TCS High Entropy Alloys Database (TCHEA5)

Technical Information

Available Starting with Thermo-Calc Version 2021b

Document created 11/15/2021

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 TCHEA5.

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 TCHEA5 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.

TCHEA5 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.
- 501 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 thermophysical 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)` **
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)` **

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
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)

TCHEA5 Systems

In this section:

TCHEA5 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	

TCHEA5 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

TCHEA5 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

Tentatively Assessed Ternary Systems					
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

TCHEA5 Phases

In this section:

TCHEA5 Models for the Included Phases

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

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

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

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

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL77W23	Unknown Structure					(Al)77(W)23	
AL7CU2FE	FeCu2Al7 (E9a)	tP40	P4/mnc			(Fe, Ni)1(Cu)2(Al)7	
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5	hR14	R-3m			(Al)1(Cu, Fe, Ni, Va)1	
AL7RH3_HT	Unknown Structure	mP*				(Al)7(Rh)3	
AL7W3	Unknown Structure					(Al)7(W)3	
AL8CR5_HT_D82	gamma-brass (Cu5Zn8, D82)	cI52	I-43m			(Al)8(Cr)5	
AL8CR5_LT_D810	Cr5Al8 (D810)	hR26	R3m			(Al)8(Cr)5	
AL8MN5_D810	Cr5Al8 (D810)	hR26	R3m			(Al, Ti, Zn)12(Mn)5(Al, Cu, Mn, Si, Ti)9	
AL8MO3	Al8Mo3	mS22	C2/m			(Al)8(Mo)3	
AL8SIC7	Unknown Structure	hP16				(Al)8(Si)1(C)7	
AL8V5_D82	gamma-brass (Cu5Zn8, D82)	cI52	I-43m			(Al, V)8(Al, V)5	
AL9CO2	Co2Al9 (D8d)	mP22	P2_1/c			(Al)9(Co, Rh)2	also Al9Rh2
AL9CR4_HT	Unknown Structure					(Al)9(Cr)4	
AL9CR4_LT	Unknown Structure					(Al)9(Cr)4	
AL9IR2	Co2Al9 (D8d)	mP22	P2_1/c			(Al)0.818(Ir)0.182	
AL9MN2ZN	Unknown Structure					(Mn)2(Zn)1(Al)9	ternary Tau2 phase
ALB12_ALPHA	alpha-AlB12	tP216	P4_12_12			(Al, Ti)1(B)12	
ALCOTI_GPHASE						(Al, Co)1(Al, Ti)16(Co)7(Ti)6	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
ALCR2C	AlCCr2	hP8	P6_3/mmc			(Al)1(C)1(Cr)2	MAX_PHASE.
ALCU_DELTA	Al5Cu8	hR52	R3m			(Al)2(Cu, Fe)3	
ALCU_EPS_B82	Ni2In (B82)	hP6	P6_3/mmc			(Al, Cu, Ni)1(Cu, Fe)1	epsilon2 HT.
ALCU_ETA	AlCu(r)	mS20	C2/m			(Al, Cu)1(Cu, Fe, Ni, Zn)1	united HT-eta1 & LT-eta2.
ALCU_PRIME	Al9Cu11(h)	oF88	Fmm2			(Al)2(Cu)1	aka THETA_PRIME.
ALCU_ZETA	Al9Cu11(h)	oF88	Fmm2			(Al)9(Cu, Fe)11	united HT-zeta1 andLT-zeta2.
ALCU3MN2_C15	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m			(Al)1(Mn)2(Cu)3	Tau3.
ALFESI_ALPHA_TAU5	Fe23Al81Si15	hP246	P6_3/mmc			(Al)0.6612(Fe)0.19(Si)0.0496(Al, Si)0.0992	
ALFESI_BETA_TAU6	Fe2Al9Si2	mS52	C2/c			(Al)14(Fe)3(Si)3	
ALFESI_DELTA_TAU4	FeAl3Si2	oP24	Pbcn			(Al)0.55(Fe)0.15(Si)0.3	
ALFESI_GAMMA_ TAU2	Unknown Structure	mS*				(Al)3(Fe)1(Si)1	
ALFESI_TAU1	Unknown Structure					(Al)2(Fe)2(Si)1	
ALFESI_TAU3	Fe(Al0.67Si0.33)3	oS128	Cmme			(Al)2(Fe)1(Si)1	
ALM3C_E21	Cubic Perovskite (CaTiO3, E21)	cP5	Pm-3m			(Al)1(Co, Fe)3(C)1	also AlCo3C, AlFe3C.
ALMNSI_TAU6	Unknown Structure					(Al, Mn)4(Si)1	
ALMNSI_TAU8	Al9Mn3Si (E9c)	hP26	P6_3/mmc			(Mn, Va)6(Mn, Va)2(Al)12(Al, Si)6(Al, Si)2	
ALMO_A2	Body-Centered Cubic (W, A2, bcc)	cI2	Im-3m			(Al, Mo)1(Al, Mo)1	improper modelling.
ALN_B4	Wurtzite (ZnS, B4)	hP4	P6_3mc			(Al)1(N)1	

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

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

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

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

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CU10SN3	Cu10Sn3	hP26	P6_3			(Cu, Ni)0.769(Sn)0.231	zeta.
CU10ZR7	Ni10Zr7	oS68	Cmce			(Cu)10(Zr)7	
CU15SI4_EPS_D86	Cu15Si4 (D86)	cI76	I-43d			(Cu, Mn)0.789474(Al, Si)0.210526	
CU2TI1	Au2V	oS12	Cmcm			(Co, Cu, Ni)2(Ti)1	
CU2TIZR	MgZn2 Hexagonal Laves (C14)	hP12	P6_3/mmc			(Cu)0.5(Ti)0.25(Zr)0.25	
CU2Y_HT	Unknown Structure	hP*				(Cu)2(Y)1	
CU2Y_LT	CeCu2	oI12	Imma			(Cu)2(Y)1	
CU33SI7_DELTA	Unknown Structure					(Cu)0.825(Si)0.175	HT phase
CU3SI_ETA	Cu3Si-h2	hR*	P-31m			(Cu, Mn, Ni)0.76(Si)0.24	United 3-allotropes:eta''-RT(oS* *), eta'-HT1(hR27 R-3), eta-HT2(hR* P-31m)
CU3SN_HT_GAMMA	BiF3 (D03)	cF16	Fm-3m			(Cu, Mn, Ni, Sn, Zn)1	Cu3Sn HT solutionphase
CU3SN_LT	Cu3Sn	oS80	Cmcm			(Cu, Sn)3(Cu, Sn)1	epsilon
CU3TI2	Cu3Ti2	tP10	P4/nmm			(Cu, Fe, Ni)3(Co, Ti)2	
CU41SN11	Cu41Sn11	cF416	F-43m			(Cu, Sn, Zn)41(Cu, Sn, Zn)11	delta.
CU46NI25SI29	Unknown Structure					(Cu)0.458(Ni)0.25(Si)0.292	
CU4MNSN_TAU1	MgCu4Sn	cF24	F-43m			(Cu)0.6666(Sn)0.1667(Mn)0.1667	
CU4TI1	Au4Zr	oP20	Pnma			(Cu, Ti)4(Cu, Ti)1	
CU4TI3	Cu4Ti3	tI14	I4/mmm			(Co, Cu, Ni)4(Ti)3	
CU4Y	Cu5Y1.25	mP16	P2_1/m			(Cu)4(Y)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CU51HF14	Ag51Gd14	hP68	P6/m			(Cu)51(Hf)14	
CU51ZR14	Ag51Gd14	hP68	P6/m			(Cu)51(Zr)14	
CU56SI11_GAMMA_A13	Mg3Ru2	cP20	P4_132			(Cu, Mn, Ni, Si)0.835821(Si)0.164179	
CU5MN4SI	Unknown Structure					(Cu)0.5(Mn)0.37(Si)0.13	
CU6NISI3	Unknown Structure					(Cu, Ni)0.732(Si)0.268	
CU6SN5_HT	Ni2In (B82)	hP6	P6_3/mmc			(Co, Cu, Mn, Ni, Va)1(Al, Cu, Ni, Sn)1(Co, Cu, Mn, Ni, Va)1	also Co3Sn2,Mn(2-x)Sn, Ni3Sn2.
CU6SN5_LT	Cu6Sn5	mS44	C2/c			(Cu)1(Cu, Sn)1(Sn)1	eta-prime.
CU7Y1	Cu7Tb	hP8	P6/mmm			(Cu2, Y)1(Cu)5	aka Cu6Y or Cu5.4Y0.8
CU7Y2	Ag51Gd14	hP68	P6/m			(Cu)7(Y)2	
CU8HF3	Cu8Hf3	oP44	Pnma			(Cu)8(Hf)3	
CU8ZR3	Cu8Hf3	oP44	Pnma			(Cu)8(Zr)3	
CUB_A13	beta-Mn (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	
CUMNZN_EPSILON_HCP	Hexagonal Close Packed (Mg, A3, hcp)	hP2	P6_3/mmc			(Cu, Mn, Zn)1(Va)0.5	
CUMNZN_TAU1	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m			(Cu)0.334(Mn)0.333(Zn)0.333	
CUTI_B11	gamma-CuTi (B11)	tP4	P4/nmm			(Co, Cu, Ni, Ti)1(Cu, Ni, Ta, Ti)1	aka B11.
CUTI3_L60	CuTi3 (L60)	tP4	P4/mmm			(Cu, Ti)1(Ti)3	
DIAMOND_A4	Diamond (A4)	cF8	Fd-3m			(Al, B, C, Si, Sn)1	Pure C, Si or solidsolution phases based on them.

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
DIS_MU	Fe7W6 (D85) mu-phase	hR13	R-3m			(Al, Co, Cr, Cu, Fe, Mn, Mo, Nb, Ni, Re, Ta, Ti, W)1	Part of thedescription for the MU_PHASE
DIS_SIG	sigma-CrFe (D8b)	tP30	P4_2/mnm			(Al, Co, Cr, Fe, Ir, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W)1	Part of thedescription for the SIGMA phase.
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	cF4	Fm-3m	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	FCC_A1 will be combined to FCC_L12 if defined.
FCC_L12	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m			(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	This phase has some contribution from FCC_A1.
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	AlNi2	hP6	P-3m1			(Fe)0.666667(Si)0.333333	
FE3SN2	Fe3Sn2	hR10	R-3m			(Fe)3(Sn)2	
FE3ZN7_GAMMA_D82	gamma-brass (Cu5Zn8,D82)	cI52	I-43m			(Fe, Zn)0.154(Fe, Zn)0.154(Fe, Zn)0.231(Zn)0.461	
FE4N_LP1	gama-Fe4N (L'10)	cP5	Pm-3m			(Co, Cr, Fe, Mn, Ni)4(C, N)1	Only stable in(Co-Cr-Fe)-N when gas suspended.
FE5SN3_B82	Ni2In (B82)	hP6	P6_3/mmc			(Fe)5(Sn)3	
FE8SI2C	Mn8Si2C	aP*	P1			(Fe)8(Si)2(C)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
FECN_CHI	Mn5C2 (Fe5C2 Hagg carbide)	mS28	C2/c			(Fe)2.2(C, N)1	Onlystable in C-Fe-N when gas suspended.
FENBZR_CFC2_C15	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m			(Fe, Nb, Zr)2(Nb, Zr)1(Nb, Zr)3	
FESI2_HT	FeSi2-h	tP3	P4/mmm			(Fe)0.3(Si)0.7	
FESI2_LT	FeSi2-l	oS48	Cmce			(Fe)0.333333(Si)0.666667	
FEZN10_DELTA	FeZn10	hP632	P6_3/mmc			(Fe)0.058(Fe, Zn)0.18(Zn)0.525(Zn)0.237	
FEZN13_ZETA	CoZn13	mS28	C2/m			(Fe, Va)0.072(Zn)0.856(Va, Zn)0.072	
FEZN4_GAMMA1_D81	Fe11Zn40	cF408	F-43m			(Fe)0.137(Fe, Zn)0.118(Zn)0.745	
G_PHASE_D8A	Th6Mn23 (D8a)	cF116	Fm-3m			(Al, Co, Fe, Mn, Ni, Ti)16(Hf, Nb, Ti, Y, Zr)6(Co, Fe, Mn, Ni, Si)7	
GAMMA_D83	gamma-brass (Cu9Al4, D83)	cP52	P-43m			(Al, Ni, Si, Zn)4(Al, Cu, Ni, Si, Zn)1(Cu, Fe, Mn, Ni, Zn)8	also Cu5Zn8, Ni5Zn8, Al5Cu8 (rt).
GAMMA_HT_D82	gamma-brass (Cu5Zn8, D82)	cI52	I-43m			(Al, Zn)4(Al, Cu, Zn)1(Cu, Fe, Mn, Ni)8	aka GAMMA_H.
GAS						(N2)1	
GRAPHITE_A9	Hexagonal Graphite (A9)	hP4	P6_3/mmc			(B, C)1	
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	hP2	P6_3/mmc			(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	Disordered HCP_A3 solution phase.
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	Heusler (L21)	cF16	Fm-3m			(Al, Cr, Ni, Sn, Ti)0.5(Al, Hf, Nb, Ni, Ta, Ti, Zr)0.5 (Co, Fe, Ni, Ru, Va)1	aka H_L21.
HF1IR1	Unknown Structure					(Hf)1(Ir)1	united HT/LT phase

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
HF2IR	NiTi2	cF96	Fd-3m			(Hf)2(Ir)1	
HF2RH	NiTi2	cF96	Fd-3m			(Hf)2(Rh)1	
HF3N2	TiS-9R	hR6	R-3m			(Hf)3(N)2	
HF3NI7	Hf3Ni7	aP20	P-1			(Hf)0.3(Ni)0.7	
HF3RH4	Unknown Structure					(Hf)3(Rh)4	
HF3RH5	Rh5Ge3	oP16	Pbam			(Hf)3(Rh)5	
HF4N3	Sc2Te3	hR8	R-3m			(Hf)4(N)3	
HF5IR3	Ir3Zr5	hP48	P6_122			(Hf)5(Ir)3	
HF5SN4	Ti5Ga4	hP18	P6_3/mcm			(Hf)5(Sn)4	
HF8NI21	Hf8Ni21	aP29	P-1			(Hf, Zr)8(Ni)21	also ZR8NI21.
HFIR3_L12	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m			(Hf)1(Ir)3	
HFMN	NiTi2	cF96	Fd-3m			(Hf)0.5(Mn)0.5	
HFN_B1	Rock Salt (NaCl, B1)	cF8	Fm-3m			(Hf)1(N, Va)1	
HFNI_ALPHA	CrB (B33)	oS8	Cmcm			(Hf)0.5(Ni)0.5	
HFNI3_ALPHA	PdRh2Ta	hP40	P6_3/mmc			(Hf)0.25(Ni)0.75	the LT phase.
HFNI3_BETA	BaPb3	hR12	R-3m			(Hf)0.25(Ni)0.75	the HT phase.
HFRE	Zr21Re25	hR92	R-3c			(Hf)1(Re)1	also Hf21Re25.
HFRH_B2	CsCl (B2)	cP2	Pm-3m			(Hf, Rh)1(Rh)1	
HFSN2_C40	CrSi2 (C40)	hP9	P6_222			(Hf)1(Sn)2	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
IR2Y3	Y3Rh2	tI140	I4/mcm			(Ir)2(Y)3	
IR2Y5	Mn5C2 (Fe5C2 Hagg carbide)	mS28	C2/c			(Ir)2(Y)5	
IR3SI1	SiU3 (D0c)	tI16	I4/mcm			(Ir)3(Si)1	
IR3SI2_B82	Ni2In (B82)	hP6	P6_3/mmc			(Ir)3(Si)2	
IR3SI4	Ru4Si3	oP28	Pnma			(Ir)3(Si)4	
IR3SI5	Ir3Si5	mP64	P2_1/c			(Ir)3(Si)5	
IR3W_D019	Ni3Sn (D019)	hP8	P6_3/mmc			(Ir, W)3(Ir, W)1	
IR3Y1	Ni3Pu	hR12	R-3m			(Ir)3(Y)1	
IR3Y5	Mavlyanovite (Mn5Si3, D88)	hP16	P6_3/mcm			(Ir)3(Y)5	unitedHT/LT phase.
IR3ZR5	Ir3Zr5	hP48	P6_122			(Ir)3(Zr)5	
IR4B3	Ir4B3	oF28	Fmm2			(Ir)4(B)3	
IR4B5	Ir4B5	mS18	Cm			(Ir)4(B)5	
IR4SI5	Ru4Si5	mP18	P2_1/m			(Ir)4(Si)5	
IR5B4	Ir5B4	tI36	I4_1/a			(Ir)5(B)4	
IRMN_L10	CuAu (L10)	tP2	P4/mmm			(Ir, Mn, Ti)0.5(Ir, Mn, Ti)0.5	also IrTi.
IRNB_L10	CuAu (L10)	tP2	P4/mmm			(Ir, Nb)1(Ir, Nb)1	
IRSI_B27	FeB (B27)	oP8	Pnma			(Ir)1(Si)1	the HT phase.
IRSI3_HT	Unknown Structure	oS*				(Ir)1(Si)3	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
IRSI3_LT	Unknown Structure	mS*				(Ir)1(Si)3	
IRV_L10	CuAu (L10)	tP2	P4/mmm			(Ir)0.5(Ir, V)0.5	aka Ir1.04V0.96 orIrV1-x.
IRV_RT	alpha-IrV	oS8	Cmmm			(Ir)1(V)1	
IRW_EPSILON_HCP	Hexagonal Close Packed (Mg, A3, hcp)	hP2	P6_3/mmc			(Ir, W)1(Ir, W)1	HT epsilon solution phase with HCP structure.
IRW_LT_B19	beta'-AuCd (B19)	oP4	Pmma			(Ir)1(Ir, W)1	
IRY3_D011	Cementite (Fe3C, D011)	oP16	Pnma			(Ir)1(Y)3	
IRZR_ALPHA	Mn3As (D0d)	oS16	Cmcm			(Ir, Zr)1(Zr)1	LT phase.
IRZR_BETA_B2	CsCl (B2)	cP2	Pm-3m			(Ir, Zr)1(Ir, Zr)1	i.e. HT- or beta- phase.
IRZR3_D0E	alpha-V3S	tI32	I-42m			(Ir)1(Zr)3	
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	Cr11Ge8	oP76	Pnma			(Cr, Nb)11(Si)8	also Cr11Si8, Nb11Si8.
M12C	Fe6W6C	cF104	Fd-3m			(Co, Ni)6(Mo, W)6(C)1	also Mo6Ni6C
M23B6_TAU_D84	Th6Mn23 (D8a)	cF116	Fm-3m			(Co, Hf, Ni, Re)20(B)6(B, Va)6(Al, Cr, Hf, Mo, Re, Ta, Ti, V, W, Zr)3	ternary boride.
M23C6_D84	Cr23C6 (D84)	cF116	Fm-3m			(Co, Cr, Fe, Mn, Ni, Re, V)20(Co, Cr, Fe, Mn, Mo, Ni, Re, V, W)3(C)6	
M2B_C16	Khatyrkite (Al2Cu, C16)	tI12	I4/mcm			(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ta, W)2(B)1	akaM2B_TETR.
M3B_D011	Cementite (Fe3C, D011)	oP16	Pnma			(Co, Cr, Fe, Mo, Ni)3(B)1	alsoNI3B_D011.
M3B2_D5A	Si2U3 (D5a)	tP10	P4/mbm			(Fe, Hf, Mo, Nb, Ta, V)3(B)2	also NB3B2, TA3B2,V3B2.

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
M3B2_T	Si2U3 (D5a)	tP10	P4/mbm			(Cr, Fe, Mo, Ni, W)0.4(Cr, Fe, Ni)0.2(B)0.4	ternary borideMo2FeB2 or Mo2CrB2.
M3B4_D7B	Ta3B4 (D7b)	oI14	Immm			(B)4(Al, Cr, Hf, Mn, Nb, Ta, Ti, V)3	also ternary X1Y2B4boride.
M3C2_D510	Tongbaite (Cr3C2, D510)	oP20	Pnma			(Co, Cr, Mo, V, W)3(C)2	
M3SI1	Ti3P	tP32	P4_2/n			(Hf, Nb, Ta, Ti, Zr)3(Si)1	also Nb3Si, Ta3Si, Ti3Si, Zr3Si.
M3SI2_D5A	Si2U3 (D5a)	tP10	P4/mbm			(Hf, Nb, Zr)3(Si)2	also Hf3Si2, Zr3Si2.
M3Y	Ni3Pu	hR12	R-3m			(Fe, Ni)3(Y)1	also Fe3Y, Ni3Y.
M4SI3	Ru4Si3	oP28	Pnma			(Cr, Ni, Ru)4(Si)3	also Cr4Si3, Nb4Si3.
M5B6	V5B6	oS22	Cmmm			(Nb, V)5(B)6	also Nb5B6.
M5C2	Mn5C2 (Fe5C2 Hagg carbide)	mS28	C2/c			(Fe, Mn)5(C)2	
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	hP16	P6_3/mcm			(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	also M5Sn3, M5Si3C.
M6C_E93	Fe3W3C (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	
M6SI5	Si5V6	oI44	Ibam			(Cr, Nb, Ti, V)6(Si)5	also Cr6Si5, Nb6Si5.
M7B3_D102	Fe3Th7 (D102)	hP20	P6_3mc			(Co, Cr, Mo, Nb, Re, Rh, Ru, Ta, W)7(B)3(B, Va)3	also RH7B3,RE7B3_D102.
M7C3_D101	C3Cr7 (D101)	oP40	Pnma			(Co, Cr, Fe, Mn, Mo, Ni, Re, V, W)7(C)3	
MB_B27	FeB (B27)	oP8	Pnma			(B)1(Co, Cr, Fe, Hf, Mn, Mo, Re, Ti, Y)1	also CoB, HfB, MnB, TiB.
MB_B33	CrB (B33)	oS8	Cmcm			(Cr, Fe, Hf, Mo, Nb, Ni, Ta, Ti, V)1(B)1	also NbB, NiB, TaB, VB.
MB2_C32	Hexagonal omega (C32)	hP3	P6/mmm			(B)2(Al, Cr, Hf, Mn, Mo, Nb, Ru, Ta, Ti, V, Y, Zr)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
MC_ETA	CMo	hP12	P6_3/mmc			(Mo, V, W)1(C, Va)1	
MC_SHP	Tungsten Carbide (Bh)	hP2	P-6m2			(Mo, W)1(C, N)1	also MoC_LT,Strukturbericht Bh
MN11SI19	Mn11Si19	tP120	P-4n2			(Mn)11(Al, Si)19	
MN12Y_D2B	Mn12Th (D2b)	tI26	I4/mmm			(Mn)12(Y)1	
MN15NI45SI40	Unknown Structure					(Mn)0.15(Ni)0.45(Si)0.4	ternary T1 orN phase
MN15NI50SI35	Unknown Structure					(Mn)0.15(Ni)0.5(Si)0.35	ternary T2 orPHI phase
MN1NI1SI1_C37	MnCuP	oP12	Pnma			(Mn)1(Ni)1(Si)1	ternary T4 or E phase
MN2B_D1F	Mg2Cu (Cb)	oF48	Fddd			(Mn)0.6707(B)0.3293	
MN2NISI	Unknown Structure					(Mn, Ni)3(Si)1	ternary T8 or S phase
MN3N2	Mn3N2	tI10	I4/mmm			(Mn)6(N)4	aka MN6N4.
MN3NI2SI	Mn3Ni2Si	cF96	Fd-3m			(Mn)3(Ni)2(Si)1	ternary T7 or Omega
MN3SI_D03	BiF3 (D03)	cF16	Fm-3m			(Fe, Mn)3(Al, Si)1	
MN3SN2	Tongbaite (Cr3C2, D510)	oP20	Pnma			(Mn)3(Sn)2	
MN3TI1	Unknown Structure					(Mn)3(Ti)1	HT phase
MN4TI	R-(Co,Cr,Mo)	hR53	R-3			(Mn)0.815(Ti)0.185	aka Ti9Mn42
MN52NI29SI19	Unknown Structure					(Mn)0.52(Ni)0.29(Si)0.19	ternary phaseT11 or W phase
MN66NI4SI30	Unknown Structure					(Mn)0.66(Ni)0.04(Si)0.3	ternary T10 orU phase
MN6N5	CoO	tI4	I4/mmm			(Mn)6(N)5	
MN6NI16SI7	Th6Mn23 (D8a)	cF116	Fm-3m			(Mn)0.206897(Ni)0.551724(Si)0.241379	ternary T3 or G phase

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
MN6NISI3	R-(Co,Cr,Mo)	hR53	R-3			(Mn)0.61(Ni)0.12(Si)0.27	ternary T9 or R'phase
MN6SI	Fe7W6 (D85) mu-phase	hR13	R-3m			(Al, Mn)17(Si, Zn)3	
MN9SI2	Mn9Si2	oI186	Immm			(Mn)33(Si)7	
MNB4	MnB4	mS10	C2/m			(Mn)0.2(B)0.8	
MNNI_L10	CuAu (L10)	tP2	P4/mmm			(Cu, Mn, Ni)0.5(Cu, Mn, Ni)0.5	
MNNI2	Unknown Structure					(Mn, Ni)1(Ni)2	
MNNISI_T5	MgZn2 Hexagonal Laves (C14)	hP12	P6_3/mmc			(Mn)1(Ni, Si)2	ternary T5 or tao_1 phase
MNNISI_T6	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m			(Mn)1(Ni, Si)2	ternary T6or tao_2 phase
MNTA	Unknown Structure					(Mn)1(Ta)1	
MNTI_HT	Unknown Structure	t**				(Mn)0.515(Ti)0.485	aka TiMn Mn+ orTi0.47Mn0.53
MNTI_LT	Zr21Re25	hR92	R-3c			(Mn)1(Ti)1	aka Ti21Mn25_RT.
MNZN9	Unknown Structure	h**				(Mn)1(Zn)9	
MO1IR3	Ni3Sn (D019)	hP8	P6_3/mmc			(Mo)1(Ir, Mo)3	
MO2B5_D8I	Mo2B5 (D8i)	hR7	R-3m			(Mo)0.32(B)0.68	
MO3IR_A15	Cr3Si (A15)	cP8	Pm-3n			(Mo)3.06(Ir)0.94	
MO7IR3	sigma-CrFe (D8b)	tP30	P4_2/mnm			(Mo)0.7(Ir)0.3	
MOB_BG	MoB (Bg)	tI16	I4_1/amd			(Cr, Fe, Mo)1(B)1	
MOB4	MoB4	hP16	P6_3/mmc			(Mo)0.2(B)0.8	
MOIR_HT	Hexagonal Close Packed	hP2	P6_3/mmc			(Ir, Mo)1(Ir, Mo)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
	(Mg, A3, hcp)						
MOIR_LT_B19	beta'-AuCd (B19)	oP4	Pmma			(Mo)1(Ir)1	
MONI_DELTA	MoNi	oP56	P2_12_12_1			(Co, Cr, Fe, Ni, Re)24(Co, Cr, Fe, Mo, Ni, Re, W)20 (Cu, Mo, W)12	
MONI4_BETA_D1A	Ni4Mo (D1a)	tI10	I4/m			(Mo, W)1(Ni)4	also WNi4.
MOSI2_C11B	MoSi2 (C11b)	tI6	I4/mmm			(Al, Co, Cu, Fe, Mo, Ni, Rh, W, Zn)1(Al, Cr, Hf, Si, Ti, Zr)2	also AlCr2, Ti2Zn,ZnZr2, CUZR2_C11B.
MOZN22	Zn93(Zn0.43Mo0.57)Mo4	cF420	F-43m			(Mo)1(Zn)22	
MOZN7	Ca7Ge	cF32	Fm-3m			(Mo)1(Zn)7	
MSI_B20	FeSi (B20)	cP8	P2_13			(Co, Cr, Fe, Mn, Ni, Re)1(Al, Si)1	also CoSi, CrSi, MnSi, ReSi.
MSI_B27	FeB (B27)	oP8	Pnma			(Hf, Nb, Ti, Y, Zr)1(Al, Si)1	also TiSi, HfSi, YSi,ZrSi(alpha).
MSI2_C1	Fluorite (CaF2, C1)	cF12	Fm-3m			(Co, Cu, Mn, Ni)1(Al, Cu, Si)2	also NiSi2, CoSi2.
MU_PHASE	Fe7W6 (D85) mu-phase	hR13	R-3m			(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	DIS_MUcontribution added onto it.
MY3_D011	Cementite (Fe3C, D011)	oP16	Pnma			(Co, Ni)1(Y)3	also CoY3, NiY3.
MZR3_E1A	MgCuAl2 (E1a)	oS16	Cmcm			(Co, Fe, Ni)1(Zr)3	also CoZr3, FeZr3.
NB13NI75TI12_XD	Unknown Structure					(Nb)0.13(Ni)0.75(Ti)0.12	
NB15NI56TI29_XA	Unknown Structure	o*100				(Nb)0.15(Ni)0.56(Ti)0.29	
NB15NI80TI5_XE	Unknown Structure					(Nb)0.15(Ni)0.8(Ti)0.05	
NB1ZN1	Unknown Structure					(Nb)0.5(Zn)0.5	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
NB2ZN3_D85	Fe7W6 (D85) mu-phase	hR13	R-3m			(Nb)0.4(Zn)0.6	
NB3RU5	Rh5Ge3	oP16	Pbam			(Nb, Ru)0.375(Ru)0.625	united Nb3Ru5_HT andNbRu3_LT phase
NB5NI75TI20_XC	Ni3Sn (D019)	hP8	P6_3/mmc			(Nb)0.05(Ni)0.75(Ti)0.2	
NB8NI9TI3_XB	Unknown Structure					(Nb)0.4(Ni)0.45(Ti)0.15	
NBSN2_CB	Mg2Cu (Cb)	oF48	Fddd			(Nb, Sn, V)1(Nb, Sn)2	
NBZN15	TiZn16	oS68	Cmcm			(Nb)0.0625(Zn)0.9376	
NBZN2_C36	MgNi2 Hexagonal Laves (C36)	hP24	P6_3/mmc			(Nb)0.333(Zn)0.667	
NBZN3_L12	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m			(Nb)0.25(Zn)0.75	
NBZN7	Unknown Structure					(Nb)0.125(Zn)0.875	
NI10ZR7	Ni10Zr7	oS68	Cmce			(Ni)23(Hf, Zr)17	also Ni10Hf7.
NI11ZR9	Pt11Zr9	tI40	I4/m			(Ni)11(Hf, Zr)9	also Ni11Hf9.
NI17Y2	Fe17Lu2	hP80	P6_3/mmc			(Al, Fe, Ni)1(Y)0.1176	also Fe17Y2.
NI2SI_THETA	AlNi2	hP6	P-3m1			(Cu, Ni)1(Ni, Va)1(Al, Si)1	aka M2SI_TETA.
NI2TA_C11B	MoSi2 (C11b)	tI6	I4/mmm			(Co, Ni)2(Ta, Ti)1	
NI2V	MoPt2	oI6	Immm			(Mo, Ni)2(Mo, Nb, Ta, V)1	
NI2Y1	Ni2Tm	cF192	F-43m			(Ni)2(Y)1	
NI2Y3	Ni2Y3	tP80	P4_12_12			(Ni)2(Y)3	
NI3SI_MONOCL	Ge9Pd25	hP34	P-3			(Ni)3(Si)1	

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

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

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
RHSN2_RT	RhSn2	tI26	I4/mmm			(Rh)0.33333(Sn)0.66667	
RHSN4	IrGe4	hP15	P3_121			(Rh)1(Sn)4	
RHZR_HT_B2	CsCl (B2)	cP2	Pm-3m			(Rh)1(Rh, Zr)1	i.e. beta_RhZr.
RHZR_LT	IrZr	oS16	Cmcm			(Rh)1(Rh, Zr)1	i.e. alpha_RhZr
RHZR2	NiTi2	cF96	Fd-3m			(Rh)1(Zr)2	
RU1B1	Unknown Structure	cI*				(Ru)1(B)1	
RU25Y44	Ru25Y44	oP276	Pnna			(Ru)0.362(Y)0.638	
RU2B3	Ru2B3	hP10	P6_3/mmc			(Ru)2(B)3	
RU2SI_C37	Co2Si (C37)	oP12	Pnma			(Ru)2(Si)1	
RU2SI3	Ge3Ru2	oP40	Pbcn			(Ru)2(Si)3	united HT/LT phase.
RU2SN3	Ru2Sn3	tP20	P-4c2			(Ru)0.4(Sn)0.6	
RU2Y3	Er3Ru2	hP10	P6_3/m			(Ru)0.4(Y)0.6	
RU2Y5	Mn5C2 (Fe5C2 Hagg carbide)	mS28	C2/c			(Ru)0.286(Y)0.714	
RU3SN7_D8F	Ir3Ge7 (D8f)	cI40	Im-3m			(Ru)0.3(Sn)0.7	
RUSI	FeSi (B20)	cP8	P2_13			(Ru)1(Si)1	united HT_B2/LT_B20 phase.
RUY3_D011	Cementite (Fe3C, D011)	oP16	Pnma			(Ru)0.25(Y)0.75	
SI3N4	Nierite (alpha-Si3N4)	hP28	P31c			(Si)3(N)4	
SIB3_D1G	B13C2 B4C (D1g)	hR15	R-3m			(B)6(Si)2(B, Si)6	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
SIB6	SiB6	oP280	Pnnm			(B)210(Si)23(B, Si)48	
SIC_B3	Zincblende (ZnS, B3)	cF8	F-43m			(Si)1(C)1	
SIGMA	sigma-CrFe (D8b)	tP30	P4_2/mnm			(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	DIS_SIGcontribution added onto it.
SN10Y11	Ge10Ho11	tI84	I4/mmm			(Sn)10(Y)11	
SN2Y_C49	ZrSi2 (C49)	oS12	Cmcm			(Sn)2(Y)1	
SN3TI2	Unknown Structure					(Sn)3(Ti)2	
SN3Y1	GdSn2.75	oS16	Amm2			(Sn)3(Y)1	
SN4Y5	Gd5Si4	oP36	Pnma			(Sn)4(Y)5	
SN5TI6	Sn5Ti6-beta	hP22	P6_3/mmc			(Al, Sn)5(Nb, Ti)6	also Sn5Nb6.
SN5Y2	Shcherbinaite (V2O5) (Revised)	oP14	Pmmn			(Sn)5(Y)2	
SNTI2_B82	Ni2In (B82)	hP6	P6_3/mmc			(Sn)1(Ti)2	
T1CUFETI_CU2TI	Au2V	oS12	Cmcm			(Cu, Fe)2(Ti)1	ternaryTi0.33FexCu0.67-x, Tau1.
T1CUNITI_C11B	MoSi2 (C11b)	tI6	I4/mmm			(Cu, Ni)2(Ti)1	the Cu-Ni-Titernary phase Tau1.
T2CUFETI_CU3TI2	Cu3Ti2	tP10	P4/nmm			(Cu, Fe)3(Ti)2	ternaryTi0.4FexCu0.6-x, Tau2.
T2CUNITI	Cu3Ti2	tP10	P4/nmm			(Cu)0.175(Ni)2.825(Ti)2	the Cu-Ni-Titernary phase Tau2.
T3CUFETI_CU4TI3	Cu4Ti3	tI14	I4/mmm			(Cu, Fe)4(Ti)3	ternaryTi0.43FexCu0.57-x, Tau3.
T4CUFETI	Unknown Structure					(Cu, Fe)0.63(Ti)0.37	ternaryTi0.37FexCu0.63-x, Tau4

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
T4CUNITI	BaPb3	hR12	R-3m			(Cu)0.05(Ni)0.7(Ti)0.25	the Cu-Ni-Ti ternaryphase Tau4.
T5CUFETI	Unknown Structure					(Cu, Fe)0.55(Ti)0.45	ternaryTi0.45FexCu0.55-x, Tau5.
T6CUNITI	Unknown Structure					(Cu)0.25(Ni)0.5(Ti)0.25	the Cu-Ni-Ti ternaryphase Tau6
TA1AL1	Al38Ta48	mP86	P2_1/c			(Ta)0.51515(Al)0.48485	
TA3SN_A15	Cr3Si (A15)	cP8	Pm-3n			(Ta)3(Sn)1	
TA41IR59	CuAu (L10)	tP2	P4/mmm			(Ta)0.41(Ir)0.59	akaTa0.82Ir1.18_rt, gamma.
TA43IR57	TaIr	oP12	Pmma			(Ta)0.43(Ir, Ta)0.57	aka Ta0.86Ir1.14, delta.
TA5SI3_D8L	Cr5B3 (D8l)	tI32	I4/mcm			(Hf, Nb, Ta)5(Al, Si)3	also alpha-Nb5Si3.
TAAL2_HT	Al69Ta39	cF444	F-43m			(Ta)0.35(Al)0.65	
TAN_EPS	TaN-eps	hP6	P-62m			(Ta)1(N)1	
TASN2_CB	Mg2Cu (Cb)	oF48	Fddd			(Ta)1(Sn)2	also SN2TA_CB.
TI25MN9AL66_L12	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m			(Al, Mn, Ti)0.25(Al, Mn)0.08(Al, Mn, Ti)0.67	also Ti25Mn8Al67 or Ti43Mn11Al66, Tau1.
TI2ALC	AlCCr2	hP8	P6_3/mmc			(Ti)2(Al)1(C, Va)1	i.e. Ti2AlC1-x.
TI2N_C4	Rutile (TiO2, C4)	tP6	P4_2/mnm			(Ti)2(N)1	
TI3ALC_E21	Cubic Perovskite (CaTiO3, E21)	cP5	Pm-3m			(Ti)3(Al)1(C, Va)1	i.e.Ti3AlC1-x.
TI3ALC2	Ti3SiC2	hP12	P6_3/mmc			(Ti)3(Al, Si)1(C, Va)2	
TI3N2	TiS-9R	hR6	R-3m			(Ti)0.71(N)0.29	
TI3SIC2	Ti3SiC2	hP12	P6_3/mmc			(Ti)3(Si)1(C)2	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
TI4N3	Sc2Te3	hR8	R-3m			(Ti)0.685(N)0.315	aka Xi-TiN0.58 HT
TISI2_C54	TiSi2 (C54)	oF24	Fddd			(Mo, Nb, Ru, Ti, Zr)1(Al, Si, Sn)2	also MoSi2, RuAl2, ZrSn2.
TIZN10	Ti3Zn22	tP100	P4_2/mbc			(Ti)1(Zn)10	
TIZN15	TiZn16	oS68	Cmcm			(Ti)1(Zn)15	
TIZN5	Unknown Structure					(Ti)1(Zn)5	
V2B3	V2B3	oS20	Cmcm			(V)0.4(B)0.6	
V3SN_A15	Cr3Si (A15)	cP8	Pm-3n			(Sn)0.205(V)0.795	
V4ZN5	V4Zn5	tI18	I4/mmm			(V)4(Zn)5	
VSN2_CB	Mg2Cu (Cb)	oF48	Fddd			(Sn)0.6(V)0.4	
VZN3_L12	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m			(V)1(Zn)3	
W2B5_D8I	Mo2B5 (D8i)	hR7	R-3m			(B, C, Va)5(W)2	nonstoichiometric W2B5.
W2B9	W2B9	hP22	P-3			(B)9(W)2	
W3MC	W10Co3C3.4	hP34	P6_3/mmc			(W)3(Co, Ni)1(C)1	also W3CoC, W3NiC.
W5SI3_D8M	W5Si3 (D8m)	tI32	I4/mcm			(Cr, Fe, Mo, Nb, Ti, V, W)4(Cr, Fe, Mo, Nb, Si, Ti, V, W)1(Al, Si, Sn)3	also Cr5Si3, Mo5Si3,Nb5Si3, V5Si3.
WB_ALPHA_BG	MoB (Bg)	tI16	I4_1/amd			(B, C, Va)1(W)1	
WB_BETA_B33	CrB (B33)	oS8	Cmcm			(B, C, Va)1(W)1	
Y13ZN58	Y13Zn58	hP146	P6_3/mmc			(Y)13(Zn)58	
Y15C19_ALPHA	alpha-Y15C19	oP18	Pbam			(C)19(Y)15	aka Y15C19_R.

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
Y15C19_BETA	Unknown Structure					(C)19(Y)15	the high temperaturebeta phase
Y1ZN3	Zn3Y	oP16	Pnma			(Y)1(Zn)3	
Y2C3_ALPHA	Sc3C4	tP70	P4/mnc			(Y)2(C)2(C, Va)1	aka Y2C3_R.
Y2C3_BETA	Unknown Structure					(Y)2(C)2(C, Va)1	HT phase
Y2ZN17	Ni17Th2	hP38	P6_3/mmc			(Y)2(Zn)17	
Y3SI5_HT_CC	alpha-ThSi2 (Cc)	tI12	I4_1/amd			(Y)3(Si)5	
Y3SI5_LT_C32	Hexagonal omega (C32)	hP3	P6/mmm			(Y)3(Si)5	
Y5SI4	Gd5Si4	oP36	Pnma			(Y)5(Si)4	
YB4_D1E	ThB4 (D1e)	tP20	P4/mbm			(Y)0.2(B)0.8	
YB6_D21	CaB6 (D21)	cP7	Pm-3m			(Y)1(B)6	
YB66	YB66	cF1936	Fm-3c			(Y)1(B)66	
YC_GAMMA_B1	Rock Salt (NaCl, B1)	cF8	Fm-3m			(Y)1(C, C2, Va)1	
YC2_C11A	CaC2-I (C11a)	tI6	I4/mmm			(C2Y1)1	
YSI2_HT_CC	alpha-ThSi2 (Cc)	tI12	I4_1/amd			(Y)1(Si)2	
YSI2_LT_C32	Hexagonal omega (C32)	hP3	P6/mmm			(Y)1(Si)2	
YZN2_HT	Unknown Structure					(Y)1(Zn)2	
YZN2_LT	Unknown Structure					(Y)1(Zn)2	
YZN5	ErZn5	hP36	P6_3/mmc			(Y)1(Zn)5	aka H_RZN5
Z_PHASE	CrNbN	tP6	P4/nmm			(Cr, Fe)1(Mo, Nb, V)1(N, Va)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
ZN11Y3	Al11La3	oI28	Immm			(Zn)11(Y)3	
ZN12Y_D2B	Mn12Th (D2b)	tI26	I4/mmm			(Zn)12(Y)1	
ZN22ZR	Zn22Zr	cF184	Fd-3m			(Zn)22(Zr)1	
ZN2ZR3	Zr3Al2	tP20	P4_2/mnm			(Zn)2(Zr)3	
ZN39ZR5	Zn39Zr5	mS88	C2/m			(Zn)39(Zr)5	
ZN3ZR_HT	Unknown Structure	c**				(Zn)3(Zr)1	
ZNZR_B2	CsCl (B2)	cP2	Pm-3m			(Zn)1(Zr)1	
ZR5SI4_TP36	Si4Zr5	tP36	P4_12_12			(Hf, Nb, Ti, Zr)5(Al, Si)4	also Hf5Si4, Ti5Si4.
ZRB12_D2F	UB12 (D2f)	cF52	Fm-3m			(B)12(Y, Zr)1	also YB12.
ZRSI2_C49	ZrSi2 (C49)	oS12	Cmcm			(Hf, Nb, Zr)1(Si)2	also HfSi2.

TCHEA5 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 thermophysical 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:	**5.1**
First release:	**TCHEA1 was released in 2015**

Changes in the Most Recent Database Release

TCHEA5.0 to TCHEA5.1

Software release 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.

Previous Releases

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.