TCS High Entropy Alloys Database (TCHEA6)

Technical Information

Available Starting with Thermo-Calc Version 2022b

Document created 6/3/2022

Contents

About the TCS High Entropy Alloys Database (TCHEA)

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

TCHEA: TCS High Entropy Alloys Database Revision History. The current version of the database is TCHEA6. See the link for any subversion release details.

The database is compatible with the TCS High Entropy Alloy Mobility Database (MOBHEA). The current version is MOBHEA2.

The CALPHAD Method

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

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

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

Use Case Examples

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

Some case examples of how the TCHEA6 database can be used include:

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

Combining Databases

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

References

[2004Yeh] J. W. Yeh, S. K. Chen, S. K. Lin, J. Y. Gan, T. S. Chin, T. T. Shun, C. H. Tsau, S. Y. Chang, Nanostructured High-Entropy Alloys with Multiple Principal Elements: Novel Alloy Design Concepts and Outcomes. Adv. Eng. Mater. 6, 299–303 (2004).

[2006Yeh] J.-W. Yeh, Recent progress in high-entropy alloys. Ann. Chim. Sci. des Matériaux. 31, 633–648 (2006).

[2013Wan] S. Wang, Atomic Structure Modeling of Multi-Principal-Element Alloys by the Principle of Maximum Entropy. Entropy. 15, 5536–5548 (2013).

[2015Sen] O. N. Senkov, J. D. Miller, D. B. Miracle, C. Woodward, Accelerated exploration of multi-principal element alloys with solid solution phases. Nat. Commun. 6, 6529 (2015).

TCS High Entropy Alloys Database (TCHEA) Resources

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

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

Database Specific Documentation

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

Go to the High Entropy Alloys Databases page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to high entropy alloys 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.

TCHEA6 Elements, Systems, Phases, and Properties Data

Included Elements

The database has been developed in a 26 element framework:

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

Assessed Systems and Phases

The most recent version of the database contains:

- 310 binary systems, with almost all of these assessed to the full range of composition and temperature. These can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 502 ternaries are assessed, and 192 of them to the full range of composition and temperature. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 518 solution and intermetallic phases, where nearly all stable phases in all assessed binary systems and most ternary systems are modeled.

About the Included Phases

The ordered B2 and $L1_2$ phases, together with BCC_A2 and FCC_A1, respectively, are modeled with the so-called partitioning model, which describes an ordered phase and its disordered counterpart using a single Gibbs energy curve. This type of description is of particular importance to be able to predict second order transformations between a disordered phase and its ordered structures.

Also note that there may be several possible composition sets for the phases named FCC_L12 and BCC_B2 designated by #1, #2, and so on (e.g. FCC_L12#1 and FCC_L12#2), due to the co-existence of disordered and ordered structures or the presence of miscibility gap. The #n suffix (where n is an integer) is generated dynamically by Thermo-Calc when using global minimization and therefore the identification of the phases should be determined from their site occupations. It can be found by LIST_EQUILIBRIUM with the VXNS option in the Console Mode or showing the site fraction in moles of the constituent elements in the Graphical Mode. When the site occupancies of the first and second sublattices are equal the phase is disordered.

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

Properties Data

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

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.

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.

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)`
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)`**

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
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 TCS Metal Oxide Solutions Database (TCOX)
** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCHEA6 Systems

In this section:

TCHEA6 Assessed Binary Systems

These are the assessed binary systems (310 in total) in the full range of composition and temperature.

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

TCHEA6 Critically Assessed Ternary Systems

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

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

TCHEA6 Tentatively Assessed Ternary Systems

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

Tentatively Assessed Ternary Systems								
C-V-Zr	C-W-Zr	Fe-Hf-Mo	Fe-Hf-Nb	Fe-Hf-Ni	Fe-Hf-Re	Fe-Hf-Si	Fe-Hf-Ta	Fe-Hf-Ti
Fe-Hf-W	Fe-Hf-Zr	Fe-Mn-Ni	Fe-Mo-N	Fe-Mo-Nb	Fe-Mo-Re	Fe-Mo-Si	Fe-Mo-Ta	Fe-Mo-Ti
Fe-Mo-W	Fe-Mo-Zr	Fe-Nb-Re	Fe-Nb-Si	Fe-Nb-Ta	Fe-Nb-Ti	Fe-Nb-W	Fe-Nb-Zr	Fe-Ni-Ta
Fe-Ni-V	Fe-Ni-Zr	Fe-Re-Ti	Fe-Re-W	Fe-Re-Zr	Fe-Si-Ta	Fe-Si-Ti	Fe-Si-W	Fe-Si-Zr
Fe-Ta-Ti	Fe-Ta-W	Fe-Ta-Zr	Fe-Ti-W	Fe-W-Zr	Hf-Mo-Ni	Hf-Mo-Si	Hf-Nb-Ni	Hf-Nb-Re
Hf-Ni-Re	Hf-Ni-Ru	Hf-Ni-Si	Hf-Ni-Ta	Hf-Ni-W	Hf-Re-Ta	Hf-Re-W	Hf-Ru-Ti	Hf-Ru-Zr
Hf-Si-Ta	Hf-Si-Ti	Hf-Si-W	Mn-Ni-Si	Mn-Ni-V	Mo-Nb-Ni	Mo-Nb-Re	Mo-Ni-Re	Mo-Ni-Ru
Mo-Ni-Si	Mo-Ni-Ti	Mo-Ni-W	Mo-Ni-Zr	Mo-N-V	Mo-Re-Ru	Mo-Re-Ta	Mo-Re-Ti	Mo-Re-V
Mo-Re-W	Mo-Re-Zr	Mo-Ru-SI	Mo-Ru-Ta	Mo-Ru-W	Mo-Si-Zr	Nb-Ni-Re	Nb-Ni-Si	Nb-Ni-Ta
Nb-Ni-V	Nb-Ni-W	Nb-Ni-Zr	Nb-Re-Ta	Nb-Re-Ti	Nb-Re-W	Nb-Re-Zr	Nb-Ru-SI	Nb-Si-Ti
Ni-Re-Ta	Ni-Re-W	NI-RE-ZR	Ni-Ru-Ta	Ni-Ru-Ti	Ni-Ru-W	Ni-Ru-Zr	Ni-Si-Ta	Ni-Si-V
Ni-Si-W	Ni-Si-Zr	Ni-Ta-Zr	Ni-W-Zr	N-Ti-V	Re-Ru-Ta	Re-Ru-Ti	Re-Ru-W	Re-Ta-Ti
Re-Ta-V	Re-Ta-Zr	Re-Ti-W	Re-W-Zr	Ru-SI-TI	Ru-Ta-Ti	Ru-Ta-W	Ru-Ti-Zr	Si-Ta-Zr
Si-Ti-Zr	Si-W-Zr	Ta-W-Zr						

TCHEA6 Phases

In this section:

TCHEA6 Models for the Included Phases

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL10CU10FE	oF116	Fmm2				(Fe)1(Al, Cu)10(Al)10	(Al10Cu10Fe)
AL10FEMN2	hP26	P6_3/mmc	Tau3.			(Fe, Mn)3(Al)10	Mn3Al10
AL11CR2	mS732	C2/c				(Al)10(Al)1(Cr)2	Al5Cr
AL11CU5MN3	oP380		Tau2			(Al)11(Mn)3(Cu)5	Unknown Structure
AL11MN3ZN2	oS152		ternary Tau3phase			(Mn)3(Zn)2(Al)11	Unknown Structure
AL11MN4_HT	oP156	Pnma				(Al, Mn)29(Mn)10	Mn6(Mn0.5Al0.5)8Al25
AL11MN4_LT	aP15	P-1				(Al)11(Fe, Mn)4	Al11Mn4
AL11RE4	aP15	P-1				(Al)11(Re)4	Al11Mn4
AL12MN_GPHASE	cI26	Im-3				(Al)12(Mn)1	Al12W
AL12W_GPHASE	cI26	Im-3	also Al12Mo, Al12Re.			(Al)12(Mo, Re, W)1	Al12W
AL13CO4	oP102	Pmn2_1				(Al)13(Co)4	Orthorhombic Co4Al13
AL13CR2	mS104	C2/m				(Al)13(Cr)2	Al45V7
AL13FE2MN2	mS102	C2/m	Tau2.			(Fe, Mn)4(Al)13	Al13Fe4
AL13FE4	mS102	C2/m	solid-solution of Al13Fe4 (aka Al3Fe) & Al13Ru4.			(Al, Cu)0.6275(Fe, Mn, Ru)0.235(Al, Si, Va)0.1375	Al13Fe4
AL13IR4						(Al)0.765(Ir)0.235	Unknown Structure
AL13NI38ZN49						(Al)0.13(Ni)0.38(Zn)0.49	Unknown Structure
AL15SI2M4_TAU9	cI168	Im-3				(Al)14(Fe, Mn)4(Al, Si)5	Al15(Mn,Fe)3Si2

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL16FEMN3	hP574	P6_3/mmc	Tau1			(Al)4(Fe, Mn)1	mu-Al4Mn
AL1MN1SI1	oF24	Fddd	Tau3			(Al)1(Mn)1(Si)1	TiSi2 (C54)
AL21V2	cF176	Fd-3m				(Al)21(V)2	Al10V
AL23CUFE4_D2H	oS28	Cmcm				(Al)23(Cu)1(Fe)4	MnAl6 (D2h)
AL23V4	hP54	P6_3/mmc				(Al)23(V)4	Al23V4
AL24MN5ZN			ternary Tau1 phase			(Mn, Zn)5(Zn)1(Al)24	Unknown Structure
AL28CU4MN7			Tau1,Mn6+xCu4+yAl29-x-y.			(Al)28(Mn)7(Cu)4	Unknown Structure
AL28IR9	hP236	P31c				(Al)0.757(Ir)0.243	Al28Ir9
AL2FE	aP18	P1				(Al, Cu)2(Fe, Mn)1	Al2Fe
AL2MN2SI3	hP21	P-6	Tau1			(Al)2(Mn)2(Si)3	(Al2Mn2Si3)
AL2MNSI3	tI24	I4/mcm	Tau10			(Al)2(Mn)1(Si)3	Ga5Pd
AL2TI_LT	tI24	I4_1/amd				(Al, Nb, Ti)2(Al, Co, Nb, Ta, Ti, V, Zr)1	Ga2Hf
AL2TI3N2	hP22	P6_3mc				(Al)2(Ti)3(N)2	(Al2Ti3N2)
AL2W_C40						(Al)2(W)1	
AL2ZR3	tP20	P4_2/mnm	also Al2Hf3, Al2Y3.			(Al)2(Hf, Ti, Y, Zr)3	Zr3Al2
AL31MN6NI2	hP574	P6_3/mmc				(Al)31(Mn)6(Ni)2	mu-Al4Mn
AL3CO1	mS34	C2/m	aka CoAl3_cub.			(Al)3(Co)1	Os4Al13
AL3IR_D018	hP8	P6_3/mmc				(Al)0.75(Ir)0.25	Na3As (D018)
AL3MN4SI2			ternary tau5 or D phase			(Al)3(Mn)4(Si)2	Unknown Structure

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL3MNSI2	tP48	P4/n	Tau4			(Al)3(Mn)1(Si)2	(Al3MnSi2)
AL3NI_D011	oP16	Pnma				(Al)0.75(Ni)0.25	Cementite (Fe3C, D011)
AL3NI2_D519	hP5	P-3m1	also Al3Ru2.			(Al, Si, Sn, Zn)3(Al, Cu, Ni, Ru)2(Ni, Ru, Va)1	Al3Ni2 (D513)
AL3NI5	oS16	Cmmm				(Al)0.375(Ni)0.625	Ga3Pt5
AL3RH_LT	oP*	Pnma				(Al)3(Rh)1	(Al3Rh)
AL3TI_D022	tI8	I4/mmm	gamma double prime,AL3TI_ D022, Al3M, Ni3V.			(Al, Co, Cr, Fe, Mo, Nb, Ni, Si, Ti, V)3(Al, Co, Cr, Mo, Nb, Ni, Si, Ta, Ti, V, Zr)1	Al3Ti (D022)
AL3TI_LT	tI32	I4/mmm				(Al, Ti)3(Al, Ti, Zr)1	Al3Ti-LT
AL3Y_HT	hR12	R-3m				(Al)0.75(Y)0.25	BaPb3
AL3Y_LT	hP8	P6_3/mmc				(Al)0.75(Y)0.25	Ni3Sn (D019)
AL3ZR_D023	tI16	I4/mmm	also Al3Hf, Zn3Zr.			(Al, Zn)3(Hf, Ti, Zr)1	Al3Zr (D023)
AL3ZR2	oF40	Fdd2	also Al3Hf2.			(Al)3(Hf, Zr)2	Zr2Al3
AL3ZR4	hP7	P6/mmm	also Al3Hf4.			(Al)3(Hf, Ti, Zr)4	Al3Zr4
AL3ZR5_D8M	tI32	I4/mcm				(Al)3(Ti, Zr)5	W5Si3 (D8m)
AL45IR13	oP236	Pnma				(Al)0.776(Ir)0.224	Al45Ir13
AL45V7	mS104	C2/m	aka Al7V			(Al)45(V)7	Al45V7
AL4C3_D71	hR7	R-3m				(Al, Si)4(C)3	Al4C3 (D71)
AL4CR	hP574	P6_3/mmc				(Al)4(Cr)1	mu-Al4Mn
AL4MN_LAMBDA	hP586	P6_3/mmc	alsoAL461MN107			(Al)461(Fe, Mn)107	lambda-Al4Mn

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL4MN_MU	hP574	P6_3/mmc				(Al)4(Mn)1	mu-Al4Mn
AL4RE	aP71	P-1				(Al)4(Re)1	Al4Re
AL4SIC4_E94	hP18	P6_3mc				(Al)4(Si)1(C)4	Al5C3N (E94)
AL4W	mS30	Cm	also Al4Mo.			(Al)4(Mo, W)1	Al4W
AL4ZR5	hP18	P6_3/mcm				(Al)4(Zr)5	Ti5Ga4
AL5CO2_D811	hP28	P6_3/mmc	also Al5Rh2.			(Al)5(Co, Rh)2	Co2Al5 (D811)
AL5CU4ZN						(Al, Cu)1(Al)4(Cu)4(Zn)1	Unknown Structure
AL5FE2	oS24	Cmcm				(Al, Cu)5(Fe, Mn)2	Al2.8Fe
AL5FE4_D82	cI52	I-43m	alsoAL8FE5_D82			(Al, Cu, Fe)1	gamma-brass (Cu5Zn8, D82)
AL5IR2	cP60	P23				(Al)0.73(Ir)0.27	Al2.75Ir
AL5MN6SI7	hP9	P6_222	Tau2			(Al)5(Mn)6(Si)7	CrSi2 (C40)
AL5RH2_HT	cP54	P23				(Al)2(Rh, Va)1	beta-Al5Rh2
AL5TI2_HT	tP28	P4/mmm				(Al, Ti)5(Al, Nb, Ta, Ti, V, Zr)2	Al5Ti2
AL5TI3	tP32	P4/mbm				(Al)5(Ta, Ti)3	Al5Ti3
AL5W	hP12	P6_322	also AL5MO.			(Al)5(Mo, W)1	Al5W
AL62CU25FE13						(Fe)0.125(Al, Cu)0.255(Al)0.62	Quasicrystal
AL63MO37			Mo3Al5_HT			(Al)63(Mo)37	Unknown Structure
AL6MN_D2H	oS28	Cmcm	also Al6Re, Al6Ru			(Al)6(Fe, Mn, Re, Ru)1	MnAl6 (D2h)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL77W23						(Al)77(W)23	Unknown Structure
AL7CU2FE	tP40	P4/mnc				(Fe, Ni)1(Cu)2(Al)7	FeCu2Al7 (E9a)
AL7CU4NI	hR14	R-3m				(Al)1(Cu, Fe, Ni, Va)1	(Cu0.8Ni0.2)2.53Al3.5
AL7RH3_HT	mP*					(Al)7(Rh)3	Unknown Structure
AL7W3						(Al)7(W)3	Unknown Structure
AL8CR5_HT_D82	cI52	I-43m				(Al)8(Cr)5	gamma-brass (Cu5Zn8, D82)
AL8CR5_LT_D810	hR26	R3m				(Al)8(Cr)5	Cr5Al8 (D810)
AL8MN5_D810	hR26	R3m				(Al, Ti, Zn)12(Mn)5(Al, Cu, Mn, Si, Ti)9	Cr5Al8 (D810)
AL8MO3	mS22	C2/m				(Al)8(Mo)3	Al8Mo3
AL8SIC7	hP16					(Al)8(Si)1(C)7	Unknown Structure
AL8V5_D82	cI52	I-43m				(Al, V)8(Al, V, Zr)5	gamma-brass (Cu5Zn8, D82)
AL9CO2	mP22	P2_1/c	also Al9Rh2			(Al)9(Co, Rh)2	Co2Al9 (D8d)
AL9CR4_HT						(Al)9(Cr)4	Unknown Structure
AL9CR4_LT						(Al)9(Cr)4	Unknown Structure
AL9IR2	mP22	P2_1/c				(Al)0.818(Ir)0.182	Co2Al9 (D8d)
AL9MN2ZN			ternary Tau2 phase			(Mn)2(Zn)1(Al)9	Unknown Structure
ALB12_ALPHA	tP216	P4_12_12				(Al, Ti)1(B)12	alpha-AlB12
ALCR2C	hP8	P6_3/mmc	MAX_PHASE.			(Al)1(C)1(Cr)2	AlCCr2

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
ALCU_DELTA	hR52	R3m				(Al)2(Cu, Fe)3	Al5Cu8
ALCU_EPS_B82	hP6	P6_3/mmc	epsilon2 HT.			(Al, Cu, Ni)1(Cu, Fe)1	Ni2In (B82)
ALCU_ETA	mS20	C2/m	united HT-eta1 & LT-eta2.			(Al, Cu)1(Cu, Fe, Ni, Zn)1	AlCu(r)
ALCU_PRIME	oF88	Fmm2	aka THETA_PRIME.			(Al)2(Cu)1	Al9Cu11(h)
ALCU_ZETA	oF88	Fmm2	united HT-zeta1 andLT-zeta2.			(Al)9(Cu, Fe)11	Al9Cu11(h)
ALCU3MN2_C15	cF24	Fd-3m	Tau3.			(Al)1(Mn)2(Cu)3	Cu2Mg Cubic Laves (C15)
ALFESI_ALPHA_ TAU5	hP246	P6_3/mmc				(Al)0.6612(Fe)0.19(Si)0.0496(Al, Si)0.0992	Fe23Al81Si15
ALFESI_BETA_TAU6	mS52	C2/c				(Al)14(Fe)3(Si)3	Fe2Al9Si2
ALFESI_DELTA_ TAU4	oP24	Pbcn				(Al)0.55(Fe)0.15(Si)0.3	FeAl3Si2
ALFESI_GAMMA_ TAU2	mS*					(Al)3(Fe)1(Si)1	Unknown Structure
ALFESI_TAU1						(Al)2(Fe)2(Si)1	Unknown Structure
ALFESI_TAU3	oS128	Cmme				(Al)2(Fe)1(Si)1	Fe(Al0.67Si0.33)3
ALM3C_E21	cP5	Pm-3m	also AlCo3C, AlFe3C.			(Al)1(Co, Fe)3(C)1	Cubic Perovskite (CaTiO3, E21)
ALMNSI_TAU6						(Al, Mn)4(Si)1	Unknown Structure
ALMNSI_TAU8	hP26	P6_3/mmc				(Mn, Va)6(Mn, Va)2(Al)12(Al, Si)6(Al, Si)2	Al9Mn3Si (E9c)
ALMO_A2	cI2	Im-3m	improper modelling.			(Al, Mo)1(Al, Mo)1	Body-Centered Cubic (W, A2, bcc)
ALN_B4	hP4	P6_3mc				(Al)1(N)1	Wurtzite (ZnS, B4)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
ALNI2ZN						(Al)0.25(Ni)0.5(Zn)0.25	Unknown Structure
ALPHA_B19	oP4	Pmma	an ordered HCP.			(Mo, Nb, Ti, V, Zr)1(Mo, Nb, Ti, V, Zr)1	beta'-AuCd (B19)
ALRE_B11	tP4	P4/nmm				(Al)1(Re)1	gamma-CuTi (B11)
ALRE2_C11B	tI6	I4/mmm				(Al)1(Re)2	MoSi2 (C11b)
ALRH2						(Al)1(Rh)2	Unknown Structure
ALSI3TI2	tI24	I4_1/amd	aka Ti7Al5Si12, Tau1			(Al)0.166667(Si)0.5(Ti)0.333333	Zr3Al4Si5
ALTI_L10	tP2	P4/mmm	Solid solution ofordered L10.			(Al, Co, Cr, Mn, Mo, Nb, Sn, Ta, Ti, V, W, Zr)1(Al, Co, Cr, Mn, Mo, Nb, Sn, Ta, Ti, V, W, Zr)1	CuAu (L10)
ALTI2N	hP8	P6_3/mmc				(Al)1(Ti)2(N)1	AlCCr2
ALTI3_D019	hP8	P6_3/mmc	also Ni3Sn_LT,Mn3Sn, Ti3Sn.			(Al, Co, Cr, Cu, Mn, Mo, Nb, Ni, Sn, Ta, Ti, V, W, Zr)3(Al, C, Cr, Mo, Nb, Ni, Si, Sn, Ta, Ti, V, W)1	Ni3Sn (D019)
ALTI3N_E21	cP5	Pm-3m				(Al)1(Ti)3(N)1	Cubic Perovskite (CaTiO3, E21)
ALY2_C37	oP12	Pnma				(Al)1(Y)2	Co2Si (C37)
ALZR_B33	oS8	Cmcm	also AlHf, ALY_B33.			(Al)1(Hf, Y, Zr)1	CrB (B33)
ALZR2_B82	hP6	P6_3/mmc				(Al)1(Ti, Zr)2	Ni2In (B82)
B4C_D1G	hR15	R-3m				(B11C, B12)1(B2, C2B, Cb2)1	B13C2 B4C (D1g)
B82_OMEGA	hP6	P6_3/mmc				(Al, Sn)1(Co, Nb, Sn, Ta, Ti)1(Ti)1	Ni2In (B82)
BCC_A2	cI2	Im-3m	BCC_A2 will be combined to BCC_B2 if defined.			(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, Va, W, Y, Zn, Zr)1(B, C, N, Va)3	Body-Centered Cubic (W, A2, bcc)
BCC_B2	cP2	Pm-3m	This phase has somecontribution from BCC_A2.			(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, Va, W, Y, Zn, Zr)0.5(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, Va, W, Y, Zn, Zr)0.5(B, C, N, Va)3	CsCl (B2)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
BCC_B2#2						(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, Va, W, Y, Zn, Zr)0.5(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, Va, W, Y, Zn, Zr)0.5(B, C, N, Va)3	
BCT_A5	tI4	I4_1/amd	Disordered BCT solutionphase.			(Al, Cu, Ni, Sn, Zn)1	beta-Sn (A5)
BETA_RHOMBO_B	hR105	R-3m				(B)93(B, C, Cu, Si)12	beta-B (R-105)
BN_B4	hP4	P6_3mc				(B)1(N)1	Wurtzite (ZnS, B4)
BNSI_RHOMBO	hR12	R-3m	aka BNSI,ALPHA_RHOMBO_B.			(B)61(Si)1(B, Si)8	alpha-B (hR12)
C14_LAVES	hP12	P6_3/mmc	also CuZn2.			(Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zn, Zr)2(Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zn, Zr)1	MgZn2 Hexagonal Laves (C14)
C15_LAVES	cF24	Fd-3m				(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zn, Zr)2(Al, Co, Cr, Cu, Fe, Hf, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zr)1	Cu2Mg Cubic Laves (C15)
C16_THETA	tI12	I4/mcm				(Al, Hf, Mn, Mo, Nb, Sn, Ta, Ti, W, Zr)2(Al, Co, Cr, Cu, Fe, Ir, Mn, Ni, Rh, Si)1	Khatyrkite (Al2Cu, C16)
C36_LAVES	hP24	P6_3/mmc				(Al, Co, Cr, Cu, Fe, Hf, Mo, Nb, Ni, Ta, Ti, W, Zr)2(Al, Co, Cr, Cu, Fe, Hf, Mo, Nb, Ni, Ta, Ti, W, Zr)1	MgNi2 Hexagonal Laves (C36)
CBCC_A12	cI58	I-43m				(Al, Co, Cr, Cu, Fe, Ir, Mn, Mo, Nb, Ni, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)1(B, C, Va)1	alpha-Mn (A12)
CEMENTITE_D011	oP16	Pnma				(Co, Cr, Fe, Mn, Mo, Ni, V, W)3(C, N)1	Cementite (Fe3C, D011)
CHI_A12	cI58	I-43m	also M5Re24,Mo2Re8, Ta3Re7, WRe3.			(Cr, Fe, Ni, Re)24(Al, Cr, Hf, Mo, Nb, Ta, Ti, W, Zr)10(Cr, Fe, Mo, Nb, Ni, Re, Ta, W)24	alpha-Mn (A12)
CO10CU57TI33	tI6	I4/mmm	Strukturbericht C11B.			(Co)0.1(Cu)0.57(Ti)0.33	MoSi2 (C11b)
CO11ZR2	oP*	Pban				(Co)11(Zr)2	(Co11Hf2)
CO17Y2	hP38	P6_3/mmc	united HT/LT phase.			(Co2, Y)1(Co2, Y)2(Co)15	Ni17Th2

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CO1SN3	oS32	Cmce				(Co)0.25(Sn)0.75	Au3Zn
CO2SI1	oP12	Pnma	also Ni2Si (delta)			(Co, Cr, Cu, Fe, Ir, Ni, Ti)2(Si)1	Co2Si (C37)
CO3SI_D019	hP8	P6_3/mmc				(Co)3(Si)1	Ni3Sn (D019)
CO3V1	hP24	P6_3/mmc				(Co, Ni, V)3(Co, V)1	Al3Pu
CO3Y1	hR12	R-3m				(Co)3(Y)1	Ni3Pu
CO3Y2	cP*					(Co)3(Y)2	Unknown Structure
CO3Y4	hP22	P6_3/m				(Co)3(Y)4	Co3Ho4
CO5Y_D2D	hP6	P6/mmm				(Co2, Y)1(Co)4(Co, Va)1	CaCu5 (D2d)
CO5Y8	mP52	P2_1/c				(Co)5(Y)8	Co5Y8
CO7HF	oP*	Pban				(Co)7(Hf)1	(Co11Hf2)
CO7NB2	mS18	C2/m				(Co)7(Nb)2	(Co7Nb2)
CO7TA2	hR12	R-3m				(Co)7(Ta)2	BaPb3
CO7Y6						(Co)7(Y)6	Unknown Structure
COSN_B35	hP6	P6/mmm	also FeSn, COSN_HP6.			(Co, Fe, Ni)0.5(Sn)0.5	CoSn (B35)
COSNTI_TAU2	cF12	F-43m	aka TiCoSn.			(Co, Ni)1(Sn)1(Ti)1	Half-Heusler (C1b)
COY_B33	oS8	Cmcm	aka COY_BF.			(Co)1(Y)1	CrB (B33)
COZN_DELTA			Zn15Co2HT phase			(Co)0.117647(Zn)0.882353	Unknown Structure
COZN_GAMMA_D82	cI52	I-43m	aka Zn11Co2, COZN4_D83.			(Co, Zn)1(Va)1	gamma-brass (Cu5Zn8, D82)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
COZN_GAMMA1	mS28	C2/m	aka CoZn7.8			(Co)0.125(Zn)0.875	Co2Zn15
COZN_GAMMA2	mS28	C2/m	akaCoZn13			(Co)0.0714286(Zn)0.9285714	CoZn13
COZN_HT						(Co, Zn)1(Va)1	Unknown Structure
COZN_LT_A13	cP20	P4_132				(Co, Zn)1(Va)1	beta-Mn (A13)
CR2B_CB	oF48	Fddd	akaCR2B_ORTH.			(Cr, Fe, Mo, Re)0.66666667(B)0.33333333	Mg2Cu (Cb)
CR2NI2SI	cF96	Fd-3m	i.e. the Tau1 phase Cr5Ni5Si3.			(Cr)5(Ni)5(Si)3	NiTi2
CR3MN5	cI58	I-43m				(Cr)3(Mn)5	alpha-Mn (A12)
CR3NI5SI2	cP20	P2_13				(Cr)3(Ni)5(Si)2(C, Va)1	AlAu4
CR3SI_A15	cP8	Pm-3n	also Cr3X, Nb3X, Ti3X,V3X.			(Cr, Fe, Ir, Mo, Nb, Ni, Re, Si, Sn, Ta, Ti, V, Zr)3(Al, Co, Cr, Ir, Nb, Ni, Rh, Ru, Si, Sn, Ta, Ti, V, Zr)1(C, Va)3	Cr3Si (A15)
CR5B3_D8L	tI32	I4/mcm	also Mo5B3.			(Cr, Mo)0.625(B)0.375	Cr5B3 (D8l)
CRB4	oI10	Immm				(Cr)0.2(B)0.8	CrB4
CRMN3_HT_SIGMA	tP30	P4_2/mnm				(Mn)8(Cr)4(Cr, Mn)18	sigma-CrFe (D8b)
CRNBSI	hP9	P-62m				(Cr)1(Nb)1(Si)1	ZrNiAl
CRNI2_OP6	oI6	Immm				(Cr, Mo, W)1(Mo, Ni, W)2	MoPt2
CRSI2_C40	hP9	P6_222	also NbSi2, TaSi2, VSi2.			(Cr, Cu, Hf, Mo, Nb, Si, Ta, Ti, V, W)1(Al, Cr, Cu, Si)2	CrSi2 (C40)
CRZN13	m**					(Cr)1(Zn)13	Unknown Structure
CRZN17	hP*					(Cr)1(Zn)17	Unknown Structure
CU10HF7	oS68	Cmce				(Cu)10(Hf)7	Ni10Zr7

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CU10SN3	hP26	P6_3	zeta.			(Cu, Ni)0.769(Sn)0.231	Cu10Sn3
CU10ZR7	oS68	Cmce				(Cu)10(Zr)7	Ni10Zr7
CU15SI4_EPS_D86	cI76	I-43d				(Cu, Mn)0.789474(Al, Si)0.210526	Cu15Si4 (D86)
CU2TI1	oS12	Cmcm				(Co, Cu, Ni)2(Ti)1	Au2V
CU2TIZR	hP12	P6_3/mmc				(Cu)0.5(Ti)0.25(Zr)0.25	MgZn2 Hexagonal Laves (C14)
CU2Y_HT	hP*					(Cu)2(Y)1	Unknown Structure
CU2Y_LT	oI12	Imma				(Cu)2(Y)1	CeCu2
CU33SI7_DELTA			HT phase			(Cu)0.825(Si)0.175	Unknown Structure
CU3SI_ETA	hR*	P-31m	United 3-allotropes:eta''-RT(oS* *), eta'-HT1(hR27 R-3), eta-HT2 (hR* P-31m)			(Cu, Mn, Ni)0.76(Si)0.24	Cu3Si-h2
CU3SN_HT_ GAMMA	cF16	Fm-3m	Cu3Sn HT solutionphase			(Cu, Mn, Ni, Sn, Zn)1	BiF3 (D03)
CU3SN_LT	oS80	Cmcm	epsilon			(Cu, Sn)3(Cu, Sn)1	Cu3Sn
CU3TI2	tP10	P4/nmm				(Cu, Fe, Ni)3(Co, Ti)2	Cu3Ti2
CU41SN11	cF416	F-43m	delta.			(Cu, Sn, Zn)41(Cu, Sn, Zn)11	Cu41Sn11
CU46NI25SI29						(Cu)0.458(Ni)0.25(Si)0.292	Unknown Structure
CU4MNSN_TAU1	cF24	F-43m				(Cu)0.6666(Sn)0.1667(Mn)0.1667	MgCu4Sn
CU4TI1	oP20	Pnma				(Cu, Ti)4(Cu, Ti)1	Au4Zr
CU4TI3	tI14	I4/mmm				(Co, Cu, Ni)4(Ti)3	Cu4Ti3

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CU4Y	mP16	P2_1/m				(Cu)4(Y)1	Cu5Y1.25
CU51HF14	hP68	P6/m				(Cu)51(Hf)14	Ag51Gd14
CU51ZR14	hP68	P6/m				(Cu)51(Zr)14	Ag51Gd14
CU56SI11_ GAMMA_A13	cP20	P4_132				(Cu, Mn, Ni, Si)0.835821(Si)0.164179	Mg3Ru2
CU5MN4SI						(Cu)0.5(Mn)0.37(Si)0.13	Unknown Structure
CU6NISI3						(Cu, Ni)0.732(Si)0.268	Unknown Structure
CU6SN5_HT	hP6	P6_3/mmc	also Co3Sn2,Mn(2-x)Sn, Ni3Sn2.			(Co, Cu, Mn, Ni, Va)1(Al, Cu, Ni, Sn)1(Co, Cu, Mn, Ni, Va)1	Ni2In (B82)
CU6SN5_LT	mS44	C2/c	eta-prime.			(Cu)1(Cu, Sn)1(Sn)1	Cu6Sn5
CU7Y1	hP8	P6/mmm	aka Cu6Y or Cu5.4Y0.8			(Cu2, Y)1(Cu)5	Cu7Tb
CU7Y2	hP68	P6/m				(Cu)7(Y)2	Ag51Gd14
CU8HF3	oP44	Pnma				(Cu)8(Hf)3	Cu8Hf3
CU8ZR3	oP44	Pnma				(Cu)8(Zr)3	Cu8Hf3
CUB_A13	cP20	P4_132				(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)1(B, C, Va)1	beta-Mn (A13)
CUMNZN_EPSILON_ HCP	hP2	P6_3/mmc				(Cu, Mn, Zn)1(Va)0.5	Hexagonal Close Packed (Mg, A3, hcp)
CUMNZN_TAU1	cF24	Fd-3m				(Cu)0.334(Mn)0.333(Zn)0.333	Cu2Mg Cubic Laves (C15)
CUTI_B11	tP4	P4/nmm	aka B11.			(Co, Cu, Ni, Ti)1(Cu, Ni, Ta, Ti)1	gamma-CuTi (B11)
CUTI3_L60	tP4	P4/mmm				(Cu, Ti)1(Ti)3	CuTi3 (L60)
DIAMOND_A4	cF8	Fd-3m	Pure C, Si or solidsolution phases based on them.			(Al, B, C, Si, Sn)1	Diamond (A4)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
DIS_MU	hR13	R-3m	Part of thedescription for the MU_PHASE			(Al, Co, Cr, Cu, Fe, Mn, Mo, Nb, Ni, Re, Ta, Ti, W)1	Fe7W6 (D85) mu-phase
DIS_SIG	tP30	P4_2/mnm	Part of thedescription for the SIGMA phase.			(Al, Co, Cr, Fe, Ir, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W)1	sigma-CrFe (D8b)
FCC_A1	cF4	Fm-3m	FCC_A1 will be combined to FCC_ L12 if defined.	A1	225	(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)1(B, C, N, Va)1	Face-Centered Cubic (Cu, A1, fcc)
FCC_L12	cP4	Pm-3m	This phase has some contribution from FCC_A1.			(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)0.75(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)0.25(B, C, N, Va)1	Bogdanovite (Cu3Au, L12)
FCC_L12#2						(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)0.75(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)0.25(B, C, N, Va)1	
FCC_L12#3						(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)0.75(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)0.25(B, C, N, Va)1	
FCC_L12#4						(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)0.75(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)0.25(B, C, N, Va)1	
FE2SI	hP6	P-3m1				(Fe)0.666667(Si)0.333333	AlNi2
FE3SN2	hR10	R-3m				(Fe)3(Sn)2	Fe3Sn2
FE3ZN7_GAMMA_ D82	cI52	I-43m				(Fe, Zn)0.154(Fe, Zn)0.154(Fe, Zn)0.231(Zn)0.461	gamma-brass (Cu5Zn8,D82)
FE4N_LP1	cP5	Pm-3m	Only stable in(Co-Cr-Fe)-N when gas suspended.			(Co, Cr, Fe, Mn, Ni)4(C, N)1	gama-Fe4N (L'10)
FE5SN3_B82	hP6	P6_3/mmc				(Fe)5(Sn)3	Ni2In (B82)
FE8SI2C	aP*	P1				(Fe)8(Si)2(C)1	Mn8Si2C
FECN_CHI	mS28	C2/c	Onlystable in C-Fe-N when gas suspended.			(Fe)2.2(C, N)1	Mn5C2 (Fe5C2 Hagg carbide)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
FENBZR_CFC2_C15	cF24	Fd-3m				(Fe, Nb, Zr)2(Nb, Zr)1(Nb, Zr)3	Cu2Mg Cubic Laves (C15)
FESI2_HT	tP3	P4/mmm				(Fe)0.3(Si)0.7	FeSi2-h
FESI2_LT	oS48	Cmce				(Fe)0.333333(Si)0.666667	FeSi2-l
FEZN10_DELTA	hP632	P6_3/mmc				(Fe)0.058(Fe, Zn)0.18(Zn)0.525(Zn)0.237	FeZn10
FEZN13_ZETA	mS28	C2/m				(Fe, Va)0.072(Zn)0.856(Va, Zn)0.072	CoZn13
FEZN4_GAMMA1_D81	cF408	F-43m				(Fe)0.137(Fe, Zn)0.118(Zn)0.745	Fe11Zn40
G_PHASE_D8A	cF116	Fm-3m				(Al, Co, Fe, Mn, Ni, Ti)16(Hf, Nb, Ti, Y, Zr)6(Co, Fe, Mn, Ni, Si)7	Th6Mn23 (D8a)
GAMMA_D83	cP52	P-43m	also Cu5Zn8, Ni5Zn8, Al5Cu8 (rt).			(Al, Ni, Si, Zn)4(Al, Cu, Ni, Si, Zn)1(Cu, Fe, Mn, Ni, Zn)8	gamma-brass (Cu9Al4, D83)
GAMMA_HT_D82	cI52	I-43m	aka GAMMA_H.			(Al, Zn)4(Al, Cu, Zn)1(Cu, Fe, Mn, Ni)8	gamma-brass (Cu5Zn8, D82)
GAS						(Al, Al1C1, Al1C2, Al1Cu1, Al1N1, Al2, Al2C2, B, B1C1, B1C2, B1N1, B2, B2C1, C, C1Ir1, C1N1, C1N2_Cnn, C1N2_Ncn, C1Rh1, C1Si1, C1Si2, C1Si3, C1Si4, C2, C2N1_Ccn, C2N1_Cnc, C2N2, C2Si1, C2Si2, C2Si3, C3, C3N1, C4, C4N1, C4N2, C5, C5N1, C60, C6N1, C6N2, C9N1, Co, Co2, Cr, Cr1N1, Cr2, Cu, Cu2, Fe, Fe2, Hf, Ir, Mn, Mo, Mo1N1, Mo2, N, N1Nb1, N1Si1, N1Si2, N1Ti1, N1V1, N1Zr1, N2, N3, Nb, Ni, Ni2, Re, Rh, Ru, Si, Si2, Si3, Sn, Sn2, Ta, Ti, Ti2, V, W, Y, Zn, Zr, Zr2)1	
GRAPHITE_A9	hP4	P6_3/mmc				(B, C)1	Hexagonal Graphite (A9)
HCP_A3	hP2	P6_3/mmc	Disordered HCP_A3 solution phase.			(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)1(B, C, N, Va)0.5	Hexagonal Close Packed (Mg, A3, hcp)
HCP_A3#2						(Al, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)1(B, C, N, Va)0.5	
HEUSLER_L21	cF16	Fm-3m	aka H_L21.			(Al, Cr, Ni, Sn, Ti)0.5(Al, Hf, Nb, Ni, Ta, Ti, Zr)0.5(Co, Fe, Ni, Ru, Va)1	Heusler (L21)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
HF1IR1			united HT/LT phase			(Hf)1(Ir)1	Unknown Structure
HF2IR	cF96	Fd-3m				(Hf)2(Ir)1	NiTi2
HF2RH	cF96	Fd-3m				(Hf)2(Rh)1	NiTi2
HF3N2	hR6	R-3m				(Hf)3(N)2	TiS-9R
HF3NI7	aP20	P-1				(Hf)0.3(Ni)0.7	Hf3Ni7
HF3RH4						(Hf)3(Rh)4	Unknown Structure
HF3RH5	oP16	Pbam				(Hf)3(Rh)5	Rh5Ge3
HF4N3	hR8	R-3m				(Hf)4(N)3	Sc2Te3
HF5IR3	hP48	P6_122				(Hf)5(Ir)3	Ir3Zr5
HF5SN4	hP18	P6_3/mcm				(Hf)5(Sn)4	Ti5Ga4
HF8NI21	aP29	P-1	also ZR8NI21.			(Hf, Zr)8(Ni)21	Hf8Ni21
HFIR3_L12	cP4	Pm-3m				(Hf)1(Ir)3	Bogdanovite (Cu3Au, L12)
HFMN	cF96	Fd-3m				(Hf)0.5(Mn)0.5	NiTi2
HFN_B1	cF8	Fm-3m				(Hf)1(N, Va)1	Rock Salt (NaCl, B1)
HFNI_ALPHA	oS8	Cmcm				(Hf)0.5(Ni)0.5	CrB (B33)
HFNI3_ALPHA	hP40	P6_3/mmc	the LT phase.			(Hf)0.25(Ni)0.75	PdRh2Ta
HFNI3_BETA	hR12	R-3m	the HT phase.			(Hf)0.25(Ni)0.75	BaPb3
HFRE	hR92	R-3c	also Hf21Re25.			(Hf)1(Re)1	Zr21Re25
HFRH_B2	cP2	Pm-3m				(Hf, Rh)1(Rh)1	CsCl (B2)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
HFSN2_C40	hP9	P6_222				(Hf)1(Sn)2	CrSi2 (C40)
IR2Y3	tI140	I4/mcm				(Ir)2(Y)3	Y3Rh2
IR2Y5	mS28	C2/c				(Ir)2(Y)5	Mn5C2 (Fe5C2 Hagg carbide)
IR3SI1	tI16	I4/mcm				(Ir)3(Si)1	SiU3 (D0c)
IR3SI2_B82	hP6	P6_3/mmc				(Ir)3(Si)2	Ni2In (B82)
IR3SI4	oP28	Pnma				(Ir)3(Si)4	Ru4Si3
IR3SI5	mP64	P2_1/c				(Ir)3(Si)5	Ir3Si5
IR3W_D019	hP8	P6_3/mmc				(Ir, W)3(Ir, W)1	Ni3Sn (D019)
IR3Y1	hR12	R-3m				(Ir)3(Y)1	Ni3Pu
IR3Y5	hP16	P6_3/mcm	unitedHT/LT phase.			(Ir)3(Y)5	Mavlyanovite (Mn5Si3, D88)
IR3ZR5	hP48	P6_122				(Ir)3(Zr)5	Ir3Zr5
IR4B3	oF28	Fmm2				(Ir)4(B)3	Ir4B3
IR4B5	mS18	Cm				(Ir)4(B)5	Ir4B5
IR4SI5	mP18	P2_1/m				(Ir)4(Si)5	Ru4Si5
IR5B4	tI36	I4_1/a				(Ir)5(B)4	Ir5B4
IRMN_L10	tP2	P4/mmm	also IrTi.			(Ir, Mn, Ti)0.5(Ir, Mn, Ti)0.5	CuAu (L10)
IRNB_L10	tP2	P4/mmm				(Ir, Nb)1(Ir, Nb)1	CuAu (L10)
IRSI_B27	oP8	Pnma	the HT phase.			(Ir)1(Si)1	FeB (B27)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
IRSI3_HT	oS*					(Ir)1(Si)3	Unknown Structure
IRSI3_LT	mS*					(Ir)1(Si)3	Unknown Structure
IRV_L10	tP2	P4/mmm	aka Ir1.04V0.96 orIrV1-x.			(Ir)0.5(Ir, V)0.5	CuAu (L10)
IRV_RT	oS8	Cmmm				(Ir)1(V)1	alpha-IrV
IRW_EPSILON_HCP	hP2	P6_3/mmc	HT epsilon solution phase with HCP structure.			(Ir, W)1(Ir, W)1	Hexagonal Close Packed (Mg, A3, hcp)
IRW_LT_B19	oP4	Pmma				(Ir)1(Ir, W)1	beta'-AuCd (B19)
IRY3_D011	oP16	Pnma				(Ir)1(Y)3	Cementite (Fe3C, D011)
IRZR_ALPHA	oS16	Cmcm	LT phase.			(Ir, Zr)1(Zr)1	Mn3As (D0d)
IRZR_BETA_B2	cP2	Pm-3m	i.e. HT- or beta- phase.			(Ir, Zr)1(Ir, Zr)1	CsCl (B2)
IRZR3_D0E	tI32	I-42m				(Ir)1(Zr)3	alpha-V3S
LIQUID						(Al, Al1N1, B, C, Co, Cr, Cu, Fe, Hf, Hf1N1, Ir, Mn, Mo, N, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)1	
M11SI8	oP76	Pnma	also Cr11Si8, Nb11Si8.			(Cr, Nb)11(Si)8	Cr11Ge8
M12C	cF104	Fd-3m	also Mo6Ni6C			(Co, Ni)6(Mo, W)6(C)1	Fe6W6C
M23B6_TAU_D84	cF116	Fm-3m	ternary boride.			(Co, Hf, Ni, Re)20(B)6(B, Va)6(Al, Cr, Hf, Mo, Re, Ta, Ti, V, W, Zr)3	Th6Mn23 (D8a)
M23C6_D84	cF116	Fm-3m				(Co, Cr, Fe, Mn, Ni, Re, V)20(Co, Cr, Fe, Mn, Mo, Ni, Re, V, W)3 (C)6	Cr23C6 (D84)
M2B_C16	tI12	I4/mcm	akaM2B_TETR.			(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ta, W)2(B)1	Khatyrkite (Al2Cu, C16)
M3B_D011	oP16	Pnma	alsoNI3B_D011.			(Co, Cr, Fe, Mo, Ni)3(B)1	Cementite (Fe3C, D011)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
M3B2_D5A	tP10	P4/mbm	also NB3B2, TA3B2,V3B2.			(Fe, Hf, Mo, Nb, Ta, V)3(B)2	Si2U3 (D5a)
M3B2_T	tP10	P4/mbm	ternary borideMo2FeB2 or Mo2CrB2.			(Cr, Fe, Mo, Ni, W)0.4(Cr, Fe, Ni)0.2(B)0.4	Si2U3 (D5a)
M3B4_D7B	oI14	Immm	also ternary X1Y2B4boride.			(B)4(Al, Cr, Hf, Mn, Nb, Ta, Ti, V)3	Ta3B4 (D7b)
M3C2_D510	oP20	Pnma				(Co, Cr, Mo, V, W)3(C)2	Tongbaite (Cr3C2, D510)
M3SI1	tP32	P4_2/n	also Nb3Si, Ta3Si, Ti3Si, Zr3Si.			(Hf, Nb, Ta, Ti, Zr)3(Si)1	Ti3P
M3SI2_D5A	tP10	P4/mbm	also Hf3Si2, Zr3Si2.			(Hf, Nb, Zr)3(Si)2	Si2U3 (D5a)
M3Y	hR12	R-3m	also Fe3Y, Ni3Y.			(Fe, Ni)3(Y)1	Ni3Pu
M4SI3	oP28	Pnma	also Cr4Si3, Nb4Si3.			(Cr, Ni, Ru)4(Si)3	Ru4Si3
M5B6	oS22	Cmmm	also Nb5B6.			(Nb, V)5(B)6	V5B6
M5C2	mS28	C2/c				(Fe, Mn)5(C)2	Mn5C2 (Fe5C2 Hagg carbide)
M5SI3_D88	hP16	P6_3/mcm	also M5Sn3, M5Si3C.			(Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Si, Ti, W, Y, Zr)2(Al, Cr, Si, Sn, Ti)3(Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Ti, Y, Zr)3(C, Sn, Va)1	Mavlyanovite (Mn5Si3, D88)
M6C_E93	cF112	Fd-3m				(Co, Fe, Ni)2(Mo, Nb, Ta, W)2(Co, Cr, Fe, Mo, Nb, Ni, Ta, V, W)2(C)1	Fe3W3C (E93)
M6SI5	oI44	Ibam	also Cr6Si5, Nb6Si5.			(Cr, Nb, Ti, V)6(Si)5	Si5V6
M7B3_D102	hP20	P6_3mc	also RH7B3,RE7B3_D102.			(Co, Cr, Mo, Nb, Re, Rh, Ru, Ta, W)7(B)3(B, Va)3	Fe3Th7 (D102)
M7C3_D101	oP40	Pnma				(Co, Cr, Fe, Mn, Mo, Ni, Re, V, W)7(C)3	C3Cr7 (D101)
MB_B27	oP8	Pnma	also CoB, HfB, MnB, TiB.			(B)1(Co, Cr, Fe, Hf, Mn, Mo, Re, Ti, Y)1	FeB (B27)
MB_B33	oS8	Cmcm	also NbB, NiB, TaB, VB.			(Cr, Fe, Hf, Mo, Nb, Ni, Ta, Ti, V)1(B)1	CrB (B33)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
MB2_C32	hP3	P6/mmm				(B)2(Al, Cr, Hf, Mn, Mo, Nb, Ru, Ta, Ti, V, Y, Zr)1	Hexagonal omega (C32)
MC_ETA	hP12	P6_3/mmc				(Mo, V, W)1(C, Va)1	CMo
MC_SHP	hP2	P-6m2	also MoC_LT,Strukturbericht Bh			(Mo, W)1(C, N)1	Tungsten Carbide (Bh)
MN11SI19	tP120	P-4n2				(Mn)11(Al, Si)19	Mn11Si19
MN12Y_D2B	tI26	I4/mmm				(Mn)12(Y)1	Mn12Th (D2b)
MN15NI45SI40			ternary T1 orN phase			(Mn)0.15(Ni)0.45(Si)0.4	Unknown Structure
MN15NI50SI35			ternary T2 orPHI phase			(Mn)0.15(Ni)0.5(Si)0.35	Unknown Structure
MN1NI1SI1_C37	oP12	Pnma	ternary T4 or E phase			(Mn)1(Ni)1(Si)1	MnCuP
MN2B_D1F	oF48	Fddd				(Mn)0.6707(B)0.3293	Mg2Cu (Cb)
MN2NISI			ternary T8 or S phase			(Mn, Ni)3(Si)1	Unknown Structure
MN3N2	tI10	I4/mmm	aka MN6N4.			(Mn)6(N)4	Mn3N2
MN3NI2SI	cF96	Fd-3m	ternary T7 or Omega			(Mn)3(Ni)2(Si)1	Mn3Ni2Si
MN3SI_D03	cF16	Fm-3m				(Fe, Mn)3(Al, Si)1	BiF3 (D03)
MN3SN2	oP20	Pnma				(Mn)3(Sn)2	Tongbaite (Cr3C2, D510)
MN3TI1			HT phase			(Mn)3(Ti)1	Unknown Structure
MN4TI	hR53	R-3	aka Ti9Mn42			(Cr, Mn)0.815(Ti)0.185	R-(Co,Cr,Mo)
MN52NI29SI19			ternary phaseT11 or W phase			(Mn)0.52(Ni)0.29(Si)0.19	Unknown Structure
MN66NI4SI30			ternary T10 orU phase			(Mn)0.66(Ni)0.04(Si)0.3	Unknown Structure
MN6N5	tI4	I4/mmm				(Mn)6(N)5	CoO

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
MN6NI16SI7	cF116	Fm-3m	ternary T3 or G phase			(Mn)0.206897(Ni)0.551724(Si)0.241379	Th6Mn23 (D8a)
MN6NISI3	hR53	R-3	ternary T9 or R'phase			(Mn)0.61(Ni)0.12(Si)0.27	R-(Co,Cr,Mo)
MN6SI	hR13	R-3m				(Al, Mn)17(Si, Zn)3	Fe7W6 (D85) mu-phase
MN9SI2	oI186	Immm				(Mn)33(Si)7	Mn9Si2
MNB4	mS10	C2/m				(Mn)0.2(B)0.8	MnB4
MNNI_L10	tP2	P4/mmm				(Cu, Mn, Ni)0.5(Cu, Mn, Ni)0.5	CuAu (L10)
MNNI2						(Mn, Ni)1(Ni)2	Unknown Structure
MNNISI_T5	hP12	P6_3/mmc	ternary T5 or tao_1 phase			(Mn)1(Ni, Si)2	MgZn2 Hexagonal Laves (C14)
MNNISI_T6	cF24	Fd-3m	ternary T6or tao_2 phase			(Mn)1(Ni, Si)2	Cu2Mg Cubic Laves (C15)
MNTA						(Mn)1(Ta)1	Unknown Structure
MNTI_HT	t**		aka TiMn Mn+ orTi0.47Mn0.53			(Mn)0.515(Ti)0.485	Unknown Structure
MNTI_LT	hR92	R-3c	aka Ti21Mn25_RT.			(Mn)1(Ti)1	Zr21Re25
MNZN9	h**					(Mn)1(Zn)9	Unknown Structure
MO1IR3	hP8	P6_3/mmc				(Mo)1(Ir, Mo)3	Ni3Sn (D019)
MO2B5_D8I	hR7	R-3m				(Mo)0.32(B)0.68	Mo2B5 (D8i)
MO3IR_A15	cP8	Pm-3n				(Mo)3.06(Ir)0.94	Cr3Si (A15)
MO7IR3	tP30	P4_2/mnm				(Mo)0.7(Ir)0.3	sigma-CrFe (D8b)
MOB_BG	tI16	I4_1/amd				(Cr, Fe, Mo)1(B)1	MoB (Bg)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
MOB4	hP16	P6_3/mmc				(Mo)0.2(B)0.8	MoB4
MOIR_HT	hP2	P6_3/mmc				(Ir, Mo)1(Ir, Mo)1	Hexagonal Close Packed (Mg, A3, hcp)
MOIR_LT_B19	oP4	Pmma				(Mo)1(Ir)1	beta'-AuCd (B19)
MONI_DELTA	oP56	P2_12_12_1				(Co, Cr, Fe, Ni, Re)24(Co, Cr, Fe, Mo, Ni, Re, W)20(Cu, Mo, W)12	MoNi
MONI4_BETA_D1A	tI10	I4/m	also WNi4.			(Mo, W)1(Ni)4	Ni4Mo (D1a)
MOSI2_C11B	tI6	I4/mmm	also AlCr2, Ti2Zn,ZnZr2, CUZR2_ C11B.			(Al, Co, Cu, Fe, Mo, Ni, Rh, W, Zn)1(Al, Cr, Hf, Si, Ti, Zr)2	MoSi2 (C11b)
MOZN22	cF420	F-43m				(Mo)1(Zn)22	Zn93(Zn0.43Mo0.57)Mo4
MOZN7	cF32	Fm-3m				(Mo)1(Zn)7	Ca7Ge
MSI_B20	cP8	P2_13	also CoSi, CrSi, MnSi, ReSi.			(Co, Cr, Fe, Mn, Ni, Re)1(Al, Si)1	FeSi (B20)
MSI_B27	oP8	Pnma	also TiSi, HfSi, YSi,ZrSi(alpha).			(Hf, Nb, Ti, Y, Zr)1(Al, Si)1	FeB (B27)
MSI2_C1	cF12	Fm-3m	also NiSi2, CoSi2.			(Co, Cu, Mn, Ni)1(Al, Cu, Si)2	Fluorite (CaF2, C1)
MU_PHASE	hR13	R-3m	DIS_MUcontribution added onto it.			(Al, Co, Cr, Cu, Fe, Mn, Mo, Nb, Ni, Re, Ta, Ti, W)1(Al, Co, Cr, Cu, Fe, Mn, Mo, Nb, Ni, Re, Ta, Ti, W)2(Al, Co, Cr, Cu, Fe, Mn, Mo, Nb, Ni, Re, Ta, Ti, W)6(Al, Co, Cr, Cu, Fe, Mn, Mo, Nb, Ni, Re, Ta, Ti, W)4	Fe7W6 (D85) mu-phase
MY3_D011	oP16	Pnma	also CoY3, NiY3.			(Co, Ni)1(Y)3	Cementite (Fe3C, D011)
MZR3_E1A	oS16	Cmcm	also CoZr3, FeZr3.			(Co, Fe, Ni)1(Zr)3	MgCuAl2 (E1a)
NB13NI75TI12_XD						(Nb)0.13(Ni)0.75(Ti)0.12	Unknown Structure
NB15NI56TI29_XA	o*100					(Nb)0.15(Ni)0.56(Ti)0.29	Unknown Structure
NB15NI80TI5_XE						(Nb)0.15(Ni)0.8(Ti)0.05	Unknown Structure

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
NB1ZN1						(Nb)0.5(Zn)0.5	Unknown Structure
NB2ZN3_D85	hR13	R-3m				(Nb)0.4(Zn)0.6	Fe7W6 (D85) mu-phase
NB3RU5	oP16	Pbam	united Nb3Ru5_HT andNbRu3_LT phase			(Nb, Ru)0.375(Ru)0.625	Rh5Ge3
NB5NI75TI20_XC	hP8	P6_3/mmc				(Nb)0.05(Ni)0.75(Ti)0.2	Ni3Sn (D019)
NB8NI9TI3_XB						(Nb)0.4(Ni)0.45(Ti)0.15	Unknown Structure
NBSN2_CB	oF48	Fddd				(Nb, Sn, V)1(Nb, Sn)2	Mg2Cu (Cb)
NBZN15	oS68	Cmcm				(Nb)0.0625(Zn)0.9376	TiZn16
NBZN2_C36	hP24	P6_3/mmc				(Nb)0.333(Zn)0.667	MgNi2 Hexagonal Laves (C36)
NBZN3_L12	cP4	Pm-3m				(Nb)0.25(Zn)0.75	Bogdanovite (Cu3Au, L12)
NBZN7						(Nb)0.125(Zn)0.875	Unknown Structure
NI10ZR7	oS68	Cmce	also Ni10Hf7.			(Ni)23(Hf, Zr)17	Ni10Zr7
NI11ZR9	tI40	I4/m	also Ni11Hf9.			(Ni)11(Hf, Zr)9	Pt11Zr9
NI17Y2	hP80	P6_3/mmc	also Fe17Y2.			(Al, Fe, Ni)1(Y)0.1176	Fe17Lu2
NI2SI_THETA	hP6	P-3m1	aka M2SI_TETA.			(Cu, Ni)1(Ni, Va)1(Al, Si)1	AlNi2
NI2TA_C11B	tI6	I4/mmm				(Co, Ni)2(Ta, Ti)1	MoSi2 (C11b)
NI2V	oI6	Immm				(Mo, Ni)2(Mo, Nb, Ta, V)1	MoPt2
NI2Y1	cF192	F-43m				(Ni)2(Y)1	Ni2Tm
NI2Y3	tP80	P4_12_12				(Ni)2(Y)3	Ni2Y3

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
NI3SI_MONOCL	hP34	P-3				(Ni)3(Si)1	Ge9Pd25
NI3SI_ORTHO_D011	oP16	Pnma				(Ni)3(Si)1	Cementite (Fe3C, D011)
NI3SI2	oP80	Cmc2_1				(Ni)3(Si)2	Ni3Si2
NI3SN4	mS14	C2/m				(Cu, Ni)0.25(Ni, Sn)0.25(Sn)0.5	delta-Ni3Sn4 (D7a)
NI3TA_D0A	oP8	Pmmn	also delta,Ni3Mo, Ni3Nb.			(Al, Co, Cr, Fe, Nb, Ni)3(Al, Fe, Mo, Nb, Ni, Ta, Ti, V, W)1	beta-TiCu3 (D0a)
NI3TI_D024	hP16	P6_3/mmc	also Eta,AlNi6Ta.			(Al, Co, Cr, Cu, Fe, Hf, Ni, Ta, Ti, W, Zr)0.75(Al, Cr, Cu, Hf, Mo, Nb, Ni, Si, Ta, Ti, W, Zr)0.25	Ni3Ti (D024)
NI4B3	mS28	C2/c				(Ni)0.57142857(B)0.42857143	m-Ni4B3
NI4Y	hR*					(Ni)4(Y)1	Unknown Structure
NI5SI2	hP42	P321				(Co, Cr, Cu, Fe, Ni)5(Si)2	Ni31S12
NI5ZR_C15B	cF24	F-43m	alsoNi5Y/Ni5Hf/Cu5Hf/Cu5Zr, aka ZRM5_C15B.			(Al, Cu, Ni)5(Hf, Y, Zr)1	AuBe5 (C15b)
NI7ZR2	mS36	C2/m	also NI7HF2, NI7Y2, CO7HF2 andCO7Y2.			(Al, Co, Cr, Ni)7(Hf, Y, Zr)2	Ni7Zr2
NI8M	tI18	I4/mmm	also Ni8Ta, Ni8Nb.			(Ni)8(Nb, Ta)1	Pt8Ti
NISI_B31	oP8	Pnma				(Ni)1(Si)1	MnP (B31)
NITI2	cF96	Fd-3m				(Co, Cr, Cu, Fe, Ni, Re, Ti)1(Al, Cr, Cu, Hf, Ni, Ta, Ti, Zr)2	NiTi2
NIY_B27	oP8	Pnma				(Ni)1(Y)1	FeB (B27)
NIZN_TP2	tP2	P4/mmm	united HT/LT phase.			(Al, Cu, Ni, Zn)0.5(Al, Ni, Zn)0.5	CuAu (L10)
NIZN8_DELTA	mS50	C2/m				(Ni)0.1111111(Al, Zn)0.8888889	Ni3Zn22
NIZR_B33	oS8	Cmcm				(Ni)1(Ti, Zr)1	CrB (B33)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
O_PHASE	oS16	Cmcm	aka Ti2NbAl, the Ophase.			(Nb, Ta, Ti)0.5(Al, Nb, Ta, Ti)0.25(Nb, Ta, Ti)0.25	NaHg
P_PHASE	oP56	Pnma				(Cr, Fe, Ni, Re)24(Cr, Fe, Mo, Ni, Re)20(Mo)12	Cr9Mo21Ni20
PI_A13	cP20	P4_132	i.e.Cr-(Fe,Ni)-N nitride.			(Cr)12.8(Fe, Ni)7.2(N)4	beta-Mn (A13)
R_PHASE	hR53	R-3				(Co, Cr, Fe, Ni, Re)27(Mo, W)14(Co, Cr, Fe, Mo, Ni, Re, W)12	R-(Co,Cr,Mo)
RE2SI	mP24	P2_1/c				(Re)2(Si)1	Re2Si
RE3B_E1A	oS16	Cmcm				(Cr, Mo, Re, Ta, W)3(B)1	Re3B
REB2	hP6	P6_3/mmc				(Re)1(B)2(B, Va)2	ReB2
RESI2_C11B	mS44	Cm				(Re)0.357(Si)0.643	Re4Si7
REZR2	hR92	R-3c	aka Zr21Re25.			(Ni, Re)1(Zr)2	Zr21Re25
RH2SN	oP12	Pnma				(Rh)2(Sn)1	Co2Si (C37)
RH3SN2	hP6	P6_3/mmc				(Rh)0.125(Rh)0.5(Sn)0.375	Ni2In (B82)
RH3ZR_L12	cP4	Pm-3m				(Rh, Zr)3(Rh, Zr)1	Bogdanovite (Cu3Au, L12)
RH4ZR3_HT			beta_Rh4Zr3			(Rh, Zr)4(Zr)3	Unknown Structure
RH4ZR3_LT	hR14	R-3	alpha_Rh4Zr3.			(Rh, Zr)4(Zr)3	Pd4Pu3
RH5TI3	oP16	Pbam				(Rh)5(Ti)3	Rh5Ge3
RH5ZR3	oS32	Cmcm				(Rh)5(Rh, Zr)3	Pd5Pu3
RHB_B81	hP4	P6_3/mmc				(Rh)1(B)1.1	NiAs (B81)
RHSN_B20	cP8	P2_13				(Rh)1(Sn)1	FeSi (B20)
RHSN2_RT	tI26	I4/mmm				(Rh)0.33333(Sn)0.66667	RhSn2

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
RHSN4	hP15	P3_121				(Rh)1(Sn)4	IrGe4
RHZR_HT_B2	cP2	Pm-3m	i.e. beta_RhZr.			(Rh)1(Rh, Zr)1	CsCl (B2)
RHZR_LT	oS16	Cmcm	i.e. alpha_RhZr			(Rh)1(Rh, Zr)1	IrZr
RHZR2	cF96	Fd-3m				(Rh)1(Zr)2	NiTi2
RU1B1	cI*					(Ru)1(B)1	Unknown Structure
RU25Y44	oP276	Pnna				(Ru)0.362(Y)0.638	Ru25Y44
RU2B3	hP10	P6_3/mmc				(Ru)2(B)3	Ru2B3
RU2SI_C37	oP12	Pnma				(Ru)2(Si)1	Co2Si (C37)
RU2SI3	oP40	Pbcn	united HT/LT phase.			(Ru)2(Si)3	Ge3Ru2
RU2SN3	tP20	P-4c2				(Ru)0.4(Sn)0.6	Ru2Sn3
RU2Y3	hP10	P6_3/m				(Ru)0.4(Y)0.6	Er3Ru2
RU2Y5	mS28	C2/c				(Ru)0.286(Y)0.714	Mn5C2 (Fe5C2 Hagg carbide)
RU3SN7_D8F	cI40	Im-3m				(Ru)0.3(Sn)0.7	Ir3Ge7 (D8f)
RUSI	cP8	P2_13	united HT_B2/LT_B20 phase.			(Ru)1(Si)1	FeSi (B20)
RUY3_D011	oP16	Pnma				(Ru)0.25(Y)0.75	Cementite (Fe3C, D011)
SI3N4	hP28	P31c				(Si)3(N)4	Nierite (alpha-Si3N4)
SIB3_D1G	hR15	R-3m				(B)6(Si)2(B, Si)6	B13C2 B4C (D1g)
SIB6	oP280	Pnnm				(B)210(Si)23(B, Si)48	SiB6

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
SIC_B3	cF8	F-43m				(Si)1(C)1	Zincblende (ZnS, B3)
SIGMA	tP30	P4_2/mnm	DIS_SIGcontribution added onto it.			(Al, Co, Cr, Fe, Ir, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W)10(Al, Co, Cr, Fe, Ir, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W)4(Al, Co, Cr, Fe, Ir, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W)16	sigma-CrFe (D8b)
SN10Y11	tI84	I4/mmm				(Sn)10(Y)11	Ge10Ho11
SN2Y_C49	oS12	Cmcm				(Sn)2(Y)1	ZrSi2 (C49)
SN3TI2						(Sn)3(Ti)2	Unknown Structure
SN3Y1	oS16	Amm2				(Sn)3(Y)1	GdSn2.75
SN4Y5	oP36	Pnma				(Sn)4(Y)5	Gd5Si4
SN5TI6	hP22	P6_3/mmc	also Sn5Nb6.			(Al, Sn)5(Nb, Ti)6	Sn5Ti6-beta
SN5Y2	oP14	Pmmn				(Sn)5(Y)2	Shcherbinaite (V2O5) (Revised)
SNTI2_B82	hP6	P6_3/mmc				(Sn)1(Ti)2	Ni2In (B82)
T1CUFETI_CU2TI	oS12	Cmcm	ternaryTi0.33FexCu0.67-x, Tau1.			(Cu, Fe)2(Ti)1	Au2V
T1CUNITI_C11B	tI6	I4/mmm	the Cu-Ni-Titernary phase Tau1.			(Cu, Ni)2(Ti)1	MoSi2 (C11b)
T2CUFETI_CU3TI2	tP10	P4/nmm	ternaryTi0.4FexCu0.6-x, Tau2.			(Cu, Fe)3(Ti)2	Cu3Ti2
T2CUNITI	tP10	P4/nmm	the Cu-Ni-Titernary phase Tau2.			(Cu)0.175(Ni)2.825(Ti)2	Cu3Ti2
T3CUFETI_CU4TI3	tI14	I4/mmm	ternaryTi0.43FexCu0.57-x, Tau3.			(Cu, Fe)4(Ti)3	Cu4Ti3
T4CUFETI			ternaryTi0.37FexCu0.63-x, Tau4			(Cu, Fe)0.63(Ti)0.37	Unknown Structure
T4CUNITI	hR12	R-3m	the Cu-Ni-Ti ternaryphase Tau4.			(Cu)0.05(Ni)0.7(Ti)0.25	BaPb3
T5CUFETI			ternaryTi0.45FexCu0.55-x, Tau5.			(Cu, Fe)0.55(Ti)0.45	Unknown Structure

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
T6CUNITI			the Cu-Ni-Ti ternaryphase Tau6			(Cu)0.25(Ni)0.5(Ti)0.25	Unknown Structure
TA1AL1	mP86	P2_1/c				(Ta)0.51515(Al)0.48485	Al38Ta48
TA3SN_A15	cP8	Pm-3n				(Ta)3(Sn)1	Cr3Si (A15)
TA41IR59	tP2	P4/mmm	akaTa0.82Ir1.18_rt, gamma.			(Ta)0.41(Ir)0.59	CuAu (L10)
TA43IR57	oP12	Pmma	aka Ta0.86Ir1.14, delta.			(Ta)0.43(Ir, Ta)0.57	TaIr
TA5SI3_D8L	tI32	I4/mcm	also alpha-Nb5Si3.			(Hf, Nb, Ta)5(Al, Si)3	Cr5B3 (D8l)
TAAL2_HT	cF444	F-43m				(Ta)0.35(Al)0.65	Al69Ta39
TAN_EPS	hP6	P-62m				(Ta)1(N)1	TaN-eps
TASN2_CB	oF48	Fddd	also SN2TA_CB.			(Ta)1(Sn)2	Mg2Cu (Cb)
TI25MN9AL66_L12	cP4	Pm-3m	also Ti25Mn8Al67 or Ti43Mn11Al66, Tau1.			(Al, Mn, Ti)0.75(Al, Mn, Ti)0.25	Bogdanovite (Cu3Au, L12)
TI2ALC	hP8	P6_3/mmc	i.e. Ti2AlC1-x.			(Ti)2(Al)1(C, Va)1	AlCCr2
TI2N_C4	tP6	P4_2/mnm				(Ti)2(N)1	Rutile (TiO2, C4)
TI3ALC_E21	cP5	Pm-3m	i.e.Ti3AlC1-x.			(Ti)3(Al)1(C, Va)1	Cubic Perovskite (CaTiO3, E21)
TI3ALC2	hP12	P6_3/mmc				(Ti)3(Al, Si)1(C, Va)2	Ti3SiC2
TI3N2	hR6	R-3m				(Ti)0.71(N)0.29	TiS-9R
TI3SIC2	hP12	P6_3/mmc				(Ti)3(Si)1(C)2	Ti3SiC2
TI4N3	hR8	R-3m	aka Xi-TiN0.58 HT			(Ti)0.685(N)0.315	Sc2Te3
TISI2_C54	oF24	Fddd	also MoSi2, RuAl2, ZrSn2.			(Mo, Nb, Ru, Ti, Zr)1(Al, Si, Sn)2	TiSi2 (C54)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
TIZN10	tP100	P4_2/mbc				(Ti)1(Zn)10	Ti3Zn22
TIZN15	oS68	Cmcm				(Ti)1(Zn)15	TiZn16
TIZN5						(Ti)1(Zn)5	Unknown Structure
V2B3	oS20	Cmcm				(V)0.4(B)0.6	V2B3
V3SN_A15	cP8	Pm-3n				(Sn)0.205(V)0.795	Cr3Si (A15)
V4ZN5	tI18	I4/mmm				(V)4(Zn)5	V4Zn5
VSN2_CB	oF48	Fddd				(Sn)0.6(V)0.4	Mg2Cu (Cb)
VZN3_L12	cP4	Pm-3m				(V)1(Zn)3	Bogdanovite (Cu3Au, L12)
W2B5_D8I	hR7	R-3m	nonstoichiometric W2B5.			(B, C, Va)5(W)2	Mo2B5 (D8i)
W2B9	hP22	P-3				(B)9(W)2	W2B9
W3MC	hP34	P6_3/mmc	also W3CoC, W3NiC.			(W)3(Co, Ni)1(C)1	W10Co3C3.4
W5SI3_D8M	tI32	I4/mcm	also Cr5Si3, Mo5Si3,Nb5Si3, V5Si3.			(Cr, Fe, Mo, Nb, Ti, V, W)4(Cr, Fe, Mo, Nb, Si, Ti, V, W)1(Al, Si, Sn)3	W5Si3 (D8m)
WB_ALPHA_BG	tI16	I4_1/amd				(B, C, Va)1(W)1	MoB (Bg)
WB_BETA_B33	oS8	Cmcm				(B, C, Va)1(W)1	CrB (B33)
Y13ZN58	hP146	P6_3/mmc				(Y)13(Zn)58	Y13Zn58
Y15C19_ALPHA	oP18	Pbam	aka Y15C19_R.			(C)19(Y)15	alpha-Y15C19
Y15C19_BETA			the high temperaturebeta phase			(C)19(Y)15	Unknown Structure
Y1ZN3	oP16	Pnma				(Y)1(Zn)3	Zn3Y

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
Y2C3_ALPHA	tP70	P4/mnc	aka Y2C3_R.			(Y)2(C)2(C, Va)1	Sc3C4
Y2C3_BETA			HT phase			(Y)2(C)2(C, Va)1	Unknown Structure
Y2ZN17	hP38	P6_3/mmc				(Y)2(Zn)17	Ni17Th2
Y3SI5_HT_CC	tI12	I4_1/amd				(Y)3(Si)5	alpha-ThSi2 (Cc)
Y3SI5_LT_C32	hP3	P6/mmm				(Y)3(Si)5	Hexagonal omega (C32)
Y5SI4	oP36	Pnma				(Y)5(Si)4	Gd5Si4
YB4_D1E	tP20	P4/mbm				(Y)0.2(B)0.8	ThB4 (D1e)
YB6_D21	cP7	Pm-3m				(Y)1(B)6	CaB6 (D21)
YB66	cF1936	Fm-3c				(Y)1(B)66	YB66
YC_GAMMA_B1	cF8	Fm-3m				(Y)1(C, C2, Va)1	Rock Salt (NaCl, B1)
YC2_C11A	tI6	I4/mmm				(C2Y1)1	CaC2-I (C11a)
YSI2_HT_CC	tI12	I4_1/amd				(Y)1(Si)2	alpha-ThSi2 (Cc)
YSI2_LT_C32	hP3	P6/mmm				(Y)1(Si)2	Hexagonal omega (C32)
YZN2_HT						(Y)1(Zn)2	Unknown Structure
YZN2_LT						(Y)1(Zn)2	Unknown Structure
YZN5	hP36	P6_3/mmc	aka H_RZN5			(Y)1(Zn)5	ErZn5
Z_PHASE	tP6	P4/nmm				(Cr, Fe)1(Mo, Nb, V)1(N, Va)1	CrNbN
ZN11Y3	oI28	Immm				(Zn)11(Y)3	Al11La3
ZN12Y_D2B	tI26	I4/mmm				(Zn)12(Y)1	Mn12Th (D2b)

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
ZN22ZR	cF184	Fd-3m				(Zn)22(Zr)1	Zn22Zr
ZN2ZR3	tP20	P4_2/mnm				(Zn)2(Zr)3	Zr3Al2
ZN39ZR5	mS88	C2/m				(Zn)39(Zr)5	Zn39Zr5
ZN3ZR_HT	c**					(Zn)3(Zr)1	Unknown Structure
ZNZR_B2	cP2	Pm-3m				(Zn)1(Zr)1	CsCl (B2)
ZR5SI4_TP36	tP36	P4_12_12	also Hf5Si4, Ti5Si4.			(Hf, Nb, Ti, Zr)5(Al, Si)4	Si4Zr5
ZRB12_D2F	cF52	Fm-3m	also YB12.			(B)12(Y, Zr)1	UB12 (D2f)
ZRSI2_C49	oS12	Cmcm	also HfSi2.			(Hf, Nb, Zr)1(Si)2	ZrSi2 (C49)
AL13NI2TI5_L12	cP4	Pm-3m	Tau1			(Al)13(Ni)2(Ti)5	AuCu3

TCHEA6 Properties Data

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

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 High Entropy Alloys 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 high entropy alloys including links to resources such as examples, publications, and more.

TCHEA: TCS High Entropy Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS High Entropy Alloys Database (TCHEA)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**6.0**
First release:	**TCHEA1 was released in 2015**

Changes in the Most Recent Database Release

TCHEA5.1 to TCHEA6.0

Software release version: 2022b (June 2022)

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

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

Previous Releases

TCHEA5.0 to TCHEA5.1

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

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

TCHEA4.2 to TCHEA5.0

Software release version: 2021b (June 2021)

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

TCHEA4.1 to TCHEA4.2

Software release version: 2021a (January 2021)

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

TCHEA4.0 to TCHEA4.1

Software release version: 2020b (June 2020)

- Crystal structure information is included for all phases.
- HCP_ZN is merged into HCP_A3. The epsilon phase with HCP structure in the Cu-Zn, Mn-Zn and Cu-Mn-Zn systems is separated from HCP_A3 and renamed as CUMNZN_EPSILON_HCP.
- Better estimation of excess energy for metastable solution phases and compound energy for metastable end-members in binary systems.

TCHEA3.1 to TCHEA4.0

Software release version: 2020a (January 2020)

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

TCHEA3.0 to TCHEA3.1

Software release 2019a (December 2018).

- The Mn-Ni-Si ternary is critically assessed in full composition and temperature ranges.
- Some bug fixes e.g. avoid the fictitious HCP_ZN phase appears in Zn-free systems, adjust the phase stability of GAMMA_D03, CRSI2_C40, C15- & C36- laves phases in some systems.

TCHEA2.0 to TCHEA3.0

Software release version: 2018a (April 2018)

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

TCHEA2.0 to TCHEA2.1

Software release version: 2017b (October 2017)

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

TCHEA1.0 to TCHEA2.0

Software release version: 2017a (March 2017)

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