

TCS Cu-based Alloys Database (TCCU7)

Technical Information

Available Starting with Thermo-Calc 2026b



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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.

TCCU7 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.

Interconnectivity with Other Products

The database can be used with our entire suite of products: Thermo-Calc, the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Additive Manufacturing Modules, and all available SDKs.

The thermodynamic database is compatible with the corresponding mobility database TCS Cu-based Alloys Mobility Database (MOBCU) that provides kinetic data for those working with the add-on kinetic modules – the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA) – as well as a few specific calculation types, such as Scheil with back diffusion. The current version of the mobility database is MOBCU6.

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 TCCU7:

- 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.

Release History

- The current version of the database is TCCU7. To review the most recent changes, see [TCCU7: Current Version Changes](#).
 - To review additional older changes, see [TCCU: Revision History](#).
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TCS Cu-based Alloys Database (TCCU) Resources

Database technical content and examples are available in different formats (html help files or PDFs).

Go to these locations to access the same content:

- **Locally Installed Help:** When in Thermo-Calc, press F1 to open the current version of the help in a local browser. You can also click **Online Help** from the **My Project** page to open the file. Then search or navigate to the **Databases** folder to browse the contents.
- **Web Help:** Go to the [Documentation](#) page to link to the most recent version of the web help. Then search or navigate to the **Databases** folder to browse the contents.
- **Website resources:** The individual database technical information and examples are also available in PDF format from the website. Download the *current version* of the PDFs for each database.

About 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. Also visit the video tutorials on our [website](#) or our [YouTube playlist](#).

Learn More



Go to the [Copper-based Alloys Databases](#) page on our website where you can access a *Validation and Calculation 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.



For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

TCCU7 Elements, Systems, and Phases

This section summarizes the available elements, assessed systems, and total number of phases in the TCS Cu-based Alloys Database (TCCU).

Included Elements

There are 34 elements included in the most recent version of the database.

Included Elements									
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	S	Se	Si	Sn
Ta	Ti	Zn	Zr						

Assessed Systems and Phases

The most recent version of the database contains:

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



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 [TCCU7 Models for the Included Phases](#) for details the models, e.g. number of sublattices and constituents on each sublattice.



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`.

TCCU7 Thermophysical Properties

This section summarizes the available thermophysical properties in this database.

Parameters and Variables

Below is a summary of the available thermophysical parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode (CM) versus Graphical Mode (GM) as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

<i>Property (Variable Name GM)</i>	<i>Model Parameters</i>	<i>Variables to Show or Plot in CM or the SDKs</i>
Molar volume	VO, VA	VM for a system VM (PHI) for phase PHI
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) **



* 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. As of 2024b, TCSLD5. ** I_{ON} is used in the TCS Metal Oxide Solutions Database (TCOX)



The examples listed for the SDKs (TC-Python and TC-Toolbox for MATLAB) are using CM syntax. The quantities can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. See the various model descriptions or the SDK help for details.

Examples

In Thermo-Calc, press F1 and search or navigate to the relevant database to discover the Validation and Calculation Examples Collection, which is also available in PDF format on our website.



Go to the [Copper-based Alloys Databases](#) page on our website where you can access a *Validation and Calculation 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



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, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what [properties can be calculated](#) with Thermo-Calc and the Add-on Modules.

TCCU7 Systems

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TCCU7 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.

<i>Assessed Ternary Systems</i>							
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	C-Cu-Fe	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-O	Cu-Fe-S
Cu-Fe-Si	Cu-Fe-Sn	Cu-Fe-Ta	Cu-Fe-Zn	Cu-La-Ni	Cu-La-Zr	Cu-Mg-Ni	Cu-Mg-Si
Cu-Mg-Sn	Cu-Mn-Ni	Cu-Mn-O	Cu-Mn-S	Cu-Mn-Si	Cu-Mn-Sn	Cu-Mn-Zn	Cu-Mo-Ni
Cu-Nb-Ni	Cu-Nb-Sn	Cu-Nb-Ti	Cu-Ni-P	Cu-Ni-Pb	Cu-Ni-S	Cu-Ni-Si	Cu-Ni-Sn
Cu-Ni-Ta	Cu-Ni-Ti	Cu-Ni-Zn	Cu-P-Sn	Cu-Pb-S	Cu-Pb-Sn	Cu-Pb-Zn	Cu-S-Sn
Cu-S-Zn	Cu-Si-Ti	Cu-Si-Zn	Cu-Sn-Zn	Cu-Ti-Zr	Fe-Mn-O	Ni-Sn-Zn	

TCCU7 Phases

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Common Phases for Copper Alloys

[TCCU7 Models for the Included Phases](#)

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

<i>Name in the Database</i>	<i>Common Name and Description</i>
BCC_B2	BCC metals as well as bcc intermetallic phase, such as β -Cu ₃ Al 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 ₃ Sn (ht) and γ -Ni ₃ Sn (ht)
GAMMA_D83	A solution phase with γ -brass structure, such as γ -Cu ₉ Al ₄ (rt), γ -Cu ₅ Zn ₈ , and γ -Ni ₅ Zn ₈
AL2CU_C16	θ -Al ₂ Cu
GAMMA_H	γ -Cu ₉ Al 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 ₂ Mg-type laves phase such as Cu ₂ Mg and Al ₂ Ca
CUPRITE_C3	Cu ₂ O
ZRM5_C15B	The Be ₅ Au-type intermetallic phase such as Cu ₅ Zr and Ni ₅ Zr
CUZR2_C11B	The CuZr ₂ -type intermetallic phase such as CuTi ₂ , CuZr ₂ , and AlZr ₂
CU6SN5_HT	η -Cu ₆ Sn ₅
CU6SN5_LT	η' -Cu ₆ Sn ₅
CU41SN11	δ -Cu ₄₁ Sn ₁₁
CU3SN	ϵ -Cu ₃ Sn (rt)
CU10SN3	ζ -Cu ₁₀ Sn ₃

<i>Name in the Database</i>	<i>Common Name and Description</i>
AL4M_D13	Al ₄ Ca
DIAMOND_A4	Si and Ge
CO2SI_C23	Co ₂ Si, Ni ₂ Si
AL2AU_C1_CAF2	CoSi ₂
M3P	Phosphide such as Fe ₃ P, Cr ₃ P, and Ni ₃ P
M2P	Phosphides such as Fe ₂ P, Cr ₂ P, and Ni ₂ P
MP	Phosphides such as FeP and CrP
R_PHASE	A high temperature Fe-Mo phase
MU_PHASE	μ phase, such as Co ₆ Nb ₇ and Mo ₆ Fe ₇
SIGMA	A chromium/molybdenum-rich intermetallic compound in Co-Cr and Fe-Mo systems

TCCU7 Models for the Included Phases



Also see the listing at the end for [Gas and Liquid Phase Models](#).

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	Metallic FCC_A1 solution, e.g. (Cu), (Al), (Ni)	2	(AG, AL, AU, AS, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, S, SE, SI, SN, TA, TI, ZN, ZR)1(B, C, O, VA)1
FCC_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	3	(AL, CU, CE, FE, GE, LA, MG, MN, MO, NI, SI, ZN, CR, SN, TA, TI, ZR, AG, CA, CO, PB, BE, BI, CD, P, AU, AS, NB, PT, S, SE)0.75(AL, CU, FE, GE, CE, LA, MG, MN, MO, NI, SI, ZN, CR, SN, TA, TI, ZR, AG, CA, CO, PB, BE, BI, CD, P, AU, AS, NB, PT, S, SE)0.25(B, C, O, VA)1
FCC_L10	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	-	2	(AL, CU, MN, NI, TI)0.5(AL, CU, MN, NI, TI)0.5
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	Metallic BCC_A2 solution	2	-
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	3	(AG, AL, AU, AS, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, S, SE, SI, SN, TA, TI, ZN, ZR, VA)0.5(AG, AL, AU, AS, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, P, PB, PT, S, SE, SI, SN, TA, TI, ZN, ZR, VA)0.5(B, C, O, VA)3
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	2	(AL, BI, CO, CU, FE, MN, NI, SI, ZN, MG, CR, TI, ZR, SN)1(B, C, O, VA)1
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)	-	2	(AL, BI, CU, CO, FE, MN, NI, SI, ZN, MG, CR, TI, ZR, SN, AG)1(B, C, O, VA)1
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)	Metallic HCP_A3 solution, alpha_Mg/Hf/Sc/Ti/Zr	2	(AG, AL, AU, AS, BE, BI, CA, CD, CE, CO, CR, CU, FE, GE, LA, MG, MN, MO, NB, NI, PB, PT, S, SI, SN, TA, TI, ZN, ZR)1(B, C, O, VA)0.5
HCP_ZN	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)	-	2	-

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RHOMBO_A7	alpha-As (A7)	A7	hR2	(166, R-3m)	-	1	(AS, AG, BI, P, PB, SN, ZN)1
DHCP	alpha-La (A3')	A3'	hP4	(194, P6_3/mmc)	-	1	(CU, CE, LA, MG, NI, ZR)1
HEXAGONAL_A8	gamma-Se (A8)	A8	hP3	(152, P3_121)	-	1	(SE)1
WHITE_P	Unknown Structure	-	-	-	-	1	(P)1
RED_P	Unknown Structure	-	-	-	-	1	(P)1
BETA_RHOMBO_B	beta-B (R-105)	-	hR105	(166, R-3m)	-	2	(B)93(CU, SI, B, C)12
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_3/mmc)	-	1	(B, C)1
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	Pure C, Ge, Si or solution phases based on them	1	(AG, AL, AU, B, C, GE, O, P, SI, SN, TI, ZN)1
BCT_A5	beta-Sn (A5)	A5	tI4	(141, I4_1/amd)	Pure Sn or its solution	1	(AG, AL, B, BI, CD, CU, NI, PB, S, SN, SI, TI, ZN)1
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	(70, Fddd)	-	1	(S)1
MONOCLINIC_S	beta-S	-	mP48	(14, P2_1/c)	-	1	(S)1
B2_BCC	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	2	(BE, CO, CU, NI)1(BE, VA)1
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	-	2	(AL, CO, CR, CU, FE, LA, MG, MN, MO, NB, NI, TA, TI, ZN, ZR)2(AL, CO, CR, CU, FE, LA, MG, MN, MO, NB, TA, TI, ZN, ZR)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	Solution of Cu2Mg-type phases	2	(AL, CA, CO, CR, CU, FE, LA, MG, MN, NB, NI, SI, SN, TA, TI, ZN, ZR)2(AL, CA, CE, CO, CR, CU, FE, LA, MG, MN, NB, NI, SI, SN, TA, TI, ZN, ZR)1
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_3/mmc)	Solution of MgNi2-type phases	2	(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

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GAMMA_D82	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(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	(215, P-43m)	solution between Al8Cu5 (rt) and Cu5Zn8	3	(AL, FE, NI, SI, SN, ZN)4(AL, CU, NI, SI, ZN)1(CU, MN, FE, NI, ZN, SN)8
CO2SI_C23	Cotunnite (PbCl2, C23)	C23	oP12	(62, Pnma)	Co2Si, Ni2Si	2	(AL, CO, CA, CU, FE, NI, SI)2(AL, CO, SI, SN, ZN)1
AG3BE8	Unknown Structure	-	-	-	-	2	(AG)2.97(BE)8.03
AG3SN_L60	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)	a binary phase in Ag-Sn system, and a ternary phase in Cu-Ni-Sn system	2	(CU, AG, CO, NI, ZN)0.75(AG, BI, NI, SN)0.25
AGZN3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)	-	1	(AG, ZN)1
AGZN_LT	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	-	2	(ZN)1(AG, ZN)2
AG5ZN8	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(AG, ZN)2(AG)2(AG, ZN)3(AG, ZN)6
ALB2_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(MG, AL, MN, CR, ZR, TI)1(B)2
ALB12	alpha-AlB12	-	tP216	(92, P4_12_12)	-	2	(AL)1(B)12
AL4C3	Al4C3 (D71)	D71	hR7	(166, R-3m)	-	2	(AL, SI)4(C)3
AL4M_D13	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	Al4Ca	2	(AL)4(CA)1
AL14CA13	Al14Ca13	-	mS54	(12, C2/m)	-	2	(AL, MG, ZN)14(CA)13
AL3CA8	Ca8In3	-	aP22	(2, P-1)	-	2	(AL)3(CA, MG)8

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL4CE	D13 (BaAl4)	D13	tl10	(139, I4/mmm)	-	2	(AL)4(CE)1
AL11CE3	Al11La3	-	ol28	(71, Immm)	-	2	(AL)11(CE)3
AL3CE_HT	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(AL)3(CE)1
AL3CE_LT	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(AL)3(CE)1
AL2CE	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(AL)2(CE)1
AL1CE1	AlCe	-	oS16	(63, Cmcm)	-	2	(AL)1(CE)1
AL1CE2	Unknown Structure	-	-	-	-	2	(AL)1(CE)2
ALCE3_HT	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(AL)1(CE)3
ALCE3_LT	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(AL)1(CE)3
AL45CR7	V7Al45	-	mS104	(11, P2_1/m)	-	2	(AL)45(CR)7
CUZR2_C11B	MoSi2 (C11b)	C11b	tl6	(139, I4/mmm)	AlCr2, CuTi2, CuZr2	2	(AL, CR, CU, NI, SI, ZN)1(AL, CR, NB, TI, ZR)2
AL5CR	Al5Cr	-	mS732	(15, C2/c)	-	2	(AL, SI)5(CR)1
AL4CR	mu-Al4Mn	-	hP574	(194, P6_3/mmc)	-	2	(CR)1(AL, SI, VA)4
ALCR_GAMMA1	Unknown Structure	-	-	-	-	4	(AL, CR, SI)2(CR)2(AL, CR)3(AL, SI)6
GAMMA_D810	Cr5Al8 (D810)	D810	hR26	(160, R3m)	A binary phase in Al-Cr system	3	(AL, SI)12(CR)5(AL, CR, SI)9
AL13CO4	Orthorhombic Co4Al13 (Approximate Quasicrystal)	-	oP102	(31, Pmn2_1)	-	2	(AL)13(CO)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3CO	Os4Al13	-	mS34	(12, C2/m)	-	2	(AL)3(CO)1
AL5CO2	Co2Al5 (D811)	D811	hP28	(194, P6 ₃ /mmc)	-	2	(AL)5(CO)2
AL9CO2	Co2Al9 (D8d)	D8d	mP22	(14, P2 ₁ /c)	-	2	(AL)9(CO)2
ALCU_DEL	Al5Cu8	-	hR52	(160, R3m)	-	2	(AL, ZN)2(CU, FE)3
ALCU_EPS	InNi2 (B82)	B82	hP6	(194, P6 ₃ /mmc)	-	2	(AL, CU, ZN, NI)1(CU, FE)1
ALCU_ETA	AlCu(r)	-	mS20	(12, C2/m)	-	2	(AL, CU)1(CU, FE, ZN, NI)1
ALCU_PRIME	Al9Cu11(h)	-	oF88	(42, Fmm2)	-	2	(AL)2(CU)1
ALCU_ZETA	Al9Cu11(h)	-	oF88	(42, Fmm2)	-	2	(AL)9(CU, FE)11
GAMMA_H	gamma-Brass (Cu5Zn8, D82)	D82	cl52	(217, I-43m)	-	3	(AL, ZN)4(AL, CU, ZN)1(CU, MN, FE, NI)8
AL2CU_C16	Khatyrkite (Al2Cu, C16)	C16	tl12	(140, I4/mcm)	Al2Cu, CoSn2, FeSn2, Mnsn2	2	(AL, NI, TA, SN, ZR)2(AL, CO, CU, FE, MN, NI, SI, TA)1
AL2FE1	Al2Fe	-	aP18	(1, P1)	-	2	(AL, CU, SI, ZN)2(FE, MN, NI)1
AL5FE2	Al2.8Fe	-	oS24	(63, Cmcm)	-	2	(AL, CU, SI, ZN)5(FE, MN, NI)2
AL5FE4	gamma-Brass (Cu5Zn8, D82)	D82	cl52	(217, I-43m)	-	1	(AL, CU, FE, MN)1
AL13FE4	Al13Fe4	-	mS102	(12, C2/m)	-	3	(AL, CU)0.6275(FE, MN, NI, ZN)0.235(AL, SI, VA, ZN)0.1375
ALMG_BETA	Al45Mg28	-	cF1832	(227, Fd-3m)	-	2	(MG)89(AL, ZN)140
ALMG_EPS	Al30Mg23	-	hR53	(148, R-3)	-	2	(MG)23(AL, ZN)30
ALMG_GAMMA	alpha-Mn (A12)	A12	cl58	(217, I-43m)	-	3	(MG)5(AL, MG, ZN)12(AL, MG, ZN)12

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL12MN	Al12W	-	cl26	(204, Im-3)	-	2	(Al)12(MN)1
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmc ₂)	-	2	(Al, ZN)6(MN, FE)1
AL4MN_R	lambda-Al4Mn	-	hP586	(176, P6 ₃ /m)	-	2	(Al)461(MN, FE)107
AL4MN_U	mu-Al4Mn	-	hP574	(194, P6 ₃ /mmc)	-	2	(Al, ZN)4(MN)1
AL11MN4_LT	Al11Mn4	-	aP15	(2, P-1)	-	2	(Al, ZN)11(MN, FE)4
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25	-	oP156	(62, Pnma)	-	2	(Al, MN)29(MN)10
AL8MN5	Cr5Al8 (D810)	D810	hR26	(160, R3m)	-	3	(Al, ZN)12(MN)5(Al, MN, Si, CU)9
AL3NI_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(Al)0.75(Fe, Ni)0.25
AL3NI2	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)	-	3	(Al, Si, ZN)3(Al, CU, FE, Ni)2(Ni, VA)1
AL3NI5	Ga3Pt5	-	oS16	(65, Cmmm)	-	2	(Al)0.375(Ni)0.625
CORUNDUM	Corundum (alpha-alumina, Al2O3, D51)	D51	hR10	(167, R-3c)	Al2O3, Cr2O3, Fe2O3	2	(Al+3, CR+3, FE+3, MN+3)2(O-2)3
ALP1	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)	-	2	(Al)1(P)1
AL2TI	Ga2Hf	-	tl24	(141, I4 ₁ /amd)	-	2	(Al)2(TI)1
AL18TI7	Al5Ti2	-	tP28	(123, P4/mmm)	-	2	(Al)0.72(TI)0.28
AL3TI_D022	Al3Ti (D022)	D022	tl8	(139, I4/mmm)	-	2	(Al, MN, Ni)3(MN, TI, ZR)1
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6 ₃ /mmc)	-	2	(Al, TI)3(Al, TI)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL2ZR1	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6 ₃ /mmc)	-	2	(AL)2(ZR)1
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	AlZr3	2	(AL, NI, SI, TI)1(AL, FE, ZR, NI, ZN)3
AL3ZR5_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	-	2	(AL, SI)3(ZR, CR, TA)5
CRB_B33	CrB (B33)	B33	oS8	(63, Cmcm)	AlZr, NiZr	2	(AL, CA, CR, NI)1(AG, B, SI, SN, ZR)1
ALZR2_B82	InNi2 (B82)	B82	hP6	(194, P6 ₃ /mmc)	-	2	(AL, MN, SN, VA)1(ZR, MN, TI, VA)2
AL4ZR5	Ti5Ga4	-	hP18	(193, P6 ₃ /mcm)	-	2	(AL)4(ZR)5
AL3ZR2_OF40	Zr2Al3	-	oF40	(43, Fdd2)	-	2	(AL)3(ZR)2
AL2ZR3_TP20	Zr3Al2	-	tP20	(136, P4 ₂ /mnm)	-	2	(AL, ZN)2(ZR)3
AL3ZR_D023	Al3Zr (D023)	D023	tI16	(139, I4/mmm)	-	2	(AL)3(TI, ZR)1
ZRB12	UB12 (D2f)	D2f	cF52	(225, Fm-3m)	-	2	(B)12(ZR)1
BIMN_LT	Nickeline (NiAs, B81)	B81	hP4	(194, P6 ₃ /mmc)	-	2	(B)0.5(MN)0.5
BIMN_HT	Mn2.23Bi1.88	-	oP10	(51, Pnma)	-	2	(B)0.481(MN)0.519
BI3NI	Bi3Ni	-	oP16	(62, Pnma)	-	2	(B)3(NI)1
CU6SN5_HT	InNi2 (B82)	B82	hP6	(194, P6 ₃ /mmc)	CU6SN5(HT), BiNi, Co6Sn5	3	(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
CA2CU	Ca2Cu	-	oP12	(62, Pnma)	-	2	(CA)2(CU)1
CA1CU1	alpha-CaCu	-	mP20	(11, P2 ₁ /m)	-	2	(CA)1(CU)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CACU5_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	-	2	(CA)1(CU, NI, ZN)5
CDCU2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	-	2	(CD)1(CU)2
CD3CU4	Cd3Cu4	-	cF1124	(216, F-43m)	-	2	-
CD8CU5	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(CU)2(CD, CU)3(CU)2(CU, CD)6
CD10CU3	Co2Al5 (D811)	D811	hP28	(194, P6_3/mmc)	-	2	-
CUR	FeB (B27)	B27	oP8	(62, Pnma)	CuLa, CuCe,	2	(CU, NI)1(LA, CE)1
CU2CE	KHg2	-	oI12	(74, Imma)	-	2	(CU)2(CE)1
CU4CE	Unknown Structure	-	oP20	-	-	2	(AL, CU)4(CE)1
CU5R	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	Cu5La, Cu5Ce, Ni5La, Ni5Ce	2	(AL, CU, NI, CE)5(LA, CE, NI)1
CU6R	CeCu6	-	oP28	(62, Pnma)	Cu6La_LT, Cu6Ce	2	(CU, NI)6(CE, LA)1
MG12R_D2B	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)	-	2	(MG)12(CE, LA)1
MG17R2	CeMg10	-	hP44	(194, P6_3/mmc)	-	2	(MG)17(CE, LA)2
MG3R_D03	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	2	(MG)3(CE, LA, MG)1
MG41R5	Ce5Mg41	-	tI92	(87, I4/m)	-	2	(MG)41(CE, LA)5
CENI2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(CE, NI)1(CE, NI)2
CENI3	CeNi3	-	hP24	(194, P6_3/mmc)	-	2	(CE)1(NI)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CE2NI7	Ce2Ni7	-	hP36	(194, P6 ₃ /mmc)	-	2	(CE)2(NI)7
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4 ₂ /mm)	A binary phase in Co-Cr and Fe-Mo systems	3	(FE, MN, NI, CO)8(CR, MO)4(CO, FE, CR, MN, MO, NI)18
CO3GE	Unknown Structure	-	-	-	-	2	(CO)0.75(GE)0.25
CO5GE2	Unknown Structure	-	-	-	-	2	(CO)0.714(GE)0.286
CO5GE3_C37	Co2Si (C37)	C37	oP12	(62, Pnma)	-	3	(CO, VA)0.125(CO)0.5(CO, GE, SN)0.375
CO5GE3_ALPHA	Unknown Structure	-	-	-	-	2	(CO)0.625(GE)0.375
CO5GE7	Co5Ge7	-	tI24	(107, I4mm)	-	2	(CO)0.417(GE)0.583
COGE	CoGe	-	mS16	(12, C2/m)	-	2	(CO, GE)0.5(CO, GE)0.5
CO1GE2	CoGe2	-	oS24	(64, Cmce)	-	2	(CO)0.333(GE)0.667
CO2SI_HT	Co2Si (C37)	C37	oP12	(62, Pnma)	-	2	(CO, SI)0.6667(CO, SI)0.3333
COSI_B20	FeSi (B20)	B20	cP8	(198, P2 ₁ 3)	-	2	(AL, CO, SI)0.5(CO, SI)0.5
CO3SI_HT	Ni3Sn (D019)	D019	hP8	(194, P6 ₃ /mmc)	-	3	(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	(225, Fm-3m)	CoSi2	2	(AG, AL, AU, CU, SI, SN)0.66667(AL, AU, CO, NI, PT)0.33333
COSN3_OS32	PdSn3	-	oS32	(64, Cmce)	-	2	(CO)0.25(SN)0.75
COSN_HP6	CoSn (B35)	B35	hP6	(191, P6/mmm)	-	2	(CO)0.5(SN)0.5
COZN_LT	beta-Mn (A13)	A13	cP20	(213, P4 ₁ 32)	-	2	(CO, ZN)1(VA)1
COZN_HT	Unknown Structure	-	-	-	-	2	(CO, ZN)1(VA)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
COZN_GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	-	2	(CO, ZN)1(VA)1
COZN_DELTA	Unknown Structure	-	-	-	-	2	(CO)0.117647(ZN)0.882353
COZN_GAMMA1	Co2Zn15	-	mS28	(12, C2/m)	-	2	(CO)0.125(ZN)0.875
COZN_GAMMA2	CoZn13	-	mS28	(12, C2/m)	-	2	(CO)0.0714286(ZN)0.9285714
CU3GE_ETA	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)	-	2	(AG, CU)0.75(GE)0.25
CU3GE_EPSILON	Na3As (D018)	D018	hP8	(194, P6_3/mmc)	-	2	(AG, CU)0.765(GE)0.235
CU3GE_THETA	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	2	(AG, CU)0.735(GE)0.265
CR5GE3	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	-	2	(CR, GE)0.625(CR, GE)0.375
LCR5GE3	Unknown Structure	-	-	-	-	2	(CR, GE)0.625(CR, GE)0.375
CR11GE8	Cr11Ge8	-	oP76	(62, Pnma)	-	2	(CR)0.579(GE)0.421
CR11GE19	Mn11Si19	-	tP120	(118, P-4n2)	-	2	(CR)0.367(GE)0.633
CR3GE	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(CR, GE)0.75(CR, GE)0.25
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)	This is Fe3O4, Mn3O4 (ht)	4	(AL+3, CR+2, CR+3, CU+2, FE+2, FE+3, MN+2)1(AL+3, CR+3, CU+2, FE+2, FE+3, MN+2, MN+3, MN+4, VA)2(CR+2, FE+2, MN+2, VA)2 (O-2)4
CU6LA_HT	Cu6La	-	mP28	(14, P2_1/c)	-	2	(CU)6(CE, LA)1
CU4LA	Cu4La	-	tI90	(119, I-4m2)	-	2	(CU)4(LA, ZR)1
CU2LA	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(CU, NI)2(LA)1
CUMG2	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	-	2	(CU, NI)1(MG)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU33SI7_DELTA	Unknown Structure	-	-	-	-	2	(AG, CU, ZN)0.825(SI)0.175
CU56SI11_GAMMA	Mg3Ru2	-	cP20	(213, P4_132)	-	2	(AG, CU, MG, MN, NI, ZN)0.835821(SI)0.164179
CUSI_ETA	Cu3Si-h2	-	hR*	(162, P-31m)	-	2	(AG, CU, MN, NI, ZN)0.76(SI)0.24
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cl76	(220, I-43d)	-	2	(AG, CU, MN, MG, ZN)0.789474(AL, SI)0.210526
CUSN_GAMMA	BiF3 (D03)	D03	cF16	(225, Fm-3m)	Cu3Sn(ht), Ni3Sn(ht)	1	(CU, MN, NB, NI, SN, ZN)1
CU10SN3	Cu10Sn3	-	hP26	(173, P6_3)	-	2	(CU, NI)0.769(SN)0.231
CU3SN	Cu3Sn	-	oS80	(63, Cmc)	-	2	(CU, SN, NI)3(CU, SN)1
CU41SN11	Cu41Sn11	-	cF416	(216, F-43m)	-	2	(CU, SN, ZN)41(CU, SN, ZN)11
CU6SN5_LT	Cu6Sn5	-	mS44	(15, C2/c)	-	3	(CU)1(CU, SN)1(SN)1
CU2TI1	Au2V	-	oS12	(63, Cmc)	-	2	(CU, NI)2(TI)1
CU3TI2	Cu3Ti2	-	tP10	(129, P4/nmm)	-	2	(CU, NI)3(NB, TI)2
CU4TI1	Au4Zr	-	oP20	(62, Pnma)	-	2	(CU, NB, NI, TI)4(CU, NB, NI, TI)1
CU4TI3	Cu4Ti3	-	tl14	(139, I4/mmm)	-	2	(CU, NI)4(NB, TI)3
CUTI_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)	-	2	(CU, NB, NI, TI)1(CU, NB, NI, TI)1
CUTI3	CuTi3 (L60)	L60	tP4	(123, P4/mmm)	-	2	(CU, TI, NB)1(TI, NB)3
CU10ZR7	Ni10Zr7	-	oS68	(64, Cmce)	-	2	(CU)10(ZR)7
ZRM5_C15B	AuBe5 (C15b)	C15b	cF24	(216, F-43m)	Cu5Zr, Ni5Zr	2	(CU, NI)5(LA, ZR)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU51ZR14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)0.7846(LA, ZR)0.2154
CU8ZR3	Cu8Hf3	-	oP44	(62, Pnma)	-	2	(CU)8(ZR)3
R_PHASE	R-(Co, Cr, Mo)	-	hR53	(148, R-3)	A binary phase in Fe-Mo system	3	(FE)27(MO)14(FE, MO)12
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	Binary phase (Mu) in Fe-Mo, Co-Nb, Fe-Ta	3	(CO, CU, FE, NB, TA)7(MO, NB, TA)2(CO, CU, FE, MO, NB, TA)4
M3P	Ni3P (D0e)	D03	tI32	(82, I-4)	Ni3P, Fe3P, Cr3P	2	(CU, NI, FE, CR)0.75(P)0.25
M2P	Barringerite (Revised Fe2P, C22)	C22	hP9	(189, P-62m)	Ni2P, Fe2P, Cr2P	2	(CU, NI, FE, CR)0.667(P)0.333
MP	Westerveldite (FeAs, B14)	B14	oP8	(62, Pnma)	FeP, CrP	2	(FE, CR)0.5(P)0.5
FEP2	Marcasite (FeS2, C18)	C18	oP6	(58, Pnnm)	-	2	(FE)0.333(P)0.667
FEP4	FeP4	-	mP30	(14, P2_1/c)	-	2	(FE)0.2(P)0.8
FE2SI	AlNi2	-	hP6	(164, P-3m1)	-	2	(FE, NI)2(AL, SI)1
FESI2_H	FeSi2-h	-	tP3	(123, P4/mmm)	-	2	(FE, NI)3(AL, SI)7
FESI2_L	FeSi2-l	-	oS48	(64, Cmce)	-	2	(FE, NI)1(AL, SI)2
FESI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	FeSi, MnSi, CrSi	2	(FE, MN, NI, CR)1(AL, GE, SI)1
MN5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	Mn5Si3, Cr3Si5, Fe5Si3, Ge3Zr5, Si3Zr5,	2	(CU, FE, MN, NI, CR, ZR, TI)5(AL, CR, SI, GE, SN)3
FE5SN3_D82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(FE)5(SN)3
FE3SN2	Fe3Sn2	-	hR10	(166, R-3m)	-	2	(FE)3(SN)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FEM_B35	CoSn (B35)	B35	hP6	(191, P6/mmm)	FeSn	2	(FE)1(SN)1
FEZN_GAMMA1	Fe11Zn40	-	cF408	(216, F-43m)	-	3	(FE)0.137(AL, CU, FE, NI, SI, ZN)0.118(MN, ZN)0.745
FEZN_DELTA	FeZn10	-	hP632	(194, P6_3/mmc)	-	4	(FE)0.058(AL, CU, FE, MN, NI, SI, ZN)0.18(ZN)0.525(ZN)0.237
FEZN_ZETA	CoZn13	-	mS28	(12, C2/m)	-	3	-
GE3NI5_C2	Ge3NI5	-	mS32	(5, C2)	-	2	(NI)0.625(GE)0.375
GE2NI5_HT	Pd5Sb2	-	hP42	(185, P6_3cm)	-	2	(NI)0.72(GE)0.28
GENI3_HT	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(NI)0.744(GE)0.256
GENI2	Co2Si (C37)	C37	oP12	(62, Pnma)	-	2	(NI)0.665(GE)0.335
GE1NI1	Westerveldite (FeAs, B14)	B14	oP8	(62, Pnma)	-	2	(GE)0.5(NI)0.5
TI6GE5	Si5V6	-	oI44	(72, Ibam)	-	2	(GE)5(TI)6
TIGE2	TiSi2 (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	-	2	(GE)2(TI)1
LA3NI	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(LA)3(NI)1
NI3R7	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)	Ni3La7, Ni3Ce7	2	(LA, CE)7(NI)3
NIR	CrB (B33)	B33	oS8	(63, Cmcm)	NiLa, NiCe	2	(CE, LA)1(CU, NI)1
LA2NI3	La2Ni3	-	oS20	(64, Cmce)	-	2	(LA)2(NI, CU)3
LA7NI16	La7Ni16	-	tI46	(121, I-42m)	-	2	(LA)7(CU, NI)16
LANI3	Ni3Pu	-	hR12	(166, R-3m)	-	2	(LA)1(CU, NI)3
LA2NI7	Ce2Ni7	-	hP36	(194, P6_	-	2	(LA)2(CU, NI)7

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				3/mmc)			
LA5Ni19	Co19Sm5	-	hP48	(194, P6_3/mmc)	-	2	(LA)5(Ni)19
MNNi2	Unknown Structure	-	-	-	-	2	(MN, Ni)1(Ni)2
MN11Si19	Mn11Si19	-	tP120	(118, P-4n2)	-	2	(MN)11(AL, Si)19
MN3Si	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	2	(Fe, MN, Ni)3(AL, Si)1
MN6Si	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	-	2	(AL, MN)17(Si, ZN)3
MN9Si2	Mn9Si2	-	oI186	(71, Immm)	-	2	(MN)33(Si)7
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)	-	2	(MN)3(SN)2
Ni3SN_D019	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(Cu, Ni, AL, SN, VA, ZN)1(Cu, MN, Fe, Ni, SN, ZN)3
MN2SN	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(MN)0.643(SN)0.357
MNZn9	Unknown Structure	-	h**	-	-	2	(MN)0.1(ZN)0.9
MONI_DELTA	MoNi	-	oP56	(19, P2_12_12_1)	-	3	(Ni)24(MO, Ni)20(Cu, MO)12
MONI4_BETA	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)	-	2	(MO)1(Ni)4
Ni3MO_D0A	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmnm)	-	2	(Ni)3(MO, Ni)1
NBNi3	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmnm)	-	2	(Cu, NB, Ni)1(Cu, NB, Ni)3
NB7Ni6	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	-	4	(NB, Ni, TA)1(NB, TA)4(NB, Ni, TA)2(Cu, NB, Ni, TA)6
NBNi8	Pt8Ti	-	tI18	(139, I4/mmm)	-	2	(NB)1(Ni)8

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NB6SN5	Sn5Ti6-alpha	-	oI44	(71, Immm)	-	3	(CU, NB)24(SN)16(NB, SN)4
NBSN2_CB	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	-	2	(CU, NB)1(SN)2
NI5P2_HT	Unknown Structure	-	-	-	-	2	(NI)0.714(P)0.286
NI5P2_LT	Pd8Sb3	-	hR44	(161, R3c)	-	2	(CU, NI)0.714(P)0.286
NI12P5_HT	Unknown Structure	-	-	-	-	2	(NI)0.706(P)0.294
NI12P5_LT	Ni12P5	-	tI34	(87, I4/m)	-	2	(NI)0.706(P)0.294
NI5P4	NI5P4	-	hP36	(194, P6_3/mmc)	-	2	(NI)0.556(P)0.444
NIP2	PdP2	-	mS12	(15, C2/c)	-	2	(NI)0.3333(P)0.6667
NI2SI_HT	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	3	(CU, NI)1(NI, VA)1(AL, SI)1
NI3SI2	Ni3Si2	-	oP80	(36, Cmc2_1)	-	2	(FE, NI)3(SI)2
NI3SI_HT	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(NI)3(SI)1
NI3SI_MT	Ge9Pd25	-	hP34	(147, P-3)	-	2	(SI)1(NI)3
NISI_B31	MnP (B31)	B31	oP8	(62, Pnma)	-	2	(FE, NI)1(SI, ZN)1
NISI2	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	-	2	(AL, CU, SI, ZN)2(CU, FE, MN, NI)1
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	(12, C2/m)	-	3	(CU, NI, ZN)0.25(NI, SN, ZN)0.25(SN, ZN)0.5
NITi2	NiT _i 2	-	cF96	(227, Fd-3m)	-	2	(CU, NI)0.3333(TI)0.6667
NI3TI	Ni3Ti (D024)	D024	hP16	(194, P6_3/mmc)	-	2	(CU, NI, TI)0.75(CU, NI, TI)0.25
NIZN_LT	delta-CuTi (L2a)	L2a	tP2	(123,	-	2	(AL, FE, MN, NI, SI, SN, ZN)0.5(AL, FE, MN, NI, SI, SN, ZN)0.5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				P4/mmm)			
NiZn8	Ni3Zn22	-	mS50	(12, C2/m)	-	2	(Ni)0.1111111(AL, ZN)0.8888889
Ni10Zr7	Ni10Zr7	-	oS68	(64, Cmce)	-	2	(Ni)23(ZR)17
Ni21Zr8	Hf8Ni21	-	aP29	(2, P-1)	-	2	(ZR)8(Ni)21
Ni11Zr9	Pt11Zr9	-	tI40	(87, I4/m)	-	2	(Ni)11(ZR)9
Ni7Zr2	Ni7Zr2	-	mS36	(12, C2/m)	-	2	(Ni)7(ZR)2
FLUORITE	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	-	2	(ZR, ZR+4)2(O-2, VA)4
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	(14, P2_1/c)	-	2	(ZR+4)2(O-2)4
ZRO2_TETR	Cocconite (Red Hgl2, C13)	C13	tP6	(137, P4_2/nmc)	-	2	(ZR+4)2(O-2)4
PSI	(SiP)	-	oS48	(36, Cmc2_1)	-	2	(P)1(Si)1
P2ZN3	Zn3P2 (D59)	D59	tP40	(137, P4_2/nmc)	-	2	(P)2(ZN)3
P2ZN1	ZnAs2	-	mP24	(14, P2_1/c)	-	2	(P)2(ZN)1
Si2ZR_C49	ZrSi2 (C49)	C49	oS12	(63, Cmc)	Si2Zr, Ge2Zr	2	(Si, GE)2(ZR)1
Si4ZR5_TP36	Si4Zr5	-	tP36	(92, P4_12_12)	Si4Zr5, Si4Ti5, Ge4Zr5	2	(Si, GE)4(Ti, ZR)5
SiZR3_TP32	Ti3P	-	tP32	(86, P4_2/n)	SiZr3, SiTi3, GeZr3, SiTa3	2	(Si, GE)1(ZR, Ti, TA)3
Si2ZR3_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	-	2	(Si)2(ZR)3
FEB_B27	FeB (B27)	B27	oP8	(62, Pnma)	ZrGe, ZrSi	2	(FE, MN, Ti, ZR)1(B, GE, Si, ZN)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SI2TI_C54	TiSi ₂ (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	Sn2Zr	2	(Si, Sn) ₂ (Ti, Zr) ₁
SN3ZR5	Mavlyanovite (Mn ₅ Si ₃ , D88)	D88	hP16	(193, P6 ₃ /mcm)	-	3	(Zr) ₅ (Sn) ₃ (Sn, VA) ₁
SNZR3_A15	Cr ₃ Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(Cu, Nb, Sn, Zr) ₃ (Nb, Sn, Zr) ₁
AGP2	CuP ₂	-	mP12	(14, P2 ₁ /c)	-	2	(Ag) ₁ (P) ₂
AG3P11	Ag ₃ P ₁₁	-	mS28	(8, Cm)	-	2	(Ag) ₃ (P) ₁₁
ALMGZN_PHI	Mg ₂₁ (Al, Zn) ₁₇	-	oP152	(57, Pbcm)	-	2	(Mg) ₆ (Al, Zn) ₅
CU3AS	H3Ho	-	hP24	(165, P-3c1)	-	2	(Cu) ₃ (Cu, AS) _{1.15}
CU7AS1	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6 ₃ /mmc)	-	2	(Cu) ₇ (AS) ₁
CU7AS3	Cu ₇ In ₃	-	aP40	(2, P-1)	-	2	(Cu) ₇ (AS) ₃
COBE3	CoBe ₃	-	hP96	(194, P6 ₃ /mmc)	-	2	(Co) ₁ (Be) ₃
CO3BE17_LT	Unknown Structure	-	cl*	-	-	2	(Co) ₃ (Be) ₁₇
CO3BE17_HT	Unknown Structure	-	cl*	-	-	2	(Co) ₃ (Be) ₁₇
BE2CU	Cu ₂ Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(Be, Cu) ₂ (Be, Cu) ₁
NIBE7	Unknown Structure	-	cl*	-	-	3	(Ni, Be) ₂ (Ni) ₂ (Be) ₉
CEMENTITE_D011	Cementite (Fe ₃ C, D011)	D011	oP16	(62, Pnma)	-	2	(Fe) ₃ (C) ₁
CE2FE17	Ni ₁₇ Th ₂	-	hP38	(194, P6 ₃ /mmc)	-	2	(Ce) ₂ (Fe) ₁₇
CO7NB2	(Co ₇ Nb ₂)	-	mS18	(12, C2/m)	-	2	(Co) ₇ (Nb) ₂

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CRNI2_OP6	MoPt2	-	ol6	(71, Immm)	-	2	(CR)1(NI)2
CR3SI	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	-
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)	-	2	(CR, SI, CU, TA)1(AL, CR, SI, CU)2
CUO	Tenorite (CuO, B26)	B26	mS8	(15, C2/c)	-	2	(CU+2)1(O-2)1
CUPRITE_C3	Cuprite (Cu2O, C3)	C3	cP6	(224, Pn-3m)	Cu2O	2	(CU+1)2(O-2)1
CU3P	Cu3P	-	hP24	(185, P6_3cm)	-	2	(CU)3(P)1
CUP2	CuP2	-	mP12	(14, P2_1/c)	-	2	(CU)1(P)2
CU2P7	Cu2P7	-	mS72	(12, C2/m)	-	2	(CU)2(P)7
CU2S_ALPHA	Cu2S-alpha	-	mP144	(14, P2_1/c)	-	2	(CU)2(S)1
CU2S_BETA	Cu2S-beta	-	hP16	(194, P6_3/mmc)	-	2	(CU)2(S)1
CU2S_GAMMA	Cu2Se	-	cF44	(225, Fm-3m)	-	3	(CU, FE, MN, NI, PB, ZN, VA)2(CU, VA)1(S)1
CU31S16	Cu31S16	-	mP376	(14, P2_1/c)	-	2	(CU)1.93(S)1
CU7S4	Cu7S4	-	oP44	(62, Pnma)	-	2	(CU)1.75(S)1
CUSE_HT	Covellite (CuS, B18)	B18	hP12	(194, P6_3/mmc)	-	2	(CU)1(S, SE)1
CU2SE_LT	Cu2Se	-	mS144	(15, C2/c)	-	2	(CU, SE)2(SE)1
CU2SE_HT	Cu2Se	-	cF44	(225, Fm-3m)	-	2	(CU, SE)2(SE)1
CU3SE2	Cu3Se2	-	tP10	(113, P-42_1m)	-	2	(CU)3(SE)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CUSE2	Marcasite (FeS ₂ , C18)	C18	oP6	(58, Pnm)	-	2	(CU)1(SE)2
CUSE_LT	Cu _{0.87} Se	-	hP26	(194, P6 ₃ /mmc)	-	2	(CU)1(SE)1
CUSE_RT	CuS	-	oS24	(63, Cmc)	-	2	(CU)1(SE)1
HALITE	Rock Salt/Halite (NaCl, B1)	B1	cF8	(225, Fm-3m)	This is FeO, MnO	2	(CU+2, FE+2, FE+3, MN+2, MN+3, VA)1(O-2)1
MS_B81	Nickeline (NiAs, B81)	B81	hP4	(194, P6 ₃ /mmc)	-	2	(CU, FE, NI, VA)1(S)1
MS2_C2	Pyrite (FeS ₂ , C2)	C2	cP12	(205, Pa-3)	-	2	(FE, MN, NI)1(S)2
FEZR3	Re3B	-	oS16	(63, Cmc)	-	2	(FE)1(ZR)3
MG2NI	Mg ₂ Ni (Ca)	Ca	hP18	(180, P6 ₂ 22)	-	2	(MG, SN)2(CU, NB, NI)1
MG2SI_C1	Fluorite (CaF ₂ , C1)	C1	cF12	(225, Fm-3m)	-	2	(MG)2(SI, SN)1
ALPHA_SPINEL	Hausmannite (Mn ₃ O ₄)	-	tI28	(141, I4 ₁ /amd)	With solubility of Cu, Fe	4	(CU+2, MN+2, MN+3)1(FE+3, MN+2, MN+3, VA)2(MN+2, VA)2(O-2)4
M2O3C	Bixbyite (Mn ₂ O ₃ , D53)	D53	cI80	(206, Ia-3)	-	3	(FE+3, MN+3)2(O-2, VA)3(O-2, VA)1
RUTILE	Rutile (TiO ₂ , C4)	C4	tP6	(136, P4 ₂ /mnm)	This is MnO ₂	2	(MN+4)1(O-2)2
MS_B1	Rock Salt/Halite (NaCl, B1)	B1	cF8	(225, Fm-3m)	-	2	(CU, MN, PB)1(S)1
NI3S2_LT	Hazelwoodite (Ni ₃ S ₂ , D5e)	D53	hR5	(155, R32)	-	2	(NI)3(S)2
NIS_LT	Millerite (NiS, B13)	B13	hR6	(160, R3m)	This is low temperature NiS.	2	(NI)1(S)1
THIOSPINEL	Spinel (Co ₃ O ₄ , D72)	D72	cF56	(227, Fd-3m)	This is a sulphur spinel: (Cu, Fe, Mn)Cr ₂ S ₄ , Co ₃ S ₄ , FeNi ₂ S ₄ and Ni ₃ S ₄ .	3	(NI)1(NI)2(S)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI9S8	Ni9S8	-	oS68	(21, C222)	-	2	(NI)9(S)8
HEAZLEWOODITE_B1	Cu1.9S	-	cF12	(216, F-43m)	This is non-stoichiometric high temperature Ni3S2.	2	(NI, VA)2(S)1
HEAZLEWOODITE_B2	Unknown Structure	-	-	-	This is non-stoichiometric high temperature Ni4S3.	2	(NI, VA)2(S)1
NI7S6	Unknown Structure	-	t**	-	-	2	(NI)7(S)6
NI19SI6	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(SI)0.24(CU, NI)0.76
NI5SI2	Ni31S12	-	hP42	(150, P321)	-	2	(CU, FE, NI)5(AL, SI)2
NI2TA_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(NI, TA)2(NI, TA)1
NI3TA	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	-	2	(NI, TA)3(NI, TA)1
SN4P3	Sn3.6As3	-	hR21	(166, R-3m)	-	2	(SN)4(P)3
SNS_B16	GeS (B16)	B16	oP8	(62, Pnma)	-	2	(SN)1(S)1
SNS_B33	CrB (B33)	B33	oS8	(63, Cmcm)	-	2	(SN)1(S)1
SN2S3	Sn2S3	-	oP20	(62, Pnma)	-	2	(SN)2(S)3
SNS2_C6	omega Phase (CdI2, C6)	C6	hP3	(164, P-3m1)	-	2	(SN)1(S)2
ZNS_B3	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)	-	2	(ZN)1(S)1
ZNS_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	-	2	(ZN)1(S)1
SI3TA5_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	-	2	(SI)3(TA)5
QUARTZ	alpha-Quartz (low Quartz)	-	hP9	(152, P3_121)	-	1	(SIO2)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CRISTOBALITE	Ideal beta-Cristobalite (SiO ₂ , C9)	C9	cF24	(227, Fd-3m)	-	1	(SiO ₂)1
TRIDYMITTE	Monoclinic (Cc) Low Tridymite (SiO ₂)	-	mS144	(9, Cc)	-	1	(SiO ₂)1
AL8CECU4	CeMn4Al8	-	tI26	(139, I4/mmm)	-	3	(Al)0.6154(CE)0.0769(CU)0.3077
ALCECU_T2	Zn17Th2	-	hR57	(166, R-3m)	-	2	(Al, CU)0.8947(CE)0.1053
ALCECU_T3	ThCr2Si2	-	tI10	(139, I4/mmm)	-	2	(Al, CU)0.8(CE)0.2
ALCECU_T4	ZrNiAl	-	hP9	(189, P-62m)	-	3	(Al)0.3333(CE)0.3333(CU)0.3334
ALCE2CU2_T5	Unknown Structure	-	-	-	-	3	(Al)0.2(CE)0.4(CU)0.4
AL23CUFE4	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)	-	3	(Al)23(CU)1(Fe)4
AL62CU25FE13	Quasicrystal	-	-	-	-	3	(Fe)0.125(Al, CU)0.255(Al)0.62
AL7CU2FE	FeCu2Al7 (E9a)	E9a	tP40	(128, P4/mnc)	-	3	(Fe, Ni)1(CU)2(Al)7
AL10CU10FE	(Al10Cu10Fe)	-	oF116	(42, Fmm2)	-	3	(Fe)1(Al, CU)10(Al)10
AL28CU4MN7	Mn6Cu4Al29	-	oS156	(63, Cmcm)	-	3	(Al)28(MN)7(CU)4
AL11CU5MN3	Unknown Structure	-	oP380	-	-	3	(Al)11(MN)3(CU)5
ALCU3MN2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	3	(Al)1(MN)2(CU)3
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5	-	hR14	(166, R-3m)	-	2	(Al)1(Fe, CU, NI, VA)1
DELAFOSSITE	Rhombohedral Delafossite (CuFeO ₂)	-	hR4	(166, R-3m)	This is Cu(Al, B, Cr, Fe, La, Mn, Y)O ₂	3	(CU+1)1(AL+3, FE+3, MN+3)1(O-2)2
AL5CU4ZN	Unknown Structure	-	-	-	-	4	(Al, CU)1(AL)4(CU)4(ZN)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL9FENI	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)	-	2	(Al)9(Fe, Ni)2
AL10FE3NI	Co2Al5 (D811)	D811	hP28	(194, P6_3/mmc)	-	2	(Al)5(Fe, Ni)2
AL71FE5NI24	Unknown Structure	-	-	-	-	3	(Al)0.71(Fe)0.05(Ni)0.24
CUFES2	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)	-	3	(Cu)1(Fe)1(S)2
CU2FESN	Unknown Structure	-	-	-	-	3	(Cu)2(Fe)1(SN)1
CU85NI5LA10	(CU85NI5LA10)	-	CF*	(225, Fm-3m)	-	3	(Cu)85(Ni)5(LA)10
CU16MG6SI7	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	3	(Cu)16(MG)6(SI)7
CU3MG2SI	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_3/mmc)	-	3	-
CUMGSN	Half-Heusler (AgAsMg, C1b)	C1b	cF12	(216, F-43m)	-	3	(Cu)0.3334(SN)0.3333(MG)0.3333
CU5MN4SI	Unknown Structure	-	-	-	-	3	(Cu)0.5(MN)0.37(SI)0.13
CU4MNSN	MgCu4Sn	-	cF24	(216, F-43m)	-	3	(Cu)0.6666(SN)0.1667(MG, MN)0.1667
CUMNZN	Unknown Structure	-	-	-	-	3	-
CUNITI_T1	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(Cu, Ni)0.6667(TI)0.3333
CUNITI_T2	Cu3Ti2	-	tP10	(129, P4/nmm)	-	3	(Cu)0.035(Ni)0.565(TI)0.4
CUNITI_T4	BaPb3	-	hR12	(166, R-3m)	-	3	(Cu, TI)0.075(Cu, Ni)0.675(TI)0.25
CUNITI_T6	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	-	3	(Cu, TI)0.25(Cu, Ni)0.5(TI)0.25

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU4SNS4	Cu4SnS4	-	oP36	(62, Pnma)	-	2	(CU2S)2(SNS2)1
CU4SN3S8	Unknown Structure	-	-	-	-	2	(CU2S)2(SNS2)3
CU2SNS3	Cu2GeS3	-	mS24	(9, Cc)	-	2	(CU2S)1(SNS2)1
CU2SN3S7	Cu4Sn7S16	-	hR84	(166, R-3m)	-	1	(CU2S, SNS2)1
CU5SN2S7	Cu5Sn2Se7	-	mS28	(5, C2)	-	3	(CU)5(SN)2(S)7
CU10SN2S13	Unknown Structure	-	-	-	-	3	(CU)10(SN)2(S)13
CUSITI	MnCuP	-	oP12	(62, Pnma)	-	3	(CU)1(SI)1(TI)1
CU2TIZR	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	-	3	(CU)0.5(TI)0.25(ZR)0.25
NISNZN_T1	Unknown Structure	-	-	-	-	3	(NI, SN, VA)0.36(NI, SN)0.38(VA, ZN)0.26
NISNZN_T2	Unknown Structure	-	-	-	-	3	(NI, VA)0.55(SN)0.26(VA, SN, ZN)0.19
NISNZN_T3	Unknown Structure	-	-	-	-	3	(NI, VA)0.482(SN)0.204(VA, SN, ZN)0.314
NISNZN_T4	Unknown Structure	-	-	-	-	3	(NI, SN, VA)0.505(SN, ZN)0.39(VA, SN, ZN)0.105

Gas and Liquid Phase Models

Phase Name	Prototype	Sublattices	Formula Unit
GAS	Gas	1	(AL, AL1AS1, AL1AU1, AL1B1O2, AL1C1, AL1C2, AL1CU1, AL1CU1S1, AL1CU1S2, AL1O1, AL1O2, AL1P1, AL1P2, AL1S1, AL1S2, AL1SE1, AL2, AL2C2, AL2O1, AL2O2, AL2O3, AL2S1, AL2S2, AL2SE1, AL2SE2, AS, AS1O1, AS1O2, AS1P1, AS1P3, AS1S1, AS1SE1, AS2, AS2P2, AS3, AS3P1, AS4, AS4O10, AS4O6, AS4O7, AS4O8, AS4O9, AS4S4, AS4SE3, AU, AU1C1, AU1CO1, AU1CU1, AU1O1, AU1S1, AU1SE1, AU1S1, AU2, B, B1BE1O2, B1C1, B1C2, B1O1, B1O2, B1S1, B1S2, B1SE1, B2, B2BE1O4, B2C1, B2O1, B2O2, B2O3, B2S1, B2S2, B2S3, B4S6, BE, BE1C2, BE1O1, BE1S1, BE2, BE2O1, BE2O2, BE3O3, BE4O4, BE5O5, BE6O6, BI, BI1O1, BI1S1, BI1SE1, BI2, BI2O1_C2V, BI2O1_DH, BI2O2, BI2O3, BI3, BI3O4, BI4, BI4O6, C,

Phase Name	Prototype	Sublattices	Formula Unit
			C1O1, C1O1S1, C1O2, C1P1, C1P1S1, C1P1S2, C1P2, C1PT1, C1S1, C1S2, C1SE1, C1SE2, C1S1, C1S2, C1S3, C1S4, C2, C2O1, C2P1, C2P2, C2S1, C2S2, C2S3, C3, C3O2, C4, C4NI1O4, C5, C5FE1O5, C60, C6MO1O6, CA, CA1O1, CA1S1, CA2, CD, CD1O1, CD1S1, CD1SE1, CE, CE1O1, CE1S1, CE1SE1, CO, CO1O1, CO1S1, CO1SE1, CO2, CR, CR1O1, CR1O2, CR1O3, CR1S1, CR1S2, CR1SE1, CR2, CR2O1, CR2O2, CR2O3, CU, CU1O1, CU1S1, CU1SE1, CU2, CU2S1, CU2SE1, FE, FE1O1, FE1O2, FE1S1, FE1SE1, FE2, GE, GE1O1, GE1O2, GE1S1, GE1S2, GE1SE1, GE2, LA, LA1O1, LA1S1, LA1SE1, LA2O1, LA2O2, MG, MG1O1, MG1S1, MG2, MN, MN1O1, MN1O2, MN1S1, MN1SE1, MO, MO1O1, MO1O2, MO1O3, MO1S1, MO1S2, MO2, MO2O6, MO3O9, MO4O12, MO5O15, NB, NB1O1, NB1O2, NB1S1, NB1SE1, NB1SE2, NI, NI1O1, NI1S1, NI2, O, O1O1, O1P1, O1PB1, O1PT1, O1S1, O1S2, O1SE1, O1S1, O1SN1, O1TA1, O1TI1, O1ZN1, O1ZR1, O2, O2P1, O2PB1, O2PT1, O2S1, O2SE1, O2S1, O2S2, O2SN1, O2TA1, O2TI1, O2ZR1, O3, O3P2, O3S1, O4P2, O5P2, O6P3, O6P4, O7P4, O8P4, O9P4, P, P1S1, P1SE1, P1S1, P1S2, P2, P2S1, P3, P4, P4S3, PB, PB1S1, PB1S2, PB1SE1, PB2, PB2S2, PT, S, S1SE1, S1S1, S1SN1, S1TA1, S1TI1, S1ZN1, S1ZR1, S2, S2S1, S2SN1, S2SN2, S2TI1, S2ZR1, S3, S4, S5, S6, S7, S8, SE, SE1S1, SE1SN1, SE1TI1, SE1ZN1, SE2, SE3, SE4, SE5, SE6, SE7, SE8, SI, SI2, SI3, SN, SN2, TA, TI, TI2, ZN, ZR, ZR2, AS2SE2, AS4SE4)1
LIQUID	Liquid	1	{AG, CU, FE, GE, LA, MN, MNS, MO, NI, SI, ZN, ZNS, SN, SNS, CO, P, PB, PBS, BE, AU, AL, AS, B, BI, C, CA, CD, CE, CR, CR3GE1, MG, MG2SN, NB, PT, S, SE, TA, TI, ZR, CU2S, CU2SE, CU2O, CUO, AL2/3O1, AL4/3O2, CRO, CRO3/2, NI12P5, NIS, ZR1/2O1, FES, SIO2, FEO, FEO3/2, MNO, MNO3/2)1

TCCU7: Current Version Changes

Current Database Version

Database name (acronym):	TCS Cu-based Alloys Database (TCCU)
Database owner:	Thermo-Calc Software AB
Database version:	7.0
First release:	TCCU1 was released in with 2016b



For earlier changes, see [TCCU: Revision History](#).

TCCU6.2 to TCCU7.0

Software release version: 2026b (June 2026)

New Elements and Phases

- 2 new elements added: S and Ta (34 total).
- 53 new phases added (368 total).

New Binary and Ternary Systems

- 26 new binary systems (175 total): Au-Si, Be-Co, C-Fe, Ce-Fe, Ce-Mg, Cr-Ta, Cu-S, Cu-Ta, Fe-La, Fe-O, Fe-S, Fe-Ta, La-Mg, Mg-Sn, Mn-O, Mn-S, Nb-Sn, Nb-Ta, Ni-S, Ni-Ta, O-Si, Pb-S, S-Sn, S-Zn, Si-Ta, Si-Ti
- 15 new ternary systems (79 total): C-Cu-Fe, Cu-Fe-O, Cu-Fe-S, Cu-Fe-Ta, Cu-Mg-Sn, Cu-Mn-O, Cu-Mn-S, Cu-Nb-Sn, Cu-Ni-Ta, Cu-Ni-S, Cu-Pb-S, Cu-S-Sn, Cu-S-Zn, Cu-Si-Ti, Fe-Mn-O

Updated Binary and Ternary Systems

- 7 updated binary systems: Al-Sn, C-Cu, Cr-Zr, Cu-Zr, Fe-Sn, Mn-Zn, Sn-Zr
- 4 updated ternary systems: Al-Cu-Sn, Cr-Cu-Zr, Cu-Fe-Sn, Cu-La-Zr

Thermophysical Properties

- Molar volumes, surface tensions, and viscosities were included with the additions of new elements of Ta and S.
 - Added viscosities of Se-containing binary interactions.
 - Updated thermal conductivity and electrical resistivity of B.
-

TCCU: Revision History



For the most recent changes, see [TCCU7: Current Version Changes](#).

TCCU6.1 to TCCU6.2

Software release version: 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.

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.
