TCS Noble Metal Alloys Database (TCNOBL3)

Technical Information

Available Starting with Thermo-Calc 2023b

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Contents

About the TCS Noble Metal Alloys Database (TCNOBL)

TCS Noble Metal Alloys Database (TCNOBL) is a thermodynamic 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.

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 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 as well as simulating general diffusion controlled phase transformations with the Diffusion Module (DICTRA) or multi-particle precipitations during aging treatment with the Precipitation Module (TC-PRISMA).

The database has been validated against many commercial noble alloys and available experimental information.

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

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.

The database is compatible with the TCS Noble Metal Alloys Mobility Database (MOBNOBL). The current version is MOBNOBL1.

TCNOBL: TCS Noble Metal Alloys Database Revision History. The current version of the database is TCNOBL3. See the link for any subversion release details.

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.

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.

Combining Databases

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

TCS 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) 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 an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to Precious Metals including links to resources such as examples, publications, and more.

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

TCNOBL3 Elements, Systems, Phases and Properties

Included Elements

There are 21 elements included in the most recent version of the database.

Ag	Al	Au	Co	Cr	Cu	Fe	Ga	Ge	In	Ir
Mn	Ni	Pd	Pt	Re	Rh	Ru	Sn	Ti	Zn	

Assessed Systems and Phases

The most recent version of the database contains:

- 204 assessed binary systems. These can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 66 ternary systems These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 324 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`.

Properties Data

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.

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

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

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

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Electrical 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
Electrical conductivity		ELCD for a system `ELCD(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)`**
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

* XI is not used in the TCOX database (all versions). As of 2023b it is also not used starting with the following versions of these databases: TCFE13, TCNI12.1, TCTI5.1, TCNOBL3, TCPMAG2, and TCCU6.

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

TCNOBL3 Systems

In this section:

TCNOBL3 Assessed Binary Systems

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

TCNOBL3 Assessed Ternary Systems

Assessed Ternary Systems					
Ag-Al-Cu	Ag-Au-Cu	Ag-Au-Ge	Ag-Au-In	Ag-Au-Ni	Ag-Au-Pd
Ag-Au-Pt	Ag-Au-Sn	Ag-Au-Zn	Ag-Cu-Ge	Ag-Cu-In	Ag-Cu-Ni
Ag-Cu-Pd	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-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
Au-Cu-Zn	Au-Ge-Sn	Au-In-Sn	Au-Ir-Pd	Au-Ir-Pt	Au-Ni-Pd
Au-Ni-Pt	Au-Ni-Sn	Au-Pd-Pt	Au-Pd-Rh	Au-Pd-Ru	Au-Pt-Rh
Au-Pt-Ru	Au-Pt-Sn	Cr-Ni-Pd	Cu-Fe-Pt	Cu-Mn-Sn	Cu-Ni-Pd
Cu-Ni-Sn	Fe-Ni-Ru	Ga-Ge-Pt	Ga-Sn-Zn	In-Ni-Sn	In-Sn-Zn
Ir-Pd-Pt	Ir-Pt-Ru	Ir-Rh-Ru	Pd-Pt-Ru	Pd-Rh-Ru	Pt-Rh-Ru

TCNOBL3 Phases

In this section:

Common Phases for Noble / Precious Metals

TCNOBL3 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

TCNOBL3 Models for the Included Phases

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
GAS	Gas						1	[1.0]	(AG, AG1AL1, AG1AU1, AG1CU1, AG2, AL, AL1AU1, AL1CU1, AL2, AU, AU1CO1, AU1CU1, AU2, CO, CO2, CR, CR2, CU, CU2, FE, FE2, GA, GA2, GE, GE2, IN, IN2, IR, MN, NI, NI2, PD, PT, RE, RH, RU, SN, SN2, TI, TI2, ZN)1
LIQUID	Liquid					Metallic LIQUID:L solutionphase	1	[1.0]	(AG, AL, AU, CO, CR, CR3GE1, CU, FE, GA, GE, IN, IR, MN, NI, PD, PT, PTSN, RE, RH, RU, SN, TI, ZN)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	Metallic FCC_A1 solution, e.g. (Al), (Cu), and MC carbides	2	[1.0, 1.0]	(AG, AL, AU, CO, CR, CU, FE, GA, GE, IN, IR, MN, NI, PD, PT, RE, RH, RU, SN, TI, ZN)1(VA)1
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221	L12phase, Ni3Si_rt, AlZr3, GeNi3, TiZn3, VZn3	2	[1.0, 3.0]	(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	P4/mmm	123	also IrTi.	2	[0.5, 0.5]	(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	Im-3m	229	Metallic BCC_A2 solution	2	[1.0, 3.0]	(AG, AL, AU, CO, CR, CU, FE, GA, GE, IN, IR, MN, NI, PD, PT, RE, RH, RU, SN, TI, VA, ZN)1 (VA)3
BCC_B2	CsCl (B2)	B2	cP2	Pm-3m	221	Solution ofordered BCC_B2, having Gibbs energy contribution from BCC_A2	3	[0.5, 0.5, 3.0]	(AG, AL, AU, CO, CR, CU, FE, GA, GE, IN, IR, MN, NI, PD, PT, RE, RH, RU, SN, TI, VA, ZN)0.5 (AG, AL, AU, CO, CR, CU, FE, GA, GE, IN, IR, MN, NI, PD, PT,

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
									RE, RH, RU, SN, TI, VA, ZN)0.5 (VA)3
CBCC_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[1.0, 1.0]	(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	P4_132	213		1	[1.0]	(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	I4_1/amd	141	Pure Sn or itssolution	1	[1.0]	(AG, AL, CU, GA, IN, NI, SN, ZN)1
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194	Metallic HCP_A3 solution alpha_ Mg/Hf/Sc/Ti/Zr, epsilon_CuZn, etc.	2	[1.0, 0.5]	(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
HCP_ZN	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		2	[1.0, 0.5]	(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	P6_3/mmc	194		2	[3.0, 1.0]	(AL, MN, TI)3(AL, PT, TI)1
BCT_D022	Al3Ti (D022)	D022	tI8	I4/mmm	139		2	[3.0, 1.0]	(AL, GA, TI)3(AL, TI)1
DIAMOND_A4	Diamond (A4)	A4	cF8	Fd-3m	227	Pure C, Ge, Si orsolution phases based on them	1	[1.0]	(AG, AU, GA, GE, SN, TI)1
ORTHORHOMBIC_GA	alpha-Ga (A11)	A11	oS8	Cmce	64		1	[1.0]	(GA)1
TETRAGONAL_A6	In (A6)	A6	tI2	I4/mmm	139		1	[1.0]	(AL, GA, IN, SN, ZN)1
DIS_SIG	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136	Part of the description for the SIGMA phase.	1	[1.0]	(CO, CR, FE, MN, RE, RU)1
SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		3	[10.0, 4.0, 16.0]	(CO, CR, FE, MN, RE, RU)10 (CO, CR, FE, MN, RE, RU)4(CO, CR, FE, MN, RE, RU)16

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
HIGH_SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		3	[8.0, 4.0, 18.0]	(MN)8(CR)4(CR, MN)18
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194	Solution of MgZn2-type phases, including MgZn2 (Eta, aka M orsigma)	2	[2.0, 1.0]	(CR, FE, MN, TI, ZN)2(CR, FE, MN, TI, ZN)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227	Solution of Cu2Mg-type phases, cF24, Fd-3m	2	[2.0, 1.0]	(CO, CR, TI)2(CO, CR, TI)1
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_3/mmc	194	Solution of MgNi2-type phases, hP24, P63/mmc	2	[2.0, 1.0]	(CO, CR, TI)2(CO, CR, TI)1
CHI_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[24.0, 10.0, 24.0]	(RE)24(TI)10(RE)24
AG2GA	Mg2In		hP9	P-62m	189		2	[2.0, 1.0]	(AG)2(AG, GA, VA)1
AG3GA2	Unknown Structure		hR*				2	[3.0, 2.0]	(AG)3(GA)2
ALCR2_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139	Same as AlCr2, CuTi2, PdTi2, RhTi2, Ti2Zn	2	[1.0, 2.0]	(AL, CU, PD, RH, ZN)1(CR, TI)2
AL2CU_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140	Al2Cu, AlHf2, Fe2B, FeGe2, FeZr2, FeSn2, Mn2B, MnSn2, NIB2, NIZr2, SiZr2	2	[0.33333, 0.66667]	(AG, AL, AU, CO, CU, FE, MN, PD, RH)0.33333(AL, IN, MN, SN)0.66667
CU5ZN8_GAMMA_D83	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		3	[4.0, 1.0, 8.0]	(AL, IN, NI, ZN)4(AG, AL, CU, IN, NI, ZN)1(AG, CU, IN, SN, ZN)8
AG15PT17	Unknown Structure		hR*				2	[0.46875, 0.53125]	(AG)0.46875(PT)0.53125
AG3SN_L60_CU3TI	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59		2	[0.75, 0.25]	(AG, AU, CO, CU, NI, ZN)0.75 (AG, AU, IN, NI, SN)0.25
AGZN_ZETA	zeta-AgZn (Bb)	Bb	hP9	P-3	147		1	[1.0]	(AG, CU, IN, SN, ZN)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AL2AU_C1_CAF2	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		2	[0.66667, 0.33333]	(AG, AL, AU, CU, GA, GE, IN, SN)0.66667(AL, AU, CO, NI, PT, SN)0.33333
ALAU_B31	AlAu		mP8	P2_1/m	11		2	[0.5, 0.5]	(AL, GA, GE, PD, SN)0.5(AU, CU, NI, PD, PT, VA)0.5
ALAU2_HT	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[1.0, 2.0]	(AL, AU)1(AL, AU)2
ALAU2_LT	AlAu2		oP12	Pnma	62		2	[1.0, 2.0]	(AL)1(AL, AU, CU)2
ALAU4_HT	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229		2	[1.0, 4.0]	(AL, AU)1(AU)4
ALAU4_LT	AlAu4		cP20	P2_13	198		2	[0.2, 0.8]	(AL)0.2(AG, AU)0.8
AL3AU8	Yb8In3		hR132	R-3c	167		2	[0.27273, 0.72727]	(AL)0.27273(AU)0.72727
AL13CO4	Orthorhombic Co4Al13		oP102	Pmn2_1	31		2	[13.0, 4.0]	(AL)13(CO)4
AL3CO	Os4Al13		mS34	C2/m	12		2	[3.0, 1.0]	(AL)3(CO)1
AL5CO2_D811	Co2Al5 (D811)	D811	hP28	P6_3/mmc	194	also Al5Rh2.	2	[5.0, 2.0]	(AL)5(CO, RH)2
AL9CO2	Co2Al9 (D8d)	D8d	mP22	P2_1/c	14		2	[9.0, 2.0]	(AL, GA)9(CO, RH)2
AL11CR2	Al5Cr		mS732	C2/c	15		3	[10.0, 1.0, 2.0]	(AL)10(AL)1(CR)2
AL13CR2	Al45V7		mS104	C2/m	12		2	[13.0, 2.0]	(AL)13(CR)2
AL4MN	mu-Al4Mn		hP574	P6_3/mmc	194		2	[4.0, 1.0]	(AL)4(CR, MN)1
AL8CR5_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		2	[8.0, 5.0]	(AL)8(CR)5
AL8CR5_L	Cr5Al8 (D810)	D810	hR26	R3m	160		2	[8.0, 5.0]	(AL)8(CR)5
AL9CR4_H	Unknown Structure						2	[9.0, 4.0]	(AL)9(CR)4

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AL9CR4_L	Unknown Structure						2	[9.0, 4.0]	(AL)9(CR)4
ALCU_GAMMA_HT	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217	aka GAMMA_H., Cu5Zn8-type Al4Cu9 (ht) phase	3	[4.0, 1.0, 8.0]	(AL, ZN)4(AL, CU, ZN)1(AG, CU)8
ALCU_ETA	AlCu(r)		mS20	C2/m	12		2	[0.5, 0.5]	(AL, CU)0.5(AG, CU, ZN)0.5
CU6SN5_HT_NIAS	Ni2In (B82)	B82	hP6	P6_3/mmc	194	AlCu_D81, AuSn_Delta, Co3Sn2, Cu2In_HT, Cu6Sn5_HT, Ge3Ni5_HT, InNi2_HT, Mn(2-x)Sn, Ni3Sn2, Pd2Sn_HT, PtSn	3	[1.0, 1.0, 1.0]	(AG, AU, CO, CU, MN, NI, PD, PT, VA)1(AG, AL, CU, GE, IN, NI, SN)1(AU, CO, CU, MN, NI, PD, VA)1
ALCU_ZETA	Al9Cu11(h)		oF88	Fmm2	42		2	[0.55, 0.45]	(AG, CU)0.55(AL, IN)0.45
AL2CU3_DELTA	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[0.4, 0.6]	(AL)0.4(AG, CU)0.6
AL2FE1	Al2Fe		aP18	P1	1		2	[2.0, 1.0]	(AL)2(FE)1
AL5FE2	Al2.8Fe		oS24	Cmcm	63		2	[5.0, 2.0]	(AL)5(FE)2
AL5FE4	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		1	[1.0]	(AL, FE)1
AL9IR2	Co2Al9 (D8d)	D8d	mP22	P2_1/c	14		2	[0.818, 0.182]	(AL)0.818(IR)0.182
AL45IR13	Al45Ir13		oP236	Pnma	62		2	[0.776, 0.224]	(AL)0.776(IR)0.224
AL13IR4	Unknown Structure						2	[0.765, 0.235]	(AL)0.765(IR)0.235
AL28IR9	Al28Ir9		hP236	P31c	159		2	[0.757, 0.243]	(AL)0.757(IR)0.243
AL3IR	Na3As (D018)	D018	hP8	P6_3/mmc	194		2	[0.75, 0.25]	(AL)0.75(IR)0.25
AL2_7IR	Al2.75Ir		cP60	P23	195		2	[0.73, 0.27]	(AL)0.73(IR)0.27
AL13FE4	Al13Fe4		mS102	C2/m	12	solution phases based	3	[0.6275, 0.235,	(AL, CU)0.6275(FE, MN,

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						on Al13Fe4, aka Al3Fe		0.1375]	RU)0.235(AL, VA)0.1375
AL12MN	Al12W		cI26	Im-3	204		2	[12.0, 1.0]	(AL)12(MN)1
AL4MN_R	lambda-Al4Mn		hP586	P6_3/mmc	194	AL461MN107	2	[0.81162, 0.18838]	(AL)0.81162(MN)0.18838
AL11MN4_LT	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(MN)4
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25		oP156	Pnma	62		2	[29.0, 10.0]	(AL, MN)29(MN)10
AL8MN5	Cr5Al8 (D810)	D810	hR26	R3m	160		3	[12.0, 5.0, 9.0]	(AL)12(MN)5(AL, MN)9
AL6MN	MnAl6 (D2h)	D2h	oS28	Cmcm	63		2	[6.0, 1.0]	(AL)6(MN, RE, RU)1
AL3NI2_D513	Al3Ni2 (D513)	D513	hP5	P-3m1	164	Al3Ni2, Al3Pd2, Al3Pt2, Al3Ru2, Au3In2, Ga3Pt2, In3Ni2, In3Pd2, In3Pt2	3	[0.6, 0.4, 0.2]	(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	Pnma	62		2	[0.75, 0.25]	(AL, PD, PT)0.75(NI)0.25
AL3NI5	Ga3Pt5		oS16	Cmmm	65		2	[0.375, 0.625]	(AL)0.375(NI)0.625
AL2PD5	Unknown Structure						2	[2.0, 5.0]	(AL)2(AL, PD)5
AL3PD	(Al3Pd)		oP*	Pna2_1	33		2	[3.0, 1.0]	(AL)3(PD)1
AL4PD	(Al4Pd)		hP*	P6_322	182		2	[4.0, 1.0]	(AL)4(PD)1
AL3PD5_OP16	Rh5Ge3		oP16	Pbam	55	Al3Pd5, Al3Pt5, In3Pd5	2	[3.0, 5.0]	(AL, IN)3(CU, PD, PT, RH)5
AL21PT8_TI116	Al21Pt8		tI116	I4_1/a	88	Al21Pd8, Al21Pt8	2	[21.0, 8.0]	(AL)21(PD, PT)8
ALPT_B20	FeSi (B20)	B20	cP8	P2_13	198		2	[1.0, 1.0]	(AL)1(NI, PT, RH)1
ALRH2	Unknown Structure						2	[1.0, 2.0]	(AL)1(RH)2

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AL3RH_LT	(Al3Rh)		oP*	Pnma	62		2	[3.0, 1.0]	(AL)3(RH)1
AL3RH_HT	Unknown Structure						2	[2.0, 1.0]	(AL)2(RH, VA)1
AL7RH3	Unknown Structure						2	[7.0, 3.0]	(AL)7(RH)3
RUAL2_C54	TiSi2 (C54)	C54	oF24	Fddd	70	also MoSi2, RuAl2, ZrSn2.	2	[1.0, 2.0]	(RU)1(AL)2
CO2SI_C23	Cotunnite (PbCl2, C23)	C23	oP12	Pnma	62	Ca2Si, NI2Si, SiSr2, SnSr2, GeSr2	2	[1.0, 2.0]	(AL, CO, IN, PD, SN, ZN)1(AL, CO, CU, NI, PD, PT)2
AL21PT5	Li21Si5		cF416	F-43m	216		2	[21.0, 5.0]	(AL)21(PT)5
AL12RE	Al12W		cI26	Im-3	204		2	[12.0, 1.0]	(AL)12(RE)1
AL4RE	Unknown Structure						2	[4.0, 1.0]	(AL)4(RE)1
AL11RE4	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(RE)4
ALRE2	CuZr2		tI6	I4/mmm	139		2	[1.0, 2.0]	(AL)1(RE)2
ALRE	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[1.0, 1.0]	(AL)1(RE)1
AL11TI5	Al3Zr (D023)	D023	tI16	I4/mmm	139		2	[17.0, 8.0]	(AL)17(TI)8
AL2TI	Ga2Hf		tI24	I4_1/amd	141		2	[2.0, 1.0]	(AL)2(TI)1
AUCU_II	CuAu		oI40	Imma	74		2	[0.5, 0.5]	(AG, AU, CU, GE, NI, PD, PT, ZN)0.5(AG, AU, CU, GE, NI, PD, PT, ZN)0.5
AU7GA2_HT	Au7Ga2		hP27	P-62m	189		2	[0.7895, 0.2105]	(AU)0.7895(GA)0.2105
AU7GA2_LT	Unknown Structure						2	[7.0, 2.0]	(AU)7(GA)2
AU7GA3	Unknown Structure						2	[7.0, 3.0]	(AU)7(GA)3

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AUGA_B31	Westerveldite (FeAs, B14)	B14	oP8	Pnma	62		2	[1.0, 1.0]	(AU)1(GA)1
AU9IN4_GAMMA_D83	Au6(Au0.5In0.5)6In		cP76	P-43m	215		4	[0.61539, 0.07692, 0.23077, 0.07692]	(AU)0.61539(AU, IN)0.07692 (AU, IN)0.23077(IN)0.07692
AUIN_BETA	Unknown Structure						2	[0.785, 0.215]	(AU)0.785(IN)0.215
AUIN_BETA_PRIME	Cu10Sb3		hP26	P6_3/m	176		2	[0.77778, 0.22222]	(AU)0.77778(IN)0.22222
AU7IN3	Au7In3		hP60	P-3	147		2	[0.7, 0.3]	(AU)0.7(IN)0.3
AUIN	Unknown Structure						2	[0.5, 0.5]	(AU)0.5(IN, SN)0.5
AU4MN	Ni4Mo (D1a)	D1a	tI10	I4/m	87		2	[0.8, 0.2]	(AU)0.8(MN)0.2
AU33MN9	Unknown Structure						2	[0.786, 0.214]	(AU)0.786(MN)0.214
AU13MN4	Unknown Structure						2	[0.765, 0.235]	(AU)0.765(MN)0.235
AU3MN	SrPb3		tp4	P4/mmm	123		2	[0.75, 0.25]	(AU)0.75(MN)0.25
AU11MN4	Au11Mn4		mS810	Cm	8		2	[0.733, 0.267]	(AU)0.733(MN)0.267
AU5MN2	Au5Mn2		mS14	C2/m	12		2	[0.714, 0.286]	(AU)0.714(MN)0.286
AU2MN	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[0.667, 0.333]	(AU)0.667(MN)0.333
AUMN2	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[0.333, 0.667]	(AU)0.333(MN)0.667
AU10SN_D024	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194	AuIn_Alpha1, AuSn_ Beta	1	[1.0]	(AG, AU, GA, GE, IN, SN)1
AUSN2_OP24	AuSn2		oP24	Pbca	61		2	[0.33333, 0.66667]	(AU, CU, PT)0.33333 (SN)0.66667

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AUSN_ZETA_PRIME	Au5Sn		hR18	R32	155	AuSn_Zeta_Prime	2	[0.84, 0.16]	(AU)0.84(IN, SN)0.16
AUSN4_OS20	PtSn4		oS20	Ccce	68	AuSn4, PdSn4, PtSn4	2	[0.2, 0.8]	(AU, CU, NI, PD, PT)0.2(IN, PD, SN)0.8
AU5ZN8_GAMMA	Cr4.5(Cr0.56Al0.44)9Al12		hR78	R3m	160		4	[2.0, 2.0, 3.0, 6.0]	(AU, ZN)2(AU, ZN)2(AU, ZN)3(ZN)6
AUTI3	Cr3Si		cP8	Pm-3m	221		2	[0.75, 0.25]	(TI)0.75(AU)0.25
AUTI	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[0.5, 0.5]	(TI, VA)0.5(AU, TI)0.5
AU2TI	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[1.0, 2.0]	(TI)1(AU)2
AU4TI	Ni4Mo (D1a)	D1a	tI10	I4/m	87		2	[0.2, 0.8]	(AU, TI)0.2(AU)0.8
AU3ZN_ALPHA1	MgAg3		cP4	Pm-3m	221		3	[3.0, 1.0, 1.0]	(AU)3(AG, AU, CU, ZN)1(CU, ZN)1
AU3ZN_ALPHA2	Au3Zn		oS32	Cmce	64		2	[0.75, 0.25]	(AU)0.75(ZN)0.25
AU4ZN_ALPHA3	Unknown Structure						3	[18.0, 7.0, 3.0]	(AU)18(AG, AU, CU, IN, ZN)7(ZN)3
AUZN3_GAMMA2	UH3		cP32	Pm-3m	221		2	[1.0, 3.0]	(AU)1(ZN)3
AUZN4_GAMMA3	Unknown Structure						3	[0.12, 0.16, 0.72]	(AU)0.12(AU, ZN)0.16(ZN)0.72
AU5ZN3	Au5Zn3		oI128	Ibam	72		2	[5.0, 3.0]	(AU)5(ZN)3
AU11ZN14	Unknown Structure						2	[11.0, 14.0]	(AU)11(ZN)14
AU15ZN85_EPSILON_PRIME	Unknown Structure						2	[0.15, 0.85]	(AU)0.15(ZN)0.85
INSN_A6	Unknown Structure					INSN_A6 solution phase	1	[1.0]	(IN, SN)1
CO3GE	Unknown Structure						2	[0.75, 0.25]	(CO)0.75(GE)0.25

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
CO5GE2	Unknown Structure						2	[0.714, 0.286]	(CO)0.714(GE)0.286
CO5GE3	Co2Si (C37)	C37	oP12	Pnma	62		3	[0.125, 0.5, 0.375]	(CO, RH, VA)0.125(CO, RH)0.5 (CO, GE, SN)0.375
CO5GE3_ALPHA	Unknown Structure						2	[0.625, 0.375]	(CO)0.625(GE)0.375
CO5GE7	Co5Ge7		tI24	I4mm	107		2	[0.417, 0.583]	(CO)0.417(GE)0.583
COGE	CoGe		mS16	C2/m	12		2	[0.5, 0.5]	(CO, GE)0.5(CO, GE)0.5
COGE2	CoGe2		oS24	Cmce	64		2	[0.333, 0.667]	(CO)0.333(GE)0.667
COSN_HP6	CoSn (B35)	B35	hP6	P6/mmm	191	CoSn, FeSn and InNi	2	[0.5, 0.5]	(CO, FE, NI)0.5(IN, SN)0.5
COSN3_OS32	PdSn3		oS32	Cmce	64		2	[0.25, 0.75]	(CO, PD)0.25(PD, SN)0.75
COZN_LT	beta-Mn (A13)	A13	cP20	P4_132	213		2	[1.0, 1.0]	(CO, ZN)1(VA)1
COZN_HT	Unknown Structure						2	[1.0, 1.0]	(CO, ZN)1(VA)1
COZN_GAMMA_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217	Zn11Co2	2	[1.0, 1.0]	(CO, ZN)1(VA)1
COZN_DELTA	Unknown Structure						2	[0.117647, 0.882353]	(CO)0.117647(ZN)0.882353
COZN_GAMMA1	Co2Zn15		mS28	C2/m	12	CoZn7	2	[0.125, 0.875]	(CO)0.125(ZN)0.875
COZN_GAMMA2	CoZn13		mS28	C2/m	12	CoZn13	2	[0.0714286, 0.9285714]	(CO)0.0714286(ZN)0.928571
CR3SI_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[3.0, 1.0]	(CR, IR, TI)3(CR, GA, GE, IR, RH, RU)1
CRGA	MnGa		hR78	R-3m	166		2	[1.0, 1.0]	(CR)1(GA)1
CR5GA6	Fe3Ga4		mS42	C2/m	12		2	[5.0, 6.0]	(CR)5(GA)6

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
CRGA4	beta-Hg4Pt		cI10	Im-3m	229		2	[1.0, 4.0]	(CR)1(GA)4
CR5GE3	W5Si3 (D8m)	D8m	tI32	I4/mcm	140	beta-Cr5Ge3	2	[0.625, 0.375]	(CR, GE)0.625(CR, GE)0.375
LCR5GE3	Unknown Structure						2	[0.625, 0.375]	(CR, GE)0.625(CR, GE)0.375
CR11GE8	Cr11Ge8		oP76	Pnma	62		2	[0.579, 0.421]	(CR)0.579(GE)0.421
CRGE	FeSi (B20)	B20	cP8	P2_13	198		2	[0.5, 0.5]	(CR)0.5(GE)0.5
CR11GE19	Mn11Si19		tP120	P-4n2	118		2	[0.367, 0.633]	(CR)0.367(GE)0.633
CR3MN5	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[3.0, 5.0]	(CR)3(MN)5
CRNI2_OP6	MoPt2		oI6	Immm	71		2	[1.0, 2.0]	(CR)1(NI)2
CRPD_L10	AuCu		tP4	P4/mmm	123		2	[0.5, 0.5]	(CR)0.5(PD)0.5
CR2PD3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.4, 0.6]	(CR)0.4(PD)0.6
CR3PT_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[4.0, 1.0]	(CR)4(PT)1
CRZN13	Unknown Structure		m**				2	[1.0, 13.0]	(CR)1(ZN)13
CRZN17	Unknown Structure		hP*				2	[1.0, 17.0]	(CR)1(ZN)17
CU9GA4_0	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215		3	[6.0, 6.0, 1.0]	(CU)6(CU, GA)6(GA)1
CU9GA4_1	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215		4	[6.0, 3.0, 3.0, 1.0]	(CU)6(CU, GA)3(CU, GA)3 (GA)1
CU9GA4_2	Cu8.2Ga4.8		cP52				4	[3.0, 3.0, 3.0, 4.0]	(CU)3(CU, VA)3(CU, GA)3 (GA)4
CU9GA4_3	Cu7.15Ga5.85		cP52				3	[6.0, 3.0, 4.0]	(CU, VA)6(CU, GA)3(GA)4

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CUGA2	FeSi2-h		tP3	P4/mmm	123		2	[1.0, 2.0]	(CU)1(GA)2
CUGA_THETA	Unknown Structure						2	[0.778, 0.222]	(CU)0.778(GA)0.222
CU3GE_ETA	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59	eta, low T, D0a	2	[0.75, 0.25]	(AG, CU)0.75(GE)0.25
CU3GE_EPSILON	Na3As (D018)	D018	hP8	P6_3/mmc	194	high T, D018	2	[0.765, 0.235]	(AG, CU)0.765(GE)0.235
CU3GE_THETA	BiF3 (D03)	D03	cF16	Fm-3m	225	high T, D03	2	[0.735, 0.265]	(AG, CU)0.735(GE)0.265
CU3IN_GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215	Cu9In4 Prototype Cu9Al4 (cP52, P-43m), with solubility of Ag, Sn.	3	[0.654, 0.115, 0.231]	(AG, AU, CU)0.654(AG, AU, CU, IN)0.115(IN, SN)0.231
CU2IN_LT	Unknown Structure						2	[0.64, 0.36]	(CU)0.64(IN)0.36
CU7IN3_DELTA	Cu7In3		aP40	P-1	2	Cu7In3_Delta	2	[0.7, 0.3]	(AU, CU)0.7(IN, SN)0.3
CUPT_L11	Rhombohedral CuPt (L11)	L11	hR2	R-3m	166	CuIn DELTAT	3	[0.5, 0.5, 1.0]	(AU, CU, PT)0.5(AU, CU, PT)0.5(VA)1
GAMMA_D03	BiF3 (D03)	D03	cF16	Fm-3m	225	Cu3Sn	1	[1.0]	(CU, MN, NI, SN, ZN)1
CU3SN	Cu3Sn		oS80	Cmcm	63		2	[3.0, 1.0]	(AU, CU, SN)3(CU, IN, SN)1
CU41SN11	Cu41Sn11		cF416	F-43m	216		2	[41.0, 11.0]	(CU, SN, ZN)41(CU, IN, SN, ZN)11
CU10SN3	Cu10Sn3		hP26	P6_3	173		2	[0.769, 0.231]	(CU, NI)0.769(SN)0.231
CU6SN5_LT	Cu6Sn5		mS44	C2/c	15		3	[1.0, 1.0, 1.0]	(CU)1(CU, SN)1(SN)1
CU2TI	Au2V		oS12	Cmcm	63		2	[2.0, 1.0]	(CU)2(TI)1
CU3TI2	Cu3Ti2		tP10	P4/nmm	129		2	[3.0, 2.0]	(CU)3(TI)2
CU4TI1	Au4Zr		oP20	Pnma	62		2	[4.0, 1.0]	(CU, TI)4(CU, TI)1

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CU4TI3	Cu4Ti3		tI14	I4/mmm	139		2	[4.0, 3.0]	(CU)4(TI)3
CUTI_B11	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[1.0, 1.0]	(CU, TI)1(CU, TI)1
CUTI3	CuTi3 (L60)	L60	tP4	P4/mmm	123		2	[1.0, 3.0]	(CU, TI)1(TI)3
FE3SN2	Fe3Sn2		hR10	R-3m	166		2	[3.0, 2.0]	(FE)3(SN)2
FE5SN3	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[5.0, 3.0]	(FE)5(SN)3
FEZN_GAMMA_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		4	[0.154, 0.154, 0.231, 0.461]	(FE, ZN)0.154(FE, ZN)0.154(FE, ZN)0.231(ZN)0.461
FEZN_GAMMA_D81	Fe11Zn40		cF408	F-43m	216		3	[0.137, 0.118, 0.745]	(FE)0.137(FE, ZN)0.118 (ZN)0.745
FEZN_DELTA	FeZn10		hP632	P6_3/mmc	194		4	[0.058, 0.18, 0.525, 0.237]	(FE)0.058(FE, ZN)0.18 (ZN)0.525(ZN)0.237
FEZN_ZETA	CoZn13		mS28	C2/m	12		3	[0.072, 0.856, 0.072]	(FE, VA)0.072(ZN)0.856(VA, ZN)0.072
NI5GA3	Ga3Pt5		oS16	Cmmm	65		2	[0.63, 0.37]	(NI)0.63(GA)0.37
NI3GA2	Unknown Structure						2	[0.6, 0.4]	(NI)0.6(GA)0.4
NI3GA4	Ga4Ni3		cI112	Ia-3d	230		2	[0.43, 0.57]	(NI)0.43(GA)0.57
NIGA4	Unknown Structure						2	[0.2, 0.8]	(NI)0.2(GA)0.8
GA5PD	Ga5Pd		tI24	I4/mcm	140		2	[0.83, 0.17]	(GA)0.83(PD)0.17
GA7PD3	Ga7Pd3		mS20	C2/m	12		2	[0.7, 0.3]	(GA)0.7(PD)0.3
GAPD_B20	FeSi (B20)	B20	cP8	P2_13	198		2	[0.5, 0.5]	(GA)0.5(PD)0.5
GA3PD5	Rh5Ge3		oP16	Pbam	55		2	[0.38, 0.62]	(GA)0.38(PD)0.62

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
GAPD2_C37	Co2Si (C37)	C37	oP12	Pnma	62		2	[0.33, 0.66]	(GA, PD)0.33(CU, PD)0.66
GE2NI5_HT	Pd5Sb2		hP42	P6_3cm	185		2	[0.72, 0.28]	(NI)0.72(GE)0.28
GENI2	Co2Si (C37)	C37	oP12	Pnma	62		2	[0.665, 0.335]	(NI)0.665(GE)0.335
GE3NI5_C2	Ge3Ni5		mS32	C2	5		2	[0.625, 0.375]	(NI, PD)0.625(GE)0.375
GA6PT	Unknown Structure						2	[0.857, 0.143]	(GA, GE)0.857(PT)0.143
GA7PT3	Ir3Ge7 (D8f)	D8f	cI40	Im-3m	229		2	[0.7, 0.3]	(GA, GE)0.7(PT)0.3
GAPT	FeSi (B20)	B20	cP8	P2_13	198		2	[0.5, 0.5]	(GA, GE)0.5(PT)0.5
GA3PT5	Ga3Pt5		oS16	Cmmm	65		2	[0.375, 0.625]	(GA, GE)0.375(PT)0.625
GAPT2	GaPt2		oP24	Pmma	51		2	[0.333, 0.667]	(GA, GE)0.333(PT)0.667
GAPT3	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.25, 0.75]	(GA, GE, PT)0.25(GA, PT)0.75
GA3RH	In3Ir		tP16	P4_2/mnm	136		2	[3.0, 1.0]	(GA)3(RH)1
GA17RH10	Rh10Ga17		tP108	P-4c2	116		2	[17.0, 10.0]	(GA)17(RH)10
GATI2	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[1.0, 2.0]	(GA)1(TI)2
GA3TI5	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[3.0, 5.0]	(GA)3(TI)5
GA4TI5	Ti5Ga4		hP18	P6_3/mcm	193		2	[4.0, 5.0]	(GA, TI)4(GA, TI)5
GA3TI2	Ti2Ge3		tP10	P4/m	83		2	[3.0, 2.0]	(GA)3(TI)2
GA2TI	Ga2Hf		tI24	I4_1/amd	141		2	[2.0, 1.0]	(GA)2(TI)1
PD21GE8	Al21Pt8		tI116	I4_1/a	88		2	[21.0, 8.0]	(PD)21(GE)8

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
PD25GE9	Ge9Pd25		hP34	P-3	147		2	[25.0, 9.0]	(PD)25(GE)9
PD2GE	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189		2	[2.0, 1.0]	(PD)2(GE)1
PD3GE	Unknown Structure						2	[3.0, 1.0]	(PD)3(GE)1
PD5GE	Pd5As		mS24	C2	5		2	[5.0, 1.0]	(PD)5(GE)1
GEPT3_MS16	GePt3		mS16	C2/m	12	GePt3, Ni25Si9, Pt3Si_ LT	2	[0.25, 0.75]	(GA, GE, PT)0.25(NI, PT)0.75
GE2PT	Hydrophilite (CaCl2, C35)	C35	oP6	Pnnm	58		2	[0.66667, 0.33333]	(GA, GE)0.66667(PT)0.33333
GE3PT2	Pt2Ge3		oP20	Pnma	62		2	[0.6, 0.4]	(GA, GE)0.6(PT)0.4
GE2PT3	Pt3Ge2		oP40	Pnma	62		2	[0.4, 0.6]	(GA, GE)0.4(PT)0.6
GEPT2	Revised Fe2P (C22)	C22(II)	hP9	P-62m	189		2	[0.333, 0.667]	(GA, GE)0.333(PT)0.667
GE7RE3	Re3Ge7		oS40	Cmcm	63		2	[7.0, 3.0]	(GE)7(RE)3
RHGE	Westerveldite (FeAs, B14)	B14	oP8	Pnma	62		2	[1.0, 1.0]	(RH)1(GE)1
RH2GE	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(RH)2(GE)1
RH5GE3	Rh5Ge3		oP16	Pbam	55	Rh5Ge3 and Rh5Ti3	2	[5.0, 3.0]	(RH)5(GE, TI)3
RH17GE22	Rh7Ge22		tI156	I-42d	122		2	[17.0, 22.0]	(RH)17(GE)22
B20_GERU	FeSi (B20)	B20	cP8	P2_13	198		2	[1.0, 1.0]	(GE)1(RU)1
ALPHA_GE3RU2	Ge3Ru2		oP40	Pbcn	60		2	[3.0, 2.0]	(GE)3(RU)2
BETA_GE3RU2	Ru2Sn3		tP20	P-4c2	116		2	[3.0, 2.0]	(GE)3(RU)2
TI5GE3	Mavlyanovite (Mn5Si3,	D88	hP16	P6_3/mcm	193		2	[3.0, 5.0]	(GE)3(TI)5

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
	D88)								
TI6GE5	Si5V6		oI44	Ibam	72		2	[5.0, 6.0]	(GE)5(TI)6
TIGE2	TiSi2 (C54)	C54	oF24	Fddd	70		2	[2.0, 1.0]	(GE)2(TI)1
IRIN2	Mg2Cu (Cb)	Cb	oF48	Fddd	70	CoIn2 and IrIn2	2	[1.0, 2.0]	(CO, IR)1(IN)2
IRIN3_LT	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[1.0, 3.0]	(IR)1(IN)3
IRIN3_HT	In3Ir		tP16	P4_2/mnm	136	CoIn3, CoGa3 and ht-IrIn3.	2	[1.0, 3.0]	(CO, IR)1(GA, IN)3
IN4MN9	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215	Formula Mn9.75In3.25	2	[4.0, 9.0]	(IN)4(MN)9
IN9NI13	Ga9Ni13		mS44	C2/m	12	In9Ni13 with solubility of Sn.	3	[1.0, 1.0, 1.0]	(NI, VA)1(IN, SN)1(NI)1
INNI_DELTA	CoSn (B35)	B35	hP6	P6/mmm	191		2	[1.0, 1.0]	(NI, VA)1(IN, NI)1
INNI2_RT	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[1.0, 1.0, 1.0]	(NI)1(NI)1(IN)1
IN7PD3	Ir3Ge7 (D8f)	D8f	cI40	Im-3m	229		2	[0.71, 0.29]	(IN)0.71(PD)0.29
INPD2_BETA	Co2Si (C37)	C37	oP12	Pnma	62		2	[0.34, 0.66]	(IN)0.34(PD)0.66
INPD3_ALPHA	CuAu (L10)	L10	tP2	P4/mmm	123	InPd3_LT	2	[0.25, 0.75]	(IN)0.25(AG, CU, PD)0.75
INPD3_BETA	Unknown Structure						2	[0.26, 0.74]	(IN)0.26(PD)0.74
IN7PT3	Ir3Ge7 (D8f)	D8f	cI40	Im-3m	229		2	[7.0, 3.0]	(IN)7(PT)3
INPT	AlCu(r)		mS20	C2/m	12		2	[1.0, 1.0]	(IN, PT)1(IN, PT)1
IN5PT6	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225		2	[5.0, 6.0]	(IN, PT)5(IN, PT)6

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
IN9PT13	Ga9Ni13		mS44	C2/m	12		2	[9.0, 13.0]	(IN)9(IN, PT)13
IN2PT3_ALPHA	Pt3Tl2		hP20	P6_3/mmc	194		2	[2.0, 3.0]	(IN)2(PT)3
IN2PT3_BETA	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[2.0, 3.0]	(IN, PT)2(IN, PT)3
INPT2	Ga3Pt5		oS16	Cmmm	65	Pt5.33In2.67 rt	2	[1.0, 2.0]	(IN)1(PT)2
IN3RH	In3Ir		tP16	P4_2/mnm	136		2	[3.0, 1.0]	(IN)3(RH)1
INSN_GAMMA	(Hg0.1Sn0.9)		hP1	P6/mmm	191		1	[1.0]	(IN, SN)1
MNNI2	Unknown Structure						2	[1.0, 2.0]	(MN, NI)1(NI)2
MN3PD5	Ga3Pt5		oS16	Cmmm	65		2	[3.0, 5.0]	(MN)3(PD)5
MNPD2	Unknown Structure						2	[1.0, 2.0]	(MN)1(PD)2
MNPT7	Ca7Ge		cF32	Fm-3m	225		3	[6.0, 1.0, 1.0]	(PT)6(PT)1(MN)1
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62		2	[3.0, 2.0]	(MN)3(SN)2
MNTI_LT	Zr21Re25		hR92	R-3c	167		2	[1.0, 1.0]	(MN)1(TI)1
MNTI_HT	Unknown Structure		t**				2	[0.515, 0.485]	(MN)0.515(TI)0.485
MN3TI	Unknown Structure						2	[3.0, 1.0]	(MN)3(TI)1
MN4TI	R-(Co, Cr, Mo)		hR53	R-3	166		2	[0.815, 0.185]	(MN)0.815(TI)0.185
MNZN9	Unknown Structure		h**				2	[1.0, 9.0]	(MN)1(ZN)9
NI3SN_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194	Ni3Sn, SnTi3, SnMn3, AlLa3	2	[0.75, 0.25]	(AU, CO, CU, MN, NI, SN, TI)0.75(GA, IN, NI, SN, TI)0.25
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	C2/m	12		3	[0.25, 0.25, 0.5]	(CU, NI)0.25(IN, NI, SN)0.25 (IN, SN)0.5

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
NITI2	NiTi2		cF96	Fd-3m	227		2	[1.0, 2.0]	(CO, NI, TI)1(NI, TI)2
NI3TI_D024	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194		2	[0.75, 0.25]	(NI, TI)0.75(NI, TI)0.25
NIZN_TP2	CuAu (L10)	L10	tP2	P4/mmm	123	united HT/LT phase.	2	[0.5, 0.5]	(CU, NI, PD, ZN)0.5(NI, PD, ZN)0.5
NIZN8_DELTA	Ni3Zn22		mS50	C2/m	12		2	[1.0, 8.0]	(NI)1(ZN)8
PD3SN	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.75, 0.25]	(PD, SN)0.75(PD, SN)0.25
PD20SN13	Unknown Structure						2	[0.6, 0.4]	(PD, SN)0.6(PD, SN)0.4
PDSN2	PdSn2		tI48	I4_1/acd	142		2	[0.333, 0.667]	(PD, SN)0.333(SN)0.667
PD3SN2_ALPHA	Unknown Structure						2	[0.6, 0.4]	(PD)0.6(SN)0.4
PD3SN2_BETA	Unknown Structure						2	[3.0, 2.0]	(PD)3(SN)2
PD3SN2_GAMMA	Unknown Structure						2	[0.59, 0.41]	(PD)0.59(SN)0.41
PDZN_GAMMA	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		2	[2.0, 9.0]	(PD, ZN)2(PD, ZN)9
PDZN_BETA	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(PD, ZN)1(PD, ZN)1
PDZN2	Zn5(Zn0.33Pd0.67)Pd2		oS48	Cmmm	65		2	[1.0, 2.0]	(PD)1(ZN)2
PDZN_ETA	Unknown Structure						2	[0.09, 0.91]	(PD)0.09(ZN)0.91
PT2SN3	Pt2Sn3 (D5b)	D5b	hP10	P6_3/mmc	194		2	[0.4, 0.6]	(PT)0.4(SN)0.6
PT3SN	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.75, 0.25]	(PT)0.75(SN)0.25
PD2TI	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(PD)2(TI)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
PD3TI2	Pd3Ti2		oS20	Cmcm	63		2	[3.0, 2.0]	(PD)3(TI)2
PD5TI3	Pd5Ti3		tP8	P4/mmm	123		2	[5.0, 3.0]	(PD)5(TI)3
PT8TI	Pt8Ti		tI18	I4/mmm	139		2	[8.0, 1.0]	(PT)8(TI)1
PT3TI_D024	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194		2	[3.0, 1.0]	(PT)3(PT, TI)1
PTTI_B19	beta'-AuCd (B19)	B19	oP4	Pmma	51		2	[1.0, 1.0]	(PT, TI)1(PT, TI)1
PT3TI4	Unknown Structure						2	[3.0, 4.0]	(PT)3(TI)4
PTTI3_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[1.0, 3.0]	(PT, TI)1(PT, TI)3
RHSN	FeSi (B20)	B20	cP8	P2_13	198		2	[1.0, 1.0]	(RH)1(SN)1
RHSN4	IrGe4		hP15	P3_121	152		2	[1.0, 4.0]	(RH)1(SN)4
RHSN2_RT	RhSn2		tI26	I4/mmm	139		2	[0.33333, 0.66667]	(RH)0.33333(SN)0.66667
RH2SN	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(RH)2(SN)1
RU3SN7	Ir3Ge7 (D8f)	D8f	cI40	Im-3m	229		2	[0.3, 0.7]	(RU)0.3(SN)0.7
RU2SN3	Ru2Sn3		tP20	P-4c2	116		2	[0.4, 0.6]	(RU)0.4(SN)0.6
SNTI2	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[1.0, 2.0]	(SN)1(TI)2
SN3TI5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193	also M5Sn3, M5Si3C.	2	[3.0, 5.0]	(SN)3(TI)5
SN5TI6	Sn5Ti6-beta		hP22	P6_3/mmc	194	also Sn5Nb6.	2	[5.0, 6.0]	(SN)5(TI)6
TIZN5	Unknown Structure						2	[1.0, 5.0]	(TI)1(ZN)5
TIZN10	Ti3Zn22		tP100	P4_2/mbc	135		2	[1.0, 10.0]	(TI)1(ZN)10

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
TIZN15	TiZn16		oS68	Cmcm	63		2	[1.0, 15.0]	(TI)1(ZN)15
HEUSLER_L21	Heusler (L21)	L21	cF16	Fm-3m	225		3	[0.5, 0.5, 1.0]	(AG, AU)0.5(AG, AU)0.5(ZN)1
AGINPD	Unknown Structure						3	[0.156, 0.26, 0.584]	(AG)0.156(IN)0.26(PD)0.584
AL3CU5ZN2	Cu3.2 (Zn0.18Al0.82)4Al0.9		hR27	R-3m	166		4	[1.0, 4.0, 4.0, 1.0]	(AL, CU)1(AL)4(CU)4(ZN)1
AUCOSN4	delta-Ni3Sn4 (D7a)	D7a	mS14	C2/m	12		3	[0.1500015, 0.249925, 0.60006]	(AU)0.150002(CO)0.249925 (SN)0.60006
AU2CUZN	(Cu0.6Zn0.4)Au		oP8	Pbam	55		2	[0.5, 0.5]	(AU)0.5(CU, ZN)0.5
AU3CUZN	Unknown Structure		o**				3	[3.0, 1.0, 1.0]	(AU)3(CU)1(ZN)1
AU4IN3SN3	Pt2Sn3 (D5b)	D5b	hP10	P6_3/mmc	194		3	[0.4, 0.3, 0.3]	(AU)0.4(IN, SN)0.3(IN, SN)0.3
AUNI2SN4	Unknown Structure						3	[0.571, 0.143, 0.286]	(SN)0.571(AU)0.143(NI)0.286
AUPT2SN4_TAO	Unknown Structure						3	[1.0, 2.0, 4.0]	(AU)1(PT)2(SN)4
CU77INSN23	Unknown Structure						2	[0.77, 0.23]	(CU)0.77(IN, SN)0.23
CU2IN3SN	Unknown Structure						3	[0.333, 0.5, 0.167]	(CU)0.333(IN)0.5(SN)0.167
CUNI2SN	Unknown Structure						3	[0.233, 0.5, 0.267]	(CU)0.233(NI)0.5(SN)0.267
CU4MNSN	MgCu4Sn		cF24	F-43m	216		3	[0.6666, 0.1667, 0.1667]	(CU)0.6666(SN)0.1667 (MN)0.1667
GA11GEPT7	Unknown Structure						3	[0.579, 0.053, 0.368]	(GA)0.579(GE)0.053(PT)0.368

Phase	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula Unit*
GA3GEPT8	Unknown Structure						2	[0.333, 0.667]	(GA, GE)0.333(PT)0.667
GAGEPT6	Ir3Si		tI16	I4/mcm	140		2	[0.25, 0.75]	(GA, GE)0.25(PT)0.75
INNI6SN5	Ni(Ga0.25Ge0.75)		oP16	Pnma	62		2	[1.0, 1.0]	(NI)1(IN, SN)1
AGTI2	CuZr2		tI6	I4/mmm	139		2	[1.0, 2.0]	(AG)1(TI)2
AGTI	CdTi		tP4	P4/nmm	129		2	[1.0, 1.0]	(AG, TI)1(AG, TI)1

TCNOBL3 Properties

Model Descriptions

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

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

Examples

Go to the Noble Metal Alloys Databases page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to Precious Metals including links to resources such as examples, publications, and more.

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:	**3.0**
First release	**TCNOBL1 was released with 2017b. Note that there is no external release of TCNOBL2**

Changes in the Most Recent Database Release

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 of 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.