Thermo-Calc Software

TCS High Entropy Alloys Database (TCHEA4)

Technical Information

Available Starting with Thermo-Calc Version 2020b

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About the TCS High Entropy Alloys Database (TCHEA)

TCHEA: TCS High Entropy Alloys Database Revision History

TCS High Entropy Alloys Database (TCHEA) is a thermodynamic database for high entropy alloys (HEA) [2004, Yeh; 2006, Yeh]. 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) [2013, Wang; 2015, Senkov] 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 viscosity of metallic liquid and molar volume.

The current version of the database is TCHEA4.

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 TCHEA4 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.

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 *TCHEA: TCS High Entropy Alloys Database Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, phases and models. It also includes a list of the included elements and summaries of the database revision history by version.
- The *TCHEA: TCS High Entropy Alloys 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 be used.

Go to the High Entropy Alloys 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 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.

TCHEA4 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.
- 493 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.
- 500 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 and viscosity of the metallic liquids is included with the database.

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.

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
Dynamic viscosity	VISC = RTLN(DVIS)	DVIS for a system `DVIS(PHI)` for phase PHI
Kinematic viscosity	VISC = RTLN(DVIS)	KVIS for a system `KVIS(PHI)` for phase PHI
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

TCHEA4 Systems

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TCHEA4 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	

TCHEA4 Critically Assessed Ternary Systems

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

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

Assessed Ternary Systems			
C-Ni-Ti	C-Ni-W	C-Ni-Zr	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	C-Ta-W
C-Ti-W	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-Nb-Ni
Fe-Ni-Ru	Fe-Ni-Si	Fe-Ni-Ti	Fe-Ni-W
Fe-N-Nb	Fe-N-Ni	Fe-N-Ti	Fe-N-V
Fe-Ti-V	Hf-Nb-Si	Hf-Ni-Ti	Ir-Rh-Ru
Mn-Si-Zn	Mo-Nb-Ti	Mo-Ni-Ta	Mo-N-Ni
Mo-Ta-Ti	Mo-Ti-V	Mo-Ti-W	Mo-Ti-Zr
Nb-Ni-Ti	Nb-Sn-Ti	Nb-Ta-Ti	Nb-Ti-V

Assessed Ternary Systems			
Nb-Ti-W	Nb-Ti-Zr	Ni-Si-Ti	Ni-Ta-Ti
Ni-Ta-W	Ni-Ti-W	Ni-Ti-Zr	N-Ni-Ti
Re-Ta-W	Si-Ti-W	Ta-Ti-V	Ta-Ti-W
Ta-Ti-Zr	Ti-V-W	Ti-V-Zr	Ti-W-Zr

TCHEA4 Tentatively Assessed Ternary Systems

Ternary Systems Tentatively Assessed			
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-Ta
C-Hf-Ti	C-Hf-W	C-Mn-V	C-Mo-N
C-Mo-Re	C-Mo-Si	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

Ternary Systems Tentatively Assessed			
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

Ternary Systems Tentatively Assessed			
C-Si-Ti	C-Ta-Ti	C-Ti-Zr	Cu-Fe-Mo
Cu-Fe-Nb	Cu-Ni-Si	C-V-W	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

Ternary Systems Tentatively Assessed			
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		

TCHEA4 Phases

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TCHEA4 Models for the Included Phases

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
AL10CU10FE	Al10Cu10Fe	oF116	Fmm2		42	(Fe)1(Cu,Al)10(Al)10	
AL10FEMN2	Mn3Al10	hP26	P63/mcm			(Mn,Fe)3(Al)10	Tau3
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	Tau2
AL11MN3ZN2	Mn3Zn2Al11	oC152				(Mn)3(Zn)2(Al)11	the Al-Mn-Zn ternary phase, Tau3
AL11MN4_HT	Al3Mn	oP156	Pnma		62	(Mn,Al)29(Mn)10	
AL11MN4_LT	Al11Mn4	aP15	P-1		2	(Al)11(Fe,Mn)4	
AL11RE4	Al11Mn4	aP15	P-1		2	(Al)11(Re)4	
AL12MN_GPHASE	Al12W	cI26	Im-3		204	(Al)12(Mn)1	
AL12W_	Al12W	cI26	Im-3		204	(Al)12(Re,W,Mo)1	also Al12Mo,

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
GPHASE							Al12Re
AL13CO4	Al19Co6	mS100	C2/m		12	(Al)13(Co)4	
AL13CR2	Al45V7	mC104	C2/m		12	(Al)13(Cr)2	
AL13CR2	Al45V7	mS104	C2/m		12	(Al)13(Cr)2	
AL13FE2MN2	Al13Fe4 (HT)	oB~50	Bmmm			(Fe,Mn)4(Al)13	Tau2
AL13FE4	Al13Fe4	mS102	C2/m		12	(Al,Cu)0.6275(Ru,Fe,Mn)0.235(Va,Al,Si)0.1375	solutions of Al13Fe4 (aka Al3Fe) & Al13Ru4
AL13IR4						(Al)0.765(Ir)0.235	
AL13NI38ZN49						(Al)0.13(Ni)0.38(Zn)0.49	
AL15SI2M4_TAU9	(Mn0.2Fe0.8)4 (Al0.9Si0.1)19	cI168	Im-3		204	(Al)14(Fe,Mn)4(Al,Si)5	
AL16FEMN3	Mn1-xFex Al4	structure unknown				(Al)4(Fe,Mn)1	Tau1
AL1MN1SI1	TiSi2	oF24	Fddd		70	(Al)1(Mn)1(Si)1	the Al-Mn-Si ternary phase, Tau3
AL23CUFE4_D2H	Al6Mn	oS28	Cmcm	D2_h	63	(Al)23(Cu)1(Fe)4	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
AL23V4	Al23V4	hP54	P6_3/mmc		194	(Al)23(V)4	
AL24MN5ZN		o**				(Zn,Mn)5(Zn)1(Al)24	the Al-Mn-Zn ternary phase, Tau1
AL28CU4MN7	Mn6Cu4Al29	oB156	Bbmm			(Al)28(Mn)7(Cu)4	Tau1, Mn6+xCu4+yAl29-x-y
AL28IR9	Al28Ir9	hP236	P31c			(Al)0.757(Ir)0.243	
AL2FE	Al2Fe	aP18	P1		1	(Al,Cu)2(Mn,Fe)1	
AL2MN2SI3	*	hP21	P-6		174	(Al)2(Mn)2(Si)3	the Al-Mn-Si ternary phase, Tau1
AL2MNSI3	Ga5Pd	tI24	I4/mcm		140	(Al)2(Mn)1(Si)3	the Al-Mn-Si ternary phase, Tau10
AL2TI_LT	Ga2Hf	tI24	I4_1/amd		141	(Ti,Al,Nb)2(V,Ta,Al,Zr,Ti,Nb,Co)1	
AL2TI3N2	Ti3Al2N2	hP22	P6_3mc		186	(Al)2(Ti)3(N)2	
AL2W_C40	CrSi2	hP9	P6_222	C40	180	(Al)2(W)1	
AL2ZR3	Al2Zr3	tP20	P4_2/mnm		136	(Al)2(Ti,Zr,Hf,Y)3	also Al2Hf3, Al2Y3

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
AL31MN6NI2	mu-Al4Mn	hP574	P6_3/mmc		194	(Al)31(Mn)6(Ni)2	
AL3CO1	Al13Os4	mS34	C2/m		12	(Al)3(Co)1	aka CoAl3_cub
AL3IR_D018	Na3As	hP8	P6_3/mmc	D018		(Al)0.75(Ir)0.25	
AL3MN4SI2	*	structure unknown				(Al)3(Mn)4(Si)2	the Al-Mn-Si ternary phase, D or Tau5
AL3MNSI2	*	tP48	P4/n		85	(Al)3(Mn)1(Si)2	the Al-Mn-Si ternary phase, Tau4
AL3NI_D011	Fe3C	oP16	Pnma	D0_11	62	(Al)0.75(Ni)0.25	
AL3NI2_D519	Al3Ni2	hP5	P-3m1	D5_19	164	(Al,Si,Zn,Sn)3(Cu,Al,Ni,Ru)2(Ru,Ni,Va)1	also Al3Ru2
AL3NI5	Ga3Pt5	oS16	Cmmm		65	(Al)0.375(Ni)0.625	
AL3RH_LT		oP*	Pnma			(Al)3(Rh)1	
AL3TI_D022	Al3Ti	tI8	I4/mmm	D022	139	(V,Co,Cr,Nb,Al,Ni,Ti,Fe,Si,Mo)3(Mo,V,Si,Ta,Nb,Co,Ni,Cr,Ti,Zr,Al)1	gamma double prime, Al3M/Ni3V, BCT_D022
AL3TI_LT	Al3Ti	tI32	I4/mmm		139	(Ti,Al)3(Ti,Zr,Al)1	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
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_D023	Al3Zr	tI16	I4/mmm	D_023	139	(Zn,Al)3(Ti,Hf,Zr)1	also Al3Hf, Zn3Zr
AL3ZR2	Al3Zr2	oF40	Fdd2		43	(Al)3(Zr,Hf)2	also Al3Hf2
AL3ZR4	Al3Zr4	hP7	P6/mmm		191	(Al)3(Zr,Hf,Ti)4	also Al3Hf4
AL3ZR5_D8M	Si3W5	tI32	I4/mcm	D8_m	140	(Al)3(Ti,Zr)5	
AL45IR13	Al45Ir13	oP236	Pnnm		62	(Al)0.776(Ir)0.224	
AL4C3_D71	Al4C3	hR21	R-3m	D7_1	166	(Al,Si)4(C)3	
AL4CR	mu-Al4Mn	hP574	P6_3/mmc		194	(Al)4(Cr)1	
AL4MN_LAMBDA	lambda-Al4Mn	hP586	P6_3/mmc		194	(Al)461(Mn,Fe)107	also AL461MN107
AL4MN_MU	mu-Al4Mn	hP574	P6_3/mmc		194	(Al)4(Mn)1	
AL4RE	Al4Re	aP71	P-1		2	(Al)4(Re)1	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
AL4SIC4_E94	Al5C3N	hP18	P6_3mc	E9_4	186	(Al)4(Si)1(C)4	
AL4W	Al4W	mS30	Cm		8	(Al)4(Mo,W)1	also Al4Mo
AL4ZR5	Ga4Ti5	hP18	P6_3/mcm		193	(Al)4(Zr)5	
AL5CO2_D811	Al5Co2	hP28	P6_3/mmc	D8_11	194	(Al)5(Rh,Co)2	also Al5Rh2
AL5CU4ZN						(Al,Cu)1(Al)4(Cu)4(Zn)1	
AL5FE2	Al2.8Fe	oS24	Cmcm		63	(Cu,Al)5(Mn,Fe)2	
AL5FE4_D82	Cu5Zn8	cI52	I-43m	D82	217	(Fe,Cu,Al)1	also AL8FE5_D82
AL5IR2	Al2.75Ir	cP60	P23			(Al)0.73(Ir)0.27	
AL5MN6SI7	CrSi2	hP9	P6_222	C40	180	(Al)5(Mn)6(Si)7	the Al-Mn-Si ternary phase, Tau2
AL5RH2_HT	RhAl2.63	cP54	P23			(Al)2(Va,Rh)1	
AL5TI2_HT	Ti1.14Al2.86	tp28	P4/mmm			(Al,Ti)5(Al,Ta,V,Zr,Ti,Nb)2	aka AL11TI5
AL5TI3	Al5Ti3	tP32	P4/mbm		127	(Al)5(Ta,Ti)3	
AL5W	Al5W	hP12	P6_322		182	(Al)5(Mo,W)1	also AL5MO

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
AL62CU25FE13	*	Quasicrystal				(Fe)0.125(Cu,Al)0.255(Al)0.62	
AL63MO37	*	structure unknown				(Al)63(Mo)37	Mo3Al5_HT
AL6MN_D2H	MnAl6	oS28	Cmcm	D2_h	63	(Al)6(Ru,Re,Fe,Mn)1	also Al6Re, Al6Ru
AL77W23	*	structure unknown				(Al)77(W)23	
AL7CU2FE	Al7Cu2Fe	tP40	P4/mnc		128	(Fe,Ni)1(Cu)2(Al)7	
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5	hR42	R-3m		166	(Al)1(Fe,Cu,Va,Ni)1	
AL7RH3_HT			mp*			(Al)7(Rh)3	
AL7V	Al45V7	mS104	C2/m		12	(Al)7(V)1	
AL7W3	*	structure unknown				(Al)7(W)3	
AL8CR5_HT_D82	Cu5Zn8	cI52	I-43m	D82	217	(Al)8(Cr)5	
AL8CR5_LT_D810	Al8Cr5	hR26	R3m	D810	160	(Al)8(Cr)5	
AL8MN5_D810	Al8Cr5	hR26	R3m	D810	160	(Al,Ti,Zn)12(Mn)5(Mn,Al,Cu,Ti,Si)9	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
AL8MO3	Al8Mo3	mS22	C2/m		12	(Al)8(Mo)3	
AL8SIC7	*	hP16	*			(Al)8(Si)1(C)7	
AL8V5_D82	Cu5Zn8	cI52	I-43m	D8_2	217	(Al)8(V)5	
AL9CO2	Al9Co2	mP22	P2_1/c		14	(Al)9(Co,Rh)2	also Al9Rh2
AL9CR4_HT	*	structure unknown				(Al)9(Cr)4	
AL9CR4_LT	Al9Cr4	cI52	I-43m?			(Al)9(Cr)4	
AL9IR2	Al9Co2	mP22	P2_1/c			(Al)0.818(Ir)0.182	
AL9MN2ZN	structure unknown					(Mn)2(Zn)1(Al)9	the Al-Mn-Zn ternary phase, Tau2
ALB12_ALPHA	AlB12-a	tP213	P4_12_12		92	(Ti,Al)1(B)12	
AlCoTi_GPHASE	Al12W	cI26	Im-3		204	(Co,Al)1(Al,Ti)16(Co)7(Ti)6	
ALCR2C	AlCCr2	hP8	P6_3/mmc		194	(Al)1(C)1(Cr)2	MAX_PHASE
ALCU_DELTA	Cu31.27(Cu0.57Al0.43)3Al16	hR156	R3m		160	(Al)2(Cu,Fe)3	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
ALCU_EPS_B82	Co1.7Ge	hP6	P6_3/mmc	B82	194	(Ni,Al,Cu)1(Cu,Fe)1	epsilon2 HT
ALCU_ETA	AlCu	mS20	C12/m1		12	(Cu,Al)1(Zn,Fe,Cu,Ni)1	united HT-eta1 & LT-eta2
ALCU_PRIME	Cu11.2Al8.88	oF88	Fmm2		42	(Al)2(Cu)1	aka THETA_PRIME
ALCU_ZETA	Al9Cu11	oI24/oF88	Imm2 / Fmm2		44/42	(Al)9(Fe,Cu)11	united HT-zeta1 and LT-zeta2
ALCU3MN2_C15	MgCu2	cF24	Fd-3m	C15	227	(Al)1(Mn)2(Cu)3	Tau3
ALFESI_ALPHA_TAU5	Fe23Al81Si15	hP246	P6_3/mmc		194	(Al)0.6612(Fe)0.19(Si)0.0496(Si,Al)0.0992	
ALFESI_BETA_TAU6	Fe2Al9Si2	mS52	A2/a		15	(Al)14(Fe)3(Si)3	
ALFESI_DELTA_TAU4	FeAl3Si2	tI24/oP24	I4/mcm / Pbcn		140/60	(Al)0.55(Fe)0.15(Si)0.3	
ALFESI_GAMMA_TAU2	Fe2Al5Si2	mS*	*			(Al)3(Fe)1(Si)1	
ALFESI_TAU1	Fe3Al2Si3	aP16	P-1		2	(Al)2(Fe)2(Si)1	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
ALFESI_TAU3	FeAl2Si	oS128	Cmma		67	(Al)2(Fe)1(Si)1	
ALM3C_E21	CaTiO3	cP5	Pm-3m	E21	221	(Al)1(Fe,Co)3(C)1	also AlCo3C, AlFe3C
ALMNSI_TAU6	*	structure unknown				(Al,Mn)4(Si)1	the Al-Mn-Si ternary phase, Tau6
ALMNSI_TAU8	Mn3Al10	hP26	P6_3/mmc		194	(Mn,Va)6(Mn,Va)2(Al)12(Si,Al)6(Si,Al)2	the Al-Mn-Si ternary phase, Tau8
ALMO_A2	W	cI2	Im-3m	A2	229	(Al,Mo)1(Al,Mo)1	improper modelling
ALN_B4	ZnO	hP4	P6_3mc	B4	186	(Al)1(N)1	
ALNI2ZN						(Al)0.25(Ni)0.5(Zn)0.25	
ALPHA_B19	AuCd	oP4	Pmma	B19	51	(Ti,V,Nb,Mo,Zr)1(Nb,V,Ti,Zr,Mo)1	an ordered HCP
ALRE_B11	CuTi-gamma	tP4	P4/nmm	B11	129	(Al)1(Re)1	
ALRE2_C11B	CuZr2	tI6	I4/mmm	C11_b	139	(Al)1(Re)2	
ALRH2						(Al)1(Rh)2	
ALSI3TI2	Zr3Al4Si5	tI24	I41/amd			(Al)0.166667(Si)0.5(Ti)0.333333	aka Ti7Al5Si12, Tau1

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
ALTI_L10	AuCu	tP2	P4/mmm	L10		(Cr,Nb,Ta,W,Co,V,Ti,Mo,Al,Zr,Sn,Mn)1 (V,Mn,Cr,Ti,Sn,Ta,Mo,Co,Al,Nb,Zr,W)1	Solution of ordered L10
ALTI2N	AlCCr2	hP8	P6_3/mmc		194	(Al)1(Ti)2(N)1	
ALTI3_D019	CdMg3	hP8	P6_3/mmc	D0_19	194	(Al,Mn,V,Ni,Sn,Nb,Ti,Ta,W,Zr,Cr,Co,Mo,Cu)3 (C,Cr,Nb,Ti,Sn,W,Mo,Al,Ta,Si,Ni,V)1	also Ni3Sn_LT, Mn3Sn, Ti3Sn
ALTI3N_E21	CaTiO3	cP5	Pm-3m	E21	221	(Al)1(Ti)3(N)1	
ALY2_C37	Co2Si	oP12	Pnma	C37	62	(Al)1(Y)2	
ALZR_B33	CrB	oC8	Cmcm	B33	63	(Al)1(Zr,Y,Hf)1	also AlHf, ALY_B33
ALZR2_B82	Ni2In	hP6	P6_3/mmc	B82	194	(Al)1(Zr,Ti)2	
B4C_D1G	B13C2	hR15	R-3m	D1G	166	(B11C,B12)1(C2B,Cb2,B2)1	
B82_OMEGA	InNi2	hP6	P6_3/mmc	B82		(Al,Sn)1(Co,Ta,Sn,Nb,Ti)1(Ti)1	
BCC_A2	W	cI2	Im-3m	A2	229	(Re,Va,Zr,V,Mn,Sn,Mo,Y,Si,Zn,Ni,Cr,Hf,W,Rh,Co,Ir,Ta,Al,Ru,Ti,Fe,Cu,Nb)1(C,B,Va,N)3	BCC_A2 will be combined to BCC_B2 if defined
BCC_B2	CsCl	cP2	Pm-3m	B2	221	(Re,Va,Zr,V,Mn,Sn,Mo,Y,Si,Zn,Ni,Cr,Hf,W,Rh,Co,Ir,Ta,Al,Ru,Ti,Fe,Cu,Nb)0.5 (Zr,Mn,Ru,Ta,Ti,Hf,W,Y,Co,Ir,Re,Cr,Rh,Zn,Sn,Si,Nb,Va,V,Cu,Mo,Al,Fe,Ni)0.5 (C,B,Va,N)3	This phase has some contribution from BCC_A2

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
BCT_A5	beta-Sn	tI4	I4_1/amd			(Sn,Al,Ni,Zn,Cu)1	Disordered BCT solution phase
BETA_RHOMBO_B	beta-B	hR105	R-3m		166	(B)93(B,Cu,C,Si)12	
BN_B4	ZnS	hP4	P6_3mc	B4	186	(B)1(N)1	
BNSI_RHOMBO	B	hR12	R-3m		166	(B)61(Si)1(Si,B)8	
C14_LAVES	MgZn2	hP12	P6_3/mmc	C14	194	(Ta,Ti,Al,Si,V,W,Cu,Cr,Mo,Y,Hf,Zn,Zr,Ru,Fe,Mn,Nb,Re,Co,Ni)2 (Ru,Si,Zr,Ta,Zn,Al,Ti,Y,Mn,V,Mo,Ni,Nb,W,Re,Hf,Fe,Co,Cu,Cr)1	also CuZn2
C15_LAVES	Cu2Mg	cF24	Fd-3m	C15	227	(Si,Cu,Zn,Ti,Cr,W,Ta,Zr,Re,Co,Mo,V,Ni,Fe,Y,Hf,Mn,Ru,Ir,Nb,Al)2 (Ta,Si,W,Cu,V,Nb,Mo,Fe,Al,Cr,Co,Y,Zr,Re,Ru,Hf,Ni,Ti)1	
C16_THETA	CuAl2	tI12	I4/mcm	C16		(W,Zr,Ta,Hf,Ti,Al,Mn,Sn,Mo,Nb)2(Ir,Mn,Al,Cr,Co,Cu,Si,Ni,Fe,Rh)1	
C36_LAVES	MgNi2	hP24	P6_3/mmc	C36	194	(Ti,Fe,Ta,Ni,Hf,Co,Al,Cu,W,Nb,Mo,Zr,Cr)2 (Zr,Mo,Cu,Co,Fe,Al,W,Hf,Ni,Cr,Ti,Nb,Ta)1	
CBCC_A12	alpha-Mn	cI58	I-43m	A12	217	(W,Ir,V,Fe,Ti,Cu,Ta,Zn,Sn,Si,Zr,Ru,Re,Al,Ni,Nb,Co,Cr,Mo,Mn,Y)1 (C,Va,B)1	
CEMENTITE_D011	Fe3C	oP16	Pnma	D011	62	(W,Mo,Mn,Co,V,Ni,Fe,Cr)3(C,N)1	
CHI_A12	a-Mn	cI58	I-43m	A12	217	(Fe,Ni,Cr,Re)24(W,Zr,Ta,Mo,Ti,Nb,Cr,Al,Hf)10	also M5Re24,

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
						(Ni,Ta,W,Mo,Re,Fe,Nb,Cr)24	Mo2Re8, Ta3Re7, WRe3
CO10CU57TI33	MoSi2	tI6	I4/mmm	C11B	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)15	united HT/LT phase
CO1SN3	PdSn3	oC32	Cmce			(Co)0.25(Sn)0.75	
CO2SI1	Co2Si	oP12	Pnma	C37	62	(Ir,Cr,Ni,Co,Cu,Ti,Fe)2(Si)1	also Ni2Si (delta)
CO3SI_D019	CdMg3	hP8	P6_3/mmc	D019	194	(Co)3(Si)1	
CO3V1	Al3Pu	hP24	P6_3/mmc		194	(V,Ni,Co)3(Co,V)1	
CO3Y1	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(Va,Co)1	
CO5Y8	Co5Y8	mP52	P2_1/c		14	(Co)5(Y)8	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
CO7HF	Co7Hf?	oP*	Pban		50	(Co)7(Hf)1	
CO7NB2	Co7Nb2	mS18	C12/m1			(Co)7(Nb)2	
CO7TA2	BaPb3	hR12	R-3m			(Co)7(Ta)2	
CO7Y6	*	structure unknown				(Co)7(Y)6	
COSN_B35	CoSn	hp6	p6/mmm	B35		(Ni,Co,Fe)0.5(Sn)0.5	also FeSn, aka COSN_HP6
COSNTI_TAU2	MgAgAs	cF12	F43m			(Co,Ni)1(Sn)1(Ti)1	aka TiCoSn
COY_B33	CrB	oC8	Cmcm	B33	63	(Co)1(Y)1	aka COY_BF
COZN_DELTA						(Co)0.117647(Zn)0.882353	Zn15Co2 HT phase
COZN_GAMMA_D82	Zn9(Zn0.5Fe0.5)2Fe2	cI52	I-43m	D83	217	(Zn,Co)1(Va)1	aka Zn11Co2, COZN4_D83
COZN_GAMMA1	Zn7.8Co	mS28	C12/m1			(Co)0.125(Zn)0.875	aka CoZn7
COZN_GAMMA2	Zn13Co	mS28	C12/m1			(Co)0.0714286(Zn)0.9285714	aka CoZn13
COZN_HT						(Zn,Co)1(Va)1	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
COZN_LT_A13	beta-Mn	cP20	P4_132	A13	213	(Zn,Co)1(Va)1	
CR2B_CB	Mg2Cu	oF48	Fddd	C_b	70	(Cr,Re,Mo,Fe)0.66666667(B)0.33333333	aka CR2B_ORTH
CR2NI2SI	NiTi2	cF96	Fd-3m		227	(Cr)5(Ni)5(Si)3	the Tau1 phase Cr5Ni5Si3
CR3MN5	a-Mn?	cI58	*	A12?		(Cr)3(Mn)5	
CR3NI5SI2	AlAu4	cP20	P2_13	G3	198	(Cr)3(Ni)5(Si)2(Va,C)1	
CR3SI_A15	Cr3Si	cP8	Pm-3n	A15	223	(Re,Ni,Fe,Mo,Cr,Zr,V,Ir,Ta,Sn,Nb,Si,Ti)3 (Ru,Sn,Ir,Co,Si,Rh,Cr,Ta,Ni,Al,Nb,Zr,V,Ti)1(C,Va)3	also Cr3X, Nb3X, Ti3X, V3X
CR5B3_D8L	CR5B3	tI32	I4/mcm	D8L	140	(Mo,Cr)0.625(B)0.375	also Mo5B3
CRB4	CrB4	oI10	Immm		71	(Cr)0.2(B)0.8	
CRMN3_HT_SIGMA	CrFe	tP30	P4_2/mnm		136	(Mn)8(Cr)4(Cr,Mn)18	
CRNBSI	ZrNiAl	hP9	P-62m		189	(Cr)1(Nb)1(Si)1	
CRNI2_OP6	MoPt2	oP6	Immm			(Cr,W,Mo)1(Ni,W,Mo)2	
CRSI2_C40	CrSi2	hP9	P6_222	C40	180	(Mo,Ta,Cr,W,Ti,Nb,Si,Cu,Hf,V)1(Cu,Cr,Si,Al)2	also NbSi2, TaSi2, VSi2
CRZN13		m**				(Cr)1(Zn)13	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
CRZN17	*	hP*	*			(Cr)1(Zn)17	
CU10HF7	Ni10Zr7	oS68	Cmce		64	(Cu)10(Hf)7	
CU10SN3	Cu10Sn3	hP26	P6_3			(Cu,Ni)0.769(Sn)0.231	
CU10ZR7	Ni10Zr7	oS68	Cmce		64	(Cu)10(Zr)7	
CU15SI4_EPS_D86	Cu15Si4	cI76	I-43d	D8_6	220	(Mn,Cu)0.789474(Al,Si)0.210526	
CU2TI	Au2V	oS12	Cmcm		63	(Cu,Co,Ni)2(Ti)1	
CU2TIZR	Cu2TiZr	hP12	P6_3/mmc		194	(Cu)0.5(Ti)0.25(Zr)0.25	
CU2Y_HT	*	hP*				(Cu)2(Y)1	
CU2Y_LT	Hg2K	oI12	Imma		74	(Cu)2(Y)1	
CU33SI7_DELTA	*	tP*	structure unknown			(Cu)0.825(Si)0.175	the HT phase
CU3SI_ETA	Cu3Si	oS*/hR27/hR*	* / R-3 / R-3m		* / 148 / 166	(Ni,Mn,Cu)0.76(Si)0.24	
CU3SN_HT_GAMMA	BiF3	cF16	Fm-3m	D03		(Mn,Ni,Zn,Cu,Sn)1	Cu3Sn HT solution
CU3SN_LT	Cu3Sn	oC80	Cmcm			(Cu,Sn)3(Cu,Sn)1	epsilon

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
CU3TI2	Cu3Ti2	tP10	P4/nmm		129	(Fe,Ni,Cu)3(Co,Ti)2	
CU41SN11	Cu41Sn11	cF416	F-43m			(Zn,Cu,Sn)41(Sn,Zn,Cu)11	delta
CU46NI25SI29	*	*	*			(Cu)0.458(Ni)0.25(Si)0.292	
CU4MNSN_TAU1	AuBe5	cF24	F3m			(Cu)0.6666(Sn)0.1667(Mn)0.1667	
CU4TI1	Au4Zr	oP20	Pnma		62	(Cu,Ti)4(Ti,Cu)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_A13	Mg3Ru2	cP20	P4_132	A13	213	(Cu,Ni,Si,Mn)0.835821(Si)0.164179	
CU5MN4SI	*	*	*			(Cu)0.5(Mn)0.37(Si)0.13	
CU6NISI3	*	*	*			(Cu,Ni)0.732(Si)0.268	
CU6SN5_HT	Co1.75Ge	hP6	P63/mmc			(Mn,Va,Cu,Ni,Co)1(Ni,Sn,Al,Cu)1(Cu,Ni,Mn,Va,Co)1	also Co3Sn2, Mn(2-x)Sn, Ni3Sn2
CU6SN5_	Cu6Sn5	mS44	C12/c1			(Cu)1(Sn,Cu)1(Sn)1	eta-prime

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
LT							
CU7Y1	Cu5.44Tb0.78	hP8	P6/mmm		191	(Cu2,Y)1(Cu)5	aka Cu6Y or Cu5.4Y0.8
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	
CUB_A13	beta-Mn	cP20	P4_132	A13	213	(Ti,Si,Hf,Y,Zn,Co,Zr,Cu,Mn,V,Mo,Ni,Ta,Al,W,Fe,Nb,Sn,Ir,Ru,Re,Cr)1 (B,Va,C)1	
CUMNZN_EPSILON_HCP	Mg	hP2	P6_3/mmc	A3	194	(Cu,Zn,Mn)1(Va)0.5	
CUMNZN_TAU1	Cu2Mg	cF24	Fd3m			(Cu)0.334(Mn)0.333(Zn)0.333	
CUTI_B11	CuTi	tP4	P4/nmm	B11	129	(Ti,Ni,Co,Cu)1(Cu,Ta,Ni,Ti)1	
CUTI3_L60	CuTi3	tP4	P4/mmm	L6_0	123	(Cu,Ti)1(Ti)3	
DIAMOND_A4	C	cF8	Fd-3m	A4	227	(B,Sn,C,Si,Al)1	Pure C, Si or solution phases based on them
DIS_FCC_A1	Cu	cF4	Fm-3m	A1	225	(Zn,Mo,Ir,Ru,Hf,Rh,Mn,V,Re,Y,Al,Ni,Ti,Nb,Sn,Zr,Co,Ta,Cu,Cr,Fe,Si,W)1(B,Va,C,N)1	A copy of the FCC_A1 phase just for the use in kinetic

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
							simulation.
DIS_MU						(Co,Ti,Mn,Nb,W,Re,Cu,Ta,Ni,Cr,Al,Mo,Fe)1	Part of the description of the MU_PHASE
DIS_SIG						(Ta,Re,Si,V,W,Nb,Ir,Al,Co,Ni,Fe,Ru,Ti,Mn,Cr,Mo)1	Part of the description of the SIGMA phase
FCC_A1	Cu	cF4	Fm-3m	A1	225	(Zn,Mo,Ir,Ru,Hf,Rh,Mn,V,Re,Y,Al,Ni,Ti,Nb,Sn,Zr,Co,Ta,Cu,Cr,Fe,Si,W)1(B,Va,C,N)1	FCC_A1 will be combined to FCC_L12 if defined
FCC_L12	AuCu3	cP4	Pm-3m	L1_2	221	(Rh,Ru,Si,W,Mn,V,Sn,Ir,Ta,Hf,Ni,Ti,Zn,Cr,Re,Co,Cu,Zr,Al,Mo,Y,Fe,Nb)0.75 (V,Sn,Ta,Re,W,Zn,Nb,Hf,Mn,Cu,Cr,Fe,Ru,Y,Mo,Rh,Ni,Si,Al,Ti,Ir,Co,Zr)0.25 (B,N,C,Va)1	This phase has some contribution from FCC_A1
FE2SI	AlNi2	hP6	P-3m1		164	(Fe)0.666667(Si)0.333333	
FE3SN2	Fe3Sn2	hR10	R-3m			(Fe)3(Sn)2	
FE3ZN7_GAMMA_D82	Cu5Zn8	cI52	I-43m	D82	217	(Fe,Zn)0.154(Zn,Fe)0.154(Fe,Zn)0.231(Zn)0.461	
FE4N_LP1	Fe4N	cP5	Pm-3m	L'1	221	(Fe,Ni,Cr,Co,Mn)4(N,C)1	Only stable in (Co-Cr-Fe)-N when gas suspended
FE5SN3_B82	InNi2	hP6	P6(3)/mmc	B82		(Fe)5(Sn)3	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
FE8SI2C	Mn8Si2C3	aP*	P1		1	(Fe)8(Si)2(C)1	
FECN_CHI	Mn5C2	mS28	C2/c		15	(Fe)2.2(C,N)1	Only stable in C-Fe-N when gas suspended.
FENBZR_CFC2_C15	MgCu2	cF24	Fd-3m	C15	227	(Fe,Zr,Nb)2(Zr,Nb)1(Zr,Nb)3	
FESI2_HT	FeSi2-h	oC48	Cmca		64	(Fe)0.3(Si)0.7	
FESI2_LT	FeSi2-l	tP3	P4/mmm		123	(Fe)0.333333(Si)0.666667	
FEZN10_DELTA	FeZn10	hP632	P6_3/mmc		194	(Fe)0.058(Fe,Zn)0.18(Zn)0.525(Zn)0.237	
FEZN13_ZETA	CoZn13	mC28	C2/m		12	(Fe,Va)0.072(Zn)0.856(Zn,Va)0.072	
FEZN4_GAMMA1_D81	Fe11Zn40	cF408	F-43m		216	(Fe)0.137(Fe,Zn)0.118(Zn)0.745	
G_PHASE_D8A	Mn23Th6	cF116	Fm-3m	D8A	225	(Ni,Fe,Al,Co,Ti,Mn)16(Ti,Zr,Nb,Y,Hf)6(Ni,Fe,Si,Mn,Co)7	
GAMMA_D83	Cu9Al4	cP52	P-43m	D83	215	(Zn,Al,Ni,Si)4(Si,Ni,Cu,Zn,Al)1(Cu,Fe,Ni,Mn,Zn)8	
GAMMA_HT_D82	Cu5Zn8	cI52	I-43m	D8_2	217	(Al,Zn)4(Al,Cu,Zn)1(Mn,Cu,Fe,Ni)8	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
GAS						(N2)1	ideal N2 gas
GRAPHITE_A9	C	hP4	P6_3/mmc	A9	194	(C,B)1	
HCP_A3	Mg	hP2	P6_3/mmc	A3	194	(Zn,Ni,Sn,W,Mo,Si,Ti,Ir,Mn,Cr,Y,Al,Ru,Re,Fe,Hf,Zr,Ta,Rh,V,Nb,Co,Cu)1(N,Va,B,C)0.5	Disordered HCP_A3 solution phase
HEUSLER_L21	AlCu2Mn	cF16	Fm-3m	L2_1	225	(Al,Cr,Ni,Ti,Sn)0.5(Ti,Ta,Nb,Al,Hf,Ni,Zr)0.5(Ru,Fe,Ni,Va,Co)1	aka H_L21
HF1IR1						(Hf)1(Ir)1	united HT/LT phase
HF2IR	NiTi2	cF96	Fd-3m			(Hf)2(Ir)1	
HF2RH	NiTi2	cF96	Fd-3m			(Hf)2(Rh)1	
HF3N2	TiS	hR6	R-3m		166	(Hf)3(N)2	
HF3NI7	Hf3Ni7	aP20	P-1		2	(Hf)0.3(Ni)0.7	
HF3RH4		o**				(Hf)3(Rh)4	
HF3RH5	Rh5Ge3	oP16	Pbam			(Hf)3(Rh)5	
HF4N3	Sc0.67Te	hR24	R-3m			(Hf)4(N)3	
HF5IR3	Zr5Ir3	hP48	P6122			(Hf)5(Ir)3	
HF5SN4	Ga4Ti5	hP18	P6_3/mcm			(Hf)5(Sn)4	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
HF8NI21	Hf8Ni21	aP29	P-1		2	(Zr,Hf)8(Ni)21	also ZR8NI21
HFIR3_L12	AuCu3	cP4	Pm-3m	L12	221	(Hf)1(Ir)3	
HFMN	NiTi2	cF96	Fd-3m		227	(Hf)0.5(Mn)0.5	
HFN_B1	NaCl	cF8	Fm-3m	B1		(Hf)1(Va,N)1	
HFNI_ ALPHA	TiI	oS8	Cmcm	B33?	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	the LT phase
HFNI3_ BETA	BaPb3	hR36	R-3m		166	(Hf)0.25(Ni)0.75	the HT phase
HFRE	Zr21Re25	hR276	R-3c		167	(Hf)1(Re)1	also Hf21Re25
HFRH_B2	CsCl	cP2	Pm-3m	B2		(Hf,Rh)1(Rh)1	
HFSN2_ C40	CrSi2	hP9	P6_222	C40		(Hf)1(Sn)2	
IR2Y3	Y3Rh2	tI140	I4/mcm			(Ir)2(Y)3	
IR2Y5	Mn5C2	mS28	C12/c1			(Ir)2(Y)5	
IR3SI1	Ir3Si	tI16	I4/mcm			(Ir)3(Si)1	
IR3SI2_	Co1.75Ge	hP6	P63/mm	B82		(Ir)3(Si)2	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
B82			c				
IR3SI4	Rh3Si4	oP28	Pnma			(Ir)3(Si)4	
IR3SI5	Ir3Si5	mP64	P121/c1			(Ir)3(Si)5	
IR3Y1	PuNi3	hR36	R-3m			(Ir)3(Y)1	
IR3Y5	Pu5Rh3	tP32	P4/ncc			(Ir)3(Y)5	united HT/LT phase
IR3ZR5	Ir3Zr5	hP48	P6_122			(Ir)3(Zr)5	
IR4B3		Of28	Fmm2			(Ir)4(B)3	
IR4B5		mC18	Cm			(Ir)4(B)5	
IR4SI5	Rh4Si5	mP18	P121/m1			(Ir)4(Si)5	
IR5B4		tI36	I41/a			(Ir)5(B)4	
IRMN_L10	AuCu	tP2	P4/mmm	L10		(Ir,Mn,Ti)0.5(Ti,Ir,Mn)0.5	also IrTi
IRNB_L10	AuCu	tP2	P4/mmm	L10		(Ir,Nb)1(Nb,Ir)1	
IRSI_B27	FeAs	oP8	Pnma	B27		(Ir)1(Si)1	the HT phase
IRSI3_HT	gamma-IrSi3	*	oS*			(Ir)1(Si)3	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
IRSI3_LT	beta-IrSi3	*	mS*			(Ir)1(Si)3	
IRV_L10	AuCu	tP2	P4/mmm	L10		(Ir)0.5(Ir,V)0.5	aka Ir1.04V0.96 or IrV1-x
IRV_RT	VIr	oS8	Cmmm			(Ir)1(V)1	
IRY3_D011	CFe3	oP16	Pnma	D0_11		(Ir)1(Y)3	
IRZR_ALPHA	ZrIr	oS16	CmCm			(Ir,Zr)1(Zr)1	the LT phase
IRZR_BETA_B2	CsCl	cP2	Pm-3m	B2		(Zr,Ir)1(Zr,Ir)1	the HT or beta phase
IRZR3_D0E	V3S	tI32	I-42m	D0E		(Ir)1(Zr)3	
LIQUID						(Ir,Hf,C,Ni,Co,Re,Nb,Al1N1,Zr,Fe,Mo,N,V,Ru,Cu,Sn,Rh,W,Cr,Ti,Si,B,Hf1N1,Y,Al,Ta,Zn,Mn)1	Liquid mixture
M11SI8	Cr8Nb3Si8	oP76	Pnma		62	(Nb,Cr)11(Si)8	also Cr11Si8, Nb11Si8
M12C	W6Fe6C	cF104	Fd-3m		227	(Ni,Co)6(Mo,W)6(C)1	also Mo6Ni6C
M23B6_TAU_D84	Cr23C6	cF116	Fm-3m	D84	225	(Co,Ni,Hf,Re)20(B)6(B,Va)6(Cr,Ta,Hf,Re,W,V,Al,Ti,Mo,Zr)3	ternary boride
M23C6_D84	Cr23C6	cF116	Fm-3m	D84	225	(Cr,Mn,Fe,Ni,Co,Re,V)20(Cr,W,Mo,V,Fe,Mn,Co,Re,Ni)3(C)6	
M2B_C16	Al2Cu	tI12	I4/mcm	C16	140	(Ni,Ta,Mn,Co,Al,Re,Nb,W,Mo,Fe,Cr)2(B)1	aka M2B_TETR

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
M3B_D011	Fe3C	oP16	Pnma	D011	62	(Co,Mo,Fe,Ni,Cr)3(B)1	also NI3B_D011
M3B2_D5A	Si2U3	tP10	P4/mbm	D5_a	127	(Nb,Hf,Fe,Ta,V,Mo)3(B)2	also NB3B2, TA3B2, V3B2
M3B2_T	Mo2FeB2	tP10	P4/mbm	D5A	127	(Cr,Ni,W,Fe,Mo)0.4(Cr,Ni,Fe)0.2(B)0.4	ternary borides Mo2FeB2 and Mo2CrB2
M3B4_D7B	Ta3B4	oI14	Immm	D7B	71	(B)4(Ti,V,Mn,Cr,Nb,Hf,Ta,Al)3	also ternary X1Y2B4 boride
M3C2_D510	Cr3C2-b	oP20	Pnma	D510	62	(Mo,V,Co,W,Cr)3(C)2	
M3SI1	Ti3P	tP32	P4_2/n		86	(Ta,Hf,Nb,Ti,Zr)3(Si)1	also Nb3Si, Ta3Si, Ti3Si, Zr3Si
M3SI2_D5A	Si2U3	tP10	P4/mbm	D5a	127	(Zr,Nb,Hf)3(Si)2	also Hf3Si2, Zr3Si2
M3Y	Ni3Pu	hR12	R-3m		166	(Ni,Fe)3(Y)1	also Fe3Y, Ni3Y
M4SI3	Ru4Si3	oP28	Pnma		62	(Ni,Cr,Ru)4(Si)3	also Cr4Si3, Nb4Si3
M5B6	V5B6	oS22	Cmmm		65	(V,Nb)5(B)6	also Nb5B6
M5C2	Mn5C2	mC28	C2/c		15	(Fe,Mn)5(C)2	
M5SI3_D88	Mn5Si3	hP16	P6_3/mcm	D88	193	(Ni,Nb,Hf,Y,Mn,Cu,Zr,Ti,Si,Cr,Mo,W,Fe)2(Al,Ti,Si,Sn,Cr)3 (Cr,Y,Mo,Zr,Ni,Hf,Fe,Nb,Ti,Cu,Mn)3(C,Va,Sn)1	also M5Sn3, M5Si3C

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
M6C_E93	W3Fe3C	cF112	Fd-3m	E93	227	(Ni,Fe,Co)2(W,Nb,Mo,Ta)2(W,Ta,Nb,V,Mo,Co,Fe,Ni,Cr)2(C)1	
M6SI5	V6Si5	oI44	Ibam		72	(Nb,Cr,Ti,V)6(Si)5	also Cr6Si5, Nb6Si5
M7B3_D102	Th7Fe3	hP20	P6_3mc	D102	186	(Ta,Nb,W,Ru,Rh,Re,Cr,Co,Mo)7(B)3(B,Va)3	also RH7B3, RE7B3_D102
M7C3_D101	Cr7C3	oP40	Pnma	D101	62	(V,Re,Cr,W,Co,Fe,Mn,Mo,Ni)7(C)3	
MB_B27	FeB	oP8	Pbnm	B27	62	(B)1(Re,Mo,Ti,Cr,Fe,Y,Mn,Hf,Co)1	also CoB, HfB, MnB, TiB
MB_B33	CrB	oC8	Cmcm	B33	63	(Mo,Fe,Ta,Cr,Nb,Hf,Ti,Ni,V)1(B)1	also NbB, NiB, TaB, VB'
MB2_C32	AlB2	hp3	P6/mmm	C32	166	(B)2(V,Ti,Al,Mn,Nb,Y,Ta,Hf,Cr,Zr,Ru,Mo)1	
MC_ETA	MoC	hP12	P63/mmc	B_i	194	(Mo,W,V)1(C,Va)1	
MC_SHP	WC	hP2	P-6m2	B_h	187	(Mo,W)1(C,N)1	also MoC_LT
MN11SI19	Mn11Si19	tP120	P-4n2		118	(Mn)11(Si,Al)19	
MN12Y_D2B	ThMn12	hI26	I4/mmm		139	(Mn)12(Y)1	
MN15NI45SI40	*	structure unknown				(Mn)0.15(Ni)0.45(Si)0.4	the Mn-Ni-Si ternary phase, T1 or N

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
MN15NI50SI35	*	structure unknown				(Mn)0.15(Ni)0.5(Si)0.35	the Mn-Ni-Si ternary phase, T2 or PHI
MN1NI1SI1_C37	NiSiTi	oP12	Pnma	C37	62	(Mn)1(Ni)1(Si)1	the Mn-Ni-Si ternary phase, T4 or E
MN2B_D1F	Mg2Cu	oF48	Fddd	C_b	70	(Mn)0.6707(B)0.3293	
MN2NISI	*	structure unknown				(Ni,Mn)3(Si)1	the Mn-Ni-Si ternary phase, T8 or S
MN3N2	Mn3N2	tI10	I4/mmm		139	(Mn)6(N)4	aka MN6N4
MN3NI2SI	Mn3Ni2Si	cF96	Fd-3m		227	(Mn)3(Ni)2(Si)1	the Mn-Ni-Si ternary phase, T7 or Omega
MN3SI_D03	BiF3	cF16	Fm-3m	D03	225	(Fe,Mn)3(Si,Al)1	
MN3SN2	Ni3Sn2	oP20	Pnma			(Mn)3(Sn)2	
MN3TI1	*	structure unknown				(Mn)3(Ti)1	the HT phase
MN4TI	Cr0.16Mo0.38Co0.46	hR159	R-3		166	(Mn)0.815(Ti)0.185	aka Ti9Mn42
MN52NI29	*	structure				(Mn)0.52(Ni)0.29(Si)0.19	the Mn-Ni-Si

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
SI19		unknown					ternary phase, T11 or W
MN66NI4SI30	*	structure unknown				(Mn)0.66(Ni)0.04(Si)0.3	the Mn-Ni-Si ternary phase, T10 or U
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	the Mn-Ni-Si ternary phase, T3 or G
MN6NISI3	Cr0.16Mo0.38Co0.46	hR159	R-3		148	(Mn)0.61(Ni)0.12(Si)0.27	the Mn-Ni-Si ternary phase, T9 or R'
MN6SI	R-(Co,Cr,Mo)	hR53	R-3		166	(Al,Mn)17(Zn,Si)3	
MN9SI2	Mn9Si2	oI186	Immm		71	(Mn)33(Si)7	
MNB4	MnB4	mS10	C2/m		12	(Mn)0.2(B)0.8	
MNNI_L10	AuCu	tP2	P4/mmm	L10		(Mn,Cu,Ni)0.5(Mn,Cu,Ni)0.5	
MNNI2	*	structure unknown				(Mn,Ni)1(Ni)2	
MNNISI_T5	MgZn2	hP12	P6_3/mmc	C14	194	(Mn)1(Si,Ni)2	the Mn-Ni-Si ternary phase, T5 or "tao 1"

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
MNNISI_T6	MgCu2	cF24	Fd-3m	C15	227	(Mn)1(Ni,Si)2	the Mn-Ni-Si ternary phase, T6 or "tao 2"
MNTA	*	structure unknown				(Mn)1(Ta)1	
MNTI_HT	*	t**				(Mn)0.515(Ti)0.485	
MNTI_LT	Zr21Re25	hR276	R-3c		167	(Mn)1(Ti)1	aka Ti21Mn25_RT
MNZN9	MnZn9?	h**	*			(Mn)1(Zn)9	
MO1IR3	Mg3Cd	hP8	P6_3/mmc			(Mo)1(Mo,Ir)3	
MO2B5_D8l	Mo2B5	hR21	R-3m	D8i	166	(Mo)0.32(B)0.68	
MO3IR_A15	Cr3Si	cP8	Pm-3n	A15		(Mo)3.06(Ir)0.94	
MO7IR3	Cr0.49Fe0.51	tP30	P42/mnm			(Mo)0.7(Ir)0.3	
MOB_BG	alpha-MoB	tI16	I4_1/amd	B_g	141	(Fe,Mo,Cr)1(B)1	
MOB4	MoB4	hP16	P6_3/mmc		194	(Mo)0.2(B)0.8	
MOIR_HT	Mg	hp2	P63/mmc	A3		(Mo,Ir)1(Mo,Ir)1	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
MOIR_LT_B19	AuCd	oP4	Pmma	B19		(Mo)1(Ir)1	
MONI_DELTA	MoNi	oP56	P2_12_12_1		19	(Re,Co,Cr,Ni,Fe)24(Cr,W,Mo,Re,Fe,Ni,Co)20(Mo,Cu,W)12	
MONI4_BETA_D1A	MoNi4	tI10	I4/m	D1a	87	(W,Mo)1(Ni)4	also WNi4
MOSI2_C11B	CuZr2	tI6	I4/mmm	C11_b	139	(Al,W,Cu,Co,Zn,Mo,Rh,Ni,Fe)1(Ti,Si,Cr,Al,Zr,Hf)2	also AlCr2, Ti2Zn, ZnZr2, CUZR2_C11B
MOZN22	Zn93(Zn0.43Mo0.57)Mo4	cF420	F-43m		216	(Mo)1(Zn)22	
MOZN7	CuPt7	cF32	Fm-3m		225	(Mo)1(Zn)7	
MSI_B20	FeSi	cP8	P2_13	B20	198	(Mn,Re,Ni,Fe,Cr,Co)1(Si,Al)1	also CoSi, CrSi, MnSi, ReSi
MSI_B27	FeB	oP8	Pnma	B27	62	(Nb,Hf,Ti,Zr,Y)1(Si,Al)1	also TiSi, HfSi, YSi, ZrSi(alpha)
MSI2_C1	CaF2	cF12	Fm-3m	C1	225	(Co,Cu,Ni,Mn)1(Al,Si,Cu)2	also NiSi2, CoSi2
MU_PHASE	Fe7W6	hR13	R-3m	D85	166	(Co,Ti,Mn,Nb,W,Re,Cu,Ta,Ni,Cr,Al,Mo,Fe)1 (Ni,Ta,W,Mo,Co,Ti,Al,Nb,Re,Mn,Fe,Cr,Cu)2 (Fe,W,Co,Nb,Ni,Ti,Cu,Cr,Mn,Ta,Mo,Al,Re)6 (Cr,Re,W,Nb,Ta,Ti,Mo,Fe,Cu,Mn,Al,Ni,Co)4	DIS_MU contribution add onto this phase

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
MY3_D011	Fe3C	oP16	Pnma	D011	62	(Ni,Co)1(Y)3	also CoY3, NiY3
MZR3_E1A	Re3B	oS16	Cmcm	E1_a	63	(Ni,Fe,Co)1(Zr)3	also CoZr3, FeZr3
NB13NI75TI12_XD	*	structure unknown				(Nb)0.13(Ni)0.75(Ti)0.12	
NB15NI56TI29_XA	*	o*100				(Nb)0.15(Ni)0.56(Ti)0.29	
NB15NI80TI5_XE	*	structure unknown				(Nb)0.15(Ni)0.8(Ti)0.05	
NB1ZN1						(Nb)0.5(Zn)0.5	
NB2ZN3_D85	Fe7W6	hR13	R-3m	D85		(Nb)0.4(Zn)0.6	
NB3RU5	*/CsCl	o**/cP2	?/Pm-3m		?/221	(Ru,Nb)0.375(Ru)0.625	united HT/LT phase
NB5NI75TI20_XC	Mg3Cd	hP8	P6_3/mmc		194	(Nb)0.05(Ni)0.75(Ti)0.2	
NB8NI9TI3_XB	*	structure unknown				(Nb)0.4(Ni)0.45(Ti)0.15	
NBCN2_CB	Mg2Cu	oF48	Fddd	CB		(V,Sn,Nb)1(Nb,Sn)2	
NBZN15	TiZn16	oC68	Cmcm			(Nb)0.0625(Zn)0.9376	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
NBZN2_C36	MgNi2	hP24	P6_3/mmc	C36		(Nb)0.333(Zn)0.667	
NBZN3_L12	AuCu3	cP4	Pm-3m	L1_2		(Nb)0.25(Zn)0.75	
NBZN7						(Nb)0.125(Zn)0.875	
NI10ZR7	Ni10Zr7	oS68	Cmce		64	(Ni)23(Zr,Hf)17	
NI11ZR9	Pt11Zr9	tI40	I4/m		87	(Ni)11(Zr,Hf)9	also Ni11Hf9
NI17Y2	Fe17Lu2	hP80	P6_3/mmc		194	(Fe,Ni,Al)1(Y)0.1176	also Fe17Y2
NI2SI_THETA	Ga3Ge6Ni13	hP66	P3_121		152	(Cu,Ni)1(Ni,Va)1(Si,Al)1	aka M2SI_TETA
NI2TA_C11B	MoSi2	tI6	I4/mmm	C11b	139	(Co,Ni)2(Ta,Ti)1	
NI2V	MoPt2	oI6	Immm		71	(Mo,Ni)2(Mo,V,Ta,Nb)1	
NI2Y1	Ni2Tm	cF192	F-43m		216	(Ni)2(Y)1	
NI2Y3	Ni2Y3	tP80	P4_12_12		92	(Ni)2(Y)3	
NI3SI_MONOCL	Ge9Pt25	hP34	P-3		147	(Ni)3(Si)1	
NI3SI_	Fe3C	oP16	Pnma	D011	62	(Ni)3(Si)1	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
ORTHO_D011							
NI3SI2	Ni3Si2	oP80	Cmc2_1		36	(Ni)3(Si)2	
NI3SN4	Ni3Sn4	mC14	C2/m			(Cu,Ni)0.25(Sn,Ni)0.25(Sn)0.5	
NI3TA_D0A	Cu3Ti	oP8	Pmmm	D0A	59	(Co,Fe,Cr,Al,Nb,Ni)3(Al,W,Ta,Ti,Mo,Ni,V,Nb,Fe)1	also delta, Ni3Mo, Ni3Nb
NI3TI_D024	Ni3Ti	hP16	P6_3/mmc	D024	194	(Cu,W,Co,Ti,Zr,Fe,Cr,Ta,Al,Hf,Ni)0.75 (Si,W,Ta,Cr,Mo,Ni,Hf,Ti,Al,Zr,Nb,Cu)0.25	also Eta, AlNi6Ta
NI4B3_M	m-Ni4B3	mS28	C2/c		15	(Ni)0.57142857(B)0.42857143	
NI4Y	*	hR*				(Ni)4(Y)1	
NI5SI2	Ni31Si12	hP42	P321		150	(Ni,Cr,Co,Fe,Cu)5(Si)2	
NI5ZR_C15B	AuBe5	cF24	F-43m	C15b	216	(Cu,Ni,Al)5(Y,Hf,Zr)1	also Ni5Y/Ni5Hf/Cu5Hf/Cu5Zr, aka ZRM5_C15B
NI7ZR2	Co7Gd2	hR18	R-3m		166	(Cr,Al,Ni,Co)7(Hf,Zr,Y)2	also NI7HF2, NI7Y2, CO7HF2 and CO7Y2
NI8M	Pt8Ti	tI18	I4/mmm		71	(Ni)8(Ta,Nb)1	also Ni8Ta, Ni8Nb
NISI_B31	MnP	oP8	Pnma	B31	62	(Ni)1(Si)1	
NITI2	NiTi2	cF96	Fd-3m		227	(Ti,Fe,Ni,Cu,Co,Re,Cr)1(Cu,Ta,Al,Ni,Hf,Zr,Cr,Ti)2	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
NIY_B27	FeB	oP8	Pnma	B27	62	(Ni)1(Y)1	
NIZN_TP2	AuCu	tP4	P4/mmm	L10	123	(Cu,Ni,Zn,Al)0.5(Zn,Ni,Al)0.5	united HT/LT phase
NIZN8_DELTA	Ni3Zn22	mC50	C2/m		12	(Ni)0.1111111(Zn,Al)0.8888889	
NIZR_B33	CrB	oS8	Cmcm	B33	63	(Ni)1(Ti,Zr)1	
O_PHASE	NaHg	oC16	Cmcm			(Nb,Ti,Ta)0.5(Nb,Ta,Al,Ti)0.25(Ta,Nb,Ti)0.25	aka Ti2NbAl
O1_DIS						(Al,Ti,Nb)0.75(Al,Nb,Ti)0.25	The HT disordered form of O phase
P_PHASE	Cr9Mo21Ni20	oP56	Pnma		62	(Cr,Fe,Ni,Re)24(Fe,Ni,Re,Mo,Cr)20(Mo)12	
PI_A13	Mo3Al2C	cP20	P4_1 32	A13	213	(Cr)12.8(Ni,Fe)7.2(N)4	the Cr-(Fe,Ni)-N nitride
R_PHASE	Co5Cr2Mo3	hR53	R-3h		148	(Ni,Co,Fe,Re,Cr)27(W,Mo)14(Co,Fe,Mo,Cr,Ni,W,Re)12	
RE2SI	Re2Si	mP24	P12_1/c1		14	(Re)2(Si)1	
RE3B_E1A	Re3B	oC16	Cmcm	E1a	63	(Mo,Ta,Re,W,Cr)3(B)1	
REB2	ReB2	hP6	P6_3/mmc		194	(Re)1(B)2(Va,B)2	
RESI2_C11B	Re4Si7	mS44	C1m1		8	(Re)0.357(Si)0.643	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
REZR2	Re25Zr21	hR276	R-3c		167	(Ni,Re)1(Zr)2	aka Zr21Re25
RH2SN	Co2Si-b	oP12	Pnma	C23 ?		(Rh)2(Sn)1	
RH3SN2	Co1.75Ge	hP6	P63/mmc			(Rh)0.125(Rh)0.5(Sn)0.375	
RH3ZR_L12	AuCu3	cP4	Pm-3m	L1_2		(Rh,Zr)3(Rh,Zr)1	
RH4ZR3_HT						(Zr,Rh)4(Zr)3	beta_Rh4Zr3
RH4ZR3_LT	Pd4Pu3	hR14	R-3			(Zr,Rh)4(Zr)3	alpha_Rh4Zr3
RH5TI3	Rh5Ge3	oP16	Pbam			(Rh)5(Ti)3	
RH5ZR3						(Rh)5(Rh,Zr)3	
RHB_B81	NiAs	hP4	P63/mmc	B81	194	(Rh)1(B)1.1	
RHSN_B20	FeSi	cP8	P2_13	B20		(Rh)1(Sn)1	
RHSN2_RT	RhSn2	tI26	I4/mmm			(Rh)0.33333(Sn)0.66667	
RHSN4	IrGe4	hP15	P3121			(Rh)1(Sn)4	
RHZR_HT_B2	CsCl	cP2	Pm-3m	B2		(Rh)1(Rh,Zr)1	beta_RhZr

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
RHZR_LT	ZrIr	oC16	CmCm			(Rh)1(Zr,Rh)1	alpha_RhZr
RHZR2	NiTi2	cF96	Fd-3m			(Rh)1(Zr)2	
RU1B1	*	cI*				(Ru)1(B)1	
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	united HT/LT phase
RU2SN3	Ru2Sn3	tP20	P-4c2			(Ru)0.4(Sn)0.6	
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	
RU3SN7_D8F	Ru3Sn7	cI40	Im-3m			(Ru)0.3(Sn)0.7	
RUSI	FeSi	cP8	P2_13	B20	198	(Ru)1(Si)1	united HT_B2/LT_B20 phase
RUY3_D011	CFe3	oP16	Pnma	D0_11	62	(Ru)0.25(Y)0.75	
SI3N4	Si3N4	hP28/hP1	P31c/P		159/	(Si)3(N)4	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
		4	6_3		173		
SIB3_D1G	B4C	hR15	R-3m	D1G	166	(B)6(Si)2(Si,B)6	
SIB6	B6Si	oP280	Pnnm		58	(B)210(Si)23(B,Si)48	
SIC_B3	ZnS	cF8	Fd-3m	B3	227	(Si)1(C)1	
SIGMA	CrFe	tP30	P4_2/mnm	D8B	136	(Ta,Re,Si,V,W,Nb,Ir,Al,Co,Ni,Fe,Ru,Ti,Mn,Cr,Mo)10 (Ti,Nb,Ni,Re,Ru,Fe,Mn,Ir,W,Ta,V,Si,Mo,Al,Co,Cr)4 (W,Ru,Nb,Mo,Fe,Co,Mn,V,Cr,Ta,Al,Si,Ni,Ir,Re,Ti)16	DIS_SIG contribution added onto it
SN10Y11	Ge10Ho11	tI84	I4/mmm			(Sn)10(Y)11	
SN2Y_C49	Si2Zr	oC12	Cmcm	C49		(Sn)2(Y)1	
SN3TI2						(Sn)3(Ti)2	
SN3Y1	GdSn2.75	oC16	Amm2			(Sn)3(Y)1	
SN4Y5	Ge4Sm5	oP36	Pnma			(Sn)4(Y)5	
SN5TI6	Sn5Ti6	hP22	P6_3/mmc			(Al,Sn)5(Ti,Nb)6	also Sn5Nb6
SN5Y2	Er2Ge5	oP14	Pmmn			(Sn)5(Y)2	
SNTI2_B82	InNi2	hP6	P6_3/mmc	B82		(Sn)1(Ti)2	
T1CUFETI_CU2TI	Au2V	oS12	Cmcm		63	(Fe,Cu)2(Ti)1	ternary Ti0.33FexCu0.67-x,

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
							Tau1
T1CUNITI_C11B	MoSi2	tI6	I4/mmm	C11_b	139	(Cu,Ni)2(Ti)1	the Cu-Ni-Ti ternary phase Tau1
T2CUFETI_CU3TI2	Cu3Ti2	tP10	P4/nmm		129	(Cu,Fe)3(Ti)2	ternary Ti0.4FexCu0.6-x, Tau2
T2CUNITI	Cu3Ti2	tP10	P4/nmm		129	(Cu)0.175(Ni)2.825(Ti)2	the Cu-Ni-Ti ternary phase Tau2
T3CUFETI_CU4TI3	Cu4Ti3	tI14	I4/mmm		139	(Cu,Fe)4(Ti)3	ternary Ti0.43FexCu0.57-x, Tau3
T4CUFETI	*	structure unknown				(Cu,Fe)0.63(Ti)0.37	the Cu-Fe-Ti ternary phase Ti0.37FexCu0.63-x, Tau4
T4CUNITI	BaPb3	hR12	R-3m		166	(Cu)0.05(Ni)0.7(Ti)0.25	the Cu-Ni-Ti ternary phase Tau4
T5CUFETI	*	structure unknown				(Cu,Fe)0.55(Ti)0.45	the Cu-Fe-Ti ternary phase Ti0.45FexCu0.55-x, Tau5
T6CUNITI	*	structure				(Cu)0.25(Ni)0.5(Ti)0.25	the Cu-Ni-Ti

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
		unknown					ternary phase Tau6
TA1AL1	Ta22Al21	mP86	P12_1/c1		14	(Ta)0.51515(Al)0.48485	
TA3SN_A15	Cr3Si	cP8	Pm-3n	A15		(Ta)3(Sn)1	
TA41IR59	AuCu	tP2	P4/mmm	L10		(Ta)0.41(Ir)0.59	aka Ta0.82Ir1.18_rt, gamma
TA43IR57	TaIr	oP12	Pmma			(Ta)0.43(Ta,Ir)0.57	aka Ta0.86Ir1.14, delta
TA5SI3_D8L	Cr5B3	tI32	I4/mcm	D8L	140	(Hf,Nb,Ta)5(Al,Si)3	also alpha-Nb5Si3
TAAL2_HT	Ta39Al69	cF444	F-43m		216	(Ta)0.35(Al)0.65	
TAN_EPS	TaN	hP6	P-62m		189	(Ta)1(N)1	
TASN2_CB	CuMg2	oF48	Fddd	C_b		(Ta)1(Sn)2	also SN2TA_CB
TI25MN9AL66_L12	AuCu3	cP4	Pm-3m	L1_2	221	(Ti,Mn,Al)0.25(Mn,Al)0.08(Al,Mn,Ti)0.67	also Ti25Mn8Al67 or Ti43Mn11Al66, Tau1
TI2ALC	Cr2AlC	hP8	P63/mmc			(Ti)2(Al)1(Va,C)1	i.e. Ti2AlC1-x
TI2N_C4	TiO2	tP6	P4_2/mnm	C4	136	(Ti)2(N)1	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
TI3ALC_E21	CaTiO3	cP5	Pm-3m	E21		(Ti)3(Al)1(Va,C)1	i.e. Ti3AlC1-x
TI3ALC2		hP12	P63/mmc			(Ti)3(Al,Si)1(C,Va)2	i.e. Ti3AlC2-x
TI3N2	TiS	hR18	R-3m		166	(Ti)0.71(N)0.29	
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	aka Xi-TiN0.58 HT
TISI2_C54	TiSi2	oF24	Fddd		70	(Nb,Ti,Ru,Mo,Zr)1(Si,Sn,Al)2	also MoSi2, RuAl2, ZrSn2
TIZN10	Ti3Zn22	tP100	P4_2/mbc		135	(Ti)1(Zn)10	
TIZN15	TiZn16	oC68	Cmcm		63	(Ti)1(Zn)15	
TIZN5	*	structure unknown				(Ti)1(Zn)5	
V2B3	V2B3	oS20	Cmcm		63	(V)0.4(B)0.6	
V3SN_A15	Cr3Si	cP8	Pm-3n	A15		(Sn)0.205(V)0.795	
V4ZN5	V4Zn5	tI18	I4/mmm		139	(V)4(Zn)5	
VSN2_CB	Mg2Cu	oF48	Fddd	CB		(Sn)0.6(V)0.4	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
VZN3_L12	AuCu3	cP4	Pm-3m	L12	221	(V)1(Zn)3	
W2B5_D8I	Mo2B5	hR21	R-3m	D8i	166	(C,Va,B)5(W)2	nonstoichiometric W2B5
W2B9	BW4	hP20	P-3		147	(B)9(W)2	
W3MC	W10Co3C3.4	hP34	P6_3/mmc		194	(W)3(Ni,Co)1(C)1	also W3CoC, W3NiC
W5SI3_D8M	W5Si3	tI32	I4/mcm	D8m	140	(V,W,Cr,Mo,Nb,Ti,Fe)4(W,Cr,V,Fe,Nb,Mo,Ti,Si)1(Sn,Si,Al)3	also Cr5Si3, Mo5Si3, Nb5Si3, V5Si3
WB_ALPHA_BG	MoB	tI16	I4_1/amd	Bg	141	(B,C,Va)1(W)1	
WB_BETA_B33	BCr	oS8	Cmcm	B33	63	(C,Va,B)1(W)1	
Y13ZN58	Y13Zn58	hP146	P6_3/mmc		194	(Y)13(Zn)58	
Y15C19_ALPHA	alpha-Y15C19	oP18	Pbam		55	(C)19(Y)15	aka Y15C19_R
Y15C19_BETA	*	structure unknown				(C)19(Y)15	the HT beta phase
Y1ZN3	YZn3	oP16	Pnma		62	(Y)1(Zn)3	
Y2C3_ALPHA	Sc3C4	tP70	P4/mnc		128	(Y)2(C)2(C,Va)1	aka Y2C3_R

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
Y2C3_BETA	*	structure unknown				(Y)2(C)2(C,Va)1	the HT beta phase
Y2ZN17	Ni17Th2	hP38	P6_3/mmc		194	(Y)2(Zn)17	
Y3SI5_HT_CC	Si2Th	tI12	I4_1/amd	CC	141	(Y)3(Si)5	
Y3SI5_LT_C32	AlB2	hP3	P6/mmm	C32	191	(Y)3(Si)5	
Y5SI4	Gd5Si4	oP36	Pnma		62	(Y)5(Si)4	
YB4_D1E	UB4	tP20	P4/mbm	D1E	127	(Y)0.2(B)0.8	
YB6_D21	CaB6	cP7	Pm-3m	D21	221	(Y)1(B)6	
YB66	YB66	cF1936	Fm-3c		226	(Y)1(B)66	
YC_GAMMA_B1	NaCl	cF8	Fm-3m	B1	225	(Y)1(C,C2,Va)1	
YC2_C11A	CaC2	tI6	I4/mmm	C11A	139	(C2Y1)1	
YSI2_HT_CC	Si2Th	tI12	I4_1/amd	CC	141	(Y)1(Si)2	
YSI2_LT_C32	AlB2	hP3	P6/mmm	C32	191	(Y)1(Si)2	

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
YZN2_HT	*	structure unknown				(Y)1(Zn)2	
YZN2_LT	*	structure unknown				(Y)1(Zn)2	
YZN5	ErZn5	hP36	P6_3/mmc		194	(Y)1(Zn)5	
Z_PHASE	CrNbN	tP6	P4/nmm		129	(Cr,Fe)1(V,Nb,Mo)1(Va,N)1	
ZN11Y3	Al11La3	oI28	Immm		71	(Zn)11(Y)3	
ZN12Y_D2B	Mn12Th	tI26	I4/mmm			(Zn)12(Y)1	
ZN22ZR	Zn22Zr	cF184	Fd-3m		227	(Zn)22(Zr)1	
ZN2ZR3	Zr3Al2	tP20	P4_2/mnm		136	(Zn)2(Zr)3	
ZN39ZR5	Zn39Zr5	mC88	C2/m		12	(Zn)39(Zr)5	
ZN3ZR_HT	*	c**	*			(Zn)3(Zr)1	
ZNZR_B2	CsCl	cP2	Pm-3m	B2	221	(Zn)1(Zr)1	
ZR5SI4_TP36	ZR5SI4	tP36	P4_12_12		92	(Nb,Hf,Zr,Ti)5(Si,Al)4	also Hf5Si4, Ti5Si4
ZRB12_D2F	UB12	cF52	Fm-3m	D2F	225	(B)12(Zr,Y)1	also YB12

Name in database	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG#*	*Thermodynamic Model and Phase constitution*	*Notes*
ZRSI2_C49	ZrSi2	oS12	Cmcm	C49	63	(Zr,Hf,Nb)1(Si)2	also HfSi2

TCHEA4 Properties Data

For more information about the models, and when in Thermo-Calc, press F1 to search the online help.

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.

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:	**4.2**
First release:	**TCHEA1 was released in 2015**

Changes in the Most Recent Database Release

TCHEA4.1 to TCHEA4.2

Software release version: 2021a (December 2020/January 2021)

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

Previous Releases

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.