TCS Cu-based Alloys Database (TCCU5)

Technical Information

Available Starting with Thermo-Calc 2022b

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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.

TCCU5 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.

TCCU: TCS Cu-based Alloys Database Revision History. The current version of the database is TCCU5. 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 TCCU5:

- Thermophysical properties, such as specific heat, enthalpy, latent heat, density as a function of temperature, and coefficients of thermal expansion.

- Phase-based properties, such as Critical transformation temperatures such as solvus temperatures of precipitates, amounts and compositions of phases, solubility limits, activities, 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.

TCCU5 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 TCCU5 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).

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*
Surface tension	SIGM, XI	`SURF(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)`
Kinematic viscosity		`KVIS(LIQUID)`
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

TCCU5 Systems

In this section:

TCCU5 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

TCCU5 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	

TCCU5 Phases

In this section:

Common Phases for Copper Alloys

TCCU5 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

TCCU5 Models for the Included Phases

Name	*Prototype*	*Pearson Symbol*	*Space Group Symbol*	*SG#*	*Strukturbericht*	*Formula Unit*	*Notes*
AG3BE8	Unknown Structure					(AG)2.97(BE)8.03	
AG3P11	Ag3P11	mS28	Cm	8		(AG)3(P)11	
AG3SN_L60	beta-TiCu3 (D0a)	oP8	Pmmn	59	D0a	(AG, CO, CU, NI, ZN)0.75 (AG, BI, NI, SN)0.25	a binary phase in Ag-Sn system, and a ternary phase in Cu-Ni-Sn system
AG5ZN8	gamma-brass (Cu5Zn8, D82)	cI52	I-43m	217	D82	(AG, ZN)2(AG)2(AG, ZN)3 (AG, ZN)6	
AGP2	CuP2	mP12	P2_1/c	14		(AG)1(P)2	
AGZN	Body-Centered Cubic (W, A2, bcc)	cI2	Im-3m	229	A2	(ZN)1(AG, ZN)2	
AGZN3	Hexagonal Close Packed (Mg, A3, hcp)	hP2	P6_3/mmc	194	A3	(AG, ZN)1	
AL10CU10FE	(Al10Cu10Fe)	oF116	Fmm2	42		(FE)1(AL, CU)10(AL)10	
AL10FE3NI	Co2Al5 (D811)	hP28	P6_3/mmc	194	D811	(AL)5(FE, NI)2	
AL11CE3	Ni3Sn (D019)	hP8	P6_3/mmc	194	D019	(AL)11(CE)3	
AL11CU5MN3	Unknown Structure	oP380				(AL)11(MN)3(CU)5	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25	oP156	Pnma	62		(AL, MN)29(MN)10	
AL11MN4_LT	Al11Mn4	aP15	P-1	2		(AL, ZN)11(FE, MN)4	
AL12MN	Al12W	cI26	Im-3	204		(AL)12(MN)1	
AL13CO4	Orthorhombic Co4Al13	oP102	Pmn2_1	31		(AL)13(CO)4	
AL13FE4	Al13Fe4	mS102	C2/m	12		(AL, CU)0.6275(FE, MN, NI, ZN)0.235(AL, SI, VA, ZN)0.1375	
AL14CA13	Al14Ca13	mS54	C2/m	12		(AL, MG, ZN)14(CA)13	
AL18TI7	Al5Ti2	tP28	P4/mmm	123		(AL)0.72(TI)0.28	
AL23CUFE4	MnAl6 (D2h)	oS28	Cmcm	63	D2h	(AL)23(CU)1(FE)4	
AL28CU4MN7	Mn6Cu4Al29	oS156	Cmcm	63		(AL)28(MN)7(CU)4	
AL2AU_C1_CAF2	Fluorite (CaF2, C1)	cF12	Fm-3m	225	C1	(AG, AL, AU, CU, SI, SN)0.66667(AL, AU, CO, NI, PT)0.33333	CoSi2
AL2CE	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m	227	C15	(AL)2(CE)1	
AL2CU_C16	Khatyrkite (Al2Cu, C16)	tI12	I4/mcm	140	C16	(AL, FE, MN, NI, SN, ZR)2 (AL, B, CO, CU, FE, MN, NI, SI)1	Al2Cu, CoSn2, FeSn2, Mnsn2

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
AL2FE1	Al2Fe	aP18	P1	1		(AL, CU, SI, ZN)2(FE, MN, NI)1	
AL2TI	Ga2Hf	tI24	I4_1/amd	141		(AL)2(TI)1	
AL2ZR	MgZn2 Hexagonal Laves (C14)	hP12	P6_3/mmc	194	C14	(AL)2(ZR)1	
AL2ZR3_TP20	Zr3Al2	tP20	P4_2/mnm	136		(AL, ZN)2(ZR)3	
AL3CA8	Ca8In3	aP22	P-1	2		(AL)3(CA, MG)8	
AL3CE_HT	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m	221	L12	(AL)3(CE)1	
AL3CE_LT	Ni3Sn (D019)	hP8	P6_3/mmc	194	D019	(AL)3(CE)1	
AL3CO	Os4Al13	mS34	C2/m	12		(AL)3(CO)1	
AL3NI_D011	Cementite (Fe3C, D011)	oP16	Pnma	62	D011	(AL, MN, NI)0.75(FE, NI)0.25	
AL3NI2	Al3Ni2 (D513)	hP5	P-3m1	164	D513	(AL, SI, ZN)3(AL, CU, FE, NI)2(NI, VA)1	
AL3NI5	Ga3Pt5	oS16	Cmmm	65		(AL)0.375(NI)0.625	
AL3TI_D022	Al3Ti (D022)	tI8	I4/mmm	139	D022	(AL, MN, NI)3(MN, TI, ZR)1	
AL3ZR_D023	Al3Zr (D023)	tI16	I4/mmm	139	D023	(AL)3(TI, ZR)1	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
AL3ZR2_OF40	Zr2Al3	oF40	Fdd2	43		(AL)3(ZR)2	
AL3ZR5_D8M	W5Si3 (D8m)	tI32	I4/mcm	140	D8m	(AL, SI)3(CR, ZR)5	
AL45CR7	V7Al45	mS104	P2_1/m	11		(AL)45(CR)7	
AL4C3	Al4C3 (D71)	hR7	R-3m	166	D71	(AL, SI)4(C)3	
AL4CE	Al4Ba (D13)	tI10	I4/mmm	139	D13	(AL)4(CE)1	
AL4CR	mu-Al4Mn	hP574	P6_3/mmc	194		(CR)1(AL, SI, VA)4	
AL4M_D13	Al4Ba (D13)	tI10	I4/mmm	139	D13	(AL)4(CA)1	Al4Ca
AL4MN_R	lambda-Al4Mn	hP586	P6_3/mmc	194		(AL)461(FE, MN)107	
AL4MN_U	mu-Al4Mn	hP574	P6_3/mmc	194		(AL, ZN)4(MN)1	
AL4ZR5	Ti5Ga4	hP18	P6_3/mcm	193		(AL)4(ZR)5	
AL5CO2	Co2Al5 (D811)	hP28	P6_3/mmc	194	D811	(AL)5(CO)2	
AL5CR	Al5Cr	mS732	C2/c	15		(AL, SI)5(CR)1	
AL5CU4ZN	Unknown Structure					(AL, CU)1(AL)4(CU)4(ZN)1	
AL5FE2	Al2.8Fe	oS24	Cmcm	63		(AL, CU, SI, ZN)5(FE, MN, NI)2	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
AL5FE4	gamma-brass (Cu5Zn8, D82)	cI52	I-43m	217	D82	(AL, CU, FE, MN)1	
AL62CU25FE13	Quasicrystal					(FE)0.125(AL, CU)0.255 (AL)0.62	
AL6MN	MnAl6 (D2h)	oS28	Cmcm	63	D2h	(AL, ZN)6(FE, MN)1	
AL71FE5NI24	Unknown Structure					(AL)0.71(FE)0.05(NI)0.24	
AL7CU2FE	FeCu2Al7 (E9a)	tP40	P4/mnc	128	E9a	(FE, NI)1(CU)2(AL)7	
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5	hR14	R-3m	166		(AL)1(CU, FE, NI, VA)1	
AL8CECU4	CeMn4Al8	tI26	I4/mmm	139		(AL)0.6154(CE)0.0769 (CU)0.3077	
AL8MN5	Cr5Al8 (D810)	hR26	R3m	160	D810	(AL, ZN)12(MN)5(AL, CU, MN, SI)9	
AL9CO2	Co2Al9 (D8d)	mP22	P2_1/c	14	D8d	(AL)9(CO)2	
AL9FENI	Co2Al9 (D8d)	mP22	P2_1/c	14	D8d	(AL)9(FE, NI)2	
ALB12	alpha-AlB12	tP216	P4_12_12	92		(AL)1(B)12	
ALB2_C32	Hexagonal omega (C32)	hP3	P6/mmm	191	C32	(AL, CR, MG, MN, TI, ZR)1 (B)2	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
ALCE	AlCe	oS16	Cmcm	63		(AL)1(CE)1	
ALCE2	Unknown Structure					(AL)1(CE)2	
ALCE2CU2	Unknown Structure					(AL)0.2(CE)0.4(CU)0.4	
ALCE3_HT	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m	221	L12	(AL)1(CE)3	
ALCE3_LT	Ni3Sn (D019)	hP8	P6_3/mmc	194	D019	(AL)1(CE)3	
ALCECU	ZrNiAl	hP9	P-62m	189		(AL)0.3333(CE)0.3333 (CU)0.3334	
ALCECU_T2	Zn17Th2	hR57	R-3m	166		(AL, CU)0.8947(CE)0.1053	
ALCECU_T3	ThCr2Si2	tI10	I4/mmm	139		(AL, CU)0.8(CE)0.2	
ALCR_GAMMA1	Unknown Structure					(AL, CR, SI)2(CR)2(AL, CR)3 (AL, SI)6	
ALCU_DEL	Al5Cu8	hR52	R3m	160		(AL, ZN)2(CU, FE)3	
ALCU_EPS	Ni2In (B82)	hP6	P6_3/mmc	194	B82	(AL, CU, NI, ZN)1(CU, FE)1	
ALCU_ETA	AlCu(r)	mS20	C2/m	12		(AL, CU)1(CU, FE, NI, ZN)1	
ALCU_PRIME	Al9Cu11(h)	oF88	Fmm2	42		(AL)2(CU)1	
ALCU_ZETA	Al9Cu11(h)	oF88	Fmm2	42		(AL)9(CU, FE)11	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
ALCU3MN2	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m	227	C15	(AL)1(MN)2(CU)3	
ALMG_BETA	Al45Mg28	cF1832	Fd-3m	227		(MG)89(AL, ZN)140	
ALMG_EPS	Al30Mg23	hR53	R-3	148		(MG)23(AL, ZN)30	
ALMG_GAMMA	alpha-Mn (A12)	cI58	I-43m	217	A12	(MG)5(AL, MG, ZN)12(AL, MG, ZN)12	
ALMGZN_PHI	Mg21(Al, Zn)17	oP152	Pbcm	57		(MG)6(AL, ZN)5	
ALP	Zincblende (ZnS, B3)	cF8	F-43m	216	B3	(AL)1(P)1	
ALTI3_D019	Ni3Sn (D019)	hP8	P6_3/mmc	194	D019	(AL, TI)3(AL, TI)1	
ALZR2_B82	Ni2In (B82)	hP6	P6_3/mmc	194	B82	(AL, MN, SN, VA)1(MN, TI, VA, ZR)2	
B2_BCC	CsCl (B2)	cP2	Pm-3m	221	B2	(AL, BE, CO, CU, FE, NI, ZN)1(BE, CO, LA, MN, TI, VA, ZR)1	
BCC_A2	Body-Centered Cubic (W, A2, bcc)	cI2	Im-3m	229	A2	(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	Metallic BCC_A2 solution
BCC_B2	CsCl (B2)	cP2	Pm-3m	221	B2	(AG, AL, AS, AU, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI,	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
						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	
BCT_A5	beta-Sn (A5)	tI4	I4_1/amd	141	A5	(AG, AL, B, BI, CD, CU, NI, PB, SI, SN, TI, ZN)1	Pure Sn or its solution
BE2CU	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m	227	C15	(BE, CU)2(BE, CU)1	
BETA_RHOMBO_B	beta-B (R-105)	hR105	R-3m	166		(B)93(B, C, CU, SI)12	
BI3NI	Bi3Ni	oP16	Pnma	62		(BI)3(NI)1	
BIMN_HT	Mn2.23Bi1.88	oP10	Pmma	51		(BI)0.481(MN)0.519	
BIMN_LT	NiAs (B81)	hP4	P6_3/mmc	194	B81	(BI)0.5(MN)0.5	
C14_LAVES	MgZn2 Hexagonal Laves (C14)	hP12	P6_3/mmc	194	C14	(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, ZN, ZR)1	
C15_LAVES	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m	227	C15	(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	Solution of Cu2Mg-type phases

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
C36_LAVES	MgNi2 Hexagonal Laves (C36)	hP24	P6_3/mmc	194	C36	(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	Solution of MgNi2-type phases
CA2CU	Ca2Cu	oP12	Pnma	62		(CA)2(CU)1	
CACU	alpha-CaCu	mP20	P2_1/m	11		(CA)1(CU)1	
CACU5_D2D	CaCu5 (D2d)	hP6	P6/mmm	191	D2d	(CA)1(CU, NI, ZN)5	
CBCC_A12	alpha-Mn (A12)	cI58	I-43m	217	A12	(AL, BI, CO, CR, CU, FE, MG, MN, NI, SI, SN, TI, ZN, ZR)1 (B, C, O, VA)1	
CD10CU3	Co2Al5 (D811)	hP28	P6_3/mmc	194	D811	(CD)0.7692(CU)0.2308	
CD3CU4	Cd3Cu4	cF1124	F-43m	216		(CD)0.4286(CU)0.5714	
CD8CU5	gamma-brass (Cu5Zn8, D82)	cI52	I-43m	217	D82	(CU)2(CD, CU)3(CU)2(CD, CU)6	
CDCU2	MgZn2 Hexagonal Laves (C14)	hP12	P6_3/mmc	194	C14	(CD)1(CU)2	
CE2NI7	Ce2Ni7	hP36	P6_3/mmc	194		(CE)2(NI)7	
CENI2	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m	227	C15	(CE, NI)1(CE, NI)2	
CENI3	CeNi3	hP24	P6_3/mmc	194		(CE)1(NI)3	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
CO2SI_C23	Cotunnite (PbCl2, C23)	oP12	Pnma	62	C23	(AL, CA, CO, CU, FE, NI, SI)2 (AL, CO, SI, SN, ZN)1	Co2Si, Ni2Si
CO2SI_HT	Co2Si (C37)	oP12	Pnma	62	C37	(CO, SI)0.6667(CO, SI)0.3333	
CO3GE	Unknown Structure					(CO)0.75(GE)0.25	
CO3SI_HT	Ni3Sn (D019)	hP8	P6_3/mmc	194	D019	(CO, CU, NI, SI, SN)0.25(CO, CU, NI, SN)0.25(CO, CU, NI)0.5	
CO5GE2	Unknown Structure					(CO)0.714(GE)0.286	
CO5GE3	Co2Si (C37)	oP12	Pnma	62	C37	(CO, VA)0.125(CO)0.5(CO, GE, SN)0.375	
CO5GE3_ALPHA	Unknown Structure					(CO)0.625(GE)0.375	
CO5GE7	Co5Ge7	tI24	I4mm	107		(CO)0.417(GE)0.583	
CO7NB2	(Co7Nb2)	mS18	C2/m	12		(CO)7(NB)2	
COGE	CoGe	mS16	C2/m	12		(CO, GE)0.5(CO, GE)0.5	
COGE2	CoGe2	oS24	Cmce	64		(CO)0.333(GE)0.667	
CORUNDUM	Corundum (Al2O3, D51)	hR10	R-3c	167	D51	(AL+3, CR+3, VA)2(VA)1(O-2)3	Al2O3

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
COSI_B20	FeSi (B20)	cP8	P2_13	198	B20	(AL, CO, SI)0.5(CO, SI)0.5	
COSN_HP6	CoSn (B35)	hP6	P6/mmm	191	B35	(CO)0.5(SN)0.5	
COSN3_OS32	PdSn3	oS32	Cmce	64		(CO)0.25(SN)0.75	
COZN_DELTA	Unknown Structure					(CO)0.117647(ZN)0.882353	
COZN_GAMMA	gamma-brass (Cu9Al4, D83)	cP52	P-43m	215	D83	(CO, ZN)1(VA)1	
COZN_GAMMA1	Co2Zn15	mS28	C2/m	12		(CO)0.125(ZN)0.875	
COZN_GAMMA2	CoZn13	mS28	C2/m	12		(CO)0.0714286 (ZN)0.928571	
COZN_HT	Unknown Structure					(CO, ZN)1(VA)1	
COZN_LT	beta-Mn (A13)	cP20	P4_132	213	A13	(CO, ZN)1(VA)1	
CR11GE19	Mn11Si19	tP120	P-4n2	118		(CR)0.367(GE)0.633	
CR11GE8	Cr11Ge8	oP76	Pnma	62		(CR)0.579(GE)0.421	
CR3GE	Cr3Si (A15)	cP8	Pm-3n	223	A15	(CR, GE)0.75(CR, GE)0.25	
CR3SI	Cr3Si (A15)	cP8	Pm-3n	223	A15	(CR, SI)3(AL, CR, SI)1	
CR5GE3	W5Si3 (D8m)	tI32	I4/mcm	140	D8m	(CR, GE)0.625(CR, GE)0.375	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
CRB_B33	CrB (B33)	oS8	Cmcm	63	B33	(AL, CA, CR, NI)1(AG, B, SI, SN, ZR)1	AlZr, NiZr
CRNI2_OP6	MoPt2	oI6	Immm	71		(CR)1(NI)2	
CRSI2_C40	CrSi2 (C40)	hP9	P6_222	180	C40	(CR, CU, SI)1(AL, CR, CU, SI)2	
CU10SN3	Cu10Sn3	hP26	P6_3	173		(CU, NI)0.769(SN)0.231	
CU10ZR7	Ni10Zr7	oS68	Cmce	64		(CU)10(ZR)7	
CU15SI4_EPSILON	Cu15Si4 (D86)	cI76	I-43d	220	D86	(AG, CU, MG, MN, ZN)0.789474(AL, SI)0.210526	
CU16MG6SI7	Th6Mn23 (D8a)	cF116	Fm-3m	225	D8a	(CU)16(MG)6(SI)7	
CU2CE	KHg2	oI12	Imma	74		(CU)2(CE)1	
CU2LA	Hexagonal omega (C32)	hP3	P6/mmm	191	C32	(CU, NI)2(LA)1	
CU2P7	Cu2P7	mS72	C2/m	12		(CU)2(P)7	
CU2SE_HT	Cu2Se	cF44	Fm-3m	225		(CU, SE)2(SE)1	
CU2SE_LT	Cu2Se	mS144	C2/c	15		(CU, SE)2(SE)1	
CU2TI	Au2V	oS12	Cmcm	63		(CU, NI)2(TI)1	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
CU2TIZR	MgZn2 Hexagonal Laves (C14)	hP12	P6_3/mmc	194	C14	(CU)0.5(TI)0.25(ZR)0.25	
CU33SI7_DELTA	Unknown Structure					(AG, CU, ZN)0.825(SI)0.175	
CU3AS	H3Ho	hP24	P-3c1	165		(CU)3(AS, CU)1.15	
CU3GE_EPSILON	Na3As (D018)	hP8	P6_3/mmc	194	D018	(AG, CU)0.765(GE)0.235	
CU3GE_ETA	beta-TiCu3 (D0a)	oP8	Pmmn	59	D0a	(AG, CU)0.75(GE)0.25	
CU3GE_THETA	BiF3 (D03)	cF16	Fm-3m	225	D03	(AG, CU)0.735(GE)0.265	
CU3MG2SI	MgNi2 Hexagonal Laves (C36)	hP24	P6_3/mmc	194	C36	(CU)2.74(MG)2(SI)1.26	
CU3P	Cu3P	hP24	P6_3cm	185		(CU)3(P)1	
CU3SE2	Cu3Se2	tP10	P-42_1m	113		(CU)3(SE)2	
CU3SN	Cu3Sn	oS80	Cmcm	63		(CU, NI, SN)3(CU, SN)1	
CU3TI2	Cu3Ti2	tP10	P4/nmm	129		(CU, NI)3(NB, TI)2	
CU41SN11	Cu41Sn11	cF416	F-43m	216		(CU, SN, ZN)41(CU, SN, ZN)11	
CU4CE	Unknown Structure	oP20				(AL, CU)4(CE)1	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
CU4LA	Cu4La	tI90	I-4m2	119		(CU)4(LA, ZR)1	
CU4MNSN	MgCu4Sn	cF24	F-43m	216		(CU)0.6666(SN)0.1667 (MN)0.1667	
CU4TI1	Au4Zr	oP20	Pnma	62		(CU, NB, NI, TI)4(CU, NB, NI, TI)1	
CU4TI3	Cu4Ti3	tI14	I4/mmm	139		(CU, NI)4(NB, TI)3	
CU51ZR14	Ag51Gd14	hP68	P6/m	175		(CU)0.7846(LA, ZR)0.2154	
CU56SI11_GAMMA	Mg3Ru2	cP20	P4_132	213		(AG, CU, MG, MN, NI, ZN)0.835821(SI)0.164179	
CU5MN4SI	Unknown Structure					(CU)0.5(MN)0.37(SI)0.13	
CU5R	CaCu5 (D2d)	hP6	P6/mmm	191	D2d	(AL, CE, CU, NI)5(CE, LA, NI)1	Cu5La, Cu5Ce, Ni5La, Ni5Ce
CU6LA_HT	Cu6La	mP28	P2_1/c	14		(CU)6(CE, LA)1	
CU6R	CeCu6	oP28	Pnma	62		(CU, NI)6(CE, LA)1	Cu6La_LT, Cu6Ce
CU6SN5_HT	Ni2In (B82)	hP6	P6_3/mmc	194	B82	(AG, CO, CU, MN, NI, VA, ZN)1(AG, AL, BI, CU, GE, NI, PB, SI, SN, ZN)1(CO, CU, MN, NI, SN, VA, ZN)1	CU6SN5(HT), BiNi, Co6Sn5
CU6SN5_LT	Cu6Sn5	mS44	C2/c	15		(CU)1(CU, SN)1(SN)1	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
CU7AS	Hexagonal Close Packed (Mg, A3, hcp)	hP2	P6_3/mmc	194	A3	(CU)7(AS)1	
CU7AS3	Cu7In3	aP40	P-1	2		(CU)7(AS)3	
CU85NI5LA10	(CU85NI5LA10)	CF*	Fm-3m	225		(CU)85(NI)5(LA)10	
CU8ZR3	Cu8Hf3	oP44	Pnma	62		(CU)8(ZR)3	
CUALO2	Rhombohedral Delafossite (CuFeO2)	hR4	R-3m	166		(CU+1)1(AL+3)1(O-2)2	
CUB_A13	beta-Mn (A13)	cP20	P4_132	213	A13	(AG, AL, BI, CO, CR, CU, FE, MG, MN, NI, SI, SN, TI, ZN, ZR)1(B, C, O, VA)1	
CUMG2	Mg2Cu (Cb)	oF48	Fddd	70	Cb	(CU, NI)1(MG)2	
CUMNZN	Unknown Structure					(CU)0.334(MN)0.333 (ZN)0.333	
CUNITI_T1	MoSi2 (C11b)	tI6	I4/mmm	139	C11b	(CU, NI)0.6667(TI)0.3333	
CUNITI_T2	Cu3Ti2	tP10	P4/nmm	129		(CU)0.035(NI)0.565(TI)0.4	
CUNITI_T4	BaPb3	hR12	R-3m	166		(CU, TI)0.075(CU, NI)0.675 (TI)0.25	
CUNITI_T6	Al3Ti (D022)	tI8	I4/mmm	139	D022	(CU, TI)0.25(CU, NI)0.5 (TI)0.25	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
CUO	Tenorite (CuO, B26)	mS8	C2/c	15	B26	(CU+2)1(O-2)1	
CUP2	CuP2	mP12	P2_1/c	14		(CU)1(P)2	
CUPRITE_C3	Cuprite (Cu2O, C3)	cP6	Pn-3m	224	C3	(CU+1)2(O-2)1	Cu2O
CUR	FeB (B27)	oP8	Pnma	62	B27	(CU, NI)1(CE, LA)1	CuLa, CuCe,
CUSE_HT	Covellite (CuS, B18)	hP12	P6_3/mmc	194	B18	(CU)1(SE)1	
CUSE_LT	Cu0.87Se	hP26	P6_3/mmc	194		(CU)1(SE)1	
CUSE_RT	CuS	oS24	Cmcm	63		(CU)1(SE)1	
CUSE2	Marcasite (FeS2, C18)	oP6	Pnnm	58	C18	(CU)1(SE)2	
CUSI_ETA	Cu3Si-h2	hR*	P-31m	162		(AG, CU, MN, NI, ZN)0.76 (SI)0.24	
CUSN_GAMMA	BiF3 (D03)	cF16	Fm-3m	225	D03	(CU, MN, NI, SN, ZN)1	Cu3Sn(ht), Ni3Sn (ht)
CUTI_B11	gamma-CuTi (B11)	tP4	P4/nmm	129	B11	(CU, NB, NI, TI)1(CU, NB, NI, TI)1	
CUTI3	CuTi3 (L60)	tP4	P4/mmm	123	L60	(CU, NB, TI)1(NB, TI)3	
CUZR2_C11B	MoSi2 (C11b)	tI6	I4/mmm	139	C11b	(AL, CR, CU, NI, SI, ZN)1(AL, CR, NB, TI, ZR)2	AlCr2, CuTi2, CuZr2

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
DHCP	alpha-La (A3')	hP4	P6_3/mmc	194	A3'	(CE, CU, LA, NI, ZR)1	
DIAMOND_A4	Diamond (A4)	cF8	Fd-3m	227	A4	(AG, AL, B, C, GE, P, SI, SN, TI, ZN)1	Pure C, Ge, Si or solution phases based on them
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	cF4	Fm-3m	225	A1	(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	Metallic FCC_A1 solution, e.g. (Cu), (Al), (Ni)
FCC_L10	CuAu (L10)	tP2	P4/mmm	123	L10	(AL, CU, MN, NI, TI)0.5(AL, CU, MN, NI, TI)0.5	
FCC_L12	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m	221	L12	(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	
FE2SI	AlNi2	hP6	P-3m1	164		(FE, NI)2(AL, SI)1	
FE3SN2	Fe3Sn2	hR10	R-3m	166		(FE)3(SN)2	
FE5SN3_D82	Ni2In (B82)	hP6	P6_3/mmc	194	B82	(FE)5(SN)3	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
FEB_B27	FeB (B27)	oP8	Pnma	62	B27	(FE, MN, TI, ZR)1(B, GE, SI, ZN)1	ZrGe, ZrSi
FEM_B35	CoSn (B35)	hP6	P6/mmm	191	B35	(FE)1(SN)1	FeSn
FEP2	Marcasite (FeS2, C18)	oP6	Pnnm	58	C18	(FE)0.333(P)0.667	
FEP4	FeP4	mP30	P2_1/c	14		(FE)0.2(P)0.8	
FESI_B20	FeSi (B20)	cP8	P2_13	198	B20	(CR, FE, MN, NI)1(AL, GE, SI)1	FeSi, MnSi, CrSi
FESI2_H	FeSi2-h	tP3	P4/mmm	123		(FE, NI)3(AL, SI)7	
FESI2_L	FeSi2-l	oS48	Cmce	64		(FE, NI)1(AL, SI)2	
FEZN_DELTA	FeZn10	hP632	P6_3/mmc	194		(FE)0.058(AL, CU, FE, MN, NI, SI, ZN)0.18(ZN)0.525 (ZN)0.237	
FEZN_GAMMA1	Fe11Zn40	cF408	F-43m	216		(FE)0.137(AL, CU, FE, NI, SI, ZN)0.118(MN, ZN)0.745	
FEZN_ZETA	CoZn13	mS28	C2/m	12		(FE, MN, NI, VA)0.072(AL, ZN)0.856(AL, CU, SI, VA, ZN)0.072	
FEZR3	Re3B	oS16	Cmcm	63		(FE)1(ZR)3	
FLUORITE	Fluorite (CaF2, C1)	cF12	Fm-3m	225	C1	(ZR, ZR+4)2(O-2, VA)4	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
GAMMA_D810	Cr5Al8 (D810)	hR26	R3m	160	D810	(AL, SI)12(CR)5(AL, CR, SI)9	A binary phase in Al- Cr system
GAMMA_D82	gamma-brass (Cu5Zn8, D82)	cI52	I-43m	217	D82	(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)	cP52	P-43m	215	D83	(AL, FE, NI, SI, SN, ZN)4(AL, CU, NI, SI, ZN)1(CU, FE, MN, NI, SN, ZN)8	solution between Al8Cu5 (rt) and Cu5Zn8
GAMMA_H	gamma-brass (Cu5Zn8, D82)	cI52	I-43m	217	D82	(AL, ZN)4(AL, CU, ZN)1(CU, FE, MN, NI)8	
GAS	Gas					(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,	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
						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, 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,	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
						I, TI2, ZN, ZR, ZR2)1	
GE2NI5_HT	Pd5Sb2	hP42	P6_3cm	185		(NI)0.72(GE)0.28	
GE3NI5_C2	Ge3Ni5	mS32	C2	5		(NI)0.625(GE)0.375	
GENI	Westerveldite (FeAs, B14)	oP8	Pnma	62	B14	(GE)0.5(NI)0.5	
GENI2	Co2Si (C37)	oP12	Pnma	62	C37	(NI)0.665(GE)0.335	
GENI3_HT	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m	221	L12	(NI)0.744(GE)0.256	
GRAPHITE	Hexagonal Graphite (A9)	hP4	P6_3/mmc	194	A9	(B, C)1	
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	hP2	P6_3/mmc	194	A3	(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	Metallic HCP_A3 solution, alpha_ Mg/Hf/Sc/Ti/Zr
HCP_ZN	Hexagonal Close Packed (Mg, A3, hcp)	hP2	P6_3/mmc	194	A3	(AG, AL, AU, BI, CO, CR, CU, FE, GE, MN, NI, PB, PT, SI, SN, ZN)1(VA)0.5	
HEXAGONAL_A8	gamma-Se (A8)	hP3	P3_121	152	A8	(SE)1	
L12_FCC	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m	221	L12	(AL, NI, SI, TI)1(AL, FE, NI, ZN, ZR)3	AlZr3
LA2NI3	La2Ni3	oS20	Cmce	64		(LA)2(CU, NI)3	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
LA2NI7	Ce2Ni7	hP36	P6_3/mmc	194		(LA)2(CU, NI)7	
LA3NI	Cementite (Fe3C, D011)	oP16	Pnma	62	D011	(LA)3(NI)1	
LA5NI19	Co19Sm5	hP48	P6_3/mmc	194		(LA)5(NI)19	
LA7NI16	La7Ni16	tI46	I-42m	121		(LA)7(CU, NI)16	
LANI3	Ni3Pu	hR12	R-3m	166		(LA)1(CU, NI)3	
LCR5GE3	Unknown Structure					(CR, GE)0.625(CR, GE)0.375	
LIQUID	Liquid					(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	
M2P	Revised Fe2P (C22)	hP9	P-62m	189	C22(II)	(CR, CU, FE, NI)0.667 (P)0.333	Ni2P, Fe2P, Cr2P
M3P	Ni3P (D0e)	tI32	I-4	82	D0e	(CR, CU, FE, NI)0.75(P)0.25	Ni3P, Fe3P, Cr3P
MG2NI	Mg2Ni (Ca)	hP18	P6_222	180	Ca	(MG, ZN)2(CU, NI, ZN)1	
MG2SI_C1	Fluorite (CaF2, C1)	cF12	Fm-3m	225	C1	(MG)2(SI, SN)1	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
MN11SI19	Mn11Si19	tP120	P-4n2	118		(MN)11(AL, SI)19	
MN2SN	Ni2In (B82)	hP6	P6_3/mmc	194	B82	(MN)0.643(SN)0.357	
MN3SI	BiF3 (D03)	cF16	Fm-3m	225	D03	(FE, MN, NI)3(AL, SI)1	
MN3SN2	Tongbaite (Cr3C2, D510)	oP20	Pnma	62	D510	(MN)3(SN)2	
MN5SI3_D88	Mavlyanovite (Mn5Si3, D88)	hP16	P6_3/mcm	193	D88	(CR, CU, FE, MN, NI, TI, ZR)5(AL, CR, GE, SI, SN)3	Mn5Si3, Cr3Si5, Fe5Si3, Ge3Zr5, Si3Zr5,
MN6SI	Fe7W6 (D85) mu-phase	hR13	R-3m	166	D85	(AL, MN)17(SI, ZN)3	
MN9SI2	Mn9Si2	oI186	Immm	71		(MN)33(SI)7	
MNNI2	Unknown Structure					(MN, NI)1(NI)2	
MNZN9	Unknown Structure	h**				(MN)0.1(ZN)0.9	
MONI_DELTA	MoNi	oP56	P2_12_12_1	19		(NI)24(MO, NI)20(CU, MO)12	
MONI4_BETA	Ni4Mo (D1a)	tI10	I4/m	87	D1a	(MO)1(NI)4	
MP	Westerveldite (FeAs, B14)	oP8	Pnma	62	B14	(CR, FE)0.5(P)0.5	FeP, CrP
MU_PHASE	Fe7W6 (D85) mu-phase	hR13	R-3m	166	D85	(CO, CU, FE, NB)7(CU, MO, NB)2(CO, FE, MO, NB)4	Binary phase (Mu) in Fe-Mo and Co-Nb systems

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
NB7NI6	Fe7W6 (D85) mu-phase	hR13	R-3m	166	D85	(NB, NI)1(NB)4(NB, NI)2 (CU, NB, NI)6	
NBNI3	beta-TiCu3 (D0a)	oP8	Pmmn	59	D0a	(CU, NB, NI)1(CU, NB, NI)3	
NBNI8	Pt8Ti	tI18	I4/mmm	139		(NB)1(NI)8	
NI10ZR7	Ni10Zr7	oS68	Cmce	64		(NI)23(ZR)17	
NI11ZR9	Pt11Zr9	tI40	I4/m	87		(NI)11(ZR)9	
NI12P5_HT	Unknown Structure					(NI)0.706(P)0.294	
NI12P5_LT	Ni12P5	tI34	I4/m	87		(NI)0.706(P)0.294	
NI19SI6	Bogdanovite (Cu3Au, L12)	cP4	Pm-3m	221	L12	(SI)0.24(CU, NI)0.76	
NI21ZR8	Hf8Ni21	aP29	P-1	2		(ZR)8(NI)21	
NI2SI_HT	Ni2In (B82)	hP6	P6_3/mmc	194	B82	(CU, NI)1(NI, VA)1(AL, SI)1	
NI3MO_D0A	beta-TiCu3 (D0a)	oP8	Pmmn	59	D0a	(NI)3(MO, NI)1	
NI3R7	Fe3Th7 (D102)	hP20	P6_3mc	186	D102	(CE, LA)7(NI)3	Ni3La7, Ni3Ce7
NI3SI_HT	Cementite (Fe3C, D011)	oP16	Pnma	62	D011	(FE, NI)3(AL, SI)1	
NI3SI_MT	Ge9Pd25	hP34	P-3	147		(SI)1(NI)3	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
NI3SI2	Ni3Si2	oP80	Cmc2_1	36		(FE, NI)3(SI)2	
NI3SN_D019	Ni3Sn (D019)	hP8	P6_3/mmc	194	D019	(AL, CU, NI, SN, VA, ZN)1 (CU, FE, MN, NI, SN, ZN)3	
NI3SN4	delta-Ni3Sn4 (D7a)	mS14	C2/m	12	D7a	(CU, NI, ZN)0.25(NI, SN, ZN)0.25(SN, ZN)0.5	
NI3TI	Ni3Ti (D024)	hP16	P6_3/mmc	194	D024	(CU, NI, TI)0.75(CU, NI, TI)0.25	
NI5P2_HT	Unknown Structure					(NI)0.714(P)0.286	
NI5P2_LT	Pd8Sb3	hR44	R3c	161		(CU, NI)0.714(P)0.286	
NI5P4	Ni5P4	hP36	P6_3/mmc	194		(NI)0.556(P)0.444	
NI5SI2	Ni31S12	hP42	P321	150		(CU, FE, NI)5(AL, SI)2	
NI7ZR2	Ni7Zr2	mS36	C2/m	12		(NI)7(ZR)2	
NIBE7	Unknown Structure	cI*				(BE, NI)2(NI)2(BE)9	
NIP2	PdP2	mS12	C2/c	15		(NI)0.3333(P)0.6667	
NIR	CrB (B33)	oS8	Cmcm	63	B33	(CE, LA)1(CU, NI)1	NiLa, NiCe
NISI_B31	MnP (B31)	oP8	Pnma	62	B31	(FE, NI)1(SI, ZN)1	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
NISI2	Fluorite (CaF2, C1)	cF12	Fm-3m	225	C1	(AL, CU, SI, ZN)2(CU, FE, MN, NI)1	
NISNZN_T1	Unknown Structure					(NI, SN, VA)0.36(NI, SN)0.38(VA, ZN)0.26	
NISNZN_T2	Unknown Structure					(NI, VA)0.55(SN)0.26(SN, VA, ZN)0.19	
NISNZN_T3	Unknown Structure					(NI, VA)0.482(SN)0.204(SN, VA, ZN)0.314	
NISNZN_T4	Unknown Structure					(NI, SN, VA)0.505(SN, ZN)0.39(SN, VA, ZN)0.105	
NITI2	NiTi2	cF96	Fd-3m	227		(CU, NI)0.3333(TI)0.6667	
NIZN_LT	delta-CuTi (L2a)	tP2	P4/mmm	123	L2a	(AL, FE, MN, NI, SI, SN, ZN)0.5(AL, FE, MN, NI, SI, SN, ZN)0.5	
NIZN8	Ni3Zn22	mS50	C2/m	12		(NI)0.111111(AL, ZN)0.888889	
P2ZN	ZnAs2	mP24	P2_1/c	14		(P)2(ZN)1	
P2ZN3	Zn3P2 (D59)	tP40	P4_2/nmc	137	D59	(P)2(ZN)3	
PSI	(SiP)	oS48	Cmc2_1	36		(P)1(SI)1	
R_PHASE	R-(Co, Cr, Mo)	hR53	R-3	166		(FE)27(MO)14(FE, MO)12	A binary phase in

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
							Fe-Mo system
RED_P	Unknown Structure					(P)1	
RHOMBO_A7	alpha-As (A7)	hR2	R-3m	166	A7	(AG, AS, BI, P, PB, SN, ZN)1	
SI2TI_C54	TiSi2 (C54)	oF24	Fddd	70	C54	(SI, SN)2(TI, ZR)1	Sn2Zr
SI2ZR_C49	ZrSi2 (C49)	oS12	Cmcm	63	C49	(GE, SI)2(ZR)1	Si2Zr, Ge2Zr
SI2ZR3_D5A	Si2U3 (D5a)	tP10	P4/mbm	127	D5a	(SI)2(ZR)3	
SI4ZR5_TP36	Cr5B3 (D8l)	tI32	I4/mcm	140	D8l	(GE, SI)4(TI, ZR)5	Si4Zr5, Si4Ti5, Ge4Zr5
SIGMA	sigma-CrFe (D8b)	tP30	P4_2/mnm	136	D8b	(CO, FE, MN, NI)8(CR, MO)4(CO, CR, FE, MN, MO, NI)18	A binary phase in Co-Cr and Fe-Mo systems
SIZR3_TP32	Ti3P	tP32	P4_2/n	86		(GE, SI)1(TI, ZR)3	SiZr3, SiTi3, GeZr3
SN3ZR5	Mavlyanovite (Mn5Si3, D88)	hP16	P6_3/mcm	193	D88	(ZR)5(SN)3(SN, VA)1	
SN4P3	Sn3.6As3	hR21	R-3m	166		(SN)4(P)3	
SNZR3_A15	Cr3Si (A15)	cP8	Pm-3n	223	A15	(SN, ZR)3(SN, ZR)1	
SPINEL	Spinel (Al2MgO4, H11)	cF56	Fd-3m	227	H11	(AL+3, CR+2, CR+3, CU+2)1 (AL+3, CR+3, CU+2, VA)2	

Name	Prototype	Pearson Symbol	Space Group Symbol	SG#	Strukturbericht	Formula Unit	Notes
						(CR+2, VA)2(O-2)4	
TI5GE3	Mavlyanovite (Mn5Si3, D88)	hP16	P6_3/mcm	193	D88	(GE)3(TI)5	
TI6GE5	Si5V6	oI44	Ibam	72		(GE)5(TI)6	
TIGE2	TiSi2 (C54)	oF24	Fddd	70	C54	(GE)2(TI)1	
WHITE_P	Unknown Structure					(P)1	
ZRB12	UB12 (D2f)	cF52	Fm-3m	225	D2f	(B)12(ZR)1	
ZRM5_C15B	AuBe5 (C15b)	cF24	F-43m	216	C15b	(CU, NI)5(LA, ZR)1	Cu5Zr, Ni5Zr
ZRO2_MONO	Baddeleyite (ZrO2, C43)	mP12	P2_1/c	14	C43	(ZR+4)2(O-2, VA)4	
ZRO2_TETR	HgI2 (C13)	tP6	P4_2/nmc	137	C13	(ZR+4)2(O-2, VA)4	

TCCU5 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:	**5.0**
First release:	**TCCU1 was released in with 2016b (November)**

Changes in the Most Recent Database Release

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.

Previous Releases

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.