TCS High Entropy Alloys Database (TCHEA8)

Technical Information

Available Starting with Thermo-Calc Version 2025b

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Contents

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

TCHEA8 Thermophysical and 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 MOBHEA3.

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 TCHEA8 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. The experts are available to make recommendations on the most suitable database to use for your needs.

Revision History

TCHEA: TCS High Entropy Alloys Database Revision History. The current version of the database is TCHEA8. See the link for any subversion release details.

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.

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[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

Information about the database is available on our website and in the Thermo-Calc software online Help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online Help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCS High Entropy Alloys Database (TCHEA) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, phases and models. It also includes details about the thermophysical and elastic properties data (e.g. viscosity, surface tension, etc.), a list of the included elements, and summaries of the database revision history by version.
- The *TCS High Entropy Alloys Database (TCHEA) Validation and Calculation Examples Collection* PDF document contains a series of validation examples using experimental data, and a set of calculation examples showing some of the ways the database can be used.

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 Solutions page on our website, that includes links to resources such as examples, publications, and more.

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-principal 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.

TCHEA8 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.
- 643 ternary systems are assessed, and 218 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.
- 713 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 $L1_2$ 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`.

TCHEA8 Models for the Included Phases

TCHEA8 Thermophysical and Elastic Properties

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

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).

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.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

Model Descriptions

For more information about the various thermophysical, thermomechanical, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

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 versus Graphical Mode as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property (and Graphical Mode Variable Name)	*Model Parameters*	*Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)****
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

Property (and Graphical Mode Variable Name)	*Model Parameters*	*Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)****
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 are using Console Mode syntax. The quantities can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. See the various model descriptions or the SDK help for details.

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 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

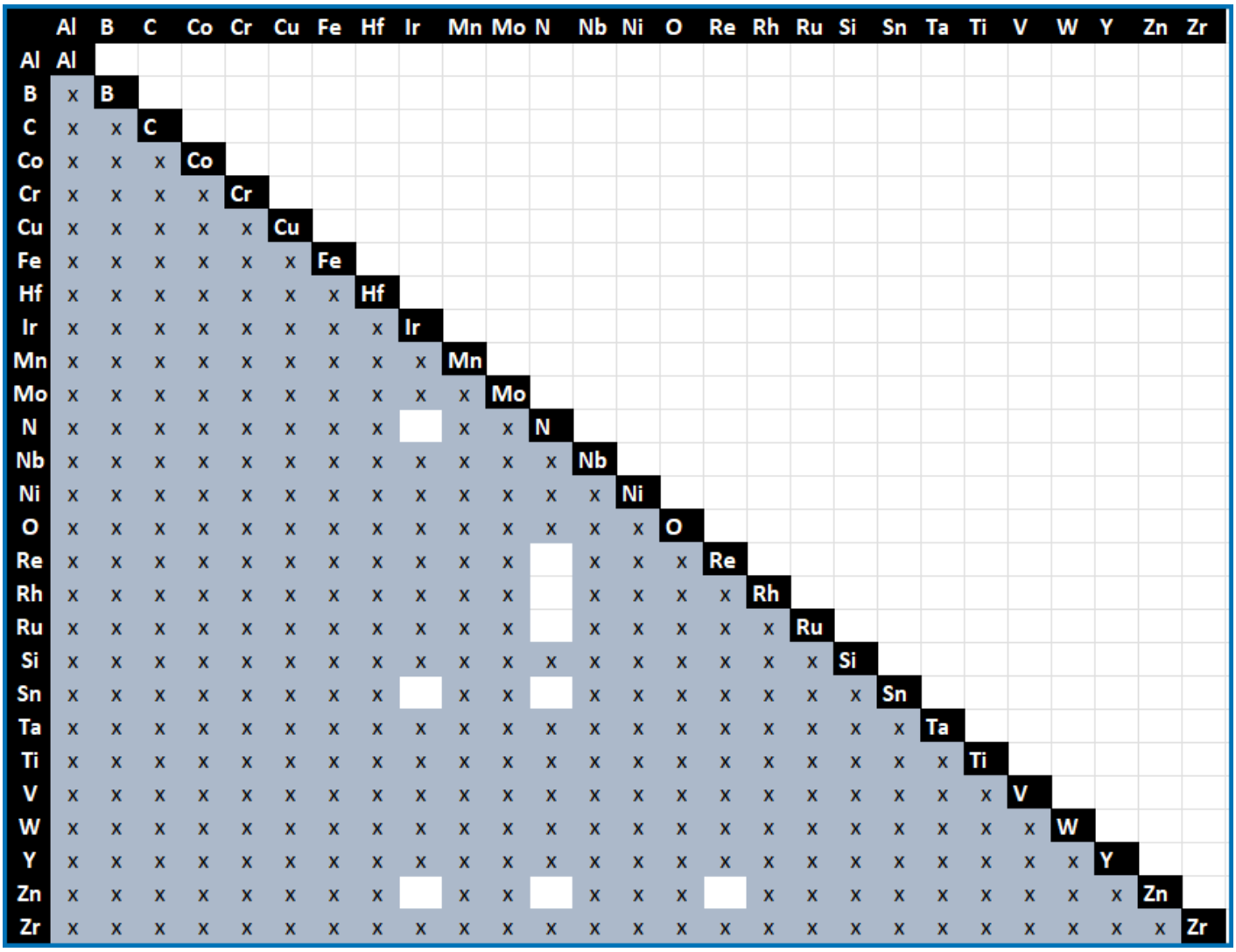
Go to the High Entropy Alloys Databases page on our website where you can access a Validation and Calculation Examples Collection and the Technical Information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to high entropy alloys and the Refractory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

TCHEA8 Systems

In this section:

TCHEA8 Assessed Binary Systems

These are the assessed binary systems (342 total) in the full range of composition and temperature.



TCHEA8 Critically Assessed Ternary Systems

These are the 218 assessed ternary systems in the full range of composition and temperature.

Critically Assessed Ternary Systems							
Al-B-Ti	Al-C-Co	Al-C-Fe	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-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-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	Cu-Fe-Ti	Cu-Fe-V	Cu-Mn-Ni	Cu-Mn-Si

Critically Assessed Ternary Systems							
Cu-Mn-Sn	Cu-Mn-Zn	Cu-Mo-Ni	Cu-Ni-Ti	Cu-Ni-Zn	Cu-Ti-Zr	Fe-Mn-N	Fe-Mn-Si
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-Ti	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						

TCHEA8 Tentatively Assessed Ternary Systems

Tentatively Assessed Ternary Systems							
Al-B-O	Al-C-Cr	Al-C-Ni	Al-Co-Cr	Al-Co-Hf	Al-Co-Mo	Al-Co-Nb	Al-Co-O
Al-Co-Ru	Al-Co-Si	Al-Co-Ta	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-Ta	Al-Fe-W	Al-Fe-Zr	Al-Hf-Ni
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-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-O	Co-Cu-Ti	Co-Fe-Hf	Co-Fe-Nb	Co-Fe-O	Co-Fe-Ta
Co-Fe-Ti	Co-Fe-V	Co-Fe-Zr	Co-Hf-Ni	Co-Hf-Si	Co-Hf-Ti	Co-Mn-O	Co-Mo-Nb
Co-Mo-Ni	Co-Mo-Re	Co-Mo-Ru	Co-Mo-Ta	Co-Mo-V	Co-Mo-W	Co-Nb-Ni	Co-Nb-O
Co-Nb-Si	Co-Nb-Ta	Co-Nb-Ti	Co-Nb-W	Co-Ni-O	Co-Ni-Re	Co-Ni-Ru	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-Ta	Co-Si-Ti

Tentatively Assessed Ternary Systems							
Co-Si-W	Co-Si-Zr	Co-Ta-W	C-O-Ti	Co-Ti-W	Co-Ti-Zr	C-O-V	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-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-O	Cu-Mn-O	Cu-Mo-O	Cu-Nb-O	Cu-Ni-O	Cu-Ni-Si	Cu-O-Si
Cu-O-Ti	Cu-O-Y	C-V-W	C-V-Zr	C-W-Zr	Fe-Hf-Mo	Fe-Hf-Nb	Fe-Hf-Ni
Fe-Hf-Re	Fe-Hf-Si	Fe-Hf-Ta	Fe-Hf-Ti	Fe-Hf-W	Fe-Hf-Zr	Fe-Mn-Ni	Fe-Mn-O
Fe-Mo-N	Fe-Mo-Nb	Fe-Mo-O	Fe-Mo-Re	Fe-Mo-Si	Fe-Mo-Ta	Fe-Mo-Ti	Fe-Mo-W
Fe-Mo-Zr	Fe-Nb-O	Fe-Nb-Re	Fe-Nb-Si	Fe-Nb-Ta	Fe-Nb-Ti	Fe-Nb-W	Fe-Nb-Zr
Fe-Ni-Ta	Fe-Ni-V	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-W
Fe-Si-Zr	Fe-Ta-Ti	Fe-Ta-W	Fe-Ta-Zr	Fe-Ti-W	Fe-W-Zr	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-Ta	Hf-Ni-W
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-O	Mn-Ni-O	Mn-Ni-V	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

Tentatively Assessed Ternary Systems							
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-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-Ta	Ni-Si-V	Ni-Si-W	Ni-Si-Zr	Ni-Ta-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							

TCHEA8 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

TCHEA8 Phases

In this section:

TCHEA8 Models for the Included Phases

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
LIQUID	Liquid					1	(AL, AL1N1, AL2/3O1, AL2O4TI, AL4/3O2, B, BO3/2, C, CO, COO, COO3/2, CR, CRO, CRO3/2, CU, CU2O, CUO, FE, FEO, FEO3/2, HF, HF1/2O1, HF1N1, IR, MN, MNO, MNO3/2, MO, MO1/2O1, MOO3, N, NB, NB1O1, NBO5/2, NI, NIO, O1TI1, O1ZN1, O2TI1, RE, RE1/2O1, REO7/2, RH, RU, RU1/2O1, SI, SI1/2O1, SI2O4, SIO2, SN, SNO, SNO2, TA, TA2/5O1, TI, TIO3/2, V, V1O1, VO2, VO3/2, VO5/2, W, W1/3O1, Y, Y2/3O1, ZN, ZR, ZR1/2O1)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, VA, W, Y, ZN, ZR)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, VA, W, Y, ZN, ZR)0.5(AL, CO, CR, CU, FE, HF, IR, MN, MO, NB, NI, RE, RH, RU, SI, SN, TA, TI, V, VA, W, Y, ZN, ZR)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

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, Cmcm)		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

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	tI16	(141, I4_ 1/amd)		2	(CR, FE, MO)1(B)1
WB_ALPHA_BG	MoB (Bg)	Bg	tI16	(141, I4_ 1/amd)		2	(B, C, VA)1(W)1
RU1B1	Unknown Structure		cI*			2	(RU)1(B)1
WB_BETA_B33	CrB (B33)	B33	oS8	(63, Cmcm)		2	(B, C, VA)1(W)1
RHB_B81	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	oI14	(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		oI10	(71, Immm)		2	(CR)0.2(B)0.8

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_ 3/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_12_ 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	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_ 3/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	AlCCr2		hP8	(194, P6_ 3/mmc)	MAX_PHASE.	3	(AL)1(C)1(CR)2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CEMENTITE_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(CO, CR, FE, MN, MO, NI, V, W)3(C, N)1
TI2ALC	AlCCr2		hP8	(194, P6_ 3/mmc)	i.e. Ti2AlC1-x.	3	(TI)2(AL)1(C, VA)1
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(FE, MN)5(C)2
M7C3_D101	C3Cr7 (D101)	D101	oP40	(62, Pnma)		2	(CO, CR, FE, MN, MO, NI, RE, V, W)7(C)3
TI3ALC2	Ti3SiC2		hP12	(194, P6_ 3/mmc)		3	(TI)3(AL, SI)1(C, VA)2
M3C2_D510	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(CO, CR, MO, V, W)3(C)2
AL4C3_D71	Al4C3 (D71)	D71	hR7	(166, R-3m)		2	(AL, SI)4(C)3
MC_ETA	CMo		hP12	(194, P6_ 3/mmc)		2	(MO, V, W)1(C, VA)1
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	(187, P-6m2)	also MoC_LT, Strukturbericht Bh	2	(MO, W)1(C, N)1
YC_GAMMA_B1	Rock Salt (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	Sc3C4		tP70	(128, P4/mnc)	aka Y2C3_R.	3	(Y)2(C)2(C, VA)1
YC2_C11A	CaC2-I (C11a)	C11a	tI6	(139, I4/mmm)		1	(C2Y1)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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FE4N_LP1	gama-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	AlCCr2		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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
HFN_B1	Rock Salt (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		oI186	(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	SiU3 (D0c)	D0c	tI16	(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	(FE, MN)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, RH, TI)2(SI)1
CRNBSI	ZrNiAl		hP9	(189, P-62m)		3	(CR)1(NB)1(SI)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
RE2SI	Re2Si		mP24	(14, P2_1/c)		2	(RE)2(SI)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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, NB, NI, SI, TI, W, Y, ZR)2(AL, CR, SI, SN, TI)3(CR, CU, FE, HF, MN, MO, NB, NI, 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, SI, TI, V, W)1 (AL, SI, SN)3
RH20SI13	Rh20Si13		hP34	(176, P6_3/m)		2	(RH)20(SI)13
IR3SI2_B82	Ni2In (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
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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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,	also AlCr2, Ti2Zn, ZnZr2,	2	(AL, CO, CU, FE, MO, NI, RH, W, ZN)1(AL, CR, HF, SI, TI,

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				I4/mmm)	CUZR2_C11B.		ZR)2
RESI2_C11B	Re4Si7		mS44	(8, Cm)		2	(RE)0.357(SI)0.643
TISI2_C54	TiSi2 (C54)	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	(HF, NB, ZR)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
ALFESI_TAU1	Unknown Structure					3	(AL)2(FE)2(SI)1
ALFESI_TAU3	Fe(Al0.67Si0.33)3		oS128	(67, Cmme)		3	(AL)2(FE)1(SI)1
AL2MN2SI3	(Al2Mn2Si3)		hP21	(174, P-6)	Tau1	3	(AL)2(MN)2(SI)3
AL5MN6SI7	CrSi2 (C40)	C40	hP9	(180, P6_222)	Tau2	3	(AL)5(MN)6(SI)7
AL1MN1SI1	TiSi2 (C54)	C54	oF24	(70, Fddd)	Tau3	3	(AL)1(MN)1(SI)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3MNSI2	(Al3MnSi2)		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	Al9Mn3Si (E9c)	E9c	hP26	(194, P6_3/mmc)		5	(MN, VA)6(MN, VA)2(AL)12(AL, SI)6(AL, SI)2
AL2MNSI3	Ga5Pd		tI24	(140, I4/mcm)	Tau10	3	(AL)2(MN)1(SI)3
MN15NI45SI40	Unknown Structure				ternary T1 or N phase	3	(MN)0.15(NI)0.45(SI)0.4
MN15NI50SI35	Unknown Structure				ternary T2 or PHI phase	3	(MN)0.15(NI)0.5(SI)0.35
MN6NI16SI7	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	ternary T3 or G phase	3	(MN)0.206897(NI)0.551724(SI)0.241379
MN1NI1SI1_C37	MnCuP		oP12	(62, Pnma)	ternary T4 or E phase	3	(MN)1(NI)1(SI)1
MNNISI_T5	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	ternary T5 or tao_1 phase	2	(MN)1(NI, SI)2
MNNISI_T6	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	ternary T6 or tao_2 phase	2	(MN)1(NI, SI)2
MN3NI2SI	Mn3Ni2Si		cF96	(227, Fd-3m)	ternary T7 or Omega	3	(MN)3(NI)2(SI)1
MN2NISI	Unknown Structure				ternary T8 or S phase	2	(MN, NI)3(SI)1
MN6NISI3	R-(Co,Cr,Mo)		hR53	(148, R-3)	ternary T9 or R' phase	3	(MN)0.61(NI)0.12(SI)0.27
MN66NI4SI30	Unknown Structure				ternary T10 or U phase	3	(MN)0.66(NI)0.04(SI)0.3
MN52NI29SI19	Unknown Structure				ternary phase T11 or W phase	3	(MN)0.52(NI)0.29(SI)0.19
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

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MEO_B1	Rock Salt (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 (hR12)		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, CR, CU, FE, MN, MO, NB, NI, RE, TA, TI, 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

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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 (L21)	L21	cF16	(225, Fm-3m)	aka H_L21.	3	(AL, CR, NI, SN, TI)0.5(AL, HF, NB, NI, TA, TI, ZR)0.5(CO, FE, NI, RU, VA)1
O_PHASE	NaHg		oS16	(63, Cmcm)	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	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		3	(AL, SN)1(CO, NB, SN, TA, TI)1(TI)1
MNNI_L10	CuAu (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 (L10)	L10	tP2	(123, P4/mmm)	also IrTi.	2	(IR, MN, TI)0.5(IR, MN, TI)0.5
ALTI_L10	CuAu (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 (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 (L10)	L10	tP2	(123, P4/mmm)	aka Ir1.04V0.96 or IrV1-x.	2	(IR)0.5(IR, V)0.5

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NBRH_L10	CuAu (L10)	L10	tP2	(123, P4/mmm)	aka Rh1.04V0.96.	2	(NB)0.96(RH)1.04
RHV_L10	CuAu (L10)	L10	tP2	(123, P4/mmm)	aka Rh1.12V0.88.	2	(RH, V)1.12(RH, V)0.88
ALCU_EPS_B82	Ni2In (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
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, Cmcm)		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

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IRZR_ALPHA	Mn3As (D0d)	D0d	oS16	(63, Cmcm)	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 (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
NIZR_B33	CrB (B33)	B33	oS8	(63, Cmcm)		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, Cmcm)	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(FE, MN, NI)1

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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	Ni2In (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, RE, RU, SI, TA, TI, V, W, Y, ZN, ZR)2(AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, RE, RU, SI, 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, RE, RH, RU, SI, TA, TI, V, W, Y, ZN, ZR)2(AL, CO, CR, CU, FE, HF, MO, NB, NI, RE, RH, RU, SI, TA, TI, V, W, Y, ZR)1
C16_THETA	Khatyrkite (Al2Cu, C16)	C16	tI12	(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	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_3/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	MoPt2		oI6	(71, Immm)		2	(CR, MO, W)1(MO, NI, W)2
CU2TI1	Au2V		oS12	(63, Cmcm)		2	(CO, CU, NI)2(TI)1
CU2Y_HT	Unknown Structure		hP*			2	(CU)2(Y)1
CU2Y_LT	CeCu2		oI12	(74, Imma)		2	(CU)2(Y)1
HF2IR	NiTi2		cF96	(227, Fd-3m)		2	(HF)2(IR)1

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HF2RH	NiTi2		cF96	(227, Fd-3m)		2	(HF)2(RH)1
HFSN2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)		2	(HF)1(SN)2
MNNI2	Unknown Structure					2	(MN, NI)1(NI)2
NBZN2_C36	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)		2	(NB)0.333(ZN)0.667
NI2V	MoPt2		oI6	(71, Immm)		2	(MO, NI)2(MO, NB, TA, V)1
NI2TA_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(CO, NI)2(TA, TI)1
NITI2	NiTi2		cF96	(227, Fd-3m)		2	(CO, CR, CU, FE, NI, RE, TI)1(AL, CR, CU, HF, NI, TA, TI, ZR)2
NI2Y1	Ni2Tm		cF192	(216, F-43m)		2	(NI)2(Y)1
REZR2	Zr21Re25		hR92	(167, R-3c)	aka Zr21Re25.	2	(NI, RE)1(ZR)2
RHSN2_RT	RhSn2		tI26	(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	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(SN)1(TI)2
SN2Y_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)		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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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	tI8	(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
AL3Y_LT	Ni3Sn (D019)	D019	hP8	(194, P6_3/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_3/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, SN)3(CU, SN)1
CUTI3_L60	CuTi3 (L60)	L60	tP4	(123, P4/mmm)		2	(CU, TI)1(TI)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
HFIR3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(HF)1(IR)3
HFNI3_ALPHA	PdRh2Ta		hP40	(194, P6_ 3/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_ 3/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_D0E	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)		oS16	(63, Cmcm)	also CoZr3, FeZr3.	2	(CO, FE, NI)1(ZR)3
MN3TI1	Unknown Structure				HT phase	2	(MN)3(TI)1
MO1IR3	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/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, FE, NB, NI)3(AL, FE, MO, NB, NI, TA, TI, V, W)1
NI3TI_D024	Ni3Ti (D024)	D024	hP16	(194, P6_ 3/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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RHY3_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(RH)1(Y)3
RH3Y1	CeNi3		hP24	(194, P6_ 3/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
AL13CO4	Orthorhombic Co4Al13		oP102	(31, Pmn2_1)		2	(AL)13(CO)4
AL5CO2_D811	Co2Al5 (D811)	D811	hP28	(194, P6_ 3/mmc)	also Al5Rh2.	2	(AL)5(CO, RH)2
AL9CO2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)	also Al9Rh2	2	(AL)9(CO, RH)2
AL9M2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)	aka Al9FeNi, metastable Al9Fe2	2	(AL)9(FE, NI)2
AL11CR2	Al5Cr		mS732	(15, C2/c)		3	(AL)10(AL)1(CR)2
AL13CR2	Al45V7		mS104	(12, C2/m)		2	(AL)13(CR)2
AL4CR	mu-Al4Mn		hP574	(194, P6_ 3/mmc)		2	(AL)4(CR)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL8CR5_LT_D810	Cr5Al8 (D810)	D810	hR26	(160, R3m)		2	(AL)8(CR, V)5
AL9CR4_HT	Unknown Structure					2	(AL)9(CR)4
AL9CR4_LT	Unknown Structure					2	(AL)9(CR)4
ALCU_DELTA	Al5Cu8		hR52	(160, R3m)		2	(AL)2(CU, FE)3
ALCU_ZETA	Al9Cu11(h)		oF88	(42, Fmm2)	united HT-zeta1 and LT-zeta2.	2	(AL)9(CU, FE)11
AL23CUFE4_D2H	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)		3	(AL)23(CU)1(FE)4
AL62CU25FE13	Quasicrystal					3	(FE)0.125(AL, CU)0.255(AL)0.62
AL7CU2FE	FeCu2Al7 (E9a)	E9a	tP40	(128, P4/mnc)		3	(FE, NI)1(CU)2(AL)7
AL10CU10FE	(Al10Cu10Fe)		oF116	(42, Fmm2)		3	(FE)1(AL, CU)10(AL)10
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5		hR14	(166, R-3m)		2	(AL)1(CU, FE, NI, VA)1
AL28CU4MN7	Mn6Cu4Al29		oS156	(63, Cmcm)	Tau1, Mn6+xCu4+yAl29-x-y.	3	(AL)28(MN)7(CU)4
AL11CU5MN3	Unknown Structure		oP380		Tau2	3	(AL)11(MN)3(CU)5
ALCU3MN2_C15	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	Tau3.	3	(AL)1(MN)2(CU)3
AL5CU4ZN	Unknown Structure					4	(AL, CU)1(AL)4(CU)4(ZN)1
AL13FE4	Al13Fe4		mS102	(12, C2/m)	solid- solution of Al13Fe4 (aka Al3Fe) & Al13Ru4.	3	(AL, CU)0.6275(FE, MN, NI, RU)0.235(AL, SI, VA)0.1375
AL5FE2	Al2.8Fe		oS24	(63, Cmcm)		2	(AL, CU)5(FE, MN, NI)2
AL5FE4_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	also AL8FE5_D82	1	(AL, CU, FE)1
AL16FEMN3	mu-Al4Mn		hP574	(194, P6_ 3/mmc)	Tau1	2	(AL)4(FE, MN)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL13FE2MN2	Al13Fe4		mS102	(12, C2/m)	Tau2.	2	(FE, MN)4(AL)13
AL10FEMN2	Mn3Al10		hP26	(194, P6_ 3/mmc)	Tau3.	2	(FE, MN)3(AL)10
AL10FE3NI	Co2Al5 (D811)	D811	hP28	(194, P6_ 3/mmc)		2	(AL)5(FE, NI)2
AL71FE5NI24	Unknown Structure					3	(AL)0.71(FE)0.05(NI)0.24
AL9IR2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)		2	(AL)0.818(IR)0.182
AL45IR13	Al45Ir13		oP236	(62, Pnma)		2	(AL)0.776(IR)0.224
AL13IR4	Unknown Structure					2	(AL)0.765(IR)0.235
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	(194, P6_ 3/mmc)	also AL461MN107	2	(AL)461(FE, MN)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(FE, MN)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(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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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(NI, RU, 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		cI168	(204, Im-3)		3	(AL)14(FE, MN)4(AL, SI)5
ALSI3TI2	Zr3Al4Si5		tI24	(141, I4_ 1/amd)	aka Ti7Al5Si12, Tau1	3	(AL)0.166667(SI)0.5(TI)0.333333

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3TI_LT	Al3Ti-LT		tI32	(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
AL8V5_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	(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		cI26	(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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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 (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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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	(CU)0.334(MN)0.333(ZN)0.333
CU6NISI3	Unknown Structure					2	(CU, NI)0.732(SI)0.268
CU46NI25SI29	Unknown Structure					3	(CU)0.458(NI)0.25(SI)0.292
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''-RT (oS* *), eta'-HT1(hR27 R-3), eta-HT2(hR* P-31m)	2	(CU, MN, NI)0.76(SI)0.24
CU6SN5_HT	Ni2In (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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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, FE, NI)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
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	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(FE)5(SN)3

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

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

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
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
NI2Y3	Ni2Y3		tP80	(92, P4_12_12)		2	(NI)2(Y)3
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
NIZN8_DELTA	Ni3Zn22		mS50	(12, C2/m)		2	(NI)0.1111111(AL, ZN)0.8888889
NI11ZR9	Pt11Zr9		tI40	(87, I4/m)	also Ni11Hf9.	2	(NI)11(HF, ZR)9
NI10ZR7	Ni10Zr7		oS68	(64, Cmce)	also Ni10Hf7.	2	(NI)23(HF, ZR)17
NI5ZR_C15B	AuBe5 (C15b)	C15b	cF24	(216, F-43m)	also Ni5Y/Ni5Hf/Cu5Hf/Cu5Zr, aka ZRM5_C15B.	2	(AL, CU, NI)5(HF, Y, ZR)1
RE3NB_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		3	(RE)24(NB, V, W)10(NB, RE, V, W)24
RHSN4	IrGe4		hP15	(152, P3_121)		2	(RH)1(SN)4

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RH3SN2	Ni2In (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
RU3SN7_D8F	Ir3Ge7 (D8f)	D8f	cI40	(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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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 (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
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, Cmcm)	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		tI14	(139, I4/mmm)	ternary Ti0.43FexCu0.57-x, Tau3.	2	(CU, FE)4(TI)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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, Cmcm)		2	(TI)1(ZN)15
V4ZN5	V4Zn5		tI18	(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
ZN12Y_D2B	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)		2	(ZN)12(Y)1
ZN11Y3	Al11La3		oI28	(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, AL1B1O2, AL1C1, AL1C2, AL1CU1, AL1N1, AL1O1,

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							AL1O2, AL2, AL2C2, AL2O1, AL2O2, AL2O3, B, B1C1, B1C2, B1N1, B1O1, B1O2, B2, B2C1, B2O1, B2O2, B2O3, C, C1IR1, C1N1, C1N1O1, C1N1O1_NCO, C1N2_CNN, C1N2_NCN, C1O1, C1O2, C1RH1, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2N1_CCN, C2N1_CNC, C2N2, C2O1, C2SI1, C2SI2, C2SI3, C3, C3N1, C3O2, C4, C4N1, C4N2, C4NI1O4, C5, C5FE1O5, C5N1, C60, C6MO1O6, C6N1, C6N2, C9N1, CO, CO1O1, CO2, CR, CR1N1, CR1O1, CR1O2, CR1O3, CR2, CR2O1, CR2O2, CR2O3, CU, CU1O1, CU2, FE, FE1O1, FE1O2, FE2, HF, HF1O1, HF1O2, IR, IR1O1, IR1O2, IR1O3, MN, MN1O1, MN1O2, MO, MO1N1, MO1O1, MO1O2, MO1O3, MO2, MO2O6, MO3O9, MO4O12, MO5O15, N, N1NB1, N1O1, N1O2, N1O3, N1SI1, N1SI2, N1TI1, N1V1, N1ZR1, N2, N2O1, N2O2, N2O3, N2O4, N2O5, N3, NB, NB1O1, NB1O2, NI, NI1O1, NI2, O, O10V4, O12W4, O15W5, O1RE1, O1RH1, O1RU1, O1SI1, O1SN1, O1TA1, O1TI1, O1V1, O1W1, O1Y1, O1Y2, O1ZN1, O1ZR1, O2, O2RE1, O2RH1, O2RU1, O2SI1, O2SI2, O2SN1, O2TA1, O2TI1, O2V1, O2W1, O2Y1, O2Y2, O2ZR1, O3, O3RE1, O3RU1, O3W1, O4RU1, O6RE2, O6W2, O7RE2, O8W3, O9W3, RE, RH, RU, SI, SI2, SI3, SN, SN2, TA, TI, TI2, V, W, Y, ZN, ZR, ZR2)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
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)		tI28	(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	(VA, Y+3, ZR+4)4(Y+3)6(SIO4-4)6(O-2, VA)2
B2O3	B2O3		hP15	(152, P3_121)		2	(B+3)2(O-2)3

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BETA_V_O	CoO		tI4	(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	hR30	(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, lt 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)	E21	cP5	(221, Pm-3m)	Ba(Hf,Zr)O3 and High-temperature Ca(Hf,Zr)O3.	3	(Y+3)1(Y+3)1(O-2)3
CLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)	This is clino-enstatite (MgSiO3), clino-ferrosilit (FeSiO3), diopside (CaMgSi2O6), niopside (CaNiSi2O6), pigeonite ((Mg,Fe,Ca)Si2O6), hedenbergite (CaFeSi2O6) dissolving Co.	4	(FE+2, NI+2)1(CO+2, FE+2, NI+2)1(SI+4)2(O-2)6
COLUMBITE	Columbite (FeNb2O6, E51)	E51	oP36	(60, Pbcn)	This is (Ca,Co,Fe,Mg,Mn)Nb2O6 with excess FeO and MgO.	3	(CO+2, FE+2, MN+2)1(FE+2, NB+5)2(O-2, VA)6
CORDIERITE	Na0.04		oS120	(66, Cccm)	This is 2Al2O3.2MgO.5SiO2,	4	(AL+3)4(FE+2, MN+2)2(SI+4)5(O-2)18

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	(Mg0.5Fe0.5)2Al4Si5O18				2Al2O3.2MnO.5SiO2 and 2Al2O3.2FeO.5SiO2		
CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	(167, R-3c)	This is Al2O3, Cr2O3, Fe2O3, Ti2O3, V2O3 + (Co,Fe,Mg,Mn,Ni)TiO3 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	Cr2P4O13		mP76	(14, P2_1/c)	This is Cr2P4O13, Cr2V4O13 and Fe2V4O13.	3	(CR+3, FE+3)2(V+5)4(O-2)13
CR2TI2O7	Unknown Structure				with solubility of Al2O3 and Fe2O3.	3	(AL+3, CR+3, FE+3)2(TI+4)2(O-2)7
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	(227, Fd-3m)	SiO2 with AlPO4 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 (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)		3	(CR+3, VA)1(CR+3, NB+5)1(O-2, VA)4
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

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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 . Mg2SiO4, 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
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

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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, VA, Y+3, ZR, ZR+4)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 (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, VA, Y+3, ZR+4)1(O-2)1
HATRURITE	Ca3(SiO4)O-b		hR81	(160, R3m)	This is 3CaO.SiO2	3	(VA, Y+3)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(VA, Y+3, ZR+4)1(O-2)3
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	La2O3 (D52)	D52	hP5	(164, P-3m1)	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

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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
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

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MNBO3	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	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
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 (FeNb2O6, E51)	E51	oP36	(60, Pbcn)		3	(NB+5, NI+2, VA)1(NB+5, NI+2)2(O-2, VA)6

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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, Pbca)	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, Cmcm)	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	Cubic Pyrochlore (Eu2Ir2O7, E81)	E81	cF88	(227, Fd-3m)	This is (Gd,La)2(Hf,Zr)2O7 and (Gd,La,Y,Yb)2Ti2O7.	5	(HF+4, TI+4, Y+3, ZR+4)2(HF+4, TI+4, Y+3, 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
RH2O3_D51	Corundum (Al2O3, D51)	D51	hR10	(167, R-3c)		2	(RH+3)2(O-2)3
RHO2_C4	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)		2	(RH+4)1(O-2)2
RHODONITE	Rhodonite (MnSiO3-b)		aP50	(2, P-1)	This is MnO.SiO2	3	(CO+2, FE+2, MN+2)1(SI+4)1(O-2)3
RUTILE	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)	This is MnO2, TiO2 and ht-VO2.	2	(AL+3, CR+3, HF+4, MN+4, RU+4, SN+4, TA+5, TI+3, TI+4, V+4, ZR+4)1(O-2, VA)2

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SILLIMANITE	Sillimanite (Al2SiO5, 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 (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)	This is MgAl2O4, Fe3O4, Mn3O4 (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	Ti20O39		aP118	(2, P-1)		2	(TI)20(O)39
TI2NB10O29	(Ti0.17Nb0.83)12O29		mS82	(12, C2/m)		3	(TI+4)2(NB+5)10(O-2)29
TI3O2	(Ti3O2)		hP5	(191, P6/mmm)		3	(TI+2)2(TI)1(O-2)2
TI5O9	Ti5O9		aP28	(2, P-1)	Ti5O9 with solubility of V.	2	(TI, V)5(O)9
TI9O17	Ti9O17		aP52	(2, P-1)		2	(TI)9(O)17
TINB24O62	(Ti0.04Nb0.96)25O62		mS174	(5, C2)		3	(TI+4)1(NB+5)24(O-2)62
TINB2O7	(Ti0.33Nb0.67)3O7		mS60	(12, C2/m)		3	(TI+4)1(NB+5)2(O-2)7
TIO_ALPHA	alpha-TiO		mS20	(12, C2/m)		2	(TI+2)1(O-2)1
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	(9, Cc)	SiO2 with AlPO4 solubility.	2	(SI+4)1(SIO4-4)1
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

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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	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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
Y3NBO7	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		3	(NB+5, VA, Y+3)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, VA, Y+3)1(NB+5, Y+3)1(O-2, VA)4
ZIRCON	Zircon (ZrSiO4, S11)	S11	tI24	(141, I4_ 1/amd)	This is HfSiO4, ZrSiO4, GdPO4, LaPO4 and YPO4.	3	(SI+4)1(HF+4, Y+3, ZR+4)1(O-2, VA)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		oI100	(46, Ima2)		3	(ZR+4)6(NB+5)2(O-2)17
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 (ZrO2, C43)	C43	mP12	(14, P2_1/c)	This is Monoclinic HfO2 and ZrO2	2	(AL+3, CR+3, HF+4, TI+4, Y+3, ZR+4)2(O-2, VA)4
ZRO2_TETR	HgI2 (C13)	C13	tP6	(137, P4_ 2/nmc)	This is Tetragonal HfO2 and ZrO2	2	(AL+3, CR+3, FE+2, HF+4, MN+2, MN+3, NB+5, NI+2, TI+4, VA, Y+3, ZR+4)2(O-2, VA)4

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZRTI2O6	Columbite (FeNb2O6, 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-Fe2N		oP12	(60, Pbcn)	This is (Hf, Zr)TiO4 solid solution with Al solubility.	3	(AL+3, HF+4, TI+4, ZR+4)2(AL+3, VA)1(O-2)4
IR1O2	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)		1	(IR1O2)1
ZNO	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)		1	(O1ZN1)1
RE2O7	Re2O7		oP72	(19, P2_12_ 12_1)		1	(O7RE2)1
REO2	ReO2		mP14	(14, P2_1/c)		1	(O2RE1)1
REO3	alpha-ReO3 (D09)	D09	cP4	(221, Pm-3m)		1	(O3RE1)1
TA2O5_HT	Ta2O5-ht		tI44	(141, I4_ 1/amd)		2	(TA)2(O)5
TA2O5_LT	beta-Ta2O5		oP14	(49, Pccm)		2	(TA)2(O)5

TCHEA: TCS High Entropy Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS High Entropy Alloys Database (TCHEA)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**8.0**
First release:	**TCHEA1 was released with 2015b**

Changes in the Most Recent Database Release

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.

Previous Releases

TCHEA6.1 to TCHEA7.0

Software release 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 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.