TCS Ni-based Superalloys Database (TCNI10)

Technical Information

Available Starting with Thermo-Calc Version 2020b

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Contents

About the TCS Ni-based Superalloys Database (TCNI)

TCNI: TCS Ni-based Superalloys Database Revision History

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, and surface tension of liquid metallic alloys.

The current version of the database is TCNI10.

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

The properties data for viscosity of the metallic liquids and surface tension of metallic liquids are included with TCS Ni-based Superalloys Database (TCNI) starting with version 10 (TCNI10).

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.

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 TCNI10 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), and/or Process Metallurgy 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 *TCNI: TCS Ni-based Superalloys Database Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, phases, models, and properties data. It also includes a list of the included elements and summaries of the database revision history by version.
- The *TCNI: TCS Ni-based Superalloys Database 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 the technical information and 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.

TCNI10 Elements, Systems, Phases and Properties Data

Included Elements

There are 30 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	Pd	Pt
Re	Ru	S	Si	Ta	Ti	V	W	Y	Zr

Assessed Systems and Phases

The most recent version of the database includes:

- Critically assessed thermodynamic descriptions for 30 elements and 680 phases.
- All possible binary systems and most Ni-containing ternary systems have been assessed to the full range of composition, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- The database also contains many assessed ternary systems, at least those being in equilibrium with γ and γ’ phase, which can be calculated with the TERNARY module in Thermo-Calc Console Mode.

TCNI10 has improved γ' precipitate solvus temperatures of industrial Ni-base superalloys compared to TCNI9.

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

TCNI10 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

[1985, Hillert] M. Hillert, B. Jansson, B. Sundman, J. Ågren, "A two-sublattice model for molten solutions with different tendency for ionization," Metall. Trans. A. 16, 261–266 (1985).

[1991, Sundman] B. Sundman, "Modification of the two-sublattice model for liquids," Calphad. 15, 109–119 (1991).

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

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

[2007, Hallstedt] 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 thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources will also be made available on our website in the near future 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.

Available Properties Data Parameters and Variables

Below is a summary of the available parameters and variables for this database 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 in TDB File	Variables to show or plot in Console Mode and TC-Python
Surface tension	SIGM, XI	`SURF(LIQUID)`
Dynamic viscosity	VICS	`DVIS(LIQUID)`

Property	Model Parameters in TDB File	Variables to show or plot in Console Mode and TC-Python
Kinematic viscosity		`KVIS(LIQUID)`
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI `VP(PHI)` volume fraction of phase PHI

TCNI10 Systems

In this section:

TCNI10 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	Pd	Pt	Re	Ru	S	Si	Ta	Ti	V	W	Y	Zr
AL																												
B	x																											
C	x	x																										
Ca	x	x	x																									
Co	x	x	x	x																								
Cr	x	x	x	x	x																							
Cu	x	x	x	x	x	x																						
Fe	x	x	x	x	x	x	x																					
Hf	x	x	x		x	x	x	x																				
Mg	x	x	x	x	x	x	x	x	x																			
Mn	x	x	x	x	x	x	x	x	x	x																		
Mo	x	x	x	x	x	x	x	x	x	x	x																	
N	x	x			x	x	x	x		x	x	x																
Nb	x	x	x	x	x	x	x	x	x	x	x	x	x															
Ni	x	x	x	x	x	x	x	x	x	x	x	x	x	x														
O	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x													
Pd	x	x	x		x	x	x	x	x		x	x		x	x	x												
Pt	x	x	x		x	x	x	x	x		x	x		x	x	x	x											
Re	x	x	x		x	x	x	x	x		x	x		x	x	x	x	x										
Ru	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x									
S	x		x	x	x	x	x	x		x	x	x		x	x		x	x	x	x								
Si	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x							
Ta	x	x	x		x	x	x	x	x		x	x	x	x	x	x	x	x	x	x		x						
Ti	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x					
V	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x				
W	x	x	x		x	x	x	x	x	x		x	x	x	x	x	x	x	x	x		x	x	x	x			
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		
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	

TCNI10 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-Hf
Al-B-Mo	Al-B-Ni	Al-B-Re	Al-B-Ta
Al-B-Ti	Al-B-Zr	Al-C-Co	Al-C-Cr
Al-C-Fe	Al-C-Hf	Al-C-Mo	Al-C-Ni
Al-C-Si	Al-C-Ta	Al-C-Ti	Al-C-W
Al-C-Zr	Al-Ca-O	Al-Ca-Si	Al-Co-Cr
Al-Co-Fe	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-Fe
Al-Cr-Hf	Al-Cr-Mo	Al-Cr-Nb	Al-Cr-Ni
Al-Cr-O	Al-Cr-Pt	Al-Cr-Ru	Al-Cr-Ta
Al-Cr-Ti	Al-Cr-W	Al-Cr-Zr	Al-Cu-Fe
Al-Cu-Mn	Al-Cu-Ni	Al-Cu-S	Al-Cu-Si
Al-Fe-Mn	Al-Fe-Mo	Al-Fe-N	Al-Fe-Nb
Al-Fe-Ni	Al-Fe-O	Al-Fe-Re	Al-Fe-Ru
Al-Fe-S	Al-Fe-Ta	Al-Fe-Ti	Al-Fe-W
Al-Hf-Mo	Al-Hf-Ni	Al-Hf-Re	Al-Hf-Ru
Al-Hf-Ta	Al-Hf-Ti	Al-Hf-W	Al-Hf-Zr
Al-Mn-Ni	Al-Mn-O	Al-Mn-Si	Al-Mn-Ti
Al-Mo-Nb	Al-Mo-Ni	Al-Mo-Re	Al-Mo-Ru

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

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

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

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

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

TCNI10 Phases

In this section:

Common Phases for the TCNI Database

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

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

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

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

Common Phase Name	
ALN_B4	M12C
BCC_B2#1 (disordered BCC A2)	M23C6
BCC_B2#2 (ordered B2, β)	M2B_TETR
BCT_D022 (γ'')	M3B2
BETA_RHOMBO_B	M3C2
C14_LAVES	M6C
CEMENTITE (Fe3C)	M7C3
CHI_A12 (χ)	MB_B33
D5A_M3B2	MB2_C32
DIAMOND_A4	MC_ETA
FCC_L12#1 (disordered FCC A1, γ, austenite)	MC_SHP
FCC_L12#2 (ordered L12 γ')	MU_PHASE (μ)
FCC_L12#3 (carbonitride)	NI3B_D011
FE4N_LP1	NI3TA_D0A (Delta δ)
FECN_CHI	NI3TI_D024 (Eta η)

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

TCNI10 Models for the Included Phases

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

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
AF	FeGaO3	oP40	Pna21		33	(AL2O3)1(FE2O3)1
AL10CU10FE	Al10Cu10Fe	oF116	Fmm2		42	(FE)1(AL,CU)10(AL)10
AL10FEMN2	MnAl6	oS28	Cmcm		63	(FE,MN)3(AL)10
AL10V	Al10V	cF176	Fd-3m		227	(AL)10(V)1
AL11CR2	Al5Cr	mS732	C2/c		15	(AL)10(AL)1(CR)2
AL11CU5MN3	*	oP380	*		*	(AL)11(MN)3(CU)5
AL11MN4_HT	Al3Mn	oP156	Pnma		62	(AL,MN)29(MN)10
AL11MN4_LT	Al11Mn4	aP15	P-1		2	(AL)11(MN,FE)4
AL11RE4	Al11Mn4	aP15	P-1		2	(AL)11(RE)4
AL11TI5	Al3Zr	tI16	I4/mmm	D0_23	139	(AL)17(TI)8
AL12MG17_A12	Mg17Al12	cI58	I-43m	A12	217	(MG)10(AL,MG)24(AL,MG)24
AL12MN	Al12W	cI26	Im-3		204	(AL)12(MN)1
AL12W	Al12W	cI26	Im-3		204	(AL)12(MO,RE,W)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
AL13CO4	Al19Co6	mS100	C2/m		12	(AL)13(CO)4
AL13CR2	Al45V7	mS104	C2/m		12	(AL)13(CR)2
AL13FE2MN2	Al13Fe4	mS102	C2/m		12	(FE,MN)4(AL)13
AL13FE4	Al13Fe4	mS102	C2/m		12	(AL,CU)0.63(FE,MN,RU)0.23(AL,SI,VA)0.14
AL15SI2M4	(Mn0.2Fe0.8)4 (Al0.9Si0.1)19	cI168	Im-3		204	(AL)14(FE,MN)4(AL,SI)5
AL16FEMN3	mu-Al4mn	hP574	P6_ 3/mmc		194	(AL)4(FE,MN)1
AL1MN1SI1	TiSi2	oF24	Fddd		70	(AL)1(MN)1(SI)1
AL21PD8	Al21Pt8	tI116	I4_1/a		88	(AL)21(PD)8
AL21PT5	Li21Si5	cF416	F-43m		216	(AL)0.8077(NI,PT)0.1923
AL21PT8	Al21Pt8	tI116	I4_1/a		88	(AL)0.7241(NI,PT)0.2759
AL23CUFE4	Al6Mn	oS28	Cmcm	D2_h	63	(AL)23(CU)1(FE)4
AL23V4	Al23V4	hP54	P6_ 3/mmc		194	(AL)23(V)4
AL28CU4MN7	*	*	*		*	(AL)28(MN)7(CU)4
AL2CA_C15	Cu2Mg	cF24	Fd-3m	C15	227	(AL)2(CA)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
AL2FE	Al2Fe	aP18	P1		1	(AL,CU)2(FE,MN)10.04
AL2MN2SI3	*	hP21	P-6		174	(AL)2(MN)2(SI)3
AL2MNSI3	Ga5Pd	tI24	I4/mcm		140	(AL)2(MN)1(SI)3
AL2N2TI3	Ti3Al2N2	hP22	P6_3mc		186	(AL)2(N)2(TI)3
AL2PD5	Ga2Pd5	oP28	Pnma		62	(AL)2(AL,PD)5
AL2PT	CaF2	cF12	Fm-3m	C1	225	(AL)2(NI,PT)1(NI,VA)1
AL2S3	Al2S3	hP30	P61		169	(AL)2(S)3
AL2TI	Ga2Hf	tI24	I4_1/amd		141	(AL)2(TI)1
AL2W	Cr2Si2	hP9	P6_222		180	(AL)2(W)1
AL2ZR3	Al2Zr3	tP20	P4_2/mnm		136	(AL)2(HF,Y,ZR)3
AL31MN6NI2	mu-Al4Mn	hP574	P6_3/mmc		194	(AL)31(MN)6(NI)2
AL3CO	Al13Os4	mS34	C2/m		12	(AL)3(CO)1
AL3MN4SI2	*	structure unknown				(AL)3(MN)4(SI)2
AL3MNSI2	*	tP48	P4/n		85	(AL)3(MN)1(SI)2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
AL3NI1	Fe3C	oP16	Pnma	D0_11	62	(AL)0.75(NI)0.25
AL3NI2	Al3Ni2	hP5	P-3m1	D5_19	164	(AL,SI)3(AL,CU,NI,PT,RU)2(RU,NI,VA)1
AL3NI5	Ga3Pt5	oS16	Cmmm		65	(AL)0.375(NI,PT)0.625
AL3PD	Al3Pd	oP*	Pna2_1		33	(AL)3(PD)1
AL3PD2	Al3Ni2	hP5	P-3m1	D5_19	164	(AL,PD)3(AL,PD)2
AL3PD5	Ge3Rh5	oP16	Pbam		55	(AL)3(PD)5
AL3PT5	Ge3Rh5	oP16	Pbam		55	(AL)0.375(NI,PT)0.625
AL3Y_HT	BaY3	hR36	R-3m		166	(AL)0.75(Y)0.25
AL3Y_LT	Mg3Cd	hP8	P6_3/mmc		194	(AL)0.75(Y)0.25
AL3ZR	Al3Zr	tI16	I4/mmm	D_023	139	(AL)3(HF,ZR)1
AL3ZR2	Al3Zr2	oF40	Fdd2		43	(AL)3(HF,ZR)2
AL3ZR4	Al3Zr4	hP7	P6/mmm		191	(AL)3(HF,ZR)4
AL3ZR5	Si3W5	tI32	I4/mcm	D8_m	140	(AL)3(ZR)5
AL4C3	Al4C3	hR21	R-3m	D7_1	166	(AL,SI)4(C)3
AL4CA_D13	Al4Ba	tI10	I4/mmm	D1_3	139	(AL)4(CA)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
AL4CR	mu-Al4Mn	hP574	P6_3/mmc		194	(AL)4(CR)1
AL4MN_R	lambda-Al4Mn	hP586	P6_3/mmc		194	(AL)461(MN,FE)107
AL4MN_U	mu-Al4Mn	hP574	P6_3/mmc		194	(AL)4(MN)1
AL4PD	Al4Pd	hP*	P6_322		182	(AL)4(PD)1
AL4RE	Al4Re	aP71	P-1		2	(AL)4(RE)1
AL4SIC4	Al5C3N	hP18	P6_3mc	E9_4	186	(AL)4(SI)1(C)4
AL4W	Al4W	mS30	Cm		8	(AL)4(MO,W)1
AL4ZR5	Ga4Ti5	hP18	P6_3/mcm		193	(AL)4(ZR)5
AL5CO2_D811	Al5Co2	hP28	P6_3/mmc	D8_11	194	(AL)5(CO)2
AL5FE2	Al2.8Fe	oS24	Cmcm		63	(AL,CU)5(FE,MN)23
AL5FE4	Cu5Zn8	cI52	I-43m		217	(AL,CU,FE)1
AL5MN6SI7	CrSi2	hP9	P6_222		180	(AL)5(MN)6(SI)7
AL5W	Al5W	hP12	P6_322		182	(AL)5(MO,W)1
AL62CU25FE1	*	Quasicryst				(FE)0.125(AL,CU)0.255(AL)0.62

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
3		al				
AL63MO37	*	structure unknown				(AL)63(MO)37
AL6MN	MnAl6	oS28	Cmcm	D2_h	63	(AL)6(FE,MN,RE,RU)1
AL77W23	*	structure unknown				(AL)77(W)23
AL7CU2FE	Al7Cu2Fe	tP40	P4/mnc		128	(FE,NI)1(CU)2(AL)7
AL7CU4NI	(Cu0.8Ni0.2)2.53 Al3.5	hR42	R-3m		166	(AL)1(FE,CU,NI,VA)1
AL7V	Al45V7	mS104	C2/m		12	(AL)7(V)1
AL7W3	*	structure unknown				(AL)7(W)3
AL8CR5_H	Cu5Zn8	cI52	I-43m	D82	217	(AL)8(CR)5
AL8CR5_L	Al8Cr5	hR26	R3m	D810	160	(AL)8(CR)5
AL8MN5	Al8Cr5	hR78	R3m	D810	160	(AL,TI)12(MN)5(AL,CU,MN,SI,TI)9
AL8MO3	Al8Mo3	mS22	C2/m		12	(AL)8(MO)3
AL8SIC7	*	hP16	*			(AL)8(SI)1(C)7
AL8V5	Cu5Zn8	cI52	I-43m	D8_2	217	(AL)8(V)5

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
AL9CO2	Al9Co2	mP22	P2_1/c		14	(AL)9(CO)2
AL9CR4_H	*	structure unknown				(AL)9(CR)4
AL9CR4_L	Al9Cr4	cI52				(AL)9(CR)4
ALABANDITE	NaCl	cF8	Fm-3m		225	(CA,CO,CR,CU,FE,MG,MN,Y,ZR)1(S)1
ALB12_ALPHA	AlB12-a	tP213	P4_12_12		92	(AL)1(B)12
ALBMO	MoAlB	oS12	Cmcm		63	(AL)1(B)1(MO)1
ALCCR2	AlCCr2	hP8	P6_3/mmc		194	(AL)1(C)1(CR)2
ALCR2	MoSi2	tI6	I4/mmm	C11_b	139	(AL)1(CR)2
ALCR2B2	AlFe2B2	oS10	Cmmm		65	(AL)1(CR)2(B)2
ALCR3B4	Cr3AlB4	oP8	Pmmm		47	(AL)1(CR)3(B)4
ALCU_DEL	Cu31.27 (Cu0.57Al0.43)3 Al16	hR156	R3m		160	(AL)2(CU,FE)3
ALCU_EPS	Co1.7Ge	hP6	P6_3/mmc	B82	194	(AL,CU,NI)1(CU,FE)1
ALCU_ETA	AlCu	mS20	C12/m1		12	(AL,CU)1(CU,FE,NI)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
ALCU_PRIME	Cu11.2Al8.88	oF88	Fmm2		42	(AL)2(CU)1
ALCU_ZETA	Al9Cu11	oI24/oF88	Imm2 / Fmm2		44/42	(AL)9(CU,FE)11
ALCU3MN2	MgCu2	cF24	Fd-3m	C15	227	(AL)1(MN)2(CU)3
ALFESI_ALPHA	*	h*	P6_3/mmc		194	(AL)0.6612(FE)0.19(SI)0.0496(AL,SI)0.0992
ALFESI_BETA		mS52	A2/a		15	(AL)14(FE)3(SI)3
ALFESI_DELTA		tI24/oP24	I4/mcm / Pbcn		140/60	(AL)0.55(FE)0.15(SI)0.3
ALFESI_GAMMA	*	m*	*			(AL)3(FE)1(SI)1
ALFESI_TAU1		aP1	P-1		2	(AL)2(FE)2(SI)1
ALFESI_TAU3		o*	Cmma		67	(AL)2(FE)1(SI)1
ALM3C_E21	CaTiO3	cP5	Pm-3m		221	(AL)1(CO,FE)3(C)1
ALMG_BETA	Al45Mg28	cF1832	Fd-3m		227	(AL)89(MG)
ALMG_EPSILON	Al30Mg23	hR53	R-3		148	(AL)30(MG)23
ALMNSI_T6	*	structure unknown				(AL,MN)4(SI)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
ALMNSI_T8	Mn3Al10	hP26	P6_3/mmc		194	(MN,VA)6(MN,VA)2(AL)12(AL,SI)6(AL,SI)2
ALMO	W	cI2	Im-3m	A2	229	(AL,MO)1(AL,MO)1
ALN_B4	ZnO	hP4	P6_3mc	B4	186	(AL)1(N)1
ALNTI2	AlCCr2	hP8	P6_3/mmc		194	(AL)1(N)1(TI)2
ALNTI3	CaTiO3	cP5	Pm-3m	E21	221	(AL)1(N)1(TI)3
ALPD2	Co2Si	oP12	Pnma	C23	62	(AL,NI,PD)1(AL,NI,PD)2
ALPHA_B19	AuCd	oP4	Pmma	B19	51	(MO,NB,PD,PT,TI,V,ZR)1(MO,NB,PD,PT,TI,V,ZR)1
ALPHA_PD2SI	Fe2P	hP9	P-62m		189	(PD,SI)2(SI)1
ALPHA_PT17SI8	Ni12P5	tI34	P4/n		85	(PT)17(SI)8
ALPHA_PT2SI	ThH2	tI6	I4/mmm	L2b	139	(PT)2(SI)1
ALPHA_PT3SI	GePt3	mC16	C12/m1		12	(PT)3(SI)1
ALPHA_SPINEL	Mn3O4	tI28	I4_1/amd		141	(CO+2,MG+2,MN+2,MN+3,NI+2)1(AL+3,CR+3,FE+3,MN+2,MN+3,VA)224
ALPT	FeSi	cP8,	P2_13	B20	198	(AL)0.5(NI,PT)0.5
ALPT2	Co2Si-b	oP12,	Pnma	C23	51	(AL)0.33333(NI,PT)0.66667

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
ALRE	CuTi-gamma	tP4	P4/nmm	B11	129	(AL)1(RE)1
ALRE2	CuZr2	tI6	I4/mmm	C11_b	139	(AL)1(RE)2
ALTI3_D019	CdMg3	hP8	P6_3/mmc	D0_19	194	(AL,CO,CR,MN,MO,NI,PT,TA,TI,W)3(AL,CR,MO,NB,NI,PT,TA,TI)1
ALZR	TlI / CrB	oS8	Cmcm	B33	63	(AL)1(HF,Y,ZR)1
ALZR2	Ni2In	hP6	P6_3/mmc	B82	194	(AL)1(Y,ZR)2
ANDALUSITE	Al2(SiO4)O	oP32	Pnnm		58	(AL+3)1(AL+3)1(SI+4)1(O-2)
ANHYDRITE	CaSo4	oS24	Cmcm		63	(CA+2,CO+2,CU+2,FE+2,MN+2,NI+2)1(SO4-2)1
ANILITE	Cu7S4	oP44	Pnma		62	(CU)1.75(S)1
ANORTHITE	Ca(Al0.5Si0.5)4O8	aP52/aP104	P-1		2	(CA+2)1(AL+3)2(SI+4)2(O-2)5
APATITE	La4.67(SiO4)3O	hP42	P6_3/m		176	(CA+2,Y+3,ZR+4,VA)4(Y+3)6(SIO4-4)6(O-2,VA)2
B11	CuTi	tP4	P4/nmm	B11	129	(CO,CU,NI,PD,TI)1(CU,NI,TA,TI)1
B12ZR	UB12	cF52	Fm-3m	D2F	225	(B)12(Y,ZR)1
B2O3	B2O3	hP15	P3_121		152	(B2O3)1
B2PD5	Mn5C2	mS28	C2/c		15	(B)2(PD)5

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
B2PT3	PtB0.67	oS8	Cmcm		63	(B)2(PT)3
B3SI	B4C	hR15	R-3m	D1G	166	(B)6(SI)2(B,SI)6
B4C	B13C2	hR15	R-3m	D1G	166	(B11C,B12)1(B2,C2B,CB2)1
B4TA3_D7B	Ta3B4	oI14	Immm	D7B	71	(B)4(CR,HF,MN,NB,TA,TI,V)3
B5W2_X	Mo2B5	hR21	R-3m	D8i	166	(B,C,VA)5(W)2
B6SI	B6Si	oP280	Pnnm		58	(B)210(SI)23(B,SI)48
B9W2	BW4	hP20	P-3		147	(B)9(W)2
BCC_A2	W	cI2	Im-3m	A2	229	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI)13
BCC_B2	CsCl	cP2	Pm-3m	B2	221	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI)0.50.53
BCT_D022	Al3Ti	tI8	I4/mmm	D0_22	139	(AL,CR,FE,MO,NB,NI,PD,PT,TI,V)3(AL,CR,MO,NB,NI,PD,PT,TA)1
BETA_PD2SI	Fe2P	hP9	P-62m	C22	189	(PD,SI)2(SI)1
BETA_PT17SI8	Ni12Pd5	tI34	I4/m		87	(PT)17(SI)8
BETA_PT2SI	Fe2P	hP9	P-62m	C22	189	(PT)2(SI)1
BETA_PT3SI	Pt3Si	oP16	C2/m	D011	12	(PT)3(SI)1
BETA_RHOMBO_B	beta-B	hR105	R-3m		166	(B)93(B,C,CU,SI)12

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
BM	FeB	oP8	Pnma	B27	62	(B,PT)1(CR,FE,HF,MN,MO,TI,Y)1
BN_B4	ZnS	hP4	P6_3mc	B4	186	(B)1(N)1
BNSI	B	hR12	R-3m		166	(B)61(SI)1(B,SI)8
BPD3	Fe3C	oP16	Pnma	D011	62	(B)1(PD)3
BPD5	UCl5	m*	P21/n		14	(B)1(PD)5
BPD6	Pd6B	mS28	C12/c1		15	(B)1(PD)6
BPT2	MoS2	hP6	P6_3/mmc	C7	194	(B)1(PT)2
BPT3	*	c*	*			(B)1(PT)3
BW_ALPHA	MoB	tI16	I4_1/amd	Bg	141	(B,C,VA)1(W)1
BW_BETA	BCr	oS8	Cmcm	B33	63	(B,C,VA)1(W)1
C12A7	Al14Ca12O33	cI152	I-43d		220	(CA+2)6(AL+3)6(AL+3,FE+3)1(O-2)
C13A6Z2	Ca7ZrAl6O18	oP104	Pmn2_1		31	(CA+2)13(AL+3)12(ZR+4)2(O-2)35
C14_LAVES	MgZn2	hP12	P63/mmc	C14	194	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,SI,RE,RU,TA,TI,V,W,Y,ZR)2 (AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,SI,RE,RU,TA,TI,V,W,Y,ZR)1
C15_LAVES	Cu2Mg	cF24	Fd-3m	C15	227	(AL,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,SI,RE,RU,TA,TI,V,W,Y,ZR)0.33 (AL,CO,CR,CU,FE,HF,MG,MO,NB,NI,SI,RE,RU,TA,TI,V,W,Y,ZR)0.67

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
C16_THETA	CuAl2	tI12				(AL,HF,MO,NB,TA,TI,W,ZR)2(AL,CO,CR,CU,FE,NI,SI)1
C1A1	Al2CaO4	mP84	P2_1/c		14	(CA+2)1(AL+3)2(AL+3,FE+3)4(O-2)
C1A1F2	*	*	*			(CA+2)1(AL+3)1(FE+3)2(AL+3,FE+3)3(O-2)10
C1A2	Al4CaO7	mC48	C2/c		15	(CA+2)1(AL+3)4(AL+3,FE+3)7(O-2)
C1A6	Fe12PbO19	hP64	P6_3/mmc		194	(CA+2)1(AL+3,FE+3)12(O-2)19
C2CA1_S	CaC2	tI6	I4/mmm	C11_a	139	(C2CA1)1
C2CA1_S2	CaC2	cF36	Fm-3m		225	(C2CA1)1
C2F	Ca2Fe2O5	oP36	Pnma		62	(CA+2)2(AL+3,FE+3)2(O-2)5
C36_LAVES	MgNi2	hP24	P6_3/mmc		194	(AL,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,TA,TI,W,ZR)2(AL,CO,CR)1
C3A1	Ca3Al2O6	cP264	Pa-3		205	(CA+2)3(AL+3,FE+3)2(O-2)6
C4WF4	Ca4Fe9O17	mS60	C2		5	(CA+2)4(FE+2)1(FE+3)8(O-2)
C4WF8	Sr2Fe2O5	oI44	Imma		74	(CA+2)4(FE+2)1(FE+3)16(O-2)17
CA15CU18O35	Ca4.8Cu6O11.6	mP92	P2/c		13	(CA+2)15(CU+2)14(CU+3)4(O-2)35
CA2ALNBO6			P121/n1		14	(CA+2)2(AL+3)1(NB+5)1(O-2)6

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
CA2CU	Ca2Cu	oP12	Pnma		62	(CA)2(CU)13
CA2CUO3	Sr2CuO3	oI12	Immm		71	(CA+2)2(CU+2)1(O-2)3
CA2NB2O7	La2Ti2O7	mP44	P2_1		4	(CA+2)2(NB+5)2(O-2)7
CA2NI7	Co7Gd2	hR18	R-3m		166	(CA)2(NI)7
CA2SI_C37	Co2Si	oP12	Pnma		62	(CA)2(SI)1
CA2SIO4_ALPHA	Ca2SiO4	hP24	P6_3/mmc		194	(CA+2,MN+2,Y+3)2(CA+2,VA)1(SIO4-4)4
CA2SIO4_ALPHA_PRIME	K2CoCl4	oP84	Pna21		33	(CA+2,FE+2,MN+2,Y+3)2(CA+2,VA)1(SIO4-4)4
CA2ZRSI4O12	Ca2ZrSi4O12	mP38	P2_1/m		11	(CA2ZRSI4O12)1
CA3CO2O6	Ca3Co2O6	hR66	R-3c		167	(CA+2)3(CO+3,CU+2)2(O-2,VA)6
CA3CO4O9	Ca2Co2.62O6.24	mS30	C2/m		12	(CA+2)3(CO+3,CU+2)4(O-2,VA)9
CA3COAL4O10	Ca3ZnAl4O10	oP72	Pca2_1		29	(CA+2)3(CO+2)1(AL+3)4(O-2)10
CA3NB2O8	Ca3Nb2O8?	hR*	space group unknown			(CA+2)3(NB+5)2(O-2)8
CA3S3FE4OX	*	*	*			(CA+2)3(S-2)3(FE+2,FE+3)4(O-2,VA)6

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
CA3Y2SI3O12			Pnma		62	(CA+2)3(Y+3)2(SI+4)3(O-2)12
CA3Y2SI6O18	(Ca0.6Y0.4)Si6O18	mS116	C2/c		15	(CA+2)3(Y+3)2(SI+4)6(O-2)18
CA3ZRSI2O9	Ca3Hf(Si2O7)O2	mP60	P2_1/c		14	(CA3ZRSI2O9)1
CA4NB2O9_HT11	Ca(Ca0.5Nd0.5)NbO6	mP20	P2_1/c		14	(CA+2)6(CA+2,NB+5)3(NB+5)3(O-2,VA)3(O-2)15
CA4NB2O9_LT21	Ca4Nb2O9	mP60	P2_1/c		14	(CA+2)6(CA+2,NB+5)4(CA+2)2(O-2,VA)3(O-2)15
CA6ZR19O44	*	hR*	*			(CA+2)6(ZR+4)19(O-2)44
CAB6	CaB6	cP7	Pm-3m	D2_1	221	(CA)1(B)6
CACR2O4_A	SrCr2O4	oP28	Pmmn		59	(CA+2)1(AL+3,CR+3,FE+3)2(O-2)4
CACRSI4O10	BaFeSi4O10	tP64	P4/ncc		130	(CA+2)1(CR+2)1(SI+4)4(O-2)10
CACU	CaCu	mP20 / oP40	P12_1/m1 / Pnma		11 / 62	(CA)1(CU)23
CACU2O3	Ca0.87Cu2.13O2.93	oP14	Pmmn		59	(CA+2)1(CU+2)2(O-2)3
CACU5_D2D	CaCu5	hP6	P6/mmm	D2_d	191	(CA)1(CU)5
CAMN2O4	CaMn2O4	oP28	Pbcm		57	(CA+2)1(MN+3)2(O-2)4

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
CAMO3	GdFeO3					(CA+2,Y+3)1(MN+4,Y+3,ZR+4)1(O-2)3
CANI2	Cu2Mg	cF24	Fd-3m	C15	227	(NI)2(CA)1
CANI3	Ni3Pu	hR12	R-3m		166	(CA)0.25(NI)0.75
CANI5	CaCu5	hP6	P6/mmm	D2D	191	(CA)1(NI)5
CASFEO	*	*	*		186?	(CA+2)2(S-2)2(FE+2,FE+3)2(O-2,VA)3
CASI_B33	CrB	oC8	Cmcm	B33	63	(CA)1(SI)1
CASI2_C12	CaSi2	hR6	R-3m	C12	166	(CA)1(SI)2
CASO4_HT	CePO4	hP18	P6_222		180	(CA+2,CO+2)1(SO4-2)1
CAV2O4	CaV2O4	oP28,	Pnma		62	(CA+2)1(AL+3,CR+3,FE+3,Y+3)2(O-2)4
CAY4O7	(Ca0.25Gd0.75)4GdO7	mS48	C2/m		12	(CA+2)1(Y+3)4(O-2)7
CAYAL3O7	(Ca0.5La0.5)2Ga3S7	tP24	P-42_1m		113	(CA+2)1(Y+3)1(AL+3)3(O-2)7
CAYALO4	K2NiF4	tI14	I4/mmm		139	(CA+2)1(Y+3)1(AL+3)1(O-2)4
CAZR4O9	CaZr4O9	mS224,	C12/c1		15	(CA+2)1(ZR+4)4(O-2)9
CAZRO3_C	CaTiO3	cP5,	Pm-3m		221	(CA+2,Y+3)1(Y+3,ZR+4)1(O-2)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
CBCC_A12	alpha-Mn	cI58	I-43m	A12	217	(AL,CO,CR,CU,FE,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W,Y,ZR)1(B)1
CEMENTITE	Fe3C	oP16	Pnma	D011	62	(CO,CR,FE,MN,MO,NI,V,W)3(C,N)1
CF2	Ca3.5Fe14O24.5	mS172	C2		5	(CA+2)1(FE+3)4(O-2)7
CFC2_FENBZR	MgCu2	cF24	Fd-3m		227	(FE,NB,ZR)2(NB,ZR)1(NB,ZR)3
CHALCOCITE_ALPHA	Cu2S-alpha	mP144	P2_1/c		14	(CU)2(S)1
CHALCOCITE_BETA	Cu2S-beta	hP16	P6_3/mmc		194	(CU)2(S)1
CHALCOPYRITE	CuFeS2	tI16	I-42d	E1_1	122	(CU,FE,VA)1(CU,VA)1(S)1
CHI_A12	a-Mn	cI58		A12	217	(CR,FE,NI,RE)24(AL,CR,HF,MO,NB,TA,TI,W,ZR)10(CR,FE,MO,NB)24
CLINO_PYROXENE	CaMgSi2O6	MS40	C2/c		15	(CA+2,FE+2,NI+2)1(CO+2,FE+2,NI+2)1(SI+4)2(O-2)
CO10CU57TI33	MoSi2	tI6	I4/mmm		139	(CO)0.1(CU)0.57(TI)0.33
CO11ZR2	Co11Zr2?	oP*	Pban		50	(CO)11(ZR)2
CO17Y2	Th2Zn17/Ni17Th2	hR19/hP38	R-3m/P6_3/mmc		166/191	(CO2 Y)1(CO2 Y)2(CO)156
CO2SI_C23	Co2Si	oP12	Pnma		62	(CO,CR,CU,FE,NI,TI)2(SI)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
CO3AL2B5	*	*	*			(CO)3(AL)2(B)5
CO3SI	CdMg3	hP8	P6_3/mmc		194	(CO)3(SI)1
CO3V	Al3Pu	hP24	P6_3/mmc		194	(CO,V)3(CO,V)1
CO3Y	Ni3Pu	hR12	R-3m		166	(CO)3(Y)1
CO3Y2	*	cP*				(CO)3(Y)2
CO3Y4	Co3Ho4	hP22	P6_3/m		176	(CO)3(Y)4
CO5Y_D2D	CaCu5	hP6	P6/mmm	D2D	191	(CO2 Y)1(CO)4(CO VA)1
CO5Y8	Co5Y8	mP52	P2_1/c		14	(CO)5(Y)8
CO7HF	Co7Hf?	oP*	Pban		50	(CO)7(HF)1
CO7M2	AuCu3/Co7Nb2	cP4/mS18	Pm-3m / C12/m1		221 / 12	(CO)7(NB,TA)2
CO7Y6	*	structure unknown				(CO)7(Y)6
CO9S8	Co9S8	cF68	Fm-3m		225	(CO,FE,NI)9(S)8
COB	FeB	oP8	Pnma	B27	62	(CO,RE)1(B)1
CORUNDUM	Al2O3	hR30	R-3c	D51	167	(AL+3,CR+2,CR+3,FE+2,FE+3,MN+3,TI+3,V+3)2(CR+3,FE+3,NI+2,VA)13

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
COVELLITE	CuS	hP12	P6_3/mmc	B18	194	(CU)1(S)1
COY_BF	CrB	oC8	Cmcm	B33	63	(CO)1(Y)1
CR1S1	CrS	mS8	C12/C1		15	(CR)1.03(S)1
CR2B_ORTH	Mg2Cu	oF48	Fddd	C_b	70	(CR,FE,MO,RE)0.66666667(B)0.33333333
CR2NI2SI	NiTi2	cF96	Fd-3m		227	(CR)5(NI)5(SI)3
CR2S3	Cr2S3	hP20/hR10	P-31c / R-3		163 / 148	(CR,FE)2(S)3
CR3MN5	a-Mn?	cI58	*			(CR)3(MN)5
CR3NI5SI2	AlAu4	cP20	P2_13		198	(CR)3(NI)5(SI)2(C,VA)1
CR3S4	Cr3S4	mS14	C2/m		12	(CR,FE,MN,NI)3(S)4
CR3SI_A15	Cr3Si	cP8	Pm-3n	A15	223	(CR,FE,MO,NB,NI,PD,PT,RE,SI,TA,TI,V)3(AL,CO,CR,MO,NB,NI)1
CR5B3	CR5B3	tI32	I4/mcm	D8L	140	(CR,MO)0.625(B)0.375
CR5S6	Cr5S6	hP22	P-31c		163	(CR)5(S)6
CR7S8	Cr7Se8	mS30	C2/m		12	(CR)7(S)8
CRB4	CrB4	oI10	Immm		71	(CR)0.2(B)0.8
CRISTOBALITE	SiO2	tP12/cF24	P4_12_12 / Fd-	*/C9	92/227	(SIO2)

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
			3m			
CRNBSI	ZrNiAl	hP9	P-62m		189	(CR)1(NB)1(SI)1
CRNI2_OP6	Mg?	hP2?	P6_3/mmc?		194?	(CR,MO,W)1(MO,NI,W)2
CRSI2_C40	CrSi2	hP9	P6_222	C40	180	(CR,CU,HF,MO,NB,SI,TA,V)1(AL,CR,CU,SI)2
CU10HF7	Ni10Zr7	oS68	Cmce		64	(CU)10(HF)7
CU10ZR7	Ni10Zr7	oS68	Cmce		64	(CU)10(ZR)7
CU15SI4_EPSILON	Cu15Si4	cI76	I-43d	D8_6	220	(CU,MN)0.789474(AL,SI)0.210526
CU2SO4	Cu2SO4	oF56	Fddd		70	(CU+1)2(SO4-2)1
CU2SO5	Cu2(SO4)O	mS32	C12/m1		12	(CU2O5S1)1
CU2TI	Au2V	oS12	Cmcm		63	(CO,CU,NI)2(TI)1
CU2TIZR	Cu2TiZr	hP12	P6_3/mmc		194	(CU)0.5(TI)0.25(ZR)0.25
CU2Y_H	*	hP*				(CU)2(Y)1
CU2Y_L	Hg2K	oI12	Imma		74	(CU)2(Y)1
CU33SI7_DELTA	*	tP*	structure unknown			(CU)0.825(SI)0.175

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
CU3TI2	Cu3Ti2	tP10	P4/nmm		129	(CU,NI,FE)3(CO,TI)2
CU46NI25SI29	*	*	*			(CU)0.458(NI)0.25(SI)0.292
CU4TI1	Au4Zr	oP20	Pnma		62	(CU,TI)4(CU,TI)1
CU4TI3	Cu4Ti3	tI14	I4/mmm		139	(CO,CU,NI)4(TI)3
CU4Y	Cu5Y1.25	mP16	P21/m:a		11	(CU)4(Y)1
CU51HF14	Ag51Gd14	hp68	P6/m		175	(CU)51(HF)14
CU51ZR14	Ag51Gd14	hp68	P6/m		175	(CU)51(ZR)14
CU56SI11_GAMMA	Mg3Ru2	cP20	P4_132	A13	213	(CU,MN,NI,SI)0.835821(SI)0.164179
CU5MN4SI	*	*	*			(CU)0.5(MN)0.37(SI)0.13
CU6NISI3	*	*	*			(CU,NI)0.732(SI)0.268
CU7Y1	Cu5.44Tb0.78	hP8	P6/mmm		191	(CU2,Y)1(CU)5
CU7Y2	Ag51Gd14	hP68	P6/m		175	(CU)7(Y)2
CU8HF3	Cu8Hf3	oP44	Pnma		62	(CU)8(HF)3
CU8ZR3	Cu8Hf3	oP44	Pnma		62	(CU)8(ZR)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
CUB_A13	beta-Mn	cP20	P4_132	A13	213	(AL,CO,CR,CU,FE,HF,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W,Y,ZR)11
CUCRS2	CuCrS2	hR12/hR15	R3m		160	(CU)1(CR)1(S)2
CUFES2_LT	CuFeS2	tI16	I-42d	E1_1	122	(CU)1(FE)1(S)2
CUMG2	CuMg2	oF48	Fddd	C_b	70	(CU,NI)1(MG)2
CUO	CuO	mS8	C2/c	B26	15	(CU+2)1(O-2)1
CUPRITE_C3	Cu2O	cP6	Pn-3m	C3	224	(CU+1)ö(O-2)1
CUPT_L11	CuPt	hR6	R-3m		166	(CU,PT)0.5(CU,PT)0.5(VA)1
CUSI_ETA	Cu3Si	oS*/hR27/hR*	* / R-3 / R-3m		* / 148 / 166	(CU,MN,NI)0.76(SI)0.24
CUTI3	CuTi3	tP4	P4/mmm	L6_0	123	(CU,TI)1(TI)3
CW3F	CaFe5O7	oS52	Cmcm		63	(CA+2)1(FE+2)3(FE+3)2(O-2)
CWF	CaFe3O5	oS36	Cmcm		63	(CA+2)1(FE+2)1(FE+3)2(O-2)7
D0l_MO2B5	Mo2B5	hR21	R-3m	D8i	166	(MO)0.32(B)0.68
D5A_M3B2	Si2U3	tP10	P4/mbm	D5_a	127	(FE,HF,MO,NB,TA,V)3(B)2
DIAMOND_A4	C	cF8	Fd-3m	A4	227	(AL,B,C,O,SI)5

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
DIGENITE	Cu2Se-beta	cF44	Fm-3m		225	(CU,FE,MG,MN,VA)2(CU,VA)1(S)1
DIS_FCC_A1	Cu	cF4	Fm-3m	A1	225	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA)11
DIS_MU	Fe7W6	hR13	R-3m	D85	166	(AL,CO,CR,CU,FE,MN,MO,NB,NI,RE,TA,TI,W)1
DIS_SIG	CrFe	tP30	P4_2/mnm	DB8	136	(AL,CO,CR,FE,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W)1
DJURLEITE	Cu31S16	mP376	P2_1/c		14	(CU)1.93(S)1
FCC_A1	Cu	cF4	Fm-3m	A1	225	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI)11
FCC_L10	AuCu	tP2	P4/mmm	L1_0	123	(AL,CR,CU,MN,MO,NI,PD,PT,TA,TI,W)0.5(AL,CR,CU,MN,MO,NI,PD,PT,TA)0.5
FCC_L12	AuCu3	cP4	Pm-3m	L1_2	221	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI,V)0.750.251
FE2O12S3	Fe2S3O12	hR102	R-3		148	(AL+3,CR+3,FE+3)2(SO4-2)3
FE2SI	AlNi2	hP6	P-3m1		164	(FE)0.67(SI)0.33
FE4N_LP1	Fe4N	cP5	Pm-3m	L'1	221	(CO,CR,FE,MN,NI)4(C,N)10.46
FE8SI2C	Mn8Si2C3	aP*	P1		1	(FE)8(SI)2(C)1
FEAL2S4	ZnIn2S4	hR21	R3m		160	(FE)1(AL)2(S)4
FECN_CHI	Mn5C2	mS28	C2/c		15	(FE)2.2(C,N)1
FESI_B20	FeSi	cP8	P2_13		198	(CO,CR,FE,MN,NI,RE)1(AL,SI)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
FESI2_H	FeSi2-h	oC48	Cmca		64	(FE)0.3(SI)0.7
FESI2_L	FeSi2-l	tP3	P4/mmm		123	(FE)0.33(SI)0.67
FEWB	NiSiTi	oP12	Pnma	C37	62	(FE)1(W)1(B)1
FLUORITE_C1	CaF2	cF12	Fm-3m	C1	225	(AL+3,CA+2,CR+3,FE+2,HF+4,MN+2,MN+3,NI+2,TI+4,Y+3,ZR)24
G_PHASE	Mn23Th6	cF116	Fm-3m	D8A	225	(AL,CO,FE,MN,NI,TI)16(HF,NB,TI,Y,ZR)6(CO,FE,MN,NI,SI)7
GAMMA_D83	Cu9Al4	cP52	P-43m	D83	215	(AL,NI,SI)4(AL,CU,NI,SI)1(CU,FE,MN,NI)8
GAMMA_H	Cu5Zn8	cI52	I-43m	D8_2	217	(AL)4(AL,CU)1(CU,FE,MN,NI)8
GARNET	Ca3(Al0.8Fe0.2)2(SiO4)3	cF320	Fddd		70	(CA+2,MN+2)3(AL+3,CR+3)2(SI+4)3(O-2)12
GAS						(AL, AL1B1O2, AL1C1, AL1C2, AL1CU1, AL1CU1S1, AL1CU1S2, AL1H1, AL1H1O1_ALOH, AL1H1O1_HALO, AL1H1O2, AL1H2, AL1H2O2, AL1H3, AL1H3O3, AL1N1, AL1O1, AL1O2, AL1S1, AL1S2, AL2, AL2C2, AL2O1, AL2O2, AL2O3, AL2S1, AL2S2, AR, B, B10H14, B1C1, B1C2, B1H1, B1H1O1_BOH, B1H1O1_HBO, B1H1O2, B1H2, B1H2O1, B1H2O2, B1H3, B1H3O1, B1H3O2, B1H3O3, B1H6N1, B1N1, B1O1, B1O2, B2, B2C1, B2H4O4, B2H6, B2O1, B2O2, B2O3, B3H3O3, B3H3O6, B3H6N3, B5H9, C, C1H1, C1H1N1O1, C1H1N1_HCN, C1H1N1_HNC, C1H1O1, C1H1O2, C1H2, C1H2N4, C1H2O1, C1H2O2_CIS, C1H2O2_DIOXIRANE, C1H2O2_TRANS, C1H3, C1H3O1_CH2OH, C1H3O1_CH3O, C1H4, C1H4N2O1, C1H4O1, C1H5N1, C1N1, C1N1O1, C1N1O1_NCO, C1N2_CNN, C1N2_NCN, C1O1, C1O1S1, C1O2, 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, C2H6O1SI1, C2H6O2, C2H8SI1, C2N1_CCN, C2N1_CNC, C2N2, C2O1, C2SI1, C2SI2, C2SI3, C3, C3H1, C3H1N1, C3H4_1, C3H4_2,

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
						C3H6O1, C3H6_1, C3H6_2, C3H8, C3N1, C3O2, C4, C4H1, C4H10_1, C4H10_2, C4H12SI1, C4H2_1, C4H2_2, C4H4_1, C4H4_2, C4H6_1, C4H6_2, C4H6_3, C4H6_4, C4H6_5, C4H8_1, C4H8_2, C4H8_3, C4H8_4, C4H8_5, C4H8_6, C4N1, C4N2, C4NI1O4, C5, C5FE1O5, C5H1N1, C5N1, C60, C6H6, C6H6O1, C6MO1O6, C6N1, C6N2, C9N1, CA, CA1O1, CA1S1, CA2, CO, CO1H1, CO1H1O1, CO1H2O2, CO1O1, CO1S1, CO2, CR, CR1H1, CR1H1O1, CR1H1O2, CR1H1O3, CR1H2O2, CR1H2O3, CR1H2O4, CR1H3O3, CR1H3O4, CR1H4O4, CR1H4O5, CR1N1, CR1O1, CR1S1, CR1S2, CR1O2, CR1O3, CR2, CR2O1, CR2O2, CR2O3, CU, CU1H1, CU1H1O1, CU1O1, CU1S1, CU2, CU2S1, FE, FE1H1, FE1H1O1, FE1H1O2, FE1H2O2, FE1O1, FE1S1, FE1O2, FE2, H, H1MN1, H1MN1O1, H1MO1O1, H1MO1O2, H1MO3, H1N1, H1N1O1, H1N1O2_CIS, H1N1O2_TRANS, H1N1O3, H1N3, H1NI1, H1NI1O1, H1O1, H1O1W1, H1O2, H1O2W1, H1PT1, H1SI1, H1ZR1, H2, H2MO1O2, H2MO1O3, H2MO1O4, H2N1, H2N2O2, H2N2_1_1N2H2, H2N2_CIS, H2N2_TRANS, H2NI1O2, H2O1, H2O2, H2O2W1, H2O3W1, H2O4W1, H2SI1, H3N1, H3N1O1, H3SI1, H4N2, H4SI1, H6SI2, HF, HF1O1, HF1O2, MN, MN1O1, MN1S1, MN1O2, MO, MO1N1, MO1O1, MO1O2, MO1O3, MO1S1, MO1S2, MO2, MO2O6, MO3O9, MO4O12, MO5O15, N, N1NB1, N1O1, N1O2, N1O3, N1SI1, N1SI2, N1TI1, N1V1, N1ZR1, N2, N2O1, N2O2, N2O3, N2O4, N2O5, N3, NB, NB1O1, NB1O2, NB1S1, NI, NI1O1, NI1S1, NI2, O10V4, O12W4, O15W5, O1PD1, O1PT1, O1RE1, O1RU1, O1S1, O1S2, O1SI1, O1TA1, O1TI1, O1V1, O1W1, O1Y1, O1Y2, O1ZR1, O2, O2PT1, O2RE1, O2RU1, O2S1, O2SI1, O2SI2, O2TA1, O2TI1, O2V1, O2W1, O2Y1, O2Y2, O2ZR1, O3, O3RE1, O3RU1, O3W1, O4RU1, O6RE2, O3S1, O6W2, O7RE2, O8W3, O9W3, PD, PT, RE, RU, S, S1SI1, S1Y1, S1ZR1, S2, S2SI1, S2ZR1, S3, S4, S5, S6, S7, S8, SI, SI2, SI3, TA, TI, TI2, V, W, Y, ZR, ZR2)
GRAPHITE	C	hP4	P6_3/mmc	A9	194	(B,C)1
H_L21	AlCu2Mn	cF16	Fm-3m	L2_1	225	(AL,CR,NI,TI)0.5(AL,HF,NB,NI,TA,TI,ZR)0.5(CO,NI,RU,VA)1
HALITE	NaCl	cF8	Fm-3m	B1	225	(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,ZR+4,Y+3)1(O-2,VA)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
HATRURITE	Ca3(SiO4)O-b	hR81	R3m		160	(CA+2,Y+3,VA)3(SIO4-4)1(O-2)5
HCP_A3	Mg	hP2	P6_3/mmc	A3	194	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V)10.5
HEAZLEWOODITE	Ni3S2	hR15	R32	D5_e	155	(CO,FE,NI,VA)2(S)1
HEAZLEWOODITE_B2	Cu1.9S	cF12	F-43m		216	(FE,NI,VA)2(S)1
HF2PD	MoSi2	tI6	I4/mmm	C11B	139	(HF)2(PD)1
HF3NI7	Hf3Ni7	aP20	P-1		2	(HF)0.3(NI)0.7
HF3PD4	*	structure unkown				(HF)3(PD)4
HF8NI21	Hf8Ni21	aP29	P-1		2	(HF,ZR)8(NI)21
HFMN	NiTi2	cF96	Fd-3m		227	(HF)0.5(MN)0.5
HFNI_ALPHA	TiI	oS8	Cmcm		63	(HF)0.5(NI)0.5
HFNI3_ALPHA	Ta (Rh0.33Pd0.67)3	hP40	P6_3/mmc		194	(HF)0.25(NI)0.75
HFNI3_BETA	BaPb3	hR36	R-3m		166	(HF)0.25(NI)0.75
HFPD2	MoSi2	tI6	I4/mmm	C11B		(HF)1(PD)2
HFRE	Zr21Re24?	hR276	R-3c		167	(HF)1(RE)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
HFSIO4	HfSiO4?	tI*	I4_1/amd		141	(HF+4)1(SI+4)1(O-2)4
HIGH_SIGMA	CrFe	tP30	P4_2/mnm		136	(MN)8(CR)4(CR,MN)18
IONIC_LIQ						(AL+3,CA+2,CO+2,CR+2,CU+1,FE+2,HF+4,MG+2,MN+2,MO+4,NB+2)11
KYANITE	Al2SiO5	aP32	P-1		2	(AL+3)1(AL+3)1(SI+4)1(O-2)
LAAP	LaAlO3	hR30	R-3c		167	(CA+2,Y+3)1(AL+3,CO+3,CU+2,FE+3,NI+2)1(O-2,VA)3
LARNITE	CaSiO3	mP60	P2_1/n		14	(CA+2)2(SI+4)1(O-2)4
LIQUID						(AL,AL1N1,B,C,CA,CO,CR,CU,FE,HF,MG,MN,MO,N,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W,Y,ZR)1
M11SI8	Cr8Nb3Si8	oP76	Pnma		62	(CR,NB)11(SI)86
M12C	W6Fe6C	cF104	Fd-3m		227	(CO,NI)6(MO,W)6(C)1
M23C6	Cr23C6	cF116	Fm-3m	D84	225	(CO,CR,FE,MN,NI,RE,V)20(CO,CR,FE,MN,MO,NI,RE,V,W)3(C)6
M2B_TETR	Al2Cu	tI12	I4/mcm	C16	140	(AL,CO,CR,FE,MN,MO,NB,NI,RE,TA,W)2(B)1
M2O3A	A-LA2O3?	hP5	P-3m1	D5_2	164	(CA+2,MG+2,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1
M2O3B	B-Sm2O3	mS30	C2/m		12	(AL+3,CA+2,CO+3,MG+2,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1
M2O3C	(Mn0.5Fe0.5)2O3	cI80	Ia-3	D53	206	(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)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
M2O3H	La2O3	hP5	P-3m1	D52	164	(CA+2,MG+2,MN+3,Y,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1
M2O3X	X-LA2O3	Ia3	Im-3m		229	(CA+2,MG+2,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1
M3B2	Mo2FeB2	tP10	P4/mbm	D5A	127	(CR,FE,MO,NI,W)0.4(CR,FE,NI)0.2(B)0.4
M3C2	Cr3C2-b	oP20	Pnma	D510	62	(CO,CR,MO,V,W)3(C)2
M3SI1	Ti3P	tP32	P4_2/n		86	(HF,NB,TA,TI,ZR)3(SI)1
M3SI2_D5A	Si2U3	tP10	P4/mbm	D5a	127	(HF,NB,ZR)3(SI)2
M4SI3	*	*	*			(CR,NI)4(SI)3
M5C2	Mn5C2	mC28	C2/c		15	(FE,MN)5(C)2
M5SI3_D88	Mn5Si3	hP16	P6_3/mcm	D88	193	(CR,CU,FE,HF,MN,MO,NI,NB,SI,TI,Y,ZR)0.62(AL,CR,SI,TI)0.38(CR)
M6C	W3Fe3C	cF112	Fd-3m	E93	227	(CO,FE,NI)2(MO,NB,TA,W)2(CO,CR,FE,MO,NB,NI,TA,V,W)2(C)1
M6SI5	V6Si5	oI44	Ibam		72	(CR,NB)6(SI)51
M7C3	Cr7C3	oP40	Pnma	D101	62	(CO,CR,FE,MN,MO,NI,RE,V,W)7(C)3
MB_B33	CrB	oC8	Cmcm	B33	63	(CR,FE,HF,MO,NB,NI,TA,TI,V)1(B)1
MB2_C32	AlB2	hp3	P6/mmm	C32	166	(B)2(AL,CR,HF,MG,MN,MO,NB,TA,TI,V,Y,ZR)1
MC_ETA	MoC	hP12	P63/mmc	B_i	194	(MO,V,W)1(C,VA)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
MC_SHP	WC	hP2	P-6m2	B_h	187	(MO,W)1(C,N)1
MELILITE	Ca2MgSi2O7	tP24	P-42_1m		113	(CA+2)2(AL+3,CO+2,FE+2,FE+3)1(AL+3,SI+4)1(SI+4)(O-2)
MG24Y5_A12	Re25Ti5	cI58	I-43m		217	(MG)24(MG Y)4(Y)1
MG2C3	Mg2C3	oP10	Pnnm		58	(MG)2(C)3
MG2NI	Mg2Ni	hP18	P6_222	Ca	180	(MG)2(CU,NI)1
MG2SI	CaF2	cF12	Fm-3m	C1	225	(MG)2(SI)1
MG3N2_D53	Mn2O3	cI180	Ia-3	D53	206	(MG)3(N)2
MG6MN3NI	*	*	*			(MG)3(MN)1(NI)2
MGB4	MgB4	oP20	Pnma		62	(MG)1(B)4
MGB7	MgB7	oI64	Imma		74	(MG)1(B)7
MGC2	MgC2	tP6	P4_2/mnm		136	(MG)1(C)2
MN11SI19	Mn11Si19	tP120	P-4n2		118	(MN)0.37(AL,SI)0.63
MN12Y	ThMn12	hI26	I4/mmm		139	(MN)12(Y)1
MN15NI45SI40	*	structure unknown				(MN)0.15(NI)0.45(SI)0.4
MN15NI50SI35	*	structure unknown				(MN)0.15(NI)0.5(SI)0.35

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
MN1NI1SI1	NiSiTi	oP12	Pnma		62	(MN)1(NI)1(SI)1
MN2B_D1F	Mg2Cu	oF48	Fddd	C_b	70	(MN)0.6707(B)0.3293
MN2NISI	*	structure unkown				(MN,NI)3(SI)1
MN2YO5	DyMn2O5	oP32	Pbam		55	(Y+3)1(MN+3)1(MN+4)1(O-2)
MN3NI2SI	Mn3Ni2Si	cF96	Fd-3m		227	(MN)3(NI)2(SI)1
MN3PD5	Pt5Ga3	oS16	Cmmm		65	(MN)3(PD)5
MN3SI	BiF3	cF16	Fm-3m		225	(MN,FE)3(AL,SI)1
MN3TI	*	structure unkown				(MN)3(TI)1
MN4TI	Cr0.16Mo0.38Co0.46	hR159	R-3		166	(MN)0.815(TI)0.185
MN52NI29SI19	*	structure unknown				(MN)0.52(NI)0.29(SI)0.19
MN66NI4SI30	*	structure unknown				(MN)0.66(NI)0.04(SI)0.3
MN6N4	Mn3N2	tI10	I4/mmm		139	(MN)6(N)4
MN6N5	CoO	tI4	I4/mmm		139	(MN)6(N)5
MN6NI16SI7	Mg6Cu16Si7	cF116	Fm-3m		225	(MN)0.206897(NI)0.551724(SI)0.241379

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
MN6NISI3	Cr0.16Mo0.38Co0.46	hR159	R-3		148	(MN)0.61(NI)0.12(SI)0.27
MN6SI	R-(Co,Cr,Mo)	hR53	R-3		166	(AL,MN)0.86(SI)0.14
MN9SI2	Mn9Si2	oI186	Immm		71	(MN)0.82(SI)0.18
MN9SI3O14S1	*	structure unkown				(MN+2)9(SI+4)3(O-2)14(S-2)1
MNB4	MnB4	mS10	C2/m		12	(MN)0.2(B)0.8
MNNI2	*	structure unkown				(MN,NI)1(NI)2
MNNISI_T5	MgZn2	hP12	P6_3/mmc		194	(MN)1(NI,SI)2
MNNISI_T6	MgCu2	cF24	Fd-3m		227	(MN)1(NI,SI)2
MNPD2	Pt5Ga3	oS16	Cmmm		65	(MN)1(PD)2
MNPT7	CuPt7	cF32,	Fm-3m		225	(PT)6(PT)1(MN)1
MNTA	unknown structure					(MN)1(TA)1
MNTI_HT	*	t**				(MN)0.515(TI)0.485
MNTI_LT	Zr21Re25	hR276	R-3c		167	(MN)1(TI)1
MNYO3_HEX	LuMnO3	hP30	P6_3cm		185	(Y+3)1(MN+3)1(O-2)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
MO1S2	MoS2	hP6	P6_3/mmc	C7	194	(MO)1(S)2
MO2S3	Mo2S3	mP10	P2_1/m		11	(MO)2(S)3
MO3NI10B11	*	oP*				(MO)3(NI)10(B)11
MO4O11	Mo4O11	oP60	Pna2_1		33	(MO)4(O)11
MO8O23	Mo8O23	mP62	P2/c		13	(MO)8(O)23
MO9O26	Mo9O26	mP70	P2/c		13	(MO)1(O)2.889
MOB	alpha-MoB	tI16	I4_1/amd	B_g	141	(CR,FE,MO)1(B)1
MOB4	MoB4	hP16	P6_3/mmc		194	(MO)0.2(B)0.8
MOCOB	TiNiSi	oP12	Pnma		62	(MO,W)1(CO)1(B)1
MONI_DELTA	MoNi	oP56	P2_12_12_1		19	(CO,CR,FE,NI,RE)24(CO,CR,FE,MO,NI,RE,W)20(CU,MO,W)12
MONI4_BETA	MoNi4	tI10	I4/m	D1a	87	(MO,W)1(CO,NI)4
MONOCLINIC_S	beta-S	mP48	P2_1/c		14	(S)1
MOO2	VO2	mP12	P2_1/c		14	(MO)1(O)2
MOO3	WO3	mP32	P2_1/c		14	(MO)1(O)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
MOSI2_C11B	MoSi2	tI6	I4/mmm	C11B	139	(CO,CU,FE,MO,NI,PD,W)1(AL,HF,SI,TI,ZR)2
MSI_B27	FeB	oP8	Pnma	B27	62	(HF,NB,TI,Y,ZR)1(SI)1
MSI2_C1	CaF2	cF12	Fm-3m	C1	225	(CO,CU,MN,NI)1(AL,CU,SI)2
MU_PHASE	Fe7W6	hR13	R-3m	D85	166	(AL,CO,CR,CU,FE,MN,MO,NB,NI,RE,TA,TI,W)1(AL,CO,CR,CU,FE)264
MULLITE	Al3SiO6.5	oP24	Pbam		55	(AL+3)1(AL+3)1(AL+3,SI+4)1(O-2,VA)5
MZR3_E1A	Re3B	oS16	Cmcm	E1_a	63	(CO,FE,NI)1(Y,ZR)3
NB13NI75TI12	*	structure unknown				(NB)0.13(NI)0.75(TI)0.12
NB15NI56TI29	*	o*100				(NB)0.15(NI)0.56(TI)0.29
NB15NI80TI5	*	structure unknown				(NB)0.15(NI)0.8(TI)0.05
NB2O5	Nb2O5	mP99	P2/m		10	(NB)2(O)5
NB3RU5	*/CsCl	o**/cP2	?/Pm-3m		?/221	(NB,RU)0.38(RU)0.62
NB5NI75TI20	Mg3Cd	hP8	P6_3/mmc		194	(NB)0.05(NI)0.75(TI)0.2
NB8NI9TI3	*	structure unknown				(NB)0.4(NI)0.45(TI)0.15

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
NBO	NbO	cP6	Pm-3m		221	(NB)1(O)1
NBO2	NbO2	tI96	I4_1/a		88	(NB)1(O)2
NI10ZR7	Ni10Zr7	oS68	Cmce		64	(NI)23(HF,ZR)17
NI11ZR9	Pt11Zr9	tI40	I4/m		87	(NI)11(HF,ZR)9
NI17Y2	Fe17Lu2	hP80	P6_3/mmc		194	(AL,FE,NI)1(Y)0.12
NI2ALY2	W2CoB2	oI10	Immm		71	(NI)2(AL)1(Y)2
NI2SI_TETA	Ga3Ge6Ni13	hP66	P3_121		152	(CU,NI)1(NI,VA)1(AL,SI)1
NI2TA	MoSi2	tI6	I4/mmm	C11b	139	(CO,NI)2(TA TI)1
NI2V	MoPt2	oI6	Immm		71	(MO,NI,PD,PT)2(MO,NB,PT,TA,V)1
NI2Y	Ni2Tm	cF192	F-43m		216	(NI)2(Y)1
NI2Y3	Ni2Y3	tP80	P4_12_12		92	(NI)2(Y)3
NI31SI12	Ni31S12	hP42	P321		150	(CO,CR,CU,FE,NI)5(SI)2
NI3ALY2	*	*	*			(NI)3(AL)1(Y)2
NI3B_D011	Fe3C	oP16	Pnma	D011	62	(CO,CR,FE,MO,NI)3(B)1
NI3CR2B6	V5B6	oS22	Cmmm		65	(NI)3(CR)2(B)6

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
NI3S2_LT	Ni3S2	hR15	R32		155	(NI)3(S)2
NI3SI_MONOCL	Ge9Pt25	hP34	P-3		147	(NI)3(SI)1
NI3SI_ORTHO	Fe3C	oP16	Pnma	D011	62	(NI)3(SI)1
NI3SI2	Ni3Si2	oP80	Cmc2_1		36	(NI)3(SI)2
NI3TA_D0A	Cu3Ti	oP8	Pmmm		59	(AL,CO,CR,FE,NI,NB,PT)3(AL,FE,MO,NB,NI,PT,TA,TI,V,W)1
NI3TI_D024	Ni3Ti	hP16	P6_3/mmc	D024	194	(AL,CO,CR,CU,FE,HF,NI,PD,PT,TA,TI,W,ZR)0.75(AL,CR,CU,HF,MO)0.25
NI3Y	Ni3Pu	hR12	R-3m		166	(FE,NI)3(Y)1
NI4B3	m-Ni4B3	mS28	C2/c		15	(NI)0.57142857(B)0.42857143
NI4SI2B	Nb5Sn2Si	tI32	I4/mcm		140	(NI)4.29(SI)2(B)1.43
NI4Y	*	hR*				(NI)4(Y)1
NI5ALB4	*	structure unknown				(NI)5(AL)1(B)4
NI5ZR	AuBe5	cF24	F-43m	C15b	216	(AL,CU,NI)5(HF,Y,ZR)1
NI6AL2Y3	Ce3Ni6Si2	cI44	Im-3m		229	(NI)6(AL)2(Y)3
NI6MNO8	NaCl	cF8	Fm-3m	B1?	225	(NI+2)6(MN+4)1(O-2)8

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
NI6SI2B	K2UF6	hP9	P-62m		189	(NI)6(SI)2(B)1
NI7S6	*	t**				(FE,NI)7(S)6
NI7ZR2	Ni7Zr2	mS36	C2/m		12	(AL,CO,CR,NI)7(HF,Y,ZR)2
NI8ALB11	*	m**				(NI)8(AL)1(B)11
NI8ALY3	Ce3Co8Si	hP24	P6_3/mmc		194	(NI)8(AL)1(Y)3
NI8TA	Pt8Ti	tI18	I4/mmm		71	(NI)8(NB,TA)1
NI9S8	Ni9S8	oS68	C222		21	(FE,NI)9(S)8
NIAL2Y	MgCuAl2	oS16	Cmcm		63	(NI)1(AL)2(Y)1
NIALY	ZrNiAL	hP9	P-62m		189	(NI)1(AL)1(Y)1
NICR3B6	V2B3	oS20	Cmcm		63	(NI)0.1(CR)0.3(B)0.6
NIMNO3	TiFeO3	hR10	R-3		148	(MN+3,MN+4,NI+2)2(O-2)3
NIMOO4	MgWO4 / CoMoO4	mP12 / mS48	P2/c / C2/m		13/12	(NI+2)1(MO+6)1(O-2)4
NIOCALITE_C10NS6	*	oS114	C222		21	(CA+2)10(NB+5)2(SI+4)6(O-2)27
NIS_LT	NiS	hR6	C2		5	(NI)1(S)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
NISI_B31	MnP	oP8	Pnma		62	(NI,PD)1(SI)1
NITI2	NiTi2	cF96	Fd-3m		227	(CO,CR,CU,FE,NI,RE,TI)0.33(AL,CR,CU,HF,NI,TA,TI,ZR)0.67
NIWO4	AgAuTe4	mP12	P2/c		13	(CO+2,FE+2,MN+2,NI+2)1(W+6)1(O-2)4
NIZR	CrB	oS8	Cmcm	B33	63	(NI)1(TI,Y,ZR)1
OLIVINE	Mg2SiO4	oP28	Pnma		62	(CA+2,CO+2,CR+2,CU+2,FE+2,MN+2,NI+2)1(CA+2,CO+2,CR+2,CU+2)11
ORTHO_PYROXENE	MgSiO3	oP80	Pbca		61	(CA+2,FE+2)1(FE+2)1(SI+4)2(O-2)4
ORTHORHOMBIC_S	alpha-S	oF128	Fddd	A16	70	(S)6
P_PHASE	Cr9Mo21Ni20	oP56	Pnma		62	(CR,FE,NI,RE)24(CR,FE,MO,NI,RE)20(MO)12
PD11ZR9	Ni11Zr9	tP44	P4/m		83	(PD)11(ZR)9
PD14SI3	*	structure unknown				(PD)14(SI)3
PD15SI4	*	aP20	P-1		2	(PD)15(SI)4
PD16S7	Pd16S7	cI46,	I-43m		217	(PD)0.696(S)0.304
PD19SI10	*	structure unknown				(PD)19(SI)10
PD21SI4	*	structure unknown				(PD,SI)21(SI)4

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
PD2TA	MoPt2	oI6	Immm		71	(PD)2(TA)1
PD2TI	MoSi2	tI6	I4/mmm	C11b	139	(PD)2(TI)1
PD2Y	*	structure unknown				(PD)2(Y)1
PD2Y3	Er3Ni2	hR15	R-3		148	(PD)2(Y)3
PD2Y5	Dy5Pd2	cF144	Fd-3m		227	(PD)2(Y)5
PD39SI20	*	structure unknown				(PD)39(SI)20
PD3S	Pd3S	oS16	Ama2		40	(PD)3(S)1
PD3SI	Fe3C	oP16	Pnma	D011	62	(PD)3(SI)1
PD3TI2	Pd3Ti2	oS20	Cmcm		63	(PD)3(TI)2
PD3Y2_HT	*	structure unknown				(PD)3(Y)2
PD3Y2_LT	*	structure unknown				(PD)3(Y)2
PD4S	Pd4Se	tP10,	P-421C		114	(PD)0.8(S)0.2
PD4Y3	Pu3Pd4	hR42	R-3		148	(PD)4(Y)3
PD4ZR3	Pu3Pd4	hR42	R-3		148	(PD)4(ZR)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
PD5SI	Pd3P0.68	mP24	P12_11		4	(PD)5(SI)1
PD5TI3	Pd5Ti3	tP8	P4/mmm		123	(PD)5(TI)3
PD7Y	CuPt7	cF32	Fm-3m		225	(PD)7(Y)1
PD9SI2	Pd9Si2	oP44	Pnma		62	(PD)9(SI)2
PDO	PtS	tP4	P4_2/mmc		131	(PD)1(O)1
PDS	PdS	tP16,	P42/m		84	(PD)0.5(S)0.5
PDY_HT	CsCl	cP2	Pm-3m	B2	221	(PD,Y)1(Y)1
PDY_LT	CrB	oS8	Cmcm	B33	63	(PD,Y)1(Y)1
PDY3	Fe3C	oP16	Pnma	D011	62	(PD)1(Y)3
PDZR_ALPHA	*	mS*	Cm		8	(PD)1(ZR)1
PDZR_BETA	CrB	oS8	Cmcm	B33	63	(PD)1(ZR)1
PDZRM	MoSi2	tI6	I4/mmm	C11b	139	(PD)1(ZR)1(PD,ZR)1
PENTLANDITE	Co9S8	cF68	Fm-3m		225	(FE,NI)8(FE,NI)1(S)8
PI	b-Mn	cP20	P4_132	A13	213	(CR)12.8(FE,NI)7.2(N)4
PROTO_PYROXENE	MgSiO3	oP40	Pbcn		60	(CA+2,CO+2,CR+2,FE+2,NI+2)1(SI+4)1(O-2)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
PSEUDO_BROOKITE	CaTi2O4	oS28	Cmcm		63	(TI+4)1(AL+3)2(O-2)5
PSEUDO_WOLLASTONITE	CaSiO3	mS120	C2/c		15	(CA+2)1(SI+4)1(O-2)3
PT10ZR7	Ni10Zr7	oS68	Cmce		64	(PT)10(ZR)7
PT25SI7	*	structure unknown				(PT)25(SI)7
PT2TA	Au2V	oS12	Cmcm		63	(PT)2(TA)1
PT2Y	MgCu2	cF24	Fd-3m		227	(PT)2(Y)1
PT3O4	Pt3O4	cI14	Im-3m		229	(PT)3(O)4
PT3TA	Pt3Nb	mP48	P2_1/m		11	(PT)3(TA)1
PT3TI4	*	structure unknown				(PT)3(TI)4
PT3Y5	Mn5Si3	hP16	P6_3/mcm		193	(PT)3(Y)5
PT3Y7	Th7Fe3	hP20	P6_3mc		186	(PT)3(Y)7
PT3ZR5	Mn5Si3	hP16	P6_3/mcm	D88	193	(PT,ZR)3(PT,ZR)5
PT4Y3	*	structure unknown				(PT)4(Y)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
PT4Y5	Sm5Ge4	oP36	Pnma		62	(PT)4(Y)5
PT4ZR	Cu3Au	cP4	Pm-3m		221	(PT,ZR)2(PT,ZR)43
PT4ZR3	Pd4Pu3	hR14	R-3		148	(PT,ZR)4(PT,ZR)3
PT5SI2	*	structure unknown				(PT)5(SI)2
PT5Y	*	o*72				(PT)5(Y)1
PT6SI5	Pt6Si5	mP22	P2_1/m		11	(PT)6(SI)5
PT8TI	Pt8Ti	tI18	I4/mmm		139	(PT)8(TI)1
PTO2	CaCl2 / TiO2 / CdI2	oP6 / tP6 / hP3	Pnnm / P4_2/mnm / P-3m1		58 / 136 / 164	(PT)1(O)2
PTS	PtS	tP4	P4_2/mmc	B17	131	(PT)1(S)1
PTS2	CdI2	hP3	P-3m1		164	(PT)1(S)2
PTSI	MnP	oP8	Pnma	B31	62	(PT)1(SI)1
PTY2	Co2Si-b	oP12	Pnma		62	(PT)1(Y)2
PTY3	Fe3C-b	oP16	Pnma	D011	62	(PT)1(Y)3
PYRITE	FeS2-b	cP12	Pa-3	C2	205	(CO,FE,MN,NI)1(S)2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
PYRRHOTITE	NiAs	hP4	P63/mmc	B8_1	194	(AL,CO,CR,CU,FE,MG,MN,NB,NI,TI,V,ZR,VA)1(S)1
QUARTZ	SiO2	hP9	P3_121 / P6_222	*/C8	152/ 180	(SIO2)
R_PHASE	Co5Cr2Mo3	hR53	R-3h		148	(CO,CR,FE,NI,RE)27(MO,W)14(CO,CR,FE,MO,NI,RE,W)12
RANKINITE	Ca3O7Si2?	m*4	P121/a1		14	(CA+2)3(SI+4)2(O-2)7
RE1S2	ReS2	aP12	P-1		2	(RE)1(S)2
RE1S3	*	*	*			(RE)1(S)3
RE2O7	Re2O7	oP72	P2_12_12_1		19	(O7RE2)1
RE2S7	Re2O7	oP72	P2_12_12_1		19	(RE)2(S)7
RE2SI	Re2Si	mP24	P12_1/c1		14	(RE)2(SI)1
RE3B	Re3B	oC16	Cmcm	E1a	63	(CR,MO,RE,TA,W)3(B)1
RE3CO3B2	Ti3P	tP32	P4_2/n		86	(RE)3(CO)3(B)2
RE5CO2B4	Re4 (Re0.5Co0.5)2Co B4	tP22	P4/mbm		127	(RE)4(CO,RE)2(CO)1(B)4
RE7B3	Th7Fe3	hP20	P6_3mc	D102	186	(CO,CR,MO,NB,RE,RU,TA,W)7(B)3(B,VA)3

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
REB2	ReB2	hP6	P6_3/mmc		194	(RE)1(B)2(B,VA)2
RECOB	Co2Si	oP12	Pnma	C37	62	(RE)1(CO)1(B)1
REO2	VO2 / ReO2	mP12 / oP12	P2_1/c / Pbcn		14 / 60	(O2RE1)1
REO3	*	6 allotropes				(O3RE1)1
RESI2_C11B	Re4Si7	mS44	C1m1		8	(RE)0.357(SI)0.643
REZR2	Re25Zr21	hR276	R-3c		167	(NI,RE)1(ZR)2
RHODONITE	MgSiO3	mP40	P2_1/c		14	(CA+2,MN+2)1(SI+4)1(O-2)3
RU1S2	FeS2	cP12	Pa-3		205	(RU)1(S)2
RU25Y44	Ru25Y44	oP276	Pnna		52	(RU)0.362(Y)0.638
RU2B3	Ru2B3	hP10	P6_3/mmc		194	(RU)2(B)3
RU2SI_C37	Co2Si	oP12	Pnma	C37	62	(RU)2(SI)1
RU2SI3	Ge3Ru2	oP40	Pbcn		60	(RU)2(SI)3
RU2Y3	Ru2Er3	hP2	P6_3/m		176	(RU)0.4(Y)0.6
RU2Y5	C2Mn5	mS28	C2/c		15	(RU)0.286(Y)0.714

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
RU4SI3	Ru4Si3	oP28	Pnma		62	(RU)4(SI)3
RUB	*	cI*				(RU)2(B)12
RUB2	RuB2	oP6	Pmmm		47	(RU)1(B)2
RUSI	FeSi	cP8	P2_13	B20	198	(RU)1(SI)1
RUTILE_MO2	TiO2	tP6	P4_2/mnm	C4	136	(AL+3,MN+4,RU+4,V+4,TI+4,ZR+4)1(O-2,VA)2
RUY3	CFe3	oP16	Pnma	D0_11	62	(RU)0.25(Y)0.75
SI3N4	Si3N4	hP28/hP14	P31c/P6_3		159/173	(SI)3(N)4
SI5V6	Si5V6	oI44	Ibam		72	(SI)5(V)6
SIC	ZnS	cF8	Fd-3m	B3	227	(SI)1(C)1
SIGMA	CrFe	tP30	P4_2/mnm	DB8	136	(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)6
SILLIMANITE	Al2(SiO4)O-a	oP32	Pnma		62	(AL+3)1(AL+3)1(SI+4)1(O-2)
SIS2	SiS2	oI12	Ibam	C42	72	(SI)(S)
SPINEL	Al2MgO4	cF56	Fd-3m	H11	227	(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

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
T1_CU2TI	Au2V	oS12	Cmcm		63	(CU,FE)2(TI)1
T1CUNITI	MoSi2	tI6	I4/mmm	C11_b	139	(CU,NI)2(TI)1
T2_CU3TI2	Cu3Ti2	tP10	P4/nmm		129	(CU,FE)3(TI)2
T2CUNITI	Cu3Ti2	tP10	P4/nmm		129	(CU)0.175(NI)2.825(TI)2
T3_CU4TI3	Cu4Ti3	tI14	I4/mmm		139	(CU,FE)4(TI)3
T4CUFETI	*	structure unknown				(CU,FE)0.63(TI)0.37
T4CUNITI	BaPb3	hR12	R-3m		166	(CU)0.05(NI)0.7(TI)0.25
T5CUFETI	*	structure unknown				(CU,FE)0.55(TI)0.45
T6CUNITI	*	structure unknown				(CU)0.25(NI)0.5(TI)0.25
TA2O5_HT	Ta2O5	tI44	I4_1/amd		141	(TA)2(O)5
TA2O5_LT	Ta2O5	oP14	Pccm		49	(TA)2(O)5
TA5SI3_D8L	Cr5B3	tI32	I4/mcm		140	(HF,NB,TA)5(AL,SI)3
TAAL	Ta22Al21	mP86	P12_1/c1		14	(TA)0.51515(AL)0.48485
TAAL2	Ta39Al69	cF444	F-43m		216	(TA)0.35(AL)0.65

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
TAN_EPS	TaN	hP6	P-62m		189	(TA)1(N)14
TAU	Cr23C6	cF116	Fm-3m	D84	225	(CO,HF,NI,RE)20(B)6(B,VA)6(AL,CR,HF,MO,RE,TA,TI,V,W,ZR)3
THIOSPINEL	Fe3O4	cF56	Fd-3m		227	(CO,CU,FE,MN,NI)1(CO,CR,NI)2(S)4
TI25MN9AL66_L12	AuCu3	cP4	Pm-3m	L1_2	221	(AL,MN,TI)0.25(AL,MN)0.08(AL,MN,TI)0.67
TI2N_C4	TiO2	tP6	P4_2/mnm	C4	136	(TI)2(N)1
TI3N2	TiS	hR18	R-3m		166	(TI)0.71(N)0.29
TI3O2	Ti3O2	hP5	P6/mmm		191	(TI+2)2(TI)1(O-2)2
TI3O5	V3O5-ht	mS32	C2/c		15	(TI+3)2(TI+4)1(O-2)5
TI3SIC2	Ti3SiC2	hP12	Pg_3/mmc		194	(TI)3(SI)1(C)2
TI4N3	Sc0.67Te	hR24	R-3m		166	(TI)0.685(N)0.315
TIO_ALPHA	alpha-TiO	mS20	C2/m		12	(TI+2)1(O-2)1
TISI2_C54	TiSi2	oF24	Fddd		70	(MO,NB,RU,TI)1(AL,SI)2
TRIDYMITE	SiO2	mS144	Cc		9	(SIO2)
V2B3	V2B3	oS20	Cmcm		63	(V)0.4(B)0.6

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
V2O_SS	V7O3	mS20	C2/m		12	(V)1(O,VA)0.5
V2O5	V2O5	oP14	Pmmn		59	(V+5)2(O-2)5
V3C2	Sc2Te3	hR20	R-3m		166	(V)3(C)2
V52O64	V13O16	tI56	I4_1/amd		141	(V)52(O)64
V5B6	V5B6	oS22	Cmmm		65	(NB,V)5(B)6
VO2_LT	VO2	mP12	P2_1/c		14	(V+4)1(O-2)2
W1S2	MoS2	hP6 / hR9	P6_3/mmc / R3m		194 / 160	(W)1(S)2
W2COB2	W2CoB2	oI10	Immm		71	(MO,W)2(CO,NI)1(B)2
W3COC	W10Co3C3.4	hP34	P6_3/mmc		194	(W)3(CO,NI)1(C)1
W5SI3_D8M	W5Si3	tI32	I4/mcm	D8m	140	(CR,FE,MO,NB,V,W)4(CR,FE,MO,NB,V,W,SI)1(AL,SI)3
WO2	VO2	mP12	P12_1/c1		14	(O2W1)1
WO2_72	*	*	*			(O2_72W1)1
WO2_90	*	*	*			(O2_90W1)1
WO2_96	*	*	*			(O2_96W1)1

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
WO3_HT	WO3	tP16	P-42_1m		113	(O3W1)1
WO3_LT	WO3	oP32	Pbcn		60	(O3W1)1
WOLLASTONITE	CaSiO3	aP30	P-1		2	(CA+2,FE+2,MN+2)1(SI+4)1(O-2)3
Y15C19_H	*	structure unknown				(C)19(Y)15
Y15C19_R	alpha-Y15C19	oP18	Pbam		55	(C)19(Y)15
Y2C3_H	*	structure unknown				(Y)2(C)2(C,VA)1
Y2C3_R	Sc3C4	tP70	P4/mnc		128	(Y)2(C)2(C,VA)1
Y2CU2O5	Cu2Ho2O5	oP36	Pna2_1		33	(Y+3)2(CU+2)2(O-2)5
Y2S2A_Y2SI2O7	La4Ge3(GeO4)O10	aP44	P-1		2	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2B_Y2SI2O7	Y2Si2O7	oP44	Pnma		62	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2D_Y2SI2O7	Ce2Si2O7	mP44	P2_1/c		14	(Y+3)1(Y+3)1(SI2O7-6)1
Y2S2G_Y2SI2O7	Y2(Si2O7)	mP22	P2_1/c		14	(Y+3)1(Y+3)1(SI2O7-6)1
Y2SIO5	Y2SiO5	mS64	C2/c		15	(Y+3)1(Y+3)1(SIO4-4)1(O-2)

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
Y3SI5_HT	GdSi1.4	oI12	Imma		74	(Y)3(SI)5
Y3SI5_LT	AlB2	hP3	P6/mmm	C32	191	(Y)3(SI)5
YAG	Al2Ca3Si3O12	cI160	Ia-3d		230	(AL+3,CR+3,FE+3)5(Y+3)3(O-2)12
YAM	Al2Y4O9	mP60	P2_1/c		14	(AL+3,SI+4)2(CA+2,Y+3)4(O-2,VA)1(O-2)
YAP	AlYO3	hP10	P6_3/mmc		194	(AL+3,CO+3,CR+3,FE+3,MN+3)1(CA+2,Y+3)1(O-2,VA)39
YB4	UB4	tP20	P4/mbm	D1E	127	(Y)1(B)4
YB6	CaB6	cP7	Pm-3m		221	(Y)1(B)6
YB66	YB66	cF1936	Fm-3c		226	(Y)1(B)66
YC_GAMMA	NaCl	cF8	Fm-3m	B1	225	(Y)1(C,C2,VA)1
YC2_C11A	CaC2	tI6	I4/mmm	C11A	139	(C2Y1)
YCUO2	AgFeO2	hP8	P6_3/mmc		194	(Y+3)1(CU+1)1(O-2)2
YSI2_HT	AlB2	hP3	P6/mmm	C32	191	(Y)1(SI)2
Z_PHASE	CrNbN	tP6	P4/nmm		129	(CR,FE)1(MO,NB,V)1(N,VA)1
ZR3Y4O12	Y6UO12	hR57	R-3		148	(ZR+4)3(Y+3)4(O-2)12

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*CEF formula*
ZR5SI4	ZR5SI4	tP36	P4_12_12		92	(HF,NB,TI,Y,ZR)5(SI)4
ZRO2_MONO	Zro2-m	mP12	P2_1/c	C43	14	(AL+3,CA+2,CR+3,HF+4,TI+4,Y+3,ZR+4)2(O-2,VA)4
ZRO2_TETR	HgI2	tP6	P4_2/nmc		137	(AL+3,CA+2,CR+3,FE+2,HF+4,MG+2,MN+2,MN+3,NI+2,TI+4,Y+3)24
ZRO8S2	Zr(SO4)2	oP44	Pnma		62	(ZR+4)1(SO4-2)2
ZRS2	CdI2	hP3	P-3m1		164	(ZR)1(S)2
ZRSI2_C49	ZrSi2	oS12	Cmcm	C49	63	(ZR,Y,HF,NB)1(SI)2
ZRSIO4	Zr(SiO4)	tI24	I4_1/amd		141	(SI+4)1(ZR+4)1(O-2)4
ZRTI2O6	Nb2FeO6	oP36	Pbcn		60	(ZR+4)1(TI+4)2(O-2)6
ZRTIO4_ALPHA	*	*	*			(ZR+4)1(TI+4)1(O-2)4
ZRTIO4_BETA	FeN0.94	oP12	Pbcn		60	(TI+4,ZR+4)2(O-2)4

TCNI10 Properties Data

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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:	**10.0**
First release:	**TCNI1 was released in 2000**

Changes in the Most Recent Database Release

TCNI9.1 to TCNI10.0

Software release 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.

References

1. P. Nash, D. R. F. West, Phase equilibria in Ni-rich region of Ni–Al–Hf system. Met. Sci. 15, 347–352 (1981).
2. M. Takeyama, C. T. Liu, Microstructures and mechanical properties of NiAl–Ni 2 AlHf alloys. J. Mater. Res. 5, 1189–1196 (1990).
3. M. Albers, M. Sai Baba, D. Kath, M. Miller, K. Hilpert, Chemical Activities in the Solid Solution of Hf in Ni3Al. Berichte der Bunsengesellschaft für Phys. Chemie. 96, 1663–1668 (1992).
4. S. Miura, Y.-M. Hong, T. Suzuki, Y. Mishima, Liquidus and solidus temperatures of Ni-solid solution in Ni-Al-X (X: Ti, Zr, and Hf) ternary systems. J. Phase Equilibria. 20, 193–198 (1999).

5. E. Copland, Partial Thermodynamic Properties of γ'-(Ni,Pt)3Al in the Ni-Al-Pt system. J. Phase Equilibria Diffus. 28, 38–48 (2007).
6. N. Volz, C. H. Zenk, R. Cherukuri, T. Kalfhaus, M. Weiser, S. K. Makineni, C. Betzing, M. Lenz, B. Gault, S. G. Fries, J. Schreuer, R. Vaßen, S. Virtanen, D. Raabe, E. Spiecker, S. Neumeier, M. Göken, Thermophysical and Mechanical Properties of Advanced Single Crystalline Co-base Superalloys. Metall. Mater. Trans. A. 49, 4099–4109 (2018).
7. K. P. Gupta, The Nb-Ni-Ti (Niobium-Nickel-Titanium) System—Update. J. Phase Equilibria Diffus. 29, 194–197 (2008).

Previous Releases

TCNI9.0 to TCNI9.1

Software release 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.