TCS Noble Metal Alloys Database (TCNOBL4)

Technical Information

Available Starting with Thermo-Calc 2025b

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Contents

About the TCS Noble Metal Alloys Database (TCNOBL)

TCS Noble Metal Alloys Database (TCNOBL) is a thermodynamic and properties database developed by Thermo-Calc software for noble (or precious) metal-based alloys. It is intended for applications in jewelry, dental alloys, decoration industries, and delicate components in scientific instruments. The database includes nearly all stable phases in the assessed systems that may form in as-cast and aged noble-based alloys.

A hybrid approach of experiments, first-principles calculations and CALPHAD modeling are used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges. The database is validated against many commercial noble alloys and available experimental information.

TCNOBL4 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 noble 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 can also be used for predicting solidification behavior of noble alloys with the Scheil Calculator in Graphical Mode or the SCHEIL_GULLIVER module in Console Mode.

In addition to thermodynamic data, it has thermophysical properties data available for:

- Molar volume with thermal expansion coefficients
- Electrical resistivity
- Thermal conductivity
- Viscosity of metallic liquids
- Surface tension of metallic liquids

TCNOBL4 Thermophysical Properties

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 also compatible with the corresponding mobility database TCS Noble Metal Alloys Mobility Database (MOBNOBL) 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 MOBNOBL2.

TCS Noble Metal Alloys Database (TCNOBL) is also integral to the Noble Metal Alloys Model Library. Noble metal alloys are frequently developed for the purpose of achieving an attractive color. In particular, the Au-Ag-Pt-Cu-Al system is of interest. The Noble Metal Alloys Model Library includes one model, the Optical Properties Model, that was designed for predicting the optical properties and apparent color of noble metal alloys as a function of incident light and other important variables. The model is intended to assist users in achieving an attractive color when developing noble metal alloys for the purpose of cosmetic applications.

The Noble Metal Alloys Model Library is available for free to all users who have the TCS Noble Metal Alloys Database (TCNOBL) (version 3 or newer) and who have a valid Maintenance & Support Subscription (M&SS).

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 areas such as process metallurgy, heat treatment, and more depending on the database. Sometimes an example is both a validation and a calculation example.

Some general use case examples of how the database can be used include the following.

For your actual alloy chemistry, use the database to calculate:

- Critical transformation temperatures such as solvus temperatures of precipitates, amounts and compositions of phases, solubility limits, activities, phase diagrams.
- Liquidus, solidus, incipient melt temperatures, freezing range, fraction solid curves, solidification path, fraction eutectic, microsegregation, partition coefficients, latent heat, shrinkage.
- Thermophysical properties for liquid and solid phases such as volume, density, thermal conductivity/resistivity, and electrical conductivity/resistivity.
- Liquid properties such as viscosity and surface tension.

Then in combination with the Add on Diffusion Module (DICTRA) or Precipitation Module (TC-PRISMA), which use a compatible mobility database, you can also calculate such things as:

- Optimal homogenization temperatures, time needed to homogenize any chemical segregation arising from solidification, and/or dissolve precipitates.
- Concurrent nucleation, growth/dissolution, coarsening of precipitate phases, volume fraction, and size distribution as a function of time.
- Simulate general diffusion controlled phase transformations with the Diffusion Module (DICTRA)
- Simulate multi-particle precipitations during aging treatment with the Precipitation Module (TC-PRISMA).

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.

Revision History

TCNOBL: TCS Noble Metal Alloys Database Revision History. The current version of the database is TCNOBL4. See the link for any subversion release details.

TCS Noble Metal Alloys Database (TCNOBL) 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 Noble Metal Alloys Database (TCNOBL) 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 Noble Metal Alloys Database (TCNOBL) Validation and Calculation 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 Noble Metal 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 Precious Metals and the Noble Metal Alloys Model Library, where there are links to resources such as examples, publications, and more.

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.

TCNOBL4 Elements, Systems, and Phases

This section summarizes the available elements, assessed systems, and total number of phases in the TCS Noble Metal Alloys Database (TCNOBL).

Included Elements

There are 26 elements included in the most recent version of the database.

Included Elements									
Ag	Al	Au	Ca	Co	Cr	Cu	Fe	Ga	Ge
In	Ir	Li	Mn	Ni	Pd	Pt	Re	Rh	Ru
Sb	Sc	Si	Sn	Ti	Zn				

Assessed Systems and Phases

The most recent version of the database contains:

- 220 assessed binary systems. These can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 71 ternary systems These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 376 solution and intermetallic phases, which includes nearly all stable phases in the assessed systems that may form in as-cast and aged noble-based alloys.

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`.

TCNOBL4 Thermophysical Properties

This section summarizes the available properties in the TCS Noble Metal Alloys Database (TCNOBL).

Molar volume with thermal expansion coefficients properties data are available starting with TCNOBL1. Electrical resistivity, thermal conductivity, viscosity of metallic liquids, and surface tension of metallic liquids properties data are available starting with TCNOBL3.

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.

Model Descriptions

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

Thermophysical 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 versus Graphical Mode as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property (and Graphical Mode Variable Name)	*Model Parameters*	*Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)****
Molar volume	V0, 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

Property (and Graphical Mode Variable Name)	*Model Parameters*	*Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)****
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.

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

*** The examples listed for the SDKs are using Console Mode 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

Go to the Noble Metal 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 Precious Metals and the Noble Metal Alloys Model Library, where there are links to resources such as examples, publications, and more.

TCNOBL4 Systems

In this section:

TCNOBL4 Assessed Binary Systems

	Ag	Al	Au	Ca	Co	Cr	Cu	Fe	Ga	Ge	In	Ir	Li	Mn	Ni	Pd	Pt	Re	Rh	Ru	Sb	Sc	Si	Sn	Ti	Zn
Ag	Ag																									
Al	x	Al																								
Au	x	x	Au																							
Ca	x		x	Ca																						
Co	x	x	x		Co																					
Cr	x	x	x		x	Cr																				
Cu	x	x	x	x	x	x	Cu																			
Fe	x	x	x		x	x	x	Fe																		
Ga	x	x	x		x	x	x		Ga																	
Ge	x	x	x		x	x	x		x	Ge																
In	x	x	x		x		x	x	x	x	In															
Ir	x	x	x		x	x	x	x	x	x	x	Ir														
Li	x		x				x						Li													
Mn	x	x	x		x	x	x	x			x	x		Mn												
Ni	x	x	x		x	x	x	x	x	x	x	x		x	Ni											
Pd	x	x	x		x	x	x	x	x	x	x	x		x	x	Pd										
Pt	x	x	x		x	x	x	x	x	x	x	x		x	x	x	Pt									
Re	x	x	x		x	x	x	x	x	x	x	x		x	x	x	x	Re								
Rh	x	x	x		x	x	x	x	x	x	x	x		x	x	x	x	x	Rh							
Ru	x	x	x		x	x	x	x	x	x	x	x		x	x	x	x	x	x	Ru						
Sb	x		x		x		x								x						Sb					
Sc	x		x				x															Sc				
Si	x		x				x									x	x						Si			
Sn	x	x	x		x	x	x	x	x	x	x			x	x	x	x	x	x	x				Sn		
Ti	x	x	x		x	x	x	x	x	x		x		x	x	x	x	x	x	x				x	Ti	
Zn	x	x	x		x	x	x	x	x	x	x			x	x	x	x		x	x				x	x	Zn

TCNOBL4 Assessed Ternary Systems

Assessed Ternary Systems				
Ag-Al-Au	Ag-Al-Cu	Ag-Au-Cu	Ag-Au-Ge	Ag-Au-In
Ag-Au-Ni	Ag-Au-Pd	Ag-Au-Pt	Ag-Au-Si	Ag-Au-Sn
Ag-Au-Zn	Ag-Cu-Ge	Ag-Cu-In	Ag-Cu-Ni	Ag-Cu-Pd
Ag-Cu-Si	Ag-Cu-Sn	Ag-Cu-Zn	Ag-Ga-Sn	Ag-In-Pd
Ag-In-Sn	Ag-In-Zn	Ag-Ir-Pd	Ag-Ni-Sn	Ag-Pd-Rh
Ag-Sn-Zn	Al-Au-Cu	Al-Cu-Sn	Al-Ga-Zn	Al-Ge-Zn
Al-In-Sn	Al-Ni-Pt	Al-Sn-Zn	Au-Co-Sn	Au-Cu-Fe
Au-Cu-Ge	Au-Cu-In	Au-Cu-Ni	Au-Cu-Pd	Au-Cu-Pt

TCNOBL4 Phases

In this section:

Common Phases for Noble / Precious Metals

TCNOBL4 Models for the Included Phases

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

Name in the Database	*Common Name and Description*
FCC_A1	Disordered solution phase. E.g. (Ag), (Au), (Cu), (Pd) and (Pt).
BCC_B2	Can be both disordered and ordered (CsCl-structure). E.g. BCC_A2 (disordered), BCC_B2 (ordered), β, β'
HCP_A3	Disordered solution phase. (Ti), A3
HCP_ZN	Disordered solution phase. (Zn), A3
BCT_A5	Disordered solution phase. (Sn), β-Sn, A5
L10_FCC	Ordered phase. E.g. CuAu, IrTi
L12_FCC	Ordered phase. Bogdanovite, Cu3Au, Ni3Si,
CBCC_A12	α-Mn
CUBIC_A13	β-Mn
ORTHORHOMBIC_GA	(Ga), α-Ga, A11
DIAMOND_A4	(Ge), A4
TETRAGONAL_A6	Disordered solution phase. (In), A6
CU3IN_GAMMA_D83	Gamma-brass, Cu9Al4, Cu9In4, D83,
CU5ZN8_GAMMA_D83	Gamma-brass, Cu5Zn8, D82
CU6SN5_HT_NIAS	AlCu_D81, AuSn_Delta, Co3Sn2, Cu2In_HT, Cu6Sn5_HT, Ge3Ni5_HT, InNi2_HT, Mn(2-x)Sn, Ni3Sn2, Pd2Sn_HT, PtSn
AG3SN_L60_CU3TI	beta-TiCu3 (D0a)
AL2CU_C16	Khatyrkite, Al2Cu, AlHf2, Fe2B, FeGe2, FeZr2, FeSn2, Mn2B, MnSn2, NIB2, NIZr2, SiZr2
AL2AU_C1_CAF2	Fluorite (CaF2, C1)
AL3NI2_D513	Al3Ni2, Al3Pd2, Al3Pt2, Al3Ru2, Au3In2, Ga3Pt2, In3Ni2, In3Pd2, In3Pt2

Name in the Database	*Common Name and Description*
AL3PD5_OP16	Rh5Ge3, Al3Pd5, Al3Pt5, In3Pd5
AL21PT8_TI116	Al21Pd8, Al21Pt8
AU10SN_D024	Ni3Ti, AuIn_Alpha1, AuSn_Beta
AUSN4_OS20	AuSn4, PdSn4, PtSn4
COSN_HP6	CoSn, FeSn and InNi
CO2SI_C23	Cotunnite, PbCl2, Ca2Si, NI2Si, SiSr2, SnSr2, GeSr2
GEPT3_MS16	GePt3, Ni25Si9, Pt3Si_LT
NI3SN_D019	Ni3Sn, SnTi3, SnMn3, AlLa3

TCNOBL4 Models for the Included Phases

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
LIQUID	Liquid				Metallic LIQUID:L solutionphase	1	(AG, AL, AU, CA, CO, CR, CR3GE1, CU, FE, GA, GE, IN, IR, LI, MN, NI, PD, PT, PTSN, RE, RH, RU, SB, SC, SI, SN, TI, ZN)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	Metallic FCC_A1 solution, e.g. (Al), (Cu), and MC carbides	2	(AG, AL, AU, CA, CO, CR, CU, FE, GA, GE, IN, IR, LI, MN, NI, PD, PT, RE, RH, RU, SB, SC, SI, SN, TI, ZN)1(VA)1
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	L12phase, Ni3Si_rt, AlZr3, GeNi3, TiZn3, VZn3	2	(AG, AL, AU, CO, CR, CU, FE, GA, GE, IR, MN, NI, PD, PT, RH, TI, ZN)1(AG, AL, AU, CO, CR, CU, FE, GA, GE, IR, MN, NI, PD, PT, RH, TI, ZN)3
L10_FCC	CuAu (L10)	L10	tP2	(123, P4/mmm)	also IrTi.	2	(AG, AL, AU, CO, CU, FE, GA, GE, IR, MN, NI, PD, PT, TI, ZN)0.5(AG, AL, AU, CO, CU, FE, GA, GE, IR, MN, NI, PD, PT, TI, ZN)0.5
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	Metallic BCC_A2 solution	2	(AG, AL, AU, CA, CO, CR, CU, FE, GA, GE, IN, IR, LI, MN, NI, PD, PT, RE, RH, RU, SB, SC, SI, SN, TI, VA, ZN)1(VA)3
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	Solution ofordered BCC_B2, having Gibbs energy contribution from BCC_A2	3	(AG, AL, AU, CA, CO, CR, CU, FE, GA, GE, IN, IR, LI, MN, NI, PD, PT, RE, RH, RU, SB, SC, SI, SN, TI, VA, ZN)0.5(AG, AL, AU, CA, CO, CR, CU, FE, GA, GE, IN, IR, LI, MN, NI, PD, PT, RE, RH, RU, SB, SC, SI, SN, TI, VA, ZN)0.5(VA)3
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(AL, CO, CR, CU, FE, IN, IR, MN, NI, PD, PT, RE, RU, SN, TI, ZN)1(VA)1
CUBIC_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		1	(AG, AL, CO, CR, CU, FE, IN, IR, MN, NI, PD, PT, RE, RU, SN, TI, ZN)1
BCT_A5	beta-Sn (A5)	A5	tI4	(141, I4_1/amd)	Pure Sn or itssolution	1	(AG, AL, CU, GA, IN, NI, SN, ZN)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	Metallic HCP_A3 solution alpha_ Mg/Hf/Sc/Ti/Zr,epsilon_CuZn, etc.	2	(AG, AL, AU, CO, CR, CU, FE, GA, GE, IN, IR, LI, MN, NI, PD, PT, RE, RH, RU, SB, SC, SI, SN, TI, ZN)1(VA)0.5
HCP_ZN	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)		2	(AG, AL, AU, CO, CR, CU, FE, GA, GE, IN, IR, MN, NI, PD, PT, RE, RH, RU, SN, TI, ZN)1(VA)0.5
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)		2	(AL, MN, TI)3(AL, PT, TI)1
BCT_D022	Al3Ti (D022)	D022	tI8	(139, I4/mmm)		2	(AL, GA, TI)3(AL, TI)1
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	Pure C, Ge, Si orsolution phases based on them	1	(AG, AU, GA, GE, SI, SN, TI)1
ORTHORHOMBIC_GA	alpha-Ga (A11)	A11	oS8	(64, Cmce)		1	(GA)1
TETRAGONAL_A6	In (A6)	A6	tI2	(139, I4/mmm)		1	(AL, GA, IN, SN, ZN)1
RHOMBOHEDRAL_A7	alpha-As (A7)	A7	hR2	(166, R-3m)		1	(SB)1
DIS_SIG	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)	Part of the description for the SIGMA phase.	1	(CO, CR, FE, MN, RE, RU)1
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		3	(CO, CR, FE, MN, RE, RU)10(CO, CR, FE, MN, RE, RU)4(CO, CR, FE, MN, RE, RU)16
HIGH_SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		3	(MN)8(CR)4(CR, MN)18
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	Solution of MgZn2-type phases, including MgZn2 (Eta, aka M orsigma)	2	(CR, FE, MN, TI, ZN)2(CR, FE, MN, TI, ZN)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	Solution of Cu2Mg-type phases, cF24, Fd-3m	2	(CO, CR, TI)2(CO, CR, TI)1
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)	Solution of MgNi2-type phases, hP24, P63/mmc	2	(CO, CR, TI)2(CO, CR, TI)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CHI_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		3	(RE)24(TI)10(RE)24
AG2GA	Mg2In		hP9	(189, P-62m)		2	(AG)2(AG, GA, VA)1
AG3GA2	Unknown Structure		hR*			2	(AG)3(GA)2
ALCR2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	Same as AlCr2, CuTi2, PdTi2, RhTi2, Ti2Zn	2	(AL, CU, PD, RH, ZN)1(CR, TI)2
AL2CU_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Al2Cu,AlHf2,Fe2B,FeGe2,FeZr2,FeSn2,Mn2B, MnSn2,NIB2,NIZr2,SiZr2	2	(AG, AL, CO, CU, FE, MN, PD, RH)0.33333(AL, IN, MN, SN)0.66667
CU5ZN8_GAMMA_D83	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		3	(AL, IN, NI, ZN)4(AG, AL, AU, CU, IN, NI, ZN)1(AG, AU, CU, IN, SN, ZN)8
AG15PT17	Unknown Structure		hR*			2	(AG)0.46875(PT)0.53125
AG3SN_L60_CU3TI	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)		2	(AG, AU, CO, CU, NI, SB, ZN)0.75(AG, AU, IN, NI, SB, SC, SN)0.25
AGZN_ZETA	zeta-AgZn (Bb)	Bb	hP9	(147, P-3)		1	(AG, CU, IN, SN, ZN)1
AL2AU_C1_CAF2	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(AG, AL, AU, CU, GA, GE, IN, SN)0.66667(AL, AU, CO, NI, PT, SN)0.33333
ALAU1	AlAu		mP8	(11, P2_1/m)		2	(AL)0.5(AU)0.5
PDSN_B31	MnP (B31)	B31	oP8	(62, Pnma)		2	(GA, GE, PD, SI, SN)0.5(AU, NI, PD, PT, VA)0.5
ALAU2_HT	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AL, AU)1(AL, AU)2
ALAU2_LT	AlAu2		oP12	(62, Pnma)		2	(AL)1(AL, AU, CU)2
ALAU4_LT	AlAu4		cP20	(198, P2_13)		2	(AL)0.2(AG, AU, CU)0.8

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3AU8	Yb8In3		hR132	(167, R-3c)		2	(AL)0.27273(AU)0.72727
AL13CO4	Orthorhombic Co4Al13		oP102	(31, Pmn2_1)		2	(AL)13(CO)4
AL3CO	Os4Al13		mS34	(12, C2/m)		2	(AL)3(CO)1
AL5CO2_D811	Co2Al5 (D811)	D811	hP28	(194, P6_ 3/mmc)	also Al5Rh2.	2	(AL)5(CO, RH)2
AL9CO2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)		2	(AL, GA)9(CO, RH)2
AL11CR2	Al5Cr		mS732	(15, C2/c)		3	(AL)10(AL)1(CR)2
AL13CR2	Al45V7		mS104	(12, C2/m)		2	(AL)13(CR)2
AL4MN	mu-Al4Mn		hP574	(194, P6_ 3/mmc)		2	(AL)4(CR, MN)1
AL8CR5_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		2	(AL)8(CR)5
AL8CR5_L	Cr5Al8 (D810)	D810	hR26	(160, R3m)		2	(AL)8(CR)5
AL9CR4_H	Unknown Structure					2	(AL)9(CR)4
AL9CR4_L	Unknown Structure					2	(AL)9(CR)4
ALCU_GAMMA_HT	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	aka GAMMA_H., Cu5Zn8-type Al4Cu9 (ht) phase	3	(AL, ZN)4(AL, CU, ZN)1(AG, CU)8
ALCU_ETA	AlCu(r)		mS20	(12, C2/m)		2	(AL, CU)0.5(AG, CU, ZN)0.5
CU6SN5_HT_NIAS	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)	AlCu_D81, AuSn_Delta, Co3Sn2, Cu2In_HT, Cu6Sn5_HT, Ge3Ni5_HT, InNi2_HT, Mn(2-x)Sn, Ni3Sn2, Pd2Sn_HT, PtSn	3	(AG, AU, CO, CU, MN, NI, PD, PT, VA)1 (AG, AL, CU, GE, IN, NI, SB, SN)1(AU, CO, CU, MN, NI, PD, VA)1
ALCU_ZETA	Al9Cu11(h)		oF88	(42, Fmm2)		2	(AG, CU)0.55(AL, IN)0.45

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL2CU3_DELTA	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(AL)0.4(AG, CU)0.6
AL2FE1	Al2Fe		aP18	(1, P1)		2	(AL)2(FE)1
AL5FE2	Al2.8Fe		oS24	(63, Cmcm)		2	(AL)5(FE)2
AL5FE4	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		1	(AL, FE)1
AL9IR2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)		2	(AL)0.818(IR)0.182
AL45IR13	Al45Ir13		oP236	(62, Pnma)		2	(AL)0.776(IR)0.224
AL13IR4	Unknown Structure					2	(AL)0.765(IR)0.235
AL28IR9	Al28Ir9		hP236	(159, P31c)		2	(AL)0.757(IR)0.243
AL3IR	Na3As (D018)	D018	hP8	(194, P6_ 3/mmc)		2	(AL)0.75(IR)0.25
AL2_7IR	Al2.75Ir		cP60	(195, P23)		2	(AL)0.73(IR)0.27
AL13FE4	Al13Fe4		mS102	(12, C2/m)	solution phases based on Al13Fe4, aka Al3Fe	3	(AL, CU)0.6275(FE, MN, RU)0.235(AL, VA)0.1375
AL12MN	Al12W		cI26	(204, Im-3)		2	(AL)12(MN)1
AL4MN_R	lambda-Al4Mn		hP586	(194, P6_ 3/mmc)	AL461MN107	2	(AL)0.81162(MN)0.18838
AL11MN4_LT	Al11Mn4		aP15	(2, P-1)		2	(AL)11(MN)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)12(MN)5(AL, MN)9
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)		2	(AL)6(MN, RE, RU)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3NI2_D513	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)	Al3Ni2, Al3Pd2, Al3Pt2, Al3Ru2, Au3In2, Ga3Pt2, In3Ni2, In3Pd2, In3Pt2	3	(AG, AL, AU, GA, GE, IN, PD, SN)0.6(AL, AU, IN, NI, PD, PT, RU)0.4(IN, NI, VA)0.2
AL3NI_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(AL, PD, PT)0.75(NI)0.25
AL3NI5	Ga3Pt5		oS16	(65, Cmmm)		2	(AL)0.375(NI)0.625
AL2PD5	Unknown Structure					2	(AL)2(AL, PD)5
AL3PD	(Al3Pd)		oP*	(33, Pna2_1)		2	(AL)3(PD)1
AL4PD	(Al4Pd)		hP*	(182, P6_322)		2	(AL)4(PD)1
AL3PD5_OP16	Rh5Ge3		oP16	(55, Pbam)	Al3Pd5, Al3Pt5, In3Pd5	2	(AL, IN)3(CU, PD, PT, RH)5
AL21PT8_TI116	Al21Pt8		tI116	(88, I4_1/a)	Al21Pd8, Al21Pt8	2	(AL)21(PD, PT)8
ALPT_B20	FeSi (B20)	B20	cP8	(198, P2_13)		2	(AL)1(NI, PT, RH)1
ALRH2	Unknown Structure					2	(AL)1(RH)2
AL3RH_LT	(Al3Rh)		oP*	(62, Pnma)		2	(AL)3(RH)1
AL3RH_HT	Unknown Structure					2	(AL)2(RH, VA)1
AL7RH3	Unknown Structure					2	(AL)7(RH)3
RUAL2_C54	TiSi2 (C54)	C54	oF24	(70, Fddd)	also MoSi2, RuAl2, ZrSn2.	2	(RU)1(AL)2
CO2SI_C23	Cotunnite (PbCl2, C23)	C23	oP12	(62, Pnma)	Ca2Si,NI2Si, SiSr2, SnSr2, GeSr2	2	(AL, IN, PD, SN, ZN)1(AL, CU, PD, PT)2
AL21PT5	Li21Si5		cF416	(216, F-43m)		2	(AL)21(PT)5
AL12RE	Al12W		cI26	(204, Im-3)		2	(AL)12(RE)1
AL4RE	Unknown Structure					2	(AL)4(RE)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL11RE4	Al11Mn4		aP15	(2, P-1)		2	(AL)11(RE)4
ALRE2	CuZr2		tI6	(139, I4/mmm)		2	(AL)1(RE)2
ALRE	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(AL)1(RE)1
AL11TI5	Al3Zr (D023)	D023	tI16	(139, I4/mmm)		2	(AL)17(TI)8
AL2TI	Ga2Hf		tI24	(141, I4_ 1/amd)		2	(AL)2(TI)1
AUCU_II	CuAu		oI40	(74, Imma)		2	(AG, AU, CU, GE, NI, PD, PT, ZN)0.5(AG, AU, CU, GE, NI, PD, PT, ZN)0.5
AU7GA2_HT	Au7Ga2		hP27	(189, P-62m)		2	(AU)0.7895(GA)0.2105
AU7GA2_LT	Unknown Structure					2	(AU)7(GA)2
AU7GA3	Unknown Structure					2	(AU)7(GA)3
AU9IN4_GAMMA_D83	Au6(Au0.5In0.5)6In		cP76	(215, P-43m)		4	(AU)0.61539(AU, IN)0.07692(AU, IN)0.23077(IN)0.07692
AUIN_BETA	Unknown Structure					2	(AU)0.785(IN)0.215
AUIN_BETA_PRIME	Cu10Sb3		hP26	(176, P6_3/m)		2	(AU)0.77778(IN)0.22222
AU7IN3	Au7In3		hP60	(147, P-3)		2	(AU)0.7(IN)0.3
AUIN	Unknown Structure					2	(AU)0.5(IN, SN)0.5
AU4MN	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)		2	(AU)0.8(MN)0.2
AU33MN9	Unknown Structure					2	(AU)0.786(MN)0.214
AU13MN4	Unknown Structure					2	(AU)0.765(MN)0.235

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AU3MN	SrPb3		tp4	(123, P4/mmm)		2	(AU)0.75(MN)0.25
AU11MN4	Au11Mn4		mS810	(8, Cm)		2	(AU)0.733(MN)0.267
AU5MN2	Au5Mn2		mS14	(12, C2/m)		2	(AU)0.714(MN)0.286
AU2MN	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AU)0.667(MN)0.333
AUMN2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AU)0.333(MN)0.667
AUSB2_C2	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)	AuSb2, NiSb2, PdSb2	2	(AU)0.33333(SB)0.66667
AU10SN_D024	Ni3Ti (D024)	D024	hP16	(194, P6_3/mmc)	AuIn_Alpha1, AuSn_Beta	1	(AG, AU, GA, GE, IN, SN)1
AUSN2_OP24	AuSn2		oP24	(61, Pbca)		2	(AU, CU, PT)0.33333(SN)0.66667
AUSN_ZETA_PRIME	Au5Sn		hR18	(155, R32)	AuSn_Zeta_Prime	2	(AU)0.84(IN, SN)0.16
AUSN4_OS20	PtSn4		oS20	(68, Ccce)	AuSn4, PdSn4, PtSn4	2	(AU, CU, NI, PD, PT)0.2(IN, PD, SN)0.8
AU5ZN8_GAMMA	Cr4.5(Cr0.56Al0.44)9Al12		hR78	(160, R3m)		4	(AU, ZN)2(AU, ZN)2(AU, ZN)3(ZN)6
AUTI3	Cr3Si		cP8	(221, Pm-3m)		2	(TI)0.75(AU)0.25
AUTI	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(TI, VA)0.5(AU, TI)0.5
AU2TI	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(TI)1(AU)2
AU4TI	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)		2	(AU, TI)0.2(AU)0.8
AU3ZN_ALPHA1	MgAg3		cP4	(221, Pm-3m)		3	(AU)3(AG, AU, CU, ZN)1(CU, ZN)1
AU3ZN_ALPHA2	Au3Zn		oS32	(64, Cmce)		2	(AU)0.75(ZN)0.25

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AU4ZN_ALPHA3	Unknown Structure					3	(AU)18(AG, AU, CU, IN, ZN)7(ZN)3
AUZN3_GAMMA2	UH3		cP32	(221, Pm-3m)		2	(AU)1(ZN)3
AUZN4_GAMMA3	Unknown Structure					3	(AU)0.12(AU, ZN)0.16(ZN)0.72
AU5ZN3	Au5Zn3		oI128	(72, Ibam)		2	(AU)5(ZN)3
AU11ZN14	Unknown Structure					2	(AU)11(ZN)14
AU15ZN85_EPSILON_PRIME	Unknown Structure					2	(AU)0.15(ZN)0.85
INSN_A6	Unknown Structure				INSN_A6 solution phase	1	(IN, SN)1
CO3GE	Unknown Structure					2	(CO)0.75(GE)0.25
CO5GE2	Unknown Structure					2	(CO)0.714(GE)0.286
CO5GE3	Co2Si (C37)	C37	oP12	(62, Pnma)		3	(CO, RH, VA)0.125(CO, RH)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
COGE2	CoGe2		oS24	(64, Cmce)		2	(CO)0.333(GE)0.667
COSN_HP6	CoSn (B35)	B35	hP6	(191, P6/mmm)	CoSn, FeSn and InNi	2	(CO, FE, NI)0.5(IN, SN)0.5
COSN3_OS32	PdSn3		oS32	(64, Cmce)		2	(CO, PD)0.25(PD, SN)0.75
COZN_LT	beta-Mn (A13)	A13	cP20	(213, P4_132)		2	(CO, ZN)1(VA)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
COZN_HT	Unknown Structure					2	(CO, ZN)1(VA)1
COZN_GAMMA_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	Zn11Co2	2	(CO, ZN)1(VA)1
COZN_DELTA	Unknown Structure					2	(CO)0.117647(ZN)0.882353
COZN_GAMMA1	Co2Zn15		mS28	(12, C2/m)	CoZn7	2	(CO)0.125(ZN)0.875
COZN_GAMMA2	CoZn13		mS28	(12, C2/m)	CoZn13	2	(CO)0.0714286(ZN)0.9285714
CR3SI_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(CR, IR, TI)3(CR, GA, GE, IR, RH, RU)1
CRGA	MnGa		hR78	(166, R-3m)		2	(CR)1(GA)1
CR5GA6	Fe3Ga4		mS42	(12, C2/m)		2	(CR)5(GA)6
CRGA4	beta-Hg4Pt		cI10	(229, Im-3m)		2	(CR)1(GA)4
CR5GE3	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	beta-Cr5Ge3	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
CRGE	FeSi (B20)	B20	cP8	(198, P2_13)		2	(CR)0.5(GE)0.5
CR11GE19	Mn11Si19		tP120	(118, P-4n2)		2	(CR)0.367(GE)0.633
CR3MN5	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(CR)3(MN)5
CRNI2_OP6	MoPt2		oI6	(71, Immm)		2	(CR)1(NI)2
CRPD_L10	AuCu		tP4	(123, P4/mmm)		2	(CR)0.5(PD)0.5
CR2PD3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(CR)0.4(PD)0.6

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CR3PT_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(CR)4(PT)1
CRZN13	Unknown Structure		m**			2	(CR)1(ZN)13
CRZN17	Unknown Structure		hP*			2	(CR)1(ZN)17
CU9GA4_0	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)		3	(CU)6(CU, GA)6(GA)1
CU9GA4_1	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)		4	(CU)6(CU, GA)3(CU, GA)3(GA)1
CU9GA4_2	Cu8.2Ga4.8		cP52			4	(CU)3(CU, VA)3(CU, GA)3(GA)4
CU9GA4_3	Cu7.15Ga5.85		cP52			3	(CU, VA)6(CU, GA)3(GA)4
CUGA2	FeSi2-h		tP3	(123, P4/mmm)		2	(CU)1(GA)2
CUGA_THETA	Unknown Structure					2	(CU)0.778(GA)0.222
CU3GE_ETA	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)	eta, low T, D0a	2	(AG, CU)0.75(GE)0.25
CU3GE_EPSILON	Na3As (D018)	D018	hP8	(194, P6_3/mmc)	high T, D018	2	(AG, CU)0.765(GE)0.235
CU3GE_THETA	BiF3 (D03)	D03	cF16	(225, Fm-3m)	high T, D03	2	(AG, CU)0.735(GE)0.265
CU3IN_GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	Cu9In4 Prototype Cu9Al4 (cP52, P-43m), with solubility of Ag, Sn.	3	(AG, AU, CU)0.654(AG, AU, CU, IN)0.115(IN, SN)0.231
CU2IN_LT	Unknown Structure					2	(CU)0.64(IN)0.36
CU7IN3_DELTA	Cu7In3		aP40	(2, P-1)	Cu7In3_Delta	2	(AU, CU)0.7(IN, SN)0.3
CUPT_L11	Rhombohedral CuPt (L11)	L11	hR2	(166, R-3m)	CuIn DELTAT	3	(AU, CU, PT)0.5(AU, CU, PT)0.5(VA)1
GAMMA_D03	BiF3 (D03)	D03	cF16	(225, Fm-3m)	Cu3Sn	1	(CU, MN, NI, SN, ZN)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU3SN	Cu3Sn		oS80	(63, Cmcm)		2	(AU, CU, SN)3(CU, IN, SN)1
CU41SN11	Cu41Sn11		cF416	(216, F-43m)		2	(CU, SN, ZN)41(CU, IN, SN, ZN)11
CU10SN3	Cu10Sn3		hP26	(173, P6_3)		2	(CU, NI)0.769(SN)0.231
CU6SN5_LT	Cu6Sn5		mS44	(15, C2/c)		3	(CU)1(CU, SN)1(SN)1
CU2TI	Au2V		oS12	(63, Cmcm)		2	(CU)2(TI)1
CU3TI2	Cu3Ti2		tP10	(129, P4/nmm)		2	(CU)3(TI)2
CU4TI1	Au4Zr		oP20	(62, Pnma)		2	(CU, TI)4(CU, TI)1
CU4TI3	Cu4Ti3		tI14	(139, I4/mmm)		2	(CU)4(TI)3
CUTI_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(CU, TI)1(CU, TI)1
CUTI3	CuTi3 (L60)	L60	tP4	(123, P4/mmm)		2	(CU, TI)1(TI)3
FE3SN2	Fe3Sn2		hR10	(166, R-3m)		2	(FE)3(SN)2
FE5SN3	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(FE)5(SN)3
FEZN_GAMMA_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		4	(FE, ZN)0.154(FE, ZN)0.154(FE, ZN)0.231(ZN)0.461
FEZN_GAMMA_D81	Fe11Zn40		cF408	(216, F-43m)		3	(FE)0.137(FE, ZN)0.118(ZN)0.745
FEZN_DELTA	FeZn10		hP632	(194, P6_ 3/mmc)		4	(FE)0.058(FE, ZN)0.18(ZN)0.525 (ZN)0.237
FEZN_ZETA	CoZn13		mS28	(12, C2/m)		3	(FE, VA)0.072(ZN)0.856(VA, ZN)0.072

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI5GA3	Ga3Pt5		oS16	(65, Cmmm)		2	(NI)0.63(GA)0.37
NI3GA2	Unknown Structure					2	(NI)0.6(GA)0.4
NI3GA4	Ga4Ni3		cI112	(230, Ia-3d)		2	(NI)0.43(GA)0.57
NIGA4	Unknown Structure					2	(NI)0.2(GA)0.8
GA5PD	Ga5Pd		tI24	(140, I4/mcm)		2	(GA)0.83(PD)0.17
GA7PD3	Ga7Pd3		mS20	(12, C2/m)		2	(GA)0.7(PD)0.3
GAPD_B20	FeSi (B20)	B20	cP8	(198, P2_13)		2	(GA)0.5(PD)0.5
GA3PD5	Rh5Ge3		oP16	(55, Pbam)		2	(GA)0.38(PD)0.62
GAPD2_C37	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(GA, PD)0.33(CU, PD)0.66
GE2NI5_HT	Pd5Sb2		hP42	(185, P6_3cm)		2	(NI)0.72(GE)0.28
GENI2	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(NI)0.665(GE)0.335
GE3NI5_C2	Ge3Ni5		mS32	(5, C2)		2	(NI, PD)0.625(GE)0.375
GA6PT	Unknown Structure					2	(GA, GE)0.857(PT)0.143
GA7PT3	Ir3Ge7 (D8f)	D8f	cI40	(229, Im-3m)		2	(GA, GE)0.7(PT)0.3
GAPT	FeSi (B20)	B20	cP8	(198, P2_13)		2	(GA, GE)0.5(PT)0.5
GA3PT5	Ga3Pt5		oS16	(65, Cmmm)		2	(GA, GE)0.375(PT)0.625
GAPT2	GaPt2		oP24	(51, Pmma)		2	(GA, GE)0.333(PT)0.667
GAPT3	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(GA, GE, PT)0.25(GA, PT)0.75

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GA3RH	In3Ir		tP16	(136, P4_2/mnm)		2	(GA)3(RH)1
GA17RH10	Rh10Ga17		tP108	(116, P-4c2)		2	(GA)17(RH)10
GATI2	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(GA)1(TI)2
GA3TI5	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)		2	(GA)3(TI)5
GA4TI5	Ti5Ga4		hP18	(193, P6_3/mcm)		2	(GA, TI)4(GA, TI)5
GA3TI2	Ti2Ge3		tP10	(83, P4/m)		2	(GA)3(TI)2
GA2TI	Ga2Hf		tI24	(141, I4_1/amd)		2	(GA)2(TI)1
PD21GE8	Al21Pt8		tI116	(88, I4_1/a)		2	(PD)21(GE)8
PD25GE9	Ge9Pd25		hP34	(147, P-3)		2	(PD)25(GE)9
PD2GE	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		2	(PD)2(GE)1
PD3GE	Unknown Structure					2	(PD)3(GE)1
PD5GE	Pd5As		mS24	(5, C2)		2	(PD)5(GE)1
GEPT3_MS16	GePt3		mS16	(12, C2/m)	GePt3, Ni25Si9, Pt3Si_LT	2	(GA, GE, PT)0.25(NI, PT)0.75
GE2PT	Hydrophilite (CaCl2, C35)	C35	oP6	(58, Pnnm)		2	(GA, GE)0.66667(PT)0.33333
GE3PT2	Pt2Ge3		oP20	(62, Pnma)		2	(GA, GE)0.6(PT)0.4
GE2PT3	Pt3Ge2		oP40	(62, Pnma)		2	(GA, GE)0.4(PT)0.6
GEPT2	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		2	(GA, GE)0.333(PT)0.667

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GE7RE3	Re3Ge7		oS40	(63, Cmcm)		2	(GE)7(RE)3
RHGE	Westerveldite (FeAs, B14)	B14	oP8	(62, Pnma)		2	(RH)1(GE)1
RH2GE	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(RH)2(GE)1
RH5GE3	Rh5Ge3		oP16	(55, Pbam)	Rh5Ge3 and Rh5Ti3	2	(RH)5(GE, TI)3
RH17GE22	Rh7Ge22		tI156	(122, I-42d)		2	(RH)17(GE)22
B20_GERU	FeSi (B20)	B20	cP8	(198, P2_13)		2	(GE)1(RU)1
ALPHA_GE3RU2	Ge3Ru2		oP40	(60, Pbcn)		2	(GE)3(RU)2
BETA_GE3RU2	Ru2Sn3		tP20	(116, P-4c2)		2	(GE)3(RU)2
TI5GE3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)		2	(GE)3(TI)5
TI6GE5	Si5V6		oI44	(72, Ibam)		2	(GE)5(TI)6
TIGE2	TiSi2 (C54)	C54	oF24	(70, Fddd)		2	(GE)2(TI)1
IRIN2	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	CoIn2 and IrIn2	2	(CO, IR)1(IN)2
IRIN3_LT	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(IR)1(IN)3
IRIN3_HT	In3Ir		tP16	(136, P4_ 2/mnm)	CoIn3, CoGa3 and ht- IrIn3.	2	(CO, IR)1(GA, IN)3
IN4MN9	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	Formula Mn9.75In3.25	2	(IN)4(MN)9
IN9NI13	Ga9Ni13		mS44	(12, C2/m)	In9Ni13 with solubility of Sn.	3	(NI, VA)1(IN, SN)1(NI)1
INNI_DELTA	CoSn (B35)	B35	hP6	(191, P6/mmm)		2	(NI, VA)1(IN, NI)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
INNI2_RT	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		3	(NI)1(NI)1(IN)1
IN7PD3	Ir3Ge7 (D8f)	D8f	cI40	(229, Im-3m)		2	(IN)0.71(PD)0.29
INPD2_BETA	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(IN)0.34(PD)0.66
INPD3_ALPHA	CuAu (L10)	L10	tP2	(123, P4/mmm)	InPd3_LT	2	(IN)0.25(AG, CU, PD)0.75
INPD3_BETA	Unknown Structure					2	(IN)0.26(PD)0.74
IN7PT3	Ir3Ge7 (D8f)	D8f	cI40	(229, Im-3m)		2	(IN)7(PT)3
INPT	AlCu(r)		mS20	(12, C2/m)		2	(IN, PT)1(IN, PT)1
IN5PT6	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)		2	(IN, PT)5(IN, PT)6
IN9PT13	Ga9Ni13		mS44	(12, C2/m)		2	(IN)9(IN, PT)13
IN2PT3_ALPHA	Pt3Tl2		hP20	(194, P6_ 3/mmc)		2	(IN)2(PT)3
IN2PT3_BETA	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(IN, PT)2(IN, PT)3
INPT2	Ga3Pt5		oS16	(65, Cmmm)	Pt5.33In2.67 rt	2	(IN)1(PT)2
IN3RH	In3Ir		tP16	(136, P4_ 2/mnm)		2	(IN)3(RH)1
INSN_GAMMA	(Hg0.1Sn0.9)		hP1	(191, P6/mmm)		1	(IN, SN)1
MNNI2	Unknown Structure					2	(MN, NI)1(NI)2
MN3PD5	Ga3Pt5		oS16	(65, Cmmm)		2	(MN)3(PD)5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MNPD2	Unknown Structure					2	(MN)1(PD)2
MNPT7	Ca7Ge		cF32	(225, Fm-3m)		3	(PT)6(PT)1(MN)1
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(MN)3(SN)2
MNTI_LT	Zr21Re25		hR92	(167, R-3c)		2	(MN)1(TI)1
MNTI_HT	Unknown Structure		t**			2	(MN)0.515(TI)0.485
MN3TI	Unknown Structure					2	(MN)3(TI)1
MN4TI	R-(Co,Cr,Mo)		hR53	(148, R-3)		2	(MN)0.815(TI)0.185
MNZN9	Unknown Structure		h**			2	(MN)1(ZN)9
NI3SN_D019	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	Ni3Sn, SnTi3,SnMn3, AlLa3	2	(AU, CO, CU, MN, NI, SN, TI)0.75(GA, IN, NI, SN, TI)0.25
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	(12, C2/m)		3	(CU, NI)0.25(IN, NI, SN)0.25(IN, SN)0.5
NITI2	NiTi2		cF96	(227, Fd-3m)		2	(CO, NI, TI)1(NI, TI)2
NI3TI_D024	Ni3Ti (D024)	D024	hP16	(194, P6_ 3/mmc)		2	(NI, TI)0.75(NI, TI)0.25
NIZN_TP2	CuAu (L10)	L10	tP2	(123, P4/mmm)	united HT/LT phase.	2	(CU, NI, PD, ZN)0.5(NI, PD, ZN)0.5
NIZN8_DELTA	Ni3Zn22		mS50	(12, C2/m)		2	(NI)1(ZN)8
PD3SN	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(PD, SN)0.75(PD, SN)0.25
PD20SN13	Unknown Structure					2	(PD, SN)0.6(PD, SN)0.4
PDSN2	PdSn2		tI48	(142, I4_ 1/acd)		2	(PD, SN)0.333(SN)0.667

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PD3SN2_ALPHA	Unknown Structure					2	(PD)0.6(SN)0.4
PD3SN2_BETA	Unknown Structure					2	(PD)3(SN)2
PD3SN2_GAMMA	Unknown Structure					2	(PD)0.59(SN)0.41
PDZN_GAMMA	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		2	(PD, ZN)2(PD, ZN)9
PDZN2	Zn5(Zn0.33Pd0.67)Pd2		oS48	(65, Cmmm)		2	(PD)1(ZN)2
PDZN_ETA	Unknown Structure					2	(PD)0.09(ZN)0.91
PT2SN3	Pt2Sn3 (D5b)	D5b	hP10	(194, P6_3/mmc)		2	(PT)0.4(SN)0.6
PT3SN	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(PT)0.75(SN)0.25
PD2TI	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(PD)2(TI)1
PD3TI2	Pd3Ti2		oS20	(63, Cmcm)		2	(PD)3(TI)2
PD5TI3	Pd5Ti3		tP8	(123, P4/mmm)		2	(PD)5(TI)3
PT8TI	Pt8Ti		tI18	(139, I4/mmm)		2	(PT)8(TI)1
PT3TI_D024	Ni3Ti (D024)	D024	hP16	(194, P6_3/mmc)		2	(PT)3(PT, TI)1
PTTI_B19	beta'-AuCd (B19)	B19	oP4	(51, Pmma)		2	(PT, TI)1(PT, TI)1
PT3TI4	Unknown Structure					2	(PT)3(TI)4
PTTI3_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(PT, TI)1(PT, TI)3

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RHSN	FeSi (B20)	B20	cP8	(198, P2_13)		2	(RH)1(SN)1
RHSN4	IrGe4		hP15	(152, P3_121)		2	(RH)1(SN)4
RHSN2_RT	RhSn2		tI26	(139, I4/mmm)		2	(RH)0.33333(SN)0.66667
RH2SN	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(RH)2(SN)1
RU3SN7	Ir3Ge7 (D8f)	D8f	cI40	(229, Im-3m)		2	(RU)0.3(SN)0.7
RU2SN3	Ru2Sn3		tP20	(116, P-4c2)		2	(RU)0.4(SN)0.6
SNTI2	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(SN)1(TI)2
SN3TI5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	also M5Sn3, M5Si3C.	2	(SN)3(TI)5
SN5TI6	Sn5Ti6-beta		hP22	(194, P6_3/mmc)	also Sn5Nb6.	2	(SN)5(TI)6
TIZN5	Unknown Structure					2	(TI)1(ZN)5
TIZN10	Ti3Zn22		tP100	(135, P4_2/mbc)		2	(TI)1(ZN)10
TIZN15	TiZn16		oS68	(63, Cmcm)		2	(TI)1(ZN)15
AG9CA2_C15B	AuBe5 (C15b)	C15b	cF24	(216, F-43m)		2	(AG)9(CA)2
AG7CA2	Ag7Yb2		oS36	(63, Cmcm)		2	(AG)7(CA)2
AU2CA	KHg2		oI12	(74, Imma)		2	(AG, AU)2(CA)1
AUCA_B33	CrB (B33)	B33	oS8	(63, Cmcm)		2	(AG, AU)1(CA)1
AG3CA5_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)		2	(AG)3(CA)5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AGCA3	Unknown Structure					2	(AG)1(CA)3
AU4CA1	AuBe5 (C15b)	C15b	cF24	(216, F-43m)		2	(AU)4(CA)1
AU3CA	Unknown Structure					2	(AU)3(CA)1
AU4CA5	Au4Ca5		mP18	(14, P2_1/c)		2	(AU)4(CA)5
AUCA2	Au3Ca7		oP80	(61, Pbca)		2	(AU)1(CA)2
CA2CU	Ca2Cu		oP12	(62, Pnma)		2	(CA)2(CU)1
CACU1	alpha-CaCu		mP20	(11, P2_1/m)	alpha-CaCu (mP20, P2_1/m) & beta-CaCu (oP40, Pnma)	2	(CA)1(CU)1
CACU5_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CA)1(CU)5
AU4LI15	Cu15Si4 (D86)	D86	cI76	(220, I-43d)		2	(AU)4(LI)15
AULI3_D03	BiF3 (D03)	D03	cF16	(225, Fm-3m)		2	(AU)0.25(LI)0.75
AULI2	Unknown Structure				United HT/LT phase	2	(AU)1(LI)2
COSB3_DELTA	Skutterudite (CoAs3, D02)	D02	cI32	(204, Im-3)		2	(CO)0.25(SB)0.75
COSB2_C18	Marcasite (FeS2, C18)	C18	oP6	(58, Pnnm)		2	(CO, NI)0.33333(SB)0.66667
CU17SB3_HT	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_3/mmc)		2	(CU)0.85(SB)0.15
CU11SB3	Cu11Sb3		oS28	(38, Amm2)		2	(CU)0.8(SB)0.2
CU10SB3_HT	Cu10Sb3		hP26	(176, P6_3/m)		2	(CU)0.77(SB)0.23
CU2SB	Cu2Sb (C38)	C38	tP6	(129, P4/nmm)		2	(CU)0.67(SB)0.33

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU33SI7_HT	Unknown Structure					2	(CU, SI)0.825(CU, SI)0.175
CU33SI7_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		2	(AU, CU, SI)0.825(AU, CU, SI)0.175
CU15SI4_D86	Cu15Si4 (D86)	D86	cI76	(220, I-43d)		2	(CU)15(SI)4
CU3SI_LT	Unknown Structure					2	(AU, CU, SI)0.76(CU, SI)0.24
CU3SI_MT	Cu3Si		hR9	(148, R-3)		2	(CU, SI)0.76(CU, SI)0.24
CU3SI_HT	Unknown Structure					2	(AU, CU, SI)0.76(CU, SI)0.24
PD5SI	Pd5Si		mP24	(4, P2_1)		2	(PD)5(SI)1
PD14SI3	Unknown Structure					2	(PD)14(SI)3
PD9SI2	Pd9Si2		oP44	(62, Pnma)		2	(PD)9(SI)2
PD15SI4	Unknown Structure					2	(PD)15(SI)4
PD39SI20	Unknown Structure					2	(PD)39(SI)20
PD19SI10	Unknown Structure					2	(PD)19(SI)10
PD21SI4	Unknown Structure					2	(PD, SI)21(SI)4
PD2SI_ALPHA	Unknown Structure					2	(PD, SI)2(SI)1
PT25SI7	Unknown Structure					2	(PT)25(SI)7
PT3SI_ALPHA	GePt3		mS16	(12, C2/m)		2	(PT)3(SI)1
PT3SI_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(PD, PT)3(SI)1
PT5SI2	Unknown Structure					2	(PT)5(SI)2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PT17SI8_ALPHA	Ni12P5		tI34	(87, I4/m)		2	(PT)17(SI)8
PT17SI8_BETA	Pt12Si5		tP68	(85, P4/n)		2	(PT)17(SI)8
PT2SI_ALPHA	ThH2 (L'2b)	L'2b	tI6	(139, I4/mmm)		2	(PT)2(SI)1
PT2SI_C22	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		2	(PD, PT)2(SI)1
PT6SI5	Pt6Si5		mP22	(11, P2_1/m)		2	(PT)6(SI)5
NI3SB_HT	BiF3 (D03)	D03	cF16	(225, Fm-3m)		3	(SB)0.25(NI, VA)0.5(NI, VA)0.25
NI5SB2_THETA	Ni5Sb2		mS28	(5, C2)		2	(NI)0.7143(NI, SB)0.2857
AU4SC_D1A	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)		2	(AG, AU, CU)4(SC)1
AU2SC_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AG, AU, CU)2(SC)1
AUSC2_C37	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(AU)1(SC)2
AU2SC7	Au2Sc7		oI142	(71, Immm)		2	(AU)2(SC)7
HEUSLER_L21	Heusler (L21)	L21	cF16	(225, Fm-3m)		3	(AG, AU)0.5(AG, AU)0.5(ZN)1
AGINPD	Unknown Structure					3	(AG)0.156(IN)0.26(PD)0.584
AL3CU5ZN2	Cu3.2 (Zn0.18Al0.82)4Al0.9		hR27	(166, R-3m)		4	(AL, CU)1(AL)4(CU)4(ZN)1
AUCOSN4	delta-Ni3Sn4 (D7a)	D7a	mS14	(12, C2/m)		3	(AU)0.1500015(CO)0.249925 (SN)0.60006
AU5CU2SI	Au5Cu2Si		oP32	(62, Pnma)		3	(AU, CU)0.625(AU, CU)0.25(SI)0.125
AU2CUZN	(Cu0.6Zn0.4)Au		oP8	(55, Pbam)		2	(AU)0.5(CU, ZN)0.5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AU3CUZN	Unknown Structure		o**			3	(AU)3(CU)1(ZN)1
AU4IN3SN3	Pt2Sn3 (D5b)	D5b	hP10	(194, P6_ 3/mmc)		3	(AU)0.4(IN, SN)0.3(IN, SN)0.3
AUNI2SN4	Unknown Structure					3	(SN)0.571(AU)0.143(NI)0.286
AUPT2SN4_TAO	Unknown Structure					3	(AU)1(PT)2(SN)4
CU77INSN23	Unknown Structure					2	(CU)0.77(IN, SN)0.23
CU2IN3SN	Unknown Structure					3	(CU)0.333(IN)0.5(SN)0.167
CUNI2SN	Unknown Structure					3	(CU)0.233(NI)0.5(SN)0.267
CU4MNSN	MgCu4Sn		cF24	(216, F-43m)		3	(CU)0.6666(SN)0.1667(MN)0.1667
GA11GEPT7	Unknown Structure					3	(GA)0.579(GE)0.053(PT)0.368
GA3GEPT8	Unknown Structure					2	(GA, GE)0.333(PT)0.667
GAGEPT6	Ir3Si		tI16	(140, I4/mcm)		2	(GA, GE)0.25(PT)0.75
INNI6SN5	Ni(Ga0.25Ge0.75)		oP16	(62, Pnma)		2	(NI)1(IN, SN)1
GAS	Gas					1	(AG, AG1AL1, AG1AU1, AG1CU1, AG2, AL, AL1AU1, AL1CU1, AL1SB1, AL2, AU, AU1CO1, AU1CU1, AU1SI1, AU2, CA, CA2, CO, CO2, CR, CR2, CU, CU2, FE, FE2, GA, GA1SB1, GA1SB2, GA2, GE, GE2, IN, IN1SB1, IN1SB2, IN2, IR, LI, LI2, MN, NI, NI2, PD, PT, RE, RH, RU, SB, SB2, SB3, SB4, SC, SI, SI2, SI3, SN, SN2, TI, TI2, ZN)1
AGTI2	CuZr2		tI6	(139, I4/mmm)		2	(AG)1(TI)2
AGTI	CdTi		tP4	(129, P4/nmm)		2	(AG, TI)1(AG, TI)1

TCNOBL: TCS Noble Metal Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS Noble Metal Alloys Database (TCNOBL)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**4.0**
First release	**TCNOBL1 was released with 2017b. Note that there is no external release of TCNOBL2**

Changes in the Most Recent Database Release

TCNOBL3.0 to TCNOBL4.0

Software release version 2025b (June 2025)

New Elements

Five (5) elements added: Ca, Li, Sb, Sc, and Si, for a 26 element framework.

Binary Systems

- Nineteen (19) new binary systems (220 total): Ag-Ca, Ag-Li, Ag-Sb, Ag-Sc, Ag-Si, Au-Ca, Au-Li, Au-Sb, Au-Sc, Au-Si, Ca-Cu, Co-Sb, Cu-Li, Cu-Sb, Cu-Sc, Cu-Si, Ni-Sb, Pd-Si, and Pt-Si.
- Reassessed four (4) binary systems: Al-Au, Al-Sn, Fe-Sn, and Pd-Zn.
- Removed three (3) binary systems (Ir-Sn, Ir-Zn, and Re-Zn) from the assessed binary systems list and the database since they are not really assessed due to a lack of experimental data.

Ternary Systems

- Five (5) new ternary systems (71 total): Ag-Al-Au, Ag-Au-Si, Ag-Cu-Si, Al-Au-Cu, and Au-Cu-Si.

Phases

- Fifty-two (52) new phases (376 total). See the technical documentation for details of all phases.

Previous Releases

TCNOBL1.0 to TCNOBL3.0

There was no external release of TCNOBL2.

Software release 2023b (June 2023)

- Binary systems – 4 re-assessments: Au-Cu, Ag-Zn, Mn-Pd, and Mn-Pt
- Ternary systems – 13 (re-)assessments: Ag-Au-Cu, Ag-Au-In, Ag-Au-Zn, Ag-Cu-Zn, Ag-In-Zn, Au-Cu-Ge, Au-Cu-In, Au-Cu-Ni, Au-Cu-Pd, Au-Cu-Pt, Au-Cu-Zn, Au-In-Zn, and Cu-In-Zn
- Viscosity/Surface tension of liquid added for 207/210 total of 210 binaries.
- Thermal conductivity (THCD) and electrical resistivity (ELRS) added for all phases.
- Complete gas description added. No need to append gas from another database.
- Volume description for all phases added.