

TCS Noble Metal Alloys Database (TCNOBL3)

Technical Information

Available Starting with Thermo-Calc 2023b



Contents

| | |
|---|-----------|
| About the TCS Noble Metal Alloys Database (TCNOBL) | 3 |
| TCS Noble Metal Alloys Database (TCNOBL) Resources | 6 |
| TCNOBL3 Elements, Systems, Phases and Properties | 7 |
| TCNOBL3 Systems | 9 |
| TCNOBL3 Assessed Binary Systems | 10 |
| TCNOBL3 Assessed Ternary Systems | 11 |
| TCNOBL3 Phases | 12 |
| Common Phases for Noble / Precious Metals | 13 |
| TCNOBL3 Models for the Included Phases | 15 |
| TCNOBL3 Properties | 36 |
| Model Descriptions | 36 |
| Examples | 36 |
| TCNOBL: TCS Noble Metal Alloys Database Revision History | 37 |
| Current Database Version | 37 |

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.

| <i>Property</i> | <i>Model Parameters</i> | <i>Variables to Show or Plot in Console Mode and TC-Python</i> |
|--|-------------------------|--|
| 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 |
| <p>* 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.</p> <p>** ION is used in the TCS Metal Oxide Solutions Database (TCOX)</p> | | |

TCNOBL3 Systems

In this section:

| | |
|--|----|
| TCNOBL3 Assessed Binary Systems | 10 |
| TCNOBL3 Assessed Ternary Systems | 11 |

TCNOBL3 Assessed Ternary Systems

| <i>Assessed Ternary Systems</i> | | | | | |
|---------------------------------|----------|----------|----------|----------|----------|
| 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 | 13 |
| TCNOBL3 Models for the Included Phases | 15 |

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.

| <i>Name in the Database</i> | <i>Common Name and Description</i> |
|-----------------------------|---|
| 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 |

| <i>Name in the Database</i> | <i>Common Name and Description</i> |
|-----------------------------|---|
| 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 of ordered 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 its solution | 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 or solution 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 | cl58 | 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 | tl6 | 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 | tl12 | 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 | cl52 | 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 (CaF ₂ , 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 | MoSi ₂ (C11b) | C11b | tI6 | I4/mmm | 139 | | 2 | [1.0, 2.0] | (AL, AU)1(AL, AU)2 |
| ALAU2_LT | AlAu ₂ | | 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 | AlAu ₄ | | cP20 | P2 ₁ -13 | 198 | | 2 | [0.2, 0.8] | (AL)0.2(AG, AU)0.8 |
| AL3AU8 | Yb ₈ In ₃ | | hR132 | R-3c | 167 | | 2 | [0.27273, 0.72727] | (AL)0.27273(AU)0.72727 |
| AL13CO4 | Orthorhombic Co ₄ Al ₁₃ | | oP102 | Pmn2 ₁ | 31 | | 2 | [13.0, 4.0] | (AL)13(CO)4 |
| AL3CO | Os ₄ Al ₁₃ | | mS34 | C2/m | 12 | | 2 | [3.0, 1.0] | (AL)3(CO)1 |
| AL5CO2_D811 | Co ₂ Al ₅ (D811) | D811 | hP28 | P6 ₃ /mmc | 194 | also Al ₅ Rh ₂ . | 2 | [5.0, 2.0] | (AL)5(CO, RH)2 |
| AL9CO2 | Co ₂ Al ₉ (D8d) | D8d | mP22 | P2 ₁ /c | 14 | | 2 | [9.0, 2.0] | (AL, GA)9(CO, RH)2 |
| AL11CR2 | Al ₅ Cr | | mS732 | C2/c | 15 | | 3 | [10.0, 1.0, 2.0] | (AL)10(AL)1(CR)2 |
| AL13CR2 | Al ₄ S ₇ | | mS104 | C2/m | 12 | | 2 | [13.0, 2.0] | (AL)13(CR)2 |
| AL4MN | mu-Al ₄ Mn | | hP574 | P6 ₃ /mmc | 194 | | 2 | [4.0, 1.0] | (AL)4(CR, MN)1 |
| AL8CR5_H | gamma-brass (Cu ₅ Zn ₈ , D82) | D82 | cI52 | I-43m | 217 | | 2 | [8.0, 5.0] | (AL)8(CR)5 |
| AL8CR5_L | Cr ₅ Al ₈ (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, |

| Phase | Prototype | Strukturbericht | Pearson Symbol | Space Group Symbol | SG# | Info | Sublattices | Sites | Formula Unit |
|---------------|------------------------|-----------------|----------------|--------------------|-----|--|-------------|--------------------|---|
| | | | | | | on Al13Fe4, aka Al3Fe | | 0.1375] | RU)0.235(AL, VA)0.1375 |
| AL12MN | Al12W | | cl26 | 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 | | cl26 | 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 | | tl6 | 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 | tl16 | I4/mmm | 139 | | 2 | [17.0, 8.0] | (AL)17(TI)8 |
| AL2TI | Ga2Hf | | tl24 | I4_1/amd | 141 | | 2 | [2.0, 1.0] | (AL)2(TI)1 |
| AUCU_II | CuAu | | ol40 | 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 | Au ₆ (Au _{0.5} In _{0.5}) ₆ In | | 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 | Cu ₁₀ Sb ₃ | | hP26 | P6 ₃ /m | 176 | | 2 | [0.77778, 0.22222] | (AU)0.77778(IN)0.22222 |
| AU7IN3 | Au ₇ In ₃ | | 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 | Ni ₄ Mo (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 | SrPb ₃ | | tp4 | P4/mmm | 123 | | 2 | [0.75, 0.25] | (AU)0.75(MN)0.25 |
| AU11MN4 | Au ₁₁ Mn ₄ | | mS810 | Cm | 8 | | 2 | [0.733, 0.267] | (AU)0.733(MN)0.267 |
| AU5MN2 | Au ₅ Mn ₂ | | mS14 | C2/m | 12 | | 2 | [0.714, 0.286] | (AU)0.714(MN)0.286 |
| AU2MN | MoSi ₂ (C11b) | C11b | tI6 | I4/mmm | 139 | | 2 | [0.667, 0.333] | (AU)0.667(MN)0.333 |
| AUMN2 | MoSi ₂ (C11b) | C11b | tI6 | I4/mmm | 139 | | 2 | [0.333, 0.667] | (AU)0.333(MN)0.667 |
| AU10SN_D024 | Ni ₃ Ti (D024) | D024 | hP16 | P6 ₃ /mmc | 194 | AuIn_Alpha1, AuSn_Beta | 1 | [1.0] | (AG, AU, GA, GE, IN, SN)1 |
| AUSN2_OP24 | AuSn ₂ | | 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 |
| CR3MNS | 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 |

| Phase | Prototype | Strukturbericht | Pearson Symbol | Space Group Symbol | SG# | Info | Sublattices | Sites | Formula Unit |
|-----------------|---------------------------|-----------------|----------------|--------------------|-----|---|-------------|--------------------------|--|
| 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 | BfF3 (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 | BfF3 (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 |

| Phase | Prototype | Strukturbericht | Pearson Symbol | Space Group Symbol | SG# | Info | Sublattices | Sites | Formula Unit |
|----------------|---------------------------|-----------------|----------------|--------------------|-----|------|-------------|------------------------------|--|
| 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 | cl40 | 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 | Pnmm | 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 | cl40 | 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 | cl40 | 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 | Pt3TI2 | | 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 | Cu _{3.2} (Zn _{0.18} Al _{0.82}) ₄ Al _{0.9} | | hR27 | R-3m | 166 | | 4 | [1.0, 4.0, 4.0, 1.0] | (AL, CU)1(AL)4(CU)4(ZN)1 |
| AUCOSN4 | delta-Ni ₃ Sn ₄ (D7a) | D7a | mS14 | C2/m | 12 | | 3 | [0.1500015, 0.249925, 0.60006] | (AU)0.150002(CO)0.249925 (SN)0.60006 |
| AU2CUZN | (Cu _{0.6} Zn _{0.4})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 | Pt ₂ Sn ₃ (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 | MgCu ₄ Sn | | 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 |

| <i>Phase</i> | <i>Prototype</i> | <i>Strukturbericht</i> | <i>Pearson Symbol</i> | <i>Space Group Symbol</i> | <i>SG#</i> | <i>Info</i> | <i>Sublattices</i> | <i>Sites</i> | <i>Formula Unit</i> |
|--------------|-------------------|------------------------|-----------------------|---------------------------|------------|-------------|--------------------|----------------|------------------------|
| 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

| | |
|---------------------------------|---|
| <i>Database name (acronym):</i> | TCS Noble Metal Alloys Database (TCNOBL) |
| <i>Database owner:</i> | Thermo-Calc Software AB |
| <i>Database version:</i> | 3.0 |
| <i>First release</i> | 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.