TCS Ni-based Superalloys Database (TCNI13)

Technical Information

Available Starting with Thermo-Calc Version 2025b

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Contents

About the TCS Ni-based Superalloys Database (TCNI)

TCS Ni-based Superalloys Database (TCNI) is a thermodynamic and properties database for Ni-based alloys and superalloys. All necessary volume data (including molar volume and thermal expansivity) for various alloy phases is available. The database also comes with the description of electrical resistivity and thermal conductivity, as well as surface tension and viscosity of the liquid. In addition, the elastic moduli and elastic constants are also included.

TCNI13 Thermophysical and Elastic Properties

Ni-based superalloys exhibit excellent mechanical strength and resistance to creep at high temperatures, good surface stability and fatigue, resistance to oxidation and hot corrosion. The nickel–aluminum system is the binary basis for Ni-based superalloy compositions. As the amount of aluminium added is large enough, an ordered L12 phase (γ') forms from the FCC matrix (γ) with the nominal composition of Ni_3Al. Today's superalloys can also be based on cobalt or nickel-iron. All these kinds of alloys usually contain at least ten alloying elements, with each one being added for a specific purpose. Due to this complexity in chemistry, it has traditionally taken a long time to optimize properties of existing alloys and to develop completely new alloys.

The database has been developed in a CALPHAD spirit with all of the constituent binary systems assessed for their full range of composition including all phases, plus all of the Ni-rich ternary systems, and many other ternary systems as well, in order to give an accurate thermodynamic description of the multicomponent systems of interest for various Ni-based alloys and superalloys including, but not limited to:

- Hastelloy and the Haynes alloys
- Inconel alloys
- Waspaloy
- René alloys
- Incoloy
- TMS alloys
- CMSX single crystal alloys
- Experimental Co-based superalloys and medium- to high-entropy alloys

Interconnectivity with Other Products

The database can be used with our entire suite of products: Thermo-Calc, the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Additive Manufacturing Modules, and all available SDKs.

The thermodynamic database is compatible with the corresponding mobility database TCS Ni-alloys Mobility Database (MOBNI) 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 MOBNI6.

TCS Ni-based Superalloys Database (TCNI) is also integral to the Nickel Model Library, which is a package of property models used to set up calculations in the Property Model Calculator that are common to those working with nickel-based alloys. The library includes models intended for those working in the nickel industry: Antiphase Boundary Energy, Coarsening, Equilibrium with Freeze-in Temperature, Solvus for Ordered Phase, and Strain-Age Cracking.

The Nickel Model Library is available for free to all users who have licenses for both of the nickel databases TCNI (version 11 or newer) and MOBNI (version 5 or newer) and valid Maintenance & Support Subscription (M&SS).

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 areas depending on the database.

Some general use case examples of how the TCNI13 database can be used include the following. Use it to calculate:

- Isothermal or vertical section phase diagrams
- Liquidus temperatures
- γ’ solvus temperatures
- Partitioning of alloying elements between γ and γ’ phases
- Amount of phases at varying temperatures
- Predict Young's modulus with elastic properties

Then in combination with the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Additive Manufacturing Modules you can also calculate such things as:

- Interdiffusion in coating/substrate systems
- Diffusion in ordered γ’ and B2 phases
- Growth or dissolution of minor phases, such as TCP phases and carbides
- Concurrent nucleation, growth/dissolution and coarsening of precipitates
- Temporal evolution of particle size distribution
- Average particle radius and number density

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.

Release History

TCNI: TCS Ni-based Superalloys Database Revision History. The current version of the database is TCNI13. See the link for any subversion release details.

Acknowledgement

Dr. Nathalie Dupin and Prof. Bo Sundman are acknowledged for many valuable discussions and important contributions during the original development, implementation and improvements to this database.

TCS Ni-based Superalloys Database (TCNI) 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 Ni-based Superalloys Database (TCNI) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, phases, models, and properties data. 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 Ni-based Superalloys Database (TCNI) 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 generally be used.

Go to the Nickel-based Superalloys 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 nickel including 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 binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

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.

TCNI13 Elements, Systems, and Phases

This section summarizes the available elements, assessed systems, and total number of phases in the TCS Ni-based Superalloys Database (TCNI).

Included Elements

There are 31 elements included in the most recent version of the database.

Included Elements									
Al	Ar*	B	C	Ca	Co	Cr	Cu	Fe	H*
Hf	Mg	Mn	Mo	N	Nb	Ni	O	P	Pd
Pt	Re	Ru	S	Si	Ta	Ti	V	W	Y
Zr									

** Ar and H are only included in the gas phase.*

Assessed Systems and Phases

The most recent version of the database contains:

- 371 assessed binary systems, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 433 assessed ternary systems mostly to their full range of composition at least those being in equilibrium with γ and γ' phase. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 732 solution and intermetallic phases, where nearly all stable phases in all assessed binary systems and most ternary systems are modeled.

About the Phases

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`.

- The database contains an extensive GAS mixture phase for the main purpose of considering oxygen/nitrogen-gas controls in alloy making processes, and different gas atmospheres under, for example, heat treatments.

  Argon (Ar) and hydrogen (H) are included in the gas phase only, and there is no solid solubility or condensed phase compounds with these elements included in the database.

- Ordered and disordered BCC (A2 and B2/β) and FCC (A1 and L12/γ′) phases are modeled with a two sub-lattice model using a single Gibbs energy curve which enables order/disorder transformations to be modeled [2001Dup].
- The sigma (σ) and mu (μ) phases—two important Topologically Close-Packed (TCP) phases—are modeled using the Effective Bond Energy Formalism (EBEF) [2018Dup]. This implementation is supported by new Density Functional Theory (DFT) data and employs a five-sublattice (5-SL) model for both phases. The use of EBEF, supported by DFT calculations, results in more physically meaningful thermodynamic descriptions of the σ and μ phases. Moreover, because only effective bond energies of the pairs involved in their configuration are required to fully describe these phases, EBEF enables the use of the 5-SL model [2018Dup; 2024San], which better reflects the actual crystallography of the σ and μ structures. Altogether, this approach enhances the modeling of these phases in binary and ternary systems, as well as across the multicomponent composition space.
- Only the phases of interest for superalloys are defined by default, which means that when retrieving the data from the database other phases will automatically be rejected and would need to be manually restored if these are required for a calculation.

There are several possible composition sets for the phases named FCC_L12 and BCC_B2; they are either disordered (A1/carbonitride and A2) or ordered (L12 (γ') and B2 (β)).

TCNI13 Models for the Included Phases has detailed descriptions of all phases, e.g. number of sub lattices and elements on each sub lattice and if available also structure, Pearson symbol and Structur Bericht.

Also see Common Phases for the TCNI Database, which lists common phase names and the corresponding Thermo-Calc database phase names for some key superalloys.

References

[2001Dup] N. Dupin, B. Sundman, A thermodynamic database for Ni-base superalloys. Scand. J. Metall. 30, 184–192 (2001).

[2001Hil] M. Hillert, The compound energy formalism (1). J. Alloys Compd. 320, 161–176 (2001).

[2018Dup] N. Dupin, U. R. Kattner, B. Sundman, M. Palumbo, S. G. Fries, Implementation of an Effective Bond Energy Formalism in the Multicomponent Calphad Approach. J. Res. Natl. Inst. Stand. Technol. 123, 123020 (2018).

[2024San] J. C. P. dos Santos, S. Griesemer, N. Dupin, U. R. Kattner, C. Liu, D. Ivanova, T. Hammerschmidt, S. G. Fries, C. Wolverton, C. E. Campbell, Applying the Effective Bond Energy Formalism (EBEF) to Describe the Sigma (σ) Phase in the Co-Cr-Ni-Re System. J. Phase Equilibria Diffus. 45, 330–357 (2024).

TCNI13 Thermophysical and Elastic Properties

This section summarizes the available thermophysical and elastic properties in the TCS Ni-based Superalloys Database (TCNI).

The thermophysical properties data is added as follows. Molar volume with thermal expansion coefficients properties data have been available since TCNI7 for the most important systems. Viscosity of the metallic liquids and surface tension of metallic liquids are included starting with version 10 (TCNI10). Electrical resistivity and thermal conductivity are included starting with version 11 (TCNI11).

The elastic properties (elastic moduli and elastic constants) are included with the database as of version 13 (TCNI13) 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.

Overview of the Thermophysical Properties

Molar Volume

Molar volume data is critically assessed for most phases of importance to Ni-based superalloys. All the necessary volume data (including molar volume and thermal expansion) for various alloy phases is incorporated, which allows for the calculation of volume fraction of phases, as well as density, thermal expansivity and lattice parameters, e.g. misfits between γ and γ', using Thermo-Calc. However, it should be noted that the molar volume data only provides rough estimations and has no pressure dependence.

Surface Tension and Viscosity

The properties data for surface tension and viscosity are available starting with TCNI10. Surface tension data is critically assessed for the liquid phase in all pure elements and binary systems. The viscosity of the liquid is described for all pure elements and 142 binary systems.

Electrical Resistivity and Thermal Conductivity

The properties data for electrical resistivity and thermal conductivity are available starting with TCNI11. Electrical resistivity and thermal conductivity data is critically assessed in all binary systems with data available, for the most important phases to Ni-base alloys. For all other phases or systems, the properties are estimated.

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
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)` **

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®)****

* 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 Nickel-based Superalloys 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 nickel including links to resources such as examples, publications, and more.

TCNI13 Systems

In this section:

TCNI13 Assessed Binary Systems

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

	AL	B	C	Ca	Co	Cr	Cu	Fe	Hf	Mg	Mn	Mo	N	Nb	Ni	O	P	Pd	Pt	Re	Ru	S	Si	Ta	Ti	V	W	Y	Zr
AL	AL																												
B	x	B																											
C	x	x	C																										
Ca	x	x	x	Ca																									
Co	x	x	x	x	Co																								
Cr	x	x	x	x	x	Cr																							
Cu	x	x	x	x	x	x	Cu																						
Fe	x	x	x	x	x	x	x	Fe																					
Hf	x	x	x		x	x	x	x	Hf																				
Mg	x	x	x	x	x	x	x	x	x	Mg																			
Mn	x	x	x	x	x	x	x	x	x	x	Mn																		
Mo	x	x	x	x	x	x	x	x	x	x	x	Mo																	
N	x	x			x	x	x	x		x	x	x	N																
Nb	x	x	x	x	x	x	x	x	x	x	x	x	x	Nb															
Ni	x	x	x	x	x	x	x	x	x	x	x	x	x	x	Ni														
O	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	O													
P	x	x	x	x	x	x	x	x			x	x		x	x		P												
Pd	x	x	x		x	x	x	x	x		x	x		x	x	x	x	Pd											
Pt	x	x	x		x	x	x	x	x		x	x		x	x	x	x	x	Pt										
Re	x	x	x		x	x	x	x	x		x	x		x	x	x		x	x	Re									
Ru	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	Ru								
S	x		x	x	x	x	x	x		x	x	x		x	x		x	x	x	x	x	S							
Si	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	Si						
Ta	x	x	x		x	x	x	x	x		x	x	x	x	x	x		x	x	x	x		x	Ta					
Ti	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	Ti				
V	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	V			
W	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	W		
Y	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x		x	x	x	x		x	x	x	x	x	Y	
Zr	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	Zr

TCNI13 Assessed Ternary Systems

These are the assessed or partially assessed ternary systems described in the full range of composition and temperature.

Assessed Ternary Systems							
Al-B-Co	Al-B-Cr	Al-B-Fe	Al-B-Mo	Al-B-Ni	Al-B-Ti	Al-B-Zr	Al-C-Co
Al-C-Cr	Al-C-Fe	Al-C-Ni	Al-C-Si	Al-Ca-O	Al-Ca-Si	Al-Co-Cr	Al-Co-Hf
Al-Co-Mo	Al-Co-Nb	Al-Co-Ni	Al-Co-O	Al-Co-Si	Al-Co-Ta	Al-Co-Ti	Al-Co-W
Al-Co-Zr	Al-Cr-Nb	Al-Cr-Ni	Al-Cr-O	Al-Cr-Pt	Al-Cr-Ru	Al-Cr-Ta	Al-Cr-Ti
Al-Cr-W	Al-Cr-Zr	Al-Cu-Fe	Al-Cu-Mn	Al-Cu-Ni	Al-Cu-S	Al-Cu-Si	Al-Fe-Mn
Al-Fe-Mo	Al-Fe-N	Al-Fe-Nb	Al-Fe-Ni	Al-Fe-O	Al-Fe-P	Al-Fe-Re	Al-Fe-Ru
Al-Fe-S	Al-Fe-Ta	Al-Fe-Ti	Al-Fe-W	Al-Hf-Ni	Al-Hf-Ru	Al-Hf-Ti	Al-Mn-Ni
Al-Mn-O	Al-Mn-Si	Al-Mn-Ti	Al-Mo-Nb	Al-Mo-Ni	Al-Mo-Re	Al-Mo-Si	Al-Mo-Ti
Al-Mo-Zr	Al-N-Ti	Al-Nb-Ni	Al-Nb-Ru	Al-Nb-Si	Al-Ni-O	Al-Ni-Pt	Al-Ni-Ru
Al-Ni-S	Al-Ni-Si	Al-Ni-Ta	Al-Ni-Ti	Al-Ni-V	Al-Ni-W	Al-Ni-Y	Al-Ni-Zr
Al-O-S	Al-O-Si	Al-O-Ti	Al-O-Y	Al-O-Zr	Al-Ru-Ti	Al-Ta-Ti	Al-Ti-W
B-C-Hf	B-C-Ti	B-C-W	B-C-Zr	B-Co-Cr	B-Co-Hf	B-Co-Mo	B-Co-Re
B-Co-Ta	B-Co-Ti	B-Co-W	B-Co-Zr	B-Cr-Fe	B-Cr-Hf	B-Cr-Mo	B-Cr-Ni
B-Cr-Re	B-Fe-Mo	B-Fe-Nb	B-Fe-Ni	B-Fe-W	B-Hf-Nb	B-Hf-Ni	B-Hf-Ta
B-Hf-Ti	B-Mo-Ni	B-Mo-Re	B-Mo-Ti	B-Nb-Re	B-Ni-P	B-Ni-Re	B-Ni-Si
B-Ni-Ta	B-Ni-Ti	B-Re-Ta	B-Re-W	B-Re-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-Mn
C-Cr-Mo	C-Cr-N	C-Cr-Nb	C-Cr-Ni	C-Cr-Re	C-Cr-Si	C-Cr-Ta	C-Cr-Ti
C-Cr-V	C-Cr-W	C-Cr-Zr	C-Cu-Fe	C-Fe-Mn	C-Fe-Mo	C-Fe-N	C-Fe-Nb
C-Fe-Ni	C-Fe-O	C-Fe-P	C-Fe-Si	C-Fe-Ti	C-Fe-V	C-Fe-W	C-Hf-Mo

Assessed Ternary Systems							
C-Hf-Ta	C-Hf-Ti	C-Hf-W	C-Mn-Si	C-Mn-V	C-Mo-N	C-Mo-Ni	C-Mo-Si
C-Mo-Ta	C-Mo-Ti	C-Mo-V	C-Mo-W	C-Mo-Zr	C-N-Nb	C-N-Ti	C-Nb-Re
C-Nb-Ti	C-Nb-V	C-Nb-W	C-Nb-Zr	C-Ni-Ta	C-Ni-Ti	C-Ni-W	C-Re-W
C-Si-Ti	C-Ta-Ti	C-Ta-W	C-Ti-W	C-Ti-Zr	C-V-W	C-W-Zr	Ca-Co-O
Ca-Cr-O	Ca-Cu-O	Ca-Cu-S	Ca-Fe-O	Ca-Fe-S	Ca-Mg-S	Ca-Mn-O	Ca-Mn-S
Ca-Nb-O	Ca-Ni-O	Ca-O-S	Ca-O-Si	Ca-O-Y	Ca-O-Zr	Ca-S-Y	Co-Cr-Cu
Co-Cr-Fe	Co-Cr-Mo	Co-Cr-Nb	Co-Cr-Ni	Co-Cr-O	Co-Cr-Re	Co-Cr-S	Co-Cr-Ta
Co-Cr-Ti	Co-Cr-W	Co-Cu-Fe	Co-Cu-Mn	Co-Cu-Nb	Co-Cu-Ni	Co-Cu-S	Co-Cu-Ti
Co-Fe-N	Co-Fe-O	Co-Fe-P	Co-Fe-S	Co-Fe-Ti	Co-Fe-W	Co-Hf-Ni	Co-Hf-Si
Co-Mn-O	Co-Mn-S	Co-Mo-Ta	Co-Nb-Ni	Co-Nb-Si	Co-Ni-O	Co-Ni-P	Co-Ni-Re
Co-Ni-Ru	Co-Ni-S	Co-Ni-Si	Co-Ni-Ta	Co-Ni-Ti	Co-Ni-V	Co-Ni-W	Co-O-S
Co-O-Si	Co-O-W	Co-P-V	Co-P-W	Co-Si-Ta	Co-Si-Ti	Co-Si-W	Co-Si-Zr
Co-Ta-Ti	Co-Ta-W	Cr-Cu-Fe	Cr-Cu-Nb	Cr-Cu-Ni	Cr-Cu-S	Cr-Cu-Si	Cr-Fe-Mn
Cr-Fe-Mo	Cr-Fe-N	Cr-Fe-Ni	Cr-Fe-O	Cr-Fe-P	Cr-Fe-S	Cr-Fe-Si	Cr-Fe-V
Cr-Fe-W	Cr-Mn-N	Cr-Mn-O	Cr-Mn-S	Cr-Mo-N	Cr-Mo-Nb	Cr-Mo-Ni	Cr-N-Nb
Cr-N-Ni	Cr-N-V	Cr-Nb-Ni	Cr-Nb-P	Cr-Nb-Si	Cr-Nb-V	Cr-Ni-O	Cr-Ni-P
Cr-Ni-Pt	Cr-Ni-Re	Cr-Ni-Ru	Cr-Ni-S	Cr-Ni-Si	Cr-Ni-Ta	Cr-Ni-Ti	Cr-Ni-V
Cr-Ni-W	Cr-Ni-Zr	Cr-O-S	Cr-O-Si	Cr-O-Ti	Cr-O-V	Cr-O-Y	Cr-O-Zr
Cr-P-Ti	Cu-Fe-Mn	Cu-Fe-Mo	Cu-Fe-N	Cu-Fe-Nb	Cu-Fe-Ni	Cu-Fe-P	Cu-Fe-S
Cu-Fe-Si	Cu-Fe-Ti	Cu-Fe-V	Cu-Mg-Ni	Cu-Mg-S	Cu-Mg-Si	Cu-Mn-Ni	Cu-Mn-S
Cu-Mn-Si	Cu-Mo-Ni	Cu-Ni-P	Cu-Ni-S	Cu-Ni-Si	Cu-Ni-Ti	Cu-O-S	Cu-O-Y
Cu-S-Si	Cu-Ti-Zr	Fe-Mg-Ni	Fe-Mg-S	Fe-Mn-N	Fe-Mn-Ni	Fe-Mn-O	Fe-Mn-P

Assessed Ternary Systems							
Fe-Mn-S	Fe-Mn-Si	Fe-Mo-N	Fe-Mo-Ni	Fe-Mo-P	Fe-Mo-W	Fe-N-Nb	Fe-N-Ti
Fe-N-V	Fe-Nb-Ni	Fe-Nb-P	Fe-Nb-S	Fe-Nb-Si	Fe-Nb-V	Fe-Nb-Zr	Fe-Ni-O
Fe-Ni-P	Fe-Ni-S	Fe-Ni-Si	Fe-Ni-Ti	Fe-Ni-W	Fe-O-S	Fe-O-Si	Fe-O-Ti
Fe-O-V	Fe-O-W	Fe-O-Y	Fe-O-Zr	Fe-P-Si	Fe-P-Ti	Fe-P-V	Fe-P-W
Fe-S-Zr	Fe-Si-Ti	Fe-Si-W	Fe-Si-Zr	Hf-Nb-Si	Hf-Ni-Si	Hf-Ni-Ta	Hf-Ni-Ti
Hf-O-Si	Mg-Mn-Ni	Mg-Mn-S	Mn-Ni-O	Mn-Ni-S	Mn-Ni-Si	Mn-O-S	Mn-O-Si
Mn-O-W	Mn-O-Y	Mn-O-Zr	Mn-S-Zr	Mo-N-Ni	Mo-N-V	Mo-Ni-O	Mo-Ni-Si
Mo-Ni-Ta	Mo-Ni-Ti	Mo-O-S	Mo-Re-Ru	Mo-Re-Ta	Mo-Ru-Ta	N-Nb-Ti	N-Ni-Ti
N-Ti-V	Nb-Ni-P	Nb-Ni-Ti	Nb-Ni-W	Nb-O-S	Nb-P-Ti	Nb-Re-Ta	Nb-Re-W
Ni-O-S	Ni-O-Si	Ni-O-Ti	Ni-O-V	Ni-O-W	Ni-O-Y	Ni-O-Zr	Ni-P-Si
Ni-P-Ti	Ni-P-V	Ni-P-W	Ni-Re-Ta	Ni-Re-W	Ni-Re-Zr	Ni-Ru-Ti	Ni-Si-Ta
Ni-Si-V	Ni-Si-W	Ni-Si-Zr	Ni-Ta-Ti	Ni-Ti-Zr	O-S-Si	O-S-Y	O-S-Zr
P-V-W							

TCNI13 Phases

In this section:

Common Phases for the TCNI Database

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key superalloys.

Only the phases of interest for superalloys are defined by default, which means that when retrieving the data from the database other phases are automatically rejected and need to be manually restored if these are required for a calculation.

The complete description of all the binary systems and many ternary systems are available using the BINARY and TERNARY modules in Thermo-Calc Console Mode.

There are several possible composition sets for the phases named FCC_L12 and BCC_B2; they are either disordered (A1/carbonitride and A2) or ordered (L12 (γ') and B2 (β)).

Common Phase Name	
ALN_B4	M12C
BCC_B2#1 (disordered BCC A2)	M23C6
BCC_B2#2 (ordered B2, β)	M2B_TETR
BCT_D022 (γ'')	M3B2
BETA_RHOMBO_B	M3C2
C14_LAVES	M6C
CEMENTITE (Fe3C)	M7C3
CHI_A12 (χ)	MB_B33
D5A_M3B2	MB2_C32
DIAMOND_A4	MC_ETA
FCC_L12#1 (disordered FCC A1, γ, austenite)	MC_SHP
FCC_L12#2 (ordered L12 γ')	MU_PHASE (μ)
FCC_L12#3 (carbonitride)	NI3B_D011
FE4N_LP1	NI3TA_D0A (Delta δ)

Common Phase Name	
FECN_CHI	NI3TI_D024 (Eta η)
G_PHASE	P_PHASE
GAS	PI (π)
GRAPHITE	R_PHASE
HCP_A3 (M2(C,N))	SIGMA (σ)
LIQUID	TAU (τ)
	Z_PHASE

TCNI13 Models for the Included Phases

The table lists all phases and the thermodynamic model used to describe the phase.

See the separate listing for Gas and Liquid Phases below.

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)		2	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, W, Y, ZR)1(B, C, N, O, VA)1
DIS_FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)		2	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, W, Y, ZR)1(B, C, N, O, VA)1
FCC_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		3	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, W, Y, ZR)0.75(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, W, Y, ZR)0.25(B, C, N, O, VA)1
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)		2	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, VA, W, Y, ZR)1(B, C, N, O, VA)3
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)		3	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, VA, W, Y, ZR)0.5(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, VA, W, Y, ZR)0.5(B, C, N, O, VA)3
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)		2	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, SI, TA, TI, V, W, Y, 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, MN, MO, NB, NI, P, PD, PT, RE, RU, SI, TA, TI, V, W, Y, ZR)1(B, C, VA)1
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		2	(AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, P, PD, PT, RE, RU, SI, TA, TI, V, W, Y, ZR)1(B, C, VA)1
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)		1	(AL, B, C, O, P, SI)1
BETA_RHOMBO_B	beta-B (R-105)		hR105	(166, R-3m)		2	(B)93(B, C, CU, SI)12

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_ 3/mmc)		1	(B, C)1
NI3TI_D024	Ni3Ti (D024)	D024	hP16	(194, P6_ 3/mmc)		2	(AL, CO, CR, CU, FE, HF, NI, PD, PT, TA, TI, W, ZR)3(AL, CR, CU, HF, MO, NB, NI, PD, PT, SI, TA, TI, W, ZR)1
NI3TA_D0A	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)		2	(AL, CO, CR, FE, NB, NI, PT)3(AL, FE, MO, NB, NI, PT, TA, TI, V, W)1
BCT_D022	Al3Ti (D022)	D022	tI8	(139, I4/mmm)		2	(AL, CO, CR, FE, MO, NB, NI, PD, PT, TI, V)3(AL, CO, CR, MO, NB, NI, PD, PT, SI, TA, TI, V)1
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W, Y, ZR)2(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W, Y, ZR)1
DIS_MU	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		1	(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, SI, TA, TI, W)1
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		5	(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, SI, TA, TI, W)1(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, SI, TA, TI, W)6(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, SI, TA, TI, W)2(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, SI, TA, TI, W)2(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, SI, TA, TI, W)2
DIS_SIG	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		1	(AL, CO, CR, FE, MN, MO, NB, NI, PD, PT, RE, RU, SI, TA, TI, V, W)1
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		5	(AL, CO, CR, FE, MN, MO, NB, NI, PD, PT, RE, RU, SI, TA, TI, V, W)2 (AL, CO, CR, FE, MN, MO, NB, NI, PD, PT, RE, RU, SI, TA, TI, V, W)4 (AL, CO, CR, FE, MN, MO, NB, NI, PD, PT, RE, RU, SI, TA, TI, V, W)8 (AL, CO, CR, FE, MN, MO, NB, NI, PD, PT, RE, RU, SI, TA, TI, V, W)8 (AL, CO, CR, FE, MN, MO, NB, NI, PD, PT, RE, RU, SI, TA, TI, V, W)8
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
P_PHASE	Cr9Mo21Ni20		oP56	(62, Pnma)		3	(CR, FE, NI, RE)24(CR, FE, MO, NI, RE)20(MO)12
CHI_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NISI_B31	MnP (B31)	B31	oP8	(62, Pnma)		2	(NI, PD)1(SI)1
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)		2	(MO, W)1(C, N)1
M23C6	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
CEMENTITE	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(CO, CR, FE, MN, MO, NI, V, W)3(C, N)1
M12C	Fe6W6C		cF104	(227, Fd-3m)		3	(CO, NI)6(MO, W)6(C)1
M3C2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(CO, CR, MO, V, W)3(C)2
M6C	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
M7C3	C3Cr7 (D101)	D101	oP40	(62, Pnma)		2	(CO, CR, FE, MN, MO, NI, RE, V, W)7(C)3
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(FE, MN)5(C)2
TAU	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)		4	(CO, HF, NI, RE)20(B)6(B, VA)6(AL, CR, HF, MO, RE, TA, TI, V, W, ZR)3
MB_B33	CrB (B33)	B33	oS8	(63, Cmcm)		2	(CR, FE, HF, MO, NB, NI, TA, TI, V)1(B)1
MB2_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(B)2(AL, CR, HF, MG, MN, MO, NB, TA, TI, V, Y, ZR)1
M3B2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		3	(CR, FE, MO, NI, W)0.4(CR, FE, NI)0.2(B)0.4
M2B_TETR	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(AL, CO, CR, FE, MN, MO, NB, NI, RE, TA, W)2(B)1
B12ZR	UB12 (D2f)	D2f	cF52	(225, Fm-3m)		2	(B)12(Y, ZR)1
MNP_B31	MnP (B31)	B31	oP8	(62, Pnma)		2	(CO, CR, FE, MN, NI, RU, W)1(P, SI)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU3P_D021	Cu3P (D021)	D021	hP24	(165, P-3c1)		2	(CU, FE)3(P)1
M2P_C22	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		2	(AL, CO, CR, FE, MN, MO, NB, NI, TI, V, W)2(B, P, SI)1
M3P_D0E	Ni3P (D0e)	D0e	tI32	(82, I-4)		2	(AL, CO, CR, CU, FE, MN, MO, NI, TI)3(B, P)1
TINIP_C37	Co2Si (C37)	C37	oP12	(62, Pnma)		3	(CO, CR, FE, NB, NI, TI, V, W)1(CO, CR, FE, NB, NI, TI, V, W)1(P)1
NI5P2_ALPHA	Pd8Sb3		hR44	(161, R3c)		2	(CO, NI)5(P)2
NI5P2_BETA	Unknown Structure					2	(CO, NI)5(P)2
NI12P5_ALPHA	Ni12P5		tI34	(87, I4/m)		2	(CO, NI)12(P)5
NI12P5_BETA	Unknown Structure					2	(CO, NI)12(P)5
NI5P4	Ni5P4		hP36	(194, P6_ 3/mmc)		2	(NI)5(P)4
NIP2	PdP2		mS12	(15, C2/c)		2	(NI)1(P)2
COP3	Skutterudite (CoAs3, D02)	D02	cI32	(204, Im-3)		2	(CO)1(P)3
NBP	NbAs		tI8	(109, I4_1md)		2	(NB)1(P)1
NB7P4	Nb7P4		mS44	(12, C2/m)		2	(NB, TI)7(P)4
TI3P	Ti3P		tP32	(86, P4_2/n)		2	(CR, NB, TI)3(P)1
TI5P3	beta-Yb5Sb3		oP32	(62, Pnma)		2	(TI)5(P)3
ZINCBLENDE_B3	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(AL)1(P)1
WP2	MoP2		oS12	(36, Cmc2_1)		2	(W)1(P)2
MO3P	alpha-V3S		tI32	(121, I-42m)		2	(MO)3(P)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MOP_BH	Tungsten Carbide (Bh)	Bh	hP2	(187, P-6m2)		2	(MO)1(P)1
NB2NI9P	MgCu4Sn		cF24	(216, F-43m)		3	(NB)2(NI)9(P)1
NBNI2P	Unknown Structure					3	(NB)1(NI)2(P)1
NB5NI4P4	Cu5Nb5Si4		tI26	(87, I4/m)		3	(NB)5(NI)4(P)4
NB3NI2P	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		3	(NB)3(NI)2(P)1
NB4NIP	Nb4CoSi		tP12	(124, P4/mcc)		3	(NB)4(NI)1(P)1
NB2NI2P3	Nb2Ni2P3		hP28	(176, P6_3/m)		3	(NB)2(NI)2(P)3
NBNIP2	NbNiP2		oP16	(62, Pnma)		3	(NB)1(NI)1(P)2
P2S5	P2S5		aP28	(2, P-1)		2	(P)2(S)5
SIP1	(SiP)		oS48	(36, Cmc2_1)		2	(P)1(SI)1
SIP2	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)		2	(P)2(SI)1
CA2P2	Na2O2		hP12	(189, P-62m)		2	(CA)1(P)1
CA5P8	Ca5P8		mS26	(12, C2/m)		2	(CA)5(P)8
CAP3	CaP3		aP8	(2, P-1)		2	(CA)1(P)3
PD15P2	P2Pd15		hR17	(148, R-3)		2	(PD)15(P)2
PD6P	PPd6		mP28	(14, P2_1/c)		2	(PD)6(P)1
PD3P_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(PD)3(P, VA)1
PD5P2	Unknown Structure					2	(PD)5(P)2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PD6FE5MN2	Unknown Structure					3	(FE)0.3846(PD)0.46154(MN)0.15385
PD7P3	P3Pd7		hR20	(148, R-3)		2	(PD)7(P)3
PDP2	PdP2		mS12	(15, C2/c)		2	(PD)1(P)2
PTP2	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)		2	(PT)1(P)2
PT5P2	Pt5P2		mS28	(15, C2/c)		2	(PT)5(P)2
RU2P	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(RU)2(P)1
RUP2	Marcasite (FeS2, C18)	C18	oP6	(58, Pnnm)		2	(RU)1(P)2
FENB2P	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		3	(FE)1(NB)2(P)1
FENB4P	Nb4CoSi		tP12	(124, P4/mcc)		3	(FE)1(NB)4(P)1
FESI4P4	FeSi4P4		aP9	(1, P1)		3	(FE)1(SI)4(P)4
CO5B2P	Mo5SiB2		tI32	(140, I4/mcm)		3	(CO)5(B)2(P)1
NB5P3	Nb5P3		oP64	(62, Pnma)		2	(NB)5(P)3
NB8P5	Nb8P5		oP54	(55, Pbam)		2	(NB)8(P)5
NB1P2	OsGe2		mS12	(12, C2/m)		2	(NB)1(P)2
ALPT_B20	FeSi (B20)	B20	cP8	(198, P2_13)		2	(AL)0.5(NI, PT)0.5
FCC_L10	CuAu (L10)	L10	tP2	(123, P4/mmm)		2	(AL, CR, CU, FE, MN, MO, NI, PD, PT, TA, TI, W)0.5(AL, CR, CU, FE, MN, MO, NI, PD, PT, TA, TI, W)0.5
NIZR	CrB (B33)	B33	oS8	(63, Cmcm)		2	(NI)1(TI, Y, ZR)1
ALZR_B33	CrB (B33)	B33	oS8	(63, Cmcm)		2	(AL)1(HF, Y, ZR)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALPHA_B19	beta'-AuCd (B19)	B19	oP4	(51, Pmma)		2	(MO, NB, PD, PT, TI, V, ZR)1(MO, NB, PD, PT, TI, V, ZR)1
B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(CO, CU, NI, PD, TI)1(CU, NI, TA, TI)1
CUPT_L11	Rhombohedral CuPt (L11)	L11	hR2	(166, R-3m)		3	(CU, PT)0.5(CU, PT)0.5(VA)1
HFMN	NiTi2		cF96	(227, Fd-3m)		2	(HF)0.5(MN)0.5
MNTA	Unknown Structure					2	(MN)1(TA)1
PDY_LT	CrB (B33)	B33	oS8	(63, Cmcm)		2	(PD, Y)1(Y)1
PDY_HT	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(PD, Y)1(Y)1
AL2PT	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		3	(AL)2(NI, PT)1(NI, VA)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(AL, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W, Y, ZR)2(AL, CO, CR, CU, FE, HF, MG, MO, NB, NI, RE, RU, SI, TA, TI, V, W, Y, ZR)1
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)		2	(AL, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, TA, TI, W, ZR)2(AL, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, TA, TI, W, ZR)1
CRNI2_OP6	MoPt2		oI6	(71, Immm)		2	(CR, MO, W)1(MO, NI, W)2
NI2TA	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(CO, NI)2(TA, TI)1
NI2V	MoPt2		oI6	(71, Immm)		2	(MO, NI, PD, PT)2(MO, NB, PT, TA, V)1
C16_THETA	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(AL, HF, MO, NB, TA, TI, W, ZR)2(AL, CO, CR, CU, FE, NI, SI)1
CU2TI1	Au2V		oS12	(63, Cmcm)		2	(CO, CU, NI)2(TI)1
CU2Y_H	Unknown Structure		hP*			2	(CU)2(Y)1
CU2Y_L	KHg2		oI12	(74, Imma)		2	(CU)2(Y)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MNNI2	Unknown Structure					2	(MN, NI)1(NI)2
NITI2	NiTi2		cF96	(227, Fd-3m)		2	(CO, CR, CU, FE, HF, NI, PT, RE, TI)1(AL, CR, CU, HF, NI, TA, TI, ZR)2
PD2Y1	Unknown Structure					2	(PD)2(Y)1
PTY2	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(PT)1(Y)2
PT2Y	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(PT)2(Y)1
REZR2	Zr21Re25		hR92	(167, R-3c)		2	(NI, RE)1(ZR)2
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)		2	(AL, CO, CR, MN, MO, NI, PT, TA, TI, W)3(AL, CR, MO, NB, NI, PT, RE, TA, TI, W)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)		2	(AL)3(HF, ZR)1
CUTI3	CuTi3 (L60)	L60	tP4	(123, P4/mmm)		2	(CU, TI)1(TI)3
MZR3_E1A	MgCuAl2 (E1a)		oS16	(63, Cmcm)		2	(CO, FE, NI)1(Y, ZR)3
PDY3	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(PD)1(Y)3
PTY3	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(PT)1(Y)3
RUY3	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(RU)0.25(Y)0.75
H_L21	Heusler (L21)	L21	cF16	(225, Fm-3m)		3	(AL, CR, NI, TI)0.5(AL, HF, NB, NI, TA, TI, ZR)0.5(CO, NI, RU, VA)1
G_PHASE	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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALCU_DEL	Al5Cu8		hR52	(160, R3m)		2	(AL)2(CU, FE)3
ALCU_EPS	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(AL, CU, NI)1(CU, FE)1
ALCU_ETA	AlCu(r)		mS20	(12, C2/m)		2	(AL, CU)1(CU, FE, NI)1
ALCU_PRIME	Al9Cu11(h)		oF88	(42, Fmm2)		2	(AL)2(CU)1
ALCU_ZETA	Al9Cu11(h)		oF88	(42, Fmm2)		2	(AL)9(CU, FE)11
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)		3	(AL, NI, SI)4(AL, CU, NI, SI)1(CU, FE, MN, NI)8
GAMMA_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		3	(AL)4(AL, CU)1(CU, FE, MN, NI)8
AL23CUFE4	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)	TAU	2	(AL)1(CU, FE, NI, VA)1
AL12MN	Al12W		cI26	(204, Im-3)		2	(AL)12(MN)1
AL4MN_R	lambda-Al4Mn		hP586	(194, P6_ 3/mmc)		2	(AL)461(FE, MN)107
AL4MN_U	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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL8MN5	Cr5Al8 (D810)	D810	hR26	(160, R3m)		3	(AL, TI)12(MN)5(AL, CU, MN, SI, TI)9
TI25MN9AL66_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		3	(AL, MN, TI)0.25(AL, MN)0.08(AL, MN, TI)0.67
AL28CU4MN7	Mn6Cu4Al29		oS156	(63, Cmcm)		3	(AL)28(MN)7(CU)4
AL11CU5MN3	Unknown Structure		oP380			3	(AL)11(MN)3(CU)5
ALCU3MN2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		3	(AL)1(MN)2(CU)3
AL16FEMN3	mu-Al4Mn		hP574	(194, P6_3/mmc)		2	(AL)4(FE, MN)1
AL13FE2MN2	Al13Fe4		mS102	(12, C2/m)		2	(FE, MN)4(AL)13
AL10FEMN2	Mn3Al10		hP26	(194, P6_3/mmc)		2	(FE, MN)3(AL)10
AL21PD8	Al21Pt8		tI116	(88, I4_1/a)		2	(AL)21(PD)8
AL2PD5	Ga2Pd5		oP28	(62, Pnma)		2	(AL)2(AL, PD)5
AL3PD1	(Al3Pd)		oP*	(33, Pna2_1)		2	(AL)3(PD)1
AL3PD2	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)		2	(AL, PD)3(AL, PD)2
AL3PD5	Rh5Ge3		oP16	(55, Pbam)		2	(AL)3(PD)5
AL4PD	(Al4Pd)		hP*	(182, P6_322)		2	(AL)4(PD)1
ALPD2	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(AL, NI, PD)1(AL, NI, PD)2
AL21PT5	Li21Si5		cF416	(216, F-43m)		2	(AL)0.8077(NI, PT)0.1923
AL21PT8	Al21Pt8		tI116	(88, I4_1/a)		2	(AL)0.7241(NI, PT)0.2759
AL3PT5	Rh5Ge3		oP16	(55, Pbam)		2	(AL)0.375(NI, PT)0.625

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALPT2	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(AL)0.33333(NI, PT)0.66667
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)		2	(AL)6(FE, MN, RE, RU)1
ALZR2	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(AL)1(Y, ZR)2
AL2ZR3	Zr3Al2		tP20	(136, P4_ 2/mnm)		2	(AL)2(HF, Y, ZR)3
AL3ZR4	Al3Zr4		hP7	(191, P6/mmm)		2	(AL)3(HF, ZR)4
AL3ZR2	Zr2Al3		oF40	(43, Fdd2)		2	(AL)3(HF, ZR)2
AL3NI2	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)		3	(AL, SI)3(AL, CU, NI, PT, RU)2(NI, RU, VA)1
AL12W	Al12W		cI26	(204, Im-3)		2	(AL)12(MO, RE, W)1
AL4W	Al4W		mS30	(8, Cm)		2	(AL)4(MO, W)1
AL1MN1SI1	TiSi2 (C54)	C54	oF24	(70, Fddd)		3	(AL)1(MN)1(SI)1
AL3MNSI2	(Al3MnSi2)		tP48	(85, P4/n)		3	(AL)3(MN)1(SI)2
AL3MN4SI2	Unknown Structure					3	(AL)3(MN)4(SI)2
ALMNSI_T6	Unknown Structure					2	(AL, MN)4(SI)1
ALMNSI_T8	Mn3Al10		hP26	(194, P6_ 3/mmc)		5	(MN, VA)6(MN, VA)2(AL)12(AL, SI)6(AL, SI)2
AL15SI2M4	Al15(Mn,Fe)3Si2		cI168	(204, Im-3)		3	(AL)14(FE, MN)4(AL, SI)5
AL2MNSI3	Ga5Pd		tI24	(140, I4/mcm)		3	(AL)2(MN)1(SI)3
HF2PD	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(HF)2(PD)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
HF3PD4	Unknown Structure					2	(HF)3(PD)4
HFPD2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(HF)1(PD)2
BPD3	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(B)1(PD)3
BPD5	Unknown Structure				Might be SG I4/mmm, Pearson tI*	2	(B)1(PD)5
BPD6	Pd6B		mS28	(15, C2/c)		2	(B)1(PD)6
B2PD5	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(B)2(PD)5
BPT3	Unknown Structure					2	(B)1(PT)3
BPT2	Molybdenite (MoS2, C7)	C7	hP6	(194, P6_ 3/mmc)		2	(B)1(PT)2
B2PT3	PtB0.67		oS8	(63, Cmcm)		2	(B)2(PT)3
YB4	ThB4 (D1e)	D1e	tP20	(127, P4/mbm)		2	(Y)1(B)4
YB6_D21	CaB6 (D21)	D21	cP7	(221, Pm-3m)		2	(Y)1(B)6
YB66	YB66		cF1936	(226, Fm-3c)		2	(Y)1(B)66
MONI4_BETA	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)		2	(MO, W)1(CO, NI)4
AL5W	Al5W		hP12	(182, P6_322)		2	(AL)5(MO, W)1
CO10CU57TI33	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		3	(CO)0.1(CU)0.57(TI)0.33
CO17Y2	Ni17Th2		hP38	(194, P6_ 3/mmc)	united HT/LT phase.	3	(CO2, Y)1(CO2, Y)2(CO)15

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CO5Y_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		3	(CO2, Y)1(CO)4(CO, VA)1
CO3Y1	Ni3Pu		hR12	(166, R-3m)		2	(CO)3(Y)1
CO3Y2	Unknown Structure		cP*			2	(CO)3(Y)2
CO7Y6	Unknown Structure					2	(CO)7(Y)6
COY_BF	CrB (B33)	B33	oS8	(63, Cmcm)		2	(CO)1(Y)1
CO3Y4	Co3Ho4		hP22	(176, P6_3/m)		2	(CO)3(Y)4
CO5Y8	Co5Y8		mP52	(14, P2_1/c)		2	(CO)5(Y)8
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
T1_CU2TI	Au2V		oS12	(63, Cmcm)		2	(CU, FE)2(TI)1
T2_CU3TI2	Cu3Ti2		tP10	(129, P4/nmm)		2	(CU, FE)3(TI)2
T3_CU4TI3	Cu4Ti3		tI14	(139, I4/mmm)		2	(CU, FE)4(TI)3
T4CUFETI	Unknown Structure					2	(CU, FE)0.63(TI)0.37
T5CUFETI	Unknown Structure					2	(CU, FE)0.55(TI)0.45
CU5MN4SI	Unknown Structure					3	(CU)0.5(MN)0.37(SI)0.13
CU6NISI3	Unknown Structure					2	(CU, NI)0.732(SI)0.268

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU46NI25SI29	Unknown Structure					3	(CU)0.458(NI)0.25(SI)0.292
T1CUNITI	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(CU, NI)2(TI)1
T2CUNITI	Cu3Ti2		tP10	(129, P4/nmm)		3	(CU)0.175(NI)2.825(TI)2
T4CUNITI	BaPb3		hR12	(166, R-3m)		3	(CU)0.05(NI)0.7(TI)0.25
T6CUNITI	Unknown Structure					3	(CU)0.25(NI)0.5(TI)0.25
CU33SI7_DELTA	Unknown Structure		tP*			2	(CU)0.825(SI)0.175
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cI76	(220, I-43d)		2	(CU, MN)0.789474(AL, SI)0.210526
CU56SI11_GAMMA	Mg3Ru2		cP20	(213, P4_132)		2	(CU, MN, NI, SI)0.835821(SI)0.164179
CUSI_ETA	Cu3Si-h2		hR*	(162, P-31m)	Structure uncertain	2	(CU, MN, NI)0.76(SI)0.24
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)		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
CU10ZR7	Ni10Zr7		oS68	(64, Cmce)		2	(CU)10(ZR)7

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU51ZR14	Ag51Gd14		hP68	(175, P6/m)		2	(CU)51(ZR)14
CU8ZR3	Cu8Hf3		oP44	(62, Pnma)		2	(CU)8(ZR)3
MN3PD5	Ga3Pt5		oS16	(65, Cmmm)		2	(MN)3(PD)5
MNPD2	Ga3Pt5		oS16	(65, Cmmm)		2	(MN)1(PD)2
MN11SI19	Mn11Si19		tP120	(118, P-4n2)		2	(MN)11(AL, SI)19
MN3SI	BiF3 (D03)	D03	cF16	(225, Fm-3m)		2	(FE, MN)3(AL, SI)1
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		2	(AL, MN)17(SI)3
MN9SI2	Mn9Si2		oI186	(71, Immm)		2	(MN)33(SI)7
MN12Y	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)		2	(MN)12(Y)1
NI2Y1	Ni2Tm		cF192	(216, F-43m)		2	(NI)2(Y)1
NI2Y3	Ni2Y3		tP80	(92, P4_12_12)		2	(NI)2(Y)3
NI3Y	Ni3Pu		hR12	(166, R-3m)		2	(FE, NI)3(Y)1
NI4Y	Unknown Structure		hR*			2	(NI)4(Y)1
NI44M56_TAU	Unknown Structure					2	(NI)0.44(HF, TI)0.56
NI7ZR2	Ni7Zr2		mS36	(12, C2/m)		2	(AL, CO, CR, NI)7(HF, Y, ZR)2
NI11ZR9	Pt11Zr9		tI40	(87, I4/m)		2	(NI)11(HF, TI, ZR)9
NI10ZR7	Ni10Zr7		oS68	(64, Cmce)		2	(NI)23(HF, TI, ZR)17
NI5ZR	AuBe5 (C15b)	C15b	cF24	(216, F-43m)		2	(AL, CU, NI)5(HF, Y, ZR)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PD21SI4	Unknown Structure					2	(PD, SI)21(SI)4
PD5SI	Pd5Si		mP24	(4, P2_1)		2	(PD)5(SI)1
PD14SI3	Unknown Structure					2	(PD)14(SI)3
PD9SI2	Pd9Si2		oP44	(62, Pnma)		2	(PD)9(SI)2
PD15SI4	Unknown Structure					2	(PD)15(SI)4
PD3SI	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(PD)3(SI)1
PD39SI20	Unknown Structure					2	(PD)39(SI)20
PD19SI10	Unknown Structure					2	(PD)19(SI)10
ALPHA_PD2SI	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		2	(PD, SI)2(SI)1
BETA_PD2SI	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		2	(PD, SI)2(SI)1
NI17Y2	Fe17Lu2		hP80	(194, P6_ 3/mmc)		2	(AL, FE, NI)1(Y)0.1176
PD2TA	MoPt2		oI6	(71, Immm)		2	(PD)2(TA)1
PD2TI	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(PD)2(TI)1
PD3TI2	Pd3Ti2		oS20	(63, Cmcm)		2	(PD, PT)3(HF, TI)2
PD5TI3	Pd5Ti3		tP8	(123, P4/mmm)		2	(PD)5(TI)3
PD7Y	Ca7Ge		cF32	(225, Fm-3m)		2	(PD)7(Y)1
PD3Y2_LT	Unknown Structure					2	(PD)3(Y)2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PD3Y2_HT	Unknown Structure					2	(PD)3(Y)2
PD4Y3	Pd4Pu3		hR14	(148, R-3)		2	(PD)4(Y)3
PD2Y3	Er3Ni2		hR15	(148, R-3)		2	(PD)2(Y)3
PD2Y5	Dy5Pd2		cF144	(227, Fd-3m)		2	(PD)2(Y)5
PD11ZR9	Ni11Zr9		tP44	(83, P4/m)		2	(PD)11(ZR)9
PD4ZR3	Pd4Pu3		hR14	(148, R-3)		2	(PD)4(ZR)3
PDZRM	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		3	(PD)1(ZR)1(PD, ZR)1
PDZR_ALPHA	(PdZr-alpha)		mS*	(8, Cm)		2	(PD)1(ZR)1
PDZR_BETA	CrB (B33)	B33	oS8	(63, Cmcm)		2	(PD)1(ZR)1
PTSI	Westerveldite (FeAs, B14)	B14	oP8	(62, Pnma)		2	(PT)1(SI)1
PT6SI5	Pt6Si5		mP22	(11, P2_1/m)		2	(PT)6(SI)5
ALPHA_PT2SI	ThH2 (L'2b)	L'2b	tI6	(139, I4/mmm)		2	(PT)2(SI)1
BETA_PT2SI	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		2	(PT)2(SI)1
ALPHA_PT17SI8	Ni12P5		tI34	(87, I4/m)		2	(PT)17(SI)8
BETA_PT17SI8	Pt12Si5		tP68	(85, P4/n)		2	(PT)17(SI)8
PT5SI2	Unknown Structure					2	(PT)5(SI)2
BETA_PT3SI	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(PT)3(SI)1
ALPHA_PT3SI	GePt3		mS16	(12, C2/m)		2	(PT)3(SI)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PT25SI7	Unknown Structure					2	(PT)25(SI)7
PT2TA	Au2V		oS12	(63, Cmcm)		2	(PT)2(TA)1
PT3TA	NbPt3		mP48	(11, P2_1/m)		2	(PT)3(TA)1
PT3TI4	Unknown Structure					2	(PT)3(TI)4
PT8TI	Pt8Ti		tI18	(139, I4/mmm)		2	(PT)8(TI)1
PT5Y	Unknown Structure					2	(PT)5(Y)1
PT4Y3	Unknown Structure					2	(PT)4(Y)3
PT4Y5	Gd5Si4		oP36	(62, Pnma)		2	(PT)4(Y)5
PT3Y5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)		2	(PT)3(Y)5
PT3Y7	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)		2	(PT)3(Y)7
PT4ZR3	Pd4Pu3		hR14	(148, R-3)		2	(HF, PT, ZR)4(HF, PT, ZR)3
PT4ZR1	Unknown Structure					2	(PT, ZR)4(PT, ZR)1
PT3ZR5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)		2	(PT, ZR)3(PT, ZR)5
PT10ZR7	Ni10Zr7		oS68	(64, Cmce)		2	(PT)10(ZR)7
HF8NI21	Hf8Ni21		aP29	(2, P-1)		2	(HF, ZR)8(NI)21
AL13FE4	Al13Fe4		mS102	(12, C2/m)		3	(AL, CU)0.6275(FE, MN, RU)0.235(AL, SI, VA)0.1375
NI8TA	Pt8Ti		tI18	(139, I4/mmm)		2	(NI)8(NB, TA)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CO7M2	(Co7Nb2)		mS18	(12, C2/m)	also L12 Co7Ta2	2	(CO, NI)7(NB, TA)2
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
NB15NI56TI29	Unknown Structure		o*100			3	(NB)0.15(NI)0.56(TI)0.29
NB8NI9TI3	Unknown Structure					3	(NB)0.4(NI)0.45(TI)0.15
NB5NI75TI20	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)		3	(NB)0.05(NI)0.75(TI)0.2
NB13NI75TI12	Unknown Structure					3	(NB)0.13(NI)0.75(TI)0.12
NB15NI80TI5	Unknown Structure					3	(NB)0.15(NI)0.8(TI)0.05
CFC2_FENBZR	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		3	(FE, NB, ZR)2(NB, ZR)1(NB, ZR)3
TI3SIC2	Ti3SiC2		hP12	(194, P6_3/mmc)		3	(TI)3(SI)1(C)2
AL31MN6NI2	mu-Al4Mn		hP574	(194, P6_3/mmc)		3	(AL)31(MN)6(NI)2
AL5MN6SI7	CrSi2 (C40)	C40	hP9	(180, P6_222)		3	(AL)5(MN)6(SI)7
ALCCR2	AlCCr2		hP8	(194, P6_3/mmc)		3	(AL)1(C)1(CR)2
AL8SIC7	Unknown Structure		hP16			3	(AL)8(SI)1(C)7
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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)		3	(AL)2(MN)2(SI)3
CO3AL2B5	Unknown Structure					3	(CO)3(AL)2(B)5
ALCR2B2	AlMn2B2		oS10	(65, Cmmm)		3	(AL)1(CR)2(B)2
ALCR3B4	AlCr3B4		oP8	(47, Pmmm)		3	(AL)1(CR)3(B)4
ALBMO	ZrSi2 (C49)	C49	oS12	(63, Cmcm)		3	(AL)1(B)1(MO)1
NI8ALB11	Unknown Structure		m**			3	(NI)8(AL)1(B)11
AL4SIC4	Al5C3N (E94)	E94	hP18	(186, P6_3mc)		3	(AL)4(SI)1(C)4
NB3RU5	Rh5Ge3		oP16	(55, Pbam)	united Nb3Ru5_HT and NbRu3_LT phase	2	(NB, RU)0.375(RU)0.625
FENBSI2	CrSi2Zr		oP48	(55, Pbam)		3	(FE)1(NB)1(SI)2
FE4NB4SI7	Co4Ge7Zr4		tI60	(139, I4/mmm)		3	(FE)4(NB)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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FENB4SI	Nb4CoSi		tP12	(124, P4/mcc)		3	(FE)1(NB)4(SI)1
FESI2_H	FeSi2-h		tP3	(123, P4/mmm)		2	(FE)0.3(SI)0.7
FESI2_L	FeSi2-l		oS48	(64, Cmce)		2	(FE)0.333333(SI)0.666667
HFNI3_ALPHA	PdRh2Ta		hP40	(194, P6_ 3/mmc)		2	(HF)0.25(NI)0.75
HF3NI7	Hf3Ni7		aP20	(2, P-1)		2	(HF)0.3(NI)0.7
HFNI_ALPHA	CrB (B33)	B33	oS8	(63, Cmcm)		2	(HF, PT)0.5(HF, NI, PT)0.5
HFRE	Zr21Re25		hR92	(167, R-3c)		2	(HF)1(RE)1
MNTI_LT	Zr21Re25		hR92	(167, R-3c)		2	(MN)1(TI)1
MNTI_HT	Unknown Structure		t**			2	(MN)0.515(TI)0.485
MN3TI	Unknown Structure					2	(MN)3(TI)1
MN4TI	R-(Co,Cr,Mo)		hR53	(148, R-3)		2	(MN)0.815(TI)0.185
NI3SI_ORTHO	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(NI)3(SI)1
FE2SI	AlNi2		hP6	(164, P-3m1)		2	(FE)0.666667(SI)0.333333
CO11ZR2	(Co11Hf2)		oP*	(50, Pban)		2	(CO)11(ZR)2
HFNI3_BETA	BaPb3		hR12	(166, R-3m)		2	(HF)0.25(NI)0.75
RUB2	RuB2		oP6	(59, Pmmn)		2	(RU)1(B)2
RU2B3	Ru2B3		hP10	(194, P6_ 3/mmc)		2	(RU)2(B)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RU1B1	Unknown Structure					2	(RU)1(B)1
B3SI	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		3	(B)6(SI)2(B, SI)6
B6SI	SiB6		oP280	(58, Pnnm)		3	(B)210(SI)23(B, SI)48
BNSI	alpha-B (hR12)		hR12	(166, R-3m)		3	(B)61(SI)1(B, SI)8
V2B3	V2B3		oS20	(63, Cmcm)		2	(V)0.4(B)0.6
B9W2	W2B9		hP22	(147, P-3)		2	(B)9(W)2
SIC	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(SI)1(C)1
V3C2	Sc2Te3		hR8	(166, R-3m)		2	(V)3(C)2
CO7HF	(Co11Hf2)		oP*	(50, Pban)		2	(CO)7(HF)1
CO3SI	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)		2	(CO)3(SI)1
CO3V	Al3Pu		hP24	(194, P6_ 3/mmc)		2	(CO, NI, TI, V)3(CO, NI, TI, V)1
AL4ZR5	Ti5Ga4		hP18	(193, P6_ 3/mcm)		2	(AL)4(ZR)5
AL2TI	Ga2Hf		tI24	(141, I4_ 1/amd)		2	(AL)2(TI)1
AL10V	Al10V		cF176	(227, Fd-3m)		2	(AL)10(V)1
AL7V	Al45V7		mS104	(12, C2/m)		2	(AL)7(V)1
AL23V4	Al23V4		hP54	(194, P6_ 3/mmc)		2	(AL)23(V)4
AL8V5	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		2	(AL)8(V)5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL77W23	Unknown Structure					2	(AL)77(W)23
AL7W3	Unknown Structure					2	(AL)7(W)3
AL2W	CrSi2 (C40)	C40	hP9	(180, P6_222)		2	(AL)2(W)1
AL3ZR5	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)		2	(AL)3(ZR)5
AL11RE4	Al11Mn4		aP15	(2, P-1)		2	(AL)11(RE)4
AL4RE	Al4Re		aP71	(2, P-1)		2	(AL)4(RE)1
ALRE2	CuZr2		tI6	(139, I4/mmm)		2	(AL)1(RE)2
ALRE_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(AL)1(RE)1
TA1AL1	Al38Ta48		mP86	(14, P2_1/c)		2	(TA)0.51515(AL)0.48485
TAAL2	Al69Ta39		cF444	(216, F-43m)		2	(TA)0.35(AL)0.65
AL11TI5	Al3Zr (D023)	D023	tI16	(139, I4/mmm)		2	(AL)17(TI)8
ALMO	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)		2	(AL, MO)1(AL, MO)1
AL3NI1	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(AL)0.75(NI)0.25
AL3NI5	Ga3Pt5		oS16	(65, Cmmm)		2	(AL)0.375(NI, PT)0.625
AL2FE	Al2Fe		aP18	(1, P1)		2	(AL, CU)2(FE, MN)1
AL5FE2	Al2.8Fe		oS24	(63, Cmcm)		2	(AL, CU)5(FE, MN)2
AL5FE4	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		1	(AL, CU, FE)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL63MO37	Unknown Structure					2	(AL)63(MO)37
AL8MO3	Al8Mo3		mS22	(12, C2/m)		2	(AL)8(MO)3
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
AL8CR5_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		2	(AL)8(CR)5
AL8CR5_L	Cr5Al8 (D810)	D810	hR26	(160, R3m)		2	(AL)8(CR)5
AL9CR4_H	Unknown Structure					2	(AL)9(CR)4
AL9CR4_L	Unknown Structure					2	(AL)9(CR)4
ALCR2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AL)1(CR)2
ALB12_ALPHA	alpha-AlB12		tP216	(92, P4_12_12)		2	(AL)1(B)12
AL13CO4	Orthorhombic Co4Al13		oP102	(31, Pmn2_1)		2	(AL)13(CO)4
AL3CO	Os4Al13		mS34	(12, C2/m)		2	(AL)3(CO)1
AL5CO2_D811	Co2Al5 (D811)	D811	hP28	(194, P6_3/mmc)		2	(AL)5(CO)2
AL9CO2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)		2	(AL)9(CO)2
W3COC	W10Co3C3.4		hP34	(194, P6_3/mmc)		3	(W)3(CO, NI)1(C)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALM3C_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(AL)1(CO, FE)3(C)1
AL4C3	Al4C3 (D71)	D71	hR7	(166, R-3m)		2	(AL, SI)4(C)3
YC2_C11A	CaC2-I (C11a)	C11a	tI6	(139, I4/mmm)		1	(C2Y1)1
Y15C19_H	Unknown Structure					2	(C)19(Y)15
Y15C19_R	alpha-Y15C19		oP18	(55, Pbam)		2	(C)19(Y)15
Y2C3_H	Unknown Structure					3	(Y)2(C)2(C, VA)1
Y2C3_R	Sc3C4		tP70	(128, P4/mnc)		3	(Y)2(C)2(C, VA)1
YC_GAMMA	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		2	(Y)1(C, C2, VA)1
BM	FeB (B27)	B27	oP8	(62, Pnma)		2	(B, PT)1(CR, FE, HF, MN, MO, TI, Y)1
COB	FeB (B27)	B27	oP8	(62, Pnma)		2	(CO, RE)1(B)1
MOB_LT	MoB (Bg)	Bg	tI16	(141, I4_ 1/amd)		2	(CR, FE, MO)1(B)1
BW_ALPHA	MoB (Bg)	Bg	tI16	(141, I4_ 1/amd)		2	(B, C, VA)1(W)1
BW_BETA	CrB (B33)	B33	oS8	(63, Cmcm)		2	(B, C, VA)1(W)1
CR2B_ORTH	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(CR, FE, MO, RE)0.66666667(B)0.33333333
MN2B_D1F	Mn2B (D1f)	D1f	oF48	(70, Fddd)		2	(MN)0.6707(B)0.3293
MNB4	MnB4		mS10	(12, C2/m)		2	(MN)0.2(B)0.8
MOCOB	MnCuP		oP12	(62, Pnma)		3	(MO, W)1(CO)1(B)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI3B_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(CO, CR, FE, MO, NI)3(B)1
RE3B	Re3B		oS16	(63, Cmcm)		2	(CR, MO, RE, TA, W)3(B)1
B4TA3_D7B	Ta3B4 (D7b)	D7b	oI14	(71, Immm)		2	(B)4(CR, HF, MN, NB, TA, TI, V)3
B5W2_X	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)		2	(B, C, VA)5(W)2
RE7B3	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)		3	(CO, CR, MO, NB, RE, RU, TA, W)7(B)3(B, VA)3
D5A_M3B2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		2	(FE, HF, MO, NB, TA, V)3(B)2
W2COB2	W2CoB2		oI10	(71, Immm)		3	(MO, W)2(CO, NI)1(B)2
CR5B3	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)		2	(CR, MO)0.625(B)0.375
V5B6	V5B6		oS22	(65, Cmmm)		2	(NB, V)5(B)6
B4C	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		2	(B11C, B12)1(B2, C2B, CB2)1
CRB4	CrB4		oI10	(71, Immm)		2	(CR)0.2(B)0.8
MOB4	MoB4		hP16	(194, P6_ 3/mmc)		2	(MO)0.2(B)0.8
REB2	ReB2		hP6	(194, P6_ 3/mmc)		3	(RE)1(B)2(B, VA)2
NI4B3	m-Ni4B3		mS28	(15, C2/c)		2	(NI)0.57142857(B)0.42857143
MO2B5_D8I	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)		2	(MO)0.32(B)0.68
RE3CO3B2	Ti3P		tP32	(86, P4_2/n)		3	(RE)3(CO)3(B)2
NI3CR2B6	V5B6		oS22	(65, Cmmm)		3	(NI)3(CR)2(B)6

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NICR3B6	V2B3		oS20	(63, Cmcm)		3	(NI)0.1(CR)0.3(B)0.6
FEWB	MnCuP		oP12	(62, Pnma)		3	(FE)1(W)1(B)1
MO3NI10B11	Unknown Structure					3	(MO)3(NI)10(B)11
RE5CO2B4	Re5Co2B4		tP22	(127, P4/mbm)		4	(RE)4(CO, RE)2(CO)1(B)4
NI5ALB4	Unknown Structure					3	(NI)5(AL)1(B)4
RECOB	MnCuP		oP12	(62, Pnma)		3	(RE)1(CO)1(B)1
Z_PHASE	CrNbN		tP6	(129, P4/nmm)		3	(CR, FE)1(MO, NB, V)1(N, VA)1
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	(221, Pm-3m)		2	(CO, CR, FE, MN, NI)4(C, N)1
FECN_CHI	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(FE)2.2(C, N)1
PI	beta-Mn (A13)	A13	cP20	(213, P4_132)		3	(CR)12.8(FE, NI)7.2(N)4
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)		2	(AL)1(N)1
SI3N4	Nierite (alpha-Si3N4)		hP28	(159, P31c)		2	(SI)3(N)4
BN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)		2	(B)1(N)1
MN6N4	Mn3N2		tI10	(139, I4/mmm)		2	(MN)6(N)4
MN6N5	CoO		tI4	(139, I4/mmm)		2	(MN)6(N)5
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mnm)		2	(TI)2(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
TI3N2	TiS-9R		hR6	(166, R-3m)		2	(TI)0.71(N)0.29
TI4N3	Sc2Te3		hR8	(166, R-3m)		2	(TI)0.685(N)0.315
ALNTI2	AlCCr2		hP8	(194, P6_ 3/mmc)		3	(AL)1(N)1(TI)2
ALNTI3	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(AL)1(N)1(TI)3
AL2N2TI3	(Al2Ti3N2)		hP22	(186, P6_3mc)		3	(AL)2(N)2(TI)3
NIAL2Y	MgCuAl2 (E1a)		oS16	(63, Cmcm)		3	(NI)1(AL)2(Y)1
NIALY	ZrNiAl		hP9	(189, P-62m)		3	(NI)1(AL)1(Y)1
NI2ALY2	W2CoB2		oI10	(71, Immm)		3	(NI)2(AL)1(Y)2
NI6AL2Y3	Ce3Ni6Si2		cI44	(229, Im-3m)		3	(NI)6(AL)2(Y)3
NI3ALY2	Unknown Structure					3	(NI)3(AL)1(Y)2
NI8ALY3	CeNi3		hP24	(194, P6_ 3/mmc)		3	(NI)8(AL)1(Y)3
HALITE	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		2	(AL+3, CA+2, CO+2, CO+3, CR+3, CU+2, FE+2, FE+3, MG+2, MN+2, MN+3, NI+2, NI+3, TI, TI+2, TI+3, V, V+2, V+3, VA, Y+3, ZR+4)1(O-2, VA)1
QUARTZ	alpha-Quartz (low Quartz)		hP9	(152, P3_121)		1	(SIO2)1
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	(9, Cc)		1	(SIO2)1
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	(227, Fd-3m)		1	(SIO2)1
B2O3	B2O3		hP15	(152, P3_121)		1	(B2O3)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CUPRITE_C3	Cuprite (Cu2O, C3)	C3	cP6	(224, Pn-3m)		2	(CU+1)2(O-2)1
CUO	Tenorite (CuO, B26)	B26	mS8	(15, C2/c)		2	(CU+2)1(O-2)1
YCUO2	Hexagonal Delafossite (CuAlO2)		hP8	(194, P6_ 3/mmc)		3	(Y+3)1(CU+1)1(O-2)2
Y2CU2O5	Cu2Ho2O5		oP36	(33, Pna2_1)		3	(Y+3)2(CU+2)2(O-2)5
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	oP28	(62, Pnma)		4	(CA+2, CO+2, CR+2, CU+2, FE+2, MN+2, NI+2)1(CA+2, CO+2, CR+2, CU+2, FE+2, MN+2, NI+2)1(SI+4)1(O-2)4
RHODONITE	Rhodonite (MnSiO3-b)		aP50	(2, P-1)		3	(CA+2, MN+2)1(SI+4)1(O-2)3
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	(58, Pnnm)		4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
SILLIMANITE	Sillimanite (Al2SiO5, S03)	S03	oP32	(62, Pnma)		4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
MULLITE	Al(Al0.7Si0.3)2O4.8		oP24	(55, Pbam)		4	(AL+3)1(AL+3)1(AL+3, SI+4)1(O-2, VA)5
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	(2, P-1)		4	(AL+3)1(AL+3)1(SI+4)1(O-2)5
CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	(167, R-3c)		3	(AL+3, CR+2, CR+3, FE+2, FE+3, MN+3, TI+3, V+3)2(CR+3, FE+3, NI+2, VA)1(O-2)3
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)		4	(AL+3, CO+2, CO+3, CR+2, CR+3, CU+2, FE+2, FE+3, MG+2, MN+2, NI+2)1(AL+3, CA+2, CO+2, CO+3, CR+3, CU+2, FE+2, FE+3, MG+2, MN+2, MN+3, MN+4, NI+2, VA)2(CR+2, FE+2, MG+2, MN+2, VA)2 (O-2)4
ALPHA_SPINEL	Hausmannite (Mn3O4)		tI28	(141, I4_ 1/amd)		4	(CO+2, MG+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
HFSIO4	(HfSiO4)		tI*	(141, I4_ 1/amd)		3	(HF+4)1(SI+4)1(O-2)4
MN2YO5	HoMn2O5		oP32	(55, Pbam)		4	(Y+3)1(MN+3)1(MN+4)1(O-2)5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MNYO3_HEX	LuMnO3		hP30	(185, P6_3cm)		3	(Y+3)1(MN+3)1(O-2)3
MO4O11	Mo4O11		oP60	(33, Pna2_1)		2	(MO)4(O)11
MO8O23	High-Temperature Mo8O23		mP62	(13, P2/c)		2	(MO)8(O)23
MO9O26	Mo9O26		mP70	(13, P2/c)		2	(MO)1(O)2.889
MOO2	VO2		mP12	(14, P2_1/c)		2	(MO)1(O)2
MOO3	gamma-WO3		mP32	(14, P2_1/c)		2	(MO)1(O)3
NIMOO4	Huanzalaite (MgWO4, H06)	H06	mP12	(13, P2/c)	Also Ni[MoO4] of type Co[MoO4] SG12	3	(NI+2)1(MO+6)1(O-2)4
NIMNO3	Ilmenite (FeTiO3, E22)	E22	hR10	(148, R-3)		2	(MN+3, MN+4, NI+2)2(O-2)3
NI6MNO8	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		3	(NI+2)6(MN+4)1(O-2)8
NIWO4	Sylvanite (AgAuTe4, E1b)	E1b	mP12	(13, P2/c)		3	(CO+2, FE+2, MN+2, NI+2)1(W+6)1(O-2)4
NB2O5	Nb2O5		mP99	(10, P2/m)		2	(NB)2(O)5
NB1O1	NbO		cP6	(221, Pm-3m)		2	(NB)1(O)1
NBO2	alpha-NbO2		tI96	(88, I4_1/a)		2	(NB)1(O)2
PDO	Cooperite (PtS, B17)	B17	tP4	(131, P4_2/mmc)		2	(PD)1(O)1
PTO2	CdI2		hP3	(164, P-3m1)	Also other variants TiO2/CaCl2	2	(PT)1(O)2
PT3O4	Pt3O4		cI14	(229, Im-3m)		2	(PT)3(O)4
REO2	ReO2		mP14	(14, P2_1/c)	Also Ht variant, SG Pbcn	1	(O2RE1)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
REO3	alpha-ReO3 (D09)	D09	cP4	(221, Pm-3m)	There are 6 allotropes	1	(O3RE1)1
RE2O7	Re2O7		oP72	(19, P2_12_12_1)		1	(O7RE2)1
RUTILE_MO2	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mnm)		2	(AL+3, MN+4, RU+4, TI+4, V+4, ZR+4)1(O-2, VA)2
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
TI3O2	(Ti3O2)		hP5	(191, P6/mmm)		3	(TI+2)2(TI)1(O-2)2
TI3O5	V3O5-ht		mS32	(15, C2/c)		3	(TI+3)2(TI+4)1(O-2)5
TIO_ALPHA	alpha-TiO		mS20	(12, C2/m)		2	(TI+2)1(O-2)1
VO2_LT	VO2		mP12	(14, P2_1/c)		2	(V+4)1(O-2)2
V2O_SS	V7O3		mS20	(12, C2/m)		2	(V)1(O, VA)0.5
V2O5	Shcherbinaite (V2O5) (Revised)		oP14	(59, Pmmn)		2	(V+5)2(O-2)5
V52O64	V13O16		tI116	(141, I4_1/amd)		2	(V)52(O)64
WO2_00	VO2		mP12	(14, P2_1/c)		1	(O2W1)1
WO2_72	Unknown Structure					1	(O2_72W1)1
WO2_90	Unknown Structure					1	(O2_90W1)1
WO2_96	Unknown Structure					1	(O2_96W1)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
WO3_HT	WO2.95		tP16	(113, P-42_ 1m)		1	(O3W1)1
WO3_LT	WO3		oP32	(60, Pbcn)		1	(O3W1)1
M2O3C	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)		3	(AL+3, CA+2, CR+3, FE+3, MG+2, MN+3, NI+2, Y, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3H	La2O3 (D52)	D52	hP5	(164, P-3m1)		3	(CA+2, MG+2, MN+3, Y, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3B	B-Sm2O3		mS30	(12, C2/m)		3	(AL+3, CA+2, CO+3, MG+2, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3A	La2O3 (D52)	D52	hP5	(164, P-3m1)		3	(CA+2, MG+2, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3X	Nd2O3		cI26	(229, Im-3m)		3	(CA+2, MG+2, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	(14, P2_1/c)		2	(AL+3, CA+2, 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)		2	(AL+3, CA+2, CR+3, FE+2, HF+4, MG+2, MN+2, MN+3, NI+2, TI+4, Y+3, ZR+4)2(O-2, VA)4
FLUORITE_C1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(AL+3, CA+2, CR+3, FE+2, HF+4, MN+2, MN+3, NI+2, TI+4, Y+3, ZR, ZR+4)2(O-2, VA)4
PSEUDO_BROOKITE	Pseudobrookite (Fe2TiO5, E41)	E41	oS32	(63, Cmcm)		3	(TI+4)1(AL+3)2(O-2)5
YAG	Garnet (Co3Al2Si3O12, S14)	S14	cI160	(230, Ia-3d)		3	(AL+3, CR+3, FE+3)5(Y+3)3(O-2)12
YAP	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)		3	(AL+3, CO+3, CR+3, FE+3, MN+3)1(CA+2, Y+3)1(O-2, VA)3
YAM	Y4Al2O9		mP60	(14, P2_1/c)		4	(AL+3, SI+4)2(CA+2, Y+3)4(O-2, VA)1(O-2)9
Y2S2D_Y2SI2O7	Possible delta-Y2Si2O7		oP44	(62, Pnma)		3	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2G_Y2SI2O7	Y2Si2O7-b		mP22	(14, P2_1/c)		3	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2B_Y2SI2O7	La4Ge3[GeO4]O10		aP44	(2, P-1)		3	(Y+3)1(Y+3)1(SI2O7-6)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
Y2S2A_Y2SI2O7	Thortveitite ([Sc,Y]2Si2O7, S21)	S21	mS22	(12, C2/m)		3	(Y+3)1(Y+3)1(SI2O7-6)1
Y2SIO5	Y2SiO5 (RE2SiO5 X2)		mS64	(15, C2/c)		4	(Y+3)1(Y+3)1(SIO4-4)1(O-2)1
ZRSIO4	Zircon (ZrSiO4, S11)	S11	tI24	(141, I4_ 1/amd)		3	(SI+4)1(ZR+4)1(O-2)4
ZRTIO4_ALPHA	Unknown Structure					3	(ZR+4)1(TI+4)1(O-2)4
ZRTIO4_BETA	zeta-Fe2N		oP12	(60, Pbcn)		2	(TI+4, ZR+4)2(O-2)4
ZRTI2O6	Columbite (FeNb2O6, E51)	E51	oP36	(60, Pbcn)		3	(ZR+4)1(TI+4)2(O-2)6
ZR3Y4O12	UY6O12		hR19	(148, R-3)		3	(ZR+4)3(Y+3)4(O-2)12
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)		4	(CR, CU, FE, HF, MN, MO, NB, NI, SI, TI, Y, ZR)2(AL, CR, SI, TI)3(CR, CU, FE, HF, MN, MO, NB, NI, TI, Y, ZR)3(C, VA)1
W5SI3_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)		3	(CR, FE, MO, NB, V, W)4(CR, FE, MO, NB, SI, V, W)1(AL, SI)3
TA5SI3_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)		2	(HF, NB, TA)5(AL, SI)3
ZR5SI4	Si4Zr5		tP36	(92, P4_12_ 12)		2	(HF, NB, TI, Y, ZR)5(SI)4
CR3SI_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		3	(CR, FE, MO, NB, NI, PD, PT, RE, SI, TA, TI, V)3(AL, CO, CR, MO, NB, NI, PD, PT, RU, SI, TA, TI, V)1(C, VA)3
M3SI1	Ti3P		tP32	(86, P4_2/n)		2	(HF, NB, TA, TI, ZR)3(SI)1
CO2SI_C23	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(CO, CR, CU, FE, NI, TI)2(SI)1
MSI_B27	FeB (B27)	B27	oP8	(62, Pnma)		2	(HF, NB, TI, Y, ZR)1(SI)1
FESI_B20	FeSi (B20)	B20	cP8	(198, P2_13)		2	(CO, CR, FE, MN, NI, RE)1(AL, SI)1
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)		2	(CR, CU, HF, MO, NB, SI, TA, V)1(AL, CR, CU, SI)2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(CO, CU, FE, MO, NI, PD, W)1(AL, HF, SI, TI, ZR)2
ZRSI2_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	Also YSi2-orth of SG Imma	2	(HF, NB, Y, ZR)1(SI)2
YSI2_HT	Unknown Structure					2	(Y)1(SI)2
Y3SI5_HT	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(Y)3(SI)5
Y3SI5_LT	Unknown Structure					2	(Y)3(SI)5
TISI2_C54	TiSi2 (C54)	C54	oF24	(70, Fddd)		2	(MO, NB, RU, TI)1(AL, SI)2
MSI2_C1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(CO, CU, MN, NI)1(AL, CU, SI)2
M3SI2_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		2	(HF, NB, ZR)3(SI)2
NI31SI12	Ni31S12		hP42	(150, P321)		2	(CO, CR, CU, FE, NI)5(SI)2
CR3NI5SI2	AlAu4		cP20	(198, P2_13)		4	(CR)3(NI)5(SI)2(C, VA)1
NI6SI2B	ZrNiAl		hP9	(189, P-62m)		3	(NI)6(SI)2(B)1
NI4SI2B	Nb5Sn2Si		tI32	(140, I4/mcm)		3	(NI)4.29(SI)2(B)1.43
FE8SI2C	Mn8Si2C		aP*	(1, P1)		3	(FE)8(SI)2(C)1
CRNBSI	ZrNiAl		hP9	(189, P-62m)		3	(CR)1(NB)1(SI)1
M11SI8	Cr11Ge8		oP76	(62, Pnma)		2	(CR, NB)11(SI)8
M6SI5	Si5V6		oI44	(72, Ibam)		2	(CR, NB)6(SI)5
CR2NI2SI	NiTi2		cF96	(227, Fd-3m)		3	(CR)5(NI)5(SI)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
M4SI3	Ru4Si3		oP28	(62, Pnma)		2	(CR, NI)4(SI)3
RU2SI_C37	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(RU)2(SI)1
RU4SI3	Ru4Si3		oP28	(62, Pnma)		2	(RU)4(SI)3
RUSI	FeSi (B20)	B20	cP8	(198, P2_13)		2	(RU)1(SI)1
RU2SI3	Ge3Ru2		oP40	(60, Pbcn)		2	(RU)2(SI)3
SI5V6	Si5V6		oI44	(72, Ibam)		2	(SI)5(V)6
NI3SI_MONOCL	Ge9Pd25		hP34	(147, P-3)		2	(NI)3(SI)1
NI3SI2	Ni3Si2		oP80	(36, Cmc2_1)		2	(NI)3(SI)2
NI2SI_TETA	AlNi2		hP6	(164, P-3m1)		3	(CU, NI)1(NI, VA)1(AL, SI)1
RE2SI	Re2Si		mP24	(14, P2_1/c)		2	(RE)2(SI)1
RESI2_C11B	Re4Si7		mS44	(8, Cm)		2	(RE)0.357(SI)0.643
MN15NI45SI40	Unknown Structure					3	(MN)0.15(NI)0.45(SI)0.4
MN15NI50SI35	Unknown Structure					3	(MN)0.15(NI)0.5(SI)0.35
MN6NI16SI7	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		3	(MN)0.206897(NI)0.551724(SI)0.241379
MN1NI1SI1	MnCuP		oP12	(62, Pnma)		3	(MN)1(NI)1(SI)1
MNNISI_T5	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(MN)1(NI, SI)2
MNNISI_T6	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(MN)1(NI, SI)2
MN3NI2SI	Mn3Ni2Si		cF96	(227, Fd-3m)		3	(MN)3(NI)2(SI)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN2NISI	Unknown Structure					2	(MN, NI)3(SI)1
MN6NISI3	R-(Co,Cr,Mo)		hR53	(148, R-3)		3	(MN)0.61(NI)0.12(SI)0.27
MN66NI4SI30	Unknown Structure					3	(MN)0.66(NI)0.04(SI)0.3
MN52NI29SI19	Unknown Structure					3	(MN)0.52(NI)0.29(SI)0.19
MONOCLINIC_S	beta-S		mP48	(14, P2_1/c)		1	(S)1
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	(70, Fddd)		1	(S)1
RED_P	Unknown Structure					1	(P)1
WHITE_P	Unknown Structure					1	(P)1
AL2S3	alpha-Al2S3		hP30	(169, P6_1)		2	(AL)2(S)3
CR1S1	CrS		mS8	(15, C2/c)		2	(CR)1.03(S)1
CR7S8	Cr7Se8		mS30	(12, C2/m)		2	(CR)7(S)8
CR5S6	Cr5S6		hP22	(163, P-31c)		2	(CR)5(S)6
CR3S4	Brezinaite (Cr3S4)		mS14	(12, C2/m)		2	(CR, FE, MN, NI)3(S)4
CR2S3	Dolomite [MgCa(CO3)2, G11]	G11	hR10	(148, R-3)	Also Cr+ variant of SG P-31c	2	(CR, FE)2(S)3
NIS_LT	Millerite (NiS, B13)	B13	hR6	(160, R3m)		2	(NI)1(S)1
NI3S2_LT	Hazelwoodite (Ni3S2, D5e)	D5e	hR5	(155, R32)		2	(NI)3(S)2
CUCRS2	CuCrS2-b		hR4	(160, R3m)	Also ht variant of pearson hR5	3	(CU)1(CR)1(S)2
FEAL2S4	ZnIn2S4		hR7	(160, R3m)		3	(FE)1(AL)2(S)4

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SIS2	SiS2 (C42)	C42	oI12	(72, Ibam)		2	(SI)1(S)2
ZRS2	CdI2		hP3	(164, P-3m1)		2	(ZR)1(S)2
ANILITE	Cu7S4		oP44	(62, Pnma)		2	(CU)1.75(S)1
CHALCOCITE_ALPHA	Cu2S-alpha		mP144	(14, P2_1/c)		2	(CU)2(S)1
CHALCOCITE_BETA	Cu2S-beta		hP16	(194, P6_ 3/mmc)		2	(CU)2(S)1
COVELLITE	Covellite (CuS, B18)	B18	hP12	(194, P6_ 3/mmc)		2	(CU)1(S)1
DJURLEITE	Cu31S16		mP376	(14, P2_1/c)		2	(CU)1.93(S)1
CUFES2_LT	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)		3	(CU)1(FE)1(S)2
MO2S3	Mo2S3		mP10	(11, P2_1/m)		2	(MO)2(S)3
MO1S2	Molybdenite (MoS2, C7)	C7	hP6	(194, P6_ 3/mmc)		2	(MO)1(S)2
HEAZLEWOODITE_B1	Cu1.9S		cF12	(216, F-43m)		2	(CO, FE, NI, VA)2(S)1
HEAZLEWOODITE_B2	Unknown Structure		cP*			2	(FE, NI, VA)2(S)1
NI7S6	Unknown Structure		t**			2	(FE, NI)7(S)6
NI9S8	Ni9S8		oS68	(21, C222)		2	(FE, NI)9(S)8
THIOSPINEL	Spinel (Co3O4, D72)	D72	cF56	(227, Fd-3m)		3	(CO, CU, FE, MN, NI)1(CO, CR, NI)2(S)4
ALABANDITE	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		2	(CA, CO, CR, CU, FE, MG, MN, Y, ZR)1(S)1
PYRRHOTITE	NiAs (B81)	B81	hP4	(194, P6_ 3/mmc)		2	(AL, CO, CR, CU, FE, MG, MN, NB, NI, TI, V, VA, ZR)1(S)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PYRITE	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)		2	(CO, FE, MN, NI)1(S)2
CO9S8	Co9S8 (D89)	D89	cF68	(225, Fm-3m)		2	(CO, FE, NI)9(S)8
PENTLANDITE	Co9S8 (D89)	D89	cF68	(225, Fm-3m)		3	(FE, NI)8(FE, NI)1(S)8
DIGENITE	Cu2Se		cF44	(225, Fm-3m)		3	(CU, FE, MG, MN, VA)2(CU, VA)1(S)1
CHALCOPYRITE	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)		3	(CU, FE, VA)1(CU, VA)1(S)1
FE2O12S3	Fe2[SO4]3		hR34	(148, R-3)		2	(AL+3, CR+3, FE+3)2(SO4-2)3
ZRO8S2	Zr[SO4]2		oP44	(62, Pnma)		2	(ZR+4)1(SO4-2)2
ANHYDRITE	Anhydrite (CaSO4, H01)	H01	oS24	(63, Cmcm)		2	(CA+2, CO+2, CU+2, FE+2, MN+2, NI+2)1(SO4-2)1
CASO4_HT	CePO4		hP18	(180, P6_222)		2	(CA+2, CO+2)1(SO4-2)1
CU2SO4	Thenardite [Na2SO4 (V), H17]	H17	oF56	(70, Fddd)		2	(CU+1)2(SO4-2)1
CU2SO5	Cu2[SO4]O		mS32	(12, C2/m)		1	(CU2O5S1)1
MN9SI3O14S1	Unknown Structure					4	(MN+2)9(SI+4)3(O-2)14(S-2)1
C1A1_AL2CAO4	Al2CaO4		mP84	(14, P2_1/c)		4	(CA+2)3(AL+3)5(AL+3, FE+3)1(O-2)12
C1A2	Al4CaO7		mS48	(15, C2/c)		4	(CA+2)1(AL+3)3(AL+3, FE+3)1(O-2)7
C1A6	Magnetoplumbite (PbFe12O19)		hP64	(194, P6_ 3/mmc)		3	(CA+2)1(AL+3, FE+3)12(O-2)19
C3A1	Ca3Al2O6		cP264	(205, Pa-3)		3	(CA+2)3(AL+3, FE+3)2(O-2)6
C12A7	Mayenite (12CaO.7Al2O3, K74, C12A7)	K74	cI152	(220, I-43d)		4	(CA+2)6(AL+3)6(AL+3, FE+3)1(O-2)16.5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AF	FeGaO3		oP40	(33, Pna2_1)		2	(AL2O3)1(FE2O3)1
CACR2O4_A	SrCr2O4		oP28	(59, Pmmn)		3	(CA+2)1(AL+3, CR+3, FE+3)2(O-2)4
CF2	Ca3.5Fe14O24.5		mS172	(5, C2)		3	(CA+2)1(FE+3)4(O-2)7
C2F	Ca2Fe2O5		oP36	(62, Pnma)		3	(CA+2)2(AL+3, FE+3)2(O-2)5
CWF	CaFe3O5		oS36	(63, Cmcm)		4	(CA+2)1(FE+2)1(FE+3)2(O-2)5
CW3F	CaFe5O7		oS52	(63, Cmcm)		4	(CA+2)1(FE+2)3(FE+3)2(O-2)7
C4WF4	Ca4Fe9O17		mS60	(5, C2)		4	(CA+2)4(FE+2)1(FE+3)8(O-2)17
C4WF8	Sr2Fe2O5		oI44	(74, Imma)		4	(CA+2)4(FE+2)1(FE+3)16(O-2)29
CAV2O4	CaV2O4		oP28	(62, Pnma)		3	(CA+2)1(AL+3, CR+3, FE+3, Y+3)2(O-2)4
CAMN2O4	CaMn2O4		oP28	(57, Pbcm)		3	(CA+2)1(MN+3)2(O-2)4
CA3CO2O6	Ca3Co2O6		hR22	(167, R-3c)		3	(CA+2)3(CO+3, CU+2)2(O-2, VA)6
CA3CO4O9	Ca3Co4O9		mS30	(12, C2/m)		3	(CA+2)3(CO+3, CU+2)4(O-2, VA)9
CA4NB2O9_HT11	Ca4Nb2O9		mP20	(14, P2_1/c)		5	(CA+2)6(CA+2, NB+5)3(NB+5)3(O-2, VA)3(O-2)15
CA4NB2O9_LT21	Ca4Nb2O9-lt		mP60	(14, P2_1/c)		5	(CA+2)6(CA+2, NB+5)4(CA+2)2(O-2, VA)3(O-2)15
LAAP	PrNiO3		hR10	(167, R-3c)	This is Rhombohedral Perovskite: La (Al,Co)O3 with solubility of Ca, Cu, Ni, Y	3	(CA+2, Y+3)1(AL+3, CO+3, CU+2, FE+3, NI+2)1(O-2, VA)3
CAMO3	CaTiO3 Pnma Perovskite		oP20	(62, Pnma)		3	(CA+2, Y+3)1(MN+4, Y+3, ZR+4)1(O-2)3
CACU2O3	Shcherbinaite (V2O5) (Revised)		oP14	(59, Pmmn)		3	(CA+2)1(CU+2)2(O-2)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CA2CUO3	Sr2CuO3		oI12	(71, Immm)		3	(CA+2)2(CU+2)1(O-2)3
CA15CU18O35	Ca4.8Cu6O11.6		mP92	(13, P2/c)		4	(CA+2)15(CU+2)14(CU+3)4(O-2)35
CASFEO	Unknown Structure					4	(CA+2)2(S-2)2(FE+2, FE+3)2(O-2, VA)3
CA3S3FE4OX	Unknown Structure					4	(CA+2)3(S-2)3(FE+2, FE+3)4(O-2, VA)6
CA2NB2O7	La2Ti2O7		mP44	(4, P2_1)		3	(CA+2)2(NB+5)2(O-2)7
CA3NB2O8	Unknown Structure					3	(CA+2)3(NB+5)2(O-2)8
CA2SIO4_ALPHA	Ca2SiO4		hP24	(194, P6_3/mmc)		3	(CA+2, MN+2, Y+3)3(CA+2, VA)1(SIO4-4)2
CA2SIO4_ALPH_PRM	K2CoCl4		oP84	(33, Pna2_1)		3	(CA+2, FE+2, MN+2, Y+3)3(CA+2, VA)1(SIO4-4)2
LARNITE	Parawollastonite (CaSiO3, S33(II))	S33(II)	mP60	(14, P2_1/c)		3	(CA+2)2(SI+4)1(O-2)4
RANKINITE	3CaO.2SiO2		mP48	(14, P2_1/c)		3	(CA+2)3(SI+4)2(O-2)7
CLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	(15, C2/c)		4	(CA+2, FE+2, NI+2)1(CO+2, FE+2, NI+2)1(SI+4)2(O-2)6
ORTHO_PYROXENE	Enstatite (MgSiO3, S43)	S43	oP80	(61, Pbca)		4	(CA+2, FE+2)1(FE+2)1(SI+4)2(O-2)6
PROTO_PYROXENE	MgSiO3		oP40	(60, Pbcn)		3	(CA+2, CO+2, CR+2, FE+2, NI+2)1(SI+4)1(O-2)3
WOLLASTONITE	Wollastonite (CaSiO3)		aP30	(2, P-1)		3	(CA+2, FE+2, MN+2)1(SI+4)1(O-2)3
PSEUDO_WOLLASTONITE	CaSiO3		mS120	(15, C2/c)		3	(CA+2)1(SI+4)1(O-2)3
HATRURITE	Ca3(SiO4)O-b		hR81	(160, R3m)		3	(CA+2, VA, Y+3)3(SIO4-4)1(O-2)1
CAZRO3_C	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)		3	(CA+2, Y+3)1(Y+3, ZR+4)1(O-2)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CAZR4O9	CaZr4O9		mS224	(15, C2/c)		3	(CA+2)1(ZR+4)4(O-2)9
CA6ZR19O44	Ca6Hf19O44		hR138	(167, R-3c)		3	(CA+2)6(ZR+4)19(O-2)44
C13A6Z2	Ca7ZrAl6O18		oP104	(31, Pmn2_1)		4	(CA+2)13(AL+3)12(ZR+4)2(O-2)35
CAY4O7	(Ca0.25Gd0.75)4GdO7		mS48	(12, C2/m)		3	(CA+2)1(Y+3)4(O-2)7
CAYALO4	K2NiF4		tI14	(139, I4/mmm)		4	(CA+2)1(Y+3)1(AL+3)1(O-2)4
CAYAL3O7	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_1m)		4	(CA+2)1(Y+3)1(AL+3)3(O-2)7
CA3COAL4O10	Ca3ZnAl4O10		oP72	(29, Pca2_1)		4	(CA+2)3(CO+2)1(AL+3)4(O-2)10
CA2ALNBO6	Ca2AlNbO6		mP24	(14, P2_1/c)		4	(CA+2)2(AL+3)1(NB+5)1(O-2)6
ANORTHITE	Ca(Al0.5Si0.5)4O8		aP104	(2, P-1)		4	(CA+2)1(AL+3)2(SI+4)2(O-2)8
CACRSI4O10	gillespite (BaFeSi4O10)		tP64	(130, P4/ncc)		4	(CA+2)1(CR+2)1(SI+4)4(O-2)10
CA2ZRSI4O12	cyclosilicate (Ca2ZrSi4O12)		mP38	(11, P2_1/m)		1	(CA2ZRSI4O12)1
CA3ZRSI2O9	Ca3Hf(Si2O7)O2		mP60	(14, P2_1/c)		1	(CA3ZRSI2O9)1
GARNET	Orthorhombic Garnet		oF320	(70, Fddd)		4	(CA+2, MN+2)3(AL+3, CR+3)2(SI+4)3(O-2)12
MELILITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	(113, P-42_1m)		5	(CA+2)2(AL+3, CO+2, FE+2, FE+3)1(AL+3, SI+4)1(SI+4)1(O-2)7
APATITE	Fluorapatite [Ca5F(PO4)3, H57]	H57	hP42	(176, P6_3/m)		4	(CA+2, VA, Y+3, ZR+4)4(Y+3)6(SIO4-4)6(O-2, VA)2
CA3Y2SI6O18	Ca0.6Y0.4Si6O18		mS116	(15, C2/c)		4	(CA+2)3(Y+3)2(SI+4)6(O-2)18
CA3Y2SI3O12	Ca3Y2Si3O12		oP100	(62, Pnma)		4	(CA+2)3(Y+3)2(SI+4)3(O-2)12

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
C1A1F2	Unknown Structure					5	(CA+2)1(AL+3)1(FE+3)2(AL+3, FE+3)3(O-2)10
CA2NI7	Co7Gd2		hR18	(166, R-3m)		2	(CA)2(NI)7
CANI2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(NI)2(CA)1
CANI3	Ni3Pu		hR12	(166, R-3m)		2	(CA)0.25(NI)0.75
CANI5	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CA)1(NI)5
CA2SI_C37	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(CA)2(SI)1
CASI_B33	CrB (B33)	B33	oS8	(63, Cmcm)		2	(CA)1(SI)1
CASI2_C12	CaSi2 (C12)	C12	hR6	(166, R-3m)		2	(CA)1(SI)2
CUMG2	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(CU, NI)1(MG)2
MG3N2_D53	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)		2	(MG)3(N)2
MG2NI	Mg2Ni (Ca)	Ca	hP18	(180, P6_222)		2	(MG)2(CU, NI)1
MG24Y5_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		3	(MG)24(MG, Y)4(Y)1
MNPT7	Ca7Ge		cF32	(225, Fm-3m)		3	(PT)6(PT)1(MN)1
PD4S	Pd4Se		tP10	(114, P-42_1c)		2	(PD)0.8(S)0.2
PD3S1	Pd3S		oS16	(40, Ama2)		2	(PD)0.75(S)0.25
PD16S7	Pd16S7		cI46	(217, I-43m)		2	(PD)0.696(S)0.304
PDS	PdS (B34)	B34	tP16	(84, P4_2/m)		2	(PD)0.5(S)0.5
PTS_B17	Cooperite (PtS, B17)	B17	tP4	(131, P4_2/mmc)		2	(PT)1(S)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PTS2	CdI2		hP3	(164, P-3m1)		2	(PT)1(S)2
RE1S2	ReS2		aP12	(2, P-1)		2	(RE)1(S)2
RE1S3	Unknown Structure					2	(RE)1(S)3
RE2S7	Re2O7		oP72	(19, P2_12_12_1)		2	(RE)2(S)7
RU1S2	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)		2	(RU)1(S)2
W1S2	Molybdenite (MoS2, C7)	C7	hP6	(194, P6_3/mmc)	also HT variant of SG R3m	2	(W)1(S)2
MG3MNNI2	Unknown Structure					3	(MG)3(MN)1(NI)2
NIOCALITE_C10NS6	Niocalite		oS114	(21, C222)		4	(CA+2)10(NB+5)2(SI+4)6(O-2)27
AL4CA_D13	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(AL)4(CA)1
AL2CA_C15	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(AL)2(CA)1
ALMG_BETA	Al45Mg28		cF1832	(227, Fd-3m)		2	(AL)140(MG)89
ALMG_EPSILON	Al30Mg23		hR53	(148, R-3)		2	(AL)30(MG)23
AL12MG17_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		3	(MG)10(AL, MG)24(AL, MG)24
CAB6	CaB6 (D21)	D21	cP7	(221, Pm-3m)		2	(CA)1(B)6
MGB4	MgB4		oP20	(62, Pnma)		2	(MG)1(B)4
MGB7	MgB7		oI64	(74, Imma)		2	(MG)1(B)7
C2CA1_C11A	CaC2-I (C11a)	C11a	tI6	(139, I4/mmm)		1	(C2CA1)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
C2CA1_S2	CaC2		cF36	(225, Fm-3m)		1	(C2CA1)1
MGC2	MgC2		tP6	(136, P4_ 2/mnm)		2	(MG)1(C)2
MG2C3	Mg2C3		oP10	(58, Pnnm)		2	(MG)2(C)3
CA2CU1	Ca2Cu		oP12	(62, Pnma)		2	(CA)2(CU)1
CA1CU1	alpha-CaCu		mP20	(11, P2_1/m)		2	(CA)1(CU)1
CACU5_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CA)1(CU)5
MG2SI	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(MG)2(SI)1

Gas and Liquid Phases

Name	Prototype	Info	Sublattices	Formula Unit
GAS	Gas	Gas mixture	1	(AL, AL1B1O2, AL1B3H12, AL1C1, AL1C2, AL1CU1, AL1CU1S1, AL1CU1S2, AL1H1, AL1H1O1_ALOH, AL1H1O1_HALO, AL1H1O2, AL1H2, AL1H2O2, AL1H3, AL1H3O3, AL1N1, AL1O1, AL1O2, AL1P1, AL1P2, AL1S1, AL1S2, AL2, AL2C2, AL2C6H18, AL2O1, AL2O2, AL2O3, AL2S1, AL2S2, AR, B, B10H14, B1C1, B1C1H3O1, B1C2, B1C2H7O2, B1C3H9, B1C3H9O3, B1C6H15, B1H1, B1H1O1_BOH, B1H1O1_HBO, B1H1O2, B1H1S1, B1H2, B1H2O1, B1H2O2, B1H3, B1H3O1, B1H3O2, B1H3O3, B1H6N1, B1N1, B1O1, B1O2, B1S1, B1S2, B2, B2C1, B2H4O4, B2H6, B2O1, B2O2, B2O3, B2S1, B2S2, B2S3, B3H3O3, B3H3O6, B3H6N3, B4S6, B5H9, C, C1H1, C1H1N1_HCN, C1H1N1_HNC, C1H1N1O1, C1H1N1S1, C1H1O1, C1H1O2, C1H1P1, C1H2, C1H2N4, C1H2O1, C1H2O2_CIS, C1H2O2_DIOXIRANE, C1H2O2_TRANS, C1H3, C1H3O1_CH2OH, C1H3O1_CH3O, C1H3P1, C1H4, C1H4N2O1, C1H4O1, C1H4S1, C1H5N1, C1H5O1P1, C1H5O3P1, C1H5P1, C1H5P1S1, C1H6N1P1_N, C1H6N1P1_P, C1H6P2, C1N1, C1N1O1, C1N1O1_NCO, C1N2_CNN, C1N2_NCN, C1O1, C1O1S1, C1O2, C1P1, C1P1SI1, C1P1SI2, C1P2, C1PT1, C1S1, C1S2, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2H1, C2H1N1, C2H2, C2H2O1, C2H3, C2H4, C2H4O1_ACETALDEHYDE, C2H4O1_OXIRANE, C2H4O2_ACETICACID, C2H4O2_DIOXETANE, C2H4O3_123TRIOXOLANE, C2H4O3_124TRIOXOLANE, C2H5, C2H6, C2H6O1_1, C2H6O1_2, C2H6O1SI1, C2H6O2, C2H7O1P1, C2H7O3P1, C2H7P1_1, C2H7P1_2, C2H7P1S1, C2H8N1P1_N, C2H8N1P1_P, C2H8SI1, C2N1_CCN, C2N1_CNC, C2N2, C2O1, C2P1, C2P2, C2SI1, C2SI2, C2SI3, C3, C3H1, C3H1N1, C3H4_1, C3H4_2, C3H6_1, C3H6_2, C3H6O1_1, C3H6O1_2, C3H8, C3N1, C3O2, C4, C4H1, C4H10_1, C4H10_2, C4H12SI1, C4H2_1, C4H2_2, C4H4_1, C4H4_2, C4H6_1, C4H6_2, C4H6_3, C4H6_4, C4H6_5, C4H8_1, C4H8_2, C4H8_3, C4H8_4, C4H8_5, C4H8_6, C4N1, C4N2, C4NI1O4, C5, C5FE1O5, C5H1N1, C5N1, C60, C6H6, C6H6O1, C6MO1O6, C6N1, C6N2, C9N1, CA, CA1H1, CA1H1O1, CA1H2O2, CA1O1, CA1S1, CA2, CO, CO1H1, CO1H1O1, CO1H2O2, CO1O1, CO1S1, CO2, CR, CR1H1, CR1H1O1, CR1H1O2, CR1H1O3, CR1H2O2, CR1H2O3, CR1H2O4, CR1H3O3, CR1H3O4, CR1H4O4, CR1H4O5, CR1N1, CR1O1, CR1O2, CR1O3, CR1S1, CR1S2, CR2, CR2O1, CR2O2, CR2O3, CU, CU1H1, CU1H1O1, CU1O1, CU1S1, CU2, CU2S1, FE, FE1H1, FE1H1O1, FE1H1O2, FE1H2O2, FE1O1, FE1O2, FE1S1, FE2, H, H1MG1, H1MG1O1, H1MN1, H1MN1O1, H1MO1O1, H1MO1O2, H1MO3, H1N1, H1N1O1, H1N1O2_CIS, H1N1O2_TRANS, H1N1O3, H1N3, H1NI1, H1NI1O1, H1O1, H1O1P1, H1O1S1_HSO, H1O1S1_SOH, H1O1W1, H1O2, H1O2W1, H1P1, H1PT1, H1S1, H1SI1, H1ZR1, H2, H2MG1O2, H2MO1O2, H2MO1O3, H2MO1O4, H2N1, H2N2_1_1N2H2, H2N2_CIS, H2N2_TRANS, H2N2O2, H2NI1O2, H2O1, H2O1S1_H2SO, H2O1S1_HSOH, H2O2, H2O2W1, H2O3SI1, H2O3W1, H2O4S1, H2O4W1, H2P1, H2S1, H2S2, H2SI1, H3N1, H3N1O1, H3P1, H3SI1, H4N2, H4O4SI1, H4SI1, H6SI2, HF, HF1O1, HF1O2, MG, MG1N1, MG1O1, MG1S1, MG2, MN, MN1O1, MN1O2, MN1S1, MO, MO1N1, MO1O1, MO1O2, MO1O3, MO1S1, MO1S2, MO2, MO2O6, MO3O9, MO4O12, MO5O15, N, N1NB1, N1O1, N1O2, N1O3, N1P1, N1S1, N1SI1, N1SI2, N1TI1, N1V1, N1ZR1, N2, N2O1, N2O2, N2O3, N2O4, N2O5, N3, NB, NB1O1, NB1O2, NB1S1, NI, NI1O1, NI1S1, NI2, O, O10P4, O10V4, O12W4, O15W5, O1P1, O1PD1, O1PT1, O1RE1, O1RU1, O1S1, O1S2, O1SI1, O1TA1, O1TI1, O1V1, O1W1, O1Y1, O1Y2, O1ZR1, O2, O2P1, O2PT1, O2RE1, O2RU1, O2S1, O2SI1, O2SI2, O2TA1, O2TI1, O2V1, O2W1, O2Y1, O2Y2, O2ZR1, O3, O3P2, O3RE1, O3RU1, O3S1, O3W1, O4P2, O4RU1, O5P2, O6P3, O6P4, O6RE2, O6W2, O7P4, O7RE2, O8P4, O8W3, O9P4, O9W3, P, P1S1, P1SI1, P1SI2, P2, P2SI2, P3, P4, P4S3, PD, PT, RE, RU, S, S1SI1, S1TA1, S1TI1, S1V1, S1W1, S1Y1, S1ZR1, S2, S2SI1, S2TI1,

Name	*Prototype*	*Info*	*Sublattices*	*Formula Unit*
				S2W1, S2ZR1, S3, S4, S5, S6, S7, S8, SI, SI2, SI3, TA, TI, TI2, V, W, Y, ZR, ZR2)1
LIQUID	Liquid	LIQUID mixture	1	(AL, AL1N1, AL2/3O1, AL2/3S, AL4/3O2, B, BO3/2, C, CA, CAO, CAS, CO, COO, COO3/2, COS, CR, CRO, CRO3/2, CRS, CU, CU2O, CU2S1, CUO, FE, FEO, FEO3/2, FES, HF, HF1/2O1, MG, MGO, MGS, MN, MNO, MNO3/2, MNS, MO, MO1/2O1, MO1/2S, MOO3, N, NB, NB1O1, NBO2, NBO5/2, NBS, NI, NIO, NIS, P, P2/5S1, PD, PDO, PT, PTO, RE, RE1/2O1, REO7/2, RU, RU1/2O1, RU1/2S1, S, SI, SI1/2O1, SI1/2S, SI2O4, SIO2, TA, TA2/5O1, TI, TIO, TIO2, TIS, V, VO, VO2, VO5/2, VS, W, W1/3O1, W1/3S1, Y, Y2/3O1, ZR, ZR1/2O1, ZR1/2S1)1

TCNI: TCS Ni-based Superalloys Database Revision History

Current Database Version

Database name (acronym):	**TCS Ni-based Superalloys Database (TCNI)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**13.0**
First release:	**TCNI1 was released in 2000**

Changes in the Most Recent Database Release

TCNI12.1 to TCNI13.0

Software release version 2025b (June 2025).

New Thermodynamic Models

- The Effective Bond Energy Formalism (EBEF) is implemented to describe the complex and important topologically close-packed (TCP) sigma (σ) and mu (μ) phases.
    - New Density Functional Theory (DFT) data is used to support the implementation of the EBEF.
    - The five-sublattice (5-SL) model is used to describe both phases, which better reflects their real crystallographic structures.

- Oxygen (O) and sulfur (S) are added in the LIQUID phase (previously only available in the IONIC_LIQ phase) and the IONIC_LIQ is removed from the database.

Binary Systems

- The Hf-Pt system is added. Previously the system was incorrectly listed as assessed in the last version of the database, TCNI12.
- The description of phase equilibria involving σ and/or μ phases is improved in several systems.
    - Co-Nb, Co-Ta, Fe-Ta, Nb-Ni, Ni-Ta, Ni-V, Pd-Ta, Pt-Ta, and Re-Ta.

Ternary Systems

- 2 new ternary systems are assessed: Cr-Ni-Pt and Hf-Ni-Ti.
- The liquidus projection of the Mg–Mn–Ni system is corrected.
- Several improvements are obtained in the description of the σ and μ phases as a result of the implementation of the EBEF. Some examples:
  - σ description in the Cr-Ni-Re, Cr-Fe-Mn, and Mo-Ni-Re.
  - μ description in the Co-Cr-W, Cr-Fe-Nb, and Fe-Mo-Nb.

Thermophysical Properties

- Added viscosity, surface tension, and THCD/ELRS descriptions for the above newly added systems.

Elastic Properties

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

Previous Releases

TCNI12.0 to TCNI12.1

Software release version: 2023b (June 2023).

- Mismatches between the two liquid descriptions (IONIC_LIQ and LIQUID) were found and fixed for:
  - Gibbs energy parameters in Al-N, Mg-Ni, Co-Ni-V, Mn-Ni-P, Mn-Ni-Si, Mo-Ni-P
  - Volume parameters in Ni-Re, Cr-Fe-Ni
- Fixed the magnetic model applied to the M2B_TETR phase
- Updated the Diamond molar volume
- The surface tension was re-assessed based on the Redlich-Kister-Muggianu (R-K-M) sub-regular solution model.
- The surface tension was added for the IONIC_LIQ.

TCNI11.0.1 to TCNI12

Software release version: 2022b (June 2022).

New Element

- Phosphorus (P) is added to make it a 31 element framework.

20 New Binary Systems

The following systems are at least partially assessed.

- Al-P, B-P, C-P, Ca-P, Co-P, Cu-P, Cr-P, Fe-P, Mn-P, Mo-P, Nb-P, Ni-P, P-Pd, Pt-P, Ru-P, S-P, Si-P, Ti-P, V-P, and W-P

30 New Ternary Systems

Al-Fe-P	B-Ni-P	B-Ni-P	C-Fe-P	Co-Fe-P	Co-Ni-P
Co-P-V	Co-P-W	Cr-Fe-P	Cr-Nb-P	Cr-Ni-P	Cr-P-Ti
Cu-Fe-P	Cu-Ni-P	Fe-Mn-P	Fe-Mo-P	Fe-Nb-P	Fe-Nb-Si
Fe-Ni-P	Fe-P-Si	Fe-P-Ti	Fe-P-V	Fe-P-W	Nb-Ni-P
Nb-P-Ti	Ni-P-Ti	Ni-P-V	Ni-P-W	Ni-SI-P	P-V-W

Binary and Ternary Updates

- Fe-Nb updated, improved MU and C14_LAVES boundaries.
- Nb-Ni, Fe-Si, Nb-Si updated metastable C14_LAVES description.
- Co-W updated so that Co3W D019 is stable to low temperature.
- Fe-Nb-Si added.
- Fe-Nb-Ni updated, improved Laves boundaries.
- Co-Ni-Ti updated to correspond better with available phase diagram data.
- Al-Co-Ni updated to better fit thermodynamic and phase diagram data.
- Al-Co-W updated to destabilize FCC_L12#2 (gamma-prime)
- Co-Ni-W updated metastable FCC_L12 towards an improved description of Al-Co-Ni-W
- Nb-Ni-Ti fixed a bug relating to a slightly destabilized ternary phase.

Thermophysical Properties

- Viscosity and Surface tension updated:
  - Viscosity is now described for the ionic liquid phase (IONIC_LIQ)
- Electrical and thermal properties improved:
  - High-temperature trends of THCD are now better for commercial alloys
  - ELRS of Cr-Fe rich Ni-base alloys were before quite over-estimated, now improved.

Phase Names/Phase Information

- AL-FE-SI ternary phases renamed to use their modern Greek letters. ALFESI_ALPHA > ALFESI_ALPHA_TAU5
- D0I_MO2B5 renamed to MO2B5_D8I, correct strukturbericht.
- All phase description updated to our new standardized crystallographic information format.

Minor Bug Fix

- Corrected minor typo in the Gibbs energy of the MUFEMO function, used in the MU_PHASE

TCNI11 to TCNI11.0.1

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

- A typographical correction was made to the molar volume of the M6C phase
- Functions corrected for consistency: F1756T, F2048T, GFECEM, THCDLQCU

TCNI10 to TCNI11

Software release version: 2021b (June 2021).

Addition of the thermophysical properties Electrical Resistivity (ELRS) and Thermal Conductivity (THCD), which can also be expressed through the derived properties Electrical Conductivity (ELCD), Thermal Resistivity (THRS) and Thermal Diffusivity (THDF). It is recommended to use the Property Model "Equilibrium with Freeze-in Temperature" to correctly predict these properties for an alloy.

TCNI9.1 to TCNI10.0

Software release version: 2020b (June 2020).

Binary and Unary System Updates

- Surface tension for the liquid phase is assessed in all unary and binary systems.
- Viscosity for the liquid phase is assessed in all unary and 142 binary systems.
- Nb-Ni metastable BCT_D022 updated to fit data on γ'' solvus temperature in commercial superalloys.
- The solubility of S in γ-Ni has been assessed.
- Bug fixed for metastable BCT_D022 destabilized in Cr-Nb and pure Cr to avoid low-temperature metastable miscibility gaps.

Ternary System Updates

- Al-Co-W system updated to fit better experimental data and no longer have stable L12 at 900 C
- Al-Hf-Ni system revised to better describe liquidus, solidus, and liquid activity as well as γ' boundaries and activity (see references 1-4 at the end of this section).
- Al-Ni-Pt system updated to better describe liquid activity and melting interval data by Copland (2007) (see reference 5 at the end of this section).
- Al-Ni-W system revised to better fit known melting interval and improve liquid/γ partitioning in higher-order alloys
- Co-Hf-Ni liquid and γ phases updated to better describe the melting intervals of high-Co Ni-base alloys. (see reference 6 at the end of this section)
- Co-Ni-W system updated to fit more recent data on the varying ternary solubility of the ALTI3_D019 phase
- Co-Ni-V has been partially assessed by adding Co to BCT-D022, and FCC and liquid have been adjusted to give approximate isothermal and isoplethal sections.
- Nb-Ni-Ti system modified to be closer to the known phase diagram (see reference 7 at the end of this section)

Ternary System Bug Fixes

- L12 destabilized in Cr-Ni-W and Cr-Ni-Si
- ALTI3_D019 destabilized in Cr-Ni-W
- Corrected M4SI3 in Cr-Ni-Si, now metastable in Cr-Si and Ni-Si
- Corrected M5Si3_D88 in C-Cr-si
- Al-Cr-Pt extrapolation corrected

Quality Improvement

- The DATABASE_INFORMATION command accessed via the DATABASE module in Console Mode now includes an exact revision number to make it easier to communicate support questions.
- The additional phase information now contains crystallographic information (if known) for all phases. The command is invoked in the DATABASE module via LIST_SYSTEM and CONSTITUENTS
- The database is automatically validated against a large range of commercial and model alloys to verify that every revision improves solidus, liquidus, γ' solvus and liquid/solid partitioning data. This ensures that no alloy should fall through the cracks.

Phase Renaming

- ALTI3_DO19 (where O is a letter) has been changed to be named ALTI3_D019 (where 0 is zero), which is consistent with the Strukturbericht designation. Users are advised to update their macros involving this phase.

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TCNI9.0 to TCNI9.1

Software release version: 2020a (January 2020).

- A new description of Al-Ni-Pt system.
- Merged all L10 phases into FCC_L10 phase.
- Revised Mn-Pt description.
- Revised default composition sets (type_defs).
- Updated the reference states of elements according to PURE5.

TCNI8.1 to TCNI9.0

Software release 2019a (December 2018).

The major updates in TCNI9 is addition of Ca, Mg and S elements. In total 58 binary and many ternary systems are added to the database. More than 150 new phases are added for a total of 680 phases.

The calculation of W-partitioning between the liquid and solid phase during the solidification of nickel alloys was improved with the help new experimental data.

The stability and composition profile of B2 phase in Ni-Al-Co-Cr alloys was improved.

The thermodynamic description of several ternary systems were revised including B-Ni-Si, Cr-Mo-Nb, Cr-Nb-V, Al-Ni-V, and Mo-Ni-Si.

The Laves phase description was modified in several system to improve the predictions of stability and composition profile of this phase.

In addition several bugs from the previous versions were fixed such as one that erroneously causes ordering in copper containing FCC_A1 phase.

TCNI8.0 to TCNI8.1

Software release version: 2017a (March 2017)

The major change in 8.1 is an update of several Y-systems. The solubility of Y in gamma phase has been increased by changing Al-Y, Co-Y, Cr-Y, Cu-Y, Fe-Y, Nb-Y, Ni-Y, Pt-Y, Re-Y and Ru-Y systems.

Al-Ni-Y and Nb-Ni-Y have also been added to the database. In Al-Ni-Y the solubility of Al in Ni5Y (called NI5ZR in TCNI8) and the addition of several ternary phases are the most significant improvements. For Nb-Ni-Y the liquid description is also greatly improved and TCNI8 now correctly predicts the liquid miscibility that occurs in this system.

TCNI7.1 to TCNI8.0

Software release version: 2015a (June 2015). Also an update released with the 2015b update in March 2016.

The major update to TCNI8.0 is the addition of Copper, Cu. In total 24 binary systems and 29 ternary systems have been added to the database and can easily be calculated using the BINARY/TERNARY module in CLASSICAL MODE or by using the BINARY/TERNARY CALCULATION template in GRAPHICAL MODE using Thermo-Calc.

The following binary systems have been added to TCNI8: Al-Cu, B-Cu, C-Cu, Co-Cu, Cr-Cu, Cu-Fe, Cu-Hf, Cu-Mn, Cu-Mo, Cu-N, Cu-Nb, Cu-Ni, Cu-O, Cu-Pd, Cu-Pt, Cu-Re, Cu-Ru, Cu-Si, Cu-Ta, Cu-Ti, Cu-V, Cu-W, Cu-Y, Cu-Zr.

The following ternary systems have been added to TCNI8: Al-Cu-Fe, Al-Cu-Mn, Al-Cu-Ni, Al-Cu-Si, C-Cu-Fe, Co-Cr-Cu, Co-Cu-Fe, Co-Cu-Mn, Co-Cu-Nb, Co-Cu-Ni, Co-Cu-Ti, Cr-Cu-Fe, Cr-Cu-Nb, Cr-Cu-Ni, Cr-Cu-Si, Cu-Fe-Mn, Cu-Fe-Mo, Cu-Fe-N, Cu-Fe-Nb, Cu-Fe-Ni, Cu-Fe-Si, Cu-Fe-Ti, Cu-Fe-V, Cu-Mn-Ni, Cu-Mn-Si, Cu-Mo-Ni, Cu-Ni-Si, Cu-Ni-Ti and Cu-Ti-Zr.

TCNI8 patch: 2015-08-27 - update to 2015a

Bug fix to TCNI8: The phase ALTI3_DO19 has been fixed in the Ni-Ti phase diagram when using the BIN module/Binary calculation in Thermo-Calc. It had been appearing incorrectly in TCNI6, TCNI7 and TCNI8.

Software release version: 2016b (November 2016)

Bug fix: Fixed a bug in TCNI8 that caused the GUI to crash on rare occasions. It was related to carbon in combination with non-Ni/Co superalloy composition.

TCNI7.0 to TCNI7.1

Software release version: 4.1 (November 2014)

By default, liquid containing no oxygen is now modeled with ordinary substitutional solution model. When oxygen is included the Ionic Liquid model will be used for the liquid phase. This change gives better performance for alloys where oxygen needs not to be considered.

The description for the M6C carbide in the C-Cr-Ni-Mo and C-Cr-Ni-W systems has been improved. The stability of M6C was underestimated, resulting in that M23C6 was predicted as primary carbide instead of M6C for some commercial alloys. This has now been fixed.

The description of the Cr-Ni-B system has been improved. The NI3B_D011 phase was too stable and resulted in wrong equilibrium with liquid. This has now fixed.

Constraint relations for parameters describing FCC_L12 phase have been added for ternary and quaternary systems containing newly introduced elements Y or/and Mn. This increases the stability of calculations.

An error concerning volume data for systems containing Fe has been fixed.

TCNI6.0 to TCNI7.0

Software release version: 4.0 (June 2014)

The major update to TCNI7.0 is the addition of Manganese, Mn. In total 23 binary systems and 19 ternary systems have been added to the database and can easily be calculated using the BINARY/TERNARY module in CLASSICAL MODE or by using the BINARY/TERNARY CALCULATION template in GRAPHICAL MODE using Thermo-Calc.

The following binary systems have been added to TCNI7: Al-Mn, B-Mn, C-Mn, Co-Mn, Cr-Mn, Fe-Mn, Hf-Mn, Mn-Mo, Mn-N, Mn-Nb, Mn-Ni, Mn-O, Mn-Pd, Mn-Pt, Mn-Re, Mn-Ru, Mn-Si, Mn-Ta, Mn-Ti, Mn-V, Mn-W, Mn-Y, Mn-Zr.

The following ternary systems have been added: Al-Fe-Mn, Al-Mn-Ni, Al-Mn-O, Al-Mn-Si, Al-Mn-Ti, C-Fe-Mn, C-Mn-V, Co-Mn-O, Cr-Mn-N, Cr-Mn-O, Fe-Mn-N, Fe-Mn-Ni, Fe-Mn-O, Fe-Mn-Si, Mn-Ni-O, Mn-Ni-Si, Mn-O-Si, Mn-O-Y, Mn-O-Zr.

Minor corrections e.g. the reappearence of phases above liquidus has been fixed for systems C-Fe, C-Mn, C-Mo, C-Ni, and Mo-Ni.