TCS Cu-based Alloys Database (TCCU6)

Technical Information

Available Starting with Thermo-Calc 2023b

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Contents

About the TCS Cu-based Alloys Database (TCCU)

TCS Cu-based Alloys Database (TCCU) is a thermodynamic and properties database for copper-based alloys. The database includes nearly all stable phases in the assessed systems that may form in as-cast and aged Cu-based alloys.

TCCU6 is based on the critical evaluation of binary and ternary systems which enables predictions to be made for multicomponent systems and alloys of industrial importance. A hybrid approach of experiments, first-principles calculations, and CALPHAD modeling has been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges.

The database can be used to calculate various phase diagrams and property diagrams in the assessed systems or even extrapolated higher-order systems. The extrapolation to higher-order systems helps to understand the phase equilibria in multicomponent industrial copper alloys, so as to predict the phase formation, phase fractions and phase compositions or to calculate the driving force of forming a phase. The database is validated where possible against commercial Cu-based alloys and available experimental information.

The properties data was gradually added to the database versions as follows. Molar volume with thermal expansion coefficients available starting with TCCU1, the viscosity of and surface tension of liquids starting with TCCU4, and electrical resistivity and thermal conductivity starting with TCCU6.

TCCU: TCS Cu-based Alloys Database Revision History. The current version of the database is TCCU6. See the link for any subversion release details.

The database is compatible with the TCS Cu-based Alloys Mobility Database (MOBCU). The current version is MOBCU5.

The CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

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

Use Case Examples

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

Calculate the following based on your actual alloy chemistry using TCCU6:

- Thermophysical properties, such as specific heat, enthalpy, latent heat, density, electrical resistivity and thermal conductivity as a function of temperature, and coefficients of thermal expansion.
- Phase-based properties, such as critical transformation temperatures e.g. solvus temperatures of precipitates, solubility limits, chemical activities, viscosity and surface tension of liquid phase, amounts and compositions of all phases and phase diagrams.
- Equilibrium and non-equilibrium solidification, such as liquidus, solidus, incipient melt temperatures, freezing range, fraction solid curves, solidification path, fraction eutectic, microsegregation, partition coefficients, latent heat, and shrinkage.
- Predict solidification behavior of Cu-alloys in Thermo-Calc using the Scheil Calculator (in Graphical Mode) or the SCHEIL module (in Console Mode).

With the addition of Add-on Modules you can also do more advanced calculations such as:

- With the addition of the Diffusion Module (DICTRA), calculate optimal homogenization temperatures, time needed to homogenize any chemical segregation arising from solidification, and/or dissolve precipitates, and much more.
- With the addition of the Precipitation Module (TC-PRISMA), calculate concurrent nucleation, growth/dissolution, coarsening of precipitate phases, volume fraction, and size distribution as a function of time. You can also simulate multi-particle precipitation during aging treatment, and much more.

Combining Databases

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

TCS Cu-based Alloys Database (TCCU) 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 Cu-based Alloys Database (TCCU) Technical Information* PDF document contains version specific information such as the binary and ternary 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 Cu-based Alloys Database (TCCU) 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 Copper-based 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 Copper 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.

TCCU6 Elements, Systems, Phases and Properties

Included Elements

There are 32 elements included in the most recent version of the database.

Ag	Al	Au	As	B	Be	Bi	C	Ca	Cd
Ce	Co	Cr	Cu	Fe	Ge	La	Mg	Mn	Mo
Nb	Ni	O	P	Pb	Pt	Se	Si	Sn	Ti
Zn	Zr								

Assessed Systems and Phases

The most recent version of the database contains:

- 148 assessed binary systems, mostly to their full range of compositions, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 64 assessed ternary systems. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 315 solution and intermetallic phases.

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

The GAS phase is rejected by default when retrieving the data from the database. You have to manually restore it when it is required for a calculation. See TCCU6 Models for the Included Phases for details the models, e.g. number of sublattices and constituents on each sublattice.

Properties Data

A variety of properties data is included with the TCS Cu-based Alloy Database (TCCU).

The properties data was gradually added to the database versions as follows. Molar volume with thermal expansion coefficients available starting with TCCU1, the viscosity of and surface tension of liquids starting with TCCU4, and electrical resistivity and thermal conductivity starting with TCCU6.

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.

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 conductivity	ELQ**	ELCD for a system `ELCD(PHI)` for phase PHI
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
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)` `SURF(ION)` **
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 TCOX database (all versions). As of 2023b it is also not used starting with the following versions of these databases: TCFE13, TCNI12.1, TCTI5.1, TCNOBL3, TCPMAG2, and TCCU6. As of 2024a, TCMG7, TCAL9, and TCHEA7.

** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCCU6 Systems

In this section:

TCCU6 Assessed Binary Systems

Low temperature ordered phases are not fully included in Au-Cu and Cu-Pt systems.

Ag	Al	Au	As	B	Be	Bi	C	Ca	Cd	Ce	Co	Cr	Fe	Ge	La	Mg	Mn	Mo	Nb	Ni	O	P	Pb	Pt	Se	Si	Sn	Ti	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	X	X	X	X	X	X	Cu
	X	X			X	X					X		X	X			X			X		X	X			X	X		X		Ag
				X	X	X	X	X	X	X	X	X	X	X		X	X			X	X	X	X			X	X	X	X	X	Al
														X																Au
																														As
																													X	B
																				X						X				Be
																	X			X			X			X	X		X	Bi
																													X	C
																														Ca
																														Cd
															X					X										Ce
												X	X	X			X		X	X			X			X	X		X		Co
													X	X	X			X	X	X	X	X				X	X			X	Cr
																	X	X		X		X	X			X	X		X	X	Fe
																				X							X	X		X	Ge
																				X										X	La
																				X						X				X	Mg
																				X			X			X	X		X	X	Mn
																				X											Mo
																				X								X			Nb
																						X	X			X	X	X	X	X	Ni
																														X	O
																										X	X		X		P
																										X	X		X		Pb
																															Pt
																															Se
																											X		X	X	Si
																													X	X	Sn
																														X	Ti
																															Zn
																															Zr

TCCU6 Assessed Ternary Systems

These are the assessed ternary systems, which are mostly in the full compositional ranges. Low temperature ordered phases are not included in Ag-Au-Cu and Au-Cu-Ge.

Assessed Ternary Systems				
Ag-Au-Cu	Ag-Cr-Cu	Ag-Cu-Ge	Ag-Cu-Ni	Ag-Cu-P
Ag-Cu-Si	Ag-Cu-Sn	Al-Ce-Cu	Al-Cu-Fe	Al-Cu-Mn
Al-Cu-Ni	Al-Cu-O	Al-Cu-Si	Al-Cu-Sn	Al-Cu-Zn
Al-Fe-Ni	Au-Cu-Ge	Be-Cu-Ni	Ce-Cu-La	Ce-Cu-Ni
Co-Cr-Cu	Co-Cu-Fe	Co-Cu-Mn	Co-Cu-Nb	Co-Cu-Ni
Co-Cu-Si	Cr-Cu-Fe	Cr-Cu-La	Cr-Cu-Mo	Cr-Cu-Nb
Cr-Cu-Ni	Cr-Cu-Si	Cr-Cu-Sn	Cr-Cu-Zr	Cu-Fe-Mn
Cu-Fe-Mo	Cu-Fe-Ni	Cu-Fe-Si	Cu-Fe-Sn	Cu-Fe-Zn
Cu-La-Ni	Cu-La-Zr	Cu-Mg-Ni	Cu-Mg-Si	Cu-Mn-Ni
Cu-Mn-Si	Cu-Mn-Sn	Cu-Mn-Zn	Cu-Mo-Ni	Cu-Nb-Ni
Cu-Nb-Ti	Cu-Ni-P	Cu-Ni-Pb	Cu-Ni-Si	Cu-Ni-Sn
Cu-Ni-Ti	Cu-Ni-Zn	Cu-Pb-Sn	Cu-Pb-Zn	Cu-P-Sn
Cu-Si-Zn	Cu-Sn-Zn	Cu-Ti-Zr	Ni-Sn-Zn	

TCCU6 Phases

In this section:

Common Phases for Copper Alloys

TCCU6 Models for the Included Phases

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

Name in the Database	*Common Name and Description*
BCC_B2	BCC metals as well as bcc intermetallic phase, such as β-Cu_3Al and β-CuZn, β-$Cu_{0.85}Sn_{0.15}$, β-$Cu_{0.85}Si_{0.15}$, and β-$Cu_{0.65}Be_{0.35}$
CUSN_GAMMA	γ-Cu_3Sn (ht) and γ-Ni_3Sn (ht)
GAMMA_D83	A solution phase with γ-brass structure, such as γ-Cu_9Al_4 (rt), γ-Cu_5Zn_8, and γ-Ni_5Zn_8
AL2CU_C16	θ-Al_2Cu
GAMMA_H	γ-Cu_9Al_4 (ht)
HCP_A3	HCP metals as well as the cph intermediate phase, such as ε-$CuZn_4$, κ-$Cu_{0.88}Si_{0.12}$, and ξ-$Cu_{0.85}Ge_{0.15}$
B2_BCC	The cubic ordered intermetallic phase, γ-CuBe
C15_LAVES	The Cu_2Mg-type laves phase such as Cu_2Mg and Al_2Ca
CUPRITE_C3	Cu_2O
ZRM5_C15B	The Be_5Au-type intermetallic phase such as Cu_5Zr and Ni_5Zr
CUZR2_C11B	The $CuZr_2$-type intermetallic phase such as $CuTi_2$, $CuZr_2$, and $AlZr_2$
CU6SN5_HT	η-Cu_6Sn_5
CU6SN5_LT	η'-Cu_6Sn_5
CU41SN11	δ-$Cu_{41}Sn_{11}$
CU3SN	ε-Cu_3Sn (rt)
CU10SN3	ζ-$Cu_{10}Sn_3$
AL4M_D13	Al_4Ca

Name in the Database	*Common Name and Description*
DIAMOND_A4	Si and Ge
CO2SI_C23	Co_2Si, Ni_2Si
AL2AU_C1_CAF2	$CoSi_2$
M3P	Phosphide such as Fe_3P, Cr_3P, and Ni_3P
M2P	Phosphides such as Fe_2P, Cr_2P, and Ni_2P
MP	Phosphides such as FeP and CrP
R_PHASE	A high temperature Fe-Mo phase
MU_PHASE	μ phase, such as Co_6Nb_7 and Mo_6Fe_7
SIGMA	A chromium/molybdenum-rich intermetallic compound in Co-Cr and Fe-Mo systems

TCCU6 Models for the Included Phases

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
LIQUID	Liquid						1	[1.0]	(AG, AL, AL2/3O1, AL4/3O2, AS, AU, B, BE, BI, C, CA, CD, CE, CO, CR, CR3GE1, CRO, CRO3/2, CU, CU2O, CU2SE, CUO, FE, GE, LA, MG, MN, MO, NB, NI, NI12P5, P, PB, PT, SE, SI, SN, TI, ZN, ZR, ZR1/2O1)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	Metallic FCC_A1 solution, e.g. (Cu), (Al), (Ni)	2	[1.0, 1.0]	(AG, AL, AS, AU, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, SE, SI, SN, TI, ZN, ZR)1(B, C, O, VA)1
FCC_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		3	[0.75, 0.25, 1.0]	(AG, AL, AS, AU, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, SE, SI, SN, TI, ZN, ZR)0.75(AG, AL, AS, AU, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, SE, SI, SN, TI, ZN, ZR)0.25(B, C, O, VA)1
FCC_L10	CuAu (L10)	L10	tP2	P4/mmm	123		2	[0.5, 0.5]	(AL, CU, MN, NI, TI)0.5(AL, CU, MN, NI, TI)0.5
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229	Metallic BCC_A2 solution	2	[1.0, 3.0]	(AG, AL, AS, AU, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, SE, SI, SN, TI, VA, ZN, ZR)1(B, C, O, VA)3
BCC_B2	CsCl (B2)	B2	cP2	Pm-3m	221		3	[0.5, 0.5, 3.0]	(AG, AL, AS, AU, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, SE, SI, SN, TI, VA, ZN, ZR)0.5(AG, AL, AS, AU, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, SE, SI, SN, TI, VA, ZN, ZR)0.5(B, C, O, VA)3
CBCC_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[1.0, 1.0]	(AL, BI, CO, CR, CU, FE, MG, MN, NI, SI, SN, TI, ZN, ZR)1(B, C, O, VA)1

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
CUB_A13	beta-Mn (A13)	A13	cP20	P4_132	213		2	[1.0, 1.0]	(AG, AL, BI, CO, CR, CU, FE, MG, MN, NI, SI, SN, TI, ZN, ZR)1(B, C, O, VA)1
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194	Metallic HCP_A3 solution, alpha_ Mg/Hf/Sc/Ti/Zr	2	[1.0, 0.5]	(AG, AL, AS, AU, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, PB, PT, SI, SN, TI, ZN, ZR)1(B, C, O, VA)0.5
HCP_ZN	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		2	[1.0, 0.5]	(AG, AL, AU, BI, CO, CR, CU, FE, GE, MN, NI, PB, PT, SI, SN, ZN)1(VA)0.5
RHOMBO_A7	alpha-As (A7)	A7	hR2	R-3m	166		1	[1.0]	(AG, AS, BI, P, PB, SN, ZN)1
DHCP	alpha-La (A3')	A3'	hP4	P6_3/mmc	194		1	[1.0]	(CE, CU, LA, NI, ZR)1
HEXAGONAL_A8	gamma-Se (A8)	A8	hP3	P3_121	152		1	[1.0]	(SE)1
WHITE_P	Unknown Structure						1	[1.0]	(P)1
RED_P	Unknown Structure						1	[1.0]	(P)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	Hexagonal Graphite (A9)	A9	hP4	P6_3/mmc	194		1	[1.0]	(B, C)1
DIAMOND_A4	Diamond (A4)	A4	cF8	Fd-3m	227	Pure C, Ge, Si or solution phases based on them	1	[1.0]	(AG, AL, B, C, GE, P, SI, SN, TI, ZN)1
BCT_A5	beta-Sn (A5)	A5	tI4	I4_1/amd	141	Pure Sn or its solution	1	[1.0]	(AG, AL, B, BI, CD, CU, NI, PB, SI, SN, TI, ZN)1
B2_BCC	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(AL, BE, CO, CU, FE, NI, ZN)1(BE, CO, LA, MN, TI, VA, ZR)1
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		2	[2.0, 1.0]	(AL, CO, CR, CU, FE, LA, MG, MN, MO, NB, NI, TI, ZN, ZR)2(AL, CO, CR, CU, FE, LA, MG, MN, MO, NB, TI,

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
									ZN, ZR)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227	Solution of Cu2Mg-type phases	2	[2.0, 1.0]	(AL, CA, CO, CR, CU, FE, LA, MG, MN, NB, NI, SI, TI, ZN, ZR)2(AL, CA, CO, CR, CU, FE, LA, MG, MN, NB, NI, SI, TI, ZN, ZR)1
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_3/mmc	194	Solution of MgNi2-type phases	2	[2.0, 1.0]	(AL, CO, CR, CU, FE, LA, MG, MN, NB, NI, ZN, ZR)2(AL, CO, CR, CU, FE, LA, MG, MN, NB, NI, ZN, ZR)1
GAMMA_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		4	[2.0, 2.0, 3.0, 6.0]	(FE, MN, ZN)2(FE, MN, NI, ZN)2(AL, CU, FE, MN, NI, SI, ZN)3(AL, ZN)6
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215	solution between Al8Cu5 (rt) and Cu5Zn8	3	[4.0, 1.0, 8.0]	(AL, FE, NI, SI, SN, ZN)4(AL, CU, NI, SI, ZN)1(CU, FE, MN, NI, SN, ZN)8
CO2SI_C23	Cotunnite (PbCl2, C23)	C23	oP12	Pnma	62	Co2Si, Ni2Si	2	[2.0, 1.0]	(AL, CA, CO, CU, FE, NI, SI)2(AL, CO, SI, SN, ZN)1
GAS	Gas						1	[1.0]	(AG, AG1AL1, AG1AU1, AG1CU1, AG1O1, AG1SE1, AG2, AG2SE1, AL, AL1AS1, AL1AU1, AL1B1O2, AL1C1, AL1C2, AL1CU1, AL1O1, AL1O2, AL1P1, AL1P2, AL1SE1, AL2, AL2C2, AL2O1, AL2O2, AL2O3, AL2SE1, AL2SE2, AS, AS1O1, AS1O2, AS1P1, AS1P3, AS1SE1, AS2, AS2P2, AS3, AS3P1, AS4, AS4O10, AS4O6, AS4O7, AS4O8, AS4O9, AS4SE3, AU, AU1C1, AU1CO1, AU1CU1, AU1O1, AU1SE1, AU1SI1, AU2, B, B1BE1O2, B1C1, B1C2, B1O1, B1O2, B1SE1, B2, B2BE1O4, B2C1, B2O1, B2O2, B2O3, BE, BE1C2, BE1O1, BE2, BE2O1, BE2O2, BE3O3, BE4O4, BE5O5, BE6O6, BI, BI1O1, BI1SE1, BI2, BI2O1_C2V, BI2O1_DH, BI2O2, BI2O3, BI3, BI3O4, BI4, BI4O6, C, C1O1, C1O2, C1P1, C1P1SI1,

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
									C1P1SI2, C1P2, C1PT1, C1SE1, C1SE2, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2O1, C2P1, C2P2, C2SI1, C2SI2, C2SI3, C3, C3O2, C4, C4NI1O4, C5, C5FE1O5, C60, C6MO1O6, CA, CA1O1, CA2, CD, CD1O1, CD1SE1, CE, CE1O1, CE1SE1, CO, CO1O1, CO1SE1, CO2, CR, CR1O1, CR1O2, CR1O3, CR1SE1, CR2, CR2O1, CR2O2, CR2O3, CU, CU1O1, CU1SE1, CU2, CU2SE1, FE, FE1O1, FE1O2, FE1SE1, FE2, GE, GE1O1, GE1O2, GE1SE1, GE2, LA, LA1O1, LA1SE1, LA2O1, LA2O2, MG, MG1O1, MG2, MN, MN1O1, MN1O2, MN1SE1, MO, MO1O1, MO1O2, MO1O3, MO2, MO2O6, MO3O9, MO4O12, MO5O15, NB, NB1O1, NB1O2, NB1SE1, NB1SE2, NI, NI1O1, NI2, O, O10P4, O1P1, O1PB1, O1PT1, O1SE1, O1SI1, O1SN1, O1TI1, O1ZN1, O1ZR1, O2, O2P1, O2PB1, O2PT1, O2SE1, O2SI1, O2SI2, O2SN1, O2TI1, O2ZR1, O3, O3P2, O4P2, O5P2, O6P3, O6P4, O7P4, O8P4, O9P4, P, P1SE1, P1SI1, P1SI2, P2, P2SI2, P3, P4, PB, PB1SE1, PB2, PT, SE, SE1SI1, SE1SN1, SE1TI1, SE1ZN1, SE2, SE3, SE4, SE5, SE6, SE7, SE8, SI, SI2, SI3, SN, SN2, TI, TI2, ZN, ZR, ZR2)1
AG3BE8	Unknown Structure						2	[2.97, 8.03]	(AG)2.97(BE)8.03
AG3SN_L60	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59	a binary phase in Ag-Sn system, and a ternary phase in Cu-Ni-Sn system	2	[0.75, 0.25]	(AG, CO, CU, NI, ZN)0.75(AG, BI, NI, SN)0.25
AGZN3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		1	[1.0]	(AG, ZN)1
AGZN_LT	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229		2	[1.0, 2.0]	(ZN)1(AG, ZN)2

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
AG5ZN8	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		4	[2.0, 2.0, 3.0, 6.0]	(AG, ZN)2(AG)2(AG, ZN)3(AG, ZN)6
ALB2_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[1.0, 2.0]	(AL, CR, MG, MN, TI, ZR)1(B)2
ALB12	alpha-AlB12		tP216	P4_12_12	92		2	[1.0, 12.0]	(AL)1(B)12
AL4C3	Al4C3 (D71)	D71	hR7	R-3m	166		2	[4.0, 3.0]	(AL, SI)4(C)3
AL4M_D13	Al4Ba (D13)	D13	tI10	I4/mmm	139	Al4Ca	2	[4.0, 1.0]	(AL)4(CA)1
AL14CA13	Al14Ca13		mS54	C2/m	12		2	[14.0, 13.0]	(AL, MG, ZN)14(CA)13
AL3CA8	Ca8In3		aP22	P-1	2		2	[3.0, 8.0]	(AL)3(CA, MG)8
AL4CE	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[4.0, 1.0]	(AL)4(CE)1
AL11CE3	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[11.0, 3.0]	(AL)11(CE)3
AL3CE_HT	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[3.0, 1.0]	(AL)3(CE)1
AL3CE_LT	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(AL)3(CE)1
AL2CE	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[2.0, 1.0]	(AL)2(CE)1
AL1CE1	AlCe		oS16	Cmcm	63		2	[1.0, 1.0]	(AL)1(CE)1
AL1CE2	Unknown Structure						2	[1.0, 2.0]	(AL)1(CE)2
ALCE3_HT	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[1.0, 3.0]	(AL)1(CE)3
ALCE3_LT	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[1.0, 3.0]	(AL)1(CE)3
AL45CR7	V7Al45		mS104	P2_1/m	11		2	[45.0, 7.0]	(AL)45(CR)7
CUZR2_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139	AlCr2, CuTi2, CuZr2	2	[1.0, 2.0]	(AL, CR, CU, NI, SI, ZN)1(AL, CR, NB, TI, ZR)2

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
AL5CR	Al5Cr		mS732	C2/c	15		2	[5.0, 1.0]	(AL, SI)5(CR)1
AL4CR	mu-Al4Mn		hP574	P6_3/mmc	194		2	[1.0, 4.0]	(CR)1(AL, SI, VA)4
ALCR_GAMMA1	Unknown Structure						4	[2.0, 2.0, 3.0, 6.0]	(AL, CR, SI)2(CR)2(AL, CR)3(AL, SI)6
GAMMA_D810	Cr5Al8 (D810)	D810	hR26	R3m	160	A binary phase in Al- Cr system	3	[12.0, 5.0, 9.0]	(AL, SI)12(CR)5(AL, CR, SI)9
AL13CO4	Orthorhombic Co4Al13		oP102	Pmn2_1	31		2	[13.0, 4.0]	(AL)13(CO)4
AL3CO	Os4Al13		mS34	C2/m	12		2	[3.0, 1.0]	(AL)3(CO)1
AL5CO2	Co2Al5 (D811)	D811	hP28	P6_3/mmc	194		2	[5.0, 2.0]	(AL)5(CO)2
AL9CO2	Co2Al9 (D8d)	D8d	mP22	P2_1/c	14		2	[9.0, 2.0]	(AL)9(CO)2
ALCU_DEL	Al5Cu8		hR52	R3m	160		2	[2.0, 3.0]	(AL, ZN)2(CU, FE)3
ALCU_EPS	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[1.0, 1.0]	(AL, CU, NI, ZN)1(CU, FE)1
ALCU_ETA	AlCu(r)		mS20	C2/m	12		2	[1.0, 1.0]	(AL, CU)1(CU, FE, NI, ZN)1
ALCU_PRIME	Al9Cu11(h)		oF88	Fmm2	42		2	[2.0, 1.0]	(AL)2(CU)1
ALCU_ZETA	Al9Cu11(h)		oF88	Fmm2	42		2	[9.0, 11.0]	(AL)9(CU, FE)11
GAMMA_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		3	[4.0, 1.0, 8.0]	(AL, ZN)4(AL, CU, ZN)1(CU, FE, MN, NI)8
AL2CU_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140	Al2Cu, CoSn2, FeSn2, Mnsn2	2	[2.0, 1.0]	(AL, FE, MN, NI, SN, ZR)2(AL, B, CO, CU, FE, MN, NI, SI)1
AL2FE1	Al2Fe		aP18	P1	1		2	[2.0, 1.0]	(AL, CU, SI, ZN)2(FE, MN, NI)1
AL5FE2	Al2.8Fe		oS24	Cmcm	63		2	[5.0, 2.0]	(AL, CU, SI, ZN)5(FE, MN, NI)2

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
AL5FE4	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		1	[1.0]	(AL, CU, FE, MN)1
AL13FE4	Al13Fe4		mS102	C2/m	12		3	[0.6275, 0.235, 0.1375]	(AL, CU)0.6275(FE, MN, NI, ZN)0.235(AL, SI, VA, ZN)0.1375
ALMG_BETA	Al45Mg28		cF1832	Fd-3m	227		2	[89.0, 140.0]	(MG)89(AL, ZN)140
ALMG_EPS	Al30Mg23		hR53	R-3	148		2	[23.0, 30.0]	(MG)23(AL, ZN)30
ALMG_GAMMA	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[5.0, 12.0, 12.0]	(MG)5(AL, MG, ZN)12(AL, MG, ZN)12
AL12MN	Al12W		cI26	Im-3	204		2	[12.0, 1.0]	(AL)12(MN)1
AL6MN	MnAl6 (D2h)	D2h	oS28	Cmcm	63		2	[6.0, 1.0]	(AL, ZN)6(FE, MN)1
AL4MN_R	lambda-Al4Mn		hP586	P6_3/mmc	194		2	[461.0, 107.0]	(AL)461(FE, MN)107
AL4MN_U	mu-Al4Mn		hP574	P6_3/mmc	194		2	[4.0, 1.0]	(AL, ZN)4(MN)1
AL11MN4_LT	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL, ZN)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	Cr5Al8 (D810)	D810	hR26	R3m	160		3	[12.0, 5.0, 9.0]	(AL, ZN)12(MN)5(AL, CU, MN, SI)9
AL3NI_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[0.75, 0.25]	(AL, MN, NI)0.75(FE, NI)0.25
AL3NI2	Al3Ni2 (D513)	D513	hP5	P-3m1	164		3	[3.0, 2.0, 1.0]	(AL, SI, ZN)3(AL, CU, FE, NI)2(NI, VA)1
AL3NI5	Ga3Pt5		oS16	Cmmm	65		2	[0.375, 0.625]	(AL)0.375(NI)0.625
CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	R-3c	167	Al2O3	3	[2.0, 1.0, 3.0]	(AL+3, CR+3, VA)2(VA)1(O-2)3
ALP	Zincblende (ZnS, B3)	B3	cF8	F-43m	216		2	[1.0, 1.0]	(AL)1(P)1

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
AL2TI	Ga2Hf		tI24	I4_1/amd	141		2	[2.0, 1.0]	(AL)2(TI)1
AL18TI7	Al5Ti2		tP28	P4/mmm	123		2	[0.72, 0.28]	(AL)0.72(TI)0.28
AL3TI_D022	Al3Ti (D022)	D022	tI8	I4/mmm	139		2	[3.0, 1.0]	(AL, MN, NI)3(MN, TI, ZR)1
ALTI3_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(AL, TI)3(AL, TI)1
AL2ZR1	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		2	[2.0, 1.0]	(AL)2(ZR)1
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	AlZr3	2	[1.0, 3.0]	(AL, NI, SI, TI)1(AL, FE, NI, ZN, ZR)3
AL3ZR5_D8M	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[3.0, 5.0]	(AL, SI)3(CR, ZR)5
CRB_B33	CrB (B33)	B33	oS8	Cmcm	63	AlZr, NiZr	2	[1.0, 1.0]	(AL, CA, CR, NI)1(AG, B, SI, SN, ZR)1
ALZR2_B82	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[1.0, 2.0]	(AL, MN, SN, VA)1(MN, TI, VA, ZR)2
AL4ZR5	Ti5Ga4		hP18	P6_3/mcm	193		2	[4.0, 5.0]	(AL)4(ZR)5
AL3ZR2_OF40	Zr2Al3		oF40	Fdd2	43		2	[3.0, 2.0]	(AL)3(ZR)2
AL2ZR3_TP20	Zr3Al2		tP20	P4_2/mnm	136		2	[2.0, 3.0]	(AL, ZN)2(ZR)3
AL3ZR_D023	Al3Zr (D023)	D023	tI16	I4/mmm	139		2	[3.0, 1.0]	(AL)3(TI, ZR)1
ZRB12	UB12 (D2f)	D2f	cF52	Fm-3m	225		2	[12.0, 1.0]	(B)12(ZR)1
BIMN_LT	NiAs (B81)	B81	hP4	P6_3/mmc	194		2	[0.5, 0.5]	(BI)0.5(MN)0.5
BIMN_HT	Mn2.23Bi1.88		oP10	Pmma	51		2	[0.481, 0.519]	(BI)0.481(MN)0.519
BI3NI	Bi3Ni		oP16	Pnma	62		2	[3.0, 1.0]	(BI)3(NI)1
CU6SN5_HT	Ni2In (B82)	B82	hP6	P6_3/mmc	194	CU6SN5(HT), BiNi, Co6Sn5	3	[1.0, 1.0, 1.0]	(AG, CO, CU, MN, NI, VA, ZN)1(AG, AL, BI, CU, GE, NI, PB, SI, SN, ZN)1

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
									(CO, CU, MN, NI, SN, VA, ZN)1
CA2CU	Ca2Cu		oP12	Pnma	62		2	[2.0, 1.0]	(CA)2(CU)1
CA1CU1	alpha-CaCu		mP20	P2_1/m	11		2	[1.0, 1.0]	(CA)1(CU)1
CACU5_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[1.0, 5.0]	(CA)1(CU, NI, ZN)5
CDCU2	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		2	[1.0, 2.0]	(CD)1(CU)2
CD3CU4	Cd3Cu4		cF1124	F-43m	216		2	[0.4286, 0.5714]	(CD)0.4286(CU)0.5714
CD8CU5	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		4	[2.0, 3.0, 2.0, 6.0]	(CU)2(CD, CU)3(CU)2(CD, CU)6
CD10CU3	Co2Al5 (D811)	D811	hP28	P6_3/mmc	194		2	[0.7692, 0.2308]	(CD)0.7692(CU)0.2308
CUR	FeB (B27)	B27	oP8	Pnma	62	CuLa, CuCe,	2	[1.0, 1.0]	(CU, NI)1(CE, LA)1
CU2CE	KHg2		oI12	Imma	74		2	[2.0, 1.0]	(CU)2(CE)1
CU4CE	Unknown Structure		oP20				2	[4.0, 1.0]	(AL, CU)4(CE)1
CU5R	CaCu5 (D2d)	D2d	hP6	P6/mmm	191	Cu5La, Cu5Ce, Ni5La, Ni5Ce	2	[5.0, 1.0]	(AL, CE, CU, NI)5(CE, LA, NI)1
CU6R	CeCu6		oP28	Pnma	62	Cu6La_LT, Cu6Ce	2	[6.0, 1.0]	(CU, NI)6(CE, LA)1
CENI2	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[1.0, 2.0]	(CE, NI)1(CE, NI)2
CENI3	CeNi3		hP24	P6_3/mmc	194		2	[1.0, 3.0]	(CE)1(NI)3
CE2NI7	Ce2Ni7		hP36	P6_3/mmc	194		2	[2.0, 7.0]	(CE)2(NI)7
SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136	A binary phase in Co-Cr and Fe-Mo systems	3	[8.0, 4.0, 18.0]	(CO, FE, MN, NI)8(CR, MO)4(CO, CR, FE, MN, MO, NI)18

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
CO3GE	Unknown Structure						2	[0.75, 0.25]	(CO)0.75(GE)0.25
CO5GE2	Unknown Structure						2	[0.714, 0.286]	(CO)0.714(GE)0.286
CO5GE3_C37	Co2Si (C37)	C37	oP12	Pnma	62		3	[0.125, 0.5, 0.375]	(CO, VA)0.125(CO)0.5(CO, GE, SN)0.375
CO5GE3_ALPHA	Unknown Structure						2	[0.625, 0.375]	(CO)0.625(GE)0.375
CO5GE7	Co5Ge7		tI24	I4mm	107		2	[0.417, 0.583]	(CO)0.417(GE)0.583
COGE	CoGe		mS16	C2/m	12		2	[0.5, 0.5]	(CO, GE)0.5(CO, GE)0.5
CO1GE2	CoGe2		oS24	Cmce	64		2	[0.333, 0.667]	(CO)0.333(GE)0.667
CO2SI_HT	Co2Si (C37)	C37	oP12	Pnma	62		2	[0.6667, 0.3333]	(CO, SI)0.6667(CO, SI)0.3333
COSI_B20	FeSi (B20)	B20	cP8	P2_13	198		2	[0.5, 0.5]	(AL, CO, SI)0.5(CO, SI)0.5
CO3SI_HT	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		3	[0.25, 0.25, 0.5]	(CO, CU, NI, SI, SN)0.25(CO, CU, NI, SN)0.25(CO, CU, NI)0.5
AL2AU_C1_CAF2	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	CoSi2	2	[0.66667, 0.33333]	(AG, AL, AU, CU, SI, SN)0.66667(AL, AU, CO, NI, PT)0.33333
COSN3_OS32	PdSn3		oS32	Cmce	64		2	[0.25, 0.75]	(CO)0.25(SN)0.75
COSN_HP6	CoSn (B35)	B35	hP6	P6/mmm	191		2	[0.5, 0.5]	(CO)0.5(SN)0.5
COZN_LT	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_ D83	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215		2	[1.0, 1.0]	(CO, ZN)1(VA)1
COZN_DELTA	Unknown Structure						2	[0.117647, 0.882353]	(CO)0.117647(ZN)0.882353

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
COZN_GAMMA1	Co2Zn15		mS28	C2/m	12		2	[0.125, 0.875]	(CO)0.125(ZN)0.875
COZN_GAMMA2	CoZn13		mS28	C2/m	12		2	[0.0714286, 0.9285714]	(CO)0.0714286(ZN)0.928571
CU3GE_ETA	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59		2	[0.75, 0.25]	(AG, CU)0.75(GE)0.25
CU3GE_EPSILON	Na3As (D018)	D018	hP8	P6_3/mmc	194		2	[0.765, 0.235]	(AG, CU)0.765(GE)0.235
CU3GE_THETA	BiF3 (D03)	D03	cF16	Fm-3m	225		2	[0.735, 0.265]	(AG, CU)0.735(GE)0.265
CR5GE3	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[0.625, 0.375]	(CR, GE)0.625(CR, GE)0.375
LCR5GE3	Unknown Structure						2	[0.625, 0.375]	(CR, GE)0.625(CR, GE)0.375
CR11GE8	Cr11Ge8		oP76	Pnma	62		2	[0.579, 0.421]	(CR)0.579(GE)0.421
CR11GE19	Mn11Si19		tP120	P-4n2	118		2	[0.367, 0.633]	(CR)0.367(GE)0.633
CR3GE	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[0.75, 0.25]	(CR, GE)0.75(CR, GE)0.25
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	Fd-3m	227		4	[1.0, 2.0, 2.0, 4.0]	(AL+3, CR+2, CR+3, CU+2)1(AL+3, CR+3, CU+2, VA)2(CR+2, VA)2(O-2)4
CU6LA_HT	Cu6La		mP28	P2_1/c	14		2	[6.0, 1.0]	(CU)6(CE, LA)1
CU4LA	Cu4La		tI90	I-4m2	119		2	[4.0, 1.0]	(CU)4(LA, ZR)1
CU2LA	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[2.0, 1.0]	(CU, NI)2(LA)1
CUMG2	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[1.0, 2.0]	(CU, NI)1(MG)2
CU33SI7_DELTA	Unknown Structure						2	[0.825, 0.175]	(AG, CU, ZN)0.825(SI)0.175
CU56SI11_GAMMA	Mg3Ru2		cP20	P4_132	213		2	[0.835821, 0.164179]	(AG, CU, MG, MN, NI, ZN)0.835821(SI)0.164179

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CUSI_ETA	Cu3Si-h2		hR*	P-31m	162		2	[0.76, 0.24]	(AG, CU, MN, NI, ZN)0.76(SI)0.24
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cI76	I-43d	220		2	[0.789474, 0.210526]	(AG, CU, MG, MN, ZN)0.789474(AL, SI)0.210526
CUSN_GAMMA	BiF3 (D03)	D03	cF16	Fm-3m	225	Cu3Sn(ht), Ni3Sn (ht)	1	[1.0]	(CU, MN, NI, SN, ZN)1
CU10SN3	Cu10Sn3		hP26	P6_3	173		2	[0.769, 0.231]	(CU, NI)0.769(SN)0.231
CU3SN	Cu3Sn		oS80	Cmcm	63		2	[3.0, 1.0]	(CU, NI, SN)3(CU, SN)1
CU41SN11	Cu41Sn11		cF416	F-43m	216		2	[41.0, 11.0]	(CU, SN, ZN)41(CU, SN, ZN)11
CU6SN5_LT	Cu6Sn5		mS44	C2/c	15		3	[1.0, 1.0, 1.0]	(CU)1(CU, SN)1(SN)1
CU2TI1	Au2V		oS12	Cmcm	63		2	[2.0, 1.0]	(CU, NI)2(TI)1
CU3TI2	Cu3Ti2		tP10	P4/nmm	129		2	[3.0, 2.0]	(CU, NI)3(NB, TI)2
CU4TI1	Au4Zr		oP20	Pnma	62		2	[4.0, 1.0]	(CU, NB, NI, TI)4(CU, NB, NI, TI)1
CU4TI3	Cu4Ti3		tI14	I4/mmm	139		2	[4.0, 3.0]	(CU, NI)4(NB, TI)3
CUTI_B11	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[1.0, 1.0]	(CU, NB, NI, TI)1(CU, NB, NI, TI)1
CUTI3	CuTi3 (L60)	L60	tP4	P4/mmm	123		2	[1.0, 3.0]	(CU, NB, TI)1(NB, TI)3
CU10ZR7	Ni10Zr7		oS68	Cmce	64		2	[10.0, 7.0]	(CU)10(ZR)7
ZRM5_C15B	AuBe5 (C15b)	C15b	cF24	F-43m	216	Cu5Zr, Ni5Zr	2	[5.0, 1.0]	(CU, NI)5(LA, ZR)1
CU51ZR14	Ag51Gd14		hP68	P6/m	175		2	[0.7846, 0.2154]	(CU)0.7846(LA, ZR)0.2154
CU8ZR3	Cu8Hf3		oP44	Pnma	62		2	[8.0, 3.0]	(CU)8(ZR)3
R_PHASE	R-(Co, Cr, Mo)		hR53	R-3	166	A binary phase in	3	[27.0, 14.0,	(FE)27(MO)14(FE, MO)12

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
						Fe-Mo system		12.0]	
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	Binary phase (Mu) in Fe-Mo and Co-Nb systems	3	[7.0, 2.0, 4.0]	(CO, CU, FE, NB)7(CU, MO, NB)2 (CO, FE, MO, NB)4
M3P	Ni3P (D0e)	D0e	tI32	I-4	82	Ni3P, Fe3P, Cr3P	2	[0.75, 0.25]	(CR, CU, FE, NI)0.75(P)0.25
M2P	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189	Ni2P, Fe2P, Cr2P	2	[0.667, 0.333]	(CR, CU, FE, NI)0.667(P)0.333
MP	Westerveldite (FeAs, B14)	B14	oP8	Pnma	62	FeP, CrP	2	[0.5, 0.5]	(CR, FE)0.5(P)0.5
FEP2	Marcasite (FeS2, C18)	C18	oP6	Pnnm	58		2	[0.333, 0.667]	(FE)0.333(P)0.667
FEP4	FeP4		mP30	P2_1/c	14		2	[0.2, 0.8]	(FE)0.2(P)0.8
FE2SI	AlNi2		hP6	P-3m1	164		2	[2.0, 1.0]	(FE, NI)2(AL, SI)1
FESI2_H	FeSi2-h		tP3	P4/mmm	123		2	[3.0, 7.0]	(FE, NI)3(AL, SI)7
FESI2_L	FeSi2-l		oS48	Cmce	64		2	[1.0, 2.0]	(FE, NI)1(AL, SI)2
FESI_B20	FeSi (B20)	B20	cP8	P2_13	198	FeSi, MnSi, CrSi	2	[1.0, 1.0]	(CR, FE, MN, NI)1(AL, GE, SI)1
MN5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193	Mn5Si3, Cr3Si5, Fe5Si3, Ge3Zr5, Si3Zr5,	2	[5.0, 3.0]	(CR, CU, FE, MN, NI, TI, ZR)5(AL, CR, GE, SI, SN)3
FE5SN3_D82	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[5.0, 3.0]	(FE)5(SN)3
FE3SN2	Fe3Sn2		hR10	R-3m	166		2	[3.0, 2.0]	(FE)3(SN)2
FEM_B35	CoSn (B35)	B35	hP6	P6/mmm	191	FeSn	2	[1.0, 1.0]	(FE)1(SN)1
FEZN_GAMMA1	Fe11Zn40		cF408	F-43m	216		3	[0.137, 0.118, 0.745]	(FE)0.137(AL, CU, FE, NI, SI, ZN)0.118(MN, ZN)0.745

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
FEZN_DELTA	FeZn10		hP632	P6_3/mmc	194		4	[0.058, 0.18, 0.525, 0.237]	(FE)0.058(AL, CU, FE, MN, NI, SI, ZN)0.18(ZN)0.525(ZN)0.237
FEZN_ZETA	CoZn13		mS28	C2/m	12		3	[0.072, 0.856, 0.072]	(FE, MN, NI, VA)0.072(AL, ZN)0.856 (AL, CU, SI, VA, ZN)0.072
GE3NI5_C2	Ge3Ni5		mS32	C2	5		2	[0.625, 0.375]	(NI)0.625(GE)0.375
GE2NI5_HT	Pd5Sb2		hP42	P6_3cm	185		2	[0.72, 0.28]	(NI)0.72(GE)0.28
GENI3_HT	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.744, 0.256]	(NI)0.744(GE)0.256
GENI2	Co2Si (C37)	C37	oP12	Pnma	62		2	[0.665, 0.335]	(NI)0.665(GE)0.335
GE1NI1	Westerveldite (FeAs, B14)	B14	oP8	Pnma	62		2	[0.5, 0.5]	(GE)0.5(NI)0.5
TI5GE3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193		2	[3.0, 5.0]	(GE)3(TI)5
TI6GE5	Si5V6		oI44	Ibam	72		2	[5.0, 6.0]	(GE)5(TI)6
TIGE2	TiSi2 (C54)	C54	oF24	Fddd	70		2	[2.0, 1.0]	(GE)2(TI)1
LA3NI	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(LA)3(NI)1
NI3R7	Fe3Th7 (D102)	D102	hP20	P6_3mc	186	Ni3La7, Ni3Ce7	2	[7.0, 3.0]	(CE, LA)7(NI)3
NIR	CrB (B33)	B33	oS8	Cmcm	63	NiLa, NiCe	2	[1.0, 1.0]	(CE, LA)1(CU, NI)1
LA2NI3	La2Ni3		oS20	Cmce	64		2	[2.0, 3.0]	(LA)2(CU, NI)3
LA7NI16	La7Ni16		tI46	I-42m	121		2	[7.0, 16.0]	(LA)7(CU, NI)16
LANI3	Ni3Pu		hR12	R-3m	166		2	[1.0, 3.0]	(LA)1(CU, NI)3
LA2NI7	Ce2Ni7		hP36	P6_3/mmc	194		2	[2.0, 7.0]	(LA)2(CU, NI)7

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
LA5NI19	Co19Sm5		hP48	P6_3/mmc	194		2	[5.0, 19.0]	(LA)5(NI)19
MNNI2	Unknown Structure						2	[1.0, 2.0]	(MN, NI)1(NI)2
MN11SI19	Mn11Si19		tP120	P-4n2	118		2	[11.0, 19.0]	(MN)11(AL, SI)19
MN3SI	BiF3 (D03)	D03	cF16	Fm-3m	225		2	[3.0, 1.0]	(FE, MN, NI)3(AL, SI)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
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62		2	[3.0, 2.0]	(MN)3(SN)2
NI3SN_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[1.0, 3.0]	(AL, CU, NI, SN, VA, ZN)1(CU, FE, MN, NI, SN, ZN)3
MN2SN	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[0.643, 0.357]	(MN)0.643(SN)0.357
MNZN9	Unknown Structure		h**				2	[0.1, 0.9]	(MN)0.1(ZN)0.9
MONI_DELTA	MoNi		oP56	P2_12_12_1	19		3	[24.0, 20.0, 12.0]	(NI)24(MO, NI)20(CU, MO)12
MONI4_BETA	Ni4Mo (D1a)	D1a	tI10	I4/m	87		2	[1.0, 4.0]	(MO)1(NI)4
NI3MO_D0A	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59		2	[3.0, 1.0]	(NI)3(MO, NI)1
NBNI3	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59		2	[1.0, 3.0]	(CU, NB, NI)1(CU, NB, NI)3
NB7NI6	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166		4	[1.0, 4.0, 2.0, 6.0]	(NB, NI)1(NB)4(NB, NI)2(CU, NB, NI)6
NBNI8	Pt8Ti		tI18	I4/mmm	139		2	[1.0, 8.0]	(NB)1(NI)8
NI5P2_HT	Unknown Structure						2	[0.714, 0.286]	(NI)0.714(P)0.286

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
NI5P2_LT	Pd8Sb3		hR44	R3c	161		2	[0.714, 0.286]	(CU, NI)0.714(P)0.286
NI12P5_HT	Unknown Structure						2	[0.706, 0.294]	(NI)0.706(P)0.294
NI12P5_LT	Ni12P5		tI34	I4/m	87		2	[0.706, 0.294]	(NI)0.706(P)0.294
NI5P4	Ni5P4		hP36	P6_3/mmc	194		2	[0.556, 0.444]	(NI)0.556(P)0.444
NIP2	PdP2		mS12	C2/c	15		2	[0.3333, 0.6667]	(NI)0.3333(P)0.6667
NI2SI_HT	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[1.0, 1.0, 1.0]	(CU, NI)1(NI, VA)1(AL, SI)1
NI3SI2	Ni3Si2		oP80	Cmc2_1	36		2	[3.0, 2.0]	(FE, NI)3(SI)2
NI3SI_HT	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(FE, NI)3(AL, SI)1
NI3SI_MT	Ge9Pd25		hP34	P-3	147		2	[1.0, 3.0]	(SI)1(NI)3
NISI_B31	MnP (B31)	B31	oP8	Pnma	62		2	[1.0, 1.0]	(FE, NI)1(SI, ZN)1
NISI2	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		2	[2.0, 1.0]	(AL, CU, SI, ZN)2(CU, FE, MN, NI)1
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	C2/m	12		3	[0.25, 0.25, 0.5]	(CU, NI, ZN)0.25(NI, SN, ZN)0.25 (SN, ZN)0.5
NITI2	NiTi2		cF96	Fd-3m	227		2	[0.3333, 0.6667]	(CU, NI)0.3333(TI)0.6667
NI3TI	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194		2	[0.75, 0.25]	(CU, NI, TI)0.75(CU, NI, TI)0.25
NIZN_LT	delta-CuTi (L2a)	L2a	tP2	P4/mmm	123		2	[0.5, 0.5]	(AL, FE, MN, NI, SI, SN, ZN)0.5(AL, FE, MN, NI, SI, SN, ZN)0.5
NIZN8	Ni3Zn22		mS50	C2/m	12		2	[0.1111111, 0.8888889]	(NI)0.111111(AL, ZN)0.888889
NI10ZR7	Ni10Zr7		oS68	Cmce	64		2	[23.0, 17.0]	(NI)23(ZR)17

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
NI21ZR8	Hf8Ni21		aP29	P-1	2		2	[8.0, 21.0]	(ZR)8(NI)21
NI11ZR9	Pt11Zr9		tI40	I4/m	87		2	[11.0, 9.0]	(NI)11(ZR)9
NI7ZR2	Ni7Zr2		mS36	C2/m	12		2	[7.0, 2.0]	(NI)7(ZR)2
FLUORITE	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		2	[2.0, 4.0]	(ZR, ZR+4)2(O-2, VA)4
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	P2_1/c	14		2	[2.0, 4.0]	(ZR+4)2(O-2, VA)4
ZRO2_TETR	HgI2 (C13)	C13	tP6	P4_2/nmc	137		2	[2.0, 4.0]	(ZR+4)2(O-2, VA)4
PSI	(SiP)		oS48	Cmc2_1	36		2	[1.0, 1.0]	(P)1(SI)1
P2ZN3	Zn3P2 (D59)	D59	tP40	P4_2/nmc	137		2	[2.0, 3.0]	(P)2(ZN)3
P2ZN1	ZnAs2		mP24	P2_1/c	14		2	[2.0, 1.0]	(P)2(ZN)1
SI2ZR_C49	ZrSi2 (C49)	C49	oS12	Cmcm	63	Si2Zr, Ge2Zr	2	[2.0, 1.0]	(GE, SI)2(ZR)1
SI4ZR5_TP36	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140	Si4Zr5, Si4Ti5, Ge4Zr5	2	[4.0, 5.0]	(GE, SI)4(TI, ZR)5
SIZR3_TP32	Ti3P		tP32	P4_2/n	86	SiZr3, SiTi3, GeZr3	2	[1.0, 3.0]	(GE, SI)1(TI, ZR)3
SI2ZR3_D5A	Si2U3 (D5a)	D5a	tP10	P4/mbm	127		2	[2.0, 3.0]	(SI)2(ZR)3
FEB_B27	FeB (B27)	B27	oP8	Pnma	62	ZrGe, ZrSi	2	[1.0, 1.0]	(FE, MN, TI, ZR)1(B, GE, SI, ZN)1
SI2TI_C54	TiSi2 (C54)	C54	oF24	Fddd	70	Sn2Zr	2	[2.0, 1.0]	(SI, SN)2(TI, ZR)1
SN3ZR5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193		3	[5.0, 3.0, 1.0]	(ZR)5(SN)3(SN, VA)1
SNZR3_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[3.0, 1.0]	(SN, ZR)3(SN, ZR)1

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
AGP2	CuP2		mP12	P2_1/c	14		2	[1.0, 2.0]	(AG)1(P)2
AG3P11	Ag3P11		mS28	Cm	8		2	[3.0, 11.0]	(AG)3(P)11
ALMGZN_PHI	Mg21(Al, Zn)17		oP152	Pbcm	57		2	[6.0, 5.0]	(MG)6(AL, ZN)5
CU3AS	H3Ho		hP24	P-3c1	165		2	[3.0, 1.15]	(CU)3(AS, CU)1.15
CU7AS1	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		2	[7.0, 1.0]	(CU)7(AS)1
CU7AS3	Cu7In3		aP40	P-1	2		2	[7.0, 3.0]	(CU)7(AS)3
BE2CU	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[2.0, 1.0]	(BE, CU)2(BE, CU)1
NIBE7	Unknown Structure		cl*				3	[2.0, 2.0, 9.0]	(BE, NI)2(NI)2(BE)9
CO7NB2	(Co7Nb2)		mS18	C2/m	12		2	[7.0, 2.0]	(CO)7(NB)2
CRNI2_OP6	MoPt2		oI6	Immm	71		2	[1.0, 2.0]	(CR)1(NI)2
CR3SI	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[3.0, 1.0]	(CR, SI)3(AL, CR, SI)1
CRSI2_C40	CrSi2 (C40)	C40	hP9	P6_222	180		2	[1.0, 2.0]	(CR, CU, SI)1(AL, CR, CU, SI)2
CUO	Tenorite (CuO, B26)	B26	mS8	C2/c	15		2	[1.0, 1.0]	(CU+2)1(O-2)1
CUPRITE_C3	Cuprite (Cu2O, C3)	C3	cP6	Pn-3m	224	Cu2O	2	[2.0, 1.0]	(CU+1)2(O-2)1
CU3P	Cu3P		hP24	P6_3cm	185		2	[3.0, 1.0]	(CU)3(P)1
CUP2	CuP2		mP12	P2_1/c	14		2	[1.0, 2.0]	(CU)1(P)2
CU2P7	Cu2P7		mS72	C2/m	12		2	[2.0, 7.0]	(CU)2(P)7
CU2SE_LT	Cu2Se		mS144	C2/c	15		2	[2.0, 1.0]	(CU, SE)2(SE)1

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CU2SE_HT	Cu2Se		cF44	Fm-3m	225		2	[2.0, 1.0]	(CU, SE)2(SE)1
CU3SE2	Cu3Se2		tP10	P-42_1m	113		2	[3.0, 2.0]	(CU)3(SE)2
CUSE2	Marcasite (FeS2, C18)	C18	oP6	Pnnm	58		2	[1.0, 2.0]	(CU)1(SE)2
CUSE_LT	Cu0.87Se		hP26	P6_3/mmc	194		2	[1.0, 1.0]	(CU)1(SE)1
CUSE_RT	CuS		oS24	Cmcm	63		2	[1.0, 1.0]	(CU)1(SE)1
CUSE_HT	Covellite (CuS, B18)	B18	hP12	P6_3/mmc	194		2	[1.0, 1.0]	(CU)1(SE)1
FEZR3	Re3B		oS16	Cmcm	63		2	[1.0, 3.0]	(FE)1(ZR)3
MG2NI	Mg2Ni (Ca)	Ca	hP18	P6_222	180		2	[2.0, 1.0]	(MG, ZN)2(CU, NI, ZN)1
MG2SI_C1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		2	[2.0, 1.0]	(MG)2(SI, SN)1
NI19SI6	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.24, 0.76]	(SI)0.24(CU, NI)0.76
NI5SI2	Ni31S12		hP42	P321	150		2	[5.0, 2.0]	(CU, FE, NI)5(AL, SI)2
SN4P3	Sn3.6As3		hR21	R-3m	166		2	[4.0, 3.0]	(SN)4(P)3
AL8CECU4	CeMn4Al8		tI26	I4/mmm	139		3	[0.6154, 0.0769, 0.3077]	(AL)0.6154(CE)0.0769(CU)0.3077
ALCECU_T2	Zn17Th2		hR57	R-3m	166		2	[0.8947, 0.1053]	(AL, CU)0.8947(CE)0.1053
ALCECU_T3	ThCr2Si2		tI10	I4/mmm	139		2	[0.8, 0.2]	(AL, CU)0.8(CE)0.2
ALCECU_T4	ZrNiAl		hP9	P-62m	189		3	[0.3333, 0.3333, 0.3334]	(AL)0.3333(CE)0.3333(CU)0.3334
ALCE2CU2_T5	Unknown Structure						3	[0.2, 0.4, 0.4]	(AL)0.2(CE)0.4(CU)0.4

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AL23CUFE4	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
AL28CU4MN7	Mn6Cu4Al29		oS156	Cmcm	63		3	[28.0, 7.0, 4.0]	(AL)28(MN)7(CU)4
AL11CU5MN3	Unknown Structure		oP380				3	[11.0, 3.0, 5.0]	(AL)11(MN)3(CU)5
ALCU3MN2	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		3	[1.0, 2.0, 3.0]	(AL)1(MN)2(CU)3
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5		hR14	R-3m	166		2	[1.0, 1.0]	(AL)1(CU, FE, NI, VA)1
CUALO2	Rhombohedral Delafossite (CuFeO2)		hR4	R-3m	166		3	[1.0, 1.0, 2.0]	(CU+1)1(AL+3)1(O-2)2
AL5CU4ZN	Unknown Structure						4	[1.0, 4.0, 4.0, 1.0]	(AL, CU)1(AL)4(CU)4(ZN)1
AL9FENI	Co2Al9 (D8d)	D8d	mP22	P2_1/c	14		2	[9.0, 2.0]	(AL)9(FE, NI)2
AL10FE3NI	Co2Al5 (D811)	D811	hP28	P6_3/mmc	194		2	[5.0, 2.0]	(AL)5(FE, NI)2
AL71FE5NI24	Unknown Structure						3	[0.71, 0.05, 0.24]	(AL)0.71(FE)0.05(NI)0.24
CU85NI5LA10	(CU85NI5LA10)		CF*	Fm-3m	225		3	[85.0, 5.0, 10.0]	(CU)85(NI)5(LA)10
CU16MG6SI7	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		3	[16.0, 6.0, 7.0]	(CU)16(MG)6(SI)7
CU3MG2SI	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_3/mmc	194		3	[2.74, 2.0, 1.26]	(CU)2.74(MG)2(SI)1.26
CU5MN4SI	Unknown Structure						3	[0.5, 0.37, 0.13]	(CU)0.5(MN)0.37(SI)0.13

Phase	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
CU4MNSN	MgCu4Sn		cF24	F-43m	216		3	[0.6666, 0.1667, 0.1667]	(CU)0.6666(SN)0.1667(MN)0.1667
CUMNZN	Unknown Structure						3	[0.334, 0.333, 0.333]	(CU)0.334(MN)0.333(ZN)0.333
CUNITI_T1	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[0.6667, 0.3333]	(CU, NI)0.6667(TI)0.3333
CUNITI_T2	Cu3Ti2		tP10	P4/nmm	129		3	[0.035, 0.565, 0.4]	(CU)0.035(NI)0.565(TI)0.4
CUNITI_T4	BaPb3		hR12	R-3m	166		3	[0.075, 0.675, 0.25]	(CU, TI)0.075(CU, NI)0.675(TI)0.25
CUNITI_T6	Al3Ti (D022)	D022	tI8	I4/mmm	139		3	[0.25, 0.5, 0.25]	(CU, TI)0.25(CU, NI)0.5(TI)0.25
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
NISNZN_T1	Unknown Structure						3	[0.36, 0.38, 0.26]	(NI, SN, VA)0.36(NI, SN)0.38(VA, ZN)0.26
NISNZN_T2	Unknown Structure						3	[0.55, 0.26, 0.19]	(NI, VA)0.55(SN)0.26(SN, VA, ZN)0.19
NISNZN_T3	Unknown Structure						3	[0.482, 0.204, 0.314]	(NI, VA)0.482(SN)0.204(SN, VA, ZN)0.314
NISNZN_T4	Unknown Structure						3	[0.505, 0.39, 0.105]	(NI, SN, VA)0.505(SN, ZN)0.39(SN, VA, ZN)0.105

TCCU6 Properties Data

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 Copper-based 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 Copper including links to resources such as examples, publications, and more.

TCCU: TCS Cu-based Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS Cu-based Alloys Database (TCCU)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**6.2**
First release:	**TCCU1 was released in with 2016b**

Changes in the Most Recent Database Release

TCCU6.1 to TCCU6.2

Software release 2024a (December 2023/January 2024)

- Corrected the default setting of major components in BCC, FCC, and HCP phases.
- Updated the surface tension of the Fe-Ni system.

Previous Releases

TCCU6.0 to TCCU6.1

Software release version: 2023b Update 1 (September 2023)

- Restored the GAS phase by default. This is for compatibility with the Additive Manufacturing (AM) Module.

TCCU5.1 to TCCU6.0

Software release version: 2023b (June 2023)

- Added electrical resistivity and thermal conductivity description
- The surface tension was re-assessed based on the Redlich-Kister-Muggianu (R-K-M) sub-regular solution model.

TCCU5.0 to TCCU5.1

Software release version: 2023a (December 2022/January 2023)

- Corrected an error in the molar volume of the B2 phase in the Al-Fe-Ni system.

TCCU4 to TCCU5

Software release version: 2022b (June 2022)

- Two new elements: Ce and La.
- 13 new binary systems: Cr-O, Cu-La, Cu-Ce, Cr-La, La-Zr, La-Ni, Ce-La, Al-Ce, Ni-Ce, Nb-Ni, Nb-Ti, Ni-Ti, Zr-O.
- 11 new ternary systems: Ag-Cu-Si, Ag-Cr-Cu, Al-Ce-Cu, Ce-Cu-La, Ce-Cu-Ni, Cr-Cu-La, Cu-La-Ni, Cu-La-Zr, Cu-Nb-Ni, Cu-Nb-Ti, and Cu-Ni-Ti.
- Volume data for the newly added phases are assessed or estimated.

TCCU3.1 to TCCU4

Software release version: 2021b (June 2021)

- Two binary systems Cr-P and Ni-P are added.
- Three ternary systems Cu-Ni-P, Cu-Co-Si, and Ni-Sn-Zn are added.
- Addition of viscosity and surface tension thermophysical property data.

TCCU3 to TCCU3.1

Software release version: 2020a (January 2020)

Revised description of liquid in Al-Cu-O system

TCCU2 TO TCCU3

Software release version: 2019b (June 2019)

- Addition of Ge.
- Ten Ge-X (X=Ag, Al, Au, Co, Cr, Cu, Ni, Sn, Ti, Zr) binary systems are added.
- Two ternary systems Ag-Cu-Ge and Au-Cu-Ge are included.
- Volume data for the newly added phases are assessed or estimated.

TCCU1 TO TCCU2

Software release version: 2017a (March 2017)

Volume data, including molar volume and thermal expansion, for most of the solution phases and intermetallic phases have been added in TCCU2. This allows for the calculations of volume fraction of phases, density, thermal expansion and lattice parameters etc.

Two elements, Mo and O, have been added in TCCU2. The thermodynamic assessments of the Ag-P, Al-O, Co-Cr, Co-Nb, Cr-Mo, Cr-Nb, Cu-Mo, Cu-O, Fe-Mo and Mo-Ni binary systems have been implemented. The following ternary systems have also been assessed: Ag-P-Sn, Al-Cu-O, Co-Cu-Nb, Co-Cr-Cu, Cr-Cu-Nb, Cr-Cu-Mo, Cu-Fe-Mo and Cu-Mo-Ni. Additionally, the Cu-P, Co-Pb, P-Zn and Cu-P-Sn descriptions have been updated.