | (0.075)(0.675) (0.25) | (Cu)(Ni)(Ti) |
| CuNiTi_T5 | CEF (ST3) | (0.25)(0.5)(0.25) | (Cu)(Ni)(Ti) |
| CuNiTi_T6 | CEF (ST3) | (0.25)(0.5)(0.25) | (Cu)(Ni)(Ti) |
| CuO | CEF (ST2) | (1)(1) | (Cu)(O) |
| CuSi12Zr12 | CEF (ST3) | (0.04)(0.48) (0.48) | (Cu)(Si)(Zr) |
| CuSi2Zr | CEF (ST3) | (0.25)(0.5)(0.25) | (Cu)(Si)(Zr) |
| CuSi4Zr2 | CEF (ST3) | (0.143)(0.571) (0.286) | (Cu)(Si)(Zr) |
| CuSiZr | CEF (ST3) | (0.3333)(0.3333) (0.3334) | (Cu)(Si)(Zr) |
| CuSn3Ti5 | CEF (ST3) | (5)(3)(1) | (Ti)(Sn)(Cu) |
| CuSnTi | CEF (ST3) | (1)(1)(1) | (Cu)(Sn)(Ti) |
| CuSn_Gamma | CEF (SLN) | (1) | (Ag,Cu,Mg,Mn,Ni,Sn) |
| CuTi | CEF (SLN) | (0.5)(0.5) | (Co,Cu,Ni,Ti)(Cu,Ni,Ti,Zr) |
| CuZn_Beta | CEF (SLN) | (1) | (Cu,Zn) |
| CuZr | CEF (SLN) | (1)(1) | (Ag,Cu,Ni)(Ti,Zr) |
| DO_19 | CEF (SLN) | (0.75)(0.25)(0.5) | (Al,Cr,Cu,Mn,Mo,Ni,Sn,Ti,V,Zr) (Al,Cr,Mn,Mo,Ni,Si,Sn,Ti)(C,Va) |
| DO_22 | CEF (SLN) | (3)(1) | (Al,Mo,Si,Ti)(Al,Cr,Mo,Ti,Zr) |
| DO_22_TiAl3_L | CEF (SLN) | (3)(1) | (Al,Ti)(Al,Cr,Ti,V) |
| Delta_AlFeSi | CEF (SLN) | (5)(1) | (Al,Si)(Fe) |
| Delta_Cu33Si7 | CEF (SLN) | (0.825)(0.175) | (Ag,Cu,Mg)(Si) |
| Diamond | CEF (SLN) | (1) | (Ag,Al,B,C,Ni,Si,Sn) |
| Eps | CEF (SLN) | (1) | (Al,Cu,Zn) |
| Epsilon_Cu15Si4 | CEF (SLN) | (0.789474) (0.210526) | (Ag,Cu,Mg,Zn)(Al,Si) |
| Eta_Cu19Si6 | CEF (SLN) | (0.76)(0.24) | (Ag,Cu,Mg)(Si) |
| Eta_MC | CEF (SLN) | (1)(1) | (Mo)(C,Va) |
| Fcc | CEF (SLN) | (1)(1) | (Ag,Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo, ,Ni,Si,Sn,Ti,V,Zn,Zr)(B,C,O,Va) |

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| Fcc_MC | CEF (SLN) | (1)(1) | (Co,Cr,Fe,Mo,Ni,Si,Ti,Zr)(C,Va) |
| Fe18Sn9Zr5 | CEF (ST3) | (18)(9)(5) | (Fe)(Sn)(Zr) |
| 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) |
| Fe2Si | CEF (ST2) | (0.666667) (0.333333) | (Fe)(Si) |
| Fe2TiZn22 | CEF (ST3) | (2)(1)(22) | (Fe)(Ti)(Zn) |
| Fe2V2Si | CEF (ST3) | (2)(2)(1) | (Fe)(V)(Si) |
| Fe3Sn2 | CEF (ST2) | (3)(2) | (Fe)(Sn) |
| Fe3Sn9Zr20 | CEF (ST3) | (3)(9)(20) | (Fe)(Sn)(Zr) |
| Fe4Sn10Zr9 | CEF (ST3) | (4)(10)(9) | (Fe)(Sn)(Zr) |
| Fe4Sn4Zr3 | CEF (ST3) | (4)(4)(3) | (Fe)(Sn)(Zr) |
| Fe4V5Si4 | CEF (ST3) | (4)(5)(4) | (Fe)(V)(Si) |
| Fe5Ni3Si2 | CEF (SLN) | (0.8)(0.2) | (Fe,Ni)(Si) |
| Fe5Sn3 | CEF (ST2) | (5)(3) | (Fe)(Sn) |
| Fe5V3Si2 | CEF (ST3) | (5)(3)(2) | (Fe)(V)(Si) |
| Fe6Sn6Zr | CEF (ST3) | (6)(6)(1) | (Fe)(Sn)(Zr) |
| Fe9Sn20Zr22 | CEF (ST3) | (9)(20)(22) | (Fe)(Sn)(Zr) |
| FeHf2 | CEF (ST2) | (0.3333)(0.6667) | (Fe)(Hf) |
| FeMn2Zn7 | CEF (ST3) | (0.1)(0.2)(0.7) | (Fe)(Mn)(Zn) |
| FeMo4Zr9 | CEF (ST3) | (1)(4)(9) | (Fe)(Mo)(Zr) |
| FeSi2_H | CEF (SLN) | (0.3)(0.7) | (Fe,V,Zr)(Al,Si) |
| FeSi2_L | CEF (SLN) | (1)(2) | (Co,Fe,Ni,V)(Al,Si) |
| FeSiZr_T1 | CEF (ST3) | (1)(1)(1) | (Fe)(Si)(Zr) |
| FeSiZr_T3 | CEF (ST3) | (4)(7)(4) | (Fe)(Si)(Zr) |
| FeSiZr_T4 | CEF (ST3) | (41)(41)(18) | (Fe)(Si)(Zr) |
| FeSiZr_T5 | CEF (SLN) | (16)(7)(6) | (Fe)(Fe,Si)(Zr) |
| FeSiZr_T8 | CEF (ST3) | (4)(2)(1) | (Fe)(Si)(Zr) |
| FeSiZr_T9 | CEF (ST3) | (29)(29)(42) | (Fe)(Zr)(Si) |
| FeSn | CEF (ST2) | (1)(1) | (Fe)(Sn) |

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| FeSn2 | CEF (ST2) | (1)(2) | (Fe)(Sn) |
| FeSn2Zr6 | CEF (ST3) | (1)(2)(6) | (Fe)(Sn)(Zr) |
| FeZn_Delta | CEF (SLN) | (0.058)(0.18) (0.525)(0.237) | (Fe)(Al,Fe,Mn,Si,Zn)(Zn)(Zn) |
| FeZn_Gamma | CEF (SLN) | (0.154)(0.154) (0.231)(0.461) | (Fe,Mn,Zn)(Fe,Mn,Zn) (Al,Fe,Mn,Si,Zn)(Zn) |
| FeZn_Gamma1 | CEF (SLN) | (0.137)(0.118) (0.745) | (Fe)(Al,Fe,Mn,Si,Zn)(Mn,Zn) |
| FeZn_Zeta | CEF (SLN) | (0.072)(0.856) (0.072) | (Fe,Mn,Va)(Al,Zn)(Al,Si,Zn,Va) |
| FeZr3 | CEF (SLN) | (1)(3) | (Al,Fe,Zr)(Fe,Ti,Zr) |
| Gamma2 | CEF (SLN) | (0.255)(0.745) | (Al,Fe,Mn,Zn)(Zn) |
| Gamma_AlFeSi | CEF (ST3) | (0.635)(0.205) (0.16) | (Al)(Fe)(Si) |
| Gamma_Cu56Si1 1 | CEF (SLN) | (0.835821) (0.164179) | (Ag,Cu,Mg,Mn,Zn)(Si) |
| Gamma_H | CEF (SLN) | (4)(1)(8) | (Al,Si,Zn)(Al,Cu,Zn)(Cu,Fe,Mn) |
| Gammabrass | CEF (SLN) | (1) | (Al,Cu,Mn,Si,Zn) |
| Gas | GAS | (1) | (Ag,Al,AlO,AlO2,Al2,Al2O,Al2O2, Al2O3,C1O1,C1O2,Fe,FeO,FeO2, Fe2,Hf,HfO,HfO2,Li,Li2,Li2O,Li2O 2, Mg,Mg2,MgO,Mn,O,O2,O3,Sn,Sn2, SnO,SnO2,Si,Si2,Si3,SiO,SiO2,Ti, TiO,TiO2,Zn,Zr,Zr2,ZrO,ZrO2) |
| Graphite | CEF (SLN) | (1) | (B,C) |
| H_CoMnSi | CEF (ST3) | (0.5)(0.25)(0.25) | (Co)(Mn)(Si) |
| H_L21 | CEF (SLN) | (0.5)(0.5)(1) | (Al,Cr,Fe,Mn,Ni,Ti) (Al,Cr,Fe,Mn,Ni,Ti) (Cr,Fe,Mn,Ni,Va) |
| Halite | CEF (SLN) | (1)(1) | (Al+3,Co+2,Cr+3,Fe+2,Fe+3,Mg+2, Mn+2,Mn+3,Ni+2,V,V+2,V+3,Va) (O-2,Va) |
| Hcp | CEF (SLN) | (1)(0.5) | (Ag,Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo , Ni,Si,Sn,Ti,V,Zn,Zr)(B,C,O,Va) |

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| Hcp_M2C | CEF (SLN) | (1)(0.5) | (Co,Cr,Fe,Mo,Ni,Ti)(C,Va) |
| Hf3Si | CEF (ST2) | (0.75)(0.25) | (Hf)(Si) |
| Hf3Si2 | CEF (ST2) | (2)(3) | (Si)(Hf) |
| Hf5Si3 | CEF (ST2) | (3)(5) | (Si)(Hf) |
| Hf5Sn3 | CEF (ST2) | (5)(3) | (Hf)(Sn) |
| Hf5Sn4 | CEF (ST2) | (5)(4) | (Hf)(Sn) |
| HfMn | CEF (ST2) | (0.5)(0.5) | (Hf)(Mn) |
| HfMn2 | CEF (SLN) | (1)(2) | (Hf,Mn)(Hf,Mn) |
| HfNiTi_Tao | CEF (SLN) | (11)(14) | (Ni)(Hf,Ti) |
| HfSi | CEF (ST2) | (0.5)(0.5) | (Hf)(Si) |
| HfSi2 | CEF (SLN) | (1)(2) | (Hf,Si)(Si) |
| HfSiO4 | CEF (ST3) | (1)(1)(4) | (Hf)(Si)(O) |
| HfSn2 | CEF (ST2) | (1)(2) | (Hf)(Sn) |
| J_Co45Si40V15 | CEF (ST3) | (0.45)(0.4)(0.15) | (Co)(Si)(V) |
| Ksi_Carbide | CEF (SLN) | (3)(1) | (Cr,Fe,Mo)(C) |
| L10_TiAl | CEF (SLN) | (1)(1)(2) | (Al,Cr,Mn,Mo,Ti,V,Zr) (Al,Cr,Mn,Mo,Ti,V,Zr)(C,Va) |
| L12_FCC | CEF (SLN) | (0.75)(0.25) | (Al,Co,Cr,Cu,Fe,Mn,Mo,Ni,Si,Ti,V, Zr) (Al,Co,Cr,Cu,Fe,Mn,Mo,Ni,Si,Ti,V, Zr) |
| L12_Ti25Mn9Al6 6 | CEF (ST3) | (0.67)(0.08) (0.25) | (Al)(Mn)(Ti) |
| L_CoMnSi | CEF (ST3) | (0.4433)(0.3333) (0.2233) | (Co)(Mn)(Si) |
| L_Sigma | CEF (SLN) | (8)(4)(18) | (Mn,Ni)(Cr)(Cr,Mn) |
| Laves_C14 | CEF (SLN) | (2)(1) | (Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo,Ni, ' Si,Ti,V,Zn,Zr) (Al,Co,Cr,Cu,Fe,Hf,Mg, Mn,Mo,Ni,Si,Ti,V,Zn,Zr) |
| Laves_C15 | CEF (SLN) | (2)(1) | (Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo,Ni, ' Si,Sn,Ti,V,Zn,Zr) (Al,Co,Cr,Cu,Fe,Hf, |

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| | | | Li,Mg,Mn,Mo,Ni,Si,Sn,Ti,V,Zn,Zr) |
| Laves_C36 | CEF (SLN) | (2)(1) | (Al,Co,Cr,Cu,Fe,Mg,Mn,Mo,Ni,Si,Ti , V,Zn,Zr)(Al,Co,Cr,Cu,Fe,Mg,Mn,Ni, Si,Sn,Ti,V,Zn,Zr) |
| Li12Mg3Si4 | CEF (ST3) | (0.631579) (0.157895) (0.210526) | (Li)(Mg)(Si) |
| Li12Si7 | CEF (ST2) | (0.6316)(0.3654) | (Li)(Si) |
| Li13Si4 | CEF (ST2) | (0.7647)(0.2353) | (Li)(Si) |
| Li13Sn5 | CEF (ST2) | (13)(5) | (Li)(Sn) |
| Li17Si4 | CEF (ST2) | (0.8095)(0.1905) | (Li)(Si) |
| Li21Si5 | CEF (ST2) | (0.80769) (0.19231) | (Li)(Si) |
| Li22Sn5 | CEF (ST2) | (22)(5) | (Li)(Sn) |
| 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) |
| Li4.13Si | CEF (ST2) | (0.80488) (0.19512) | (Li)(Si) |
| Li5Sn2 | CEF (ST2) | (5)(2) | (Li)(Sn) |
| Li7Si3 | CEF (ST2) | (0.7)(0.3) | (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) |
| LiSi | CEF (ST2) | (0.5)(0.5) | (Li)(Si) |
| LiSn | CEF (ST2) | (1)(1) | (Li)(Sn) |
| LiZn2 | CEF (ST2) | (1)(2) | (Li)(Zn) |
| Liquid | CEF (SLN) | (1) | (Ag,Al,B,C,Co,Cr,Cu,Fe,Hf,Li,Mg, |

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| | | | Mg ₂ Sn, Mn, Mo, Ni, Si, Sn, Ti, V, Zn, Zr, Al ₂ O ₃ , B ₂ O ₃ , CoO, Co ₂ O ₃ , Cr ₂ /3O, CuO, Cu ₂ O, Cu ₂ O ₃ , FeO, FeO ₃ /2, HfO ₂ , Li ₂ O, MgO, MnO, MnO ₃ /2, MoO ₂ , MoO ₃ , NiO, O, SiO ₂ , SnO, SnO ₂ , TiO, TiO ₃ /2, TiO ₂ , VO, VO ₂ , VO ₃ /2, VO ₅ /2, Zr ₁ /2O) |
| M10X7_oS68 | CEF (SLN) | (10)(7) | (Ag, Al, Cu, Fe, Ni)(Hf, Ti, Zr) |
| M11X2_mS36 | CEF (SLN) | (11)(2) | (Co, Fe)(Hf, Zr) |
| M11X9_ti40 | CEF (SLN) | (11)(9) | (Cu, Ni)(Hf, Ti, Zr) |
| M21X8_aP29 | CEF (SLN) | (21)(8) | (Cu, Ni)(Hf, Zr) |
| M23C6 | CEF (SLN) | (20)(3)(6) | (Co, Cr, Fe, Mn, Ni, V) (Co, Cr, Fe, Mn, Mo, Ni, V)(C) |
| M23X6_cF116 | CEF (SLN) | (23)(6) | (Co, Cu, Fe, Si)(Hf, Zr) |
| M2B_ti12 | CEF (SLN) | (2)(1) | (Co, Fe, Mn, Mo, Ni)(B) |
| M2O3_cI80 | CEF (SLN) | (2)(3)(1) | (Mn+3, Va)(O-2)(O-2, Va) |
| M2SiO4 | CEF (SLN) | (2)(1) | (FeO, MnO, NiO)(SiO ₂) |
| M2X_ti12 | CEF (SLN) | (0.333)(0.667) | (Al, Si)(Cr, Fe, Hf, Mn, Mo, Ti, V, Zr) |
| M3C2 | CEF (SLN) | (3)(2) | (Co, Cr, Mo, V)(C) |
| M51X14_hP68 | CEF (SLN) | (51)(14) | (Ag, Cu, Ni)(Hf, Ti, Zr) |
| M5C2 | CEF (SLN) | (5)(2) | (Fe, Mn, V)(C) |
| M5Si3_ti32 | CEF (SLN) | (0.625)(0.375) | (Cr, Fe, Mo, Si, Ti, V, Zr)(Al, Mo, Ni, Si) |
| M5Si4_tP36 | CEF (SLN) | (0.555556) (0.444444) | (Cr, Hf, Mo, Ti, Zr)(Al, Si) |
| M5X3_hP16 | CEF (SLN) | (2)(3)(3) | (Al, Co, Cr, Cu, Fe, Mn, Mo, Ni, Si, Ti, V, Zr) (Al, Cr, Ni, Si, Sn, Ti) (Co, Cr, Cu, Fe, Mn, Mo, Ni, Ti, V) |
| M5X_cF24 | CEF (SLN) | (5)(1) | (Cr, Cu, Fe, Ni)(Hf, Ti, Zr) |
| M6C | CEF (SLN) | (2)(2)(2)(1) | (Co, Fe, Ni)(Cr, Mo) (Co, Cr, Fe, Mo, Ni, Si, V)(C) |
| M6Sn5 | CEF (SLN) | (1)(1)(1) | (Cu, Ni)(Cu, Sn, Ni, Va)(Sn) |
| M7C3 | CEF (SLN) | (7)(3) | (Co, Cr, Fe, Mn, Mo, Ni, V)(C) |

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| M7X2_mS36 | CEF (SLN) | (7)(2) | (Al,Cr,Cu,Fe,Ni,V)(Cr,Hf,Ti,Zr) |
| M8X3_oP44 | CEF (SLN) | (8)(3) | (Ag,Cu)(Hf,Zr) |
| MA13Si3Zr5 | CEF (SLN) | (3)(5) | (Al,Cu,Si)(Zr) |
| MB2_hP3 | CEF (SLN) | (1)(2) | (Al,Cr,Hf,Mg,Mn,Mo,Ti,V,Zr,Va) (B,Va) |
| MB_oP8 | CEF (SLN) | (1)(1) | (Co,Fe,Mn,Ti)(B) |
| MB_oS8 | CEF (SLN) | (1)(1) | (Cr,Mo,Ni,V)(B,Va) |
| MO2_cF12 | CEF (SLN) | (1)(2) | (Hf,Zr)(O,Va) |
| MO2_mP12 | CEF (SLN) | (1)(2) | (Hf,Mo,V,Zr)(O) |
| MO2_tP6 | CEF (SLN) | (1)(2) | (Hf,Zr)(O,Va) |
| MSi | CEF (SLN) | (0.5)(0.5) | (Co,Cr,Fe,Mg,Mn,Ni,Si,V,Zr) (Al,Co,Cr,Si) |
| MSi2 | CEF (SLN) | (1)(2) | (Co,Fe,Mn,Ni,Zr)(Al,Si) |
| MX2_cF96 | CEF (SLN) | (1)(2) | (Co,Cr,Cu,Fe,Hf,Ni,Si,Ti) (Al,Cu,Fe,Hf,Ni,Ti,V,Zr) |
| MX2_tI12 | CEF (SLN) | (1)(2) | (Al,Co,Cu,Fe,Ni,Si,Zr)(Fe,Hf,Ti,Zr) |
| MX2_tI6 | CEF (SLN) | (1)(2) | (Ag,Co,Cu,Fe,Ni)(Al,Hf,Ti,Zr) |
| MX_oS8 | CEF (SLN) | (1)(1) | (Cu,Ni)(Hf,Ti,Zr) |
| Mg2C3 | CEF (ST2) | (0.4)(0.6) | (Mg)(C) |
| Mg2CrNi | CEF (SLN) | (0.12)(0.33) (0.55) | (Cr,Ni)(Mg,Ni)(Cr,Mg) |
| Mg2M | CEF (SLN) | (0.5)(0.25)(0.25) | (Mg)(Al,Si,Sn)(Li,Va) |
| Mg2Ni | CEF (SLN) | (2)(1) | (Cr,Mg)(Cu,Ni,Zn) |
| Mg2SiNi3 | CEF (ST3) | (2)(1)(3) | (Mg)(Si)(Ni) |
| Mg2Zn11 | CEF (SLN) | (5)(6)(2) | (Al,Zn)(Cu,Zn)(Mg) |
| Mg2Zn3 | CEF (SLN) | (2)(3) | (Mg)(Al,Zn) |
| Mg3MnNi2 | CEF (ST3) | (3)(1)(2) | (Mg)(Mn)(Ni) |
| Mg3Ni11Si6 | CEF (ST3) | (3)(11)(6) | (Mg)(Ni)(Si) |
| Mg5Ni17Si7 | CEF (SLN) | (5)(17)(7) | (Mg)(Ni,Si)(Ni,Si) |
| Mg7Zn3 | CEF (ST2) | (51)(20) | (Mg)(Zn) |
| MgB4 | CEF (ST2) | (1)(4) | (Mg)(B) |
| MgB7 | CEF (ST2) | (1)(7) | (Mg)(B) |

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| MgC2 | CEF (ST2) | (0.333333) (0.666667) | (Mg)(C) |
| MgNi8Si6 | CEF (ST3) | (1)(8)(5.5) | (Mg)(Ni)(Si) |
| MgZn | CEF (SLN) | (12)(13) | (Mg)(Al,Zn) |
| Mn11Si19 | CEF (SLN) | (11)(19) | (Mn,Ni)(Al,Si) |
| Mn13NiSi6 | CEF (ST3) | (13)(1)(6) | (Mn)(Ni)(Si) |
| Mn19Sn6 | CEF (ST2) | (19)(6) | (Mn)(Sn) |
| Mn2Ni3Si | CEF (ST3) | (1)(1.56)(0.44) | (Mn)(Ni)(Si) |
| Mn2NiSi | CEF (SLN) | (2)(1)(1) | (Mn,Ni)(Mn,Ni)(Si) |
| Mn2Sn | CEF (ST2) | (2)(1) | (Mn)(Sn) |
| Mn3B4 | CEF (ST2) | (0.428571) (0.571429) | (Mn)(B) |
| Mn3Ni10Si7 | CEF (ST3) | (3)(10)(7) | (Mn)(Ni)(Si) |
| Mn3Ni2Si | CEF (ST3) | (3)(2)(1) | (Mn)(Ni)(Si) |
| Mn3Ni9Si8 | CEF (ST3) | (3)(9)(8) | (Mn)(Ni)(Si) |
| Mn3Si | CEF (SLN) | (3)(1) | (Cr,Fe,Mn,Ni)(Al,Si) |
| Mn3Ti | CEF (SLN) | (3)(1) | (Mn,V)(Ti) |
| Mn4Ti | CEF (SLN) | (0.815)(0.185) | (Mn,V)(Ti) |
| Mn52Ni29Si19 | CEF (ST3) | (52)(29)(19) | (Mn)(Ni)(Si) |
| Mn61Ni12Si27 | CEF (ST3) | (61)(12)(27) | (Mn)(Ni)(Si) |
| Mn6Ni16Si7 | CEF (ST3) | (6)(16)(7) | (Mn)(Ni)(Si) |
| Mn6Si | CEF (SLN) | (0.85)(0.15) | (Al,Mn)(Si) |
| Mn9Si2 | CEF (ST2) | (0.825)(0.175) | (Mn)(Si) |
| MnB4 | CEF (ST2) | (0.2)(0.8) | (Mn)(B) |
| MnNi2 | CEF (SLN) | (1)(2) | (Mn,Ni)(Ni) |
| MnNiSi | CEF (ST3) | (1)(1)(1) | (Mn)(Ni)(Si) |
| MnNiSi_P | CEF (SLN) | (1)(1)(1) | (Mn)(Ni)(Ni,Si) |
| MnNi_Beta | CEF (SLN) | (1)(1) | (Co,Cr,Fe,Mg,Mn,Ni) (Co,Cr,Fe,Mn,Ni) |
| MnSi | CEF (ST2) | (1)(1) | (Mn)(Si) |
| MnSn2 | CEF (ST2) | (1)(2) | (Mn)(Sn) |

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| MnZn9 | CEF (ST2) | (0.1)(0.9) | (Mn)(Zn) |
| Mo2B5 | CEF (SLN) | (2)(5) | (Mo)(B,Va) |
| Mo2Hf | CEF (SLN) | (2)(1) | (Hf,Mo)(Hf,Mo) |
| Mo2Ti | CEF (ST2) | (2)(1) | (Mo)(Ti) |
| Mo3Si5Zr2 | CEF (ST3) | (3)(5)(2) | (Mo)(Si)(Zr) |
| Mo3Sn | CEF (ST2) | (3)(1) | (Mo)(Sn) |
| Mo3Ti2 | CEF (ST2) | (3)(2) | (Mo)(Ti) |
| Mo4O11 | CEF (ST2) | (0.266667) (0.733333) | (Mo)(O) |
| Mo4Si9Ti7 | CEF (SLN) | (0.55)(0.45) | (Mo,Ti)(Si) |
| Mo4Ti | CEF (ST2) | (4)(1) | (Mo)(Ti) |
| Mo5Si9Zr6 | CEF (ST3) | (5)(9)(6) | (Mo)(Si)(Zr) |
| Mo5Ti | CEF (ST2) | (5)(1) | (Mo)(Ti) |
| Mo7Ti | CEF (ST2) | (7)(1) | (Mo)(Ti) |
| Mo8O23 | CEF (ST2) | (0.258064) (0.741935) | (Mo)(O) |
| Mo9O26 | CEF (ST2) | (0.257143) (0.742857) | (Mo)(O) |
| Mo9Ti | CEF (ST2) | (9)(1) | (Mo)(Ti) |
| MoB4 | CEF (ST2) | (0.8)(0.2) | (B)(Mo) |
| MoNi | CEF (SLN) | (24)(20)(12) | (Co,Cr,Fe,Ni) (Al,Co,Cr,Fe,Mn,Mo,Ni)(Mo) |
| MoNi3 | CEF (SLN) | (0.75)(0.25) | (Mo,Ni)(Mo,Ni,Ti) |
| MoNi4 | CEF (ST2) | (0.2)(0.8) | (Mo)(Ni) |
| MoO3 | CEF (ST2) | (1)(3) | (Mo)(O) |
| MoSi2 | CEF (SLN) | (1)(2) | (Co,Cr,Mo,V)(Al,Si) |
| MoSi6Ti2 | CEF (SLN) | (1)(2) | (Mo,Ti)(Si) |
| MoSiZr | CEF (ST3) | (1)(1)(1) | (Mo)(Si)(Zr) |
| MoSn | CEF (ST2) | (1)(1) | (Mo)(Sn) |
| MoSn2 | CEF (ST2) | (1)(2) | (Mo)(Sn) |
| MoTi | CEF (ST2) | (1)(2) | (Mo)(Ti) |
| MoTi2 | CEF (ST2) | (1)(2) | (Mo)(Ti) |

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| Mu_PHASE | CEF (SLN) | (7)(2)(4) | (Al,Co,Cr,Fe,Mo,Mn,Ni,Si,Ti,V,Zr) (Mo)(Al,Co,Cr,Fe,Mo,Ni,Si,Ti,V,Zr) |
| Ni11Si31Zr8 | CEF (ST3) | (0.22)(0.62) (0.16) | (Ni)(Si)(Zr) |
| Ni11Si5Zr4 | CEF (ST3) | (0.55)(0.25)(0.2) | (Ni)(Si)(Zr) |
| Ni16Si7Ti6 | CEF (SLN) | (16)(7)(6) | (Ni)(Si)(Si,Ti) |
| Ni2Si2Zr | CEF (ST3) | (0.4)(0.4)(0.2) | (Ni)(Si)(Zr) |
| Ni2Si9Zr14 | CEF (ST3) | (0.08)(0.36) (0.56) | (Ni)(Si)(Zr) |
| Ni2SiO4 | CEF (ST3) | (2)(1) | (NiO)(SiO2) |
| Ni2SiZn | CEF (ST3) | (2)(1)(1) | (Ni)(Si)(Zn) |
| Ni2SiZn3 | CEF (ST3) | (2)(1)(3) | (Ni)(Si)(Zn) |
| Ni2Si_H | CEF (SLN) | (1)(1)(1) | (Ni)(Ni,Va)(Al,Si) |
| Ni2Si_L | CEF (SLN) | (2)(1) | (Fe,Ni)(Al,Si) |
| Ni2SnTi | CEF (SLN) | (0.25)(0.5)(0.25) | (Ti)(Ni,Va)(Sn,Ti) |
| Ni2Ti2Sn | CEF (ST3) | (0.4)(0.4)(0.2) | (Ti)(Ni)(Sn) |
| Ni2V | CEF (SLN) | (0.6667)(0.3333) | (Ni)(Al,V) |
| Ni2Zr | CEF (SLN) | (0.04)(0.66)(0.3) | (Cu,Zr)(Ni)(Zr) |
| Ni3B | CEF (ST2) | (3)(1) | (Ni)(B) |
| Ni3Hf_Alpha | CEF (SLN) | (3)(1) | (Ni)(Hf,Ti) |
| Ni3Hf_Beta | CEF (ST2) | (3)(1) | (Ni)(Hf) |
| Ni3Si2 | CEF (SLN) | (3)(2) | (Fe,Mn,Ni)(Si) |
| Ni3Si2Zn | CEF (ST3) | (3)(2)(1) | (Ni)(Si)(Zn) |
| Ni3SiTi2 | CEF (SLN) | (3)(1)(2) | (Ni,Si)(Ni,Si)(Ti) |
| Ni3Si_H | CEF (SLN) | (3)(1) | (Ni)(Al,Si) |
| Ni3Si_L | CEF (SLN) | (3)(1) | (Ni)(Si,Ti) |
| Ni3Sn2 | CEF (SLN) | (0.5)(0.25)(0.25) | (Ni,Sn)(Ni)(Ni) |
| Ni3Sn4 | CEF (SLN) | (0.4286)(0.5714) | (Cu,Ni)(Ni,Sn) |
| Ni3Ti | CEF (SLN) | (0.75)(0.25) | (Co,Cr,Cu,Fe,Ni,Ti) (Cr,Cu,Fe,Hf,Mo,Ni,Si,Ti,V) |
| Ni3V | CEF (SLN) | (3)(1) | (Fe,Ni,V)(Al,Ni,Ti,V) |
| Ni3Zr | CEF (ST2) | (3)(1) | (Ni)(Zr) |

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| Ni4Si3Ti | CEF (SLN) | (4)(3)(1) | (Ni,Ti)(Si)(Ti) |
| Ni4Si7Ti4 | CEF (SLN) | (4)(7)(4) | (Ni)(Si,Ti)(Si,Ti) |
| Ni4Si9Zr7 | CEF (ST3) | (0.2)(0.45)(0.35) | (Ni)(Si)(Zr) |
| Ni5Si2 | CEF (SLN) | (5)(2) | (Fe,Ni)(Al,Si) |
| Ni5SiTi6 | CEF (ST3) | (5)(1)(6) | (Ni)(Si)(Ti) |
| Ni7Hf3 | CEF (ST2) | (7)(3) | (Ni)(Hf) |
| Ni9Si2Zn | CEF (ST3) | (9)(2)(1) | (Ni)(Si)(Zn) |
| NiSi | CEF (SLN) | (1)(1) | (Fe,Ni,Zn)(Si) |
| NiSi4Ti4 | CEF (ST3) | (1)(4)(4) | (Ni)(Si)(Ti) |
| NiSiTi | CEF (SLN) | (1)(1)(1) | (Ni,Ti)(Si)(Ni,Ti) |
| NiSiZr | CEF (ST3) | (0.3333)(0.3333) (0.3334) | (Ni)(Si)(Zr) |
| NiSnTi | CEF (ST3) | (0.333)(0.333) (0.333) | (Ti)(Ni)(Sn) |
| NiTizr | CEF (SLN) | (1)(1)(1) | (Ni,Ti,Zr)(Ni,Ti,Zr)(Ni,Ti,Zr) |
| NiV3 | CEF (ST2) | (0.25)(0.75) | (Ni)(V) |
| NiZn8 | CEF (ST2) | (0.111)(0.889) | (Ni)(Zn) |
| NiZn_Beta1 | CEF (SLN) | (1)(1) | (Al,Cu,Ni,Zn)(Ni,Zn) |
| NiZn_Gamma | CEF (SLN) | (1) | (Ni,Zn) |
| P_Phase | CEF (SLN) | (24)(12)(20) | (Co,Cr,Fe,Ni)(Mo)(Co,Cr,Fe,Mo,Ni) |
| Phi_Al2Mg5Zn2 | CEF (SLN) | (6)(5) | (Mg)(Al,Zn) |
| Q | CEF (ST3) | (0.4375)(0.375) (0.1875) | (Al)(Mg)(Cu) |
| Q_Al5Cu2Mg8Si6 | CEF (ST4) | (0.2381)(0.0952) (0.381)(0.2857) | (Al)(Cu)(Mg)(Si) |
| Quartz | CEF (ST2) | (1)(2) | (Si)(O) |
| R_Al5CuLi3 | CEF (ST3) | (0.55)(0.117) (0.333) | (Al)(Cu)(Li) |
| R_Co40Si15V45 | CEF (ST3) | (0.4)(0.15)(0.45) | (Co)(Si)(V) |
| R_CoMnSi | CEF (ST3) | (0.2)(0.53)(0.27) | (Co)(Mn)(Si) |
| R_Phase | CEF (SLN) | (27)(14)(12) | (Co,Cr,Fe,Mo,Mn,Ni,V)(Cr,Mo) (Co,Cr,Fe,Mn,Mo,Ni,Si,V) |

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| Rutile | CEF (SLN) | (1)(2) | (Mn+4,Sn+4,Ti+3,Ti+4,V+4)(O-2,Va) |
| S | CEF (ST3) | (0.5)(0.25)(0.25) | (Al)(Mg)(Cu) |
| Shp_MC | CEF (ST2) | (1)(1) | (Mo)(C) |
| Si2Ti | CEF (SLN) | (0.666667) (0.333333) | (Al,Si)(Co,Cr,Mo,Ti,V) |
| Si2TiV | CEF (SLN) | (1)(1) | (Si)(Ti,V) |
| Si2V | CEF (SLN) | (0.666667) (0.333333) | (Al,Si)(Fe,Mo,Ti,V) |
| Si2Zr | CEF (SLN) | (2)(1) | (Si,Al)(Al,Co,Fe,Zr) |
| Si2Zr3 | CEF (SLN) | (2)(3) | (Co,Si)(Zr) |
| Si3Zr5 | CEF (SLN) | (3)(5) | (Al,Mo,Si)(Zr) |
| Si4Ti5 | CEF (SLN) | (0.444444) (0.555556) | (Si)(Mo,Ti) |
| Si4Zr5 | CEF (SLN) | (4)(5) | (Al,Co,Si)(Zr) |
| Si5V6 | CEF (SLN) | (0.454545) (0.545455) | (Si)(Cr,V) |
| SiB3 | CEF (SLN) | (6)(2)(6) | (B)(Si)(B,Si) |
| SiB6 | CEF (SLN) | (210)(23)(48) | (B)(Si)(B,Si) |
| SiBn | CEF (SLN) | (61)(1)(8) | (B)(Si)(B,Si) |
| SiC | CEF (ST2) | (1)(1) | (C)(Si) |
| SiTi | CEF (SLN) | (0.5)(0.5) | (Al,Si)(Co,Ti) |
| SiTi3 | CEF (SLN) | (0.25)(0.75) | (Si)(Ti,V) |
| SiZr | CEF (SLN) | (1)(1) | (Si,Al)(Zr) |
| SiZr3 | CEF (ST2) | (1)(3) | (Si)(Zr) |
| Sigma | CEF (SLN) | (8)(4)(18) | (Al,Co,Cr,Cu,Fe,Mn,Ni,Si) (Cr,Fe,Hf,Mo,Si,Ti,V) (Al,Co,Cr,Fe,Hf,Mn,Mo,Ni,Si,Ti,V) |
| Sn2V | CEF (ST2) | (1)(2) | (V)(Sn) |
| Sn2Zr | CEF (ST2) | (2)(1) | (Sn)(Zr) |
| Sn3Ti2 | CEF (ST2) | (0.6)(0.4) | (Sn)(Ti) |
| Sn3Zr5_hP18 | CEF (SLN) | (5)(3)(1) | (Ti,Zr)(Sn)(Sn,Va) |
| Sn5Ti6 | CEF (SLN) | (0.455)(0.545) | (Sn)(Cr,Cu,Ni,Ti) |

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| SnTi2 | CEF (SLN) | (0.333)(0.667) | (Sn)(Co,Cr,Ti,Zr) |
| 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, 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) |
| 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) |
| T1_Al2CuLi | CEF (ST3) | (0.5)(0.25)(0.25) | (Al)(Cu)(Li) |
| T1_AlCuMo | CEF (ST3) | (2.5)(0.5)(1) | (Al)(Cu)(Mo) |
| T1_AlFeMo | CEF (ST3) | (2.72)(0.28)(1) | (Al)(Fe)(Mo) |
| T1_AlFeSi | CEF (SLN) | (5)(3) | (Al,Si)(Fe) |
| T1_Co5Si3V4 | CEF (ST3) | (0.4167)(0.25) (0.3333) | (Co)(Si)(V) |
| T1_CoMnSi | CEF (ST3) | (0.08)(0.64) (0.28) | (Co)(Mn)(Si) |
| T1_CuFeTi | CEF (SLN) | (0.63)(0.37) | (Cu,Fe)(Ti) |
| T2_Al6CuLi3 | CEF (ST3) | (0.57)(0.11) (0.32) | (Al)(Cu)(Li) |
| T2_AlCuMo | CEF (ST3) | (7.7)(2.3)(1) | (Al)(Cu)(Mo) |
| T2_CoMnSi | CEF (ST3) | (0.2456)(0.5088) (0.2456) | (Co)(Mn)(Si) |
| T2_CuFeTi | CEF (SLN) | (0.55)(0.45) | (Cu,Fe)(Ti) |
| T3_AlFeSi | CEF (ST3) | (0.55)(0.25)(0.2) | (Al)(Fe)(Si) |
| T7_AlFeSi | CEF (SLN) | (0.75)(0.25) | (Al,Si)(Fe) |
| T8_AlFeSi | CEF (SLN) | (0.66667) (0.33333) | (Al,Si)(Fe) |
| TA13Zr | CEF (ST3) | (0.65)(0.1)(0.25) | (Al)(Si)(Zr) |

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| T_AlCoMo | CEF (ST3) | (2.72)(0.28)(1) | (Al)(Co)(Mo) |
| T_AlCuMg | CEF (SLN) | (26)(6)(48)(1) | (Mg)(Al,Mg)(Al,Cu,Mg)(Al) |
| T_AlMgZn | CEF (SLN) | (26)(6)(48)(1) | (Mg)(Al,Mg)(Al,Cu,Mg,Zn)(Al) |
| T_Cu5Li2Mg11 | CEF (ST3) | (0.278)(0.111) (0.611) | (Cu)(Li)(Mg) |
| T_FeNiZn | CEF (SLN) | (1)(5) | (Fe,Ni,Zn)(Zn) |
| Tau10_AlCuZr | CEF (ST3) | (0.241)(0.552) (0.207) | (Al)(Cu)(Zr) |
| Tau1_AlCrSi | CEF (ST3) | (13)(4)(4) | (Al)(Cr)(Si) |
| Tau1_AlCuZr | CEF (ST3) | (0.14)(0.71) (0.15) | (Al)(Cu)(Zr) |
| Tau1_AlFeZr | CEF (SLN) | (12)(1) | (Al,Fe)(Zr) |
| Tau1_AlNiZr | CEF (ST3) | (1)(1)(1) | (Al)(Ni)(Zr) |
| Tau1_AlSiZr | CEF (ST3) | (0.35)(0.39) (0.26) | (Al)(Si)(Zr) |
| Tau1_CoSiZr | CEF (ST3) | (1)(1)(1) | (Co)(Si)(Zr) |
| Tau1_NiSiV | CEF (SLN) | (1)(1)(1) | (Ni,Si)(Si)(V) |
| Tau2_AlCrSi | CEF (ST3) | (9)(3)(1) | (Al)(Cr)(Si) |
| Tau2_AlCuZr | CEF (ST3) | (0.13)(0.14) (0.73) | (Al)(Cu)(Zr) |
| Tau2_AlFeZr | CEF (SLN) | (1)(2)(6) | (Fe)(Al,Zr)(Zr) |
| Tau2_AlNiZr | CEF (ST3) | (1)(2)(1) | (Al)(Ni)(Zr) |
| Tau2_AlSiZr | CEF (ST3) | (0.65)(0.1)(0.25) | (Al)(Si)(Zr) |
| Tau2_Co5Si3Zr | CEF (ST3) | (5)(3)(1) | (Co)(Si)(Zr) |
| Tau2_NiSiV | CEF (SLN) | (2)(1)(3) | (Ni)(Ni,Si)(Ni,V) |
| Tau3_AlCrSi | CEF (SLN) | (11)(4) | (Al,Si)(Cr) |
| Tau3_AlCuZr | CEF (ST3) | (0.21)(0.28) (0.51) | (Al)(Cu)(Zr) |
| Tau3_AlFeZr | CEF (ST3) | (7)(67)(26) | (Fe)(Al)(Zr) |
| Tau3_AlNiZr | CEF (ST3) | (1)(4)(5) | (Al)(Ni)(Zr) |
| Tau3_CoSi2Zr | CEF (ST3) | (1)(2)(1) | (Co)(Si)(Zr) |
| Tau3_NiSiV | CEF (ST3) | (12)(5)(3) | (Ni)(Si)(V) |

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| Tau4_AlCrSi | CEF (ST3) | (0.58)(0.315) (0.105) | (Al)(Cr)(Si) |
| Tau4_AlCuZr | CEF (ST3) | (0.25)(0.5)(0.25) | (Al)(Cu)(Zr) |
| Tau4_AlNiZr | CEF (ST3) | (2)(1)(6) | (Al)(Ni)(Zr) |
| Tau4_CoSi2Zr2 | CEF (ST3) | (1)(2)(2) | (Co)(Si)(Zr) |
| Tau4_NiSiV | CEF (SLN) | (11)(3)(6) | (Ni)(Si)(Ni,V) |
| Tau5_AlNiZr | CEF (SLN) | (15)(8)(6) | (Al)(Al,Ni)(Zr) |
| Tau5_Co2Si2Zr | CEF (ST3) | (2)(2)(1) | (Co)(Si)(Zr) |
| Tau5_NiSiV | CEF (ST3) | (5)(3)(4) | (Ni)(Si)(V) |
| Tau6_AlCuZr | CEF (ST3) | (0.375)(0.5) (0.125) | (Al)(Cu)(Zr) |
| Tau6_AlNiZr | CEF (ST3) | (5)(2)(1) | (Al)(Ni)(Zr) |
| Tau6_Co7Si9Zr4 | CEF (ST3) | (7)(9)(4) | (Co)(Si)(Zr) |
| Tau6_NiSiV | CEF (ST3) | (36)(23)(41) | (Ni)(Si)(V) |
| Tau7_AlCuZr | CEF (SLN) | (0.5)(0.423) (0.077) | (Al,Cu)(Cu)(Zr) |
| Tau7_CoSi10Zr9 | CEF (ST3) | (1)(10)(9) | (Co)(Si)(Zr) |
| Tau8_AlCuZr | CEF (ST3) | (0.625)(0.125) (0.25) | (Al)(Cu)(Zr) |
| Tau9_AlCuZr | CEF (ST3) | (0.672)(0.157) (0.171) | (Al)(Cu)(Zr) |
| Tau_AlSiV | CEF (ST3) | (0.6)(1.4)(1) | (Al)(Si)(V) |
| Tb_Al7Cu4Li | CEF (ST3) | (0.6)(0.32)(0.08) | (Al)(Cu)(Li) |
| Ti10O19 | CEF (ST2) | (10)(19) | (Ti)(O) |
| Ti20O39 | CEF (ST2) | (20)(39) | (Ti)(O) |
| Ti2Zn | CEF (ST2) | (2)(1) | (Ti)(Zn) |
| Ti3B4 | CEF (ST2) | (3)(4) | (Ti)(B) |
| Ti3O2 | CEF (ST2) | (3)(2) | (Ti)(O) |
| Ti3O5 | CEF (ST2) | (3)(5) | (Ti)(O) |
| Ti3Zn22 | CEF (ST2) | (3)(22) | (Ti)(Zn) |
| Ti4O7 | CEF (ST2) | (4)(7) | (Ti)(O) |
| Ti5O9 | CEF (ST2) | (5)(9) | (Ti)(O) |

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| Ti6O11 | CEF (ST2) | (6)(11) | (Ti)(O) |
| Ti7O13 | CEF (ST2) | (7)(13) | (Ti)(O) |
| Ti8O15 | CEF (ST2) | (8)(15) | (Ti)(O) |
| Ti9O17 | CEF (ST2) | (9)(17) | (Ti)(O) |
| TiAlSi_Tau1 | CEF (SLN) | (8)(16) | (Al,Ti)(Al,Si) |
| TiAlSi_Tau2 | CEF (SLN) | (1)(2) | (Ti)(Al,Si) |
| TiOx | CEF (SLN) | (1)(1)(1) | (Ti+2,Ti+3,Va)(Ti,Va)(O-2) |
| TiZn | CEF (ST2) | (1)(1) | (Ti)(Zn) |
| TiZn16 | CEF (ST2) | (1)(16) | (Ti)(Zn) |
| TiZn2 | CEF (ST2) | (1)(2) | (Ti)(Zn) |
| TiZn3 | CEF (ST2) | (1)(3) | (Ti)(Zn) |
| Tridymite | CEF (ST2) | (1)(2) | (Si)(O) |
| V | CEF (ST3) | (0.38461) (0.15385) (0.46154) | (Al)(Mg)(Cu) |
| V2B3 | CEF (ST2) | (2)(3) | (V)(B) |
| V2O5 | CEF (ST2) | (2)(5) | (V)(O) |
| V2O_SS | CEF (SLN) | (1)(0.5) | (V)(O,Va) |
| 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) |
| 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) |

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| 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) |
| W_CoMnSi | CEF (ST3) | (0.3333)(0.3333) (0.3333) | (Co)(Mn)(Si) |
| X_Co52Co20V28 | CEF (ST3) | (0.52)(0.2)(0.28) | (Co)(Si)(V) |
| X_CoMnSi | CEF (ST3) | (0.4)(0.4459) (0.1541) | (Co)(Mn)(Si) |
| 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_1 | 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) |
| 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) |
| m_Ni4B3 | CEF (ST2) | (0.564)(0.436) | (Ni)(B) |
| o_Ni4B3 | CEF (ST2) | (0.586)(0.414) | (Ni)(B) |