TCS Ni-based Superalloys Database (TCNI12)

Technical Information

Available Starting with Thermo-Calc Version 2022b

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About the TCS Ni-based Superalloys Database (TCNI)

TCS Ni-based Superalloys Database (TCNI) is a thermodynamic database developed for different kinds of Ni-based superalloys. In addition to thermodynamic data, it has properties data available for molar volume with thermal expansion coefficients, viscosity of the metallic liquids, surface tension of liquid metallic alloys, electrical resistivity, thermal conductivity.

Molar volume with thermal expansion coefficients properties data have been available since TCNI7 for the most important systems.

The properties data for TCS Ni-based Superalloys Database (TCNI) is added as follows. Viscosity of the metallic liquids and surface tension of metallic liquids are included starting with version 10 (TCNI10) and electrical resistivity and thermal conductivity are included starting with version 11 (TCNI11).

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 10 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.

TCNI: TCS Ni-based Superalloys Database Revision History. The current version of the database is TCNI12. See the link for any subversion release details.

The database is compatible with the TCS Ni-alloys Mobility Database (MOBNI). The current version is MOBNI6.

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.

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 TCNI12 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

Then in combination with the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), Process Metallurgy, 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.

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 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) 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 an 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.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

TCNI12 Elements, Systems, Phases and Properties Data

Included Elements

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

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									

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.
- 431 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.
- 733 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].
- Topologically Close-Packed (TCP) phases are modeled using more complex and physically correct models, which gives the ability to correctly predict site-fractions etc. [2007Hal].
- Oxygen has been implemented in an ambitious way using the Compound Energy Formalism (CEF) [2001Hil] for the solution phases, e.g. spinel, halite, corundum etc., and the ionic two-sublattice model [1985Hil; 1991Sun] for the metallic and ionized liquid.
- 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)).

TCNI12 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

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[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).

[2007Hal] B. Hallstedt, N. Dupin, M. Hillert, L. Höglund, H. L. Lukas, J. C. Schuster, and N. Solak. "Thermodynamic models for crystalline phases. Composition dependent models for volume, bulk modulus and thermal expansion," Calphad 31.1, 28-37 (2007).

Properties Data

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.

Molar Volume

Molar volume with thermal expansion coefficients properties data have been available since TCNI7 for the most important systems.

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.

Available Properties Data Parameters and Variables

Below is a summary of the available 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 the TC-Python SDK. More details are described in the online help.

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
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
Electrical conductivity		ELCD for a system `ELCD(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)` **
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

* 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.

** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCNI12 Systems

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TCNI12 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

TCNI12 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-Ca-O
Al-Ca-Si	Al-C-Co	Al-C-Cr	Al-C-Fe	Al-C-Ni	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-C-Si	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-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-N-Ti
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-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-C-Ti	B-C-W
B-C-Zr	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	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	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

Assessed Ternary Systems							
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
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-Nb-Re	C-Nb-Ti	C-Nb-V
C-Nb-W	C-Nb-Zr	C-Ni-Ta	C-Ni-Ti	C-Ni-W	C-N-Nb	C-N-Ti	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	C-Re-W
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-Nb-Ni	Cr-Nb-P	Cr-Nb-Si	Cr-Nb-V	Cr-Ni-O	Cr-Ni-P	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-N-Nb
Cr-N-Ni	Cr-N-V	Cr-O-S	Cr-O-Si	Cr-O-Ti	Cr-O-V	Cr-O-Y	Cr-O-Zr
Cr-P-Ti	C-Si-Ti	C-Ta-Ti	C-Ta-W	C-Ti-W	C-Ti-Zr	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	C-V-W

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

TCNI12 Phases

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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

TCNI12 Models for the Included Phases

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

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
LIQUID	Liquid					LIQUID mixture.	1	[1.0]	(AL, AL1N1, B, C, CA, CO, CR, CU, FE, HF, MG, MN, MO, N, NB, NI, P, PD, PT, RE, RU, SI, TA, TI, V, W, Y, ZR)1
IONIC_LIQ	Liquid					IONIC_LIQ mixture modeled by the ionic two-sublattice model	2	[1.0, 1.0]	(AL+3, CA+2, CO+2, CR+2, CU+1, FE+2, HF+4, MG+2, MN+2, MO+4, NB+2, NI+2, P+5, PD+2, PT+2, RE+4, RU+4, SI+4, TA+5, TI+2, V+2, W+6, Y+3, ZR+4)1(ALN, ALO2-1, B, BO3/2, C, C3S2Z_1/6, COO3/2, CRO3/2, CUO, FEO3/2, MNO3/2, MOO3, N, NBO2, NBO5/2, O-2, REO7/2, S, S-2, SIO2, SIO4-4, TIO2, VA, VO2, VO5/2)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225		2	[1.0, 1.0]	(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	Fm-3m	225		2	[1.0, 1.0]	(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	Pm-3m	221		3	[0.75, 0.25, 1.0]	(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	Im-3m	229		2	[1.0, 3.0]	(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

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
									(B, C, N, O, VA)3
BCC_B2	CsCl (B2)	B2	cP2	Pm-3m	221		3	[0.5, 0.5, 3.0]	(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	P6_3/mmc	194		2	[1.0, 0.5]	(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	I-43m	217		2	[1.0, 1.0]	(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	P4_132	213		2	[1.0, 1.0]	(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	Fd-3m	227		1	[1.0]	(AL, B, C, O, P, SI)1
BETA_RHOMBO_B	beta-B (R-105)		hR105	R-3m	166		2	[93.0, 12.0]	(B)93(B, C, CU, SI)12
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	P6_3/mmc	194		1	[1.0]	(B, C)1
NI3TI_D024	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194		2	[3.0, 1.0]	(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	Pmmn	59		2	[3.0, 1.0]	(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	I4/mmm	139		2	[3.0, 1.0]	(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

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		2	[2.0, 1.0]	(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	R-3m	166		1	[1.0]	(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, SI, TA, TI, W)1
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166		4	[1.0, 2.0, 6.0, 4.0]	(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)2(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)4
DIS_SIG	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		1	[1.0]	(AL, CO, CR, FE, MN, MO, NB, NI, PD, PT, RE, RU, SI, TA, TI, V, W)1
SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		3	[10.0, 4.0, 16.0]	(AL, CO, CR, FE, MN, MO, NB, NI, PD, PT, RE, RU, SI, TA, TI, V, W)10 (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)16
R_PHASE	R-(Co, Cr, Mo)		hR53	R-3	166		3	[27.0, 14.0, 12.0]	(CO, CR, FE, NI, RE)27(MO, W)14 (CO, CR, FE, MO, NI, RE, W)12
P_PHASE	Cr9Mo21Ni20		oP56	Pnma	62		3	[24.0, 20.0, 12.0]	(CR, FE, NI, RE)24(CR, FE, MO, NI, RE)20(MO)12
CHI_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[24.0, 10.0, 24.0]	(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	P2_12_12_1	19		3	[24.0, 20.0, 12.0]	(CO, CR, FE, NI, RE)24(CO, CR, FE, MO, NI, RE, W)20(CU, MO, W)12
NISI_B31	MnP (B31)	B31	oP8	Pnma	62		2	[1.0, 1.0]	(NI, PD)1(SI)1

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MC_ETA	CMo		hP12	P6_3/mmc	194		2	[1.0, 1.0]	(MO, V, W)1(C, VA)1
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	P-6m2	187		2	[1.0, 1.0]	(MO, W)1(C, N)1
M23C6	Cr23C6 (D84)	D84	cF116	Fm-3m	225		3	[20.0, 3.0, 6.0]	(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	Pnma	62		2	[3.0, 1.0]	(CO, CR, FE, MN, MO, NI, V, W)3 (C, N)1
M12C	Fe6W6C		cF104	Fd-3m	227		3	[6.0, 6.0, 1.0]	(CO, NI)6(MO, W)6(C)1
M3C2	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62		2	[3.0, 2.0]	(CO, CR, MO, V, W)3(C)2
M6C	Fe3W3C (E93)	E93	cF112	Fd-3m	227		4	[2.0, 2.0, 2.0, 1.0]	(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	Pnma	62		2	[7.0, 3.0]	(CO, CR, FE, MN, MO, NI, RE, V, W)7(C)3
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[5.0, 2.0]	(FE, MN)5(C)2
TAU	Cr23C6 (D84)	D84	cF116	Fm-3m	225		4	[20.0, 6.0, 6.0, 3.0]	(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	Cmcm	63		2	[1.0, 1.0]	(CR, FE, HF, MO, NB, NI, TA, TI, V)1(B)1
MB2_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[2.0, 1.0]	(B)2(AL, CR, HF, MG, MN, MO, NB, TA, TI, V, Y, ZR)1
M3B2	Si2U3 (D5a)	D5a	tP10	P4/mbm	127		3	[0.4, 0.2, 0.4]	(CR, FE, MO, NI, W)0.4(CR, FE, NI)0.2(B)0.4
M2B_TETR	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[2.0, 1.0]	(AL, CO, CR, FE, MN, MO, NB, NI, RE, TA, W)2(B)1

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B12ZR	UB12 (D2f)	D2f	cF52	Fm-3m	225		2	[12.0, 1.0]	(B)12(Y, ZR)1
MNP_B31	MnP (B31)	B31	oP8	Pnma	62		2	[1.0, 1.0]	(CO, CR, FE, MN, NI, RU, W)1(P, SI)1
CU3P_D021	Cu3P (D021)	D021	hP24	P-3c1	165		2	[3.0, 1.0]	(CU, FE)3(P)1
M2P_C22	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189		2	[2.0, 1.0]	(AL, CO, CR, FE, MN, MO, NB, NI, TI, V, W)2(B, P, SI)1
M3P_D0E	Ni3P (D0e)	D0e	tI32	I-4	82		2	[3.0, 1.0]	(AL, CO, CR, CU, FE, MN, MO, NI, TI)3(B, P)1
TINIP_C37	Co2Si (C37)	C37	oP12	Pnma	62		3	[1.0, 1.0, 1.0]	(CO, CR, FE, NB, NI, TI, V, W)1(CO, CR, FE, NB, NI, TI, V, W)1(P)1
NI5P2_ALPHA	Pd8Sb3		hR44	R3c	161		2	[5.0, 2.0]	(CO, NI)5(P)2
NI5P2_BETA	Unknown Structure						2	[5.0, 2.0]	(CO, NI)5(P)2
NI12P5_ALPHA	Ni12P5		tI34	I4/m	87		2	[12.0, 5.0]	(CO, NI)12(P)5
NI12P5_BETA	Unknown Structure						2	[12.0, 5.0]	(CO, NI)12(P)5
NI5P4	Ni5P4		hP36	P6_3/mmc	194		2	[5.0, 4.0]	(NI)5(P)4
NIP2	PdP2		mS12	C2/c	15		2	[1.0, 2.0]	(NI)1(P)2
COP3	Skutterudite (CoAs3, D02)	D02	cI32	Im-3	204		2	[1.0, 3.0]	(CO)1(P)3
NBP	NbAs		tI8	I4_1md	109		2	[1.0, 1.0]	(NB)1(P)1
NB7P4	Nb7P4		mS44	C2/m	12		2	[7.0, 4.0]	(NB, TI)7(P)4
TI3P	Ti3P		tP32	P4_2/n	86		2	[3.0, 1.0]	(CR, NB, TI)3(P)1
TI5P3	beta-Yb5Sb3		oP32	Pnma	62		2	[5.0, 3.0]	(TI)5(P)3

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
ZINCBLENDE_B3	Zincblende (ZnS, B3)	B3	cF8	F-43m	216		2	[1.0, 1.0]	(AL)1(P)1
WP2	MoP2		oS12	Cmc2_1	36		2	[1.0, 2.0]	(W)1(P)2
MO3P	alpha-V3S		tI32	I-42m	121		2	[3.0, 1.0]	(MO)3(P)1
MOP_BH	Tungsten Carbide (Bh)	Bh	hP2	P-6m2	187		2	[1.0, 1.0]	(MO)1(P)1
NB2NI9P	MgCu4Sn		cF24	F-43m	216		3	[2.0, 9.0, 1.0]	(NB)2(NI)9(P)1
NBNI2P	Unknown Structure						3	[1.0, 2.0, 1.0]	(NB)1(NI)2(P)1
NB5NI4P4	Cu5Nb5Si4		tI26	I4/m	87		3	[5.0, 4.0, 4.0]	(NB)5(NI)4(P)4
NB3NI2P	Si2U3 (D5a)	D5a	tP10	P4/mbm	127		3	[3.0, 2.0, 1.0]	(NB)3(NI)2(P)1
NB4NIP	Nb4CoSi		tP12	P4/mcc	124		3	[4.0, 1.0, 1.0]	(NB)4(NI)1(P)1
NB2NI2P3	Nb2Ni2P3		hP28	P6_3/m	176		3	[2.0, 2.0, 3.0]	(NB)2(NI)2(P)3
NBNIP2	NbNiP2		oP16	Pnma	62		3	[1.0, 1.0, 2.0]	(NB)1(NI)1(P)2
P2S5	P2S5		aP28	P-1	2		2	[2.0, 5.0]	(P)2(S)5
SIP1	(SiP)		oS48	Cmc2_1	36		2	[1.0, 1.0]	(P)1(SI)1
SIP2	Pyrite (FeS2, C2)	C2	cP12	Pa-3	205		2	[2.0, 1.0]	(P)2(SI)1
CA2P2	Na2O2		hP12	P-62m	189		2	[1.0, 1.0]	(CA)1(P)1
CA5P8	Ca5P8		mS26	C2/m	12		2	[5.0, 8.0]	(CA)5(P)8
CAP3	CaP3		aP8	P-1	2		2	[1.0, 3.0]	(CA)1(P)3
PD15P2	P2Pd15		hR17	R-3	148		2	[15.0, 2.0]	(PD)15(P)2

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PD6P	PPd6		mP28	P2_1/c	14		2	[6.0, 1.0]	(PD)6(P)1
PD3P_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(PD)3(P, VA)1
PD5P2	Unknown Structure						2	[5.0, 2.0]	(PD)5(P)2
PD7P3	P3Pd7		hR20	R-3	148		2	[7.0, 3.0]	(PD)7(P)3
PDP2	PdP2		mS12	C2/c	15		2	[1.0, 2.0]	(PD)1(P)2
PTP2	Pyrite (FeS2, C2)	C2	cP12	Pa-3	205		2	[1.0, 2.0]	(PT)1(P)2
PT5P2	Pt5P2		mS28	C2/c	15		2	[5.0, 2.0]	(PT)5(P)2
RU2P	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(RU)2(P)1
RUP2	Marcasite (FeS2, C18)	C18	oP6	Pnnm	58		2	[1.0, 2.0]	(RU)1(P)2
FENB2P	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		3	[1.0, 2.0, 1.0]	(FE)1(NB)2(P)1
FENB4P	Nb4CoSi		tP12	P4/mcc	124		3	[1.0, 4.0, 1.0]	(FE)1(NB)4(P)1
FESI4P4	FeSi4P4		aP9	P1	1		3	[1.0, 4.0, 4.0]	(FE)1(SI)4(P)4
CO5B2P	Mo5SiB2		tI32	I4/mcm	140		3	[5.0, 2.0, 1.0]	(CO)5(B)2(P)1
NB5P3	Nb5P3		oP64	Pnma	62		2	[5.0, 3.0]	(NB)5(P)3
NB8P5	Nb8P5		oP54	Pbam	55		2	[8.0, 5.0]	(NB)8(P)5
NB1P2	OsGe2		mS12	C2/m	12		2	[1.0, 2.0]	(NB)1(P)2
ALPT	FeSi (B20)	B20	cP8	P2_13	198		2	[0.5, 0.5]	(AL)0.5(NI, PT)0.5
FCC_L10	CuAu (L10)	L10	tP2	P4/mmm	123		2	[0.5, 0.5]	(AL, CR, CU, MN, MO, NI, PD, PT, TA, TI, W)0.5(AL, CR, CU, MN, MO, NI, PD, PT, TA, TI, W)0.5

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NIZR	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(NI)1(TI, Y, ZR)1
ALZR	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(AL)1(HF, Y, ZR)1
ALPHA_B19	beta'-AuCd (B19)	B19	oP4	Pmma	51		2	[1.0, 1.0]	(MO, NB, PD, PT, TI, V, ZR)1(MO, NB, PD, PT, TI, V, ZR)1
B11	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[1.0, 1.0]	(CO, CU, NI, PD, TI)1(CU, NI, TA, TI)1
CUPT_L11	Rhombohedral CuPt (L11)	L11	hR2	R-3m	166		3	[0.5, 0.5, 1.0]	(CU, PT)0.5(CU, PT)0.5(VA)1
HFMN	NiTi2		cF96	Fd-3m	227		2	[0.5, 0.5]	(HF)0.5(MN)0.5
MNTA	Unknown Structure						2	[1.0, 1.0]	(MN)1(TA)1
PDY_LT	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(PD, Y)1(Y)1
PDY_HT	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(PD, Y)1(Y)1
AL2PT	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		3	[2.0, 1.0, 1.0]	(AL)2(NI, PT)1(NI, VA)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[2.0, 1.0]	(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	P6_3/mmc	194		2	[2.0, 1.0]	(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	Immm	71		2	[1.0, 2.0]	(CR, MO, W)1(MO, NI, W)2
NI2TA	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(CO, NI)2(TA, TI)1
NI2V	MoPt2		oI6	Immm	71		2	[2.0, 1.0]	(MO, NI, PD, PT)2(MO, NB, PT, TA, V)1

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C16_THETA	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[2.0, 1.0]	(AL, HF, MO, NB, TA, TI, W, ZR)2 (AL, CO, CR, CU, FE, NI, SI)1
CU2TI	Au2V		oS12	Cmcm	63		2	[2.0, 1.0]	(CO, CU, NI)2(TI)1
CU2Y_H	Unknown Structure		hP*				2	[2.0, 1.0]	(CU)2(Y)1
CU2Y_L	KHg2		oI12	Imma	74		2	[2.0, 1.0]	(CU)2(Y)1
MNNI2	Unknown Structure						2	[1.0, 2.0]	(MN, NI)1(NI)2
NITI2	NiTi2		cF96	Fd-3m	227		2	[1.0, 2.0]	(CO, CR, CU, FE, NI, RE, TI)1(AL, CR, CU, HF, NI, TA, TI, ZR)2
PD2Y	Unknown Structure						2	[2.0, 1.0]	(PD)2(Y)1
PTY2	Co2Si (C37)	C37	oP12	Pnma	62		2	[1.0, 2.0]	(PT)1(Y)2
PT2Y	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[2.0, 1.0]	(PT)2(Y)1
REZR2	Zr21Re25		hR92	R-3c	167		2	[1.0, 2.0]	(NI, RE)1(ZR)2
ALTI3_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(AL, CO, CR, MN, MO, NI, PT, TA, TI, W)3(AL, CR, MO, NB, NI, PT, TA, TI, W)1
AL3Y_HT	BaPb3		hR12	R-3m	166		2	[0.75, 0.25]	(AL)0.75(Y)0.25
AL3Y_LT	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[0.75, 0.25]	(AL)0.75(Y)0.25
AL3ZR	Al3Zr (D023)	D023	tI16	I4/mmm	139		2	[3.0, 1.0]	(AL)3(HF, ZR)1
CUTI3	CuTi3 (L60)	L60	tP4	P4/mmm	123		2	[1.0, 3.0]	(CU, TI)1(TI)3
MZR3_E1A	MgCuAl2 (E1a)		oS16	Cmcm	63		2	[1.0, 3.0]	(CO, FE, NI)1(Y, ZR)3
PDY3	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[1.0, 3.0]	(PD)1(Y)3

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
PTY3	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[1.0, 3.0]	(PT)1(Y)3
RUY3	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[0.25, 0.75]	(RU)0.25(Y)0.75
H_L21	Heusler (L21)	L21	cF16	Fm-3m	225		3	[0.5, 0.5, 1.0]	(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	Fm-3m	225		3	[16.0, 6.0, 7.0]	(AL, CO, FE, MN, NI, TI)16(HF, NB, TI, Y, ZR)6(CO, FE, MN, NI, SI)7
ALCU_DEL	Al5Cu8		hR52	R3m	160		2	[2.0, 3.0]	(AL)2(CU, FE)3
ALCU_EPS	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[1.0, 1.0]	(AL, CU, NI)1(CU, FE)1
ALCU_ETA	AlCu(r)		mS20	C2/m	12		2	[1.0, 1.0]	(AL, CU)1(CU, FE, NI)1
ALCU_PRIME	Al9Cu11(h)		oF88	Fmm2	42		2	[2.0, 1.0]	(AL)2(CU)1
ALCU_ZETA	Al9Cu11(h)		oF88	Fmm2	42		2	[9.0, 11.0]	(AL)9(CU, FE)11
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215		3	[4.0, 1.0, 8.0]	(AL, NI, SI)4(AL, CU, NI, SI)1(CU, FE, MN, NI)8
GAMMA_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		3	[4.0, 1.0, 8.0]	(AL)4(AL, CU)1(CU, FE, MN, NI)8
AL23CUFE4	MnAl6 (D2h)	D2h	oS28	Cmcm	63		3	[23.0, 1.0, 4.0]	(AL)23(CU)1(FE)4
AL62CU25FE13	Quasicrystal						3	[0.125, 0.255, 0.62]	(FE)0.125(AL, CU)0.255(AL)0.62
AL7CU2FE	FeCu2Al7 (E9a)	E9a	tP40	P4/mnc	128		3	[1.0, 2.0, 7.0]	(FE, NI)1(CU)2(AL)7
AL10CU10FE	(Al10Cu10Fe)		oF116	Fmm2	42		3	[1.0, 10.0, 10.0]	(FE)1(AL, CU)10(AL)10
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5		hR14	R-3m	166	TAU	2	[1.0, 1.0]	(AL)1(CU, FE, NI, VA)1
AL12MN	Al12W		cI26	Im-3	204		2	[12.0, 1.0]	(AL)12(MN)1

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
AL4MN_R	lambda-Al4Mn		hP586	P6_3/mmc	194		2	[461.0, 107.0]	(AL)461(FE, MN)107
AL4MN_U	mu-Al4Mn		hP574	P6_3/mmc	194		2	[4.0, 1.0]	(AL)4(MN)1
AL11MN4_LT	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(FE, MN)4
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25		oP156	Pnma	62		2	[29.0, 10.0]	(AL, MN)29(MN)10
AL8MN5	Cr5Al8 (D810)	D810	hR26	R3m	160		3	[12.0, 5.0, 9.0]	(AL, TI)12(MN)5(AL, CU, MN, SI, TI)9
TI25MN9AL66_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		3	[0.25, 0.08, 0.67]	(AL, MN, TI)0.25(AL, MN)0.08(AL, MN, TI)0.67
AL28CU4MN7	Mn6Cu4Al29		oS156	Cmcm	63		3	[28.0, 7.0, 4.0]	(AL)28(MN)7(CU)4
AL11CU5MN3	Unknown Structure		oP380				3	[11.0, 3.0, 5.0]	(AL)11(MN)3(CU)5
ALCU3MN2	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		3	[1.0, 2.0, 3.0]	(AL)1(MN)2(CU)3
AL16FEMN3	mu-Al4Mn		hP574	P6_3/mmc	194		2	[4.0, 1.0]	(AL)4(FE, MN)1
AL13FE2MN2	Al13Fe4		mS102	C2/m	12		2	[4.0, 13.0]	(FE, MN)4(AL)13
AL10FEMN2	Mn3Al10		hP26	P6_3/mmc	194		2	[3.0, 10.0]	(FE, MN)3(AL)10
AL21PD8	Al21Pt8		tI116	I4_1/a	88		2	[21.0, 8.0]	(AL)21(PD)8
AL2PD5	Ga2Pd5		oP28	Pnma	62		2	[2.0, 5.0]	(AL)2(AL, PD)5
AL3PD	(Al3Pd)		oP*	Pna2_1	33		2	[3.0, 1.0]	(AL)3(PD)1
AL3PD2	Al3Ni2 (D513)	D513	hP5	P-3m1	164		2	[3.0, 2.0]	(AL, PD)3(AL, PD)2
AL3PD5	Rh5Ge3		oP16	Pbam	55		2	[3.0, 5.0]	(AL)3(PD)5

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
AL4PD	(Al4Pd)		hP*	P6_322	182		2	[4.0, 1.0]	(AL)4(PD)1
ALPD2	Co2Si (C37)	C37	oP12	Pnma	62		2	[1.0, 2.0]	(AL, NI, PD)1(AL, NI, PD)2
AL21PT5	Li21Si5		cF416	F-43m	216		2	[0.8077, 0.1923]	(AL)0.8077(NI, PT)0.1923
AL21PT8	Al21Pt8		tI116	I4_1/a	88		2	[0.7241, 0.2759]	(AL)0.7241(NI, PT)0.2759
AL3PT5	Rh5Ge3		oP16	Pbam	55		2	[0.375, 0.625]	(AL)0.375(NI, PT)0.625
ALPT2	Co2Si (C37)	C37	oP12	Pnma	62		2	[0.33333, 0.66667]	(AL)0.33333(NI, PT)0.66667
AL6MN	MnAl6 (D2h)	D2h	oS28	Cmcm	63		2	[6.0, 1.0]	(AL)6(FE, MN, RE, RU)1
ALZR2	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[1.0, 2.0]	(AL)1(Y, ZR)2
AL2ZR3	Zr3Al2		tP20	P4_2/mnm	136		2	[2.0, 3.0]	(AL)2(HF, Y, ZR)3
AL3ZR4	Al3Zr4		hP7	P6/mmm	191		2	[3.0, 4.0]	(AL)3(HF, ZR)4
AL3ZR2	Zr2Al3		oF40	Fdd2	43		2	[3.0, 2.0]	(AL)3(HF, ZR)2
AL3NI2	Al3Ni2 (D513)	D513	hP5	P-3m1	164		3	[3.0, 2.0, 1.0]	(AL, SI)3(AL, CU, NI, PT, RU)2(NI, RU, VA)1
AL12W	Al12W		cI26	Im-3	204		2	[12.0, 1.0]	(AL)12(MO, RE, W)1
AL4W	Al4W		mS30	Cm	8		2	[4.0, 1.0]	(AL)4(MO, W)1
AL1MN1SI1	TiSi2 (C54)	C54	oF24	Fddd	70		3	[1.0, 1.0, 1.0]	(AL)1(MN)1(SI)1
AL3MNSI2	(Al3MnSi2)		tP48	P4/n	85		3	[3.0, 1.0, 2.0]	(AL)3(MN)1(SI)2
AL3MN4SI2	Unknown Structure						3	[3.0, 4.0, 2.0]	(AL)3(MN)4(SI)2

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
ALMNSI_T6	Unknown Structure						2	[4.0, 1.0]	(AL, MN)4(SI)1
ALMNSI_T8	Mn3Al10		hP26	P6_3/mmc	194		5	[6.0, 2.0, 12.0, 6.0, 2.0]	(MN, VA)6(MN, VA)2(AL)12(AL, SI)6(AL, SI)2
AL15SI2M4	Al15(Mn, Fe)3Si2		cI168	Im-3	204		3	[14.0, 4.0, 5.0]	(AL)14(FE, MN)4(AL, SI)5
AL2MNSI3	Ga5Pd		tI24	I4/mcm	140		3	[2.0, 1.0, 3.0]	(AL)2(MN)1(SI)3
HF2PD	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(HF)2(PD)1
HF3PD4	Unknown Structure						2	[3.0, 4.0]	(HF)3(PD)4
HFPD2	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[1.0, 2.0]	(HF)1(PD)2
BPD3	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[1.0, 3.0]	(B)1(PD)3
BPD5	Unknown Structure					Might be SG I4/mmm, Pearson tI*	2	[1.0, 5.0]	(B)1(PD)5
BPD6	Pd6B		mS28	C2/c	15		2	[1.0, 6.0]	(B)1(PD)6
B2PD5	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[2.0, 5.0]	(B)2(PD)5
BPT3	Unknown Structure						2	[1.0, 3.0]	(B)1(PT)3
BPT2	Molybdenite (MoS2, C7)	C7	hP6	P6_3/mmc	194		2	[1.0, 2.0]	(B)1(PT)2
B2PT3	PtB0.67		oS8	Cmcm	63		2	[2.0, 3.0]	(B)2(PT)3
YB4	ThB4 (D1e)	D1e	tP20	P4/mbm	127		2	[1.0, 4.0]	(Y)1(B)4
YB6	CaB6 (D21)	D21	cP7	Pm-3m	221		2	[1.0, 6.0]	(Y)1(B)6
YB66	YB66		cF1936	Fm-3c	226		2	[1.0, 66.0]	(Y)1(B)66

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
MONI4_BETA	Ni4Mo (D1a)	D1a	tI10	I4/m	87		2	[1.0, 4.0]	(MO, W)1(CO, NI)4
AL5W	Al5W		hP12	P6_322	182		2	[5.0, 1.0]	(AL)5(MO, W)1
CO10CU57TI33	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		3	[0.1, 0.57, 0.33]	(CO)0.1(CU)0.57(TI)0.33
CO17Y2	Ni17Th2		hP38	P6_3/mmc	194	united HT/LT phase.	3	[1.0, 2.0, 15.0]	(CO2, Y)1(CO2, Y)2(CO)15
CO5Y_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		3	[1.0, 4.0, 1.0]	(CO2, Y)1(CO)4(CO, VA)1
CO3Y	Ni3Pu		hR12	R-3m	166		2	[3.0, 1.0]	(CO)3(Y)1
CO3Y2	Unknown Structure		cP*				2	[3.0, 2.0]	(CO)3(Y)2
CO7Y6	Unknown Structure						2	[7.0, 6.0]	(CO)7(Y)6
COY_BF	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(CO)1(Y)1
CO3Y4	Co3Ho4		hP22	P6_3/m	176		2	[3.0, 4.0]	(CO)3(Y)4
CO5Y8	Co5Y8		mP52	P2_1/c	14		2	[5.0, 8.0]	(CO)5(Y)8
CU51HF14	Ag51Gd14		hP68	P6/m	175		2	[51.0, 14.0]	(CU)51(HF)14
CU8HF3	Cu8Hf3		oP44	Pnma	62		2	[8.0, 3.0]	(CU)8(HF)3
CU10HF7	Ni10Zr7		oS68	Cmce	64		2	[10.0, 7.0]	(CU)10(HF)7
T1_CU2TI	Au2V		oS12	Cmcm	63		2	[2.0, 1.0]	(CU, FE)2(TI)1
T2_CU3TI2	Cu3Ti2		tP10	P4/nmm	129		2	[3.0, 2.0]	(CU, FE)3(TI)2
T3_CU4TI3	Cu4Ti3		tI14	I4/mmm	139		2	[4.0, 3.0]	(CU, FE)4(TI)3
T4CUFETI	Unknown Structure						2	[0.63, 0.37]	(CU, FE)0.63(TI)0.37

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T5CUFETI	Unknown Structure						2	[0.55, 0.45]	(CU, FE)0.55(TI)0.45
CU5MN4SI	Unknown Structure						3	[0.5, 0.37, 0.13]	(CU)0.5(MN)0.37(SI)0.13
CU6NISI3	Unknown Structure						2	[0.732, 0.268]	(CU, NI)0.732(SI)0.268
CU46NI25SI29	Unknown Structure						3	[0.458, 0.25, 0.292]	(CU)0.458(NI)0.25(SI)0.292
T1CUNITI	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(CU, NI)2(TI)1
T2CUNITI	Cu3Ti2		tP10	P4/nmm	129		3	[0.175, 2.825, 2.0]	(CU)0.175(NI)2.825(TI)2
T4CUNITI	BaPb3		hR12	R-3m	166		3	[0.05, 0.7, 0.25]	(CU)0.05(NI)0.7(TI)0.25
T6CUNITI	Unknown Structure						3	[0.25, 0.5, 0.25]	(CU)0.25(NI)0.5(TI)0.25
CU33SI7_DELTA	Unknown Structure		tP*				2	[0.825, 0.175]	(CU)0.825(SI)0.175
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cI76	I-43d	220		2	[0.789474, 0.210526]	(CU, MN)0.789474(AL, SI)0.210526
CU56SI11_GAMMA	Mg3Ru2		cP20	P4_132	213		2	[0.835821, 0.164179]	(CU, MN, NI, SI)0.835821 (SI)0.164179
CUSI_ETA	Cu3Si-h2		hR*	P-31m	162	Structure uncertain	2	[0.76, 0.24]	(CU, MN, NI)0.76(SI)0.24
CU3TI2	Cu3Ti2		tP10	P4/nmm	129		2	[3.0, 2.0]	(CU, FE, NI)3(CO, TI)2
CU4TI1	Au4Zr		oP20	Pnma	62		2	[4.0, 1.0]	(CU, TI)4(CU, TI)1
CU4TI3	Cu4Ti3		tI14	I4/mmm	139		2	[4.0, 3.0]	(CO, CU, NI)4(TI)3
CU2TIZR	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		3	[0.5, 0.25, 0.25]	(CU)0.5(TI)0.25(ZR)0.25

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
CU7Y1	Cu7Tb		hP8	P6/mmm	191		2	[1.0, 5.0]	(CU2, Y)1(CU)5
CU4Y	Cu5Y1.25		mP16	P2_1/m	11		2	[4.0, 1.0]	(CU)4(Y)1
CU7Y2	Ag51Gd14		hP68	P6/m	175		2	[7.0, 2.0]	(CU)7(Y)2
CU10ZR7	Ni10Zr7		oS68	Cmce	64		2	[10.0, 7.0]	(CU)10(ZR)7
CU51ZR14	Ag51Gd14		hP68	P6/m	175		2	[51.0, 14.0]	(CU)51(ZR)14
CU8ZR3	Cu8Hf3		oP44	Pnma	62		2	[8.0, 3.0]	(CU)8(ZR)3
MN3PD5	Ga3Pt5		oS16	Cmmm	65		2	[3.0, 5.0]	(MN)3(PD)5
MNPD2	Ga3Pt5		oS16	Cmmm	65		2	[1.0, 2.0]	(MN)1(PD)2
MN11SI19	Mn11Si19		tP120	P-4n2	118		2	[11.0, 19.0]	(MN)11(AL, SI)19
MN3SI	BiF3 (D03)	D03	cF16	Fm-3m	225		2	[3.0, 1.0]	(FE, MN)3(AL, SI)1
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166		2	[17.0, 3.0]	(AL, MN)17(SI)3
MN9SI2	Mn9Si2		oI186	Immm	71		2	[33.0, 7.0]	(MN)33(SI)7
MN12Y	Mn12Th (D2b)	D2b	tI26	I4/mmm	139		2	[12.0, 1.0]	(MN)12(Y)1
NI2Y	Ni2Tm		cF192	F-43m	216		2	[2.0, 1.0]	(NI)2(Y)1
NI2Y3	Ni2Y3		tP80	P4_12_12	92		2	[2.0, 3.0]	(NI)2(Y)3
NI3Y	Ni3Pu		hR12	R-3m	166		2	[3.0, 1.0]	(FE, NI)3(Y)1
NI4Y	Unknown Structure		hR*				2	[4.0, 1.0]	(NI)4(Y)1
NI7ZR2	Ni7Zr2		mS36	C2/m	12		2	[7.0, 2.0]	(AL, CO, CR, NI)7(HF, Y, ZR)2

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
NI11ZR9	Pt11Zr9		tI40	I4/m	87		2	[11.0, 9.0]	(NI)11(HF, ZR)9
NI10ZR7	Ni10Zr7		oS68	Cmce	64		2	[23.0, 17.0]	(NI)23(HF, ZR)17
NI5ZR	AuBe5 (C15b)	C15b	cF24	F-43m	216		2	[5.0, 1.0]	(AL, CU, NI)5(HF, Y, ZR)1
PD21SI4	Unknown Structure						2	[21.0, 4.0]	(PD, SI)21(SI)4
PD5SI	Pd5Si		mP24	P2_1	4		2	[5.0, 1.0]	(PD)5(SI)1
PD14SI3	Unknown Structure						2	[14.0, 3.0]	(PD)14(SI)3
PD9SI2	Pd9Si2		oP44	Pnma	62		2	[9.0, 2.0]	(PD)9(SI)2
PD15SI4	Unknown Structure						2	[15.0, 4.0]	(PD)15(SI)4
PD3SI	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(PD)3(SI)1
PD39SI20	Unknown Structure						2	[39.0, 20.0]	(PD)39(SI)20
PD19SI10	Unknown Structure						2	[19.0, 10.0]	(PD)19(SI)10
ALPHA_PD2SI	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189		2	[2.0, 1.0]	(PD, SI)2(SI)1
BETA_PD2SI	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189		2	[2.0, 1.0]	(PD, SI)2(SI)1
NI17Y2	Fe17Lu2		hP80	P6_3/mmc	194		2	[1.0, 0.1176]	(AL, FE, NI)1(Y)0.1176
PD2TA	MoPt2		oI6	Immm	71		2	[2.0, 1.0]	(PD)2(TA)1
PD2TI	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(PD)2(TI)1
PD3TI2	Pd3Ti2		oS20	Cmcm	63		2	[3.0, 2.0]	(PD)3(TI)2
PD5TI3	Pd5Ti3		tP8	P4/mmm	123		2	[5.0, 3.0]	(PD)5(TI)3

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
PD7Y	Ca7Ge		cF32	Fm-3m	225		2	[7.0, 1.0]	(PD)7(Y)1
PD3Y2_LT	Unknown Structure						2	[3.0, 2.0]	(PD)3(Y)2
PD3Y2_HT	Unknown Structure						2	[3.0, 2.0]	(PD)3(Y)2
PD4Y3	Pd4Pu3		hR14	R-3	148		2	[4.0, 3.0]	(PD)4(Y)3
PD2Y3	Er3Ni2		hR15	R-3	148		2	[2.0, 3.0]	(PD)2(Y)3
PD2Y5	Dy5Pd2		cF144	Fd-3m	227		2	[2.0, 5.0]	(PD)2(Y)5
PD11ZR9	Ni11Zr9		tP44	P4/m	83		2	[11.0, 9.0]	(PD)11(ZR)9
PD4ZR3	Pd4Pu3		hR14	R-3	148		2	[4.0, 3.0]	(PD)4(ZR)3
PDZRM	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		3	[1.0, 1.0, 1.0]	(PD)1(ZR)1(PD, ZR)1
PDZR_ALPHA	(PdZr-alpha)		mS*	Cm	8		2	[1.0, 1.0]	(PD)1(ZR)1
PDZR_BETA	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(PD)1(ZR)1
PTSI	Westerveldite (FeAs, B14)	B14	oP8	Pnma	62		2	[1.0, 1.0]	(PT)1(SI)1
PT6SI5	Pt6Si5		mP22	P2_1/m	11		2	[6.0, 5.0]	(PT)6(SI)5
ALPHA_PT2SI	ThH2 (L'2b)	L'2b	tI6	I4/mmm	139		2	[2.0, 1.0]	(PT)2(SI)1
BETA_PT2SI	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189		2	[2.0, 1.0]	(PT)2(SI)1
ALPHA_PT17SI8	Ni12P5		tI34	I4/m	87		2	[17.0, 8.0]	(PT)17(SI)8
BETA_PT17SI8	Pt12Si5		tP68	P4/n	85		2	[17.0, 8.0]	(PT)17(SI)8
PT5SI2	Unknown Structure						2	[5.0, 2.0]	(PT)5(SI)2

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
BETA_PT3SI	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(PT)3(SI)1
ALPHA_PT3SI	GePt3		mS16	C2/m	12		2	[3.0, 1.0]	(PT)3(SI)1
PT25SI7	Unknown Structure						2	[25.0, 7.0]	(PT)25(SI)7
PT2TA	Au2V		oS12	Cmcm	63		2	[2.0, 1.0]	(PT)2(TA)1
PT3TA	NbPt3		mP48	P2_1/m	11		2	[3.0, 1.0]	(PT)3(TA)1
PT3TI4	Unknown Structure						2	[3.0, 4.0]	(PT)3(TI)4
PT8TI	Pt8Ti		tI18	I4/mmm	139		2	[8.0, 1.0]	(PT)8(TI)1
PT5Y	Unknown Structure						2	[5.0, 1.0]	(PT)5(Y)1
PT4Y3	Unknown Structure						2	[4.0, 3.0]	(PT)4(Y)3
PT4Y5	Gd5Si4		oP36	Pnma	62		2	[4.0, 5.0]	(PT)4(Y)5
PT3Y5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193		2	[3.0, 5.0]	(PT)3(Y)5
PT3Y7	Fe3Th7 (D102)	D102	hP20	P6_3mc	186		2	[3.0, 7.0]	(PT)3(Y)7
PT4ZR3	Pd4Pu3		hR14	R-3	148		2	[4.0, 3.0]	(PT, ZR)4(PT, ZR)3
PT4ZR	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[4.0, 1.0]	(PT, ZR)4(PT, ZR)1
PT3ZR5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193		2	[3.0, 5.0]	(PT, ZR)3(PT, ZR)5
PT10ZR7	Ni10Zr7		oS68	Cmce	64		2	[10.0, 7.0]	(PT)10(ZR)7
HF8NI21	Hf8Ni21		aP29	P-1	2		2	[8.0, 21.0]	(HF, ZR)8(NI)21
AL13FE4	Al13Fe4		mS102	C2/m	12		3	[0.6275, 0.235,	(AL, CU)0.6275(FE, MN, RU)0.235

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
								0.1375]	(AL, SI, VA)0.1375
NI8TA	Pt8Ti		tI18	I4/mmm	139		2	[8.0, 1.0]	(NI)8(NB, TA)1
CO7M2	(Co7Nb2)		mS18	C2/m	12	also L12 Co7Ta2	2	[7.0, 2.0]	(CO)7(NB, TA)2
RU2Y3	Er3Ru2		hP10	P6_3/m	176		2	[0.4, 0.6]	(RU)0.4(Y)0.6
RU25Y44	Ru25Y44		oP276	Pnna	52		2	[0.362, 0.638]	(RU)0.362(Y)0.638
RU2Y5	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[0.286, 0.714]	(RU)0.286(Y)0.714
NB15NI56TI29	Unknown Structure		o*100				3	[0.15, 0.56, 0.29]	(NB)0.15(NI)0.56(TI)0.29
NB8NI9TI3	Unknown Structure						3	[0.4, 0.45, 0.15]	(NB)0.4(NI)0.45(TI)0.15
NB5NI75TI20	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		3	[0.05, 0.75, 0.2]	(NB)0.05(NI)0.75(TI)0.2
NB13NI75TI12	Unknown Structure						3	[0.13, 0.75, 0.12]	(NB)0.13(NI)0.75(TI)0.12
NB15NI80TI5	Unknown Structure						3	[0.15, 0.8, 0.05]	(NB)0.15(NI)0.8(TI)0.05
CFC2_FENBZR	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		3	[2.0, 1.0, 3.0]	(FE, NB, ZR)2(NB, ZR)1(NB, ZR)3
TI3SIC2	Ti3SiC2		hP12	P6_3/mmc	194		3	[3.0, 1.0, 2.0]	(TI)3(SI)1(C)2
AL31MN6NI2	mu-Al4Mn		hP574	P6_3/mmc	194		3	[31.0, 6.0, 2.0]	(AL)31(MN)6(NI)2
AL5MN6SI7	CrSi2 (C40)	C40	hP9	P6_222	180		3	[5.0, 6.0, 7.0]	(AL)5(MN)6(SI)7
ALCCR2	AlCCr2		hP8	P6_3/mmc	194		3	[1.0, 1.0, 2.0]	(AL)1(C)1(CR)2
AL8SIC7	Unknown Structure		hP16				3	[8.0, 1.0, 7.0]	(AL)8(SI)1(C)7
ALFESI_ALPHA_TAU5	Fe23Al81Si15		hP246	P6_3/mmc	194		4	[0.6612, 0.19,	(AL)0.6612(FE)0.19(SI)0.0496(AL,

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
								0.0496, 0.0992]	SI)0.0992
ALFESI_BETA_TAU6	Fe2Al9Si2		mS52	C2/c	15		3	[14.0, 3.0, 3.0]	(AL)14(FE)3(SI)3
ALFESI_GAMMA_TAU2	Unknown Structure		mS*				3	[3.0, 1.0, 1.0]	(AL)3(FE)1(SI)1
ALFESI_DELTA_TAU4	FeAl3Si2		oP24	Pbcn	60		3	[0.55, 0.15, 0.3]	(AL)0.55(FE)0.15(SI)0.3
ALFESI_TAU1	Unknown Structure						3	[2.0, 2.0, 1.0]	(AL)2(FE)2(SI)1
ALFESI_TAU3	Fe(Al0.67Si0.33)3		oS128	Cmme	67		3	[2.0, 1.0, 1.0]	(AL)2(FE)1(SI)1
AL2MN2SI3	(Al2Mn2Si3)		hP21	P-6	174		3	[2.0, 2.0, 3.0]	(AL)2(MN)2(SI)3
CO3AL2B5	Unknown Structure						3	[3.0, 2.0, 5.0]	(CO)3(AL)2(B)5
ALCR2B2	AlMn2B2		oS10	Cmmm	65		3	[1.0, 2.0, 2.0]	(AL)1(CR)2(B)2
ALCR3B4	AlCr3B4		oP8	Pmmm	47		3	[1.0, 3.0, 4.0]	(AL)1(CR)3(B)4
ALBMO	ZrSi2 (C49)	C49	oS12	Cmcm	63		3	[1.0, 1.0, 1.0]	(AL)1(B)1(MO)1
NI8ALB11	Unknown Structure		m**				3	[8.0, 1.0, 11.0]	(NI)8(AL)1(B)11
AL4SIC4	Al5C3N (E94)	E94	hP18	P6_3mc	186		3	[4.0, 1.0, 4.0]	(AL)4(SI)1(C)4
NB3RU5	Rh5Ge3		oP16	Pbam	55	united Nb3Ru5_HT and NbRu3_LT phase	2	[0.375, 0.625]	(NB, RU)0.375(RU)0.625
FENBSI2	CrSi2Zr		oP48	Pbam	55		3	[1.0, 1.0, 2.0]	(FE)1(NB)1(SI)2
FE4NB4SI7	Co4Ge7Zr4		tI60	I4/mmm	139		3	[4.0, 4.0, 7.0]	(FE)4(NB)4(SI)7
FENBSI_C23	MnCuP		oP12	Pnma	62		3	[1.0, 1.0, 1.0]	(FE)1(NB)1(SI)1

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
FE3NB4SI5	Fe3Nb4Si5		oP72	Pmn2_1	31		3	[3.0, 4.0, 5.0]	(FE)3(NB)4(SI)5
FENB2SI2	FeNb2Si2		tP198	P4_2/mcm	132		3	[1.0, 2.0, 2.0]	(FE)1(NB)2(SI)2
FENB4SI	Nb4CoSi		tP12	P4/mcc	124		3	[1.0, 4.0, 1.0]	(FE)1(NB)4(SI)1
FESI2_H	FeSi2-h		tP3	P4/mmm	123		2	[0.3, 0.7]	(FE)0.3(SI)0.7
FESI2_L	FeSi2-l		oS48	Cmce	64		2	[0.333333, 0.666667]	(FE)0.333333(SI)0.666667
HFNI3_ALPHA	PdRh2Ta		hP40	P6_3/mmc	194		2	[0.25, 0.75]	(HF)0.25(NI)0.75
HF3NI7	Hf3Ni7		aP20	P-1	2		2	[0.3, 0.7]	(HF)0.3(NI)0.7
HFNI_ALPHA	CrB (B33)	B33	oS8	Cmcm	63		2	[0.5, 0.5]	(HF)0.5(NI)0.5
HFRE	Zr21Re25		hR92	R-3c	167		2	[1.0, 1.0]	(HF)1(RE)1
MNTI_LT	Zr21Re25		hR92	R-3c	167		2	[1.0, 1.0]	(MN)1(TI)1
MNTI_HT	Unknown Structure		t**				2	[0.515, 0.485]	(MN)0.515(TI)0.485
MN3TI	Unknown Structure						2	[3.0, 1.0]	(MN)3(TI)1
MN4TI	R-(Co, Cr, Mo)		hR53	R-3	166		2	[0.815, 0.185]	(MN)0.815(TI)0.185
NI3SI_ORTHO	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(NI)3(SI)1
CR3MN5	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[3.0, 5.0]	(CR)3(MN)5
HIGH_SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		3	[8.0, 4.0, 18.0]	(MN)8(CR)4(CR, MN)18
FE2SI	AlNi2		hP6	P-3m1	164		2	[0.666667, 0.333333]	(FE)0.666667(SI)0.333333

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
CO11ZR2	(Co11Hf2)		oP*	Pban	50		2	[11.0, 2.0]	(CO)11(ZR)2
HFNI3_BETA	BaPb3		hR12	R-3m	166		2	[0.25, 0.75]	(HF)0.25(NI)0.75
RUB2	RuB2		oP6	Pmmn	59		2	[1.0, 2.0]	(RU)1(B)2
RU2B3	Ru2B3		hP10	P6_3/mmc	194		2	[2.0, 3.0]	(RU)2(B)3
RUB	Unknown Structure						2	[1.0, 1.0]	(RU)1(B)1
B3SI	B13C2 B4C (D1g)	D1g	hR15	R-3m	166		3	[6.0, 2.0, 6.0]	(B)6(SI)2(B, SI)6
B6SI	SiB6		oP280	Pnnm	58		3	[210.0, 23.0, 48.0]	(B)210(SI)23(B, SI)48
BNSI	alpha-B (hR12)		hR12	R-3m	166		3	[61.0, 1.0, 8.0]	(B)61(SI)1(B, SI)8
V2B3	V2B3		oS20	Cmcm	63		2	[0.4, 0.6]	(V)0.4(B)0.6
B9W2	W2B9		hP22	P-3	147		2	[9.0, 2.0]	(B)9(W)2
SIC	Zincblende (ZnS, B3)	B3	cF8	F-43m	216		2	[1.0, 1.0]	(SI)1(C)1
V3C2	Sc2Te3		hR8	R-3m	166		2	[3.0, 2.0]	(V)3(C)2
CO7HF	(Co11Hf2)		oP*	Pban	50		2	[7.0, 1.0]	(CO)7(HF)1
CO3SI	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(CO)3(SI)1
CO3V	Al3Pu		hP24	P6_3/mmc	194		2	[3.0, 1.0]	(CO, NI, TI, V)3(CO, NI, TI, V)1
AL4ZR5	Ti5Ga4		hP18	P6_3/mcm	193		2	[4.0, 5.0]	(AL)4(ZR)5
AL2TI	Ga2Hf		tI24	I4_1/amd	141		2	[2.0, 1.0]	(AL)2(TI)1
AL10V	Al10V		cF176	Fd-3m	227		2	[10.0, 1.0]	(AL)10(V)1

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
AL7V	Al45V7		mS104	C2/m	12		2	[7.0, 1.0]	(AL)7(V)1
AL23V4	Al23V4		hP54	P6_3/mmc	194		2	[23.0, 4.0]	(AL)23(V)4
AL8V5	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		2	[8.0, 5.0]	(AL)8(V)5
AL77W23	Unknown Structure						2	[77.0, 23.0]	(AL)77(W)23
AL7W3	Unknown Structure						2	[7.0, 3.0]	(AL)7(W)3
AL2W	CrSi2 (C40)	C40	hP9	P6_222	180		2	[2.0, 1.0]	(AL)2(W)1
AL3ZR5	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[3.0, 5.0]	(AL)3(ZR)5
AL11RE4	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(RE)4
AL4RE	Al4Re		aP71	P-1	2		2	[4.0, 1.0]	(AL)4(RE)1
ALRE2	CuZr2		tI6	I4/mmm	139		2	[1.0, 2.0]	(AL)1(RE)2
ALRE	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[1.0, 1.0]	(AL)1(RE)1
TAAL	Al38Ta48		mP86	P2_1/c	14		2	[0.51515, 0.48485]	(TA)0.51515(AL)0.48485
TAAL2	Al69Ta39		cF444	F-43m	216		2	[0.35, 0.65]	(TA)0.35(AL)0.65
AL11TI5	Al3Zr (D023)	D023	tI16	I4/mmm	139		2	[17.0, 8.0]	(AL)17(TI)8
ALMO	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229		2	[1.0, 1.0]	(AL, MO)1(AL, MO)1
AL3NI1	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[0.75, 0.25]	(AL)0.75(NI)0.25
AL3NI5	Ga3Pt5		oS16	Cmmm	65		2	[0.375, 0.625]	(AL)0.375(NI, PT)0.625

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
AL2FE	Al2Fe		aP18	P1	1		2	[2.0, 1.0]	(AL, CU)2(FE, MN)1
AL5FE2	Al2.8Fe		oS24	Cmcm	63		2	[5.0, 2.0]	(AL, CU)5(FE, MN)2
AL5FE4	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		1	[1.0]	(AL, CU, FE)1
AL63MO37	Unknown Structure						2	[63.0, 37.0]	(AL)63(MO)37
AL8MO3	Al8Mo3		mS22	C2/m	12		2	[8.0, 3.0]	(AL)8(MO)3
AL11CR2	Al5Cr		mS732	C2/c	15		3	[10.0, 1.0, 2.0]	(AL)10(AL)1(CR)2
AL13CR2	Al45V7		mS104	C2/m	12		2	[13.0, 2.0]	(AL)13(CR)2
AL4CR	mu-Al4Mn		hP574	P6_3/mmc	194		2	[4.0, 1.0]	(AL)4(CR)1
AL8CR5_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		2	[8.0, 5.0]	(AL)8(CR)5
AL8CR5_L	Cr5Al8 (D810)	D810	hR26	R3m	160		2	[8.0, 5.0]	(AL)8(CR)5
AL9CR4_H	Unknown Structure						2	[9.0, 4.0]	(AL)9(CR)4
AL9CR4_L	Unknown Structure						2	[9.0, 4.0]	(AL)9(CR)4
ALCR2	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[1.0, 2.0]	(AL)1(CR)2
ALB12_ALPHA	alpha-AlB12		tP216	P4_12_12	92		2	[1.0, 12.0]	(AL)1(B)12
AL13CO4	Orthorhombic Co4Al13		oP102	Pmn2_1	31		2	[13.0, 4.0]	(AL)13(CO)4
AL3CO	Os4Al13		mS34	C2/m	12		2	[3.0, 1.0]	(AL)3(CO)1
AL5CO2_D811	Co2Al5 (D811)	D811	hP28	P6_3/mmc	194		2	[5.0, 2.0]	(AL)5(CO)2

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
AL9CO2	Co2Al9 (D8d)	D8d	mP22	P2_1/c	14		2	[9.0, 2.0]	(AL)9(CO)2
W3COC	W10Co3C3.4		hP34	P6_3/mmc	194		3	[3.0, 1.0, 1.0]	(W)3(CO, NI)1(C)1
ALM3C_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221		3	[1.0, 3.0, 1.0]	(AL)1(CO, FE)3(C)1
AL4C3	Al4C3 (D71)	D71	hR7	R-3m	166		2	[4.0, 3.0]	(AL, SI)4(C)3
YC2_C11A	CaC2-I (C11a)	C11a	tI6	I4/mmm	139		1	[1.0]	(C2Y1)1
Y15C19_H	Unknown Structure						2	[19.0, 15.0]	(C)19(Y)15
Y15C19_R	alpha-Y15C19		oP18	Pbam	55		2	[19.0, 15.0]	(C)19(Y)15
Y2C3_H	Unknown Structure						3	[2.0, 2.0, 1.0]	(Y)2(C)2(C, VA)1
Y2C3_R	Sc3C4		tP70	P4/mnc	128		3	[2.0, 2.0, 1.0]	(Y)2(C)2(C, VA)1
YC_GAMMA	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		2	[1.0, 1.0]	(Y)1(C, C2, VA)1
BM	FeB (B27)	B27	oP8	Pnma	62		2	[1.0, 1.0]	(B, PT)1(CR, FE, HF, MN, MO, TI, Y)1
COB	FeB (B27)	B27	oP8	Pnma	62		2	[1.0, 1.0]	(CO, RE)1(B)1
MOB	MoB (Bg)	Bg	tI16	I4_1/amd	141		2	[1.0, 1.0]	(CR, FE, MO)1(B)1
BW_ALPHA	MoB (Bg)	Bg	tI16	I4_1/amd	141		2	[1.0, 1.0]	(B, C, VA)1(W)1
BW_BETA	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(B, C, VA)1(W)1
CR2B_ORTH	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[0.66666667, 0.33333333]	(CR, FE, MO, RE)0.666667 (B)0.333333
MN2B_D1F	Mn2B (D1f)	D1f	oF48	Fddd	70		2	[0.6707, 0.3293]	(MN)0.6707(B)0.3293

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
MNB4	MnB4		mS10	C2/m	12		2	[0.2, 0.8]	(MN)0.2(B)0.8
MOCOB	MnCuP		oP12	Pnma	62		3	[1.0, 1.0, 1.0]	(MO, W)1(CO)1(B)1
NI3B_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(CO, CR, FE, MO, NI)3(B)1
RE3B	Re3B		oS16	Cmcm	63		2	[3.0, 1.0]	(CR, MO, RE, TA, W)3(B)1
B4TA3_D7B	Ta3B4 (D7b)	D7b	oI14	Immm	71		2	[4.0, 3.0]	(B)4(CR, HF, MN, NB, TA, TI, V)3
B5W2_X	Mo2B5 (D8i)	D8i	hR7	R-3m	166		2	[5.0, 2.0]	(B, C, VA)5(W)2
RE7B3	Fe3Th7 (D102)	D102	hP20	P6_3mc	186		3	[7.0, 3.0, 3.0]	(CO, CR, MO, NB, RE, RU, TA, W)7 (B)3(B, VA)3
D5A_M3B2	Si2U3 (D5a)	D5a	tP10	P4/mbm	127		2	[3.0, 2.0]	(FE, HF, MO, NB, TA, V)3(B)2
W2COB2	W2CoB2		oI10	Immm	71		3	[2.0, 1.0, 2.0]	(MO, W)2(CO, NI)1(B)2
CR5B3	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140		2	[0.625, 0.375]	(CR, MO)0.625(B)0.375
V5B6	V5B6		oS22	Cmmm	65		2	[5.0, 6.0]	(NB, V)5(B)6
B4C	B13C2 B4C (D1g)	D1g	hR15	R-3m	166		2	[1.0, 1.0]	(B11C, B12)1(B2, C2B, CB2)1
CRB4	CrB4		oI10	Immm	71		2	[0.2, 0.8]	(CR)0.2(B)0.8
MOB4	MoB4		hP16	P6_3/mmc	194		2	[0.2, 0.8]	(MO)0.2(B)0.8
REB2	ReB2		hP6	P6_3/mmc	194		3	[1.0, 2.0, 2.0]	(RE)1(B)2(B, VA)2
NI4B3	m-Ni4B3		mS28	C2/c	15		2	[0.57142857, 0.42857143]	(NI)0.571429(B)0.428571
MO2B5_D8l	Mo2B5 (D8i)	D8i	hR7	R-3m	166		2	[0.32, 0.68]	(MO)0.32(B)0.68

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
RE3CO3B2	Ti3P		tP32	P4_2/n	86		3	[3.0, 3.0, 2.0]	(RE)3(CO)3(B)2
NI3CR2B6	V5B6		oS22	Cmmm	65		3	[3.0, 2.0, 6.0]	(NI)3(CR)2(B)6
NICR3B6	V2B3		oS20	Cmcm	63		3	[0.1, 0.3, 0.6]	(NI)0.1(CR)0.3(B)0.6
FEWB	MnCuP		oP12	Pnma	62		3	[1.0, 1.0, 1.0]	(FE)1(W)1(B)1
MO3NI10B11	Unknown Structure						3	[3.0, 10.0, 11.0]	(MO)3(NI)10(B)11
RE5CO2B4	Re5Co2B4		tP22	P4/mbm	127		4	[4.0, 2.0, 1.0, 4.0]	(RE)4(CO, RE)2(CO)1(B)4
NI5ALB4	Unknown Structure						3	[5.0, 1.0, 4.0]	(NI)5(AL)1(B)4
RECOB	MnCuP		oP12	Pnma	62		3	[1.0, 1.0, 1.0]	(RE)1(CO)1(B)1
Z_PHASE	CrNbN		tP6	P4/nmm	129		3	[1.0, 1.0, 1.0]	(CR, FE)1(MO, NB, V)1(N, VA)1
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	Pm-3m	221		2	[4.0, 1.0]	(CO, CR, FE, MN, NI)4(C, N)1
FECN_CHI	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[2.2, 1.0]	(FE)2.2(C, N)1
PI	beta-Mn (A13)	A13	cP20	P4_132	213		3	[12.8, 7.2, 4.0]	(CR)12.8(FE, NI)7.2(N)4
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186		2	[1.0, 1.0]	(AL)1(N)1
SI3N4	Nierite (alpha-Si3N4)		hP28	P31c	159		2	[3.0, 4.0]	(SI)3(N)4
BN_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186		2	[1.0, 1.0]	(B)1(N)1
MN6N4	Mn3N2		tI10	I4/mmm	139		2	[6.0, 4.0]	(MN)6(N)4
MN6N5	CoO		tI4	I4/mmm	139		2	[6.0, 5.0]	(MN)6(N)5
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136		2	[2.0, 1.0]	(TI)2(N)1

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TAN_EPS	TaN-eps		hP6	P-62m	189		2	[1.0, 1.0]	(TA)1(N)1
TI3N2	TiS-9R		hR6	R-3m	166		2	[0.71, 0.29]	(TI)0.71(N)0.29
TI4N3	Sc2Te3		hR8	R-3m	166		2	[0.685, 0.315]	(TI)0.685(N)0.315
ALNTI2	AlCCr2		hP8	P6_3/mmc	194		3	[1.0, 1.0, 2.0]	(AL)1(N)1(TI)2
ALNTI3	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221		3	[1.0, 1.0, 3.0]	(AL)1(N)1(TI)3
AL2N2TI3	(Al2Ti3N2)		hP22	P6_3mc	186		3	[2.0, 2.0, 3.0]	(AL)2(N)2(TI)3
NIAL2Y	MgCuAl2 (E1a)		oS16	Cmcm	63		3	[1.0, 2.0, 1.0]	(NI)1(AL)2(Y)1
NIALY	ZrNiAl		hP9	P-62m	189		3	[1.0, 1.0, 1.0]	(NI)1(AL)1(Y)1
NI2ALY2	W2CoB2		oI10	Immm	71		3	[2.0, 1.0, 2.0]	(NI)2(AL)1(Y)2
NI6AL2Y3	Ce3Ni6Si2		cI44	Im-3m	229		3	[6.0, 2.0, 3.0]	(NI)6(AL)2(Y)3
NI3ALY2	Unknown Structure						3	[3.0, 1.0, 2.0]	(NI)3(AL)1(Y)2
NI8ALY3	CeNi3		hP24	P6_3/mmc	194		3	[8.0, 1.0, 3.0]	(NI)8(AL)1(Y)3
HALITE	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		2	[1.0, 1.0]	(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	P3_121	152		1	[1.0]	(SIO2)1
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	Cc	9		1	[1.0]	(SIO2)1
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	Fd-3m	227		1	[1.0]	(SIO2)1

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
B2O3	B2O3		hP15	P3_121	152		1	[1.0]	(B2O3)1
CUPRITE_C3	Cuprite (Cu2O, C3)	C3	cP6	Pn-3m	224		2	[2.0, 1.0]	(CU+1)2(O-2)1
CUO	Tenorite (CuO, B26)	B26	mS8	C2/c	15		2	[1.0, 1.0]	(CU+2)1(O-2)1
YCUO2	Hexagonal Delafossite (CuAlO2)		hP8	P6_3/mmc	194		3	[1.0, 1.0, 2.0]	(Y+3)1(CU+1)1(O-2)2
Y2CU2O5	Cu2Ho2O5		oP36	Pna2_1	33		3	[2.0, 2.0, 5.0]	(Y+3)2(CU+2)2(O-2)5
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	oP28	Pnma	62		4	[1.0, 1.0, 1.0, 4.0]	(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	P-1	2		3	[1.0, 1.0, 3.0]	(CA+2, MN+2)1(SI+4)1(O-2)3
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	Pnnm	58		4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(SI+4)1(O-2)5
SILLIMANITE	Sillimanite (Al2SiO5, S03)	S03	oP32	Pnma	62		4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(SI+4)1(O-2)5
MULLITE	Al(Al0.7Si0.3)2O4.8		oP24	Pbam	55		4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(AL+3, SI+4)1(O-2, VA)5
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	P-1	2		4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(SI+4)1(O-2)5
CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	R-3c	167		3	[2.0, 1.0, 3.0]	(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	Fd-3m	227		4	[1.0, 2.0, 2.0, 4.0]	(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

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
ALPHA_SPINEL	Hausmannite (Mn3O4)		tI28	I4_1/amd	141		4	[1.0, 2.0, 2.0, 4.0]	(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*	I4_1/amd	141		3	[1.0, 1.0, 4.0]	(HF+4)1(SI+4)1(O-2)4
MN2YO5	HoMn2O5		oP32	Pbam	55		4	[1.0, 1.0, 1.0, 5.0]	(Y+3)1(MN+3)1(MN+4)1(O-2)5
MNYO3_HEX	LuMnO3		hP30	P6_3cm	185		3	[1.0, 1.0, 3.0]	(Y+3)1(MN+3)1(O-2)3
MO4O11	Mo4O11		oP60	Pna2_1	33		2	[4.0, 11.0]	(MO)4(O)11
MO8O23	High-Temperature Mo8O23		mP62	P2/c	13		2	[8.0, 23.0]	(MO)8(O)23
MO9O26	Mo9O26		mP70	P2/c	13		2	[1.0, 2.889]	(MO)1(O)2.889
MOO2	VO2		mP12	P2_1/c	14		2	[1.0, 2.0]	(MO)1(O)2
MOO3	gamma-WO3		mP32	P2_1/c	14		2	[1.0, 3.0]	(MO)1(O)3
NIMOO4	Huanzalaite (MgWO4, H06)	H06	mP12	P2/c	13	Also Ni[MoO4] of type Co [MoO4] SG12	3	[1.0, 1.0, 4.0]	(NI+2)1(MO+6)1(O-2)4
NIMNO3	Ilmenite (FeTiO3, E22)	E22	hR10	R-3	148		2	[2.0, 3.0]	(MN+3, MN+4, NI+2)2(O-2)3
NI6MNO8	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		3	[6.0, 1.0, 8.0]	(NI+2)6(MN+4)1(O-2)8
NIWO4	Sylvanite (AgAuTe4, E1b)	E1b	mP12	P2/c	13		3	[1.0, 1.0, 4.0]	(CO+2, FE+2, MN+2, NI+2)1 (W+6)1(O-2)4
NB2O5	Nb2O5		mP99	P2/m	10		2	[2.0, 5.0]	(NB)2(O)5
NBO	NbO		cP6	Pm-3m	221		2	[1.0, 1.0]	(NB)1(O)1
NBO2	alpha-NbO2		tI96	I4_1/a	88		2	[1.0, 2.0]	(NB)1(O)2

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
PDO	Cooperite (PtS, B17)	B17	tP4	P4_2/mmc	131		2	[1.0, 1.0]	(PD)1(O)1
PTO2	CdI2		hP3	P-3m1	164	Also other variants TiO2/CaCl2	2	[1.0, 2.0]	(PT)1(O)2
PT3O4	Pt3O4		cI14	Im-3m	229		2	[3.0, 4.0]	(PT)3(O)4
REO2	ReO2		mP14	P2_1/c	14	Also Ht variant, SG Pbcn	1	[1.0]	(O2RE1)1
REO3	alpha-ReO3 (D09)	D09	cP4	Pm-3m	221	There are 6 allotropes	1	[1.0]	(O3RE1)1
RE2O7	Re2O7		oP72	P2_12_12_1	19		1	[1.0]	(O7RE2)1
RUTILE_MO2	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136		2	[1.0, 2.0]	(AL+3, MN+4, RU+4, TI+4, V+4, ZR+4)1(O-2, VA)2
TA2O5_HT	Ta2O5-ht		tI44	I4_1/amd	141		2	[2.0, 5.0]	(TA)2(O)5
TA2O5_LT	beta-Ta2O5		oP14	Pccm	49		2	[2.0, 5.0]	(TA)2(O)5
TI3O2	(Ti3O2)		hP5	P6/mmm	191		3	[2.0, 1.0, 2.0]	(TI+2)2(TI)1(O-2)2
TI3O5	V3O5-ht		mS32	C2/c	15		3	[2.0, 1.0, 5.0]	(TI+3)2(TI+4)1(O-2)5
TIO_ALPHA	alpha-TiO		mS20	C2/m	12		2	[1.0, 1.0]	(TI+2)1(O-2)1
VO2_LT	VO2		mP12	P2_1/c	14		2	[1.0, 2.0]	(V+4)1(O-2)2
V2O_SS	V7O3		mS20	C2/m	12		2	[1.0, 0.5]	(V)1(O, VA)0.5
V2O5	Shcherbinaite (V2O5) (Revised)		oP14	Pmmn	59		2	[2.0, 5.0]	(V+5)2(O-2)5
V52O64	V13O16		tI116	I4_1/amd	141		2	[52.0, 64.0]	(V)52(O)64

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
WO2	VO2		mP12	P2_1/c	14		1	[1.0]	(O2W1)1
WO2_72	Unknown Structure						1	[1.0]	(O2_72W1)1
WO2_90	Unknown Structure						1	[1.0]	(O2_90W1)1
WO2_96	Unknown Structure						1	[1.0]	(O2_96W1)1
WO3_HT	WO2.95		tP16	P-42_1m	113		1	[1.0]	(O3W1)1
WO3_LT	WO3		oP32	Pbcn	60		1	[1.0]	(O3W1)1
M2O3C	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	206		3	[2.0, 3.0, 1.0]	(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	P-3m1	164		3	[2.0, 3.0, 1.0]	(CA+2, MG+2, MN+3, Y, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3B	B-Sm2O3		mS30	C2/m	12		3	[2.0, 3.0, 1.0]	(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	P-3m1	164		3	[2.0, 3.0, 1.0]	(CA+2, MG+2, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2O3X	Nd2O3		cI26	Im-3m	229		3	[2.0, 3.0, 1.0]	(CA+2, MG+2, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	P2_1/c	14		2	[2.0, 4.0]	(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	P4_2/nmc	137		2	[2.0, 4.0]	(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	Fm-3m	225		2	[2.0, 4.0]	(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

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
PSEUDO_BROOKITE	Pseudobrookite (Fe2TiO5, E41)	E41	oS32	Cmcm	63		3	[1.0, 2.0, 5.0]	(TI+4)1(AL+3)2(O-2)5
YAG	Garnet (Co3Al2Si3O12, S14)	S14	cI160	Ia-3d	230		3	[5.0, 3.0, 12.0]	(AL+3, CR+3, FE+3)5(Y+3)3(O-2)12
YAP	GdFeO3		oP20	Pnma	62		3	[1.0, 1.0, 3.0]	(AL+3, CO+3, CR+3, FE+3, MN+3)1 (CA+2, Y+3)1(O-2, VA)3
YAM	Y4Al2O9		mP60	P2_1/c	14		4	[2.0, 4.0, 1.0, 9.0]	(AL+3, SI+4)2(CA+2, Y+3)4(O-2, VA)1(O-2)9
Y2S2D_Y2SI2O7	Possible delta-Y2Si2O7		oP44	Pnma	62		3	[1.0, 1.0, 1.0]	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2G_Y2SI2O7	Y2Si2O7-b		mP22	P2_1/c	14		3	[1.0, 1.0, 1.0]	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2B_Y2SI2O7	La4Ge3[GeO4]O10		aP44	P-1	2		3	[1.0, 1.0, 1.0]	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2A_Y2SI2O7	Thortveitite ([Sc, Y]2Si2O7, S21)	S21	mS22	C2/m	12		3	[1.0, 1.0, 1.0]	(Y+3)1(Y+3)1(SI2O7-6)1
Y2SIO5	Y2SiO5 (RE2SiO5 X2)		mS64	C2/c	15		4	[1.0, 1.0, 1.0, 1.0]	(Y+3)1(Y+3)1(SIO4-4)1(O-2)1
ZRSIO4	Zircon (ZrSiO4, S11)	S11	tI24	I4_1/amd	141		3	[1.0, 1.0, 4.0]	(SI+4)1(ZR+4)1(O-2)4
ZRTIO4_ALPHA	Unknown Structure						3	[1.0, 1.0, 4.0]	(ZR+4)1(TI+4)1(O-2)4
ZRTIO4_BETA	zeta-Fe2N		oP12	Pbcn	60		2	[2.0, 4.0]	(TI+4, ZR+4)2(O-2)4
ZRTI2O6	Columbite (FeNb2O6, E51)	E51	oP36	Pbcn	60		3	[1.0, 2.0, 6.0]	(ZR+4)1(TI+4)2(O-2)6
ZR3Y4O12	UY6O12		hR19	R-3	148		3	[3.0, 4.0, 12.0]	(ZR+4)3(Y+3)4(O-2)12
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193		4	[2.0, 3.0, 3.0, 1.0]	(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

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
W5SI3_D8M	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		3	[4.0, 1.0, 3.0]	(CR, FE, MO, NB, V, W)4(CR, FE, MO, NB, SI, V, W)1(AL, SI)3
TA5SI3_D8L	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140		2	[5.0, 3.0]	(HF, NB, TA)5(AL, SI)3
ZR5SI4	Si4Zr5		tP36	P4_12_12	92		2	[5.0, 4.0]	(HF, NB, TI, Y, ZR)5(SI)4
CR3SI_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		3	[3.0, 1.0, 3.0]	(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	P4_2/n	86		2	[3.0, 1.0]	(HF, NB, TA, TI, ZR)3(SI)1
CO2SI_C23	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(CO, CR, CU, FE, NI, TI)2(SI)1
MSI_B27	FeB (B27)	B27	oP8	Pnma	62		2	[1.0, 1.0]	(HF, NB, TI, Y, ZR)1(SI)1
FESI_B20	FeSi (B20)	B20	cP8	P2_13	198		2	[1.0, 1.0]	(CO, CR, FE, MN, NI, RE)1(AL, SI)1
CRSI2_C40	CrSi2 (C40)	C40	hP9	P6_222	180		2	[1.0, 2.0]	(CR, CU, HF, MO, NB, SI, TA, V)1 (AL, CR, CU, SI)2
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[1.0, 2.0]	(CO, CU, FE, MO, NI, PD, W)1(AL, HF, SI, TI, ZR)2
ZRSI2_C49	ZrSi2 (C49)	C49	oS12	Cmcm	63	Also YSi2-orth of SG Imma	2	[1.0, 2.0]	(HF, NB, Y, ZR)1(SI)2
YSI2_HT	Unknown Structure						2	[1.0, 2.0]	(Y)1(SI)2
Y3SI5_HT	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[3.0, 5.0]	(Y)3(SI)5
Y3SI5_LT	Unknown Structure						2	[3.0, 5.0]	(Y)3(SI)5
TISI2_C54	TiSi2 (C54)	C54	oF24	Fddd	70		2	[1.0, 2.0]	(MO, NB, RU, TI)1(AL, SI)2
MSI2_C1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		2	[1.0, 2.0]	(CO, CU, MN, NI)1(AL, CU, SI)2

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
M3SI2_D5A	Si2U3 (D5a)	D5a	tP10	P4/mbm	127		2	[3.0, 2.0]	(HF, NB, ZR)3(SI)2
NI31SI12	Ni31S12		hP42	P321	150		2	[5.0, 2.0]	(CO, CR, CU, FE, NI)5(SI)2
CR3NI5SI2	AlAu4		cP20	P2_13	198		4	[3.0, 5.0, 2.0, 1.0]	(CR)3(NI)5(SI)2(C, VA)1
NI6SI2B	ZrNiAl		hP9	P-62m	189		3	[6.0, 2.0, 1.0]	(NI)6(SI)2(B)1
NI4SI2B	Nb5Sn2Si		tI32	I4/mcm	140		3	[4.29, 2.0, 1.43]	(NI)4.29(SI)2(B)1.43
FE8SI2C	Mn8Si2C		aP*	P1	1		3	[8.0, 2.0, 1.0]	(FE)8(SI)2(C)1
CRNBSI	ZrNiAl		hP9	P-62m	189		3	[1.0, 1.0, 1.0]	(CR)1(NB)1(SI)1
M11SI8	Cr11Ge8		oP76	Pnma	62		2	[11.0, 8.0]	(CR, NB)11(SI)8
M6SI5	Si5V6		oI44	Ibam	72		2	[6.0, 5.0]	(CR, NB)6(SI)5
CR2NI2SI	NiTi2		cF96	Fd-3m	227		3	[5.0, 5.0, 3.0]	(CR)5(NI)5(SI)3
M4SI3	Ru4Si3		oP28	Pnma	62		2	[4.0, 3.0]	(CR, NI)4(SI)3
RU2SI_C37	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(RU)2(SI)1
RU4SI3	Ru4Si3		oP28	Pnma	62		2	[4.0, 3.0]	(RU)4(SI)3
RUSI	FeSi (B20)	B20	cP8	P2_13	198		2	[1.0, 1.0]	(RU)1(SI)1
RU2SI3	Ge3Ru2		oP40	Pbcn	60		2	[2.0, 3.0]	(RU)2(SI)3
SI5V6	Si5V6		oI44	Ibam	72		2	[5.0, 6.0]	(SI)5(V)6
NI3SI_MONOCL	Ge9Pd25		hP34	P-3	147		2	[3.0, 1.0]	(NI)3(SI)1
NI3SI2	Ni3Si2		oP80	Cmc2_1	36		2	[3.0, 2.0]	(NI)3(SI)2

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NI2SI_TETA	AlNi2		hP6	P-3m1	164		3	[1.0, 1.0, 1.0]	(CU, NI)1(NI, VA)1(AL, SI)1
RE2SI	Re2Si		mP24	P2_1/c	14		2	[2.0, 1.0]	(RE)2(SI)1
RESI2_C11B	Re4Si7		mS44	Cm	8		2	[0.357, 0.643]	(RE)0.357(SI)0.643
MN15NI45SI40	Unknown Structure						3	[0.15, 0.45, 0.4]	(MN)0.15(NI)0.45(SI)0.4
MN15NI50SI35	Unknown Structure						3	[0.15, 0.5, 0.35]	(MN)0.15(NI)0.5(SI)0.35
MN6NI16SI7	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		3	[0.206897, 0.551724, 0.241379]	(MN)0.206897(NI)0.551724 (SI)0.241379
MN1NI1SI1	MnCuP		oP12	Pnma	62		3	[1.0, 1.0, 1.0]	(MN)1(NI)1(SI)1
MNNISI_T5	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		2	[1.0, 2.0]	(MN)1(NI, SI)2
MNNISI_T6	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[1.0, 2.0]	(MN)1(NI, SI)2
MN3NI2SI	Mn3Ni2Si		cF96	Fd-3m	227		3	[3.0, 2.0, 1.0]	(MN)3(NI)2(SI)1
MN2NISI	Unknown Structure						2	[3.0, 1.0]	(MN, NI)3(SI)1
MN6NISI3	R-(Co, Cr, Mo)		hR53	R-3	166		3	[0.61, 0.12, 0.27]	(MN)0.61(NI)0.12(SI)0.27
MN66NI4SI30	Unknown Structure						3	[0.66, 0.04, 0.3]	(MN)0.66(NI)0.04(SI)0.3
MN52NI29SI19	Unknown Structure						3	[0.52, 0.29, 0.19]	(MN)0.52(NI)0.29(SI)0.19
MONOCLINIC_S	beta-S		mP48	P2_1/c	14		1	[1.0]	(S)1
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	Fddd	70		1	[1.0]	(S)1
RED_P	Unknown Structure						1	[1.0]	(P)1

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
WHITE_P	Unknown Structure						1	[1.0]	(P)1
AL2S3	alpha-Al2S3		hP30	P6_1	169		2	[2.0, 3.0]	(AL)2(S)3
CR1S1	CrS		mS8	C2/c	15		2	[1.03, 1.0]	(CR)1.03(S)1
CR7S8	Cr7Se8		mS30	C2/m	12		2	[7.0, 8.0]	(CR)7(S)8
CR5S6	Cr5S6		hP22	P-31c	163		2	[5.0, 6.0]	(CR)5(S)6
CR3S4	Brezinaite (Cr3S4)		mS14	C2/m	12		2	[3.0, 4.0]	(CR, FE, MN, NI)3(S)4
CR2S3	Dolomite [MgCa(CO3)2, G11]	G11	hR10	R-3	148	Also Cr+ variant of SG P-31c	2	[2.0, 3.0]	(CR, FE)2(S)3
NIS_LT	Millerite (NiS, B13)	B13	hR6	R3m	160		2	[1.0, 1.0]	(NI)1(S)1
NI3S2_LT	Hazelwoodite (Ni3S2, D5e)	D5e	hR5	R32	155		2	[3.0, 2.0]	(NI)3(S)2
CUCRS2	CuCrS2-b		hR4	R3m	160	Also ht variant of pearson hR5	3	[1.0, 1.0, 2.0]	(CU)1(CR)1(S)2
FEAL2S4	ZnIn2S4		hR7	R3m	160		3	[1.0, 2.0, 4.0]	(FE)1(AL)2(S)4
SIS2	SiS2 (C42)	C42	oI12	Ibam	72		2	[1.0, 2.0]	(SI)1(S)2
ZRS2	CdI2		hP3	P-3m1	164		2	[1.0, 2.0]	(ZR)1(S)2
ANILITE	Cu7S4		oP44	Pnma	62		2	[1.75, 1.0]	(CU)1.75(S)1
CHALCOCITE_ALPHA	Cu2S-alpha		mP144	P2_1/c	14		2	[2.0, 1.0]	(CU)2(S)1
CHALCOCITE_BETA	Cu2S-beta		hP16	P6_3/mmc	194		2	[2.0, 1.0]	(CU)2(S)1
COVELLITE	Covellite (CuS, B18)	B18	hP12	P6_3/mmc	194		2	[1.0, 1.0]	(CU)1(S)1

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DJURLEITE	Cu31S16		mP376	P2_1/c	14		2	[1.93, 1.0]	(CU)1.93(S)1
CUFES2_LT	Chalcopyrite (CuFeS2, E11)	E11	tI16	I-42d	122		3	[1.0, 1.0, 2.0]	(CU)1(FE)1(S)2
MO2S3	Mo2S3		mP10	P2_1/m	11		2	[2.0, 3.0]	(MO)2(S)3
MO1S2	Molybdenite (MoS2, C7)	C7	hP6	P6_3/mmc	194		2	[1.0, 2.0]	(MO)1(S)2
HEAZLEWOODITE_B1	Cu1.9S		cF12	F-43m	216		2	[2.0, 1.0]	(CO, FE, NI, VA)2(S)1
HEAZLEWOODITE_B2	Unknown Structure		cP*				2	[2.0, 1.0]	(FE, NI, VA)2(S)1
NI7S6	Unknown Structure		t**				2	[7.0, 6.0]	(FE, NI)7(S)6
NI9S8	Ni9S8		oS68	C222	21		2	[9.0, 8.0]	(FE, NI)9(S)8
THIOSPINEL	Spinel (Co3O4, D72)	D72	cF56	Fd-3m	227		3	[1.0, 2.0, 4.0]	(CO, CU, FE, MN, NI)1(CO, CR, NI)2 (S)4
ALABANDITE	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		2	[1.0, 1.0]	(CA, CO, CR, CU, FE, MG, MN, Y, ZR)1(S)1
PYRRHOTITE	NiAs (B81)	B81	hP4	P6_3/mmc	194		2	[1.0, 1.0]	(AL, CO, CR, CU, FE, MG, MN, NB, NI, TI, V, VA, ZR)1(S)1
PYRITE	Pyrite (FeS2, C2)	C2	cP12	Pa-3	205		2	[1.0, 2.0]	(CO, FE, MN, NI)1(S)2
CO9S8	Co9S8 (D89)	D89	cF68	Fm-3m	225		2	[9.0, 8.0]	(CO, FE, NI)9(S)8
PENTLANDITE	Co9S8 (D89)	D89	cF68	Fm-3m	225		3	[8.0, 1.0, 8.0]	(FE, NI)8(FE, NI)1(S)8
DIGENITE	Cu2Se		cF44	Fm-3m	225		3	[2.0, 1.0, 1.0]	(CU, FE, MG, MN, VA)2(CU, VA)1 (S)1
CHALCOPYRITE	Chalcopyrite (CuFeS2, E11)	E11	tI16	I-42d	122		3	[1.0, 1.0, 1.0]	(CU, FE, VA)1(CU, VA)1(S)1
FE2O12S3	Fe2[SO4]3		hR34	R-3	148		2	[2.0, 3.0]	(AL+3, CR+3, FE+3)2(SO4-2)3

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
ZRO8S2	Zr[SO4]2		oP44	Pnma	62		2	[1.0, 2.0]	(ZR+4)1(SO4-2)2
ANHYDRITE	Anhydrite (CaSO4, H01)	H01	oS24	Cmcm	63		2	[1.0, 1.0]	(CA+2, CO+2, CU+2, FE+2, MN+2, NI+2)1(SO4-2)1
CASO4_HT	CePO4		hP18	P6_222	180		2	[1.0, 1.0]	(CA+2, CO+2)1(SO4-2)1
CU2SO4	Thenardite [Na2SO4 (V), H17]	H17	oF56	Fddd	70		2	[2.0, 1.0]	(CU+1)2(SO4-2)1
CU2SO5	Cu2[SO4]O		mS32	C2/m	12		1	[1.0]	(CU2O5S1)1
MN9SI3O14S1	Unknown Structure						4	[9.0, 3.0, 14.0, 1.0]	(MN+2)9(SI+4)3(O-2)14(S-2)1
C1A1	Al2CaO4		mP84	P2_1/c	14		4	[3.0, 5.0, 1.0, 12.0]	(CA+2)3(AL+3)5(AL+3, FE+3)1(O-2)12
C1A2	Al4CaO7		mS48	C2/c	15		4	[1.0, 3.0, 1.0, 7.0]	(CA+2)1(AL+3)3(AL+3, FE+3)1(O-2)7
C1A6	Magnetoplumbite (PbFe12O19)		hP64	P6_3/mmc	194		3	[1.0, 12.0, 19.0]	(CA+2)1(AL+3, FE+3)12(O-2)19
C3A1	Ca3Al2O6		cP264	Pa-3	205		3	[3.0, 2.0, 6.0]	(CA+2)3(AL+3, FE+3)2(O-2)6
C12A7	Mayenite (12CaO.7Al2O3, K74, C12A7)	K74	cI152	I-43d	220		4	[6.0, 6.0, 1.0, 16.5]	(CA+2)6(AL+3)6(AL+3, FE+3)1(O-2)16.5
AF	FeGaO3		oP40	Pna2_1	33		2	[1.0, 1.0]	(AL2O3)1(FE2O3)1
CACR2O4_A	SrCr2O4		oP28	Pmmn	59		3	[1.0, 2.0, 4.0]	(CA+2)1(AL+3, CR+3, FE+3)2(O-2)4
CF2	Ca3.5Fe14O24.5		mS172	C2	5		3	[1.0, 4.0, 7.0]	(CA+2)1(FE+3)4(O-2)7
C2F	Ca2Fe2O5		oP36	Pnma	62		3	[2.0, 2.0, 5.0]	(CA+2)2(AL+3, FE+3)2(O-2)5

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
CWF	CaFe3O5		oS36	Cmcm	63		4	[1.0, 1.0, 2.0, 5.0]	(CA+2)1(FE+2)1(FE+3)2(O-2)5
CW3F	CaFe5O7		oS52	Cmcm	63		4	[1.0, 3.0, 2.0, 7.0]	(CA+2)1(FE+2)3(FE+3)2(O-2)7
C4WF4	Ca4Fe9O17		mS60	C2	5		4	[4.0, 1.0, 8.0, 17.0]	(CA+2)4(FE+2)1(FE+3)8(O-2)17
C4WF8	Sr2Fe2O5		oI44	Imma	74		4	[4.0, 1.0, 16.0, 29.0]	(CA+2)4(FE+2)1(FE+3)16(O-2)29
CAV2O4	CaV2O4		oP28	Pnma	62		3	[1.0, 2.0, 4.0]	(CA+2)1(AL+3, CR+3, FE+3, Y+3)2 (O-2)4
CAMN2O4	CaMn2O4		oP28	Pbcm	57		3	[1.0, 2.0, 4.0]	(CA+2)1(MN+3)2(O-2)4
CA3CO2O6	Ca3Co2O6		hR22	R-3c	167		3	[3.0, 2.0, 6.0]	(CA+2)3(CO+3, CU+2)2(O-2, VA)6
CA3CO4O9	Ca3Co4O9		mS30	C2/m	12		3	[3.0, 4.0, 9.0]	(CA+2)3(CO+3, CU+2)4(O-2, VA)9
CA4NB2O9_HT11	Ca4Nb2O9		mP20	P2_1/c	14		5	[6.0, 3.0, 3.0, 3.0, 15.0]	(CA+2)6(CA+2, NB+5)3(NB+5)3(O-2, VA)3(O-2)15
CA4NB2O9_LT21	Ca4Nb2O9-lt		mP60	P2_1/c	14		5	[6.0, 4.0, 2.0, 3.0, 15.0]	(CA+2)6(CA+2, NB+5)4(CA+2)2(O-2, VA)3(O-2)15
LAAP	LaAlO3		hR10	R-3c	167		3	[1.0, 1.0, 3.0]	(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	Pnma	62		3	[1.0, 1.0, 3.0]	(CA+2, Y+3)1(MN+4, Y+3, ZR+4)1 (O-2)3
CACU2O3	Shcherbinaite (V2O5) (Revised)		oP14	Pmmn	59		3	[1.0, 2.0, 3.0]	(CA+2)1(CU+2)2(O-2)3
CA2CUO3	Sr2CuO3		oI12	Immm	71		3	[2.0, 1.0, 3.0]	(CA+2)2(CU+2)1(O-2)3
CA15CU18O35	Ca4.8Cu6O11.6		mP92	P2/c	13		4	[15.0, 14.0, 4.0, 35.0]	(CA+2)15(CU+2)14(CU+3)4(O-2)35

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
CASFEO	Unknown Structure						4	[2.0, 2.0, 2.0, 3.0]	(CA+2)2(S-2)2(FE+2, FE+3)2(O-2, VA)3
CA3S3FE4OX	Unknown Structure						4	[3.0, 3.0, 4.0, 6.0]	(CA+2)3(S-2)3(FE+2, FE+3)4(O-2, VA)6
CA2NB2O7	La2Ti2O7		mP44	P2_1	4		3	[2.0, 2.0, 7.0]	(CA+2)2(NB+5)2(O-2)7
CA3NB2O8	Unknown Structure						3	[3.0, 2.0, 8.0]	(CA+2)3(NB+5)2(O-2)8
CA2SIO4_ALPHA	Ca2SiO4		hP24	P6_3/mmc	194		3	[3.0, 1.0, 2.0]	(CA+2, MN+2, Y+3)3(CA+2, VA)1 (SIO4-4)2
CA2SIO4_ALPHA_ PRIME	K2CoCl4		oP84	Pna2_1	33		3	[3.0, 1.0, 2.0]	(CA+2, FE+2, MN+2, Y+3)3(CA+2, VA)1(SIO4-4)2
LARNITE	Parawollastonite (CaSiO3, S33(II))	S33(II)	mP60	P2_1/c	14		3	[2.0, 1.0, 4.0]	(CA+2)2(SI+4)1(O-2)4
RANKINITE	3CaO.2SiO2		mP48	P2_1/c	14		3	[3.0, 2.0, 7.0]	(CA+2)3(SI+4)2(O-2)7
CLINO_PYROXENE	Diopside [CaMg(SiO3)2, S41]	S41	mS40	C2/c	15		4	[1.0, 1.0, 2.0, 6.0]	(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	Pbca	61		4	[1.0, 1.0, 2.0, 6.0]	(CA+2, FE+2)1(FE+2)1(SI+4)2(O-2)6
PROTO_PYROXENE	MgSiO3		oP40	Pbcn	60		3	[1.0, 1.0, 3.0]	(CA+2, CO+2, CR+2, FE+2, NI+2)1 (SI+4)1(O-2)3
WOLLASTONITE	Wollastonite (CaSiO3)		aP30	P-1	2		3	[1.0, 1.0, 3.0]	(CA+2, FE+2, MN+2)1(SI+4)1(O-2)3
PSEUDO_ WOLLASTONITE	CaSiO3		mS120	C2/c	15		3	[1.0, 1.0, 3.0]	(CA+2)1(SI+4)1(O-2)3
HATRURITE	Ca3(SiO4)O-b		hR81	R3m	160		3	[3.0, 1.0, 1.0]	(CA+2, VA, Y+3)3(SIO4-4)1(O-2)1
CAZRO3_C	Cubic Perovskite (CaTiO3,	E21	cP5	Pm-3m	221		3	[1.0, 1.0, 3.0]	(CA+2, Y+3)1(Y+3, ZR+4)1(O-2)3

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
	E21)								
CAZR4O9	CaZr4O9		mS224	C2/c	15		3	[1.0, 4.0, 9.0]	(CA+2)1(ZR+4)4(O-2)9
CA6ZR19O44	Ca6Hf19O44		hR138	R-3c	167		3	[6.0, 19.0, 44.0]	(CA+2)6(ZR+4)19(O-2)44
C13A6Z2	Ca7ZrAl6O18		oP104	Pmn2_1	31		4	[13.0, 12.0, 2.0, 35.0]	(CA+2)13(AL+3)12(ZR+4)2(O-2)35
CAY4O7	(Ca0.25Gd0.75)4GdO7		mS48	C2/m	12		3	[1.0, 4.0, 7.0]	(CA+2)1(Y+3)4(O-2)7
CAYALO4	K2NiF4		tI14	I4/mmm	139		4	[1.0, 1.0, 1.0, 4.0]	(CA+2)1(Y+3)1(AL+3)1(O-2)4
CAYAL3O7	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	P-42_1m	113		4	[1.0, 1.0, 3.0, 7.0]	(CA+2)1(Y+3)1(AL+3)3(O-2)7
CA3COAL4O10	Ca3ZnAl4O10		oP72	Pca2_1	29		4	[3.0, 1.0, 4.0, 10.0]	(CA+2)3(CO+2)1(AL+3)4(O-2)10
CA2ALNBO6	Ca2AlNbO6		mP24	P2_1/c	14		4	[2.0, 1.0, 1.0, 6.0]	(CA+2)2(AL+3)1(NB+5)1(O-2)6
ANORTHITE	Ca(Al0.5Si0.5)4O8		aP104	P-1	2		4	[1.0, 2.0, 2.0, 8.0]	(CA+2)1(AL+3)2(SI+4)2(O-2)8
CACRSI4O10	gillespite (BaFeSi4O10)		tP64	P4/ncc	130		4	[1.0, 1.0, 4.0, 10.0]	(CA+2)1(CR+2)1(SI+4)4(O-2)10
CA2ZRSI4O12	cyclosilicate (Ca2ZrSi4O12)		mP38	P2_1/m	11		1	[1.0]	(CA2ZRSI4O12)1
CA3ZRSI2O9	Ca3Hf(Si2O7)O2		mP60	P2_1/c	14		1	[1.0]	(CA3ZRSI2O9)1
GARNET	Orthorhombic Garnet		oF320	Fddd	70		4	[3.0, 2.0, 3.0, 12.0]	(CA+2, MN+2)3(AL+3, CR+3)2 (SI+4)3(O-2)12
MELILITE	Akermanite (Ca2MgSi2O7, S53)	S53	tP24	P-42_1m	113		5	[2.0, 1.0, 1.0, 1.0, 7.0]	(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	P6_3/m	176		4	[4.0, 6.0, 6.0, 2.0]	(CA+2, VA, Y+3, ZR+4)4(Y+3)6 (SIO4-4)6(O-2, VA)2

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
CA3Y2SI6O18	Ca0.6Y0.4Si6O18		mS116	C2/c	15		4	[3.0, 2.0, 6.0, 18.0]	(CA+2)3(Y+3)2(SI+4)6(O-2)18
CA3Y2SI3O12	Ca3Y2Si3O12		oP100	Pnma	62		4	[3.0, 2.0, 3.0, 12.0]	(CA+2)3(Y+3)2(SI+4)3(O-2)12
C1A1F2	Unknown Structure						5	[1.0, 1.0, 2.0, 3.0, 10.0]	(CA+2)1(AL+3)1(FE+3)2(AL+3, FE+3)3(O-2)10
CA2NI7	Co7Gd2		hR18	R-3m	166		2	[2.0, 7.0]	(CA)2(NI)7
CANI2	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[2.0, 1.0]	(NI)2(CA)1
CANI3	Ni3Pu		hR12	R-3m	166		2	[0.25, 0.75]	(CA)0.25(NI)0.75
CANI5	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[1.0, 5.0]	(CA)1(NI)5
CA2SI_C37	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(CA)2(SI)1
CASI_B33	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(CA)1(SI)1
CASI2_C12	CaSi2 (C12)	C12	hR6	R-3m	166		2	[1.0, 2.0]	(CA)1(SI)2
CUMG2	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[1.0, 2.0]	(CU, NI)1(MG)2
MG3N2_D53	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	206		2	[3.0, 2.0]	(MG)3(N)2
MG2NI	Mg2Ni (Ca)	Ca	hP18	P6_222	180		2	[2.0, 1.0]	(MG)2(CU, NI)1
MG24Y5_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[24.0, 4.0, 1.0]	(MG)24(MG, Y)4(Y)1
MNPT7	Ca7Ge		cF32	Fm-3m	225		3	[6.0, 1.0, 1.0]	(PT)6(PT)1(MN)1
PD4S	Pd4Se		tP10	P-42_1c	114		2	[0.8, 0.2]	(PD)0.8(S)0.2
PD3S	Pd3S		oS16	Ama2	40		2	[0.75, 0.25]	(PD)0.75(S)0.25

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
PD16S7	Pd16S7		cI46	I-43m	217		2	[0.696, 0.304]	(PD)0.696(S)0.304
PDS	PdS (B34)	B34	tP16	P4_2/m	84		2	[0.5, 0.5]	(PD)0.5(S)0.5
PTS	Cooperite (PtS, B17)	B17	tP4	P4_2/mmc	131		2	[1.0, 1.0]	(PT)1(S)1
PTS2	CdI2		hP3	P-3m1	164		2	[1.0, 2.0]	(PT)1(S)2
RE1S2	ReS2		aP12	P-1	2		2	[1.0, 2.0]	(RE)1(S)2
RE1S3	Unknown Structure						2	[1.0, 3.0]	(RE)1(S)3
RE2S7	Re2O7		oP72	P2_12_12_1	19		2	[2.0, 7.0]	(RE)2(S)7
RU1S2	Pyrite (FeS2, C2)	C2	cP12	Pa-3	205		2	[1.0, 2.0]	(RU)1(S)2
W1S2	Molybdenite (MoS2, C7)	C7	hP6	P6_3/mmc	194	also HT variant of SG R3m	2	[1.0, 2.0]	(W)1(S)2
MG6MN3NI	Unknown Structure						3	[3.0, 1.0, 2.0]	(MG)3(MN)1(NI)2
NIOCALITE_C10NS6	Niocalite		oS114	C222	21		4	[10.0, 2.0, 6.0, 27.0]	(CA+2)10(NB+5)2(SI+4)6(O-2)27
AL4CA_D13	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[4.0, 1.0]	(AL)4(CA)1
AL2CA_C15	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[2.0, 1.0]	(AL)2(CA)1
ALMG_BETA	Al45Mg28		cF1832	Fd-3m	227		2	[140.0, 89.0]	(AL)140(MG)89
ALMG_EPSILON	Al30Mg23		hR53	R-3	148		2	[30.0, 23.0]	(AL)30(MG)23
AL12MG17_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[10.0, 24.0, 24.0]	(MG)10(AL, MG)24(AL, MG)24
CAB6	CaB6 (D21)	D21	cP7	Pm-3m	221		2	[1.0, 6.0]	(CA)1(B)6

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
MGB4	MgB4		oP20	Pnma	62		2	[1.0, 4.0]	(MG)1(B)4
MGB7	MgB7		oI64	Imma	74		2	[1.0, 7.0]	(MG)1(B)7
C2CA1_S	CaC2-I (C11a)	C11a	tI6	I4/mmm	139		1	[1.0]	(C2CA1)1
C2CA1_S2	CaC2		cF36	Fm-3m	225		1	[1.0]	(C2CA1)1
MGC2	MgC2		tP6	P4_2/mnm	136		2	[1.0, 2.0]	(MG)1(C)2
MG2C3	Mg2C3		oP10	Pnnm	58		2	[2.0, 3.0]	(MG)2(C)3
CA2CU	Ca2Cu		oP12	Pnma	62		2	[2.0, 1.0]	(CA)2(CU)1
CACU	alpha-CaCu		mP20	P2_1/m	11		2	[1.0, 1.0]	(CA)1(CU)1
CACU5_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[1.0, 5.0]	(CA)1(CU)5
MG2SI	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		2	[2.0, 1.0]	(MG)2(SI)1
GAS	Gas					Gas mixture	1	[1.0]	(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,

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*
									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,

	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	CEF Formula
									H2O2, 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,

	Prototype	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*CEF Formula*

TCNI12 Properties Data

Model Descriptions

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

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.

Examples

Go to the Nickel-based Superalloys Databases page on our website where you can access an 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.

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:	**12.1**
First release:	**TCNI1 was released in 2000**

Changes in the Most Recent Database Release

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.

Previous Releases

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.