TCS High Entropy Alloys Database (TCHEA6)

Technical Information

Available Starting with Thermo-Calc Version 2022b

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Contents

About the TCS High Entropy Alloys Database (TCHEA) **3**

TCS High Entropy Alloys Database (TCHEA) Resources **6**

TCHEA6 Elements, Systems, Phases, and Properties Data **7**

TCHEA6 Systems **10**

TCHEA6 Assessed Binary Systems 11

TCHEA6 Critically Assessed Ternary Systems 12

TCHEA6 Tentatively Assessed Ternary Systems 14

TCHEA6 Phases **16**

TCHEA6 Models for the Included Phases 17

TCHEA6 Properties Data **38**

Model Descriptions 38

Examples 38

TCHEA: TCS High Entropy Alloys Database Revision History **39**

About the TCS High Entropy Alloys Database (TCHEA)

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

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

The database is compatible with the TCS High Entropy Alloy Mobility Database (MOBHEA). The current version is MOBHEA3.

The CALPHAD Method

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

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

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

Use Case Examples

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

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

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

Combining Databases

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

References

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Suggested References to Cite this Database

[2017Mao] H. Mao, H.-L. Chen, Q. Chen, TCHEA1: A Thermodynamic Database Not Limited for "High Entropy" Alloys. J. Phase Equilibria Diffus. 38 (2017) 353–368.

[2018Chen] H.-L. Chen, H. Mao, Q. Chen, Database development and Calphad calculations for high entropy alloys: Challenges, strategies, and tips. Mater. Chem. Phys. 210 (2018) 279-290.

TCS High Entropy Alloys Database (TCHEA) Resources

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

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

Database Specific Documentation

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

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

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

TCHEA6 Elements, Systems, Phases, and Properties Data

Included Elements

The database has been developed in a 26 element framework:

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

Assessed Systems and Phases

The most recent version of the database contains:

- 310 binary systems, with almost all of these assessed to the full range of composition and temperature. These can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 511 ternaries are assessed, and 201 of them to the full range of composition and temperature. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 515 solution and intermetallic phases, where nearly all stable phases in all assessed binary systems and most ternary systems are modeled.

About the Included Phases

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

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

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

Properties Data

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

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

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

Below is a summary of the available parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use the TC-Python SDK. More details are described in the online help.

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Electrical conductivity		ELCD for a system `ELCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI*	`SURF(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)`**

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)`**
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

* XI is not used in the TCS Metal Oxide Solutions Database (TCOX)
** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCHEA6 Systems

In this section:

TCHEA6 Assessed Binary Systems 11
TCHEA6 Critically Assessed Ternary Systems 12
TCHEA6 Tentatively Assessed Ternary Systems 14

TCHEA6 Assessed Binary Systems

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

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

TCHEA6 Critically Assessed Ternary Systems

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

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

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

TCHEA6 Tentatively Assessed Ternary Systems

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

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

TCHEA6 Phases

In this section:

TCHEA6 Models for the Included Phases 17

TCHEA6 Models for the Included Phases

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
LIQUID	Liquid						1	[1.0]	(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
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	FCC_A1 will be combined to FCC_L12 if defined.	2	[1.0, 1.0]	(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_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	This phase has some contribution from FCC_ A1.	3	[0.75, 0.25, 1.0]	(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
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229	BCC_A2 will be combined to BCC_B2 if defined.	2	[1.0, 3.0]	(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_B2	CsCl (B2)	B2	cP2	Pm-3m	221	This phase has some contribution from BCC_ A2.	3	[0.5, 0.5, 3.0]	(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
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_ 3/mmc	194	Disordered HCP_A3 solution phase.	2	[1.0, 0.5]	(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
CBCC_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[1.0, 1.0]	(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
CUB_A13	beta-Mn (A13)	A13	cP20	P4_132	213		2	[1.0, 1.0]	(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
DIS_FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	A copy of the FCC_A1 phase just for the use in kinetic simulation.	2	[1.0, 1.0]	(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
DIAMOND_A4	Diamond (A4)	A4	cF8	Fd-3m	227	Pure C, Si or solid solution phases based on them.	1	[1.0]	(AL, B, C, SI, SN)1
BETA_ RHOMBO_B	beta-B (R-105)		hR105	R-3m	166		2	[93.0, 12.0]	(B)93(B, C, CU, SI)12
GRAPHITE_A9	Hexagonal Graphite (A9)	A9	hP4	P6_ 3/mmc	194		1	[1.0]	(B, C)1
BCT_A5	beta-Sn (A5)	A5	tI4	I4_1/amd	141	Disordered BCT solution phase.	1	[1.0]	(AL, CU, NI, SN, ZN)1
M23B6_TAU_ D84	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225	ternary boride.	4	[20.0, 6.0, 6.0, 3.0]	(CO, HF, NI, RE)20(B)6(B, VA)6(AL, CR, HF, MO, RE, TA, TI, V, W, ZR)3
M3B_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62	also NI3B_D011.	2	[3.0, 1.0]	(CO, CR, FE, MO, NI)3(B)1
RE3B_E1A	Re3B		oS16	Cmcm	63		2	[3.0, 1.0]	(CR, MO, RE, TA, W)3(B)1
M7B3_D102	Fe3Th7 (D102)	D102	hP20	P6_3mc	186	also RH7B3, RE7B3_D102.	3	[7.0, 3.0, 3.0]	(CO, CR, MO, NB, RE, RH, RU, TA, W)7(B)3(B, VA)3

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M2B_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140	aka M2B_TETR.	2	[2.0, 1.0]	(AL, CO, CR, FE, MN, MO, NB, NI, RE, TA, W)2(B)1
CR2B_CB	Mg2Cu (Cb)	Cb	oF48	Fddd	70	aka CR2B_ORTH.	2	[0.66666667, 0.33333333]	(CR, FE, MO, RE)0.666667(B)0.333333
MN2B_D1F	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[0.6707, 0.3293]	(MN)0.6707(B)0.3293
CR5B3_D8L	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140	also Mo5B3.	2	[0.625, 0.375]	(CR, MO)0.625(B)0.375
M3B2_D5A	Si2U3 (D5a)	D5a	tP10	P4/mbm	127	also NB3B2, TA3B2, V3B2.	2	[3.0, 2.0]	(FE, HF, MO, NB, TA, V)3(B)2
M3B2_T	Si2U3 (D5a)	D5a	tP10	P4/mbm	127	ternary boride Mo2FeB2 or Mo2CrB2.	3	[0.4, 0.2, 0.4]	(CR, FE, MO, NI, W)0.4(CR, FE, NI)0.2(B)0.4
IR4B3	Ir4B3		oF28	Fmm2	42		2	[4.0, 3.0]	(IR)4(B)3
NI4B3	m-Ni4B3		mS28	C2/c	15		2	[0.57142857, 0.42857143]	(NI)0.571429(B)0.428571
IR5B4	Ir5B4		tI36	I4_1/a	88		2	[5.0, 4.0]	(IR)5(B)4
MB_B27	FeB (B27)	B27	oP8	Pnma	62	also CoB, HfB, MnB, TiB.	2	[1.0, 1.0]	(B)1(CO, CR, FE, HF, MN, MO, RE, TI, Y)1
MB_B33	CrB (B33)	B33	oS8	Cmcm	63	also NbB, NiB, TaB, VB.	2	[1.0, 1.0]	(CR, FE, HF, MO, NB, NI, TA, TI, V)1(B)1
MOB_BG	MoB (Bg)	Bg	tI16	I4_1/amd	141		2	[1.0, 1.0]	(CR, FE, MO)1(B)1
WB_ALPHA_BG	MoB (Bg)	Bg	tI16	I4_1/amd	141		2	[1.0, 1.0]	(B, C, VA)1(W)1
RU1B1	Unknown Structure		cI*				2	[1.0, 1.0]	(RU)1(B)1
WB_BETA_B33	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(B, C, VA)1(W)1
RHB_B81	NiAs (B81)	B81	hP4	P6_ 3/mmc	194		2	[1.0, 1.1]	(RH)1(B)1.1
M5B6	V5B6		oS22	Cmmm	65	also Nb5B6.	2	[5.0, 6.0]	(NB, V)5(B)6
IR4B5	Ir4B5		mS18	Cm	8		2	[4.0, 5.0]	(IR)4(B)5
M3B4_D7B	Ta3B4 (D7b)	D7b	oI14	Immm	71	also ternary X1Y2B4 boride.	2	[4.0, 3.0]	(B)4(AL, CR, HF, MN, NB, TA, TI, V)3
RU2B3	Ru2B3		hP10	P6_ 3/mmc	194		2	[2.0, 3.0]	(RU)2(B)3
V2B3	V2B3		oS20	Cmcm	63		2	[0.4, 0.6]	(V)0.4(B)0.6
MB2_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[2.0, 1.0]	(B)2(AL, CR, HF, MN, MO, NB, RU, TA, TI, V, Y, ZR)1
REB2	ReB2		hP6	P6_ 3/mmc	194		3	[1.0, 2.0, 2.0]	(RE)1(B)2(B, VA)2
MO2B5_D8I	Mo2B5 (D8i)	D8i	hR7	R-3m	166		2	[0.32, 0.68]	(MO)0.32(B)0.68
W2B5_D8I	Mo2B5 (D8i)	D8i	hR7	R-3m	166	nonstoichiometric W2B5.	2	[5.0, 2.0]	(B, C, VA)5(W)2
CRB4	CrB4		oI10	Immm	71		2	[0.2, 0.8]	(CR)0.2(B)0.8
MNB4	MnB4		mS10	C2/m	12		2	[0.2, 0.8]	(MN)0.2(B)0.8

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MOB4	MoB4		hP16	P6_ 3/mmc	194		2	[0.2, 0.8]	(MO)0.2(B)0.8
YB4_D1E	ThB4 (D1e)	D1e	tP20	P4/mbm	127		2	[0.2, 0.8]	(Y)0.2(B)0.8
W2B9	W2B9		hP22	P-3	147		2	[9.0, 2.0]	(B)9(W)2
YB6_D21	CaB6 (D21)	D21	cP7	Pm-3m	221		2	[1.0, 6.0]	(Y)1(B)6
ZRB12_D2F	UB12 (D2f)	D2f	cF52	Fm-3m	225	also YB12.	2	[12.0, 1.0]	(B)12(Y, ZR)1
ALB12_ALPHA	alpha-AlB12		tP216	P4_12_ 12	92		2	[1.0, 12.0]	(AL, TI)1(B)12
YB66	YB66		cF1936	Fm-3c	226		2	[1.0, 66.0]	(Y)1(B)66
M12C	Fe6W6C		cF104	Fd-3m	227	also Mo6Ni6C	3	[6.0, 6.0, 1.0]	(CO, NI)6(MO, W)6(C)1
M6C_E93	Fe3W3C (E93)	E93	cF112	Fd-3m	227		4	[2.0, 2.0, 2.0, 1.0]	(CO, FE, NI)2(MO, NB, TA, W)2(CO, CR, FE, MO, NB, NI, TA, V, W)2(C)1
ALM3C_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221	also AlCo3C, AlFe3C.	3	[1.0, 3.0, 1.0]	(AL)1(CO, FE)3(C)1
TI3ALC_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221	i.e. Ti3AlC1-x.	3	[3.0, 1.0, 1.0]	(TI)3(AL)1(C, VA)1
W3MC	W10Co3C3.4		hP34	P6_ 3/mmc	194	also W3CoC, W3NiC.	3	[3.0, 1.0, 1.0]	(W)3(CO, NI)1(C)1
M23C6_D84	Cr23C6 (D84)	D84	cF116	Fm-3m	225		3	[20.0, 3.0, 6.0]	(CO, CR, FE, MN, NI, RE, V)20(CO, CR, FE, MN, MO, NI, RE, V, W)3(C)6
ALCR2C	AlCCr2		hP8	P6_ 3/mmc	194	MAX_PHASE.	3	[1.0, 1.0, 2.0]	(AL)1(C)1(CR)2
CEMENTITE_ D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(CO, CR, FE, MN, MO, NI, V, W)3(C, N)1
TI2ALC	AlCCr2		hP8	P6_ 3/mmc	194	i.e. Ti2AlC1-x.	3	[2.0, 1.0, 1.0]	(TI)2(AL)1(C, VA)1
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[5.0, 2.0]	(FE, MN)5(C)2
M7C3_D101	C3Cr7 (D101)	D101	oP40	Pnma	62		2	[7.0, 3.0]	(CO, CR, FE, MN, MO, NI, RE, V, W)7(C)3
TI3ALC2	Ti3SiC2		hP12	P6_ 3/mmc	194		3	[3.0, 1.0, 2.0]	(TI)3(AL, SI)1(C, VA)2
M3C2_D510	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62		2	[3.0, 2.0]	(CO, CR, MO, V, W)3(C)2
AL4C3_D71	Al4C3 (D71)	D71	hR7	R-3m	166		2	[4.0, 3.0]	(AL, SI)4(C)3
MC_ETA	CMo		hP12	P6_ 3/mmc	194		2	[1.0, 1.0]	(MO, V, W)1(C, VA)1
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	P-6m2	187	also MoC_LT, Strukturbericht Bh	2	[1.0, 1.0]	(MO, W)1(C, N)1

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YC_GAMMA_B1	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		2	[1.0, 1.0]	(Y)1(C, C2, VA)1
Y15C19_BETA	Unknown Structure					the high temperature beta phase	2	[19.0, 15.0]	(C)19(Y)15
Y15C19_ALPHA	alpha-Y15C19		oP18	Pbam	55	aka Y15C19_R.	2	[19.0, 15.0]	(C)19(Y)15
Y2C3_BETA	Unknown Structure					HT phase	3	[2.0, 2.0, 1.0]	(Y)2(C)2(C, VA)1
Y2C3_ALPHA	Sc3C4		tP70	P4/mnc	128	aka Y2C3_R.	3	[2.0, 2.0, 1.0]	(Y)2(C)2(C, VA)1
YC2_C11A	CaC2-I (C11a)	C11a	tI6	I4/mmm	139		1	[1.0]	(C2Y1)1
PI_A13	beta-Mn (A13)	A13	cP20	P4_132	213	i.e. Cr-(Fe,Ni)-N nitride.	3	[12.8, 7.2, 4.0]	(CR)12.8(FE, NI)7.2(N)4
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	Pm-3m	221	Only stable in (Co-Cr-Fe)-N when gas suspended.	2	[4.0, 1.0]	(CO, CR, FE, MN, NI)4(C, N)1
ALTI3N_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221		3	[1.0, 3.0, 1.0]	(AL)1(TI)3(N)1
ALTI2N	AlCCr2		hP8	P6_ 3/mmc	194		3	[1.0, 2.0, 1.0]	(AL)1(TI)2(N)1
AL2TI3N2	(Al2Ti3N2)		hP22	P6_3mc	186		3	[2.0, 3.0, 2.0]	(AL)2(TI)3(N)2
FECN_CHI	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15	Only stable in C-Fe-N when gas suspended.	2	[2.2, 1.0]	(FE)2.2(C, N)1
TI4N3	Sc2Te3		hR8	R-3m	166	aka Xi-TiN0.58 HT	2	[0.685, 0.315]	(TI)0.685(N)0.315
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	P4_ 2/mnm	136		2	[2.0, 1.0]	(TI)2(N)1
Z_PHASE	CrNbN		tP6	P4/nmm	129		3	[1.0, 1.0, 1.0]	(CR, FE)1(MO, NB, V)1(N, VA)1
HF3N2	TiS-9R		hR6	R-3m	166		2	[3.0, 2.0]	(HF)3(N)2
MN3N2	Mn3N2		tI10	I4/mmm	139	aka MN6N4.	2	[6.0, 4.0]	(MN)6(N)4
TI3N2	TiS-9R		hR6	R-3m	166		2	[0.71, 0.29]	(TI)0.71(N)0.29
HF4N3	Sc2Te3		hR8	R-3m	166		2	[4.0, 3.0]	(HF)4(N)3
MN6N5	CoO		tI4	I4/mmm	139		2	[6.0, 5.0]	(MN)6(N)5
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186		2	[1.0, 1.0]	(AL)1(N)1
TAN_EPS	TaN-eps		hP6	P-62m	189		2	[1.0, 1.0]	(TA)1(N)1
HFN_B1	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		2	[1.0, 1.0]	(HF)1(N, VA)1
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166		2	[17.0, 3.0]	(AL, MN)17(SI, ZN)3
MN9SI2	Mn9Si2		oI186	Immm	71		2	[33.0, 7.0]	(MN)33(SI)7
CR3NI5SI2	AlAu4		cP20	P2_13	198		4	[3.0, 5.0, 2.0, 1.0]	(CR)3(NI)5(SI)2(C, VA)1
CR2NI2SI	NiTi2		cF96	Fd-3m	227	i.e. the Tau1 phase Cr5Ni5Si3.	3	[5.0, 5.0, 3.0]	(CR)5(NI)5(SI)3

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CR3SI_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223	also Cr3X, Nb3X, Ti3X, V3X.	3	[3.0, 1.0, 3.0]	(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
CO3SI_D019	Ni3Sn (D019)	D019	hP8	P6_ 3/mmc	194		2	[3.0, 1.0]	(CO)3(SI)1
IR3SI1	SiU3 (D0c)	D0c	tI16	I4/mcm	140		2	[3.0, 1.0]	(IR)3(SI)1
M3SI1	Ti3P		tP32	P4_2/n	86	also Nb3Si, Ta3Si, Ti3Si, Zr3Si.	2	[3.0, 1.0]	(HF, NB, TA, TI, ZR)3(SI)1
MN3SI_D03	BiF3 (D03)	D03	cF16	Fm-3m	225		2	[3.0, 1.0]	(FE, MN)3(AL, SI)1
NI3SI_ORTHO_ D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(NI)3(SI)1
NI3SI_MONOCL	Ge9Pd25		hP34	P-3	147		2	[3.0, 1.0]	(NI)3(SI)1
NI5SI2	Ni31S12		hP42	P321	150		2	[5.0, 2.0]	(CO, CR, CU, FE, NI)5(SI)2
CO2SI1	Co2Si (C37)	C37	oP12	Pnma	62	also Ni2Si (delta)	2	[2.0, 1.0]	(CO, CR, CU, FE, IR, NI, TI)2(SI)1
CRNBSI	ZrNiAl		hP9	P-62m	189		3	[1.0, 1.0, 1.0]	(CR)1(NB)1(SI)1
FE2SI	AlNi2		hP6	P-3m1	164		2	[0.666667, 0.333333]	(FE)0.666667(SI)0.333333
NI2SI_THETA	AlNi2		hP6	P-3m1	164	aka M2SI_TETA.	3	[1.0, 1.0, 1.0]	(CU, NI)1(NI, VA)1(AL, SI)1
RE2SI	Re2Si		mP24	P2_1/c	14		2	[2.0, 1.0]	(RE)2(SI)1
RU2SI_C37	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(RU)2(SI)1
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_ 3/mcm	193	also M5Sn3, M5Si3C.	4	[2.0, 3.0, 3.0, 1.0]	(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
TA5SI3_D8L	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140	also alpha-Nb5Si3.	2	[5.0, 3.0]	(HF, NB, TA)5(AL, SI)3
W5SI3_D8M	W5Si3 (D8m)	D8m	tI32	I4/mcm	140	also Cr5Si3, Mo5Si3, Nb5Si3, V5Si3.	3	[4.0, 1.0, 3.0]	(CR, FE, MO, NB, TI, V, W)4(CR, FE, MO, NB, SI, TI, V, W)1(AL, SI, SN)3
IR3SI2_B82	Ni2In (B82)	B82	hP6	P6_ 3/mmc	194		2	[3.0, 2.0]	(IR)3(SI)2
M3SI2_D5A	Si2U3 (D5a)	D5a	tP10	P4/mbm	127	also Hf3Si2, Zr3Si2.	2	[3.0, 2.0]	(HF, NB, ZR)3(SI)2
NI3SI2	Ni3Si2		oP80	Cmc2_1	36		2	[3.0, 2.0]	(NI)3(SI)2
M11SI8	Cr11Ge8		oP76	Pnma	62	also Cr11Si8, Nb11Si8.	2	[11.0, 8.0]	(CR, NB)11(SI)8
M4SI3	Ru4Si3		oP28	Pnma	62	also Cr4Si3, Nb4Si3.	2	[4.0, 3.0]	(CR, NI, RU)4(SI)3
ZR5SI4_TP36	Si4Zr5		tP36	P4_12_ 12	92	also Hf5Si4, Ti5Si4.	2	[5.0, 4.0]	(HF, NB, TI, ZR)5(AL, SI)4
Y5SI4	Gd5Si4		oP36	Pnma	62		2	[5.0, 4.0]	(Y)5(SI)4
M6SI5	Si5V6		oI44	Ibam	72	also Cr6Si5, Nb6Si5.	2	[6.0, 5.0]	(CR, NB, TI, V)6(SI)5
MSI_B20	FeSi (B20)	B20	cP8	P2_13	198	also CoSi, CrSi, MnSi, ReSi.	2	[1.0, 1.0]	(CO, CR, FE, MN, NI, RE)1(AL, SI)1
IRSI_B27	FeB (B27)	B27	oP8	Pnma	62	the HT phase.	2	[1.0, 1.0]	(IR)1(SI)1
MSI_B27	FeB (B27)	B27	oP8	Pnma	62	also TiSi, HfSi, YSi, ZrSi (alpha).	2	[1.0, 1.0]	(HF, NB, TI, Y, ZR)1(AL, SI)1

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NISI_B31	MnP (B31)	B31	oP8	Pnma	62		2	[1.0, 1.0]	(NI)1(SI)1
RUSI	FeSi (B20)	B20	cP8	P2_13	198	united HT_B2/LT_B20 phase.	2	[1.0, 1.0]	(RU)1(SI)1
IR4SI5	Ru4Si5		mP18	P2_1/m	11		2	[4.0, 5.0]	(IR)4(SI)5
IR3SI4	Ru4Si3		oP28	Pnma	62		2	[3.0, 4.0]	(IR)3(SI)4
RU2SI3	Ge3Ru2		oP40	Pbcn	60	united HT/LT phase.	2	[2.0, 3.0]	(RU)2(SI)3
IR3SI5	Ir3Si5		mP64	P2_1/c	14		2	[3.0, 5.0]	(IR)3(SI)5
Y3SI5_HT_CC	alpha-ThSi2 (Cc)	Cc	tI12	I4_1/amd	141		2	[3.0, 5.0]	(Y)3(SI)5
Y3SI5_LT_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[3.0, 5.0]	(Y)3(SI)5
MN11SI19	Mn11Si19		tP120	P-4n2	118		2	[11.0, 19.0]	(MN)11(AL, SI)19
CRSI2_C40	CrSi2 (C40)	C40	hP9	P6_222	180	also NbSi2, TaSi2, VSi2.	2	[1.0, 2.0]	(CR, CU, HF, MO, NB, SI, TA, TI, V, W)1(AL, CR, CU, SI)2
FESI2_HT	FeSi2-h		tP3	P4/mmm	123		2	[0.3, 0.7]	(FE)0.3(SI)0.7
FESI2_LT	FeSi2-l		oS48	Cmce	64		2	[0.333333, 0.666667]	(FE)0.333333(SI)0.666667
MSI2_C1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	also NiSi2, CoSi2.	2	[1.0, 2.0]	(CO, CU, MN, NI)1(AL, CU, SI)2
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139	also AlCr2, Ti2Zn, ZnZr2, CUZR2_C11B.	2	[1.0, 2.0]	(AL, CO, CU, FE, MO, NI, RH, W, ZN)1(AL, CR, HF, SI, TI, ZR)2
RESI2_C11B	Re4Si7		mS44	Cm	8		2	[0.357, 0.643]	(RE)0.357(SI)0.643
TISI2_C54	TiSi2 (C54)	C54	oF24	Fddd	70	also MoSi2, RuAl2, ZrSn2.	2	[1.0, 2.0]	(MO, NB, RU, TI, ZR)1(AL, SI, SN)2
YSI2_HT_CC	alpha-ThSi2 (Cc)	Cc	tI12	I4_1/amd	141		2	[1.0, 2.0]	(Y)1(SI)2
YSI2_LT_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[1.0, 2.0]	(Y)1(SI)2
ZRSI2_C49	ZrSi2 (C49)	C49	oS12	Cmcm	63	also HfSi2.	2	[1.0, 2.0]	(HF, NB, ZR)1(SI)2
IRSI3_LT	Unknown Structure		mS*				2	[1.0, 3.0]	(IR)1(SI)3
IRSI3_HT	Unknown Structure		oS*				2	[1.0, 3.0]	(IR)1(SI)3
ALFESI_ALPHA_ TAU5	Fe23Al81Si15		hP246	P6_ 3/mmc	194		4	[0.6612, 0.19, 0.0496, 0.0992]	(AL)0.6612(FE)0.19(SI)0.0496(AL, SI)0.0992
ALFESI_BETA_ TAU6	Fe2Al9Si2		mS52	C2/c	15		3	[14.0, 3.0, 3.0]	(AL)14(FE)3(SI)3
ALFESI_ GAMMA_TAU2	Unknown Structure		mS*				3	[3.0, 1.0, 1.0]	(AL)3(FE)1(SI)1
ALFESI_DELTA_ TAU4	FeAl3Si2		oP24	Pbcn	60		3	[0.55, 0.15, 0.3]	(AL)0.55(FE)0.15(SI)0.3
ALFESI_TAU1	Unknown Structure						3	[2.0, 2.0, 1.0]	(AL)2(FE)2(SI)1
ALFESI_TAU3	Fe(Al0.67Si0.33)3		oS128	Cmme	67		3	[2.0, 1.0, 1.0]	(AL)2(FE)1(SI)1

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AL2MN2SI3	(Al2Mn2Si3)		hP21	P-6	174	Tau1	3	[2.0, 2.0, 3.0]	(AL)2(MN)2(SI)3
AL5MN6SI7	CrSi2 (C40)	C40	hP9	P6_222	180	Tau2	3	[5.0, 6.0, 7.0]	(AL)5(MN)6(SI)7
AL1MN1SI1	TiSi2 (C54)	C54	oF24	Fddd	70	Tau3	3	[1.0, 1.0, 1.0]	(AL)1(MN)1(SI)1
AL3MNSI2	(Al3MnSi2)		tP48	P4/n	85	Tau4	3	[3.0, 1.0, 2.0]	(AL)3(MN)1(SI)2
AL3MN4SI2	Unknown Structure					ternary tau5 or D phase	3	[3.0, 4.0, 2.0]	(AL)3(MN)4(SI)2
ALMNSI_TAU6	Unknown Structure						2	[4.0, 1.0]	(AL, MN)4(SI)1
ALMNSI_TAU8	Al9Mn3Si (E9c)	E9c	hP26	P6_ 3/mmc	194		5	[6.0, 2.0, 12.0, 6.0, 2.0]	(MN, VA)6(MN, VA)2(AL)12(AL, SI)6(AL, SI)2
AL2MNSI3	Ga5Pd		tI24	I4/mcm	140	Tau10	3	[2.0, 1.0, 3.0]	(AL)2(MN)1(SI)3
MN15NI45SI40	Unknown Structure					ternary T1 or N phase	3	[0.15, 0.45, 0.4]	(MN)0.15(NI)0.45(SI)0.4
MN15NI50SI35	Unknown Structure					ternary T2 or PHI phase	3	[0.15, 0.5, 0.35]	(MN)0.15(NI)0.5(SI)0.35
MN6NI16SI7	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225	ternary T3 or G phase	3	[0.206897, 0.551724, 0.241379]	(MN)0.206897(NI)0.551724(SI)0.241379
MN1NI1SI1_ C37	MnCuP		oP12	Pnma	62	ternary T4 or E phase	3	[1.0, 1.0, 1.0]	(MN)1(NI)1(SI)1
MNNISI_T5	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_ 3/mmc	194	ternary T5 or tao_1 phase	2	[1.0, 2.0]	(MN)1(NI, SI)2
MNNISI_T6	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227	ternary T6 or tao_2 phase	2	[1.0, 2.0]	(MN)1(NI, SI)2
MN3NI2SI	Mn3Ni2Si		cF96	Fd-3m	227	ternary T7 or Omega	3	[3.0, 2.0, 1.0]	(MN)3(NI)2(SI)1
MN2NISI	Unknown Structure					ternary T8 or S phase	2	[3.0, 1.0]	(MN, NI)3(SI)1
MN6NISI3	R-(Co,Cr,Mo)		hR53	R-3	166	ternary T9 or R' phase	3	[0.61, 0.12, 0.27]	(MN)0.61(NI)0.12(SI)0.27
MN66NI4SI30	Unknown Structure					ternary T10 or U phase	3	[0.66, 0.04, 0.3]	(MN)0.66(NI)0.04(SI)0.3
MN52NI29SI19	Unknown Structure					ternary phase T11 or W phase	3	[0.52, 0.29, 0.19]	(MN)0.52(NI)0.29(SI)0.19
B4C_D1G	B13C2 B4C (D1g)	D1g	hR15	R-3m	166		2	[1.0, 1.0]	(B11C, B12)1(B2, C2B, CB2)1
BN_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186		2	[1.0, 1.0]	(B)1(N)1
SIB3_D1G	B13C2 B4C (D1g)	D1g	hR15	R-3m	166		3	[6.0, 2.0, 6.0]	(B)6(SI)2(B, SI)6
SIB6	SiB6		oP280	Pnnm	58		3	[210.0, 23.0, 48.0]	(B)210(SI)23(B, SI)48
BNSI_RHOMBO	alpha-B (hR12)		hR12	R-3m	166	aka BNSI, ALPHA_ RHOMBO_B.	3	[61.0, 1.0, 8.0]	(B)61(SI)1(B, SI)8
SIC_B3	Zincblende (ZnS, B3)	B3	cF8	F-43m	216		2	[1.0, 1.0]	(SI)1(C)1

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SI3N4	Nierite (alpha-Si3N4)		hP28	P31c	159		2	[3.0, 4.0]	(SI)3(N)4
AL4SIC4_E94	Al5C3N (E94)	E94	hP18	P6_3mc	186		3	[4.0, 1.0, 4.0]	(AL)4(SI)1(C)4
AL8SIC7	Unknown Structure		hP16				3	[8.0, 1.0, 7.0]	(AL)8(SI)1(C)7
FE8SI2C	Mn8Si2C		aP*	P1	1		3	[8.0, 2.0, 1.0]	(FE)8(SI)2(C)1
TI3SIC2	Ti3SiC2		hP12	P6_ 3/mmc	194		3	[3.0, 1.0, 2.0]	(TI)3(SI)1(C)2
DIS_MU	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	Part of the description for the MU_PHASE	1	[1.0]	(AL, CO, CR, CU, FE, MN, MO, NB, NI, RE, TA, TI, W)1
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	DIS_MU contribution added onto it.	4	[1.0, 2.0, 6.0, 4.0]	(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_SIG	sigma-CrFe (D8b)	D8b	tP30	P4_ 2/mnm	136	Part of the description for the SIGMA phase.	1	[1.0]	(AL, CO, CR, FE, IR, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W)1
SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_ 2/mnm	136	DIS_SIG contribution added onto it.	3	[10.0, 4.0, 16.0]	(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
CHI_A12	alpha-Mn (A12)	A12	cI58	I-43m	217	also M5Re24, Mo2Re8, Ta3Re7, WRe3.	3	[24.0, 10.0, 24.0]	(CR, FE, NI, RE)24(AL, CR, HF, MO, NB, TA, TI, W, ZR)10(CR, FE, MO, NB, NI, RE, TA, W)24
G_PHASE_D8A	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		3	[16.0, 6.0, 7.0]	(AL, CO, FE, MN, NI, TI)16(HF, NB, TI, Y, ZR)6(CO, FE, MN, NI, SI)7
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215	also Cu5Zn8, Ni5Zn8, Al5Cu8 (rt).	3	[4.0, 1.0, 8.0]	(AL, NI, SI, ZN)4(AL, CU, NI, SI, ZN)1(CU, FE, MN, NI, ZN)8
GAMMA_HT_ D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217	aka GAMMA_H.	3	[4.0, 1.0, 8.0]	(AL, ZN)4(AL, CU, ZN)1(CU, FE, MN, NI)8
HEUSLER_L21	Heusler (L21)	L21	cF16	Fm-3m	225	aka H_L21.	3	[0.5, 0.5, 1.0]	(AL, CR, NI, SN, TI)0.5(AL, HF, NB, NI, TA, TI, ZR)0.5(CO, FE, NI, RU, VA)1
O_PHASE	NaHg		oS16	Cmcm	63	aka Ti2NbAl, the O phase.	3	[0.5, 0.25, 0.25]	(NB, TA, TI)0.5(AL, NB, TA, TI)0.25(NB, TA, TI)0.25
P_PHASE	Cr9Mo21Ni20		oP56	Pnma	62		3	[24.0, 20.0, 12.0]	(CR, FE, NI, RE)24(CR, FE, MO, NI, RE)20(MO)12
R_PHASE	R-(Co,Cr,Mo)		hR53	R-3	166		3	[27.0, 14.0, 12.0]	(CO, CR, FE, NI, RE)27(MO, W)14(CO, CR, FE, MO, NI, RE, W)12
B82_OMEGA	Ni2In (B82)	B82	hP6	P6_ 3/mmc	194		3	[1.0, 1.0, 1.0]	(AL, SN)1(CO, NB, SN, TA, TI)1(TI)1
MNNI_L10	CuAu (L10)	L10	tP2	P4/mmm	123		2	[0.5, 0.5]	(CO, CR, CU, FE, MN, NI)0.5(CO, CR, CU, FE, MN, NI)0.5
IRMN_L10	CuAu (L10)	L10	tP2	P4/mmm	123	also IrTi.	2	[0.5, 0.5]	(IR, MN, TI)0.5(IR, MN, TI)0.5
ALTI_L10	CuAu (L10)	L10	tP2	P4/mmm	123	Solid solution of ordered L10.	2	[1.0, 1.0]	(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
IRNB_L10	CuAu (L10)	L10	tP2	P4/mmm	123		2	[0.5, 0.5]	(IR, NB)0.5(IR, NB)0.5
IRW_EPSILON_	Hexagonal Close	A3	hP2	P6_	194	HT epsilon solution phase	2	[1.0, 1.0]	(IR, W)1(IR, W)1

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HCP	Packed (Mg, A3, hcp)			3/mmc		with HCP structure.			
IRW_LT_B19	beta'-AuCd (B19)	B19	oP4	Pmma	51		2	[1.0, 1.0]	(IR)1(IR, W)1
IRV_L10	CuAu (L10)	L10	tP2	P4/mmm	123	aka Ir1.04V0.96 or IrV1-x.	2	[0.5, 0.5]	(IR)0.5(IR, V)0.5
ALCU_EPS_B82	Ni2In (B82)	B82	hP6	P6_ 3/mmc	194	epsilon2 HT.	2	[1.0, 1.0]	(AL, CU, NI)1(CU, FE)1
ALCU_ETA	AlCu(r)		mS20	C2/m	12	united HT-eta1 & LT-eta2.	2	[1.0, 1.0]	(AL, CU)1(CU, FE, NI, ZN)1
ALPHA_B19	beta'-AuCd (B19)	B19	oP4	Pmma	51	an ordered HCP.	2	[1.0, 1.0]	(MO, NB, TI, V, ZR)1(MO, NB, TI, V, ZR)1
ALRE_B11	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[1.0, 1.0]	(AL)1(RE)1
ALZR_B33	CrB (B33)	B33	oS8	Cmcm	63	also AlHf, ALY_B33.	2	[1.0, 1.0]	(AL)1(HF, Y, ZR)1
COSN_B35	CoSn (B35)	B35	hP6	P6/mmm	191	also FeSn, COSN_HP6.	2	[0.5, 0.5]	(CO, FE, NI)0.5(SN)0.5
COY_B33	CrB (B33)	B33	oS8	Cmcm	63	aka COY_BF.	2	[1.0, 1.0]	(CO)1(Y)1
CUTI_B11	gamma-CuTi (B11)	B11	tP4	P4/nmm	129	aka B11.	2	[1.0, 1.0]	(CO, CU, NI, TI)1(CU, NI, TA, TI)1
HF1IR1	Unknown Structure					united HT/LT phase	2	[1.0, 1.0]	(HF)1(IR)1
HFMN	NiTi2		cF96	Fd-3m	227		2	[0.5, 0.5]	(HF)0.5(MN)0.5
HFNI_ALPHA	CrB (B33)	B33	oS8	Cmcm	63		2	[0.5, 0.5]	(HF)0.5(NI)0.5
HFRE	Zr21Re25		hR92	R-3c	167	also Hf21Re25.	2	[1.0, 1.0]	(HF)1(RE)1
HFRH_B2	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(HF, RH)1(RH)1
IRV_RT	alpha-IrV		oS8	Cmmm	65		2	[1.0, 1.0]	(IR)1(V)1
IRZR_BETA_B2	CsCl (B2)	B2	cP2	Pm-3m	221	i.e. HT- or beta- phase.	2	[1.0, 1.0]	(IR, ZR)1(IR, ZR)1
IRZR_ALPHA	Mn3As (D0d)	D0d	oS16	Cmcm	63	LT phase.	2	[1.0, 1.0]	(IR, ZR)1(ZR)1
MNTA	Unknown Structure						2	[1.0, 1.0]	(MN)1(TA)1
MNTI_LT	Zr21Re25		hR92	R-3c	167	aka Ti21Mn25_RT.	2	[1.0, 1.0]	(MN)1(TI)1
MOIR_HT	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_ 3/mmc	194		2	[1.0, 1.0]	(IR, MO)1(IR, MO)1
MOIR_LT_B19	beta'-AuCd (B19)	B19	oP4	Pmma	51		2	[1.0, 1.0]	(MO)1(IR)1
NB1ZN1	Unknown Structure						2	[0.5, 0.5]	(NB)0.5(ZN)0.5
NIZN_TP2	CuAu (L10)	L10	tP2	P4/mmm	123	united HT/LT phase.	2	[0.5, 0.5]	(AL, CU, NI, ZN)0.5(AL, NI, ZN)0.5
NIY_B27	FeB (B27)	B27	oP8	Pnma	62		2	[1.0, 1.0]	(NI)1(Y)1
NIZR_B33	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(NI)1(TI, ZR)1
RHSN_B20	FeSi (B20)	B20	cP8	P2_13	198		2	[1.0, 1.0]	(RH)1(SN)1
RHZR_LT	IrZr		oS16	Cmcm	63	i.e. alpha_RhZr	2	[1.0, 1.0]	(RH)1(RH, ZR)1
RHZR_HT_B2	CsCl (B2)	B2	cP2	Pm-3m	221	i.e. beta_RhZr.	2	[1.0, 1.0]	(RH)1(RH, ZR)1
ZNZR_B2	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(ZN)1(ZR)1
ALCU_PRIME	Al9Cu11(h)		oF88	Fmm2	42	aka THETA_PRIME.	2	[2.0, 1.0]	(AL)2(CU)1
AL2FE	Al2Fe		aP18	P1	1		2	[2.0, 1.0]	(AL, CU)2(FE, MN)1
ALRE2_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[1.0, 2.0]	(AL)1(RE)2

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ALRH2	Unknown Structure						2	[1.0, 2.0]	(AL)1(RH)2
AL2TI_LT	Ga2Hf		tI24	I4_1/amd	141		2	[2.0, 1.0]	(AL, NB, TI)2(AL, CO, NB, TA, TI, V, ZR)1
Al2W_C40	CrSi2 (C40)	C40	hP9	P6_222	180		2	[2.0, 1.0]	(AL)2(W)1
ALY2_C37	Co2Si (C37)	C37	oP12	Pnma	62		2	[1.0, 2.0]	(AL)1(Y)2
ALZR2_B82	Ni2In (B82)	B82	hP6	P6_ 3/mmc	194		2	[1.0, 2.0]	(AL)1(TI, ZR)2
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_ 3/mmc	194	also CuZn2.	2	[2.0, 1.0]	(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
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[2.0, 1.0]	(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)	C16	tI12	I4/mcm	140		2	[2.0, 1.0]	(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)	C36	hP24	P6_ 3/mmc	194		2	[2.0, 1.0]	(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
CRNI2_OP6	MoPt2		oI6	Immm	71		2	[1.0, 2.0]	(CR, MO, W)1(MO, NI, W)2
CU2TI1	Au2V		oS12	Cmcm	63		2	[2.0, 1.0]	(CO, CU, NI)2(TI)1
CU2Y_HT	Unknown Structure		hP*				2	[2.0, 1.0]	(CU)2(Y)1
CU2Y_LT	CeCu2		oI12	Imma	74		2	[2.0, 1.0]	(CU)2(Y)1
HF2IR	NiTi2		cF96	Fd-3m	227		2	[2.0, 1.0]	(HF)2(IR)1
HF2RH	NiTi2		cF96	Fd-3m	227		2	[2.0, 1.0]	(HF)2(RH)1
HFSN2_C40	CrSi2 (C40)	C40	hP9	P6_222	180		2	[1.0, 2.0]	(HF)1(SN)2
MNNI2	Unknown Structure						2	[1.0, 2.0]	(MN, NI)1(NI)2
NBZN2_C36	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_ 3/mmc	194		2	[0.333, 0.667]	(NB)0.333(ZN)0.667
NI2V	MoPt2		oI6	Immm	71		2	[2.0, 1.0]	(MO, NI)2(MO, NB, TA, V)1
NI2TA_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(CO, NI)2(TA, TI)1
NITI2	NiTi2		cF96	Fd-3m	227		2	[1.0, 2.0]	(CO, CR, CU, FE, NI, RE, TI)1(AL, CR, CU, HF, NI, TA, TI, ZR)2
NI2Y1	Ni2Tm		cF192	F-43m	216		2	[2.0, 1.0]	(NI)2(Y)1
REZR2	Zr21Re25		hR92	R-3c	167	aka Zr21Re25.	2	[1.0, 2.0]	(NI, RE)1(ZR)2
RHSN2_RT	RhSn2		tI26	I4/mmm	139		2	[0.33333, 0.66667]	(RH)0.33333(SN)0.66667
RH2SN	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(RH)2(SN)1
SNTI2_B82	Ni2In (B82)	B82	hP6	P6_ 3/mmc	194		2	[1.0, 2.0]	(SN)1(TI)2
SN2Y_C49	ZrSi2 (C49)	C49	oS12	Cmcm	63		2	[2.0, 1.0]	(SN)2(Y)1
RHZR2	NiTi2		cF96	Fd-3m	227		2	[1.0, 2.0]	(RH)1(ZR)2

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
TASN2_CB	Mg2Cu (Cb)	Cb	oF48	Fddd	70	also SN2TA_CB.	2	[1.0, 2.0]	(TA)1(SN)2
VSN2_CB	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[0.6, 0.4]	(SN)0.6(V)0.4
YZN2_LT	Unknown Structure						2	[1.0, 2.0]	(Y)1(ZN)2
YZN2_HT	Unknown Structure						2	[1.0, 2.0]	(Y)1(ZN)2
AL3CO1	Os4Al13		mS34	C2/m	12	aka CoAl3_cub.	2	[3.0, 1.0]	(AL)3(CO)1
AL3IR_D018	Na3As (D018)	D018	hP8	P6_ 3/mmc	194		2	[0.75, 0.25]	(AL)0.75(IR)0.25
AL3NI_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[0.75, 0.25]	(AL)0.75(NI)0.25
AL3RH_LT	(Al3Rh)		oP*	Pnma	62		2	[3.0, 1.0]	(AL)3(RH)1
ALTI3_D019	Ni3Sn (D019)	D019	hP8	P6_ 3/mmc	194	also Ni3Sn_LT, Mn3Sn, Ti3Sn.	2	[3.0, 1.0]	(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
AL3TI_D022	Al3Ti (D022)	D022	tI8	I4/mmm	139	gamma double prime, AL3TI_D022, Al3M, Ni3V.	2	[3.0, 1.0]	(AL, CO, CR, FE, MO, NB, NI, SI, TI, V)3(AL, CO, CR, MO, NB, NI, SI, TA, TI, V, ZR)1
AL3Y_HT	BaPb3		hR12	R-3m	166		2	[0.75, 0.25]	(AL)0.75(Y)0.25
AL3Y_LT	Ni3Sn (D019)	D019	hP8	P6_ 3/mmc	194		2	[0.75, 0.25]	(AL)0.75(Y)0.25
AL3ZR_D023	Al3Zr (D023)	D023	tI16	I4/mmm	139	also Al3Hf, Zn3Zr.	2	[3.0, 1.0]	(AL, ZN)3(HF, TI, ZR)1
CO1SN3	Au3Zn		oS32	Cmce	64		2	[0.25, 0.75]	(CO)0.25(SN)0.75
CO3V1	Al3Pu		hP24	P6_ 3/mmc	194		2	[3.0, 1.0]	(CO, NI, V)3(CO, V)1
CO3Y1	Ni3Pu		hR12	R-3m	166		2	[3.0, 1.0]	(CO)3(Y)1
CU3SN_LT	Cu3Sn		oS80	Cmcm	63	epsilon	2	[3.0, 1.0]	(CU, SN)3(CU, SN)1
CUTI3_L60	CuTi3 (L60)	L60	tP4	P4/mmm	123		2	[1.0, 3.0]	(CU, TI)1(TI)3
HFIR3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[1.0, 3.0]	(HF)1(IR)3
HFNI3_ALPHA	PdRh2Ta		hP40	P6_ 3/mmc	194	the LT phase.	2	[0.25, 0.75]	(HF)0.25(NI)0.75
HFNI3_BETA	BaPb3		hR12	R-3m	166	the HT phase.	2	[0.25, 0.75]	(HF)0.25(NI)0.75
IRNB_ALPHA2	TaIr		oP12	Pmma	51		2	[1.0, 1.0]	(IR)1(IR, NB)1
IR3W_D019	Ni3Sn (D019)	D019	hP8	P6_ 3/mmc	194		2	[3.0, 1.0]	(IR, W)3(IR, W)1
IRY3_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[1.0, 3.0]	(IR)1(Y)3
IR3Y1	Ni3Pu		hR12	R-3m	166		2	[3.0, 1.0]	(IR)3(Y)1
IRZR3_D0E	alpha-V3S		tI32	I-42m	121		2	[1.0, 3.0]	(IR)1(ZR)3
MY3_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62	also CoY3, NiY3.	2	[1.0, 3.0]	(CO, NI)1(Y)3

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
MZR3_E1A	MgCuAl2 (E1a)		oS16	Cmcm	63	also CoZr3, FeZr3.	2	[1.0, 3.0]	(CO, FE, NI)1(ZR)3
MN3TI1	Unknown Structure					HT phase	2	[3.0, 1.0]	(MN)3(TI)1
MO1IR3	Ni3Sn (D019)	D019	hP8	P6_ 3/mmc	194		2	[1.0, 3.0]	(MO)1(IR, MO)3
MO3IR_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[3.06, 0.94]	(MO)3.06(IR)0.94
NBZN3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.25, 0.75]	(NB)0.25(ZN)0.75
NI3TA_D0A	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59	also delta, Ni3Mo, Ni3Nb.	2	[3.0, 1.0]	(AL, CO, CR, FE, NB, NI)3(AL, FE, MO, NB, NI, TA, TI, V, W)1
NI3TI_D024	Ni3Ti (D024)	D024	hP16	P6_ 3/mmc	194	also Eta, AlNi6Ta.	2	[0.75, 0.25]	(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
M3Y	Ni3Pu		hR12	R-3m	166	also Fe3Y, Ni3Y.	2	[3.0, 1.0]	(FE, NI)3(Y)1
RH3ZR_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[3.0, 1.0]	(RH, ZR)3(RH, ZR)1
RUY3_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[0.25, 0.75]	(RU)0.25(Y)0.75
SN3Y1	GdSn2.75		oS16	Amm2	38		2	[3.0, 1.0]	(SN)3(Y)1
TA3SN_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[3.0, 1.0]	(TA)3(SN)1
V3SN_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[0.205, 0.795]	(SN)0.205(V)0.795
VZN3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[1.0, 3.0]	(V)1(ZN)3
Y1ZN3	Zn3Y		oP16	Pnma	62		2	[1.0, 3.0]	(Y)1(ZN)3
ZN3ZR_HT	Unknown Structure		c**				2	[3.0, 1.0]	(ZN)3(ZR)1
AL13CO4	Orthorhombic Co4Al13		oP102	Pmn2_1	31		2	[13.0, 4.0]	(AL)13(CO)4
AL5CO2_D811	Co2Al5 (D811)	D811	hP28	P6_ 3/mmc	194	also Al5Rh2.	2	[5.0, 2.0]	(AL)5(CO, RH)2
AL9CO2	Co2Al9 (D8d)	D8d	mP22	P2_1/c	14	also Al9Rh2	2	[9.0, 2.0]	(AL)9(CO, RH)2
AL11CR2	Al5Cr		mS732	C2/c	15		3	[10.0, 1.0, 2.0]	(AL)10(AL)1(CR)2
AL13CR2	Al45V7		mS104	C2/m	12		2	[13.0, 2.0]	(AL)13(CR)2
AL4CR	mu-Al4Mn		hP574	P6_ 3/mmc	194		2	[4.0, 1.0]	(AL)4(CR)1
AL8CR5_LT_ D810	Cr5Al8 (D810)	D810	hR26	R3m	160		2	[8.0, 5.0]	(AL)8(CR, V)5
AL9CR4_HT	Unknown Structure						2	[9.0, 4.0]	(AL)9(CR)4
AL9CR4_LT	Unknown Structure						2	[9.0, 4.0]	(AL)9(CR)4
ALCU_DELTA	Al5Cu8		hR52	R3m	160		2	[2.0, 3.0]	(AL)2(CU, FE)3

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ALCU_ZETA	Al9Cu11(h)		oF88	Fmm2	42	united HT-zeta1 and LT-zeta2.	2	[9.0, 11.0]	(AL)9(CU, FE)11
AL23CUFE4_ D2H	MnAl6 (D2h)	D2h	oS28	Cmcm	63		3	[23.0, 1.0, 4.0]	(AL)23(CU)1(FE)4
AL62CU25FE13	Quasicrystal						3	[0.125, 0.255, 0.62]	(FE)0.125(AL, CU)0.255(AL)0.62
AL7CU2FE	FeCu2Al7 (E9a)	E9a	tP40	P4/mnc	128		3	[1.0, 2.0, 7.0]	(FE, NI)1(CU)2(AL)7
AL10CU10FE	(Al10Cu10Fe)		oF116	Fmm2	42		3	[1.0, 10.0, 10.0]	(FE)1(AL, CU)10(AL)10
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5		hR14	R-3m	166		2	[1.0, 1.0]	(AL)1(CU, FE, NI, VA)1
AL28CU4MN7	Unknown Structure					Tau1, Mn6+xCu4+yAl29-x-y.	3	[28.0, 7.0, 4.0]	(AL)28(MN)7(CU)4
AL11CU5MN3	Unknown Structure		oP380			Tau2	3	[11.0, 3.0, 5.0]	(AL)11(MN)3(CU)5
ALCU3MN2_ C15	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227	Tau3.	3	[1.0, 2.0, 3.0]	(AL)1(MN)2(CU)3
AL5CU4ZN	Unknown Structure						4	[1.0, 4.0, 4.0, 1.0]	(AL, CU)1(AL)4(CU)4(ZN)1
AL13FE4	Al13Fe4		mS102	C2/m	12	solid- solution of Al13Fe4 (aka Al3Fe) & Al13Ru4.	3	[0.6275, 0.235, 0.1375]	(AL, CU)0.6275(FE, MN, RU)0.235(AL, SI, VA)0.1375
AL5FE2	Al2.8Fe		oS24	Cmcm	63		2	[5.0, 2.0]	(AL, CU)5(FE, MN)2
AL5FE4_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217	also AL8FE5_D82	1	[1.0]	(AL, CU, FE)1
AL16FEMN3	mu-Al4Mn		hP574	P6_ 3/mmc	194	Tau1	2	[4.0, 1.0]	(AL)4(FE, MN)1
AL13FE2MN2	Al13Fe4		mS102	C2/m	12	Tau2.	2	[4.0, 13.0]	(FE, MN)4(AL)13
AL10FEMN2	Mn3Al10		hP26	P6_ 3/mmc	194	Tau3.	2	[3.0, 10.0]	(FE, MN)3(AL)10
AL9IR2	Co2Al9 (D8d)	D8d	mP22	P2_1/c	14		2	[0.818, 0.182]	(AL)0.818(IR)0.182
AL45IR13	Al45Ir13		oP236	Pnma	62		2	[0.776, 0.224]	(AL)0.776(IR)0.224
AL13IR4	Unknown Structure						2	[0.765, 0.235]	(AL)0.765(IR)0.235
AL28IR9	Al28Ir9		hP236	P31c	159		2	[0.757, 0.243]	(AL)0.757(IR)0.243
AL5IR2	Al2.75Ir		cP60	P23	195		2	[0.73, 0.27]	(AL)0.73(IR)0.27
AL12MN_	Al12W		cI26	Im-3	204		2	[12.0, 1.0]	(AL)12(MN)1

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GPHASE									
AL4MN_ LAMBDA	lambda-Al4Mn		hP586	P6_ 3/mmc	194	also AL461MN107	2	[461.0, 107.0]	(AL)461(FE, MN)107
AL4MN_MU	mu-Al4Mn		hP574	P6_ 3/mmc	194		2	[4.0, 1.0]	(AL)4(MN)1
AL11MN4_LT	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(FE, MN)4
AL11MN4_HT	Mn6 (Mn0.5Al0.5)8Al25		oP156	Pnma	62		2	[29.0, 10.0]	(AL, MN)29(MN)10
AL8MN5_D810	Cr5Al8 (D810)	D810	hR26	R3m	160		3	[12.0, 5.0, 9.0]	(AL, TI, ZN)12(MN)5(AL, CU, MN, SI, TI)9
AL6MN_D2H	MnAl6 (D2h)	D2h	oS28	Cmcm	63	also Al6Re, Al6Ru	2	[6.0, 1.0]	(AL)6(FE, MN, RE, RU)1
AL31MN6NI2	mu-Al4Mn		hP574	P6_ 3/mmc	194		3	[31.0, 6.0, 2.0]	(AL)31(MN)6(NI)2
TI25MN9AL66_ L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	also Ti25Mn8Al67 or Ti43Mn11Al66, Tau1.	2	[0.75, 0.25]	(AL, MN, TI)0.75(AL, MN, TI)0.25
AL24MN5ZN	Unknown Structure					ternary Tau1 phase	3	[5.0, 1.0, 24.0]	(MN, ZN)5(ZN)1(AL)24
AL9MN2ZN	Unknown Structure					ternary Tau2 phase	3	[2.0, 1.0, 9.0]	(MN)2(ZN)1(AL)9
AL11MN3ZN2	Unknown Structure		oS152			ternary Tau3 phase	3	[3.0, 2.0, 11.0]	(MN)3(ZN)2(AL)11
AL63MO37	Unknown Structure					Mo3Al5_HT	2	[63.0, 37.0]	(AL)63(MO)37
AL8MO3	Al8Mo3		mS22	C2/m	12		2	[8.0, 3.0]	(AL)8(MO)3
ALMO_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229	improper modelling.	2	[1.0, 1.0]	(AL, MO)1(AL, MO)1
AL3NI5	Ga3Pt5		oS16	Cmmm	65		2	[0.375, 0.625]	(AL)0.375(NI)0.625
AL3NI2_D519	Al3Ni2 (D513)	D513	hP5	P-3m1	164	also Al3Ru2.	3	[3.0, 2.0, 1.0]	(AL, SI, SN, ZN)3(AL, CU, NI, RU)2(NI, RU, VA)1
AL13NI2TI5_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	Tau1	3	[13.0, 2.0, 5.0]	(AL)13(NI)2(TI)5
ALNI2ZN	Unknown Structure						3	[0.25, 0.5, 0.25]	(AL)0.25(NI)0.5(ZN)0.25
AL13NI38ZN49	Unknown Structure						3	[0.13, 0.38, 0.49]	(AL)0.13(NI)0.38(ZN)0.49
AL11RE4	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(RE)4
AL4RE	Al4Re		aP71	P-1	2		2	[4.0, 1.0]	(AL)4(RE)1
AL5RH2_HT	beta-Al5Rh2		cP54	P23	195		2	[2.0, 1.0]	(AL)2(RH, VA)1
AL7RH3_HT	Unknown Structure		mP*				2	[7.0, 3.0]	(AL)7(RH)3
AL15SI2M4_ TAU9	Al15(Mn,Fe)3Si2		cI168	Im-3	204		3	[14.0, 4.0, 5.0]	(AL)14(FE, MN)4(AL, SI)5

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ALSI3TI2	Zr3Al4Si5		tI24	I4_1/amd	141	aka Ti7Al5Si12, Tau1	3	[0.166667, 0.5, 0.333333]	(AL)0.166667(SI)0.5(TI)0.333333
AL3TI_LT	Al3Ti-LT		tI32	I4/mmm	139		2	[3.0, 1.0]	(AL, TI)3(AL, TI, ZR)1
AL5TI2_HT	Al5Ti2		tP28	P4/mmm	123		2	[5.0, 2.0]	(AL, TI)5(AL, NB, TA, TI, V, ZR)2
AL5TI3	Al5Ti3		tP32	P4/mbm	127		2	[5.0, 3.0]	(AL)5(TA, TI)3
AL21V2	Al10V		cF176	Fd-3m	227		2	[21.0, 2.0]	(AL)21(V)2
AL45V7	Al45V7		mS104	C2/m	12	aka Al7V	2	[45.0, 7.0]	(AL)45(V)7
AL23V4	Al23V4		hP54	P6_ 3/mmc	194		2	[23.0, 4.0]	(AL)23(V)4
AL8V5_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		2	[8.0, 5.0]	(AL, V)8(AL, CR, V, Zr)5
AL77W23	Unknown Structure						2	[77.0, 23.0]	(AL)77(W)23
AL7W3	Unknown Structure						2	[7.0, 3.0]	(AL)7(W)3
AL12W_ GPHASE	Al12W		cI26	Im-3	204	also Al12Mo, Al12Re.	2	[12.0, 1.0]	(AL)12(MO, RE, W)1
AL4W	Al4W		mS30	Cm	8	also Al4Mo.	2	[4.0, 1.0]	(AL)4(MO, W)1
AL5W	Al5W		hP12	P6_322	182	also AL5MO.	2	[5.0, 1.0]	(AL)5(MO, W)1
AL2ZR3	Zr3Al2		tP20	P4_ 2/mnm	136	also Al2Hf3, Al2Y3.	2	[2.0, 3.0]	(AL)2(HF, TI, Y, ZR)3
AL3ZR2	Zr2Al3		oF40	Fdd2	43	also Al3Hf2.	2	[3.0, 2.0]	(AL)3(HF, ZR)2
AL3ZR4	Al3Zr4		hP7	P6/mmm	191	also Al3Hf4.	2	[3.0, 4.0]	(AL)3(HF, TI, ZR)4
AL3ZR5_D8M	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[3.0, 5.0]	(AL)3(TI, ZR)5
AL4ZR5	Ti5Ga4		hP18	P6_ 3/mcm	193		2	[4.0, 5.0]	(AL)4(ZR)5
CO10CU57TI33	MoSi2 (C11b)	C11b	tI6	I4/mmm	139	Strukturbericht C11B.	3	[0.1, 0.57, 0.33]	(CO)0.1(CU)0.57(TI)0.33
CO7HF	(Co11Hf2)		oP*	Pban	50		2	[7.0, 1.0]	(CO)7(HF)1
COSNTI_TAU2	Half-Heusler (C1b)	C1b	cF12	F-43m	216	aka TiCoSn.	3	[1.0, 1.0, 1.0]	(CO, NI)1(SN)1(TI)1
CO3Y2	Unknown Structure		cP*				2	[3.0, 2.0]	(CO)3(Y)2
CO3Y4	Co3Ho4		hP22	P6_3/m	176		2	[3.0, 4.0]	(CO)3(Y)4
CO5Y_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		3	[1.0, 4.0, 1.0]	(CO2, Y)1(CO)4(CO, VA)1
CO5Y8	Co5Y8		mP52	P2_1/c	14		2	[5.0, 8.0]	(CO)5(Y)8
CO7NB2	(Co7Nb2)		mS18	C2/m	12		2	[7.0, 2.0]	(CO)7(NB)2
CO7TA2	BaPb3		hR12	R-3m	166		2	[7.0, 2.0]	(CO)7(TA)2
CO7Y6	Unknown Structure						2	[7.0, 6.0]	(CO)7(Y)6
CO17Y2	Ni17Th2		hP38	P6_ 3/mmc	194	united HT/LT phase.	3	[1.0, 2.0, 15.0]	(CO2, Y)1(CO2, Y)2(CO)15

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COZN_LT_A13	beta-Mn (A13)	A13	cP20	P4_132	213		2	[1.0, 1.0]	(CO, ZN)1(VA)1
COZN_HT	Unknown Structure						2	[1.0, 1.0]	(CO, ZN)1(VA)1
COZN_ GAMMA_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217	aka Zn11Co2, COZN4_ D83.	2	[1.0, 1.0]	(CO, ZN)1(VA)1
COZN_DELTA	Unknown Structure					Zn15Co2 HT phase	2	[0.117647, 0.882353]	(CO)0.117647(ZN)0.882353
COZN_ GAMMA1	Co2Zn15		mS28	C2/m	12	aka CoZn7.8	2	[0.125, 0.875]	(CO)0.125(ZN)0.875
COZN_ GAMMA2	CoZn13		mS28	C2/m	12	aka CoZn13	2	[0.0714286, 0.9285714]	(CO)0.0714286(ZN)0.928571
CO11ZR2	(Co11Hf2)		oP*	Pban	50		2	[11.0, 2.0]	(CO)11(ZR)2
CRMN3_HT_ SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_ 2/mnm	136		3	[8.0, 4.0, 18.0]	(MN)8(CR)4(CR, MN)18
CR3MN5	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[3.0, 5.0]	(CR)3(MN)5
CRZN13	Unknown Structure		m**				2	[1.0, 13.0]	(CR)1(ZN)13
CRZN17	Unknown Structure		hP*				2	[1.0, 17.0]	(CR)1(ZN)17
CU51HF14	Ag51Gd14		hP68	P6/m	175		2	[51.0, 14.0]	(CU)51(HF)14
CU8HF3	Cu8Hf3		oP44	Pnma	62		2	[8.0, 3.0]	(CU)8(HF)3
CU10HF7	Ni10Zr7		oS68	Cmce	64		2	[10.0, 7.0]	(CU)10(HF)7
CU5MN4SI	Unknown Structure						3	[0.5, 0.37, 0.13]	(CU)0.5(MN)0.37(SI)0.13
CU4MNSN_ TAU1	MgCu4Sn		cF24	F-43m	216		3	[0.6666, 0.1667, 0.1667]	(CU)0.6666(SN)0.1667(MN)0.1667
CUMNZN_TAU1	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		3	[0.334, 0.333, 0.333]	(CU)0.334(MN)0.333(ZN)0.333
CU6NISI3	Unknown Structure						2	[0.732, 0.268]	(CU, NI)0.732(SI)0.268
CU46NI25SI29	Unknown Structure						3	[0.458, 0.25, 0.292]	(CU)0.458(NI)0.25(SI)0.292
CU33SI7_DELTA	Unknown Structure					HT phase	2	[0.825, 0.175]	(CU)0.825(SI)0.175
CU15SI4_EPS_ D86	Cu15Si4 (D86)	D86	cI76	I-43d	220		2	[0.789474, 0.210526]	(CU, MN)0.789474(AL, SI)0.210526
CU56SI11_ GAMMA_A13	Mg3Ru2		cP20	P4_132	213		2	[0.835821, 0.164179]	(CU, MN, NI, SI)0.835821(SI)0.164179
CU3SI_ETA	Cu3Si-h2		hR*	P-31m	162	United 3-allotropes: eta''-RT(oS* *), eta'-HT1(hR27 R-3), eta-HT2(hR* P-31m)	2	[0.76, 0.24]	(CU, MN, NI)0.76(SI)0.24

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CU6SN5_HT	Ni2In (B82)	B82	hP6	P6_ 3/mmc	194	also Co3Sn2, Mn(2-x)Sn, Ni3Sn2.	3	[1.0, 1.0, 1.0]	(CO, CU, MN, NI, VA)1(AL, CU, NI, SN)1(CO, CU, MN, NI, VA)1
CU6SN5_LT	Cu6Sn5		mS44	C2/c	15	eta-prime.	3	[1.0, 1.0, 1.0]	(CU)1(CU, SN)1(SN)1
CU10SN3	Cu10Sn3		hP26	P6_3	173	zeta.	2	[0.769, 0.231]	(CU, NI)0.769(SN)0.231
CU41SN11	Cu41Sn11		cF416	F-43m	216	delta.	2	[41.0, 11.0]	(CU, SN, ZN)41(CU, SN, ZN)11
CU3TI2	Cu3Ti2		tP10	P4/nmm	129		2	[3.0, 2.0]	(CU, FE, NI)3(CO, TI)2
CU4TI1	Au4Zr		oP20	Pnma	62		2	[4.0, 1.0]	(CU, TI)4(CU, TI)1
CU4TI3	Cu4Ti3		tI14	I4/mmm	139		2	[4.0, 3.0]	(CO, CU, NI)4(TI)3
CU2TIZR	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_ 3/mmc	194		3	[0.5, 0.25, 0.25]	(CU)0.5(TI)0.25(ZR)0.25
CU7Y1	Cu7Tb		hP8	P6/mmm	191	aka Cu6Y or Cu5.4Y0.8	2	[1.0, 5.0]	(CU2, Y)1(CU)5
CU4Y	Cu5Y1.25		mP16	P2_1/m	11		2	[4.0, 1.0]	(CU)4(Y)1
CU7Y2	Ag51Gd14		hP68	P6/m	175		2	[7.0, 2.0]	(CU)7(Y)2
CUMNZN_ EPSILON_HCP	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_ 3/mmc	194		2	[1.0, 0.5]	(CU, MN, ZN)1(VA)0.5
CU10ZR7	Ni10Zr7		oS68	Cmce	64		2	[10.0, 7.0]	(CU)10(ZR)7
CU51ZR14	Ag51Gd14		hP68	P6/m	175		2	[51.0, 14.0]	(CU)51(ZR)14
CU8ZR3	Cu8Hf3		oP44	Pnma	62		2	[8.0, 3.0]	(CU)8(ZR)3
FENBZR_CFC2_ C15	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		3	[2.0, 1.0, 3.0]	(FE, NB, ZR)2(NB, ZR)1(NB, ZR)3
FE3SN2	Fe3Sn2		hR10	R-3m	166		2	[3.0, 2.0]	(FE)3(SN)2
FE5SN3_B82	Ni2In (B82)	B82	hP6	P6_ 3/mmc	194		2	[5.0, 3.0]	(FE)5(SN)3
FE3ZN7_ GAMMA_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		4	[0.154, 0.154, 0.231, 0.461]	(FE, ZN)0.154(FE, ZN)0.154(FE, ZN)0.231(ZN)0.461
FEZN4_ GAMMA1_D81	Fe11Zn40		cF408	F-43m	216		3	[0.137, 0.118, 0.745]	(FE)0.137(FE, ZN)0.118(ZN)0.745
FEZN10_DELTA	FeZn10		hP632	P6_ 3/mmc	194		4	[0.058, 0.18, 0.525, 0.237]	(FE)0.058(FE, ZN)0.18(ZN)0.525(ZN)0.237
FEZN13_ZETA	CoZn13		mS28	C2/m	12		3	[0.072, 0.856, 0.072]	(FE, VA)0.072(ZN)0.856(VA, ZN)0.072
CU3SN_HT_ GAMMA	BiF3 (D03)	D03	cF16	Fm-3m	225	Cu3Sn HT solution phase	1	[1.0]	(CU, MN, NI, SN, ZN)1
HF5IR3	Ir3Zr5		hP48	P6_122	178		2	[5.0, 3.0]	(HF)5(IR)3
HF3NI7	Hf3Ni7		aP20	P-1	2		2	[0.3, 0.7]	(HF)0.3(NI)0.7
HF8NI21	Hf8Ni21		aP29	P-1	2	also ZR8NI21.	2	[8.0, 21.0]	(HF, ZR)8(NI)21
HF3RH4	Unknown Structure						2	[3.0, 4.0]	(HF)3(RH)4

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HF3RH5	Rh5Ge3		oP16	Pbam	55		2	[3.0, 5.0]	(HF)3(RH)5
HF5SN4	Ti5Ga4		hP18	P6_ 3/mcm	193		2	[5.0, 4.0]	(HF)5(SN)4
IR2Y3	Y3Rh2		tI140	I4/mcm	140		2	[2.0, 3.0]	(IR)2(Y)3
IR2Y5	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[2.0, 5.0]	(IR)2(Y)5
IR3Y5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_ 3/mcm	193	united HT/LT phase.	2	[3.0, 5.0]	(IR)3(Y)5
IR3ZR5	Ir3Zr5		hP48	P6_122	178		2	[3.0, 5.0]	(IR)3(ZR)5
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62		2	[3.0, 2.0]	(MN)3(SN)2
MNTI_HT	Unknown Structure		t**			aka TiMn Mn+ or Ti0.47Mn0.53	2	[0.515, 0.485]	(MN)0.515(TI)0.485
MN4TI	R-(Co,Cr,Mo)		hR53	R-3	166	aka Ti9Mn42	2	[0.815, 0.185]	(CR, MN)0.815(TI)0.185
MN12Y_D2B	Mn12Th (D2b)	D2b	tI26	I4/mmm	139		2	[12.0, 1.0]	(MN)12(Y)1
MNZN9	Unknown Structure		h**				2	[1.0, 9.0]	(MN)1(ZN)9
MO7IR3	sigma-CrFe (D8b)	D8b	tP30	P4_ 2/mnm	136		2	[0.7, 0.3]	(MO)0.7(IR)0.3
MONI4_BETA_ D1A	Ni4Mo (D1a)	D1a	tI10	I4/m	87	also WNi4.	2	[1.0, 4.0]	(MO, W)1(NI)4
MONI_DELTA	MoNi		oP56	P2_12_ 12_1	19		3	[24.0, 20.0, 12.0]	(CO, CR, FE, NI, RE)24(CO, CR, FE, MO, NI, RE, W)20(CU, MO, W)12
MOZN7	Ca7Ge		cF32	Fm-3m	225		2	[1.0, 7.0]	(MO)1(ZN)7
MOZN22	Zn93 (Zn0.43Mo0.57)Mo4		cF420	F-43m	216		2	[1.0, 22.0]	(MO)1(ZN)22
NB15NI56TI29_ XA	Unknown Structure		o*100				3	[0.15, 0.56, 0.29]	(NB)0.15(NI)0.56(TI)0.29
NB8NI9TI3_XB	Unknown Structure						3	[0.4, 0.45, 0.15]	(NB)0.4(NI)0.45(TI)0.15
NB5NI75TI20_ XC	Ni3Sn (D019)	D019	hP8	P6_ 3/mmc	194		3	[0.05, 0.75, 0.2]	(NB)0.05(NI)0.75(TI)0.2
NB13NI75TI12_ XD	Unknown Structure						3	[0.13, 0.75, 0.12]	(NB)0.13(NI)0.75(TI)0.12
NB15NI80TI5_ XE	Unknown Structure						3	[0.15, 0.8, 0.05]	(NB)0.15(NI)0.8(TI)0.05
NB3RU5	Rh5Ge3		oP16	Pbam	55	united Nb3Ru5_HT and NbRu3_LT phase	2	[0.375, 0.625]	(NB, RU)0.375(RU)0.625

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NBSN2_CB	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[1.0, 2.0]	(NB, SN, V)1(NB, SN)2
NBZN7	Unknown Structure						2	[0.125, 0.875]	(NB)0.125(ZN)0.875
NBZN15	TiZn16		oS68	Cmcm	63		2	[0.0625, 0.9376]	(NB)0.0625(ZN)0.9376
NB2ZN3_D85	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166		2	[0.4, 0.6]	(NB)0.4(ZN)0.6
NI8M	Pt8Ti		tI18	I4/mmm	139	also Ni8Ta, Ni8Nb.	2	[8.0, 1.0]	(NI)8(NB, TA)1
NI7ZR2	Ni7Zr2		mS36	C2/m	12	also NI7HF2, NI7Y2, CO7HF2 and CO7Y2.	2	[7.0, 2.0]	(AL, CO, CR, NI)7(HF, Y, ZR)2
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	C2/m	12		3	[0.25, 0.25, 0.5]	(CU, NI)0.25(NI, SN)0.25(SN)0.5
NI2Y3	Ni2Y3		tP80	P4_12_12	92		2	[2.0, 3.0]	(NI)2(Y)3
NI4Y	Unknown Structure		hR*				2	[4.0, 1.0]	(NI)4(Y)1
NI17Y2	Fe17Lu2		hP80	P6_3/mmc	194	also Fe17Y2.	2	[1.0, 0.1176]	(AL, FE, NI)1(Y)0.1176
NIZN8_DELTA	Ni3Zn22		mS50	C2/m	12		2	[0.1111111, 0.8888889]	(NI)0.111111(AL, ZN)0.888889
NI11ZR9	Pt11Zr9		tI40	I4/m	87	also Ni11Hf9.	2	[11.0, 9.0]	(NI)11(HF, ZR)9
NI10ZR7	Ni10Zr7		oS68	Cmce	64	also Ni10Hf7.	2	[23.0, 17.0]	(NI)23(HF, ZR)17
NI5ZR_C15B	AuBe5 (C15b)	C15b	cF24	F-43m	216	also Ni5Y/Ni5Hf/Cu5Hf/Cu5Zr, aka ZRM5_C15B.	2	[5.0, 1.0]	(AL, CU, NI)5(HF, Y, ZR)1
RE3NB_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[24.0, 10.0, 24.0]	(RE)24(NB, V, W)10(NB, RE, V, W)24
RHSN4	IrGe4		hP15	P3_121	152		2	[1.0, 4.0]	(RH)1(SN)4
RH3SN2	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[0.125, 0.5, 0.375]	(RH)0.125(RH)0.5(SN)0.375
RH5TI3	Rh5Ge3		oP16	Pbam	55		2	[5.0, 3.0]	(RH)5(TI)3
RH4ZR3_LT	Pd4Pu3		hR14	R-3	148	alpha_Rh4Zr3.	2	[4.0, 3.0]	(RH, ZR)4(ZR)3
RH4ZR3_HT	Unknown Structure					beta_Rh4Zr3	2	[4.0, 3.0]	(RH, ZR)4(ZR)3
RH5ZR3	Pd5Pu3		oS32	Cmcm	63		2	[5.0, 3.0]	(RH)5(RH, ZR)3
RU3SN7_D8F	Ir3Ge7 (D8f)	D8f	cI40	Im-3m	229		2	[0.3, 0.7]	(RU)0.3(SN)0.7
RU2SN3	Ru2Sn3		tP20	P-4c2	116		2	[0.4, 0.6]	(RU)0.4(SN)0.6
RU2Y3	Er3Ru2		hP10	P6_3/m	176		2	[0.4, 0.6]	(RU)0.4(Y)0.6
RU25Y44	Ru25Y44		oP276	Pnna	52		2	[0.362, 0.638]	(RU)0.362(Y)0.638

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RU2Y5	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[0.286, 0.714]	(RU)0.286(Y)0.714
SN3TI2	Unknown Structure						2	[3.0, 2.0]	(SN)3(TI)2
SN5TI6	Sn5Ti6-beta		hP22	P6_ 3/mmc	194	also Sn5Nb6.	2	[5.0, 6.0]	(AL, SN)5(NB, TI)6
SN5Y2	Shcherbinaite (V2O5) (Revised)		oP14	Pmmn	59		2	[5.0, 2.0]	(SN)5(Y)2
SN10Y11	Ge10Ho11		tI84	I4/mmm	139		2	[10.0, 11.0]	(SN)10(Y)11
SN4Y5	Gd5Si4		oP36	Pnma	62		2	[4.0, 5.0]	(SN)4(Y)5
TA1AL1	Al38Ta48		mP86	P2_1/c	14		2	[0.51515, 0.48485]	(TA)0.51515(AL)0.48485
TAAL2_HT	Al69Ta39		cF444	F-43m	216		2	[0.35, 0.65]	(TA)0.35(AL)0.65
TA41IR59	CuAu (L10)	L10	tP2	P4/mmm	123	aka Ta0.82Ir1.18_rt, gamma.	2	[0.41, 0.59]	(TA)0.41(IR)0.59
TA43IR57	TaIr		oP12	Pmma	51	aka Ta0.86Ir1.14, delta.	2	[0.43, 0.57]	(TA)0.43(IR, TA)0.57
T1CUNITI_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139	the Cu-Ni-Ti ternary phase Tau1.	2	[2.0, 1.0]	(CU, NI)2(TI)1
T2CUNITI	Cu3Ti2		tP10	P4/nmm	129	the Cu-Ni-Ti ternary phase Tau2.	3	[0.175, 2.825, 2.0]	(CU)0.175(NI)2.825(TI)2
T4CUNITI	BaPb3		hR12	R-3m	166	the Cu-Ni-Ti ternary phase Tau4.	3	[0.05, 0.7, 0.25]	(CU)0.05(NI)0.7(TI)0.25
T6CUNITI	Unknown Structure					the Cu-Ni-Ti ternary phase Tau6	3	[0.25, 0.5, 0.25]	(CU)0.25(NI)0.5(TI)0.25
T1CUFETI_ CU2TI	Au2V		oS12	Cmcm	63	ternary Ti0.33FexCu0.67-x, Tau1.	2	[2.0, 1.0]	(CU, FE)2(TI)1
T2CUFETI_ CU3TI2	Cu3Ti2		tP10	P4/nmm	129	ternary Ti0.4FexCu0.6-x, Tau2.	2	[3.0, 2.0]	(CU, FE)3(TI)2
T3CUFETI_ CU4TI3	Cu4Ti3		tI14	I4/mmm	139	ternary Ti0.43FexCu0.57-x, Tau3.	2	[4.0, 3.0]	(CU, FE)4(TI)3
T4CUFETI	Unknown Structure					ternary Ti0.37FexCu0.63-x, Tau4	2	[0.63, 0.37]	(CU, FE)0.63(TI)0.37
T5CUFETI	Unknown Structure					ternary Ti0.45FexCu0.55-x, Tau5.	2	[0.55, 0.45]	(CU, FE)0.55(TI)0.45
TIZN5	Unknown Structure						2	[1.0, 5.0]	(TI)1(ZN)5
TIZN10	Ti3Zn22		tP100	P4_ 2/mbc	135		2	[1.0, 10.0]	(TI)1(ZN)10
TIZN15	TiZn16		oS68	Cmcm	63		2	[1.0, 15.0]	(TI)1(ZN)15
V4ZN5	V4Zn5		tI18	I4/mmm	139		2	[4.0, 5.0]	(V)4(ZN)5
Y2ZN17	Ni17Th2		hP38	P6_	194		2	[2.0, 17.0]	(Y)2(ZN)17

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				3/mmc					
Y13ZN58	Y13Zn58		hP146	P6_ 3/mmc	194		2	[13.0, 58.0]	(Y)13(ZN)58
YZN5	ErZn5		hP36	P6_ 3/mmc	194	aka H_RZN5	2	[1.0, 5.0]	(Y)1(ZN)5
ZN12Y_D2B	Mn12Th (D2b)	D2b	tI26	I4/mmm	139		2	[12.0, 1.0]	(ZN)12(Y)1
ZN11Y3	Al11La3		oI28	Immm	71		2	[11.0, 3.0]	(ZN)11(Y)3
ZN22ZR	Zn22Zr		cF184	Fd-3m	227		2	[22.0, 1.0]	(ZN)22(ZR)1
ZN39ZR5	Zn39Zr5		mS88	C2/m	12		2	[39.0, 5.0]	(ZN)39(ZR)5
ZN2ZR3	Zr3Al2		tP20	P4_ 2/mnm	136		2	[2.0, 3.0]	(ZN)2(ZR)3
GAS	Gas						1	[1.0]	(AL, AL1C1, AL1C2, AL1CU1, AL1N1, AL2, AL2C2, B, B1C1, B1C2, B1N1, B2, B2C1, C, C1IR1, C1N1, C1N2_CNN, C1N2_NCN, C1RH1, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2N1_CCN, C2N1_CNC, C2N2, C2SI1, C2SI2, C2SI3, C3, C3N1, C4, C4N1, C4N2, C5, C5N1, C60, C6N1, C6N2, C9N1, CO, CO2, CR, CR1N1, CR2, CU, CU2, FE, FE2, HF, IR, MN, MO, MO1N1, MO2, N, N1NB1, N1SI1, N1SI2, N1TI1, N1V1, N1ZR1, N2, N3, NB, NI, NI2, RE, RH, RU, SI, SI2, SI3, SN, SN2, TA, TI, TI2, V, W, Y, ZN, ZR, ZR2)1

TCHEA6 Properties Data

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

Model Descriptions

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

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

Examples

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

TCHEA: TCS High Entropy Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS High Entropy Alloys Database (TCHEA)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**6.1**
First release:	**TCHEA1 was released in 2015**

Changes in the Most Recent Database Release

TCHEA6.0 to TCHEA6.1

Software release 2023a (December 2022/January 2023)

Reassessed Binary, Ternary, and Quinary Systems

- Binary: Two reassessments, Cr-Mn, Ir-Nb.
- Ternary: Seventeen (re-)assessments: Al-Cr-V, Co-Cr-Fe, Co-Cr-Mn, Co-Cr-Ni, Co-Fe-Mn, Co-Fe-Ni, Co-Mn-Ni, Cr-Fe-Mn, Cr-Mn-Ni, Cr-Mo-Nb, Cr-Mo-Ti, Cr-Nb-V, Fe-Mn-Ni, Fe-Ni-W, Mo-Nb-V, Re-Nb-V, and Re-V-W.
- Quinary: Validation of the Co-Cr-Fe-Mn-Ni system in full temperature and composition space (7 isopleths).

Previous Releases

TCHEA5.1 to TCHEA6.0

Software release version: 2022b (June 2022)

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

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

TCHEA5.0 to TCHEA5.1

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

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

TCHEA4.2 to TCHEA5.0

Software release version: 2021b (June 2021)

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

TCHEA4.1 to TCHEA4.2

Software release version: 2021a (January 2021)

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

TCHEA4.0 to TCHEA4.1

Software release version: 2020b (June 2020)

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

TCHEA3.1 to TCHEA4.0

Software release version: 2020a (January 2020)

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

TCHEA3.0 to TCHEA3.1

Software release 2019a (December 2018).

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

TCHEA2.0 to TCHEA3.0

Software release version: 2018a (April 2018)

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

TCHEA2.0 to TCHEA2.1

Software release version: 2017b (October 2017)

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

TCHEA1.0 to TCHEA2.0

Software release version: 2017a (March 2017)

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