TCS Cu-based Alloys Database (TCCU4)

Technical Information

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About the TCS Cu-based Alloys Database (TCCU)

TCCU: TCS Cu-based Alloys Database Revision History

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. The current version of the database is TCCU4.

TCCU4 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 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 TCCU4:

- 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.

TCCU4 Elements, Systems, Phases and Properties

Included Elements

There are 30 elements included in the most recent version of the database.

Ag	Al	Au	As	B	Be	Bi	C	Ca	Cd
Co	Cr	Cu	Fe	Ge	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:

- 135 assessed binary systems, mostly to their full range of compositions, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 53 assessed ternary systems. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 268 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 TCCU4 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 thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

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

Property	Model Parameters	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

TCCU4 Systems

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TCCU4 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	Co	Cr	Fe	Ge	Mg	Mn	Mo	Nb	Ni	O	P	Pb	Pt	Se	Si	Sn	Ti	Zn	Zr	
2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	Cu
--	2	2			2	2				2		2	2		2			2		2	2			2	2		2		Ag
	--			2	2	2	2	2	2	2	2	2	2	2	2			2	2	2	2			2	2	2	2	2	Al
		--											2																Au
			--																										As
				--																								2	B
					--													2						2				Be
						--									2			2			2			2	2		2		Bi
							--																				2	C
								--																				Ca
									--																			Cd
										--	2	2	2		2		2	2			2			2	2		2		Co
											--	2	2			2	2	2		2				2	2			2	Cr
												--			2	2		2		2	2			2	2		2	2	Fe
													--					2							2	2		2	Ge
														--				2						2				2	Mg
															--			2			2			2	2		2	2	Mn
																--		2											Mo
																	--												Nb
																		--		2	2			2	2		2	2	Ni
																			--										O
																				--				2	2		2		P
																					--			2	2		2		Pb
																						--							Pt
																							--						Se
																								--	2		2	2	Si
																									--		2	2	Sn
																										--		2	Ti
																											--		Zn
																												--	Zr

TCCU4 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.

and

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

TCCU4 Phases

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Common Phases for Copper Alloys

TCCU4 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
DIAMOND_A4	Si and Ge

Name in the Database	Common Name and Description
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

TCCU4 Models for the Included Phases

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
LIQUID						(AG CU FE GE MN MO NI SI ZN SN CO P PB BE AU AL AS B BI C CA CD CR CR3GE1 MG NB PT SE TI ZR CU2SE CU2O CUO AL2/3O1 AL4/3O2 NI12P5)1	
FCC_A1	Cu	cF4	Fm-3m	A1	225	(AG AL AU AS BE BI CA CD CO CR CU FE GE 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_L12						(AL CU FE GE MG MN MO NI SI ZN CR SN TI ZR AG CA CO PB BE BI CD P AU AS NB PT SE)0.75(AL CU FE GE MG MN MO NI SI ZN CR SN TI ZR AG CA CO PB BE BI CD P AU AS NB PT SE)0.25(B C O VA)1	
BCC_A2	W	cI2	I m -3 m	BCC_A2	229	(AG AL AU AS BE BI CA CD CO CR CU FE GE MG MN MO NB NI P PB PT SE SI SN TI ZN ZR VA)1(B C O VA)3	Metallic BCC_A2 solution
BCC_B2						(AG AL AU AS BE BI CA CD CO CR CU FE GE MG MN MO NB NI P PB PT SE SI SN TI ZN ZR VA)0.5(AG AL AU AS BE BI CA CD CO CR CU FE GE MG MN MO NB NI P PB PT SE SI SN TI ZN ZR VA)0.5(B C O VA)3	
CBCC_A12	Mn	cI58	I -4 3 m	A12	217	(AL BI CO CU FE MN NI SI ZN MG CR TI ZR SN)1(B C O VA)1	
CUB_A13	Mn	cP20	P 4_1 3 2	A13	213	(AL BI CU CO FE MN NI SI ZN MG CR TI ZR SN AG)1(B C O VA)1	
HCP_A3	Mg	hP2	P 6_3/m m c	A3	194	(AG AL AU AS BE BI CA CD CO CR CU FE GE 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						(AG AU BI AL CO CR CU FE GE NI MN PB SI ZN SN PT)1 (VA)0.5	
RHOMBO_A7	As	hR6	R -3 m	A7	166	(AS AG BI P PB SN ZN)	
HEXAGONAL_A8	Se	hP3	P3121	A8	152	(SE)1	
WHITE_P	P	aP24	P -1		2	(P)1	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
RED_P	P	mP84	mP84		13	(P)1	
BETA_RHOMBO_B	B	hR423	R -3 m		166	(B)93(CU SI B C)12	
DIAMOND_A4	C	cF8	F d -3 m	A4	227	(AG B C P AL GE SI ZN SN TI)	Pure C, Ge, Si or solution phases based on them
BCT_A5	C	cF8	F d -3 m	A4	227	(AG AL B BI CD CU NI PB ZN SN SI TI)	Pure Sn or its solution
B2_BCC						(AL CO FE CU ZN BE NI)1(BE CO MN TI VA ZR)	
C14_LAVES	MgZn2	hP12	P6_3/m m c	C14	194	(AL CO CU CR FE MG MN MO NB NI TI ZN ZR)2(AL CO CU CR FE MG MN MO NB TI ZN ZR)1	
C15_LAVES	Cu2Mg	cF24	F d -3 m	C15	227	(AL CA CO CU FE MG MN NB NI SI ZN CR TI ZR)2(AL CA CO CU FE MG MN NB NI SI ZN CR TI ZR)1	Solution of Cu2Mg-type phases
C36_LAVES	MgNi2	hP24	P 6_3/m m c	C36	194	(AL CO CU CR FE MG MN NB NI ZN ZR)2(AL CO CU CR FE MG MN NB NI ZN ZR)1	Solution of MgNi2-type phases
GAMMA_D83	*	cP52	*	D83		(AL FE NI SI SN ZN)4(AL CU NI SI ZN)1(CU MN FE NI ZN SN)8	solution between Al8Cu5 (rt) and Cu5Zn8
CO2SI_C23	Co2Si-b	oP12	P n m a		62	(AL CO CA CU FE NI SI)2(AL CO SI SN ZN)1	Co2Si, Ni2Si
GAS						(AG AG2 AL AL2 AL1O1 AL1O2 AL2O1 AL2O2 AL2O3 AS AS2 AS3 AS4 AU AU2 B B2 BE BE2 BI BI2 BI3 BI4 CD CO CO2 CU CU2 FE FE2 MN MO MO2 NB NI NI2 O O2 O3 P P2 P3 P4 PB PB2 PT SE SE2 SE3 SE4 SE5 SE6 SE7 SE8 SI SI2 SI3 SN SN2 ZN ZR ZR2)	
AG3BE8						(AG)2.97(BE)8.03	
AG3SN_L60	Cu3Ti	oP8	Pmmn		47	(CU AG CO 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
AGZN3	Mg	hP24	P6-3/mmc		194	(AG ZN)1	
AGZN	W	cI2	Im-3m		229	(ZN)1(AG ZN)2	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AG5ZN8	Cu5Zn8	cI52	I-43m	D82	217	(AG ZN)2(AG)2(AG ZN)3 (AG ZN)6	
ALB2_C32	AlB2	hP3	P6/mmm	C32	191	(MG AL MN CR ZR TI)1(B)2	
ALB12		tP208	P4-12-12		92	(AL)1(B)12	
AL4C3	Al4C3	hR21	R-3m		166	(AL SI)4(C)3	
AL4M_D13	Al4Ba	tI10	I4/mmm	D13	139	(AL)4(CA)1	Al4Ca
AL14CA13	Al14Ca13	mS54	C2/m		12	(AL MG ZN)14(CA)13	
AL3CA8	Ca8In3	aP22	P-1		2	(AL)3(CA MG)8	
AL45CR7	Al45V7	mC104		C 2/m	12	(AL)45(CR)7	
CUZR2_C11B	MoSi2/ CuZr2	tI6	I4/mmm	C11b	139	(AL CR CU SI ZN)1(AL CR TI ZR)2	AlCr2, CuTi2, CuZr2
AL5CR	Al11Cr2	mS*	C2/c	orth	15	(AL SI)5(CR)1	
AL4CR	Al4Mn	hP574	P6_3/mmc		194	(CR)1(AL SI VA)4	
ALCR_GAMMA1						(AL CR SI)2(CR)2(AL CR)3(AL SI)6	
GAMMA_D810	Cr4.5(Cr0.56Al0.44)9Al12	hR26/hR78	R3m	D810	160	(AL SI)12(CR)5(AL CR SI)9	A binary phase in Al-Cr system
AL13CO4	Al19Co6	mS100	C2/m		12	(AL)13(CO)4	
AL3CO				cub		(AL)3(CO)1	
AL5CO2	Al5Co2	hP28	P6-3/mmc		194	(AL)5(CO)2	
AL9CO2	Al9Co2	mP22	P2-1/c		14	(AL)9(CO)2	
ALCU_DEL						(AL ZN)2(CU FE)3	
ALCU_EPS	Co1.75Ge	hP6	P6-3/mmc		194	(AL CU ZN NI)1(CU FE)1	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
ALCU_ETA	CuAl	mS20	C2/m		12	(AL CU)1(CU FE ZN NI)1	
ALCU_ZETA						(AL)9(CU FE)11	
GAMMA_H	Cu5Zn8			D82		(AL ZN)4(AL CU ZN)1(CU MN FE NI)8	Cu5Zn8-type Al8Cu5 (ht) phase
AL2CU_C16	Al2Cu	tI12	I4/mcm	C16	140	(AL FE SN ZR MN NI)2(AL CU FE NI B MN SI CO)1	Al2Cu, CoSn2, FeSn2, Mnsn2
AL2FE1	FeAl2	aP18	P1		1	(AL CU SI ZN)2(FE MN NI)1	
AL5FE2	FeAl2.8	oS24	Cmcm		63	(AL CU SI ZN)5(FE MN NI)2	
AL5FE4						(AL CU FE MN)1	
AL13FE4	Al13Fe4	mS102	C2/m		12	(AL CU)0.63(FE MN NI ZN)0.23(AL SI VA ZN)0.14	
ALMG_BETA	Mg28Al45	cF1832	Fd-3m		227	(MG)89(AL ZN)140	
ALMG_EPS	Mg23Al30	hR159	R-3		148	(MG)23(AL ZN)30	
ALMG_GAMMA	Mg24Y5 / Al12Mg17	cI58	I-43m		217	(MG)5(AL MG ZN)12(AL MG ZN)12	
AL12MN	Al12W	cI26	Im-3m		229	(AL)12(MN)1	
AL6MN	Al6Mn	oS28	Cmcm		63	(AL ZN)6(MN FE)1	
AL4MN_R	Al230.8Mn53.3	hP586	P63/m		176	(AL)461(MN FE)107	
AL4MN_U	Mn55Al226.58	hP574	P6-3/mmc		194	(AL ZN)4(MN)1	
AL11MN4_LT	Mn4Al11	aP15	P-1		2	(AL ZN)11(MN FE)4	
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25	oP156	Pnma		62	(AL MN)29(MN)10	
AL8MN5	Cr4.5(Cr0.56Al0.44)9Al12	hR26 / hR78	R3m	D810	160	(AL ZN)12(MN)5(AL MN SI CU)9	
AL3NI_D011	CFe3	oP16	I4/mmm	D022	139	(AL MN NI)0.75(FE NI)0.25	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL3NI2	Ni2Al3	hP5	P-3m1		164	(AL SI ZN)3(AL CU FE NI)2(NI VA)1	
AL3NI5	Pt5Ga3	oS16	Cmmm		65	(AL)0.38(NI)0.62	
CORUNDUM						(AL+3 VA)2(VA)1(O-2)3	Al2O3
ALP		cF8	Fm-3m		225	(AL)1(P)1	
AL2TI	Gd2Hf	tI24	I4-1/amd		141	(AL)2(TI)1	
AL18TI7	Al5Ti2	tP28	P 4/mmm		123	(AL)0.72(TI)0.28	
AL3TI_D022	Al3Ti	tI8	I 4/mmm	D022	139	(AL MN NI)3(MN TI ZR)1	
ALTI3_DO19	CdMg3	hP8	P6-3/mmc		194	(AL TI)3(AL TI)1	
AL2ZR	MgZn2	hP12	P6-3/mmc	C14	194	(AL)2(ZR)1	
L12_FCC	AuCu3	cP4	Pm-3m			(AL NI SI TI)1(AL FE ZR NI ZN)3	AlZr3
AL3ZR5_D8M	W5Si3	tI32	I4/mcm	D8m	140	(AL SI)3(ZR CR)5	
CRB_B33	CrB / TlI	oC8 / oS8	Cmcm	B33 / Bf	63	(AL CA CR NI)1(AG B SI SN ZR)1	AlZr, NiZr
ALZR2_B82	Ni2In / C01.75Ge	hP6	P6-3/m	B82	194	(AL MN SN VA)1(ZR MN TI VA)2	
AL4ZR5	Ga4Ti5	hP18	P6-3/mcm		193	(AL)4(ZR)5	
AL3ZR2_OF40	Al3Zr2	oF40	Fdd2		43	(AL)3(ZR)2	
AL2ZR3_TP20	Al2Zr3	tP20	P4-2/mnm		136	(AL ZN)2(ZR)3	
AL3ZR_D023	Al3Zr	tI16	I4/m m m		139	(AL)3(TI ZR)1	
ZRB12	UB12	cF52	Fm-3m	D2F	225	(B)12(ZR)1	
BIMN_LT	NiAs	hP4	P63/mmc		194	(BI)0.5(MN)0.5	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
BIMN_HT						(BI)0.48(MN)0.52	
BI3NI	RhBi3		Pnma		62	(BI)3(NI)1	
CU6SN5_HT	Co1.75Ge	hP6	P6-3/mmc		194	(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
CA2CU	Ca2Cu	oP12	Pnma		62	(CA)2(CU)1	
CACU	CaCu (h)	oP40	Pnma		62	(CA)1(CU)1	
CACU5_D2D	CaCu5	hP6	P6/mmm	D2d	191	(CA)1(CU NI ZN)5	
CDCU2	MgZn2	hP12	P6-3/mmc	C14	194	(CD)1(CU)2	
CD3CU4	Cd121Cu160	cF1124	F-43m		216	(CD)0.43(CU)0.57	
CD8CU5	Cu5Zn8	cI52	I-43m	D82	217	(CU)2(CD CU)3(CU)2(CU CD)6	
CD10CU3	Al5Co2	hP28	P6-3/mmc		194	(CD)0.77(CU)0.23	
SIGMA	Cr0.49Fe0.51	tP30	P4-2/mnm	D8b	136	(FE MN NI CO)8(CR MO)4(CO FE CR MN MO NI)18	A binary phase in Co-Cr and Fe-Mo systems
CO3GE	C	cP8	Pm-3n		223	(CO)0.75(GE)0.25	
CO5GE2						(CO)0.71(GE)0.29	
CO5GE3	Ni2In	hP6	P63/mmc		194	(CO VA)0.12(CO)0.50(CO GE SN)0.38	
CO5GE3_ALPHA		oP	Pbnm		62	(CO)0.62(GE)0.38	
CO5GE7	Co5Ge7	tI24	I4mm		107	(CO)0.42(GE)0.58	
COGE	CoGe	mC16	C2/m		12	(CO GE)0.5(CO GE)0.5	
COGE2	PdSn2	oC24	Aba2		41	(CO)0.33(GE)0.67	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CO2SI_HT	Co2Si-b	oP12	Pnma		62	(CO SI)0.67(CO SI)0.33	
COSI_B20	FeSi	cP8	P213	B20	198	(AL CO SI)0.5(CO SI)0.5	
CO3SI_HT						(CO CU NI SI SN)0.25(CO CU NI SN)0.25(CO CU NI)0.5	
AL2AU_C1_CAF2	CaF2	cF12	Fm-3m	C1	225	(AG AL AU CU SI SN)0.67(AL AU CO NI PT)0.33	CoSi2
COSN3_OS32			I41/acd		142	(CO)0.25(SN)0.75	
COSN_HP6	CoSn	hP6	P6/mmm	B35	191	(CO)0.5(SN)0.5	
COZN_LT		cP20	P4132		213	(CO ZN)1(VA)1	
COZN_HT						(CO ZN)1(VA)1	
COZN_GAMMA	Cu9Al4	cP52	P-43m	D83	215	(CO ZN)1(VA)1	
COZN_DELTA						(CO)0.125(ZN)0.875	
COZN_GAMMA1						(CO)0.1176 (ZN)0.8824	
COZN_GAMMA2	CoZn13	mC28	C2/m		12	(CO)0.0714(ZN)0.9286	
CU3GE_ETA	Cu3Ti	oP8	Pmmn		59	(AG CU)0.75(GE)0.25	
CU3GE_EPSILON						(AG CU)0.77(GE)0.23	
CU3GE_THETA						(AG CU)0.73(GE)0.27	
CR5GE3	W5Si3	hP16	I4/mcm	D8m	140	(CR GE)0.625(CR GE)0.375	
LCR5GE3						(CR GE)0.625(CR GE)0.375	
CR11GE8	Ge18Mn11	oP76	Pnma		62	(CR)0.579(GE)0.421	
CR11GE19	Mn11Si19	tP120	P-4n2		118	(CR)0.633(GE)0.367	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CR3GE	Cr3Si	cP8	Pm-3n	A15	223	(CR)0.75(GE)0.25	
CUMG2	CuMg2	oF48	Fddd		70	(CU NI)(MG)2	
CU33SI7_DELTA		tP*				(CU ZN)0.825(SI)0.175	
CU56SI11_GAMMA	Mg3Ru2	cP20	P4-132		213	(CU MG MN NI ZN) 0.835821(SI)0.164179	
CUSI_ETA		tP*				(CU MN NI ZN)0.76(SI)0.24	
CU15SI4_EPSILON	Cu15Si4	cI76	I-43d		220	(CU, MN, MG, ZN) 0.789474 (AL, SI) 0.210526	
CUSN_GAMMA	BiF3	cF16	Fm-3m	L21	225	(CU MN NI SN ZN)	Cu3Sn(ht), Ni3Sn(ht)
CU10SN3	Cu10Sn3	hP26	P6-3		173	(CU NI)0.769(SN)0.231	
CU3SN	Cu3Sn	oS80	Cmcm		63	(CU SN NI)3(CU SN)1	
CU41SN11	Cu41Sn11	cF416	F-43m		216	(CU SN ZN)41(CU SN ZN)11	
CU6SN5_LT	Cu6Sn5	mS44	C2/c		15	(CU)1(CU SN)1(SN)1	
CU2TI		oS12	Cmcm		63	(CU)2(TI)1	
CU3TI2	Cu3Ti2	tP10	P4/nmm		129	(CU)3(TI)2	
CU4TI1		oP20	Pnma		62	(CU)4(TI)1	
CU4TI3		tI14	I4/mmm		139	(CU)4(TI)3	
CUTI_B11	CuTi	tP4	P4/nmm		129	(CU TI)1(CU TI)1	
CUTI3	CuTi3	tP4	P4/mmm		123	(CU)1(TI)3	
CU10ZR7	Zr7Ni10	oS68	Cmca		64	(CU)10(ZR)7	
ZRM5_C15B	Be5Au	cF24	F-43m		216	(CU NI)5(ZR)1	Cu5Zr, Ni5Zr

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CU51ZR14		hP65	P6/m		175	(CU)51(ZR)14	
CU8ZR3	Cu8Hf3	oP44	Pnma		62	(CU)8(ZR)3	
R_PHASE						(FE)27(MO)14(FE MO)12	A binary phase in Fe-Mo system
MU_PHASE	W6Fe7	hR39	R-3m		166	(CU CO NB FE)7(CU MO NB)2(CO NB FE MO)4	Binary phase (Mu) in Fe-Mo and Co-Nb systems
M3P	Ni3P	tI32	I-4		82	(CU NI FE CR)0.75(P)0.25	Ni3P, Fe3P, Cr3P
M2P	Fe2P	hP9	P-62m		189	(CU NI FE CR)0.667(P)0.333	Ni2P, Fe2P, Cr2P
MP	FeAs	oP8	Pnma		62	(FE CR)0.5(P)0.5	FeP, CrP
FEP2	FeS2	oP6	Pnnm		58	(FE)0.333(P)0.667	
FEP4	FeP4	mP30	P21/c		14	(FE)0.2(P)0.8	
FE2SI	AlNi2	hP6	P-3m1		164	(FE NI)2(AL SI)1	
FESI2_H	Fe0.92Si2	tP36	P4/mmm		123	(FE NI)3(AL SI)7	
FESI2_L	FeSi2	oS48	Cmca		64	(FE NI)1(AL SI)2	
FESI_B20	FeSi	cP16	P2-13		198	(FE MN NI CR)1(AL GE SI)1	FeSi, MnSi, CrSi
MN5SI3_D88	Mn5Si3	hP16	P6-3/mcm	D88	193	(CU FE MN NI CR ZR TI)5(AL CR SI GE SN)3	Mn5Si3, Cr3Si5, Fe5Si3, Ge3Zr5, Si3Zr5,
FE5SN3_D82	Co1.75Ge	hP6	P6-3/mmc		194	(FE)5(SN)3	
FE3SN2	Fe3Sn2	hR30	R-3m		166	(FE)3(SN)2	
FEM_B35	CoSn	hP6	P6/mmm	B35	191	(FE)1(SN)1	FeSn
FEZN_GAMMA1						(FE)0.137(AL CU FE NI SI ZN)0.118(MN ZN)0.745	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
FEZN_DELTA	FeZn10	hP63	P6-3/m		194	(FE)0.058 (AL CU FE MN NI SI ZN)0.18 (ZN)0.525 (ZN)0.237	
FEZN_ZETA	Zn13Co	mS28	C2/m		12	(FE MN NI VA)0.072(AL ZN)0.856(AL CU SI VA ZN)0.072	
GE3NI5_C2	Ni5Ge3	mS32	C2		5	(NI)0.625(GE)0.375	
GE2NI5_HT	Pd5Sb2	hP42	P63cm		185	(NI)0.72(GE)0.28	
GENI3_HT						(NI)0.744(GE)0.256	
GENI2	Co2Si-b	oP12	Pnma		62	(NI)0.665(GE)0.335	
GENI	FeAs	oP8	Pnma		62	(NI)0. (GE)0. 5	
TI5GE3	Mn5Si3	hP16	P63/mcm		193	(GE)3(TI)5	
TI6GE5	V6Si5	oI44	Ibam		72	(GE)5(TI)6	
TIGE2	TiSi2	oF24	Fddd		70	(GE)2(TI)1	
MNNI2	CuAu	tP20	P4/mmm	L10	123	(MN NI)1(NI)2	
MN11SI19	Mn11Si9	tP20	P-4n2		118	(MN)11(AL SI)19	
MN3SI	AlFe3 or BiF3	cF16	Fm-3m	D03 or L21	225	(FE MN NI)3(AL SI)1	
MN6SI	(Cr0.16Mo0.38Co0.46)	hR159	R-3		148	(AL MN)17(SI ZN)3	
MN9SI2	Mn19(Mn0.62Si0.38)10Si2	oI186	Immm		71	(MN)33(SI)7	
MN3SN2	Ni3Sn	oP20	Pnma		62	(MN)3(SN)2	
NI3SN_D019	Ni3Sn / Mg3Cd	hP8	P6-3/mmc	D019	194	(CU NI AL SN VA ZN)1(CU MN FE NI SN ZN)3	
MN2SN	Co1.75Ge	hP6	P6-3/mmc		194	(MN)0.643(SN)0.357	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
MNZN9						(MN)0.1(ZN)0.9	
MONI_DELTA	Mo3(Mo0.8Ni0.2)5Ni6	oP56	P212121		19	(NI)24(MO NI)20(CU MO)12	
MONI4_BETA	MoNi4	tI10	I4/m		87	(MO)1(NI)4	
NI3MO_D0A	Cu3Ti	oP8	Pmmn		59	(NI)3(MO NI)1	
NI5P2_HT						(NI)0.714(P)0.286	
NI5P2_LT						(NI)0.714(P)0.286	
NI12P5_HT						(NI)0.706(P)0.294	
NI12P5_LT	Ni12P5	tI34	I4/m		87	(NI)0.706(P)0.294	
NI5P4	Ni5P4	hP36	P63mc		186	(NI)0.556(P)0.444	
NIP2	PdP2	mS12	C2/c		15	(NI)0.333(P)0.667	
NI2SI_HT	Co1.75Ge	hP6	P6-3/mmc		194	(CU NI)1(NI VA)1(AL SI)1	
NI3SI2	Ni3Si2	oS80	Cmc2-1		36	(FE NI)3(SI)2	
NI3SI_HT	Fe3C	oP16	Pnma		62	(FE NI)3(AL SI)1	
NI3SI_MT	Pd25Ge9	hP34	P-3		147	(SI)1(NI)3	
NISI_B31	MnP/FeAs	oP8	Pnma	B31	62	(FE NI)1(SI ZN)1	
NISI2	CaF2	cF12	Fm-3m	C1	225	(AL CU SI ZN)2(CU FE MN NI)1	
NI3SN4	Ni3Sn4	mS14	C2/m		12	(CU NI ZN)0.25(NI SN ZN)0.25(SN ZN)0.25	
NIZN_LT	CuTi	tP2	P4/mmm		123	(AL FE MN NI SI SN ZN)0.5(AL FE MN NI SI SN ZN)0.5	
NIZN8	Zn22Ni3	mS50	C2/m		12	(NI)0.111(AL ZN)0.889	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
NI10ZR7	Ni10Zr7	oS68	Cmca		64	(NI)23(ZR)17	
NI21ZR8	Hf8Ni21	aP29	P-1		2	(ZR)8 (NI)21	
NI11ZR9	Ni11Zr9	tI40	I4/m		87	(NI)11(ZR)9	
NI7ZR2	Ni7Zr2	mS36	C2/m		12	(NI)7(ZR)2	
PSI	SiP	oS48	Cmc21		36	(P)1(SI)1	
P2ZN3	Zn3P2	tP40	P4-2/nmc		137	(P)2(ZN)3	
P2ZN	ZnAs2	mP24	P2-1/c		14	(P)2(ZN)1	
SI2ZR_C49	Si2Zr	oC12	Cmcm		63	(SI GE)2(ZR)1	Si2Zr, Ge2Zr
SI4ZR5_TP36	Cr5B3	tI32	I4/mcm	D8l	140	(SI GE)4(TI ZR)5	Si4Zr5, Si4Ti5, Ge4Zr5
SIZR3_TP32	Ti3P	tP32	P4-2/n		86	(SI GE)1(ZR TI)3	SiZr3, SiTi3, GeZr3
SI2ZR3_D5A	U3Si2	tP10	P4/mbm	D5a	127	(SI)2(ZR)3	
FEB_B27	FeB	oP8	Pnma	B27	62	(FE MN TI ZR)1(B GE SI ZN)1	ZrGe, ZrSi
SI2TI_C54	Si2Ti	oF24	Fddd	C54	70	(SI SN)2(TI ZR)1	Sn2Zr
SN3ZR5	Mn5Si3	hP16	P6-3/mcm	D88	193	(ZR)5(SN)3(SN VA)1	
SNZR3_A15	Cr3Si	cP8	P m -3 n	A15	223	(SN ZR)3(SN ZR)1	
AGP2	CuP2	mP12	P21/c		14	(AG)1(P)2	
AG3P11	Ag3P11	mS28	Cm		8	(AG)3(P)11	
CU3AS	Cu3As	hP24	P-3c1		165	(CU)3(CU AS)1.15	
CU7AS	Mg	hP2	P63/mmc	A3	194	(CU)7(AS)1	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CU7AS3	BiF3	cF16	Fm3m		225	(CU)7(AS)3	
BE2CU	MgCu2	cF24	Fd-3m		227	(BE CU)2(BE CU)1	
NIBE7		cI*				(NI BE)2(NI)2(BE)9	
CO7NB2						(CO)7(NB)2	
CRNI2_OP6	MoPt2	oI6	Immm		71	(CR)1(NI)2	
CR3SI	Cr3Si	cP8	Pm-3n	A15	223	(CR SI)3(AL CR SI)1	
CRSI2_C40	CrSi2	hP9	P6-222	C40	180	(CR SI CU)1(AL CR SI CU)2	
CUO						(CU+2)1(O-2)1	
CUPRITE_C3						(CU+2)2(O-2)1	Cu2O
CU3P	Cu3P	hP24	P63cm		185	(CU)3(P)1	
CUP2	CuP2	mP12	P21/c		14	(CU)2(P)1	
CU2P7	Cu2P7	mS72	C2/m		12	(CU)2(P)7	
CU2SE_LT						(CU SE)2(SE)1	
CU2SE_HT	Cu2Se	cF44	Fm-3m		225	(CU SE)2(SE)1	
CU3SE2	Cu3Se2	tP10	P-421m		113	(CU)3(SE)2	
CUSE2	FeS2	oP6	Pnnm		58	(CU)1(SE)2	
CUSE_LT	Cu0.87Se	hP26	P63/mmc		194	(CU)1(SE)1	
CUSE_RT						(CU)1(SE)1	
CUSE_HT	CuS	hP12	P63/mmc		194	(CU)1(SE)1	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
FEZR3	Re3B	oC16/oS16	Cmcm	E1a	63	(FE)1(ZR)3	
MG2NI	Mg2Ni	hP18	P6-222	Ca	180	(MG ZN)2(CU NI ZN)1	
MG2SI_C1	CaF2	cF12	Fm-3m	C1	225	(MG)2(SI SN)1	
NI19SI6						(SI)0.24(CU NI)0.76	
NI5SI2	Ni31Si12	hP43	P321		150	(CU FE NI)5(AL SI)2	
SN4P3	Sn3.6As3	hR21	R-3m		166	(SN)4(P)3	
AL23CUFE4						(AL)23(CU)1(FE)4	
AL62CU25FE13						(FE)0.125(AL CU) 0.255 (AL)0.62	
AL7CU2FE		tP40	P 4/mnc		128	(FE NI)1(CU)2(AL)7	
AL10CU10FE		oF*	Fmm2		42	(FE)1(AL CU)10(AL)10	
AL28CU4MN7	Mn6Cu4Al29	oC156	Cmcm		63	(AL)28(MN)7(CU)4	
AL11CU5MN3		oP380				(AL)11(MN)3(CU)5	
ALCU3MN2						(AL)1(MN)2(CU)3	
AL7CU4NI		hP*/hR*				(AL)1(CU NI VA)1	
CUALO2						(CU+1)1(AL+3)1(O-2)2	
SPINEL						(AL+3 CU+2)1(AL+3 CU+2 VA)2(VA)2(O-2)4	
AL5CU4ZN						(AL CU)1(AL)4(CU)4(ZN)1	
AL9FENI	Co2Al9	mP22	P2-1/c		14	(AL)9(FE NI)2	
AL10FE3NI	Co2Al5	hP28	P6-3/mmc		194	(AL)5(FE NI)2	

Name	*Prototype*	*Pearson*	*Space group*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL71FE5NI24						(AL)0.71(FE)0.05(NI)0.24	
CU16MG6SI7						(CU)16(MG)6(SI)7	
CU3MG2SI	MgNi2	hP24	P6-3/mmc		194	(CU)2.74(MG)(SI)1.26	
CU5MN4SI						(CU)0.5(MN)0.37(SI)0.13	
CU4MNSN						(CU)0.666(SN)0.167(MN)0.167	
CUMNZN						(CU)0.334(MN)0.333(ZN)0.333	
CU2TIZR						(CU)0.5(TI)0.25(ZR)0.25	
NISNZN_T1						(NI SN VA)0.36(NI SN)0.38(VA ZN)0.26	
NISNZN_T2						(NI VA)0.55(SN)0.26(VA SN ZN)0.19	
NISNZN_T3						(NI VA)0.48(SN)0.20(VA SN ZN)0.31	
NISNZN_T4						(NI SN VA)0.51(SN ZN)0.39(VA SN ZN)0.10	

TCCU4 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 thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

Examples

Go to the 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:	**4.0**
First release:	**TCCU1 was released in with 2016b (November)**

Changes in the Most Recent Database Release

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.

Previous Releases

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.