

# TCS High Entropy Alloys Database (TCHEA9)

## Technical Information

*Available Starting with Thermo-Calc Version 2026b*



---

# Contents

---

<b>About the TCS High Entropy Alloys Database (TCHEA)</b> .....	<b>4</b>
<i>Interconnectivity with Other Products</i> .....	4
<i>Use Case Examples</i> .....	5
<i>Combining Databases</i> .....	5
<i>Release History</i> .....	5
<i>References</i> .....	5
<i>Suggested References to Cite this Database</i> .....	6
<b>TCS High Entropy Alloys Database (TCHEA) Resources</b> .....	<b>7</b>
<i>About the CALPHAD Method</i> .....	7
<i>Learn More</i> .....	8
<b>TCHEA9 Elements, Systems, and Phases</b> .....	<b>9</b>
<i>Included Elements</i> .....	9
<i>Assessed Systems and Phases</i> .....	9
<i>About the Included Phases</i> .....	9
<b>TCHEA9 Properties Data</b> .....	<b>11</b>
<i>TCHEA9 Thermophysical Properties</i> .....	12
<i>TCHEA9 Elastic Properties</i> .....	14
<b>TCHEA9 Systems</b> .....	<b>16</b>
<i>TCHEA9 Assessed Binary Systems</i> .....	17
<i>TCHEA9 Critically Assessed Ternary Systems</i> .....	18
<i>TCHEA9 Tentatively Assessed Ternary Systems</i> .....	20
<i>TCHEA9 Assessed Quaternary and Higher Order Systems</i> .....	23
<b>TCHEA9 Phases</b> .....	<b>24</b>
<i>TCHEA9 Models for the Included Phases</i> .....	25
<b>TCHEA9: Current Version Changes</b> .....	<b>71</b>

---

<i>TCHEA8.1 to TCHEA9.0</i> .....	71
<b>TCHEA: Revision History</b> .....	<b>73</b>
<i>TCHEA8.0 to TCHEA8.1</i> .....	73
<i>TCHEA7.0 to TCHEA8.0</i> .....	73
<i>TCHEA6.1 to TCHEA7.0</i> .....	74
<i>TCHEA6.0 to TCHEA6.1</i> .....	75
<i>TCHEA5.1 to TCHEA6.0</i> .....	75
<i>TCHEA5.0 to TCHEA5.1</i> .....	76
<i>TCHEA4.2 to TCHEA5.0</i> .....	76
<i>TCHEA4.1 to TCHEA4.2</i> .....	76
<i>TCHEA4.0 to TCHEA4.1</i> .....	76
<i>TCHEA3.1 to TCHEA4.0</i> .....	77
<i>TCHEA3.0 to TCHEA3.1</i> .....	77
<i>TCHEA2.0 to TCHEA3.0</i> .....	77
<i>TCHEA2.0 to TCHEA2.1</i> .....	77
<i>TCHEA1.0 to TCHEA2.0</i> .....	78

## About the TCS High Entropy Alloys Database (TCHEA)

---

TCS High Entropy Alloys Database (TCHEA) is a thermodynamic database for high entropy alloys (HEA) [2004Yeh; 2006Yeh]. HEAs are a new class of materials consisting of more than one principal element in a multi-component system. They are also known as multi-principal element alloys (MPEAs) [2013Wan; 2015Sen] or complex concentrated alloys (CCAs). The coupling of our CALPHAD based computational tools and databases allows a high fidelity calculation of thermodynamic properties and phase equilibria in multi-component HEAs, thus shedding light on the formation mechanism and thermodynamic and kinetic stability of HEAs, providing an efficient way to design HEAs for desired materials properties based on the prediction of microstructures through process optimization.

In addition to thermodynamic data, the database has thermophysical and elastic properties data available for:

- Molar volume with thermal expansion coefficients
- Viscosity of the metallic liquids
- Surface tension of liquid metallic alloys
- Electrical resistivity
- Thermal conductivity
- Elastic moduli and elastic constants



[TCHEA9 Thermophysical Properties](#) and [TCHEA9 Elastic Properties](#)

### Interconnectivity with Other Products

The database can be used with other products: Thermo-Calc, the Add-on Diffusion Module (DICTRA), Precipitation Module (TC-PRISMA), and/or Additive Manufacturing (AM) Module, and all available SDKs.

The thermodynamic database is compatible with the corresponding TCS High Entropy Alloy Mobility Database (MOBHEA) that provides kinetic data for those working with the add-on kinetic modules – the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA) – as well as a few specific calculation types, such as Scheil with back diffusion. The current version of the mobility database is MOBHEA4.

---

## Use Case Examples

There are examples available to both demonstrate the *validation* of the database and to showcase the types of *calculations* that can be used for different materials or application area.

Some case examples of how the TCHEA9 database can be used include:

- Calculate various phase diagrams and property diagrams in the assessed systems and higher-order systems.
- Predict solidification behavior of HEAs with a Scheil-Gulliver calculation.
- Predict a wide variety of equilibrium properties such as phase amount and constitution as a function of composition or temperature, homogeneity range, or thermo-stability of HEAs.
- Study the oxidation behaviors of HEAs at various temperatures and compositions.
- Use the Add-on Diffusion Module (DICTRA) and combine it with TCHEA and compatible kinetic databases to simulate typical diffusion-controlled phase transformations in HEAs under arbitrary heat treatment conditions.
- Use the Precipitation Module (TC-PRISMA) and combine it with TCHEA and compatible kinetic databases, to simulate the concurrent nucleation, growth and coarsening of precipitates.

## Combining Databases

It is possible to combine several databases to make calculations using Thermo-Calc. For more information related to a specific type of problem, contact one of our support specialists at [info@thermocalc.com](mailto:info@thermocalc.com). The experts are available to make recommendations on the most suitable database to use for your needs.

## Release History

- The current version of the database is TCHEA9. To review the most recent changes, see [TCHEA9: Current Version Changes](#).
- To review additional older changes, see [TCHEA: Revision History](#).

## References

[2004Can] B. Cantor, I.T.H. Chang, P. Knight, A.J.B. Vincent, Microstructural development in equiatomic multicomponent alloys. Mater. Sci. Eng. A 375–377 (2004) 213–218.

---

- [2004Yeh] J. W. Yeh, S. K. Chen, S. K. Lin, J. Y. Gan, T. S. Chin, T. T. Shun, C. H. Tsau, S. Y. Chang, Nanostructured High-Entropy Alloys with Multiple Principal Elements: Novel Alloy Design Concepts and Outcomes. *Adv. Eng. Mater.* 6, 299–303 (2004).
- [2006Yeh] J.-W. Yeh, Recent progress in high-entropy alloys. *Ann. Chim. Sci. des Matériaux.* 31, 633–648 (2006).
- [2013Wan] S. Wang, Atomic Structure Modeling of Multi-Principal-Element Alloys by the Principle of Maximum Entropy. *Entropy.* 15, 5536–5548 (2013).
- [2015Sen] O. N. Senkov, J. D. Miller, D. B. Miracle, C. Woodward, Accelerated exploration of multi-principal element alloys with solid solution phases. *Nat. Commun.* 6, 6529 (2015).
- [2017Mir] D.B. Miracle, O.N. Senkov, A critical review of high entropy alloys and related concepts, *Acta Mater.* 122 (2017) 448–511.

## **| Suggested References to Cite this Database**

- [2017Mao] H. Mao, H.-L. Chen, Q. Chen, TCHEA1: A Thermodynamic Database Not Limited for “High Entropy” Alloys. *J. Phase Equilibria Diffus.* 38 (2017) 353–368.
- [2018Chen] H.-L. Chen, H. Mao, Q. Chen, Database development and Calphad calculations for high entropy alloys: Challenges, strategies, and tips. *Mater. Chem. Phys.* 210 (2018) 279-290.
-

## TCS High Entropy Alloys Database (TCHEA) Resources

---

Database technical content and examples are available in different formats (html help files or PDFs).

Go to these locations to access the same content:

- **Locally Installed Help:** When in Thermo-Calc, press F1 to open the current version of the help in a local browser. You can also click **Online Help** from the **My Project** page to open the file. Then search or navigate to the **Databases** folder to browse the contents.
- **Web Help:** Go to the [Documentation](#) page to link to the most recent version of the web help. Then search or navigate to the **Databases** folder to browse the contents.
- **Website resources:** The individual database technical information and examples are also available in PDF format from the website. Download the *current version* of the PDFs for each database.

### About the CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of all the binary systems and many ternary systems. A hybrid approach of experiments, first-principles calculations and CALPHAD modeling has been used to obtain reliable thermodynamic descriptions of the BCC, FCC and HCP solutions. That enables predictions to be made for multicomponent alloy systems, especially for HEAs.

The extrapolation to higher-order systems helps to understand the phase equilibria in HEAs, so as to predict the phase formation, phase fractions and phase compositions or to calculate the driving force of forming a phase. All necessary molar volume data and thermal expansion data are assessed or estimated for most of the phases.



Learn more on our website about the [CALPHAD Method](#) and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our [website](#) or our [YouTube playlist](#).

## Learn More



Go to the [High Entropy Alloys Databases](#) page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information* plus learn more about the compatible kinetic database. Also explore further [applications of Thermo-Calc to high entropy alloys](#) and the [Refractory Alloys](#) page on our website, that includes links to resources such as examples, publications, and more.



Read more on our website about applications for [Sustainability](#). The webpage highlights several examples demonstrating how Thermo-Calc has been applied to address key sustainability challenges.



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

## TCHEA9 Elements, Systems, and Phases

This section summarizes the available elements, assessed systems, and total number of phases in the TCS High Entropy Alloys Database (TCHEA).

### Included Elements

The database is developed in a 27 element framework:

Elements									
Al	B	C	Co	Cr	Cu	Fe	Hf	Ir	Mn
Mo	N	Nb	Ni	O	Re	Rh	Ru	Si	Sn
Ta	Ti	V	W	Y	Zn	Zr			

### Assessed Systems and Phases

The most recent version of the database contains:

- 342 binary systems, with almost all of these assessed to the full range of composition and temperature. These can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 729 ternary systems are assessed, with 227 of them to the full range of composition and temperature. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 54 quaternary systems and 3 higher order systems are assessed.
- 730 solution and intermetallic phases, where nearly all stable phases in all assessed binary systems and most ternary systems are modeled.

### About the Included Phases

The ordered B2 and L1<sub>2</sub> phases, together with BCC\_A2 and FCC\_A1, respectively, are modeled with the so-called partitioning model, which describes an ordered phase and its disordered counterpart using a single Gibbs energy curve. This type of description is of particular importance to be able to predict second order transformations between a disordered phase and its ordered structures.

Also note that there may be several possible composition sets for the phases named FCC\_L12 and BCC\_B2 designated by #1, #2, and so on (e.g. FCC\_L12#1 and FCC\_L12#2), due to the co-existence of disordered and ordered structures or the presence of miscibility gap. The #n suffix (where n is an integer) is generated dynamically by Thermo-Calc when using global minimization and therefore the identification of the phases should be determined from their site occupations. It can be found by LIST\_EQUILIBRIUM with the VXNS option in the Console Mode or showing the site fraction in moles of the constituent elements in the Graphical Mode. When the site occupancies of the first and second sublattices are equal the phase is disordered.



In Console Mode, you can list phases and constituents in the Database (TDB) module and the Gibbs (GES) module. For some phases, supplementary information is included in the definitions. To show the information, it is recommended in the Database (TDB) module to use the command LIST\_SYSTEM with the option `Constituents`.



[TCHEA9 Models for the Included Phases](#)

# TCHEA9 Properties Data

In this section:

- TCHEA9 Thermophysical Properties ..... 12
- TCHEA9 Elastic Properties ..... 14

## TCHEA9 Thermophysical Properties

This section summarizes the thermophysical properties available in the TCS High Entropy Alloys Database (TCHEA).

### Thermophysical Properties Parameters and Variables

Below is a summary of the available thermophysical parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode (CM) versus Graphical Mode (GM) as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property (Variable Name GM)	Model Parameters	Variables to Show or Plot in CM or the SDKs
Molar volume	V0, VA	VM for a system $VM(PHI)$ for phase PHI
Electrical conductivity	ELQ**	ELCD for a system $ELCD(PHI)$ for phase PHI
Electrical resistivity	ELRS, ESPD	ELRS for a system $ELRS(PHI)$ for a phase PHI
Thermal conductivity	THCD	THCD for a system $THCD(PHI)$ for phase PHI
Thermal resistivity		THRS for a system $THRS(PHI)$ for phase PHI
Thermal diffusivity		THDF for a system $THDF(PHI)$ for phase PHI
Surface tension	SIGM, XI*	SURF (LIQUID) SURF (ION) **
Dynamic viscosity	VISC	DVIS (LIQUID) DVIS (ION) **
Kinematic viscosity		KVIS (LIQUID) KVIS (ION) **



\* XI is not used in the TCOX database (all versions). As of 2023b it is also not used starting with the following versions of these databases: TCFE13, TCNI12.1, TCTI5.1, TCNOBL3, TCPMAG2, and TCCU6. As of 2024a, TCMG7, TCAL9, and TCHEA7. As of 2024b, TCSLD5. \*\* ION is used in the TCS Metal Oxide Solutions Database (TCOX)



The examples listed for the SDKs (TC-Python and TC-Toolbox for MATLAB) are using CM syntax. The quantities can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. See the various model descriptions or the SDK help for details.

## Examples

In Thermo-Calc, press F1 and search or navigate to the relevant database to discover the Validation and Calculation Examples Collection, which is also available in PDF format on our website.



Go to the [High Entropy Alloys Databases](#) page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information* plus learn more about the compatible kinetic database. Also explore further [applications of Thermo-Calc to high entropy alloys](#) and the [Refractory Alloys](#) page on our website, that includes links to resources such as examples, publications, and more.

## Learn More



The thermophysical properties data for molar volume, viscosity, surface tension, electrical resistivity, and thermal conductivity are included with the database. Molar volume is available starting with version 1 (TCHEA1), viscosity is available starting with version 4 (TCHEA4), and surface tension, electrical resistivity, and thermal conductivity are available starting with version 5 (TCHEA5).



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

## TCHEA9 Elastic Properties

---

This section summarizes the elastic properties in the TCS High Entropy Alloys Database (TCHEA).

### Elastic Properties Parameters and Variables



Elastic properties are only available for cubic BCC (A2 and B2), cubic FCC (A1 and L12), and hexagonal HCP (A3) phases.

#### Graphical Mode

In the **Plot Renderer** in Graphical Mode, elastic constants and moduli can be selected from the drop-down list of axis variables.

The independent elastic constants are selected on the **Plot Renderer** as an axis variable **Elastic constant** and then choose an option (**C11**, **C12**, **C13**, **C33**, or **C44**) from the drop-down list.

The elastic moduli, **Bulk modulus**, **Shear modulus**, and **Young's modulus**, are directly available from the **Axis variable** list.

All can be tabulated and plotted using the quantity names, with options for a specific phase or all phases.

#### Console Mode

The quantities corresponding to the individual elastic constants and elastic moduli (derived from the elastic constants) can be calculated in Console Mode for individual phases or all phases. The results can be shown in the POLY module with the command `SHOW_VALUE` or shown as a plot in the POST module with the command `PLOT_DIAGRAM` using:

- `Cij(<phase name>)` or `Cij(*)`
- **Bulk modulus:** `BULKMOD(<phase name>)` or `BULKMOD(*)`
- **Shear modulus:** `SHEARMOD(<phase name>)` or `SHEARMOD(*)`
- **Young's modulus:** `YOUNGMOD(<phase name>)` or `YOUNGMOD(*)`

#### TC-Python and TC-Toolbox for MATLAB®

For the Software Development Kits (SDKs), i.e. TC-Python and TC-Toolbox, the quantities of elastic constants, bulk modulus, shear modulus, and Young's modulus can be retrieved for individual phases or all phases via `get_value_of()` or `get_values_of()` from any equilibrium calculation types using:

- `Cij (<phase name>)` **OR** `Cij (ALL_PHASES/*)`
- `ThermodynamicQuantity.bulk_modulus (<phase name>)` **OR** `ThermodynamicQuantity.bulk_modulus (ALL_PHASES/*)`
- `ThermodynamicQuantity.shear_modulus (<phase name>)` **OR** `ThermodynamicQuantity.shear_modulus (ALL_PHASES/*)`
- `ThermodynamicQuantity.youngs_modulus (<phase name>)` **OR** `ThermodynamicQuantity.youngs_modulus (ALL_PHASES/*)`



See the relevant SDK documentation for details.

## Examples

In Thermo-Calc, press F1 and search or navigate to the relevant database to discover the Validation and Calculation Examples Collection, which is also available in PDF format on our website.



Go to the [High Entropy Alloys Databases](#) page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information* plus learn more about the compatible kinetic database. Also explore further [applications of Thermo-Calc to high entropy alloys](#) and the [Refractory Alloys](#) page on our website, that includes links to resources such as examples, publications, and more.

## Learn More



The elastic properties (elastic moduli and elastic constants) are included with the database as of TCHEA8 and are only available for cubic BCC (A2 and B2), cubic FCC (A1 and L12), and hexagonal HCP (A3) phases.



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

## TCHEA9 Systems

In this section:

<b>TCHEA9 Assessed Binary Systems .....</b>	<b>17</b>
<b>TCHEA9 Critically Assessed Ternary Systems .....</b>	<b>18</b>
<b>TCHEA9 Tentatively Assessed Ternary Systems .....</b>	<b>20</b>
<b>TCHEA9 Assessed Quaternary and Higher Order Systems .....</b>	<b>23</b>

---



## TCHEA9 Critically Assessed Ternary Systems

These are the 227 critically assessed ternary systems in the full range of composition and temperature.

<i>Critically Assessed Ternary Systems</i>							
Al-B-Ti	Al-C-Co	Al-C-Fe	Al-Co-Fe	Al-Co-Mn	Al-Co-Ni	Al-Co-Ti	Al-Co-W
Al-Co-Zr	Al-Cr-Ni	Al-Cr-Sn	Al-Cr-Ti	Al-Cr-V	Al-C-Ti	Al-Cu-Fe	Al-Cu-Mn
Al-Cu-Ni	Al-Cu-Si	Al-Cu-Sn	Al-Cu-Zn	Al-Fe-Mn	Al-Fe-N	Al-Fe-Ni	Al-Fe-Si
Al-Fe-Ti	Al-Hf-Ni	Al-Mn-Ni	Al-Mn-Si	Al-Mn-Ti	Al-Mn-Zn	Al-Mo-Ni	Al-Mo-Ti
Al-Nb-Ni	Al-Nb-Ti	Al-Ni-Ru	Al-Ni-Si	Al-Ni-Ta	Al-Ni-Ti	Al-Ni-W	Al-Ni-Zn
Al-N-Ti	Al-Ru-Ti	Al-Si-Sn	Al-Si-Ti	Al-Si-Zn	Al-Sn-Ti	Al-Sn-Zn	Al-Ta-Ti
Al-Ti-V	Al-Ti-W	Al-Ti-Y	Al-Ti-Zr	Al-V-Zr	C-Co-Cr	C-Co-Fe	C-Co-Mo
C-Co-Nb	C-Co-Ni	C-Co-Ta	C-Co-Ti	C-Co-W	C-Cr-Fe	C-Cr-Hf	C-Cr-Si
C-Cr-Ti	C-Cr-V	C-Cr-Zr	C-Cu-Fe	C-Fe-Mn	C-Fe-Mo	C-Fe-N	C-Fe-Ni
C-Fe-Si	C-Fe-Ti	C-Fe-V	C-Fe-W	C-Hf-Mo	C-Hf-Ni	C-Mn-Si	C-Mo-Ni
C-Mo-Ta	C-Mo-Ti	C-Mo-V	C-Mo-W	C-Mo-Zr	C-Nb-Ni	C-Nb-Re	C-Nb-Ti
C-Nb-W	C-Ni-Ta	C-Ni-Ti	C-Ni-W	C-Ni-Zr	Co-Cr-Cu	Co-Cr-Fe	Co-Cr-Mn
Co-Cr-Ni	Co-Cr-Ti	Co-Cr-W	Co-Cu-Fe	Co-Cu-Mn	Co-Cu-Nb	Co-Cu-Ni	Co-Cu-Si
Co-Fe-Mn	Co-Fe-Mo	Co-Fe-N	Co-Fe-Ni	Co-Fe-W	Co-Mn-Ni	Co-Mo-Ti	Co-Ni-Si
Co-Ni-V	Co-Ni-W	Co-Sn-Ti	Co-Ta-Ti	Co-W-Zr	Cr-Cu-Fe	Cr-Cu-Mo	Cr-Cu-Nb
Cr-Cu-Si	Cr-Cu-Sn	Cr-Cu-Zr	Cr-Fe-Mn	Cr-Fe-Mo	Cr-Fe-N	Cr-Fe-Ni	Cr-Fe-O
Cr-Fe-Si	Cr-Fe-Ti	Cr-Fe-V	Cr-Mn-N	Cr-Mn-Ni	Cr-Mn-Ti	Cr-Mo-Nb	Cr-Mo-Ni
Cr-Mo-Ti	Cr-Nb-Ni	Cr-Nb-Ti	Cr-Nb-V	Cr-Nb-W	Cr-Ni-O	Cr-Ni-Re	Cr-Ni-Si
Cr-Ni-Ta	Cr-Ni-Ti	Cr-Ni-W	Cr-Ni-Zr	Cr-N-Ni	Cr-Si-Ti	Cr-Ti-Zr	C-Ta-W
C-Ti-W	Cu-Fe-Mn	Cu-Fe-Mo	Cu-Fe-N	Cu-Fe-Nb	Cu-Fe-Ni	Cu-Fe-Si	Cu-Fe-Sn

*Critically Assessed Ternary Systems*

Cu-Fe-Ti	Cu-Fe-V	Cu-Mn-Ni	Cu-Mn-Si	Cu-Mn-Sn	Cu-Mn-Zn	Cu-Mo-Ni	Cu-Ni-Sn
Cu-Ni-Ti	Cu-Ni-Zn	Cu-Ti-Zr	Fe-Mn-N	Fe-Mn-Si	Fe-Mn-Ti	Fe-Mo-Ni	Fe-Nb-Ni
Fe-Ni-O	Fe-Ni-Ru	Fe-Ni-Si	Fe-Ni-Ti	Fe-Ni-W	Fe-N-Nb	Fe-N-Ni	Fe-N-Ti
Fe-N-V	Fe-Ti-V	Hf-Nb-Si	Hf-Ni-Ti	Ir-Rh-Ru	Mn-Ni-Si	Mn-Si-Zn	Mo-Nb-Ti
Mo-Nb-V	Mo-Ni-Ta	Mo-N-Ni	Mo-Ta-Ti	Mo-Ti-V	Mo-Ti-W	Mo-Ti-Zr	Nb-Ni-Ti
Nb-Ni-W	Nb-Re-V	Nb-Sn-Ti	Nb-Ta-Ti	Nb-Ti-V	Nb-Ti-W	Nb-Ti-Zr	Nb-V-Zr
Ni-Si-Ta	Ni-Si-Ti	Ni-Sn-Ti	Ni-Sn-Zr	Ni-Ta-Ti	Ni-Ta-W	Ni-Ti-W	Ni-Ti-Zr
N-Ni-Ti	Re-Ta-W	Re-V-W	Si-Ti-W	Ta-Ti-V	Ta-Ti-W	Ta-Ti-Zr	Ti-V-W
Ti-V-Zr	Ti-W-Zr	V-W-Zr					

## TCHEA9 Tentatively Assessed Ternary Systems

These are the 502 tentatively assessed ternary systems.

<i>Tentatively Assessed Ternary Systems</i>							
Al-B-O	Al-C-Cr	Al-C-Ni	Al-Co-Cr	Al-Co-Cu	Al-Co-Hf	Al-Co-Mo	Al-Co-Nb
Al-Co-O	Al-Co-Ru	Al-Co-Si	Al-Co-Sn	Al-Co-Ta	Al-Co-V	Al-Cr-Fe	Al-Cr-Mo
Al-Cr-Nb	Al-Cr-O	Al-Cr-Re	Al-Cr-Ru	Al-Cr-Si	Al-Cr-Ta	Al-Cr-W	Al-Cr-Zr
Al-C-Si	Al-Cu-O	Al-Fe-Hf	Al-Fe-Mo	Al-Fe-Nb	Al-Fe-O	Al-Fe-Re	Al-Fe-Sn
Al-Fe-Ta	Al-Fe-V	Al-Fe-W	Al-Fe-Zr	Al-Hf-O	Al-Hf-Ru	Al-Hf-Si	Al-Hf-Ti
Al-Mn-O	Al-Mo-Nb	Al-Mo-O	Al-Mo-Re	Al-Mo-Ru	Al-Mo-Si	Al-Mo-Ta	Al-Mo-W
Al-Mo-Zr	Al-Nb-O	Al-Nb-Re	Al-Nb-Ru	Al-Nb-Si	Al-Nb-Ta	Al-Nb-W	Al-Ni-O
Al-Ni-Re	Al-Ni-Sn	Al-Ni-V	Al-Ni-Zr	Al-O-Si	Al-O-Ti	Al-O-V	Al-O-W
Al-O-Y	Al-O-Zr	Al-Re-Ru	Al-Re-Ta	Al-Re-Ti	Al-Re-W	Al-Ru-Ta	Al-Ru-W
Al-Ru-Zr	Al-Si-Zr	Al-Ta-W	B-Co-O	B-Cu-O	B-Fe-O	B-Mn-O	B-Nb-O
B-Ni-O	B-O-Si	B-O-Ti	B-O-V	B-O-W	B-O-Y	B-O-Zr	C-Co-Re
C-Co-V	C-Cr-Mn	C-Cr-Mo	C-Cr-N	C-Cr-Nb	C-Cr-Ni	C-Cr-O	C-Cr-Re
C-Cr-Ta	C-Cr-W	C-Fe-Nb	C-Fe-O	C-Fe-Re	C-Fe-Ta	C-Hf-Nb	C-Hf-Ta
C-Hf-Ti	C-Hf-V	C-Hf-W	C-Mn-V	C-Mo-N	C-Mo-Re	C-Mo-Si	C-Nb-Ta
C-Nb-V	C-Nb-Zr	C-Ni-O	C-Ni-V	C-N-Nb	C-N-Ti	Co-Cr-Hf	Co-Cr-Mo
Co-Cr-Nb	Co-Cr-O	Co-Cr-Re	Co-Cr-Ru	Co-Cr-Si	Co-Cr-Ta	Co-Cr-V	Co-Cu-Hf
Co-Cu-O	Co-Cu-Ta	Co-Cu-Ti	Co-Cu-V	Co-Cu-Zr	Co-Fe-Hf	Co-Fe-Nb	Co-Fe-O
Co-Fe-Si	Co-Fe-Ta	Co-Fe-Ti	Co-Fe-V	Co-Fe-Zr	Co-Hf-Mn	Co-Hf-Mo	Co-Hf-Nb
Co-Hf-Ni	Co-Hf-Si	Co-Hf-Sn	Co-Hf-Ta	Co-Hf-Ti	Co-Hf-V	Co-Hf-Zr	Co-Mn-Nb
Co-Mn-O	Co-Mn-Si	Co-Mn-Sn	Co-Mn-Ta	Co-Mn-Ti	Co-Mn-Zr	Co-Mo-Nb	Co-Mo-Ni

**Tentatively Assessed Ternary Systems**

Co-Mo-Re	Co-Mo-Ru	Co-Mo-Si	Co-Mo-Ta	Co-Mo-V	Co-Mo-W	Co-Nb-Ni	Co-Nb-O
Co-Nb-Si	Co-Nb-Sn	Co-Nb-Ta	Co-Nb-Ti	Co-Nb-W	Co-Nb-Zr	Co-Ni-O	Co-Ni-Re
Co-Ni-Ru	Co-Ni-Sn	Co-Ni-Ta	Co-Ni-Ti	Co-Ni-Zr	Co-O-Si	Co-O-Ti	Co-O-V
Co-O-W	Co-O-Y	Co-O-Zr	Co-Re-Ta	Co-Re-Ti	Co-Re-V	Co-Re-W	Co-Ru-Ta
Co-Ru-W	Co-Si-Sn	Co-Si-Ta	Co-Si-Ti	Co-Si-V	Co-Si-W	Co-Si-Zr	Co-Sn-Ta
Co-Sn-V	Co-Sn-Zr	Co-Ta-V	Co-Ta-W	Co-Ta-Zr	C-O-Ti	Co-Ti-V	Co-Ti-W
Co-Ti-Zr	C-O-V	Co-V-Zr	C-O-Zr	Cr-Cu-Ni	Cr-Cu-O	C-Re-Ta	C-Re-V
C-Re-W	Cr-Fe-Hf	Cr-Fe-Nb	Cr-Fe-Re	Cr-Fe-Ta	Cr-Fe-W	Cr-Fe-Zr	Cr-Hf-Mo
Cr-Hf-Nb	Cr-Hf-Ni	Cr-Hf-Re	Cr-Hf-Si	Cr-Hf-Ta	Cr-Hf-W	Cr-Mn-O	Cr-Mo-N
Cr-Mo-Re	Cr-Mo-Ru	Cr-Mo-Si	Cr-Mo-Ta	Cr-Mo-W	Cr-Mo-Zr	Cr-Nb-O	Cr-Nb-Re
Cr-Nb-Si	Cr-Nb-Ta	Cr-Nb-Zr	Cr-Ni-Ru	Cr-Ni-Sn	Cr-Ni-V	Cr-N-Nb	Cr-N-V
Cr-O-Si	Cr-O-Ta	Cr-O-Ti	Cr-O-V	Cr-O-Y	Cr-O-Zr	Cr-Re-Ru	Cr-Re-Ta
Cr-Re-Ti	Cr-Re-V	Cr-Re-W	Cr-Re-Zr	Cr-Ru-Ta	Cr-Ru-Ti	Cr-Ru-W	Cr-Si-Ta
Cr-Si-W	Cr-Si-Zr	Cr-Ta-Ti	Cr-Ta-W	Cr-Ta-Zr	Cr-Ti-V	Cr-Ti-W	Cr-W-Zr
C-Si-Ti	C-Ta-Ti	C-Ta-V	C-Ta-Zr	C-Ti-V	C-Ti-Zr	Cu-Fe-Hf	Cu-Fe-O
Cu-Fe-Ta	Cu-Hf-Ni	Cu-Mn-O	Cu-Mo-O	Cu-Nb-Ni	Cu-Nb-O	Cu-Ni-O	Cu-Ni-Si
Cu-Ni-Ta	Cu-Ni-V	Cu-Ni-Zr	Cu-O-Si	Cu-O-Ti	Cu-O-Y	C-V-W	C-V-Zr
C-W-Zr	Fe-Hf-Mn	Fe-Hf-Mo	Fe-Hf-Nb	Fe-Hf-Ni	Fe-Hf-Re	Fe-Hf-Si	Fe-Hf-Sn
Fe-Hf-Ta	Fe-Hf-Ti	Fe-Hf-V	Fe-Hf-W	Fe-Hf-Zr	Fe-Mn-Nb	Fe-Mn-Ni	Fe-Mn-O
Fe-Mn-Ta	Fe-Mn-V	Fe-Mo-N	Fe-Mo-Nb	Fe-Mo-O	Fe-Mo-Re	Fe-Mo-Si	Fe-Mo-Ta
Fe-Mo-Ti	Fe-Mo-V	Fe-Mo-W	Fe-Mo-Zr	Fe-Nb-O	Fe-Nb-Re	Fe-Nb-Si	Fe-Nb-Sn
Fe-Nb-Ta	Fe-Nb-Ti	Fe-Nb-V	Fe-Nb-W	Fe-Nb-Zr	Fe-Ni-Sn	Fe-Ni-Ta	Fe-Ni-V

<i>Tentatively Assessed Ternary Systems</i>							
Fe-Ni-Zr	Fe-O-Si	Fe-O-Ti	Fe-O-V	Fe-O-W	Fe-O-Y	Fe-O-Zr	Fe-Re-Ta
Fe-Re-Ti	Fe-Re-W	Fe-Re-Zr	Fe-Si-Ta	Fe-Si-Ti	Fe-Si-V	Fe-Si-W	Fe-Si-Zr
Fe-Sn-Ta	Fe-Sn-Ti	Fe-Sn-V	Fe-Sn-Zr	Fe-Ta-Ti	Fe-Ta-V	Fe-Ta-W	Fe-Ta-Zr
Fe-Ti-W	Fe-Ti-Zr	Fe-V-Zr	Fe-W-Zr	Hf-Mn-Ni	Hf-Mo-Ni	Hf-Mo-Re	Hf-Mo-Si
Hf-Nb-Ni	Hf-Nb-Re	Hf-Ni-Re	Hf-Ni-Ru	Hf-Ni-Si	Hf-Ni-Sn	Hf-Ni-Ta	Hf-Ni-V
Hf-Ni-W	Hf-Ni-Zr	Hf-O-Si	Hf-O-Ti	Hf-O-W	Hf-O-Y	Hf-O-Zr	Hf-Re-Ta
Hf-Re-W	Hf-Ru-Ti	Hf-Ru-Zr	Hf-Si-Ta	Hf-Si-Ti	Hf-Si-W	Mn-Nb-Ni	Mn-Nb-O
Mn-Ni-O	Mn-Ni-Sn	Mn-Ni-Ta	Mn-Ni-Ti	Mn-Ni-V	Mn-Ni-Zr	Mn-O-Si	Mn-O-Ti
Mn-O-V	Mn-O-W	Mn-O-Y	Mn-O-Zr	Mo-Nb-Ni	Mo-Nb-Re	Mo-Nb-Ta	Mo-Ni-Re
Mo-Ni-Ru	Mo-Ni-Si	Mo-Ni-Ti	Mo-Ni-W	Mo-Ni-Zr	Mo-N-V	Mo-O-Ti	Mo-O-W
Mo-Re-Ru	Mo-Re-Ta	Mo-Re-Ti	Mo-Re-V	Mo-Re-W	Mo-Re-Zr	Mo-Ru-Si	Mo-Ru-Ta
Mo-Ru-W	Mo-Si-Zr	Nb-Ni-O	Nb-Ni-Re	Nb-Ni-Si	Nb-Ni-Sn	Nb-Ni-Ta	Nb-Ni-V
Nb-Ni-Zr	Nb-O-Si	Nb-O-Ti	Nb-O-V	Nb-O-Y	Nb-O-Zr	Nb-Re-Ta	Nb-Re-Ti
Nb-Re-W	Nb-Re-Zr	Nb-Ru-Si	Nb-Si-Ti	Ni-O-Si	Ni-O-Ti	Ni-O-V	Ni-O-W
Ni-O-Y	Ni-O-Zr	Ni-Re-Ta	Ni-Re-Ti	Ni-Re-W	Ni-Re-Zr	Ni-Ru-Ta	Ni-Ru-Ti
Ni-Ru-W	Ni-Ru-Zr	Ni-Si-Sn	Ni-Si-V	Ni-Si-W	Ni-Si-Zr	Ni-Sn-Ta	Ni-Sn-V
Ni-Ta-V	Ni-Ta-Zr	Ni-Ti-V	Ni-V-Zr	Ni-W-Zr	N-Nb-Ti	N-Ti-V	O-Si-Ti
O-Si-V	O-Si-W	O-Si-Y	O-Si-Zr	O-Ta-Ti	O-Ti-V	O-Ti-W	O-Ti-Y
O-Ti-Zr	O-V-Y	O-V-Zr	O-W-Y	O-W-Zr	O-Y-Zr	Re-Ru-Ta	Re-Ru-Ti
Re-Ru-W	Re-Ta-Ti	Re-Ta-V	Re-Ta-Zr	Re-Ti-W	Re-W-Zr	Ru-Si-Ti	Ru-Ta-Ti
Ru-Ta-W	Ru-Ti-Zr	Si-Ta-Zr	Si-Ti-Zr	Si-W-Zr	Ta-W-Zr		

## TCHEA9 Assessed Quaternary and Higher Order Systems

These are the assessed quaternary systems (54 total) and higher order systems (3 total).

### Quaternary Systems

#### Critically Assessed Quaternary Systems

Al-B-O-Si	Al-Co-O-Si	Al-Co-O-Ti	Al-Cr-Fe-O	Al-Cr-O-Si
Al-Cr-O-Ti	Al-Cr-O-Y	Al-Cu-O-Si	Al-Fe-Mn-O	Al-Fe-O-Si
Al-Fe-O-Ti	Al-Fe-O-Y	Al-Hf-O-Y	Al-Mn-O-Si	Al-Mn-O-Ti
Al-Ni-O-Ti	Al-O-Si-Ti	Al-O-Si-Y	Al-O-Si-Zr	Al-O-Ti-Zr
Al-O-Y-Zr	Co-Cr-Fe-Mn	Co-Cr-Fe-Ni	Co-Cr-Mn-Ni	Co-Cr-O-Si
Co-Cr-O-Ti	Co-Cu-O-Si	Co-Fe-Mn-Ni	Co-Fe-Mn-O	Co-Fe-O-Si
Co-Mn-O-Si	Co-Mn-O-Y	Co-Ni-O-Si	Cr-Fe-Mn-Ni	Cr-Fe-Mn-O
Cr-Fe-Ni-O	Cr-Fe-O-Si	Cr-Fe-O-Ti	Cr-Fe-O-Y	Cr-Mn-Ni-O
Cr-Mn-O-Si	Cr-Mn-O-Ti	Cr-Ni-O-Si	Cr-Ni-O-Ti	Cu-Fe-O-Si
Fe-Mn-O-Si	Fe-Mn-O-Ti	Fe-Ni-O-Si	Fe-Ni-O-Ti	Fe-O-Si-Ti
Mn-Ni-O-V	Mn-O-Y-Zr	Mo-Nb-Ta-W	O-Ti-Y-Zr	

### Higher Order Systems

#### Critically Assessed Higher Order Systems

Al-Fe-Mn-O-Si	C-Cr-Fe-Mn-Ni-O	Co-Cr-Fe-Mn-Ni
---------------	-----------------	----------------

## TCHEA9 Phases

In this section:

TCHEA9 Models for the Included Phases .....	25
---	----

---

## TCHEA9 Models for the Included Phases

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LIQUID	Liquid	-	-	-	-	1	{AL, AL1N1, B, C, CO, CR, CU, FE, HF, HF1N1, IR, MN, MO, N, NB, NI, RH, RE, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR, AL2/3O1, AL4/3O2, BO3/2, COO, COO3/2, CRO, CRO3/2, CU2O, CUO, FEO, FEO3/2, HF1/2O1, MNO, MNO3/2, MO1/2O1, MOO3, NB1O1, NBO5/2, NIO, RE1/2O1, REO7/2, RU1/2O1, S1/2O1, SiO2, Si2O4, SNO, SNO2, TA2/5O1, O1Ti1, TiO3/2, O2Ti1, V1O1, VO2, VO3/2, VO5/2, W1/3O1, Y2/3O1, O1ZN1, ZR1/2O1, AL2O4Ti}1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	FCC_A1 will be combined to FCC_L12 if defined.	2	{AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR}1(B, C, N, O, VA)1
FCC_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	This phase has some contribution from FCC_A1.	3	{AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR}0.75(AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR)0.25(B, C, N, O, VA)1
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	BCC_A2 will be combined to BCC_B2 if defined.	2	{AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR, VA}1(B, C, N, O, VA)3
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	This phase has some contribution from BCC_A2.	3	{AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR, VA}0.5(AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR, VA)0.5(B, C, N, O, VA)3
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)	Disordered HCP_A3 solution phase.	2	{AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR}1(B, C, N, O, VA)0.5
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	2	{AL, CO, CR, CU, FE, IR, MN, MO, NB, NI, RE, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR}1(B, C, VA)1
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)	-	2	{AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR}1(B, C, VA)1
DIS_FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	A copy of the FCC_A1 phase just for the use in kinetic simulation.	2	{AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, W, Y, ZN, ZR}1(B, C, N, O, VA)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	Pure C, Si or solid solution phases based on them.	1	(AL, B, C, SI, SN)1
BETA_RHOMBO_B	beta-B (R-105)	-	hR105	(166, R-3m)	-	2	(B)93(B, C, CU, SI)12
GRAPHITE_A9	Hexagonal Graphite (A9)	A9	hP4	(194, P6_3/mmc)	-	1	(B, C)1
BCT_A5	beta-Sn (A5)	A5	tI4	(141, I4_1/amd)	Disordered BCT solution phase.	1	(AL, CU, NI, SN, ZN)1
M23B6_TAU_D84	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	ternary boride.	4	(CO, HF, NI, RE)20(B)6(B, VA)6(AL, CR, HF, MO, RE, TA, TI, V, W, ZR)3
M3B_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	also NI3B_D011.	2	(CO, CR, FE, MO, NI)3(B)1
RE3B_E1A	Re3B	-	oS16	(63, Cmcmm)	-	2	(CR, MO, RE, TA, W)3(B)1
M7B3_D102	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)	also RH7B3, RE7B3_D102.	3	(CO, CR, MO, NB, RE, RH, RU, TA, W)7(B)3(B, VA)3
M2B_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	aka M2B_TETR.	2	(AL, CO, CR, FE, MN, MO, NB, NI, RE, TA, W)2(B)1
CR2B_CB	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	aka CR2B_ORTH.	2	(CR, FE, MO, RE)0.66666667(B)0.33333333
MN2B_D1F	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	-	2	(MN)0.6707(B)0.3293
CR5B3_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	also Mo5B3.	2	(CR, MO)0.625(B)0.375
M3B2_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	also NB3B2, TA3B2, V3B2.	2	(FE, HF, MO, NB, TA, V)3(B)2
M3B2_T	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	ternary boride Mo2FeB2 or Mo2CrB2.	3	(CR, FE, MO, NI, W)0.4(CR, FE, NI)0.2(B)0.4
IR4B3	Ir4B3	-	oF28	(42, Fmm2)	-	2	(IR)4(B)3
NI4B3	m-Ni4B3	-	mS28	(15, C2/c)	-	2	(NI)0.57142857(B)0.42857143
IR5B4	Ir5B4	-	tI36	(88, I4_1/a)	-	2	(IR)5(B)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MB_B27	FeB (B27)	B27	oP8	(62, Pnma)	also CoB, HfB, MnB, TiB.	2	(B)1(CO, CR, FE, HF, MN, MO, RE, TI, Y)1
MB_B33	CrB (B33)	B33	oS8	(63, Cmcm)	also NbB, NiB, TaB, VB.	2	(CR, FE, HF, MO, NB, NI, TA, TI, V)1(B)1
MOB_BG	MoB (Bg)	Bg	tl16	(141, I4_1/amd)	-	2	(CR, FE, MO)1(B)1
WB_ALPHA_BG	MoB (Bg)	Bg	tl16	(141, I4_1/amd)	-	2	(B, C, VA)1(W)1
RU1B1	Unknown Structure	-	cl*	-	-	2	(RU)1(B)1
WB_BETA_B33	CrB (B33)	B33	oS8	(63, Cmcm)	-	2	(B, C, VA)1(W)1
RHB_B81	Nickeline (NiAs, B81)	B81	hP4	(194, P6_3/mmc)	-	2	(RH)1(B)1.1
M5B6	V5B6	-	oS22	(65, Cmmm)	also Nb5B6.	2	(NB, V)5(B)6
IR4B5	Ir4B5	-	mS18	(8, Cm)	-	2	(IR)4(B)5
M3B4_D7B	Ta3B4 (D7b)	D7b	ol14	(71, Immm)	also ternary X1Y2B4 boride.	2	(B)4(AL, CR, HF, MN, NB, TA, TI, V)3
RU2B3	Ru2B3	-	hP10	(194, P6_3/mmc)	-	2	(RU)2(B)3
V2B3	V2B3	-	oS20	(63, Cmcm)	-	2	(V)0.4(B)0.6
MB2_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(B)2(AL, CR, HF, MN, MO, NB, RU, TA, TI, V, Y, ZR)1
REB2	ReB2	-	hP6	(194, P6_3/mmc)	-	3	(RE)1(B)2(B, VA)2
MO2B5_D8i	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)	-	2	(MO)0.32(B)0.68
W2B5_D8i	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)	nonstoichiometric W2B5.	2	(B, C, VA)5(W)2
CRB4	CrB4	-	ol10	(71, Immm)	-	2	(CR)0.2(B)0.8

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN1B4	MnB4	-	mS10	(12, C2/m)	-	2	(MN)0.2(B)0.8
MOB4	MoB4	-	hP16	(194, P6 <sub>3</sub> /mmc)	-	2	(MO)0.2(B)0.8
YB4_D1E	ThB4 (D1e)	D1e	tP20	(127, P4/mbm)	-	2	(Y)0.2(B)0.8
W2B9	W2B9	-	hP22	(147, P-3)	-	2	(B)9(W)2
YB6_D21	CaB6 (D21)	D21	cP7	(221, Pm-3m)	-	2	(Y)1(B)6
ZRB12_D2F	UB12 (D2f)	D2f	cF52	(225, Fm-3m)	also YB12.	2	(B)12(Y, ZR)1
ALB12_ALPHA	alpha-AlB12	-	tP216	(92, P4 <sub>12</sub> -12)	-	2	(AL, TI)1(B)12
YB66	YB66	-	cF1936	(226, Fm-3c)	-	2	(Y)1(B)66
M12C	Fe6W6C	-	cF104	(227, Fd-3m)	also Mo6Ni6C	3	(CO, NI)6(MO, W)6(C)1
M6C_E93	eta-carbide (Fe3W3C, E93)	E93	cF112	(227, Fd-3m)	-	4	(CO, FE, NI)2(MO, NB, TA, W)2(CO, CR, FE, MO, NB, NI, TA, V, W)2(C)1
ALM3C_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	also AlCo3C, AlFe3C.	3	(AL)1(CO, FE)3(C)1
TI3ALC_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	i.e. Ti3AlC1-x.	3	(TI)3(AL)1(C, VA)1
W3MC	W10Co3C3.4	-	hP34	(194, P6 <sub>3</sub> /mmc)	also W3CoC, W3NiC.	3	(W)3(CO, NI)1(C)1
M23C6_D84	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)	-	3	(CO, CR, FE, MN, NI, RE, V)20(CO, CR, FE, MN, MO, NI, RE, V, W)3(C)6
ALCR2C	AlCr2	-	hP8	(194, P6 <sub>3</sub> /mmc)	MAX_PHASE.	3	(AL)1(C)1(CR)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CEMENTITE_D011	Cementite (Fe <sub>3</sub> C, D011)	D011	oP16	(62, Pnma)	-	2	(CO, CR, FE, MN, MO, NI, V, W)3(C, N)1
TI2ALC	AlCr <sub>2</sub>	-	hP8	(194, P6 <sub>3</sub> /mmc)	i.e. Ti <sub>2</sub> AlC <sub>1-x</sub> .	3	(TI)2(AL)1(C, VA)1
M5C2	Mn <sub>5</sub> C <sub>2</sub> (Fe <sub>5</sub> C <sub>2</sub> Hagg carbide)	-	mS28	(15, C2/c)	-	2	(FE, MN)5(C)2
M7C3_D101	C <sub>3</sub> Cr <sub>7</sub> (D101)	D101	oP40	(62, Pnma)	-	2	(CO, CR, FE, MN, MO, NI, RE, V, W)7(C)3
TI3ALC2	Ti <sub>3</sub> SiC <sub>2</sub>	-	hP12	(194, P6 <sub>3</sub> /mmc)	-	3	(TI)3(AL, SI)1(C, VA)2
M3C2_D510	Tungbaite (Cr <sub>3</sub> C <sub>2</sub> , D510)	D510	oP20	(62, Pnma)	-	2	(CO, CR, MO, V, W)3(C)2
AL4C3_D71	Al <sub>4</sub> C <sub>3</sub> (D71)	D71	hR7	(166, R-3m)	-	2	(AL, SI)4(C)3
MC_ETA	CMo	-	hP12	(194, P6 <sub>3</sub> /mmc)	-	2	(MO, V, W)1(C, VA)1
MC_SHP	Tungsten Carbide (WC, Bh)	Bh	hP2	(187, P-6m2)	also MoC_LT, Strukturbericht Bh	2	(MO, W)1(C, N)1
YC_GAMMA_B1	Rock Salt/Halite (NaCl, B1)	B1	cF8	(225, Fm-3m)	-	2	(Y)1(C, C2, VA)1
Y15C19_BETA	Unknown Structure	-	-	-	the high temperature beta phase	2	(C)19(Y)15
Y15C19_ALPHA	alpha-Y15C19	-	oP18	(55, Pbam)	aka Y15C19_R.	2	(C)19(Y)15
Y2C3_BETA	Unknown Structure	-	-	-	HT phase	3	(Y)2(C)2(C, VA)1
Y2C3_ALPHA	Sc <sub>3</sub> C <sub>4</sub>	-	tP70	(128, P4/mnc)	aka Y2C3_R.	3	(Y)2(C)2(C, VA)1
YC2_C11A	CaC <sub>2</sub> -I (C11a)	C11a	tI6	(139, I4/mmm)	-	1	(C2Y)1
PI_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)	i.e. Cr-(Fe, Ni)-N nitride.	3	(CR)12.8(FE, NI)7.2(N)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FE4N_LP1	gamma'-Fe4N (L'10)	L'10	cP5	(221, Pm-3m)	Only stable in (Co-Cr-Fe)-N when gas suspended.	2	(CO, CR, FE, MN, NI)4(C, N)1
ALTI3N_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	-	3	(AL)1(TI)3(N)1
ALTI2N	AlCr2	-	hP8	(194, P6_3/mmc)	-	3	(AL)1(TI)2(N)1
AL2TI3N2	(Al2Ti3N2)	-	hP22	(186, P6_3mc)	-	3	(AL)2(TI)3(N)2
FECN_CHI	Mn5C2 (Fe5C2 Hagg carbide)	-	mS28	(15, C2/c)	Only stable in C-Fe-N when gas suspended.	2	(FE)2.2(C, N)1
TI4N3	Sc2Te3	-	hR8	(166, R-3m)	aka Xi-TiN0.58 HT	2	(TI)0.685(N)0.315
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mnm)	-	2	(TI)2(N)1
Z_PHASE	CrNbN	-	tP6	(129, P4/nmm)	-	3	(CR, FE)1(MO, NB, V)1(N, VA)1
HF3N2	TiS-9R	-	hR6	(166, R-3m)	-	2	(HF)3(N)2
MN3N2	Mn3N2	-	tI10	(139, I4/mmm)	aka MN6N4.	2	(MN)6(N)4
TI3N2	TiS-9R	-	hR6	(166, R-3m)	-	2	(TI)0.71(N)0.29
HF4N3	Sc2Te3	-	hR8	(166, R-3m)	-	2	(HF)4(N)3
MN6N5	CoO	-	tI4	(139, I4/mmm)	-	2	(MN)6(N)5
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	-	2	(AL)1(N)1
TAN_EPS	TaN-eps	-	hP6	(189, P-62m)	-	2	(TA)1(N)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
HFN_B1	Rock Salt/Halite (NaCl, B1)	B1	cf8	(225, Fm-3m)	-	2	(HF)1(N, VA)1
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	-	2	(AL, MN)17(SI, ZN)3
MN9SI2	Mn9SI2	-	ol186	(71, Immm)	-	2	(MN)33(SI)7
CR3NI5SI2	AlAu4	-	cP20	(198, P2_13)	-	4	(CR)3(NI)5(SI)2(C, VA)1
CR2NI2SI	NiTi2	-	cF96	(227, Fd-3m)	i.e. the Tau1 phase Cr5Ni5Si3.	3	(CR)5(NI)5(SI)3
CR3SI_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	also Cr3X, Nb3X, Ti3X, V3X.	3	(CR, FE, IR, MO, NB, NI, RE, RH, SI, SN, TA, TI, V, ZR)3(AL, CO, CR, IR, NB, NI, RH, RU, SI, SN, TA, TI, V, ZR)1(C, VA)3
CO3SI_D019	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(CO)3(SI)1
IR3SI1	alpha-SiU3 (D0c)	D0c	tl16	(140, I4/mcm)	-	2	(IR)3(SI)1
M3SI1	Ti3P	-	tP32	(86, P4_2/n)	also Nb3Si, Ta3Si, Ti3Si, Zr3Si.	2	(HF, NB, TA, TI, ZR)3(SI)1
MN3SI_D03	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	2	(MN, FE)3(AL, SI)1
NI3SI_ORTHO_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(NI)3(SI)1
NI3SI_MONOCL	Ge9Pd25	-	hP34	(147, P-3)	-	2	(NI)3(SI)1
NI5SI2	Ni31S12	-	hP42	(150, P321)	-	2	(CO, CR, CU, FE, NI)5(SI)2
CO2SI1	Co2Si (C37)	C37	oP12	(62, Pnma)	also Ni2Si (delta)	2	(CO, CR, CU, FE, IR, NI, TI, RH)2(SI)1
CRNBSI	ZrNiAl	-	hP9	(189, P-62m)	-	3	(CR)1(NB)1(SI)1
FESITI	TiFeSi	-	ol36	(46, Ima2)	-	3	(FE)1(SI)1(TI)1
FE2SI	AlNi2	-	hP6	(164, P-3m1)	-	2	(FE)0.666667(SI)0.333333
NI2SI_THETA	AlNi2	-	hP6	(164, P-3m1)	aka M2SI_TETA.	3	(CU, NI)1(NI, VA)1(AL, SI)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RE2Si	Re2Si	-	mP24	(14, P2_1/c)	-	2	(RE)2(Si)1
RU2Si_C37	Co2Si (C37)	C37	oP12	(62, Pnma)	-	2	(RU)2(Si)1
M5Si3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	also M5Sn3, M5Si3C.	4	(CR, CU, FE, HF, MN, MO, NI, NB, SI, TI, W, Y, ZR)2(AL, CR, SI, SN, TI)3(CR, CU, FE, HF, MN, MO, NI, NB, TI, Y, ZR)3(C, SN, VA)1
RH5Si3	Rh5Ge3	-	oP16	(55, Pbam)	-	2	(RH)5(Si)3
TA5Si3_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	also alpha-Nb5Si3.	2	(HF, NB, TA)5(AL, SI)3
W5Si3_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	also Cr5Si3, Mo5Si3, Nb5Si3, V5Si3.	3	(CR, FE, MO, NB, TI, V, W)4(CR, FE, MO, NB, TI, V, W, SI)1 (AL, SI, SN)3
FE4Si3TI	Pd40Sn31Y13	-	hP168	(191, P6/mmm)	-	3	(FE)0.5(SI)0.375(TI)0.125
RH20Si13	Rh20Si13	-	hP34	(176, P6_3/m)	-	2	(RH)20(SI)13
IR3Si2_B82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(IR)3(SI)2
M3Si2_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	also Hf3Si2, Zr3Si2.	2	(HF, NB, ZR)3(SI)2
NI3Si2	Ni3Si2	-	oP80	(36, Cmc2_1)	-	2	(NI)3(SI)2
M11Si8	Cr11Ge8	-	oP76	(62, Pnma)	also Cr11Si8, Nb11Si8.	2	(CR, NB)11(SI)8
M4Si3	Ru4Si3	-	oP28	(62, Pnma)	also Cr4Si3, Nb4Si3.	2	(CR, NI, RU)4(SI)3
ZR5Si4_TP36	Si4Zr5	-	tP36	(92, P4_12_12)	also Hf5Si4, Ti5Si4.	2	(HF, NB, TI, ZR)5(AL, SI)4
Y5Si4	Gd5Si4	-	oP36	(62, Pnma)	-	2	(Y)5(SI)4
M6Si5	Si5V6	-	oI44	(72, Ibam)	also Cr6Si5, Nb6Si5.	2	(CR, NB, TI, V)6(SI)5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MSI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	also CoSi, CrSi, MnSi, ReSi.	2	(CO, CR, FE, MN, NI, RE)1(AL, SI)1
FESI2M	CrSi2Zr	-	oP48	(55, Pbam)	-	3	(FE)1(SI)2(TI)1
IRSI_B27	FeB (B27)	B27	oP8	(62, Pnma)	the HT phase.	2	(IR)1(SI)1
MSI_B27	FeB (B27)	B27	oP8	(62, Pnma)	also TiSi, HfSi, YSi, ZrSi(alpha).	2	(HF, NB, TI, Y, ZR)1(AL, SI)1
NISI_B31	MnP (B31)	B31	oP8	(62, Pnma)	-	2	(NI)1(SI)1
RHSI_B31	MnP (B31)	B31	oP8	(62, Pnma)	-	2	(RH)1(SI)1
RHSI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	-	2	(RH)1(SI)1
RUSI	FeSi (B20)	B20	cP8	(198, P2_13)	united HT_B2/LT_B20 phase.	2	(RU)1(SI)1
IR4SI5	Ru4Si5	-	mP18	(11, P2_1/m)	-	2	(IR)4(SI)5
RH4SI5	Ru4Si5	-	mP18	(11, P2_1/m)	-	2	(RH)4(SI)5
IR3SI4	Ru4Si3	-	oP28	(62, Pnma)	-	2	(IR)3(SI)4
RH3SI4	Rh3Si4	-	oP28	(62, Pnma)	-	2	(RH)3(SI)4
RU2SI3	Ge3Ru2	-	oP40	(60, Pbcn)	united HT/LT phase.	2	(RU)2(SI)3
IR3SI5	Ir3Si5	-	mP64	(14, P2_1/c)	-	2	(IR)3(SI)5
Y3SI5_HT_CC	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_1/amd)	-	2	(Y)3(SI)5
Y3SI5_LT_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(Y)3(SI)5
MN11SI19	Mn11Si19	-	tP120	(118, P-4n2)	-	2	(MN)11(AL, SI)19
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)	also NbSi2, TaSi2, VSi2.	2	(CR, CU, HF, MO, NB, SI, TA, TI, V, W)1(AL, CR, CU, SI)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FESI2_HT	FeSi2-h	-	tP3	(123, P4/mmm)	-	2	(FE)0.3(SI)0.7
FESI2_LT	FeSi2-l	-	oS48	(64, Cmce)	-	2	(FE)0.333333(SI)0.666667
MSI2_C1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	also NiSi2, CoSi2.	2	(CO, CU, MN, NI)1(AL, CU, SI)2
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	also AlCr2, Ti2Zn, ZnZr2, CUZR2_C11B.	2	(AL, CO, CU, FE, MO, NI, RH, W, ZN)1(AL, CR, HF, SI, TI, ZR)2
RESI2_C11B	Re4Si7	-	mS44	(8, Cm)	-	2	(RE)0.357(SI)0.643
TISI2_C54	TiSi2 (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	also MoSi2, RuAl2, ZrSn2.	2	(MO, NB, RU, TI, ZR)1(AL, SI, SN)2
YSI2_HT_CC	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_1/amd)	-	2	(Y)1(SI)2
YSI2_LT_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(Y)1(SI)2
ZRSI2_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	also HfSi2.	2	(ZR, HF, NB)1(SI)2
IRSI3_LT	Unknown Structure	-	mS*	-	-	2	(IR)1(SI)3
IRSI3_HT	Unknown Structure	-	oS*	-	-	2	(IR)1(SI)3
ALFESI_ALPHA_TAU5	Fe23Al81Si15	-	hP246	(194, P6_3/mmc)	-	4	(AL)0.6612(FE)0.19(SI)0.0496(AL, SI)0.0992
ALFESI_BETA_TAU6	Fe2Al9Si2	-	mS52	(15, C2/c)	-	3	(AL)14(FE)3(SI)3
ALFESI_GAMMA_TAU2	Unknown Structure	-	mS*	-	-	3	(AL)3(FE)1(SI)1
ALFESI_DELTA_TAU4	FeAl3Si2	-	oP24	(60, Pbcn)	-	3	(AL)0.55(FE)0.15(SI)0.3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALFESI_TAU1	Unknown Structure	-	-	-	-	3	(AL)2(Fe)2(Si)1
ALFESI_TAU3	Fe(Al <sub>0.67</sub> Si <sub>0.33</sub> ) <sub>3</sub>	-	oS128	(67, Cmme)	-	3	(AL)2(Fe)1(Si)1
AL2MN2SI3	(Al <sub>2</sub> Mn <sub>2</sub> Si <sub>3</sub> )	-	hP21	(174, P-6)	Tau1	3	(AL)2(MN)2(SI)3
AL5MN6SI7	CrSi <sub>2</sub> (C40)	C40	hP9	(180, P6_222)	Tau2	3	(AL)5(MN)6(SI)7
AL1MN1SI1	TiSi <sub>2</sub> (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	Tau3	3	(AL)1(MN)1(SI)1
AL3MNSI2	(Al <sub>3</sub> MnSi <sub>2</sub> )	-	tP48	(85, P4/n)	Tau4	3	(AL)3(MN)1(SI)2
AL3MN4SI2	Unknown Structure	-	-	-	ternary tau5 or D phase	3	(AL)3(MN)4(SI)2
ALMNSI_TAU6	Unknown Structure	-	-	-	-	2	(AL, MN)4(SI)1
ALMNSI_TAU8	Al <sub>9</sub> Mn <sub>3</sub> Si (E9c)	E9c	hP26	(194, P6_3/mmc)	-	5	(MN, VA)6(MN, VA)2(AL)12(AL, SI)6(AL, SI)2
AL2MNSI3	Ga <sub>5</sub> Pd	-	tI24	(140, I4/mcm)	Tau10	3	(AL)2(MN)1(SI)3
MN15NI45SI40	Unknown Structure	-	-	-	ternary T1 or N phase	3	-
MN15NI50SI35	Unknown Structure	-	-	-	ternary T2 or PHI phase	3	-
MN6NI16SI7	Th <sub>6</sub> Mn <sub>23</sub> (D8a)	D8a	cF116	(225, Fm-3m)	ternary T3 or G phase	3	-
MN1NI1SI1_C37	MnCuP	-	oP12	(62, Pnma)	ternary T4 or E phase	3	-
MNNISI_T5	MgZn <sub>2</sub> Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	ternary T5 or tao_1 phase	2	-
MNNISI_T6	Cu <sub>2</sub> Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	ternary T6 or tao_2 phase	2	-
MN3NI2SI	Mn <sub>3</sub> Ni <sub>2</sub> Si	-	cF96	(227, Fd-3m)	ternary T7 or Omega	3	-

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN2NISI	Unknown Structure	-	-	-	ternary T8 or S phase	2	-
MN6NISI3	R-(Co, Cr, Mo)	-	hR53	(148, R-3)	ternary T9 or R' phase	3	-
MN66NI4SI30	Unknown Structure	-	-	-	ternary T10 or U phase	3	-
MN52NI29SI19	Unknown Structure	-	-	-	ternary phase T11 or W phase	3	-
B4C_D1G	B13C2 "B4C" (D1g)	D1g	hR15	(166, R-3m)	-	2	(B11C, B12)1(B2, C2B, CB2)1
BN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	-	2	(B)1(N)1
MEO_B1	Rock Salt/Halite (NaCl, B1)	B1	cF8	(225, Fm-3m)	TiO	2	(Ti, V, VA)1(O, VA)1
SIB3_D1G	B13C2 "B4C" (D1g)	D1g	hR15	(166, R-3m)	-	3	(B)6(SI)2(B, SI)6
SIB6	SiB6	-	oP280	(58, Pnnm)	-	3	(B)210(SI)23(B, SI)48
BNSI_RHOMBO	alpha-B (R-12)	-	hR12	(166, R-3m)	aka BNSI, ALPHA_RHOMBO_B.	3	(B)61(SI)1(B, SI)8
SIC_B3	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)	-	2	(SI)1(C)1
SI3N4	Nierite (alpha-Si3N4)	-	hP28	(159, P31c)	-	2	(SI)3(N)4
AL4SIC4_E94	Al5C3N (E94)	E94	hP18	(186, P6_3mc)	-	3	(AL)4(SI)1(C)4
AL8SIC7	Unknown Structure	-	hP16	-	-	3	(AL)8(SI)1(C)7
FE8SI2C	Mn8Si2C	-	aP*	(1, P1)	-	3	(FE)8(SI)2(C)1
TI3SIC2	Ti3SiC2	-	hP12	(194, P6_3/mmc)	-	3	(TI)3(SI)1(C)2
DIS_MU	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	Part of the description for the MU_PHASE	1	(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, TA, TI, W)1
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	DIS_MU contribution added onto it.	4	(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, TA, TI, W)1(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, TA, TI, W)2(AL, CO,

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							CR, CU, FE, MN, MO, NB, NI, RE, TI, TA, W)6(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, TA, TI, W)4
DIS_SIG	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)	Part of the description for the SIGMA phase.	1	(AL, CO, CR, FE, IR, MN, MO, NB, NI, RE, RH, RU, SI, TA, TI, V, W)1
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)	DIS_SIG contribution added onto it.	3	(AL, CO, CR, FE, IR, MN, MO, NB, NI, RE, RH, RU, SI, TA, TI, V, W)10(AL, CO, CR, FE, IR, MN, MO, NB, NI, RE, RH, RU, SI, TA, TI, V, W)4(AL, CO, CR, FE, IR, MN, MO, NB, NI, RE, RH, RU, SI, TA, TI, V, W)16
CHI_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)	also M5Re24, Mo2Re8, Ta3Re7, WRe3.	3	(CR, FE, NI, RE)24(AL, CR, HF, MO, NB, TA, TI, W, ZR)10 (CR, FE, MO, NB, NI, RE, TA, W)24
G_PHASE_D8A	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	3	(AL, CO, FE, MN, NI, TI)16(HF, NB, TI, Y, ZR)6(CO, FE, MN, NI, SI)7
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	also Cu5Zn8, Ni5Zn8, Al5Cu8 (rt).	3	(AL, NI, SI, ZN)4(AL, CU, NI, SI, ZN)1(CU, FE, MN, NI, ZN)8
GAMMA_HT_D82	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	aka GAMMA_H.	3	(AL, ZN)4(AL, CU, ZN)1(CU, FE, MN, NI)8
HEUSLER_L21	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	-	3	(CO, FE, NI)0.5(AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, SI, SN, TA, TI, V, ZR)0.25(AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, SI, SN, TA, TI, V, ZR)0.25
O_PHASE	NaHg	-	oS16	(63, Cmc)	aka Ti2NbAl, the O phase.	3	(NB, TA, TI)0.5(AL, NB, TA, TI)0.25(NB, TA, TI)0.25
P_PHASE	Cr9Mo21Ni20	-	oP56	(62, Pnma)	-	3	(CR, FE, NI, RE)24(CR, FE, MO, NI, RE)20(MO)12
R_PHASE	R-(Co, Cr, Mo)	-	hR53	(148, R-3)	-	3	(CO, CR, FE, NI, RE)27(MO, W)14(CO, CR, FE, MO, NI, RE, W)12
B82_OMEGA	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	3	(AL, SN)1(CO, NB, SN, TA, TI)1(TI)1
MNNI_L10	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	-	2	(CO, CR, CU, FE, MN, NI)0.5(CO, CR, CU, FE, MN, NI)0.5
IRMN_L10	CuAu(I) (L10)	L10	tP2	(123,	also IrTi.	2	(IR, MN, TI)0.5(IR, MN, TI)0.5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				P4/mmm)			
ALTI_L10	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	Solid solution of ordered L10.	2	(AL, CO, CR, MN, MO, NB, SN, TA, TI, V, W, ZR)1(AL, CO, CR, MN, MO, NB, SN, TA, TI, V, W, ZR)1
IRNB_L10	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	-	2	(IR, NB)0.5(IR, NB)0.5
IRW_EPSILON_HCP	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)	HT epsilon solution phase with HCP structure.	2	(IR, W)1(IR, W)1
IRW_LT_B19	beta'-AuCd (B19)	B19	oP4	(51, Pmma)	-	2	(IR)1(IR, W)1
IRV_L10	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	aka Ir1.04V0.96 or IrV1-x.	2	(IR)0.5(IR, V)0.5
NBRH_L10	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	aka Rh1.04V0.96.	2	(NB)0.96(RH)1.04
RHV_L10	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	aka Rh1.12V0.88.	2	(RH, V)1.12(RH, V)0.88
ALCU_EPS_B82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	epsilon2 HT.	2	(AL, CU, NI)1(CU, FE)1
ALCU_ETA	AlCu(r)	-	mS20	(12, C2/m)	united HT-eta1 & LT-eta2.	2	(AL, CU)1(CU, FE, NI, ZN)1
ALPHA_B19	beta'-AuCd (B19)	B19	oP4	(51, Pmma)	an ordered HCP.	2	(MO, NB, TI, V, ZR)1(MO, NB, TI, V, ZR)1
ALRE_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)	-	2	(AL)1(RE)1
ALZR_B33	CrB (B33)	B33	oS8	(63, Cmcm)	also AlHf, ALY_B33.	2	(AL)1(HF, Y, ZR)1
COSN_B35	CoSn (B35)	B35	hP6	(191, P6/mmm)	also FeSn, COSN_HP6.	2	(CO, FE, NI)0.5(SN)0.5
COY_B33	CrB (B33)	B33	oS8	(63, Cmcm)	aka COY_BF.	2	(CO)1(Y)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CUTI_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)	aka B11.	2	(CO, CU, NI, TI)1(CU, NI, TA, TI)1
HF1IR1	Unknown Structure	-	-	-	united HT/LT phase	2	(HF)1(IR)1
HFMN	NiTi2	-	cF96	(227, Fd-3m)	-	2	(HF)0.5(MN)0.5
HFNI_ALPHA	CrB (B33)	B33	oS8	(63, Cmcmm)	-	2	(HF)0.5(NI)0.5
HFRE	Zr21Re25	-	hR92	(167, R-3c)	also Hf21Re25.	2	(HF)1(RE)1
HFRH_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	2	(HF, RH)1(RH)1
IRV_RT	alpha-IrV	-	oS8	(65, Cmmm)	-	2	(IR)1(V)1
IRZR_BETA_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	i.e. HT- or beta- phase.	2	(IR, ZR)1(IR, ZR)1
IRZR_ALPHA	Mn3As (D0d)	D0d	oS16	(63, Cmcmm)	LT phase.	2	(IR, ZR)1(ZR)1
MNTA	Unknown Structure	-	-	-	-	2	(MN)1(TA)1
MNTI_LT	Zr21Re25	-	hR92	(167, R-3c)	aka Ti21Mn25_RT.	2	(MN)1(TI)1
MOIR_HT	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)	-	2	(IR, MO)1(IR, MO)1
MOIR_LT_B19	beta'-AuCd (B19)	B19	oP4	(51, Pmma)	-	2	(MO)1(IR)1
NBRH_HT	Unknown Structure	-	-	-	-	2	(NB, RH)1(NB, RH)1
NB1ZN1	Unknown Structure	-	-	-	-	2	(NB)0.5(ZN)0.5
NIZN_TP2	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	united HT/LT phase.	2	(AL, CU, NI, ZN)0.5(AL, NI, ZN)0.5
NIY_B27	FeB (B27)	B27	oP8	(62, Pnma)	-	2	(NI)1(Y)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NIZR_B33	CrB (B33)	B33	oS8	(63, Cmc <sub>2</sub> )	-	2	(NI)1(TI, ZR)1
RHSN_B20	FeSi (B20)	B20	cP8	(198, P2_13)	-	2	(RH)1(SN)1
RHZR_LT	IrZr	-	oS16	(63, Cmc <sub>2</sub> )	i.e. alpha_RhZr	2	(RH)1(RH, ZR)1
RHV_RT	alpha-IrV	-	oS8	(65, Cmmm)	-	2	(RH)1(V)1
RHV_HT	Unknown Structure	-	-	-	-	2	(RH, V)1(V)1
RHZR_HT_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	i.e. beta_RhZr.	2	(RH)1(RH, ZR)1
ZNZR_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	2	(ZN)1(ZR)1
ALCU_PRIME	Al9Cu11(h)	-	oF88	(42, Fmm2)	aka THETA_PRIME.	2	(AL)2(CU)1
AL2FE	Al2Fe	-	aP18	(1, P1)	-	2	(AL, CU)2(CO, FE, MN, NI)1
ALRE2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(AL)1(RE)2
ALRH2	Unknown Structure	-	-	-	-	2	(AL)1(RH)2
AL2TI_LT	Ga2Hf	-	tI24	(141, I4_1/amd)	-	2	(AL, NB, TI)2(AL, CO, NB, TA, TI, V, ZR)1
Al2W_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)	-	2	(AL)2(W)1
ALY2_C37	Co2Si (C37)	C37	oP12	(62, Pnma)	-	2	(AL)1(Y)2
ALZR2_B82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(AL)1(TI, ZR)2
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	also CuZn2.	2	(AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, SI, RE, RU, TA, TI, V, W, Y, ZN, ZR)2(AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, SI, RE, RU, TA, TI, V, W, Y, ZN, ZR)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, SI, RE, RH,

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							RU, TA, TI, V, W, Y, ZN, ZR)2(AL, CO, CR, CU, FE, HF, MO, NB, NI, SI, RE, RH, RU, TA, TI, V, W, Y, ZR)1
C16_THETA	Khatyrkite (Al <sub>2</sub> Cu, C16)	C16	tl12	(140, I4/mcm)	-	2	(AL, HF, MN, MO, NB, SN, TA, TI, W, ZR)2(AL, CO, CR, CU, FE, IR, MN, NI, RH, SI)1
C36_LAVES	MgNi <sub>2</sub> Hexagonal Laves (C36)	C36	hP24	(194, P6 <sub>3</sub> /mmc)	-	2	(AL, CO, CR, CU, FE, HF, MO, NB, NI, TA, TI, W, ZR)2(AL, CO, CR, CU, FE, HF, MO, NB, NI, TA, TI, W, ZR)1
CRNI2_OP6	MoPt <sub>2</sub>	-	oI6	(71, Immm)	-	2	(CR, MO, W)1(MO, NI, W)2
CU2TI1	Au <sub>2</sub> V	-	oS12	(63, Cmcn)	-	2	(CO, CU, NI)2(TI)1
CU2Y_HT	Unknown Structure	-	hP*	-	-	2	(CU)2(Y)1
CU2Y_LT	CeCu <sub>2</sub>	-	oI12	(74, Imma)	-	2	(CU)2(Y)1
HF2IR	NiTi <sub>2</sub>	-	cF96	(227, Fd-3m)	-	2	(HF)2(IR)1
HF2RH	NiTi <sub>2</sub>	-	cF96	(227, Fd-3m)	-	2	(HF)2(RH)1
HFSN2_C40	CrSi <sub>2</sub> (C40)	C40	hP9	(180, P6 <sub>2</sub> 222)	-	2	(HF)1(SN)2
MNNI2	Unknown Structure	-	-	-	-	2	(MN, NI)1(NI)2
NBZN2_C36	MgNi <sub>2</sub> Hexagonal Laves (C36)	C36	hP24	(194, P6 <sub>3</sub> /mmc)	-	2	(NB)0.333(ZN)0.667
NI2V	MoPt <sub>2</sub>	-	oI6	(71, Immm)	-	2	(MO, NI)2(MO, NB, TA, V)1
NI2TA_C11B	MoSi <sub>2</sub> (C11b)	C11b	tl6	(139, I4/mmm)	-	2	(CO, NI)2(TA, TI)1
NITI2	NiTi <sub>2</sub>	-	cF96	(227, Fd-3m)	-	2	(CO, CR, CU, FE, NI, RE, TI)1(AL, CR, CU, HF, NI, TA, TI, ZR)2
NI2Y1	Ni <sub>2</sub> Tm	-	cF192	(216, F-43m)	-	2	(NI)2(Y)1
REZR2	Zr <sub>21</sub> Re <sub>25</sub>	-	hR92	(167, R-3c)	aka Zr <sub>21</sub> Re <sub>25</sub> .	2	(NI, RE)1(ZR)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RHSN2_RT	RhSn2	-	tl26	(139, I4/mmm)	-	2	(RH)0.33333(SN)0.66667
RH2SN	Co2Si (C37)	C37	oP12	(62, Pnma)	-	2	(RH)2(SN)1
RH2TA	Co2Si (C37)	C37	oP12	(62, Pnma)	-	2	(RH)2(TA)1
SNTI2_B82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(SN)1(TI)2
SN2Y_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcn)	-	2	(SN)2(Y)1
RHZR2	NiTi2	-	CF96	(227, Fd-3m)	-	2	(RH)1(ZR)2
TASN2_CB	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	also SN2TA_CB.	2	(TA)1(SN)2
VSN2_CB	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	-	2	(SN)0.6(V)0.4
YZN2_LT	Unknown Structure	-	-	-	-	2	(Y)1(ZN)2
YZN2_HT	Unknown Structure	-	-	-	-	2	(Y)1(ZN)2
AL3CO1	Os4Al13	-	mS34	(12, C2/m)	aka CoAl3_cub.	2	(AL)3(CO)1
AL3IR_D018	Na3As (D018)	D018	hP8	(194, P6_3/mmc)	-	2	(AL)0.75(IR)0.25
AL3NI_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(AL, NI)0.75(Fe, NI)0.25
AL3RH_LT	(Al3Rh)	-	oP*	(62, Pnma)	-	2	(AL)3(RH)1
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	also Ni3Sn_LT, Mn3Sn, Ti3Sn.	2	(AL, CO, CR, CU, MN, MO, NB, NI, SN, TA, TI, V, W, ZR)3 (AL, C, CR, MO, NB, NI, SI, SN, TA, TI, V, W)1
AL3TI_D022	Al3Ti (D022)	D022	tl8	(139, I4/mmm)	gamma double prime, AL3TI_D022, Al3M, Ni3V.	2	(AL, CO, CR, FE, MO, NB, NI, SI, TI, V)3(AL, CO, CR, MO, NB, NI, SI, TA, TI, V, ZR)1
AL3Y_HT	BaPb3	-	hR12	(166, R-3m)	-	2	(AL)0.75(Y)0.25

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3Y_LT	Ni3Sn (D019)	D019	hP8	(194, P6 <sub>3</sub> /mmc)	-	2	(AL)0.75(Y)0.25
AL3ZR_D023	Al3Zr (D023)	D023	tI16	(139, I4/mmm)	also Al3Hf, Zn3Zr.	2	(AL, ZN)3(HF, TI, ZR)1
CO1SN3	Au3Zn	-	oS32	(64, Cmce)	-	2	(CO)0.25(SN)0.75
CO3V1	Al3Pu	-	hP24	(194, P6 <sub>3</sub> /mmc)	-	2	(CO, NI, V)3(CO, V)1
CO3Y1	Ni3Pu	-	hR12	(166, R-3m)	-	2	(CO)3(Y)1
CU3SN_LT	Cu3Sn	-	oS80	(63, Cmcm)	epsilon	2	(CU, NI, SN)3(CU, SN)1
CUTi3_L60	CuTi3 (L60)	L60	tP4	(123, P4/mmm)	-	2	(CU, TI)1(TI)3
HFIR3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(HF)1(IR)3
HFNI3_ALPHA	PdRh2Ta	-	hP40	(194, P6 <sub>3</sub> /mmc)	the LT phase.	2	(HF)0.25(NI)0.75
HFNI3_BETA	BaPb3	-	hR12	(166, R-3m)	the HT phase.	2	(HF)0.25(NI)0.75
IRNB_ALPHA2	TaIr	-	oP12	(51, Pmma)	-	2	(IR)1(IR, NB)1
IR3W_D019	Ni3Sn (D019)	D019	hP8	(194, P6 <sub>3</sub> /mmc)	-	2	(IR, W)3(IR, W)1
IRY3_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(IR)1(Y)3
IR3Y1	Ni3Pu	-	hR12	(166, R-3m)	-	2	(IR)3(Y)1
IRZR3_DOE	alpha-V3S	-	tI32	(121, I-42m)	-	2	(IR)1(ZR)3
MY3_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	also CoY3, NiY3.	2	(CO, NI)1(Y)3
MZR3_E1A	MgCuAl2 (E1a)	E1a	oS16	(63, Cmcm)	also CoZr3, FeZr3.	2	(CO, FE, NI)1(ZR)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN3TI1	Unknown Structure	-	-	-	HT phase	2	(MN)3(TI)1
MO1IR3	Ni3Sn (D019)	D019	hP8	(194, P6 <sub>3</sub> /mmc)	-	2	(MO)1(IR, MO)3
MO3IR_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(MO)3.06(IR)0.94
NBZN3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(NB)0.25(ZN)0.75
NI3TA_D0A	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)	also delta, Ni3Mo, Ni3Nb.	2	(AL, CO, CR, CU, FE, NI, NB)3(AL, FE, MO, NB, NI, TA, TI, V, W)1
NI3TI_D024	Ni3Ti (D024)	D024	hP16	(194, P6 <sub>3</sub> /mmc)	also Eta, AlNi6Ta.	2	(AL, CO, CR, CU, FE, HF, NI, TA, TI, W, ZR)0.75(AL, CR, CU, HF, MO, NB, NI, SI, TA, TI, W, ZR)0.25
M3Y	Ni3Pu	-	hR12	(166, R-3m)	also Fe3Y, Ni3Y.	2	(FE, NI)3(Y)1
RHY3_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(RH)1(Y)3
RH3Y1	CeNi3	-	hP24	(194, P6 <sub>3</sub> /mmc)	-	2	(RH)3(Y)1
RH3ZR_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(RH, ZR)3(RH, ZR)1
RUY3_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(RU)0.25(Y)0.75
SN3Y1	GdSn2.75	-	oS16	(38, Amm2)	-	2	(SN)3(Y)1
TA3SN_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(TA)3(SN)1
V3SN_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(SN)0.205(V)0.795
VZN3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(V)1(ZN)3
Y1ZN3	Zn3Y	-	oP16	(62, Pnma)	-	2	(Y)1(ZN)3
ZN3ZR_HT	Unknown Structure	-	c**	-	-	2	(ZN)3(ZR)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AG35N_L60	beta-TiCu <sub>3</sub> (D0a)	D0a	oP8	(59, Pmmn)	a binary phase in Ag-Sn system, and a ternary phase in Cu-Ni-Sn system	2	(Cu, Ni) <sub>0.75</sub> (Ni, Sn) <sub>0.25</sub>
AL13CO4	Orthorhombic Co <sub>4</sub> Al <sub>13</sub> (Approximate Quasicrystal)	-	oP102	(31, Pmn2 <sub>1</sub> )	-	2	(Al) <sub>13</sub> (Co, Fe, Mn) <sub>4</sub>
AL5CO2_D811	Co <sub>2</sub> Al <sub>5</sub> (D811)	D811	hP28	(194, P6 <sub>3</sub> /mmc)	also Al <sub>5</sub> Rh <sub>2</sub> .	2	(Al) <sub>5</sub> (Al, Co, Fe, Mn, Rh) <sub>2</sub>
AL9CO2	Co <sub>2</sub> Al <sub>9</sub> (D8d)	D8d	mP22	(14, P2 <sub>1</sub> /c)	also Al <sub>9</sub> Rh <sub>2</sub>	2	(Al) <sub>9</sub> (Co, Fe, Rh) <sub>2</sub>
AL9M2	Co <sub>2</sub> Al <sub>9</sub> (D8d)	D8d	mP22	(14, P2 <sub>1</sub> /c)	aka Al <sub>9</sub> FeNi, metastable Al <sub>9</sub> Fe <sub>2</sub>	2	(Al) <sub>9</sub> (Fe, Ni) <sub>2</sub>
ALCOMN_T	Mn <sub>6</sub> Cu <sub>4</sub> Al <sub>29</sub>	-	oS156	(63, Cmcm)	-	3	(Al) <sub>0.794</sub> (Co) <sub>0.02</sub> (Mn) <sub>0.186</sub>
AL11CR2	Al <sub>5</sub> Cr	-	mS732	(15, C2/c)	-	3	(Al) <sub>10</sub> (Al) <sub>1</sub> (Cr) <sub>2</sub>
AL13CR2	Al <sub>4</sub> V <sub>7</sub>	-	mS104	(12, C2/m)	-	2	(Al) <sub>13</sub> (Cr) <sub>2</sub>
AL4CR	mu-Al <sub>4</sub> Mn	-	hP574	(194, P6 <sub>3</sub> /mmc)	-	2	(Al) <sub>4</sub> (Cr) <sub>1</sub>
AL8CR5_LT_D810	Cr <sub>5</sub> Al <sub>8</sub> (D810)	D810	hR26	(160, R3m)	-	2	(Al) <sub>8</sub> (Cr, V) <sub>5</sub>
AL9CR4_HT	Unknown Structure	-	-	-	-	2	(Al) <sub>9</sub> (Cr) <sub>4</sub>
AL9CR4_LT	Unknown Structure	-	-	-	-	2	(Al) <sub>9</sub> (Cr) <sub>4</sub>
ALCU_DELTA	Al <sub>5</sub> Cu <sub>8</sub>	-	hR52	(160, R3m)	-	2	(Al) <sub>2</sub> (Cu, Fe) <sub>3</sub>
ALCU_ZETA	Al <sub>9</sub> Cu <sub>11</sub> (h)	-	oF88	(42, Fmm2)	united HT-zeta1 and LT-zeta2.	2	(Al) <sub>9</sub> (Cu, Fe) <sub>11</sub>
AL23CUFE4_D2H	MnAl <sub>6</sub> (D2h)	D2h	oS28	(63, Cmcm)	-	3	(Al) <sub>23</sub> (Cu) <sub>1</sub> (Fe) <sub>4</sub>
AL62CU25FE13	Quasicrystal	-	-	-	-	3	(Fe) <sub>0.125</sub> (Al, Cu) <sub>0.255</sub> (Al) <sub>0.62</sub>
AL7CU2FE	FeCu <sub>2</sub> Al <sub>7</sub> (E9a)	E9a	tP40	(128, P4/mnc)	-	3	(Fe, Ni) <sub>1</sub> (Cu) <sub>2</sub> (Al) <sub>7</sub>

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL10CU10FE	(Al <sub>10</sub> Cu <sub>10</sub> Fe)	-	oF116	(42, Fmm2)	-	3	(FE) <sub>1</sub> (AL, CU) <sub>10</sub> (AL) <sub>10</sub>
AL7CU4NI	(Cu <sub>0.8</sub> Ni <sub>0.2</sub> ) <sub>2.53</sub> Al <sub>3.5</sub>	-	hR14	(166, R-3m)	-	2	(AL) <sub>1</sub> (FE, CU, NI, VA) <sub>1</sub>
AL28CU4MN7	Mn <sub>6</sub> Cu <sub>4</sub> Al <sub>29</sub>	-	oS156	(63, Cmcn)	Tau <sub>1</sub> , Mn <sub>6</sub> +xCu <sub>4</sub> +yAl <sub>29</sub> -x-y.	3	(AL) <sub>28</sub> (MN) <sub>7</sub> (CU) <sub>4</sub>
AL11CU5MN3	Unknown Structure	-	oP380	-	Tau <sub>2</sub>	3	(AL) <sub>11</sub> (MN) <sub>3</sub> (CU) <sub>5</sub>
ALCU3MN2_C15	Cu <sub>2</sub> Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	Tau <sub>3</sub> .	3	(AL) <sub>1</sub> (MN) <sub>2</sub> (CU) <sub>3</sub>
AL5CU4ZN	Unknown Structure	-	-	-	-	4	(AL, CU) <sub>1</sub> (AL) <sub>4</sub> (CU) <sub>4</sub> (ZN) <sub>1</sub>
AL13FE4	Al <sub>13</sub> Fe <sub>4</sub>	-	mS102	(12, C2/m)	solid- solution of Al <sub>13</sub> Fe <sub>4</sub> (aka Al <sub>3</sub> Fe) & Al <sub>13</sub> Ru <sub>4</sub> .	3	(AL, CU) <sub>0.6275</sub> (CO, FE, MN, NI, RU) <sub>0.235</sub> (AL, SI, VA) <sub>0.1375</sub>
AL5FE2	Al <sub>2.8</sub> Fe	-	oS24	(63, Cmcn)	-	2	(AL, CU) <sub>5</sub> (CO, FE, MN, NI) <sub>2</sub>
AL5FE4_D82	gamma-Brass (Cu <sub>5</sub> Zn <sub>8</sub> , D82)	D82	cl52	(217, I-43m)	also AL <sub>8</sub> FE <sub>5</sub> _D82	1	(AL, CU, FE) <sub>1</sub>
AL16FEMN3	mu-Al <sub>4</sub> Mn	-	hP574	(194, P6 <sub>3</sub> /mmc)	Tau <sub>1</sub>	2	(AL) <sub>4</sub> (FE, MN) <sub>1</sub>
AL13FE2MN2	Al <sub>13</sub> Fe <sub>4</sub>	-	mS102	(12, C2/m)	Tau <sub>2</sub> .	2	(FE, MN) <sub>4</sub> (AL) <sub>13</sub>
AL10FEMN2	Mn <sub>3</sub> Al <sub>10</sub>	-	hP26	(194, P6 <sub>3</sub> /mmc)	Tau <sub>3</sub> .	2	(FE, MN) <sub>3</sub> (AL) <sub>10</sub>
AL10FE3NI	Co <sub>2</sub> Al <sub>5</sub> (D811)	D811	hP28	(194, P6 <sub>3</sub> /mmc)	-	2	(AL) <sub>5</sub> (FE, NI) <sub>2</sub>
AL71FE5NI24	Unknown Structure	-	-	-	-	3	(AL) <sub>0.71</sub> (FE) <sub>0.05</sub> (NI) <sub>0.24</sub>
AL9IR2	Co <sub>2</sub> Al <sub>9</sub> (D8d)	D8d	mP22	(14, P2 <sub>1</sub> /c)	-	2	(AL) <sub>0.818</sub> (IR) <sub>0.182</sub>
AL45IR13	Al <sub>45</sub> Ir <sub>13</sub>	-	oP236	(62, Pnma)	-	2	(AL) <sub>0.776</sub> (IR) <sub>0.224</sub>
AL13IR4	Unknown Structure	-	-	-	-	2	(AL) <sub>0.765</sub> (IR) <sub>0.235</sub>

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL28IR9	Al28Ir9	-	hP236	(159, P31c)	-	2	(AL)0.757(IR)0.243
AL5IR2	Al2.75Ir	-	cP60	(195, P23)	-	2	(AL)0.73(IR)0.27
AL12MN_GPHASE	Al12W	-	cI26	(204, Im-3)	-	2	(AL)12(MN)1
AL4MN_LAMBDA	lambda-Al4Mn	-	hP586	(176, P6_3/m)	also AL461MN107	2	(AL)461(MN, FE)107
AL4MN_MU	mu-Al4Mn	-	hP574	(194, P6_3/mmc)	-	2	(AL)4(MN)1
AL11MN4_LT	Al11Mn4	-	aP15	(2, P-1)	-	2	(AL)11(MN, FE)4
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25	-	oP156	(62, Pnma)	-	2	(AL, MN)29(MN)10
AL8MN5_D810	Cr5Al8 (D810)	D810	hR26	(160, R3m)	-	3	(AL, Ti, ZN)12(CO, MN)5(AL, CU, MN, SI, TI)9
AL6MN_D2H	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)	also Al6Re, Al6Ru	2	(AL)6(FE, MN, RE, RU)1
AL31MN6NI2	mu-Al4Mn	-	hP574	(194, P6_3/mmc)	-	3	(AL)31(MN)6(NI)2
TI25MN9AL66_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	also Ti25Mn8Al67 or Ti43Mn11Al66, Tau1.	2	(AL, MN, TI)0.75(AL, MN, TI)0.25
AL24MN5ZN	Unknown Structure	-	-	-	ternary Tau1 phase	3	(MN, ZN)5(ZN)1(AL)24
AL9MN2ZN	Unknown Structure	-	-	-	ternary Tau2 phase	3	(MN)2(ZN)1(AL)9
AL11MN3ZN2	Unknown Structure	-	oS152	-	ternary Tau3 phase	3	(MN)3(ZN)2(AL)11
AL63MO37	Unknown Structure	-	-	-	Mo3Al5_HT	2	(AL)63(MO)37
AL8MO3	Al8Mo3	-	mS22	(12, C2/m)	-	2	(AL)8(MO)3
ALMO_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	improper modelling.	2	(AL, MO)1(AL, MO)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3NI5	Ga3Pt5	-	oS16	(65, Cmmm)	-	2	(AL)0.375(NI)0.625
AL3NI2_D519	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)	also Al3Ru2.	3	(AL, SI, SN, ZN)3(AL, CU, FE, NI, RU)2(RU, NI, VA)1
AL13NI2TI5_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	Tau1	3	(AL)13(NI)2(TI)5
ALNI2ZN	Unknown Structure	-	-	-	-	3	(AL)0.25(NI)0.5(ZN)0.25
AL13NI38ZN49	Unknown Structure	-	-	-	-	3	(AL)0.13(NI)0.38(ZN)0.49
AL11RE4	Al11Mn4	-	aP15	(2, P-1)	-	2	(AL)11(RE)4
AL4RE	Al4Re	-	aP71	(2, P-1)	-	2	(AL)4(RE)1
AL5RH2_HT	beta-Al5Rh2	-	cP54	(195, P23)	-	2	(AL)2(RH, VA)1
AL7RH3_HT	Unknown Structure	-	mP*	-	-	2	(AL)7(RH)3
AL15SI2M4_TAU9	Al15(Mn, Fe)3Si2	-	cl168	(204, Im-3)	-	3	(AL)14(FE, MN)4(AL, SI)5
ALS13TI2	Zr3Al4Si5	-	tl24	(141, I4_1/amd)	aka Ti7Al5Si12, Tau1	3	(AL)0.166667(SI)0.5(TI)0.333333
AL3TI_LT	Al3Ti-LT	-	tl32	(139, I4/mmm)	-	2	(AL, TI)3(AL, TI, ZR)1
AL5TI2_HT	Al5Ti2	-	tP28	(123, P4/mmm)	-	2	(AL, TI)5(AL, NB, TA, TI, V, ZR)2
AL5TI3	Al5Ti3	-	tP32	(127, P4/mbm)	-	2	(AL)5(TA, TI)3
AL21V2	Al10V	-	cF176	(227, Fd-3m)	-	2	(AL)21(V)2
AL45V7	Al45V7	-	mS104	(12, C2/m)	aka Al7V	2	(AL)45(V)7
AL23V4	Al23V4	-	hP54	(194, P6_3/mmc)	-	2	(AL)23(V)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL8V5_D82	gamma-Brass (Cu5Zn8, D82)	D82	cl52	(217, I-43m)	-	2	(AL, V)8(AL, CR, V, Zr)5
AL77W23	Unknown Structure	-	-	-	-	2	(AL)77(W)23
AL7W3	Unknown Structure	-	-	-	-	2	(AL)7(W)3
AL12W_GPHASE	Al12W	-	cl26	(204, Im-3)	also Al12Mo, Al12Re.	2	(AL)12(MO, RE, W)1
AL4W	Al4W	-	mS30	(8, Cm)	also Al4Mo.	2	(AL)4(MO, W)1
AL5W	Al5W	-	hP12	(182, P6_322)	also Al5MO.	2	(AL)5(MO, W)1
AL2ZR3	Zr3Al2	-	tP20	(136, P4_2/mnm)	also Al2Hf3, Al2Y3.	2	(AL)2(HF, TI, Y, ZR)3
AL3ZR2	Zr2Al3	-	oF40	(43, Fdd2)	also Al3Hf2.	2	(AL)3(HF, ZR)2
AL3ZR4	Al3Zr4	-	hP7	(191, P6/mmm)	also Al3Hf4.	2	(AL)3(HF, TI, ZR)4
AL3ZR5_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	-	2	(AL)3(TI, ZR)5
AL4ZR5	Ti5Ga4	-	hP18	(193, P6_3/mcm)	-	2	(AL)4(ZR)5
CO10CU57TI33	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	Strukturbericht C11B.	3	(CO)0.1(CU)0.57(TI)0.33
CO7HF	(Co11Hf2)	-	oP*	(50, Pban)	-	2	(CO)7(HF)1
COSNTI_TAU2	Half-Heusler (AgAsMg, C1b)	C1b	cF12	(216, F-43m)	aka TiCoSn.	3	(CO, NI)1(SN)1(TI)1
CO3Y2	Unknown Structure	-	cP*	-	-	2	(CO)3(Y)2
CO3Y4	Co3Ho4	-	hP22	(176, P6_3/m)	-	2	(CO)3(Y)4
CO5Y_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	-	3	(CO2, Y)1(CO)4(CO, VA)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CO5Y8	Co5Y8	-	mP52	(14, P2_1/c)	-	2	(CO)5(Y)8
CO7NB2	(Co7Nb2)	-	mS18	(12, C2/m)	-	2	(CO)7(NB)2
CO7TA2	BaPb3	-	hR12	(166, R-3m)	-	2	(CO)7(TA)2
CO7Y6	Unknown Structure	-	-	-	-	2	(CO)7(Y)6
CO17Y2	Ni17Th2	-	hP38	(194, P6_3/mmc)	united HT/LT phase.	3	(CO2, Y)1(CO2, Y)2(CO)15
COZN_LT_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)	-	2	(CO, ZN)1(VA)1
COZN_HT	Unknown Structure	-	-	-	-	2	(CO, ZN)1(VA)1
COZN_GAMMA_D82	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	aka Zn11Co2, COZN4_D83.	2	(CO, ZN)1(VA)1
COZN_DELTA	Unknown Structure	-	-	-	Zn15Co2 HT phase	2	(CO)0.117647(ZN)0.882353
COZN_GAMMA1	Co2Zn15	-	mS28	(12, C2/m)	aka CoZn7.8	2	(CO)0.125(ZN)0.875
COZN_GAMMA2	CoZn13	-	mS28	(12, C2/m)	aka CoZn13	2	(CO)0.0714286(ZN)0.9285714
CO11ZR2	(Co11Hf2)	-	oP*	(50, Pban)	-	2	(CO)11(ZR)2
CRZN13	Unknown Structure	-	m**	-	-	2	(CR)1(ZN)13
CRZN17	Unknown Structure	-	hP*	-	-	2	(CR)1(ZN)17
CU51HF14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)51(HF)14
CU8HF3	Cu8HF3	-	oP44	(62, Pnma)	-	2	(CU)8(HF)3
CU10HF7	Ni10Zr7	-	oS68	(64, Cmce)	-	2	(CU)10(HF)7
CU5MN4SI	Unknown Structure	-	-	-	-	3	(CU)0.5(MN)0.37(SI)0.13

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU4MNSN_TAU1	MgCu4Sn	-	cF24	(216, F-43m)	-	3	(CU)0.6666(SN)0.1667(MN)0.1667
CUMNZN_TAU1	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	3	-
CU6NISI3	Unknown Structure	-	-	-	-	2	-
CU46NI25SI29	Unknown Structure	-	-	-	-	3	-
CU33SI7_DELTA	Unknown Structure	-	-	-	HT phase	2	(CU)0.825(SI)0.175
CU15SI4_EPS_D86	Cu15Si4 (D86)	D86	cI76	(220, I-43d)	-	2	(CU, MN)0.789474(AL, SI)0.210526
CU56SI11_GAMMA_A13	Mg3Ru2	-	cP20	(213, P4_132)	-	2	(CU, MN, NI, SI)0.835821(SI)0.164179
CU3SI_ETA	Cu3Si-h2	-	hR*	(162, P-31m)	United 3-allotropes: eta <sup>1</sup> -RT (oS* *), eta <sup>1</sup> -HT1(hR27 R-3), eta-HT2(hR* P-31m)	2	(CU, MN, NI)0.76(SI)0.24
CU6SN5_HT	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	also Co3Sn2, Mn(2-x)Sn, Ni3Sn2.	3	(CO, CU, MN, NI, VA)1(AL, CU, NI, SN)1(CO, CU, MN, NI, VA)1
CU6SN5_LT	Cu6Sn5	-	mS44	(15, C2/c)	eta-prime.	3	(CU)1(CU, SN)1(SN)1
CU10SN3	Cu10Sn3	-	hP26	(173, P6_3)	zeta.	2	(CU, NI)0.769(SN)0.231
CU41SN11	Cu41Sn11	-	cF416	(216, F-43m)	delta.	2	(CU, SN, ZN)41(CU, SN, ZN)11
CU3TI2	Cu3Ti2	-	tP10	(129, P4/nmm)	-	2	(CU, NI, FE)3(CO, TI)2
CU4TI1	Au4Zr	-	oP20	(62, Pnma)	-	2	(CU, TI)4(CU, TI)1
CU4TI3	Cu4Ti3	-	tI14	(139, I4/mmm)	-	2	(CO, CU, NI)4(TI)3
CU2TIZR	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	-	3	(CU)0.5(TI)0.25(ZR)0.25

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU7Y1	Cu7Tb	-	hP8	(191, P6/mmm)	aka Cu6Y or Cu5.4Y0.8	2	(CU2, Y)1(CU)5
CU4Y	Cu5Y1.25	-	mP16	(11, P2_1/m)	-	2	(CU)4(Y)1
CU7Y2	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)7(Y)2
CUMNZN_EPSILON_HCP	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)	-	2	(CU, MN, ZN)1(VA)0.5
CU10ZR7	Ni10Zr7	-	oS68	(64, Cmce)	-	2	(CU)10(ZR)7
CU51ZR14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)51(ZR)14
CU8ZR3	Cu8Hf3	-	oP44	(62, Pnma)	-	2	(CU)8(ZR)3
FENBZR_CFC2_C15	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	3	(FE, NB, ZR)2(NB, ZR)1(NB, ZR)3
FE3SN2	Fe3Sn2	-	hR10	(166, R-3m)	-	2	(FE)3(SN)2
FE5SN3_B82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(FE)5(SN)3
FENBSI2	CrSi2Zr	-	oP48	(55, Pbam)	-	3	(FE)1(NB)1(SI)2
FE4NB4SI7	Co4Ge7Zr4	-	tI60	(139, I4/mmm)	-	3	(FE)4(NB, TA)4(SI)7
FENBSI_C23	MnCuP	-	oP12	(62, Pnma)	-	3	(FE)1(NB)1(SI)1
FE3NB4SI5	Fe3Nb4Si5	-	oP72	(31, Pmn2_1)	-	3	(FE)3(NB)4(SI)5
FENB2SI2	FeNb2Si2	-	tP198	(132, P4_2/mcm)	-	3	(FE)1(NB)2(SI)2
FENB4SI	Nb4CoSi	-	tP12	(124, P4/mcc)	-	3	(FE)1(NB)4(SI)1
FE3TA3SI4	Unknown Structure	-	-	-	-	3	(FE)3(TA)3(SI)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FE3ZN7_GAMMA_D82	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(FE, ZN)0.154(FE, ZN)0.154(FE, ZN)0.231(ZN)0.461
FEZN4_GAMMA1_D81	Fe11Zn40	-	cF408	(216, F-43m)	-	3	(FE)0.137(FE, ZN)0.118(ZN)0.745
FEZN10_DELTA	FeZn10	-	hP632	(194, P6_3/mmc)	-	4	(FE)0.058(FE, ZN)0.18(ZN)0.525(ZN)0.237
FEZN13_ZETA	CoZn13	-	mS28	(12, C2/m)	-	3	(FE, VA)0.072(ZN)0.856(VA, ZN)0.072
CU3SN_HT_GAMMA	BiF3 (D03)	D03	cF16	(225, Fm-3m)	Cu3Sn HT solution phase	1	(CU, MN, NI, SN, ZN)1
HF5IR3	Ir3Zr5	-	hP48	(178, P6_122)	-	2	(HF)5(IR)3
HF3NI7	Hf3Ni7	-	aP20	(2, P-1)	-	2	(HF)0.3(NI)0.7
HF8NI21	Hf8Ni21	-	aP29	(2, P-1)	also ZR8NI21.	2	(HF, ZR)8(NI)21
HF3RH4	Unknown Structure	-	-	-	-	2	(HF)3(RH)4
HF3RH5	Rh5Ge3	-	oP16	(55, Pbam)	-	2	(HF)3(RH)5
HF5SN4	Ti5Ga4	-	hP18	(193, P6_3/mcm)	-	2	(HF)5(SN)4
IR2Y3	Y3Rh2	-	tI140	(140, I4/mcm)	-	2	(IR)2(Y)3
IR2Y5	Mn5C2 (Fe5C2 Hagg carbide)	-	mS28	(15, C2/c)	-	2	(IR)2(Y)5
IR3Y5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	united HT/LT phase.	2	(IR)3(Y)5
IR3ZR5	Ir3Zr5	-	hP48	(178, P6_122)	-	2	(IR)3(ZR)5
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)	-	2	(MN)3(SN)2
MNTI_HT	Unknown Structure	-	t**	-	aka TiMn Mn+ or Ti0.47Mn0.53	2	(MN)0.515(TI)0.485

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN4TI	R-(Co, Cr, Mo)	-	hR53	(148, R-3)	aka Ti9Mn42	2	(CR, MN)0.815(TI)0.185
MN12Y_D2B	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)	-	2	(MN)12(Y)1
MNZN9	Unknown Structure	-	h**	-	-	2	(MN)1(ZN)9
MO7IR3	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)	-	2	(MO)0.7(IR)0.3
MONI4_BETA_D1A	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)	also WNi4.	2	(MO, W)1(NI)4
MONI_DELTA	MoNi	-	oP56	(19, P2_12_12_1)	-	3	(CO, CR, FE, NI, RE)24(CO, CR, FE, MO, NI, RE, W)20(CU, MO, W)12
MOZN7	Ca7Ge	-	cF32	(225, Fm-3m)	-	2	(MO)1(ZN)7
MOZN22	Zn93(Zn0.43Mo0.57)Mo4	-	cF420	(216, F-43m)	-	2	(MO)1(ZN)22
NB15NI56TI29_XA	Unknown Structure	-	o*100	-	-	3	(NB)0.15(NI)0.56(TI)0.29
NB8NI9TI3_XB	Unknown Structure	-	-	-	-	3	(NB)0.4(NI)0.45(TI)0.15
NB5NI75TI20_XC	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	3	(NB)0.05(NI)0.75(TI)0.2
NB13NI75TI12_XD	Unknown Structure	-	-	-	-	3	(NB)0.13(NI)0.75(TI)0.12
NB15NI80TI5_XE	Unknown Structure	-	-	-	-	3	(NB)0.15(NI)0.8(TI)0.05
NB3RU5	Rh5Ge3	-	oP16	(55, Pbam)	united Nb3Ru5_HT and NbRu3_LT phase	2	(NB, RU)0.375(RU)0.625
NBRH_ETA	Al3Pu	-	hP24	(194, P6_3/mmc)	-	2	(NB, RH)1.3(RH)2.7
NBRH_ZETA	Unknown Structure	-	-	-	-	2	(NB)3(NB, RH)5
NBRH_EPSILON	beta'-AuCd (B19)	B19	oP4	(51, Pmma)	-	2	(NB, RH)0.85(RH)1.15

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NBRH_DELTA	TaIr	-	oP12	(51, Pmma)	-	2	(NB)0.9(RH)1.1
NBSN2_CB	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	-	2	(NB, SN, V)1(NB, SN)2
NBZN7	Unknown Structure	-	-	-	-	2	(NB)0.125(ZN)0.875
NBZN15	TiZn16	-	oS68	(63, Cmcm)	-	2	(NB)0.0625(ZN)0.9376
NB2ZN3_D85	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	-	2	(NB)0.4(ZN)0.6
NI5TA8SI7	Unknown Structure	-	-	-	-	3	(NI)5(TA)8(SI)7
NI8M	Pt8Ti	-	tI18	(139, I4/mmm)	also Ni8Ta, Ni8Nb.	2	(NI)8(NB, TA)1
NI7ZR2	Ni7Zr2	-	mS36	(12, C2/m)	also Ni7HF2, Ni7Y2, CO7HF2 and CO7Y2.	2	(AL, CO, CR, NI)7(HF, Y, ZR)2
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	(12, C2/m)	-	3	(CU, NI)0.25(NI, SN)0.25(SN)0.5
NISNZR	Half-Heusler (AgAsMg, C1b)	C1b	cF12	(216, F-43m)	-	3	(NI)1(SN)1(ZR)1
NISN2ZR6	Barringerite (Revised Fe2P, C22)	C22	hP9	(189, P-62m)	-	3	(NI)1(SN, ZR)2(ZR)6
NI2SNZR2	U2Pt2Sn	-	tP20	(136, P4_2/mnm)	-	3	(NI)2(SN, ZR)1(ZR)2
NI2Y3	Ni2Y3	-	tP80	(92, P4_12_12)	-	2	(NI)2(Y)3
NI44M56_TAU	Unknown Structure	-	-	-	-	2	(NI)0.44(HF, TI)0.56
NI4Y	Unknown Structure	-	hR*	-	-	2	(NI)4(Y)1
NI17Y2	Fe17Lu2	-	hP80	(194, P6_3/mmc)	also Fe17Y2.	2	(AL, FE, NI)1(Y)0.1176
NI3N8_DELTA	Ni3Zn22	-	mS50	(12, C2/m)	-	2	(NI)0.111111(AL, ZN)0.888889

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI11ZR9	Pt11Zr9	-	tI40	(87, I4/m)	also Ni11Hf9.	2	(NI)11(HF, TI, ZR)9
NI10ZR7	Ni10Zr7	-	oS68	(64, Cmce)	also Ni10Hf7.	2	(NI)23(HF, TI, ZR)17
NI5ZR_C15B	AuBe5 (C15b)	C15b	cF24	(216, F-43m)	also Ni5Y/Ni5Hf/Cu5Hf/Cu5Zr, aka ZRM5_C15B.	2	(AL, CU, NI, SN)5(HF, Y, ZR)1
RE3NB_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	3	(RE)24(NB, V, W)10(NB, V, RE, W)24
RHSN4	IrGe4	-	hP15	(152, P3_121)	-	2	(RH)1(SN)4
RH3SN2	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	3	(RH)0.125(RH)0.5(SN)0.375
RH12TA8	Rh12Ta8	-	oP12	(51, Pmma)	-	2	(RH, TA)1.2(TA)0.8
RH5TA4	Unknown Structure	-	-	-	-	2	(RH, TA)5(TA)4
RH5TI3	Rh5Ge3	-	oP16	(55, Pbam)	-	2	(RH)5(TI)3
RH5V3	Rh5V3	-	oS16	(63, Cmcm)	-	2	(RH)5(V)3
RH5Y_HT	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	-	2	(RH)5(Y)1
RH2Y3	Y3Rh2	-	tI140	(140, I4/mcm)	-	2	(RH)2(Y)3
RH3Y5	Unknown Structure	-	-	-	-	2	(RH)3(Y)5
RH3Y7	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)	-	2	(RH)3(Y)7
RH4ZR3_LT	Pd4Pu3	-	hR14	(148, R-3)	alpha_Rh4Zr3.	2	(RH, ZR)4(ZR)3
RH4ZR3_HT	Unknown Structure	-	-	-	beta_Rh4Zr3	2	(RH, ZR)4(ZR)3
RH5ZR3	Pd5Pu3	-	oS32	(63, Cmcm)	-	2	(RH)5(RH, ZR)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RU3SN7_D8F	Ir3Ge7 (D8f)	D8f	cl40	(229, Im-3m)	-	2	(RU)0.3(SN)0.7
RU2SN3	Ru2Sn3	-	tP20	(116, P-4c2)	-	2	(RU)0.4(SN)0.6
RU2Y3	Er3Ru2	-	hP10	(176, P6_3/m)	-	2	(RU)0.4(Y)0.6
RU25Y44	Ru25Y44	-	oP276	(52, Pnna)	-	2	(RU)0.362(Y)0.638
RU2Y5	Mn5C2 (Fe5C2 Hagg carbide)	-	mS28	(15, C2/c)	-	2	(RU)0.286(Y)0.714
SN3TI2	Unknown Structure	-	-	-	-	2	(SN)3(TI)2
SN5TI6	Sn5Ti6-beta	-	hP22	(194, P6_3/mmc)	also Sn5Nb6.	2	(AL, SN)5(NB, TI)6
SN5Y2	Shcherbinaite (V2O5) (Revised)	-	oP14	(59, Pmmn)	-	2	(SN)5(Y)2
SN10Y11	Ge10Ho11	-	tI84	(139, I4/mmm)	-	2	(SN)10(Y)11
SN4Y5	Gd5Si4	-	oP36	(62, Pnma)	-	2	(SN)4(Y)5
TA1AL1	Al38Ta48	-	mP86	(14, P2_1/c)	-	2	(TA)0.51515(AL)0.48485
TAAL2_HT	Al69Ta39	-	cF444	(216, F-43m)	-	2	(TA)0.35(AL)0.65
TA41IR59	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	aka Ta0.82Ir1.18_rt, gamma.	2	(TA)0.41(IR)0.59
TA43IR57	TaIr	-	oP12	(51, Pmma)	aka Ta0.86Ir1.14, delta.	2	(TA)0.43(IR, TA)0.57
T1CUNITI_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	the Cu-Ni-Ti ternary phase Tau1.	2	(CU, NI)2(TI)1
T2CUNITI	Cu3Ti2	-	tP10	(129, P4/nmm)	the Cu-Ni-Ti ternary phase Tau2.	3	(CU)0.175(NI)2.825(TI)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
T4CUNITI	BaPb3	-	hR12	(166, R-3m)	the Cu-Ni-Ti ternary phase Tau4.	3	(CU)0.05(NI)0.7(TI)0.25
T6CUNITI	Unknown Structure	-	-	-	the Cu-Ni-Ti ternary phase Tau6	3	(CU)0.25(NI)0.5(TI)0.25
T1CUFETI_CU2TI	Au2V	-	oS12	(63, Cmc)	ternary Ti0.33FexCu0.67-x, Tau1.	2	(CU, FE)2(TI)1
T2CUFETI_CU3TI2	Cu3Ti2	-	tP10	(129, P4/nmm)	ternary Ti0.4FexCu0.6-x, Tau2.	2	(CU, FE)3(TI)2
T3CUFETI_CU4TI3	Cu4Ti3	-	tl14	(139, I4/mmm)	ternary Ti0.43FexCu0.57-x, Tau3.	2	(CU, FE)4(TI)3
T4CUFETI	Unknown Structure	-	-	-	ternary Ti0.37FexCu0.63-x, Tau4	2	(CU, FE)0.63(TI)0.37
T5CUFETI	Unknown Structure	-	-	-	ternary Ti0.45FexCu0.55-x, Tau5.	2	(CU, FE)0.55(TI)0.45
TIZN5	Unknown Structure	-	-	-	-	2	(TI)1(ZN)5
TIZN10	Ti3Zn22	-	tP100	(135, P4_2/mbc)	-	2	(TI)1(ZN)10
TIZN15	TiZn16	-	oS68	(63, Cmc)	-	2	(TI)1(ZN)15
V4ZN5	V4Zn5	-	tl18	(139, I4/mmm)	-	2	(V)4(ZN)5
Y2ZN17	Ni17Th2	-	hP38	(194, P6_3/mmc)	-	2	(Y)2(ZN)17
Y13ZN58	Y13Zn58	-	hP146	(194, P6_3/mmc)	-	2	(Y)13(ZN)58
YZN5	ErZn5	-	hP36	(194, P6_3/mmc)	aka H_RZN5	2	(Y)1(ZN)5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZN12Y_D2B	Mn12Th (D2b)	D2b	ti26	(139, I4/mmm)	-	2	(ZN)12(Y)1
ZN11Y3	Al11La3	-	ol28	(71, Immm)	-	2	(ZN)11(Y)3
ZN22ZR	Zn22Zr	-	cF184	(227, Fd-3m)	-	2	(ZN)22(ZR)1
ZN39ZR5	Zn39Zr5	-	mS88	(12, C2/m)	-	2	(ZN)39(ZR)5
ZN2ZR3	Zr3Al2	-	tP20	(136, P4_2/mnm)	-	2	(ZN)2(ZR)3
GAS	Gas	-	-	-	-	1	(AL, AL1C1, AL1C2, AL1CU1, AL1N1, AL2, AL2C2, B, B1C1, B1C2, B1N1, B2, B2C1, C, C1R1, C1N1, C1N2_CNN, C1N2_NCN, C1RH1, C1S1, C1S2, C1S3, C1S4, C2, C2N1_CCN, C2N1_CNC, C2N2, C2S1, C2S2, C2S3, C3, C3N1, C4, C4N1, C4N2, C5, C5N1, C6, C6N1, C6N2, C9N1, CO, CO2, CR, CR1N1, CR2, CU, CU2, FE, FE2, HF, IR, MN, MO, MO1N1, MO2, N, N1NB1, N1S1, N1S2, N1T1, N1V1, N1ZR1, N2, N3, NB, NI, NI2, RE, RH, RU, SI, SI2, SI3, SN, SN2, TA, TI, TI2, V, W, Y, ZN, ZR, ZR2, AL1B1O2, AL1O1, AL1O2, AL2O1, AL2O2, AL2O3, B1O1, B1O2, B2O1, B2O2, B2O3, C1N1O1_NCO, C1N1O1, C1O1, C1O2, C2O1, C3O2, C4N1O4, C5FE1O5, C6MO1O6, CO1O1, CR1O1, CR1O2, CR1O3, CR2O1, CR2O2, CR2O3, CU1O1, FE1O1, FE1O2, HF1O1, HF1O2, MN1O1, MN1O2, MO1O1, MO1O2, MO1O3, MO2O6, MO3O9, MO4O12, MO5O15, N1O1, N1O2, N1O3, N2O1, N2O2, N2O3, N2O4, N2O5, NB1O1, NB1O2, N1O1, O, O10V4, O12W4, O15W5, O1S1, O1T1, O1V1, O1W1, O1Y1, O1Y2, O1ZR1, O2, O2S1, O2S2, O2T1, O2V1, O2W1, O2Y1, O2Y2, O2ZR1, O3, O3W1, O6W2, O8W3, O9W3, IR1O1, IR1O2, IR1O3, O1RE1, O1RH1, O1RU1, O1SN1, O1TA1, O1ZN1, O2RE1, O2RH1, O2RU1, O2SN1, O2TA1, O3RE1, O3RU1, O4RU1, O6RE2, O7RE2)1
AF	FeGaO3	-	oP40	(33, Pna2_1)	This is Al2O3.Fe2O3.	3	(AL+3)2(FE+3)2(O-2)6
AL18B4O33	Al5BO9	-	oS60	(36, Cmc2_1)	-	3	(AL+3)18(B+3)4(O-2)33
AL4B2O9	Al4B1.5[BO3]0.5O7.5	-	mS124	(12, C2/m)	-	3	(AL+3)4(B+3)2(O-2)9

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALNB11O29	(Ti0.17Nb0.83)12O29	-	mS82	(12, C2/m)	-	3	(AL+3)1(NB+5)11(O-2)29
ALNB49O124	Unknown Structure	-	-	-	-	3	(AL+3)1(NB+5)49(O-2)124
ALPHA_SPINEL	Hausmannite (Mn3O4)	-	tl28	(141, I4_1/amd)	With solubility of Al, Co, Cr, Cu, Fe, Mg and Ni.	4	(CO+2, CU+2, MN+2, MN+3, NI+2)1(AL+3, CR+3, FE+3, MN+2, MN+3, VA)2(MN+2, VA)2(O-2)4
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	(58, Pnnm)	This is a high-pressure phase	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
APATITE	Fluorapatite [Ca5F(PO4)3, H57]	H57	hP42	(176, P6_3/m)	This is Ca2(Gd, Y)8(SiO4)6O2 and Mg2(Gd, Y)8(SiO4)6O2	4	(Y+3, ZR+4, VA)4(Y+3)6(SIO4-4)6(O-2, VA)2
B2O3	B2O3	-	hP15	(152, P3_121)	-	2	(B+3)2(O-2)3
BETA_V_O	CoO	-	tl4	(139, I4/mmm)	-	2	(V)1(O, VA)1
BRONZE	Unknown Structure	-	-	-	-	3	(V+4, V+5)2(O-2)5(FE+2, VA)1
CA2SIO4_ALPHA_A	Ca2SiO4	-	hP24	(194, P6_3/mmc)	This is 2CaO.SiO2 and 3CaO.P2O5.	3	(MN+2, Y+3)3(VA)1(BO3-3, SIO4-4)2
CA2SIO4_ALPHA_PRIME	K2CoCl4	-	oP84	(33, Pna2_1)	This is Ca2SiO4.	3	(FE+2, MN+2, Y+3)3(VA)1(BO3-3, SIO4-4)2
CACO3	Calcite (CaCO3, G01)	G01	hR10	(167, R-3c)	This is (Ca, Fe, Mg)CO3.	2	(FE+2)1(CO3-2)1
CAF2_S1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is low temperature CaF2.	2	(MN+2)1(O-2, VA)2
CAF2_S2	Cotunnite (PbCl2, C23)	C23	oP12	(62, Pnma)	This is high temperature CaF2.	2	(MN+2)1(O-2, VA)2
CAMO3	CaTiO3 Pnma Perovskite	-	oP20	(62, Pnma)	This is CaHfO3, CaMnO3, CaTiO3, It CaZrO3.	3	(Y+3)1(Y+3)1(O-2)3
CAV2O6	ThTi2O6	-	mS18	(12, C2/m)	This is CaV2O6, CoV2O6, MgV2O6, MnV2O6 and NiV2O6.	3	(CO+2, MN+2, NI+2)1(V+5)2(O-2)6
CAZRO3_C	Cubic Perovskite (CaTiO3,	E21	cP5	(221, Pm-3m)	Ba(Hf, Zr)O3 and High-	3	(Y+3)1(Y+3)1(O-2)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
	E21)				temperature Ca(Hf, Zr)O <sub>3</sub> .		
CLINO_PYROXENE	Diopside [CaMg(SiO <sub>3</sub> ) <sub>2</sub> , S41]	S41	mS40	(15, C2/c)	This is clino-enstatite (MgSiO <sub>3</sub> ), clino-ferrosilit (FeSiO <sub>3</sub> ), diopside (CaMgSi <sub>2</sub> O <sub>6</sub> ), niopside (CaNiSi <sub>2</sub> O <sub>6</sub> ), pigeonite ((Mg, Fe, Ca)Si <sub>2</sub> O <sub>6</sub> ), hedenbergite (CaFeSi <sub>2</sub> O <sub>6</sub> ) dissolving Co.	4	(FE+2, NI+2)1(CO+2, FE+2, NI+2)1(SI+4)2(O-2)6
COLUMBITE	Columbite (FeNb <sub>2</sub> O <sub>4</sub> , E51)	E51	oP36	(60, Pbcn)	This is (Ca, Co, Fe, Mg, Mn)Nb <sub>2</sub> O <sub>6</sub> with excess FeO and MgO.	3	(CO+2, FE+2, MN+2)1(FE+2, NB+5)2(O-2, VA)6
CORDIERITE	Na <sub>0.04</sub> (Mg <sub>0.5</sub> Fe <sub>0.5</sub> ) <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub>	-	oS120	(66, Cccm)	This is 2Al <sub>2</sub> O <sub>3</sub> .2MgO.5SiO <sub>2</sub> , 2Al <sub>2</sub> O <sub>3</sub> .2MnO.5SiO <sub>2</sub> and 2Al <sub>2</sub> O <sub>3</sub> .2FeO.5SiO <sub>2</sub>	4	(AL+3)4(FE+2, MN+2)2(SI+4)5(O-2)18
CORUNDUM	Corundum (alpha-alumina, Al <sub>2</sub> O <sub>3</sub> , D51)	D51	hR10	(167, R-3c)	This is Al <sub>2</sub> O <sub>3</sub> , Cr <sub>2</sub> O <sub>3</sub> , Fe <sub>2</sub> O <sub>3</sub> , Ti <sub>2</sub> O <sub>3</sub> , V <sub>2</sub> O <sub>3</sub> + (Co, Fe, Mg, Mn, Ni)TiO <sub>3</sub> Ilmenite.	2	(AL+3, CO+2, CR+3, FE+2, FE+3, MN+2, MN+3, NI+2, TI+3, TI+4, V+3, V+4, VA)2(O-2)3
CR2P4O13	Cr <sub>2</sub> P <sub>4</sub> O <sub>13</sub>	-	mP76	(14, P2 <sub>1</sub> /c)	This is Cr <sub>2</sub> P <sub>4</sub> O <sub>13</sub> , Cr <sub>2</sub> V <sub>4</sub> O <sub>13</sub> and Fe <sub>2</sub> V <sub>4</sub> O <sub>13</sub> .	3	(CR+3, FE+3)2(V+5)4(O-2)13
CR2TI2O7	Unknown Structure	-	-	-	with solubility of Al <sub>2</sub> O <sub>3</sub> and Fe <sub>2</sub> O <sub>3</sub> .	3	(AL+3, CR+3, FE+3)2(TI+4)2(O-2)7
CRISTOBALITE	Ideal beta-Cristobalite (SiO <sub>2</sub> , C9)	C9	cF24	(227, Fd-3m)	SiO <sub>2</sub> with AlPO <sub>4</sub> solubility.	2	(SI+4)1(SIO4-4)1
CRNB25O64	Unknown Structure	-	-	-	-	3	(CR+3)1(NB+5)25(O-2)64
CRNB49O124	Unknown Structure	-	-	-	-	3	(CR+3)1(NB+5)49(O-2)124
CRNB9O24	Unknown Structure	-	-	-	-	3	(CR+3)1(NB+5)9(O-2)24
CRNBO4	Rutile (TiO <sub>2</sub> , C4)	C4	tP6	(136, P4 <sub>2</sub> /mnm)	-	3	(CR+3, VA)1(CR+3, NB+5)1(O-2, VA)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CRVO4	MgSO4	-	oS24	(63, Cmcm)	-	3	(CR+3)1(V+5)1(O-2)4
CU2B4O7	Unknown Structure	-	-	-	-	3	(CU+1)2(B+3)4(O-2)7
CU2COO3	CaCu2O3	-	oP12	(59, Pmmn)	-	3	(CO+2)1(CU+2)2(O-2)3
CU2Y2O5	Cu2Ho2O5	-	oP36	(33, Pna2_1)	-	3	(CU+2)2(Y+3)2(O-2)5
CU3B2O6	Cu3B2O6	-	aP110	(2, P-1)	-	3	(CU+2)3(B+3)2(O-2)6
CU3NB2O8	Cu3(Ta0.5Nb0.5)2O8	-	aP13	(2, P-1)	-	3	(CU+2)3(NB+5)2(O-2)8
CUB2O4	CuB2O4	-	tI84	(122, I-42d)	-	3	(CU+2)1(B+3)2(O-2)4
CUB8O13	Unknown Structure	-	-	-	-	3	(CU+2)1(B+3)8(O-2)13
CUNB2O6	CuNb2O6	-	mP36	(14, P2_1/c)	-	3	(CU+2)1(NB+5)2(O-2)6
CUO	Tenorite (CuO, B26)	B26	mS8	(15, C2/c)	-	2	(CO+2, CU+2)1(O-2)1
CUPRITE	Cuprite (Cu2O, C3)	C3	cP6	(224, Pn-3m)	This is Cu2O with solubility of Na.	2	(CU+1)2(O-2)1
DELAFOSSITE	Rhombohedral Delafossite (CuFeO2)	-	hR4	(166, R-3m)	This is Cu(Al, B, Cr, Fe, La, Mn, Y)O2	3	(CU+1)1(AL+3, B+3, CR+3, FE+3, MN+3, Y+3)1(O-2)2
DYMN2O5	HoMn2O5	-	oP32	(55, Pbam)	This is Mn2(Gd, Y)O5.	4	(Y+3)1(MN+3)1(MN+4)1(O-2)5
FE3BO5	Fe3[BO3]O2	-	oP36	(55, Pbam)	-	4	(FE+2)2(FE+3)1(B+3)1(O-2)5
FE3BO6	Norbergite [Mg(F, OH)2. Mg2SiO6, S07]	S07	oP40	(62, Pnma)	-	3	(FE+3)3(B+3)1(O-2)6
FEB4O7	ZnB4O7	-	oS48	(63, Cmcm)	-	3	(FE+2)1(B+3)4(O-2)7
FEBO3	Calcite (CaCO3, G01)	G01	hR10	(167, R-3c)	-	3	(FE+3)1(B+3)1(O-2)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FENB14O36	Unknown Structure	-	-	-	This is (Co, Fe)Nb14O36	3	(CO+2, FE+2)1(NB+5)14(O-2)36
FENB25O64	Unknown Structure	-	-	-	-	3	(FE+3)1(NB+5)25(O-2)64
FENB36O91	Unknown Structure	-	-	-	This is (Co, Fe)Nb36O91	3	(CO+2, FE+2)1(NB+5)36(O-2)91
FENB49O124	Unknown Structure	-	-	-	-	3	(FE+3)1(NB+5)49(O-2)124
FENB68O171	Unknown Structure	-	-	-	This is (Co, Fe)Nb68O171	3	(CO+2, FE+2)1(NB+5)68(O-2)171
FENB9O24	Unknown Structure	-	-	-	-	3	(FE+3)1(NB+5)9(O-2)24
FEV2O6	Unknown Structure	-	-	-	-	3	(FE+2)1(V+5)2(O-2)6
FEVO4	Zn[MoO4]	-	aP36	(2, P-1)	This is FeVO4 and AlVO4.	3	(AL+3, FE+3)1(V+5)1(O-2)4
FLUORITE	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is cubic high temp HfO2 and ZrO2	2	(AL+3, CR+3, FE+2, HF+4, MN+2, MN+3, NB+5, NI+2, SI+4, TI+4, Y+3, ZR, ZR+4, VA)2(O-2, VA)4
GARNET	Orthorhombic Garnet	-	oF320	(70, Fddd)	This is Grossular, Uvarovite, Spessartine and Goldmanite Garnets and (Gd, Y, Yb)3(Al, Fe)5O12.	4	(FE+2, MN+2, Y+3)3(AL+3, CR+3, FE+3, V+3)2(AL+3, CR+3, FE+3, SI+4)3(O-2)12
HALITE	Rock Salt/Halite (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is BaO, CaO, CoO, FeO, MgO, MnO and NiO	2	(AL+3, CO+2, CO+3, CR+3, CU+2, FE+2, FE+3, MN+2, MN+3, NI+2, NI+3, TI+4, V+3, Y+3, ZR+4, VA)1(O-2)1
HATRURITE	Ca3(SiO4)O-b	-	hR81	(160, R3m)	This is 3CaO.SiO2	3	(Y+3, VA)3(SiO4-4)1(O-2)1
HFW2O8	Zr[WO4]2	-	cP44	(198, P2_13)	-	3	(HF+4)1(W+6)2(O-2)8
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	(2, P-1)	This is Al2O3.SiO2	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
LAAP	PrNiO3	-	hR10	(167, R-3c)	This is Rhombohedral Perovskite: La(Al, Co)O3 with solubility of Ca, Cu, Ni, Y	3	(Y+3)1(AL+3, CO+3, CU+2, FE+3, NI+2)1(O-2, VA)3
LAYP	CaTiO3 Pnma Perovskite	-	oP20	(62, Pnma)	This is an Orthorhombic Perovskite, La(Y, Yb)O3.	3	(Y+3)1(Y+3, ZR+4, VA)1(O-2)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
M2O3A	La2O3 (D52)	D52	hP5	(164, P-3m1)	A-LA2O3. Also hexagonal A-type structure of Gd2O3.	3	(HF+4, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3B	B-Sm2O3	-	mS30	(12, C2/m)	This is monoclinic B-type structure of R2O3	3	(AL+3, CO+3, HF+4, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3C	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)	This is also cubic Gd2O3, Y2O3 and Yb2O3	3	(AL+3, CO+3, CR+3, FE+3, HF+4, MN+3, NI+2, TI+4, Y, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3H	H-La2O3	-	hP10	(194, P6_3/mmc)	H-La2O3. This is also hexagonal (Gd, Y, Yb)2O3.	3	(HF+4, MN+3, Y, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3X	Nd2O3	-	cI26	(229, Im-3m)	X-LA2O3. This is also HT cubic X-type structure of Gd2O3.	3	(HF+4, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M4O7	Ti4O7-a	-	aP22	(2, P-1)	This is Ti4O7 and V4O7 with solubility of Al and Mn.	2	(AL, MN, TI, V)4(O)7
M6O11	Ti6O11	-	aP34	(2, P-1)	This is Ti6O11 and V6O11.	2	(TI, V)6(O)11
M7O13	Ti7O13	-	aP40	(2, P-1)	This is Ti7O13 and V7O13.	2	(TI, V)7(O)13
M8O15	Ti8O15	-	aP46	(2, P-1)	This is Ti8O15 and V8O15.	2	(TI, V)8(O)15
MG2B2O5	Co2B2O5	-	aP18	(2, P-1)	This is (Co, Fe, Mg, Ni)2B2O5	3	(CO+2, FE+2, NI+2)2(B+3)2(O-2)5
MG2V2O7	Co2[V2O7]	-	mP44	(14, P2_1/c)	This is Co2V2O7, Mg2V2O7 and Ni2V2O7.	3	(CO+2, NI+2)2(V+5)2(O-2)7
MG3V2O8	Ni3[VO4]2	-	oS52	(64, Cmce)	This is Co3V2O8, Mg3V2O8 and Ni3V2O8.	3	(CO+2, NI+2)3(V+5)2(O-2)8
MGWO4_TYPE	Huanzalaite (MgWO4, H06)	H06	mP12	(13, P2/c)	This is (Al, Fe)NbO4 and (Co, Fe, Mg, Mn, Ni)WO4.	3	(AL+3, CO+2, FE+2, FE+3, MN+2, NB+5, NI+2, VA)1(NB+5, W+6)1(O-2)4
MN2B4O9	Unknown Structure	-	-	-	-	3	(MN+3)2(B+3)4(O-2)9
MN2V2O7	Thortveitite ([Sc, Y]2Si2O7, S21)	S21	mS22	(12, C2/m)	-	3	(MN+2)2(V+5)2(O-2)7

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN4NB2O9	Nb2Mn4O9	-	hP30	(165, P-3c1)	This is (Co, Fe, Mg, Mn)4Nb2O9.	3	(CO+2, FE+2, MN+2)4(NB+5)2(O-2)9
MNB2O4	Unknown Structure	-	-	-	-	3	(MN+2)1(B+3)2(O-2)4
MNB3O6	Unknown Structure	-	-	-	-	3	(MN+3)1(B+3)3(O-2)6
MNB4O7	Unknown Structure	-	-	-	-	3	(MN+2)1(B+3)4(O-2)7
MNB6O10	Unknown Structure	-	-	-	-	3	(MN+2)1(B+3)6(O-2)10
MNB03	Unknown Structure	-	-	-	-	3	(MN+3)1(B+3)1(O-2)3
MNYO3_HEX	LuMnO3	-	hP30	(185, P6_3cm)	-	3	(Y+3)1(MN+3)1(O-2)3
MO4O11	Mo4O11	-	oP60	(33, Pna2_1)	-	3	(MO+4)1(MO+6)3(O-2)11
MO8O23	Approximate High Temperature Mo8O23	-	mP62	(13, P2/c)	-	3	(MO+4)1(MO+6)7(O-2)23
MO9O26	Mo9O26	-	mP70	(13, P2/c)	-	3	(MO+4)1(MO+6)8(O-2)26
MOO3	gamma-WO3	-	mP32	(14, P2_1/c)	-	2	(MO+6)1(O-2)3
MULLITE	Al(Al0.7Si0.3)2O4.8	-	oP24	(55, Pbam)	With solubility of B, Cr and Fe.	4	(AL+3)1(AL+3, CR+3, FE+3)1(AL+3, B+3, SI+4)1(O-2, VA)5
NB2O5	Nb2O5	-	mP99	(10, P2/m)	-	2	(NB+5, V+5, ZR+4)2(O-2, VA)5
NB3BO9	Unknown Structure	-	-	-	-	3	(NB+5)3(B+3)1(O-2)9
NBO1	NbO	-	cP6	(221, Pm-3m)	-	2	(NB+2)1(O-2)1
NBO2	alpha-NbO2	-	tI96	(88, I4_1/a)	This is NbO2	2	(FE+2, NB+4, NB+5)1(O-2)2
NI3B2O6	Kotoite (Mg3(BO3)2)	-	oP22	(58, Pnnm)	This is (Co, Mg, Ni)3B2O6	3	(CO+2, NI+2)3(B+3)2(O-2)6
NI4NB2O9	Nb2Ni4O9	-	oF480	(43, Fdd2)	-	3	(NI+2)4(NB+5)2(O-2)9

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
Ni6MnO8_TYPE	Mg6MnO8	-	cf60	(225, Fm-3m)	This is (Mg, Ni)6MnO8, with an ordered NaCl-type structure.	3	(Ni+2)6(MN+4)1(O-2)8
NiMnO3	Ilmenite (FeTiO3, E22)	E22	hR10	(148, R-3)	This is NiMnO3 with Ilmenite structure	2	(MN+3, MN+4, Ni+2)2(O-2)3
NiNb14O36	Unknown Structure	-	-	-	-	3	(Ni+2)1(NB+5)14(O-2)36
NiNb2O6	Columbite (FeNb2O4, E51)	E51	oP36	(60, Pbcn)	-	3	(NB+5, Ni+2, VA)1(NB+5, Ni+2)2(O-2, VA)6
NiNb36O91	Unknown Structure	-	-	-	-	3	(Ni+2)1(NB+5)36(O-2)91
NiNb68O171	Unknown Structure	-	-	-	-	3	(Ni+2)1(NB+5)68(O-2)171
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	oP28	(62, Pnma)	This is Calcio-olivine (Ca2SiO4) - Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephroite (Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4) solid solution dissolving Cr and Cu.	4	(CO+2, CR+2, CU+2, FE+2, MN+2, Ni+2)1(CO+2, CR+2, CU+2, FE+2, MN+2, Ni+2)1(Si+4)1(O-2)4
ORTHO_PYROXENE	Enstatite (MgSiO3, S43)	S43	oP80	(61, Pbcn)	This is enstatite (MgSiO3) and ortho-diopside (CaMgSi2O6) with Fe solubility.	4	(FE+2)1(FE+2)1(Si+4)2(O-2)6
PROTO_PYROXENE	MgSiO3	-	oP40	(60, Pbcn)	This is proto- enstatite (MgSiO3) and proto-diopside (CaMgSi2O6) dissolving Co, Cr, and Fe.	3	(CO+2, CR+2, FE+2, Ni+2)1(Si+4)1(O-2)3
PSEUDO_BROOKITE	Pseudobrookite (Fe2TiO5, E41)	E41	oS32	(63, Cmcn)	This is Fe2TiO5, Ti3O5, Al2TiO5 and (Co, Fe, Mg, Mn)Ti2O5.	3	(AL+3, CO+2, FE+2, FE+3, MN+2, Ni+2, Si+4, Ti+3, Ti+4, V+3)1(AL+3, FE+3, Si+4, Ti+3, Ti+4)2(O-2)5
PYROCHLORE	Pyrochlore Iridate (Eu2Ir2O7, E81)	E81	cf88	(227, Fd-3m)	This is (Gd, La)2(Hf, Zr)2O7 and (Gd, La, Y, Yb)2Ti2O7.	5	(HF+4, Y+3, Ti+4, ZR+4)2(HF+4, Y+3, Ti+4, ZR+4)2(O-2, VA)6(O-2)1(O-2, VA)1
QUARTZ	alpha-Quartz (low Quartz)	-	hP9	(152, P3_121)	SiO2 with AlPO4 solubility.	2	(Si+4)1(SiO4-4)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RH2O3_D51	Corundum (alpha-alumina, Al <sub>2</sub> O <sub>3</sub> , D51)	D51	hR10	(167, R-3c)	-	2	(RH+3)2(O-2)3
RHO2_C4	Rutile (TiO <sub>2</sub> , C4)	C4	tP6	(136, P4 <sub>2</sub> /mnm)	-	2	(RH+4)1(O-2)2
RHODONITE	Rhodonite (MnSiO <sub>3</sub> -b)	-	aP50	(2, P-1)	This is MnO.SiO <sub>2</sub>	3	(CO+2, FE+2, MN+2)1(SI+4)1(O-2)3
RUTILE	Rutile (TiO <sub>2</sub> , C4)	C4	tP6	(136, P4 <sub>2</sub> /mnm)	This is MnO <sub>2</sub> , TiO <sub>2</sub> and ht-VO <sub>2</sub> .	2	(AL+3, HF+4, MN+4, RU+4, SN+4, TI+3, TI+4, V+4, ZR+4, CR+3, TA+5)1(O-2, VA)2
SILLIMANITE	Sillimanite (Al <sub>2</sub> SiO <sub>5</sub> , S03)	S03	oP32	(62, Pnma)	This is a high-pressure phase	4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
SPINEL	Spinel (Al <sub>2</sub> MgO <sub>4</sub> , H11)	H11	cF56	(227, Fd-3m)	This is MgAl <sub>2</sub> O <sub>4</sub> , Fe <sub>3</sub> O <sub>4</sub> , Mn <sub>3</sub> O <sub>4</sub> (ht) and many more.	4	(AL+3, CO+2, CO+3, CR+2, CR+3, CU+2, FE+2, FE+3, MN+2, NI+2)1(AL+3, CO+2, CO+3, CR+3, CU+2, FE+2, FE+3, MN+2, MN+3, MN+4, MO+4, NI+2, TI+3, TI+4, V+3, VA)2(CR+2, FE+2, MN+2, VA)2(O-2)4
TI10O19	Unknown Structure	-	-	-	-	2	(TI)10(O)19
TI20O39	Ti <sub>20</sub> O <sub>39</sub>	-	aP118	(2, P-1)	-	2	(TI)20(O)39
TI2NB10O29	(Ti <sub>0.17</sub> Nb <sub>0.83</sub> ) <sub>12</sub> O <sub>29</sub>	-	mS82	(12, C <sub>2</sub> /m)	-	3	(TI+4)2(NB+5)10(O-2)29
TI3O2	(Ti <sub>3</sub> O <sub>2</sub> )	-	hP5	(191, P6/mmm)	-	3	(TI+2)2(TI)1(O-2)2
TI5O9	Ti <sub>5</sub> O <sub>9</sub>	-	aP28	(2, P-1)	Ti <sub>5</sub> O <sub>9</sub> with solubility of V.	2	(TI, V)5(O)9
TI9O17	Ti <sub>9</sub> O <sub>17</sub>	-	aP52	(2, P-1)	-	2	(TI)9(O)17
TINB24O62	(Ti <sub>0.04</sub> Nb <sub>0.96</sub> ) <sub>25</sub> O <sub>62</sub>	-	mS174	(5, C <sub>2</sub> )	-	3	(TI+4)1(NB+5)24(O-2)62
TINB2O7	(Ti <sub>0.33</sub> Nb <sub>0.67</sub> ) <sub>3</sub> O <sub>7</sub>	-	mS60	(12, C <sub>2</sub> /m)	-	3	(TI+4)1(NB+5)2(O-2)7
TIO_ALPHA	alpha-TiO	-	mS20	(12, C <sub>2</sub> /m)	-	2	(TI+2)1(O-2)1
TRIDYMITTE	Monoclinic (Cc) Low Tridymite (SiO <sub>2</sub> )	-	mS144	(9, Cc)	SiO <sub>2</sub> with AlPO <sub>4</sub> solubility.	2	(SI+4)1(SIO4-4)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
V2O5	Shcherbinaite (V2O5) (Revised)	-	oP14	(59, Pmmn)	-	2	(V+5)2(O-2)5
V2O_SS	V7O3	-	mS20	(12, C2/m)	-	2	(V)1(O, VA)0.5
V3O5_HT	V3O5-ht	-	mS32	(15, C2/c)	This is ht-V3O5 with solubility of Al, Cr, Mg, Mn and Ti.	2	(AL, CR, MN, TI, V)3(O)5
V3O5_LT	V3O5-lt	-	mP32	(13, P2/c)	-	2	(V)3(O)5
V3O7	V3O7	-	mS120	(15, C2/c)	-	2	(V)3(O)7
V52O64	V13O16	-	tI116	(141, I4_1/amd)	-	2	(V)52(O)64
V5O9	Ti5O9	-	aP28	(2, P-1)	V5O9 with solubility of Ti.	2	(TI, V)5(O)9
V6O13	V6O13	-	mS38	(12, C2/m)	-	2	(V)6(O)13
VO2_LT	VO2	-	mP12	(14, P2_1/c)	This is lt-VO2, MoO2 and WO2.	2	(MO+4, V+4, W+4)1(O-2)2
WO2_72	Unknown Structure	-	-	-	-	1	(O2_72W1)1
WO2_90	Unknown Structure	-	-	-	-	1	(O2_90W1)1
WO2_96	Unknown Structure	-	-	-	-	1	(O2_96W1)1
WO3_HT	WO2.95	-	tP16	(113, P-42_1m)	-	2	(W+6)1(O-2)3
WO3_LT	beta-WO3	-	oP32	(60, Pbcn)	-	2	(W+6)1(O-2)3
WOLLASTONITE	Wollastonite (CaSiO3)	-	aP30	(2, P-1)	This is CaO.SiO2 with Ba, Fe, Mg and Mn solubility	3	(FE+2, MN+2)1(SI+4)1(O-2)3
Y2S2A_Y2SI2O7	Thortveitite ([Sc, Y]2Si2O7, S21)	S21	mS22	(12, C2/m)	Y2Si2O7	3	(Y+3)1(Y+3)1(SI2O7-6)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
Y2S2B_Y2Si2O7	La4Ge3[GeO4]O10	-	aP44	(2, P-1)	(Y, Yb)2Si2O7 solid solution.	2	(Y+3)2(Si2O7-6)1
Y2S2D_Y2Si2O7	Possible delta-Y2Si2O7	-	oP44	(62, Pnma)	Y2Si2O7 with Yb solubility.	2	(Y+3)2(Si2O7-6)1
Y2S2G_Y2Si2O7	Y2Si2O7-b	-	mP22	(14, P2_1/c)	Y2Si2O7-b with Yb solubility.	2	(Y+3)2(Si2O7-6)1
Y2SiO5	Y2SiO5 (RE2SiO5 X2)	-	mS64	(15, C2/c)	This is (Y, Yb)2SiO5	3	(Y+3)2(SiO4-4)1(O-2)1
Y2TiO5	La2TiO5	-	oP32	(62, Pnma)	This is (Gd, La, Y)2TiO5	3	(Y+3)2(Ti+4)1(O-2)5
Y3NbO7	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	-	3	(NB+5, Y+3, VA)3(NB+5, Y+3)1(O-2, VA)7
YAM	Y4Al2O9	-	mP60	(14, P2_1/c)	This is Y4Al2O9, Gd4Al2O9 and Ca2Y2Si2O9 (Cuspidine)	4	(Al+3, Si+4)2(Y+3)4(O-2, VA)1(O-2)9
YAP	CaTiO3 Pnma Perovskite	-	oP20	(62, Pnma)	This is Y(Al, Co, Cr, Fe)O3, YbFeO3 and Gd(Al, Co, Cr, Fe)O3.	3	(Al+3, Co+3, Cr+3, Fe+3, Mn+3)1(Y+3)1(O-2)3
YBO3	Unknown Structure	-	-	-	This is (Y, Yb)BO3 solid solution.	3	(Y+3)1(B+3)1(O-2)3
YNBO4	LaNbO4	-	mS24	(15, C2/c)	-	3	(NB+5, Y+3, VA)1(NB+5, Y+3)1(O-2, VA)4
ZIRCON	Zircon (ZrSiO4, S11)	S11	tl24	(141, I4_1/amd)	This is HfSiO4, ZrSiO4, GdPO4, LaPO4 and YPO4.	3	(Si+4)1(HF+4, Y+3, ZR+4)1(VA, O-2)4
ZR11NB4O32	Unknown Structure	-	-	-	-	3	(ZR+4)11(NB+5)4(O-2)32
ZR13NB4O36	Unknown Structure	-	-	-	-	3	(ZR+4)13(NB+5)4(O-2)36
ZR15NB4O40	Unknown Structure	-	-	-	-	3	(ZR+4)15(NB+5)4(O-2)40
ZR3Y4O12	UY6O12	-	hR19	(148, R-3)	Zr3(Y, Yb)4O12 and Hf3Yb4O12.	3	(HF+4, ZR+4)3(Y+3)4(O-2)12
ZR5NB2O15	Unknown Structure	-	-	-	-	3	(ZR+4)5(NB+5)2(O-2)15
ZR6NB2O17	Nb2Zr6O17	-	ol100	(46, Ima2)	-	3	(ZR+4)6(NB+5)2(O-2)17

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZR7NB2O19	Unknown Structure	-	-	-	-	3	(ZR+4)7(NB+5)2(O-2)19
ZR8NB2O21	Unknown Structure	-	-	-	-	3	(ZR+4)8(NB+5)2(O-2)21
ZRO2_MONO	Baddeleyite (ZrO <sub>2</sub> , C43)	C43	mP12	(14, P2_1/c)	This is Monoclinic HfO <sub>2</sub> and ZrO <sub>2</sub>	2	(AL+3, CR+3, HF+4, TI+4, Y+3, ZR+4)2(O-2, VA)4
ZRO2_TETR	Cocconite (Red Hgl <sub>2</sub> , C13)	C13	tP6	(137, P4_2/nmc)	This is Tetragonal HfO <sub>2</sub> and ZrO <sub>2</sub>	2	(AL+3, CR+3, FE+2, HF+4, MN+2, MN+3, NB+5, NI+2, TI+4, Y+3, ZR+4, VA)2(O-2, VA)4
ZRTi2O6	Columbite (FeNb <sub>2</sub> O <sub>4</sub> , E51)	E51	oP36	(60, Pbcn)	-	3	(ZR+4)1(TI+4)2(O-2)6
ZRTiO4_ALPHA	Unknown Structure	-	-	-	-	3	(ZR+4)1(TI+4)1(O-2)4
ZRTiO4_BETA	zeta-Fe <sub>2</sub> N	-	oP12	(60, Pbcn)	This is (Hf, Zr)TiO <sub>4</sub> solid solution with Al solubility.	3	(AL+3, HF+4, TI+4, ZR+4)2(AL+3, VA)1(O-2)4
IR1O2	Rutile (TiO <sub>2</sub> , C4)	C4	tP6	(136, P4_2/mnm)	-	1	(IR1O2)1
ZNO	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	-	1	(O1ZN1)1
RE2O7	Re <sub>2</sub> O <sub>7</sub>	-	oP72	(19, P2_12_12_1)	-	1	(O7RE2)1
REO2	ReO <sub>2</sub>	-	mP14	(14, P2_1/c)	-	1	(O2RE1)1
REO3	alpha-ReO <sub>3</sub> (D09)	D09	cP4	(221, Pm-3m)	-	1	(O3RE1)1
TA2O5_HT	Ta <sub>2</sub> O <sub>5</sub> -ht	-	tI44	(141, I4_1/amd)	-	2	(TA)2(O)5
TA2O5_LT	beta-Ta <sub>2</sub> O <sub>5</sub>	-	oP14	(49, Pccm)	-	2	(TA)2(O)5

## TCHEA9: Current Version Changes

### Current Database Version

Database name (acronym):	TCS High Entropy Alloys Database (TCHEA)
Database owner:	Thermo-Calc Software AB
Database version:	9.0
First release:	TCHEA1 was released with 2015b



For earlier changes, see [TCHEA: Revision History](#).

### TCHEA8.1 to TCHEA9.0

Software release version: 2026b (June 2026)

#### Improvements to the Heusler Phase

- Remodeled the Heusler phase as  $(\text{Co, Fe, Ni})_{0.5}(\text{Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Si, Sn, Ta, Ti, V, Zr})_{0.25}$ . DFT-calculated formation energy is applied for all the end-members. All the related binary and ternary systems are checked with necessary modifications.

#### Updated Binary Systems

- In total, 49 binaries are updated. Particularly, the binary Mo-Ti (for BCC miscibility gap) and Re-Ta (for B2 phase stability) are improved in full temperature range.

## **New and Updated Ternary Systems**

- In total, 86 new ternaries (9 critical + 77 tentative) are added. 167 ternaries (72 critical + 95 tentative) are updated.
- New critically assessed ternary systems (9): Al-Co-Fe, Al-Co-Mn, Al-Hf-Ni, Co-Cu-Si, Cu-Ni-Sn, Fe-Mn-Ti, Ni-Si-Ta, Ni-Sn-Ti, Ni-Sn-Zr.
- Updated critically assessed systems with new ternary phases or improved ternary solubility: Al-Co-Ti, Al-Fe-Ti, Al-Ni-Ti, Co-Sn-Ti, Hf-Ni-Ti and many more.
- New tentatively assessed ternary systems with stable or metastable Heusler phase: Al-Fe-V, Co-Fe-Si, Cu-Nb-Ni, Fe-Sn-Ti and many more.
- Updated tentatively assessed systems with improved ternary solubility and phase stability: Al-Fe-Ta, Fe-Nb-Si, Fe-Si-Ta, Fe-Si-Ti, and many more.

## **Thermophysical Properties**

- Updated thermal conductivity and electrical resistivity of B.
-

# TCHEA: Revision History



For the most recent changes, see [TCHEA9: Current Version Changes](#).

## TCHEA8.0 to TCHEA8.1

Software release version: 2026a (January 2026)

- Corrected a typo in L(LIQUID,MNO,FeO3/2;O) of the [Fe, Mn, O] system.
- Corrected the crystal structure information for M2O3H. It is the high temperature La2O3, its structure is now fixed: #H-La2O3 #hP10 #P6\_3/mmc.

## TCHEA7.0 to TCHEA8.0

Software release version: 2025b (June 2025)

### Elements and Phases

- Added O (oxygen) making it a 27 element framework.
- 173 new phases (713 phases in total)

### Elastic Properties

- Added elastic properties for BCC (A2 & B2), FCC (A1 & L12), and HCP (A3) phases.

### Binary Systems

- 26 newly assessed M-O binaries, where M = Al, B, C, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, N, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, and Zr.
- Updated 11 assessed binaries: Al-Fe, Al-Ni, B-Nb, Cr-Ti, Fe-Ni, Fe-Ti, Mo-Nb, Mo-Ta, Mo-W, Nb-W, and Ta-W.

## Ternary Systems

- 117 new ternary assessments, mainly related to O containing systems especially in oxide pseudo-binaries.
- Reassessed 3 metallic ternary systems: Al-Fe-Ni, Cr-Fe-Ti, and Cr-Nb-Ti.

## Quaternary Systems

- Added 54 quaternary assessments, mainly related to O containing systems especially in oxide pseudo-ternaries, but also for metallic systems e.g. Mo-Nb-Ta-W.

## Higher Order Systems

- 3 new higher order systems added: Al-Fe-Mn-O-Si, C-Cr-Fe-Mn-Ni-O, and Co-Cr-Fe-Mn-Ni.

## Thermophysical Properties

- Added/updated viscosity, surface tension and THCD/ELRS descriptions of the liquid phase for the above newly-added/updated systems.
- Added/updated ELRS-THCD description for all the phases including intermetallic phases in addition of BCC (A2 & B2), FCC (A1 & L12) and HCP (A3) solution phases.

## TCHEA6.1 to TCHEA7.0

Software release version: 2024a (December 2023/January 2024)

## Binary Systems

- Newly assessed Mo-Sn, N-Y, Rh-Nb, Rh-Si, Rh-Ta, Rh-V, and Rh-Y.
- Reassessed Mn-W.

## Ternary Systems

- Newly assessed Nb-V-Zr and V-W-Zr
- Revision of SIGMA phase stability: Al-Co-Cr, Al-Co-V, Al-Cr-Ni, Al-Cr-V, Al-Fe-Ni, Al-Fe-V, Al-Mo-Ni, Al-Mo-V, Al-Ni-V, Co-Cr-V, Co-Fe-V, Co-Mo-V, Cr-Fe-V, Fe-Mo-Ni, Fe-Mo-V, and Mo-Ni-V.
- Revision of BCC phase stability: Co-Cr-Ti, Co-Cu-Nb, Co-Cu-Ni, Co-Ni-Si, Co-Ni-V, Co-Ni-W, Cr-Cu-Si, Cr-Mo-Ni, Cr-Ni-Si, Cu-Fe-Ni, Cu-Mo-Ni, Fe-Ni-Ti, Fe-Ni-W, and Ni-Si-Ti.

- Revision of FCC phase stability: Al-Co-Zr, Al-Cr-Ti, Al-Fe-Ti, Al-Hf-Ti, Al-Mn-Ti, Al-Mo-Ti, Al-Nb-Ti, Al-Si-Ti, Al-Sn-Ti, Al-Ta-Ti, Al-Ti-Zr, Al-V-Zr, Co-Ta-Ti, Cr-Cu-Mo, Cr-Cu-Zr, Cr-Fe-Si, Cr-Fe-V, Cr-Mo-Nb, Cr-Ti-Zr, Fe-Ni-V, Fe-Ti-V, Mo-Nb-Ti, Mo-Ni-Ti, Mo-Re-Ta, Mo-Ta-Ti, Mo-Ti-W, Mo-Ti-Zr, Nb-Ti-W, Si-Ti-W, Ta-Ti-V, Ti-V-W, and Ti-V-Zr.
- Revision of HCP phase stability: Al-Co-Ni, Al-Co-W, Al-Co-Zr, Al-Cr-Ni, Al-Cu-Ni, Al-Fe-Mn, Al-Fe-Ni, Al-Nb-Ni, Al-Ni-Si, Al-Ni-Ti, Al-Ni-W, Al-Ni-Zn, Co-Cr-Ti, Co-Cu-Fe, Co-Cu-Nb, Co-Cu-Ni, Co-Ni-V, Co-Ni-W, Co-Ta-Ti, Cr-Cu-Mo, Cr-Cu-Nb, Cr-Cu-Si, Cr-Cu-Zr, Cr-Fe-Mo, Cr-Fe-Ni, Cr-Fe-Si, Cr-Fe-V, Cr-Mo-Nb, Cr-Mo-Ni, Cr-Ni-Re, Cr-Ni-Si, Cr-Ni-W, Cr-Ti-Zr, Cu-Fe-Mn, Cu-Fe-Ni, Cu-Fe-Si, Cu-Fe-Sn, Cu-Fe-V, Cu-Mn-Ni, Cu-Mn-Si, Cu-Mn-Sn, Cu-Mo-Ni, Cu-Ni-Ti, Cu-Ni-Zn, Fe-Mo-Ni, Fe-Ni-Ti, Fe-Ni-V, Fe-Ni-W, Hf-Ni-Ti, Mo-Nb-Ti, Mo-Ni-Ti, Mo-Re-Ta, Mo-Ti-W, Mo-Ti-Zr, Ni-Si-Ti, Si-Ti-W, Ta-Ti-V, and Ti-V-W.
- Revision of LIQUID phase stability: Al-Cr-Ti, Mo-Nb-Ti, Mo-Ni-Ti, Mo-Re-Ru, Mo-Re-Ta, Mo-Ta-Ti, Ta-Ti-V, and Ti-V-W.

## Surface Tension Re-assessed

The surface tension was re-assessed based on the Redlich-Kister-Muggianu (R-K-M) sub-regular solution model.

## TCHEA6.0 to TCHEA6.1

Software release version: 2023a (December 2022/January 2023)

### Reassessed Binary, Ternary, and Quinary Systems

- Binary: Two reassessments, Cr-Mn, Ir-Nb.
- Ternary: Seventeen (re-)assessments: Al-Cr-V, Co-Cr-Fe, Co-Cr-Mn, Co-Cr-Ni, Co-Fe-Mn, Co-Fe-Ni, Co-Mn-Ni, Cr-Fe-Mn, Cr-Mn-Ni, Cr-Mo-Nb, Cr-Mo-Ti, Cr-Nb-V, Fe-Mn-Ni, Fe-Ni-W, Mo-Nb-V, Re-Nb-V, and Re-V-W.
- Quinary: Validation of the Co-Cr-Fe-Mn-Ni system in full temperature and composition space (7 isopleths).

## TCHEA5.1 to TCHEA6.0

Software release version: 2022b (June 2022)

In this release of the database, there is one new ternary system assessment plus major changes to 18 critically assessed systems. In addition, 19 ternary systems also had some minor changes and a complete description of the gas phase is added.

- 1 new ternary assessment added: Al-V-Zr.
- Reassessed 18 ternary systems: Al-Co-Ti, Al-Cr-Ti, Al-Mn-Ti, Al-Mo-Ti, Al-Ni-Ti, Al-Sn-Ti, Al-Ta-Ti, Al-V-Zr, Co-Mo-Ti, Cr-Mn-Ti, Cr-Ti-Zr, Fe-Ti-V, Mo-Ti-V, Mo-Ti-Zr, Nb-Ti-W, Ta-Ti-V, Ti-V-W, and Ti-V-Zr.
- Minor modifications to 19 ternary systems: Al-B-Ti, Al-C-Ti, Al-Fe-Ti, Al-N-Ti, Al-Si-Ti, Co-Sn-Ti, Cr-Si-Ti, Cu-Ti-Zr, Mo-Nb-Ti, Mo-Ta-Ti, Mo-Ti-W, Nb-Sn-Ti, Nb-Ta-Ti, Nb-Ti-V, Nb-Ti-Zr, Si-Ti-W, Ta-Ti-W, Ta-Ti-Zr, and Ti-W-Zr.
- Added a complete description of the gas phase in the 26 element framework.

## TCHEA5.0 to TCHEA5.1

Software release version: 2022a (December 2021/January 2022)

- Improved the BCC (A2/B2) phase descriptions in the framework of the Al-Cr-Nb-Ti-V-Zr system. Updated assessments of the Al-V, Mo-V, and Ti-V binaries. Updated assessments of the Al-Nb-Ti, Al-Ti-V, and Al-Ti-Zr ternaries.
- Improved the MC carbide description in the framework of the (Hf, Nb, Ta, Ti, V, Zr)C system. Added assessments of the C-Hf-Nb, C-Hf-V, C-Nb-Ta, C-Ta-V, C-Ta-Zr, C-Ti-V, and C-V-Zr ternaries. Updated assessment of the C-Hf-Ta, C-Hf-Ti, C-Nb-Ti, C-Nb-V, C-Nb-Zr, and C-Ti-Zr ternaries.
- Minor bug fixed for ternary-related calculations of the Al-Fe-W, Al-Hf-Nb, Al-Mo-Nb, and Al-Mo-Ni systems.

## TCHEA4.2 to TCHEA5.0

Software release version: 2021b (June 2021)

- Addition of surface tension of liquid phase.
- Addition of electrical resistivity and thermal conductivity of liquid, BCC (A2, B2), FCC (A1, L12), and HCP solution phases.

## TCHEA4.1 to TCHEA4.2

Software release version: 2021a (January 2021)

- Added the assessment of three binary systems- Ir-W, Mo-Rh, and Rh-W.

## TCHEA4.0 to TCHEA4.1

Software release version: 2020b (June 2020)

---

- Crystal structure information is included for all phases.
- HCP\_ZN is merged into HCP\_A3. The epsilon phase with HCP structure in the Cu-Zn, Mn-Zn and Cu-Mn-Zn systems is separated from HCP\_A3 and renamed as CUMNZN\_EPSILON\_HCP.
- Better estimation of excess energy for metastable solution phases and compound energy for metastable end-members in binary systems.

## TCHEA3.1 to TCHEA4.0

Software release version: 2020a (January 2020)

- 49 ternaries added.
- 12 ternaries improved.
- 13 binaries added (mainly Ir-, or Rh-).
- 1 binary updated (Al-Ti).
- Includes the viscosity of metallic liquid data.

## TCHEA3.0 to TCHEA3.1

Software release 2019a (December 2018).

- The Mn-Ni-Si ternary is critically assessed in full composition and temperature ranges.
- Some bug fixes e.g. avoid the fictitious HCP\_ZN phase appears in Zn-free systems, adjust the phase stability of GAMMA\_D03, CRSI2\_C40, C15- & C36- laves phases in some systems.

## TCHEA2.0 to TCHEA3.0

Software release version: 2018a (April 2018)

- 6 new elements (B, Ir, Rh, Sn, Y and Zn) added.
- More than 100 new binary systems and >150 new phases added.

## TCHEA2.0 to TCHEA2.1

Software release version: 2017b (October 2017)

- The database has improved stability description of the sigma phase.
-

## TCHEA1.0 to TCHEA2.0

Software release version: 2017a (March 2017)

- Added 5 new elements (C, N, Re, Ru, Si) and 100 phases.
  - Assessed most of new binary systems that contain one or two of these 5 new elements in the 20-element framework of this database.
  - Assessed 200 additional ternary systems relevant to the 5 new elements.
  - The application of TCHEA2 extends from BCC and FCC HEAs to HCP HEA as well.
  - Revised some subsystems based on the validation against updated experimental information. This includes the phase stability of solid solutions such as BCC and FCC and intermetallic phases such as sigma and laves in some ternary and quaternary systems.
-