TCS Al-based Alloy Database (TCAL9)

Technical Information

Available Starting with Thermo-Calc Version 2024a

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Contents

About the TCS Al-based Alloy Database (TCAL)

TCS Al-based Alloy Database (TCAL) is a thermodynamic database developed for aluminum-based alloys, including but not limited to, the industrial grades.

In addition to thermodynamic data, it has 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 TCAL2. Electrical resistivity, thermal conductivity, viscosity of metallic liquids, and surface tension of metallic liquids properties data are available starting with TCAL7.

TCAL: TCS Aluminium-based Alloys Database Revision History. The current version of the database is TCAL9. See the link for any subversion release details.

The database is compatible with the TCS Al-alloys Mobility Database (MOBAL). The current version is MOBAL8.

The CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

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

Use Case Examples

There are examples available to both demonstrate the *validation* of the database and to showcase the types of *calculations* that can be used for different materials or application 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 use case examples of how this database can be used include the following. Use it to:

- Calculate various phase diagrams and property diagrams in the assessed systems as well as to extrapolate higher-order systems, and predict phase formation, phase fractions and phase compositions in multicomponent aluminum alloys.
- Predict non-equilibrium solidification behavior of aluminum alloys. This can be at specific cooling rates when you take into account back diffusion using the Scheil calculation options in Thermo-Calc.
- Integrate with a compatible atomic mobility database and use it to simulate diffusion-controlled phase transformations with the add-on Diffusion Module (DICTRA) and multi-particle precipitation kinetics with the add-on Precipitation Module (TC-PRISMA).

Calculations and simulations for higher-order systems might not be valid beyond the Al-rich region.

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 Al-based Alloy Database (TCAL) 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 Al-based Alloy Database (TCAL) Technical Information* PDF document contains version specific information such as the binary, ternary, and higher-order assessed 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 Al-based Alloy Database (TCAL) 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 Aluminum-based Alloys Databases page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to aluminum including links to resources such as publications, webinars, videos, and more.

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

TCAL9 Elements, Systems, Phases and Properties

Included Elements

There are 48 elements included in the most recent version of the database.

Ag	Al	B	Ba	Be	Bi	C	Ca	Cd	Ce
Co	Cr	Cu	Er	Fe	Ga	Ge	H	Hf	In
K	La	Li	Mg	Mn	Mo	Na	Nb	Nd	Ni
P	Pb	Pr	S	Sb	Sc	Se	Si	Sn	Sr
Te	Ta	Ti	V	W	Y	Zn	Zr		

Assessed Systems and Phases

The most recent version of the database contains:

- 313 assessed binary systems, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 119 assessed ternary systems, mostly to their full range of composition. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 14 quaternaries are assessed within the Al-rich region.
- 722 solution and intermetallic phases. This includes nearly all stable phases in the assessed systems and the most important metastable phases that may form in as-cast and aged Al-based alloys.

The GAS phase is restored by default when retrieving the data from the database. In order to reject it when it is not required for a calculation, you now have to manually reject it.

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 TCAL2. Electrical resistivity, thermal conductivity, viscosity of metallic liquids, and surface tension of metallic liquids properties data are available starting with TCAL7.

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 conductivity	ELQ**	ELCD for a system `ELCD(PHI)` for phase PHI
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI*	`SURF(LIQUID)` `SURF(ION)` **
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)` **
Kinematic viscosity		`KVIS(LIQUID)`

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
		`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. As of 2024a, TCMG7, TCAL9, and TCHEA7.

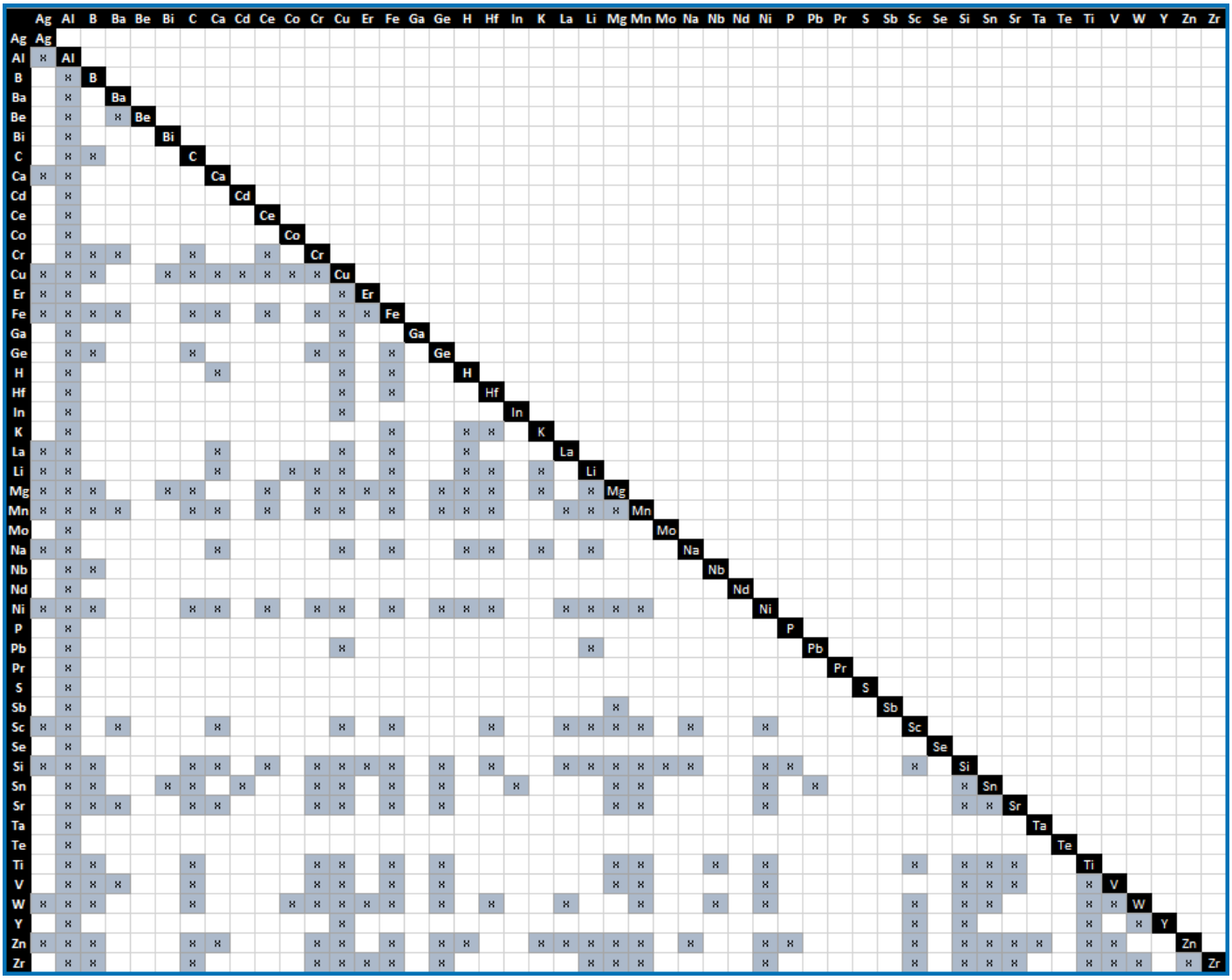
** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCAL9 Systems

In this section:

TCAL9 Assessed Binary Systems

These are the assessed binary systems, which are mostly in the full range of composition and temperature.



TCAL9 Assessed Ternary Systems

The assessed ternary systems that are mostly in full compositional ranges.

Assessed Ternary Systems				
Ag-Al-Cu	Al-B-Nb	Al-Bi-Mg	Al-Bi-Sn	Al-C-Cr
Al-C-Mg	Al-C-Si	Al-C-Ti	Al-C-V	Al-Cd-Sn
Al-Ce-Cr	Al-Ce-Cu	Al-Ce-Fe	Al-Ce-Mg	Al-Ce-Mn
Al-Ce-Ni	Al-Ce-Si	Al-Cr-Mg	Al-Cr-Si	Al-Cr-Sn
Al-Cu-Er	Al-Cu-Fe	Al-Cu-Li	Al-Cu-Mg	Al-Cu-Mn
Al-Cu-Ni	Al-Cu-Sc	Al-Cu-Si	Al-Cu-Sn	Al-Cu-Ti
Al-Cu-W	Al-Cu-Y	Al-Cu-Zn	Al-Er-Fe	Al-Er-Mg
Al-Fe-Mg	Al-Fe-Mn	Al-Fe-Ni	Al-Fe-Si	Al-Fe-Zn
Al-In-Sn	Al-Li-Mg	Al-Li-Pb	Al-Li-Si	Al-Li-Zn
Al-Li-Zr	Al-Mg-Mn	Al-Mg-Ni	Al-Mg-Sb	Al-Mg-Sc
Al-Mg-Si	Al-Mg-Sn	Al-Mg-Sr	Al-Mg-Ti	Al-Mg-Zn
Al-Mg-Zr	Al-Mn-Ni	Al-Mn-Si	Al-Mn-Ti	Al-Mn-Zn
Al-Mo-Si	Al-Nb-Ti	Al-Ni-Si	Al-Ni-Ti	Al-Ni-Zn
Al-P-Si	Al-P-Zn	Al-Pb-Sn	Al-Sc-Si	Al-Sc-Ti
Al-Sc-Y	Al-Sc-Zr	Al-Si-Sn	Al-Si-Sr	Al-Si-Ti
Al-Si-Y	Al-Si-Zn	Al-Sn-Zn	Al-Ta-Zn	Al-Ti-Y
Bi-Mg-Sn	Cu-Fe-Mg	Cu-Fe-Mn	Cu-Fe-Ni	Cu-Fe-Si
Cu-Fe-Zn	Cu-Li-Mg	Cu-Mg-Mn	Cu-Mg-Ni	Cu-Mg-Si
Cu-Mg-Zn	Cu-Mn-Ni	Cu-Mn-Si	Cu-Mn-Zn	Cu-Ni-Si
Cu-Ni-Zn	Cu-Si-Zn	Fe-Mg-Mn	Fe-Mg-Ni	Fe-Mg-Si

Assessed Ternary Systems				
Fe-Mg-Zn	Fe-Mn-Ni	Fe-Mn-Si	Fe-Mn-Zn	Fe-Ni-Si
Fe-Ni-Zn	Fe-Si-Zn	Mg-Mn-Ni	Mg-Mn-Si	Mg-Mn-Zn
Mg-Ni-Si	Mg-Ni-Zn	Mg-Sc-Si	Mg-Si-Sn	Mg-Si-Zn
Mn-Ni-Si	Mn-Ni-Zn	Mn-Si-Zn	Ni-Si-Zn	

TCAL9 Assessed Quaternary Systems

Quaternary Systems
Al-Cu-Fe-Mn
Al-Cu-Fe-Ni
Al-Cu-Mg-Ni
Al-Cu-Mg-Si
Al-Cu-Mg-Zn
Al-Cu-Mn-Si
Al-Cu-Ni-Si
Al-Fe-Mg-Mn
Al-Fe-Mg-Si
Al-Fe-Mn-Si
Al-Fe-Ni-Si
Al-Mg-Mn-Si
Al-Bi-Mg-Sn
Al-Mg-Sc-Si

TCAL9 Phases

In this section:

Common Phases for Aluminum Alloys

TCAL9 Models for the Included Phases

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

Name in the Database	*Common Name and Description*
AL15SI2M4	A cubic precipitate, which originates from the Al-Mn-Si ternary system, aka τ9, Al15Mn3Si2, Al16Mn4Si3 or Al15Mn4Si2. Mn can be substituted by Fe, as well as Cr and Mo. The phase observed in aluminum alloys is also designated as α.
AL13FE4	An iron aluminide, which often forms as a primary phase during casting, aka Al3Fe.
AL2CU_C16	The so-called θ-Al2Cu phase that forms in many Cu-containing aluminum alloys.
AL2CU_OMEGA	Ω-Al2Cu, a metastable precipitate and the coherent version of the θ phase
THETA_PRIME	A semi-coherent precipitate with a stoichiometry of Al2Cu in α-(Al), i.e. the GPI zones.
THETA_DPRIME	Coherent metastable precipitates in α-(Al), also referred to as GPII zones. It has a stoichiometry close to Al3Cu.
BETA_DPRIME	Metastable precipitate β'' related to Mg2Si that forms in Al-Mg-Si based alloys. It may contain Al atoms (Al2Mg5Si4) or be Al-free (Mg5Si6).
BETA_PRIME	Metastable precipitate β' related to Mg2Si, aka Mg9Si5/Mg1.8Si
U1_AL2MGSI2	An Al-containing pre-β Al-Mg-Si metastable precipitate, U1_Al2MgSi2
U2_AL4MG4SI4	An Al-containing pre-β Al-Mg-Si metastable precipitate, U2_Al4Mg4Si4
AL18FE2MG7SI10	A quaternary phase, aka Al8FeMg3Si6, Q, PHI and H_PHASE
Al4Fe	A metastable Al-Fe phase that forms in solidification of some aluminum alloys. Also known as AlmFe.
AL9M2	A metastable Al-Fe phase that forms in solidification of some aluminum alloys and it can be stabilized in the Al-Fe-Ni system
AL6MN	A common Al-Mn compound that forms in Mn-containing aluminum alloys. Mn could be substituted by Cu and Fe, especially to a larger extent by the latter.
AL28CU4MN7	An Al-Cu-Mn intermetallic phase that forms in aluminum alloys
Q_ALCUMGSI	A stable Al-Cu-Mg-Si quaternary phase, aka Q, Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 and Al4Cu2Mg8Si7

Name in the Database	*Common Name and Description*
QPRIME	The coherent / semi-coherent version of Q_ALCUMGSI
MG2SI_C1	Mg2Si, which forms in Mg- and Si-containing aluminum alloys
AL9FE2SI2	A common Al-Fe-Si ternary phase in aluminum alloys, aka τ6, Al5FeSi, β-AlFeSi
AL8FE2SI	A common Al-Fe-Si ternary phase in aluminum alloys, aka τ5, α-AlFeSi
AL7CU2FE	An Al-Cu-Fe ternary compound that may form in some aluminum alloys
DIAMOND_A4	Si, as well as C and Ge
C14_LAVES	A common stable precipitate in 7000 series aluminum alloys, aka. the η (MgZn2) phase, eta and the M phase. This phase includes all MgZn2-type phases.
ETA_PRIME	The metastable η' phase, which is related to the η-MgZn2 phase.
T_PHASE	A stable phase in Al-Mg-Zn, Al-Cu-Mg and Al-Cu-Mg-Zn. It is modeled as (Al,Cu,Zn)49Mg32 and is often designated as Al2Mg3Zn3 in aluminum alloys.
T_PRIME	The metastable form of T phase, T’
S_PHASE	The S phase, Al2CuMg
S_PRIME	The metastable S’ phase, precursor to the S phase
Q_ALCUMGSI	The Al-Cu-Mg-Si quaternary phase, i.e. the Q Phase, aka Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 and Al4Cu2Mg8Si7
Q_AL7CU3MG6	An Al-Cu-Mg ternary phase, aka, Al7Cu3Mg6 and the Q phase

TCAL9 Models for the Included Phases

See the separate listing for Gas and Liquid Phases below.

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	(70, Fddd)		1	(S)1.0
RED_P	Unknown Structure					1	(P)1.0
WHITE_P	Unknown Structure					1	(P)1.0
HEXAGONAL_A8	gamma-Se (A8)	A8	hP3	(152, P3_121)	Se, Te	1	(SE, TE)1.0
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	Metallic FCC_A1 solution, e.g. (Al), (Cu), and MC carbides	2	(AG, AL, BA, BE, BI, CA, CD, CE, CO, CR, CU, ER, FE, GA, GE, HF, IN, K, LA, LI, MG, MN, MO, NA, NB, ND, NI, P, PB, PR, S, SB, SC, SE, SI, SN, SR, TA, TE, TI, V, W, Y, ZN, ZR)1.0(B, C, H, VA)1.0
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	L12, Ni3Si_rt, AlZr3, GeNi3, TiZn3, VZn3, Ag3Mg, AlNi3, FeNi3, MnNi3, AlPr3(ht), (Al,Cu)3Ti, (Al,Mn)3Ti	2	(AG, AL, FE, GE, MG, MN, NI, SI, TI, V, ZN)1.0(AG, AL, CU, FE, MG, MN, NI, PR, TI, ZN, ZR)3.0
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	Metallic BCC_A2 solution	2	(AG, AL, BA, BE, BI, CA, CD, CE, CO, CR, CU, ER, FE, GA, GE, HF, IN, K, LA, LI, MG, MN, MO, NA, NB, ND, NI, P, PB, PR, SC, SI, SN, SR, TA, TI, V, VA, W, Y, ZN, ZR)1.0(B, C, H, VA)3.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	Solution of ordered BCC_B2, having Gibbs energy contribution from BCC_A2	3	(AG, AL, BA, BE, BI, CA, CD, CE, CO, CR, CU, ER, FE, GA, GE, HF, IN, K, LA, LI, MG, MN, MO, NA, NB, ND, NI, P, PB, PR, SC, SI, SN, SR, TA, TI, V, VA, W, Y, ZN, ZR)0.5(AG, AL, BA, BE, BI, CA, CD, CE, CO, CR, CU, ER, FE, GA, GE, HF, IN, K, LA, LI, MG, MN, MO, NA, NB, ND, NI, P, PB, PR, SC, SI, SN, SR, TA, TI, V, VA, W, Y, ZN, ZR)0.5 (B, C, H, VA)3.0
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(AL, CO, CR, CU, FE, GE, LI, MG, MN, NI, SI, SN, SR, TI, V, W, ZN, ZR)1.0(B, C, H, VA)1.0
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		2	(AG, AL, CE, CR, CU, FE, GE, HF, LI, MG, MN, NI, SI, SN, SR, TI, V, W, ZN, ZR)1.0 (B, C, H, VA)1.0
DHCP	alpha-La (A3')	A3'	hP4	(194, P6_ 3/mmc)		1	(AL, CE, CU, LA, ND, NI, PR, SC)1.0
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	Metallic HCP_A3 solution, alpha_Mg/Hf/Sc/Ti/Zr, epsilon_CuZn, etc.	2	(AG, AL, BE, BI, CA, CD, CE, CO, CR, CU, ER, FE, GA, GE, HF, IN, K, LA, LI, MG, MN, MO, NA, NB, ND, NI, PB, PR, SB, SC, SI, SN, SR, TI, V, W, Y, ZN, ZR)1.0(B, C, H, VA)0.5
BETA_RHOMBO_B	beta-B (R-105)		hR105	(166, R-3m)		2	(B)93.0(B, C, CU, NB, SI)12.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_ 3/mmc)		1	(B, C)1.0
RHOMBO_A7	alpha-As (A7)	A7	hR2	(166, R-3m)	Bi	1	(BI, IN, SB, SN)1.0
TETRA_A6	In (A6)	A6	tI2	(139, I4/mmm)		1	(IN, SN)1.0
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	Solution of MgZn2-type phases, including MgZn2 (Eta, aka M or sigma)	2	(AL, CR, CU, FE, HF, LI, MG, MN, NI, TI, W, ZN, ZR)2.0(AL, CR, CU, ER, FE, HF, MG, MN, NI, SC, TI, W, ZN, ZR)1.0
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	Solution of Cu2Mg-type phases, cF24, Fd-3m, Al2Nd, Al2Pr	2	(AL, CA, CR, CU, FE, HF, LA, LI, MG, ND, NI, SC, SI, TI, W, ZN, ZR)2.0(AL, CA, CE, CR, CU, ER, FE, HF, LA, LI, MG, ND, NI, PR, SC, SI, TI, W, ZN, ZR)1.0
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)	Solution of MgNi2-type phases, hP24, P63/mmc	2	(AL, CR, CU, FE, HF, MG, MN, NI, ZN, ZR)2.0(AL, CR, CU, FE, HF, MG, NI, SC, ZN, ZR)1.0
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	Pure C, Ge, Si or solution phases based on them	1	(AL, B, C, GA, GE, P, SI, SN, SR, TI, ZN)1.0
BCT_A5	beta-Sn (A5)	A5	tI4	(141, I4_ 1/amd)	Pure Sn or its solution	1	(AL, B, BI, CD, CU, GA, GE, IN, PB, SN, TI, ZN)1.0
ORTHORHOMBIC_GA	alpha-Ga (A11)	A11	oS8	(64, Cmce)		1	(GA)1.0
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		3	(FE, MN, NI)8.0(CR, V)4.0(CR, FE, MN, NI, V)18.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL45V7	Al45V7		mS104	(12, C2/m)	Al45Cr7, Al45V7	2	(AL)45.0(CR, V)7.0
CUZR2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	AlCr2, CuTi2, CuZr2, Ti2Zn, ZnZr2	2	(AL, CR, CU, SI, ZN)1.0(AL, CR, TI, ZR)2.0
B2_BCC	CsCl (B2)	B2	cP2	(221, Pm-3m)	AlCo, CuZr, FeTi, TiZn, ZnZr, MgSc, MnZn(rt)	2	(AG, AL, CO, CU, FE, MG, ZN)1.0(AG, CO, MG, MN, SC, TI, VA, ZR)1.0
ALB2_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	AlB2, B2Cr, B2Mg, B2Mn, B2Ti, B2V, B2Zr	2	(AL, CR, MG, MN, NB, TI, V, ZR)1.0 (B)2.0
FEB_B27	FeB (B27)	B27	oP8	(62, Pnma)	BFe, BMn, BTi, GeZr, SiTi, SrZn, SiZr	2	(FE, MN, SR, TI, ZR)1.0(B, GE, SI, ZN)1.0
AL3TI_D022	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	Al3Ti, Ni3V, GeMn3, Al3V	2	(AL, CU, MN, NB, NI, SI, TI)3.0(AL, GE, MN, NB, SC, TA, TI, V, ZR)1.0
ALZR2_B82	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)	SnTi2, GeMn2, AlZr2, AlSc2	2	(AL, GE, MN, SN, VA)1.0(MN, SC, TI, VA, Y, ZR)2.0
AL2ZR3_TP20	Zr3Al2		tP20	(136, P4_ 2/mnm)	Al2Zr3, Al2Hf3, ZN2Zr3	2	(AL, ZN)2.0(HF, SC, Y, ZR)3.0
CAZN13_CF112	NaZn13 (D23)	D23	cF112	(226, Fm-3c)	CaZn13, SrZn13	2	(CA, SR)1.0(ZN)13.0
NI3SN_D019	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	Ni3Sn, SnTi3, SnMn3, AlLa3	2	(AL, GE, SN, VA)1.0 (FE, LA, MN, NI, TI)3.0
CRB_B33	CrB (B33)	B33	oS8	(63, Cmcm)	AgCa, AlHf, AlZr, BNi, BV, GeSr, NiZr, SiSr, SnSr	2	(AL, CA, CR, NB, NI, SR, V)1.0(AG, B, GE, HF, SC, SI, SN, ZR)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3ZR5_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	Al3Zr5, Cr3Si5, Ge3V5, Si3V5	2	(AL, GE, SI)3.0(CR, V, ZR)5.0
AL2SR_OI12	CeCu2		oI12	(74, Imma)	Al2Sr, SrZn2	2	(AL, MG, ZN)2.0 (SR)1.0
CACU5_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	CaCu5, CaNi5, CaZn5, Cu5Sr, ScNi5, SrZn5	2	(CA, SC, SR)1.0(CU, NI, ZN)5.0
M3B4_D7B	Ta3B4 (D7b)	D7b	oI14	(71, Immm)	V3B4, Ti3B4, Mn3B4, Cr3B4	2	(B)4.0(AL, CR, MN, NB, TI, V)3.0
SI2ZR3_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	Si2Zr3, B2V3	2	(B, SI)2.0(NB, V, ZR)3.0
CO2SI_C23	Cotunnite (PbCl2, C23)	C23	oP12	(62, Pnma)	Ca2Si, Ni2Si, SiSr2, SnSr2, GeSr2	2	(CA, CU, FE, NI, SR)2.0(AL, GE, SI, SN, ZN)1.0
CR5B3_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	Ca5Si3, Sn3Sr5, Si4Sr5, Ge3Sr5, B3Cr5	2	(CA, CR, SR)0.625 (AG, B, GE, SI, SN)0.375
M11GE8_OP76	Cr11Ge8		oP76	(62, Pnma)	Cr11Ge8, V11Ge8	2	(CR, V)0.579 (GE)0.421
SIZR3_TP32	Ti3P		tP32	(86, P4_2/n)	SiZr3, SiTi3, GeZr3	2	(GE, SI)1.0(TI, ZR)3.0
SI4ZR5_TP36	Si4Zr5		tP36	(92, P4_12_12)	Si4Zr5, Si4Ti5, Ge4Zr5	2	(GE, SI)4.0(TI, ZR)5.0
SI2ZR_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	Si2Zr, Ge2Zr	2	(GE, SI)2.0(ZR)1.0
SI2TI_C54	TiSi2 (C54)	C54	oF24	(70, Fddd)	Ge2Ti, Si2Ti, Sn2Zr	2	(AL, GE, SI, SN)2.0 (TI, ZR)1.0
ZRM5_C15B	AuBe5 (C15b)	C15b	cF24	(216, F-43m)	Cu5Zr, Ni5Zr	2	(CU, NI)5.0(ZR)1.0
FEM_B35	CoSn (B35)	B35	hP6	(191,	FeSn, FeGe	2	(FE)1.0(GE, SN)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				P6/mmm)			
SN5TI6_OI44	Sn5Ti6-alpha		oI44	(71, Immm)	Sn5Ti6, Si5V6, Ge5Ti6	2	(GE, SI, SN)5.0(TI, V)6.0
M7C3_D101	C3Cr7 (D101)	D101	oP40	(62, Pnma)	Cr7C3, Mn7C3	2	(CR, MN)7.0(C)3.0
M23C6_D84	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)	Cr23C6, Mn23C6, Mn23SC6	2	(CR, MN)23.0(C, SC)6.0
V_PHASE	Mg2Zn11 (D8c)	D8c	cP39	(200, Pm-3)	solution of Mg2Zn11, Al5Cu6Mg2; aka Z	3	(AL, SI, ZN)5.0(CU, ZN)6.0(MG)2.0
AG9CA2	Unknown Structure					2	(AG)0.818182 (CA)0.181818
AG7CA2	Ag7Yb2		oS36	(63, Cmcm)		2	(AG)0.777778 (CA)0.222222
AG2CA	KHg2		oI12	(74, Imma)		2	(AG)0.666667 (CA)0.333333
AGCA3	Unknown Structure					2	(AG)0.25(CA)0.75
AGER	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(AG)1.0(ER)1.0
AG2ER	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AG)2.0(ER)1.0
AG51ER14	Ag51Gd14		hP68	(175, P6/m)		2	(AG)0.77(ER)0.23
AGLA	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(LA)1.0(AG)1.0
AG2LA	KHg2		oI12	(74, Imma)		2	(LA)1.0(AG)2.0
AG51LA14	Ag51Gd14		hP68	(175, P6/m)		2	(LA)14.0(AG)51.0
AG5LA	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(LA)1.0(AG)5.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AGMG3	Hf54Os17		oI142	(71, Immm)	Ag17Mg54	2	(AG)0.23(MG)0.77
AGMG4	Ag9Mg37		hP116	(176, P6_3/m)	Ag9Mg37	2	(AG)0.2(MG)0.8
AG2NA	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(AG)2.0(NA)1.0
AG4SC	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)		2	(AG)0.8(SC)0.2
AGSC	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(AG)0.5(SC)0.5
AGZN3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)		1	(AG, ZN)1.0
AGZN_HP9	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)		2	(ZN)1.0(AG, ZN)2.0
AG5ZN8	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		4	(AG, ZN)2.0(AG)2.0 (AG, ZN)3.0(AG, ZN)6.0
ALB12	alpha-AlB12		tP216	(92, P4_12_ 12)		2	(AL, NB)1.0(B)12.0
AL4BA_D13	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(AL)4.0(BA)1.0
AL13BA7	Al13Ba7		hP20	(164, P-3m1)		2	(AL)13.0(BA)7.0
AL5BA3	Al5Ba3		hP16	(194, P6_ 3/mmc)		2	(AL)5.0(BA)3.0
AL5BA4	Al5Ba4		hP18	(194, P6_ 3/mmc)		2	(AL)5.0(BA)4.0
AL4C3	Al4C3 (D71)	D71	hR7	(166, R-3m)		3	(AL, SI)2.0(AL, MG, SI)2.0(C)3.0
AL14CA13	Al14Ca13		mS54	(12, C2/m)		2	(AL, MG, ZN)14.0 (CA)13.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3CA8	Ca8In3		aP22	(2, P-1)		2	(AL)3.0(CA, MG)8.0
AL4CE1	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(AL)0.8(CE)0.2
AL11CE3	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)		2	(AL, MG)0.7857 (CE)0.2143
AL3CE_H	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)		2	(AL)0.75(CE)0.25
AL3CE_L	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)		2	(AL, SI)0.75(CE)0.25
ALCE_OC16	AlCe		oS16	(63, Cmcm)		2	(AL)0.5(CE)0.5
AL1CE2	Unknown Structure					2	(AL)0.3333 (CE)0.6667
ALCE3_H	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(AL)0.25(CE)0.75
ALCE3_L	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)		2	(AL)0.25(CE)0.75
AL13CO4	Orthorhombic Co4Al13		oP102	(31, Pmn2_1)		2	(AL)13.0(CO)4.0
AL3CO	Os4Al13		mS34	(12, C2/m)		2	(AL)3.0(CO)1.0
AL5CO2	Co2Al5 (D811)	D811	hP28	(194, P6_3/mmc)		2	(AL)5.0(CO)2.0
AL9CO2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)		2	(AL)9.0(CO)2.0
AL5CR	Al5Cr		mS732	(15, C2/c)		2	(AL, SI)5.0(CR)1.0
AL4CR	mu-Al4Mn		hP574	(194, P6_3/mmc)		2	(CR)1.0(AL, SI, VA)4.0
ALCR_GAMMA1	Unknown Structure					4	(AL, CR, SI)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							(CR)2.0(AL, CR)3.0 (AL, SI)6.0
GAMMA_D810	Cr5Al8 (D810)	D810	hR26	(160, R3m)		3	(AL, SI)12.0(CR)5.0 (AL, CR, SI)9.0
ALCU_DEL	Al5Cu8		hR52	(160, R3m)		2	(AL, ZN)2.0(CU, FE)3.0
ALCU_EPS	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(AL, CU, NI, ZN)1.0 (CU, FE)1.0
ALCU_ETA	AlCu(r)		mS20	(12, C2/m)		2	(AL, CU)1.0(CU, FE, NI, ZN)1.0
AL2CU_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Al2Cu,AlHf2,Fe2B,FeGe2,FeZr2,FeSn2,Mn2B,MnSn2,NiB2,NiZr2,SiZr2	2	(AL, FE, GE, HF, MN, NI, SN, ZR)2.0(AL, B, CU, FE, MN, NI, SI)1.0
AL2CU_OMEGA	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Al2Cu- OMEGA metastable precipitate	2	(AL)2.0(CU)1.0
THETA_PRIME	(Al2Cu)		tP*	(123, P4/mmm)	metal stable Al2Cu, theta prime	2	(AL)2.0(CU)1.0
THETA_DPRIME	(Al3Cu)		tP8	(123, P4/mmm)	GII zones, theta double prime, Al3Cu, metastable	2	(AL)3.0(CU)1.0
ALCU_ZETA	Al9Cu11(h)		oF88	(42, Fmm2)		2	(AL)9.0(CU, FE)11.0
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	solution between Al8Cu5 (rt) and Cu5Zn8	3	(AL, FE, NI, SI, ZN)4.0(AL, CU, NI, SI, ZN)1.0(AG, CU, FE, MN, NI, ZN)8.0
GAMMA_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	Cu5Zn8-type Al8Cu5 (ht) phase	3	(AL, ZN)4.0(AL, CU, ZN)1.0(CU, FE, MN, NI)8.0
ALR_OP16	DyAl		oP16	(57, Pbcm)	AlEr, AlNd, AlPr(ht)	2	(AL, MG)1.0(ER, ND, PR)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL2ER3	Zr3Al2		tP20	(136, P4_2/mnm)		2	(AL, MG)0.4(ER)0.6
ALR2_C37	Co2Si (C37)	C37	oP12	(62, Pnma)	AlEr2, AlNd2, AlPr2	2	(AL, MG)1.0(ER, ND, PR)2.0
AL2FE1	Al2Fe		aP18	(1, P1)		2	(AL, CU, SI, ZN)2.0 (FE, MN, NI)1.0
AL5FE2	Al2.8Fe		oS24	(63, Cmcm)		2	(AL, CU, SI, ZN)5.0 (FE, MN, NI)2.0
AL8FE5	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	aka Al5Fe4	1	(AL, CU, FE, MN)1.0
AL13FE4	Al13Fe4		mS102	(12, C2/m)	solution phases based on Al13Fe4, aka Al3Fe	3	(AL, CU)0.6275(FE, MN, NI, ZN)0.235 (AL, SI, VA, ZN)0.1375
AL4FE	AlmFe		tI110	(121, I-42m)		2	(AL)4.2(FE)1.0
AL3HF4	Al3Zr4		hP7	(191, P6/mmm)		2	(AL)3.0(HF)4.0
AL3LA	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	Al3La	2	(AL)3.0(LA)1.0
ALR_OS16	AlCe		oS16	(63, Cmcm)	AlLa, AlPr(rt)	2	(AL)1.0(LA, PR)1.0
AL53LA22	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(AL)0.707(LA)0.293
AL11R3_LT	Al11La3		oI28	(71, Immm)	Al11La3(rt), Al11Nd3(rt), Al11Pr3(rt)	2	(AL)11.0(LA, ND, PR)3.0
AL11R3_HT	Al4Ba (D13)	D13	tI10	(139, I4/mmm)	Al11La3(ht), Al11Nd3(ht), Al11Pr3(ht)	2	(AL)11.0(LA, ND, PR)3.0
AL2LI3	Li3Al2		hr5	(166, R-3m)		2	(AL, MG, ZN)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							(LI)3.0
AL1LI2	Li2Ga		oS12	(63, Cmcm)		2	(AL)1.0(LI)2.0
AL4LI9	Al4Li9		mS26	(12, C2/m)		2	(AL, ZN)4.0(LI)9.0
B32_ALLI	NaTl (B32)	B32	cF16	(227, Fd-3m)		2	(AL, LI, MG, ZN)1.0 (LI, MG, VA)1.0
ALMG_BETA	Al45Mg28		cF1832	(227, Fd-3m)		2	(LI, MG)89.0(AL, ZN)140.0
ALMG_EPS	Al30Mg23		hR53	(148, R-3)		2	(MG)23.0(AL, ZN)30.0
ALMG_GAMMA	alpha-Mn (A12)	A12	cI58	(217, I-43m)		3	(LI, MG)5.0(AL, MG, ZN)12.0(AL, MG, ZN)12.0
ALMGZN_PHI	Mg21(Al,Zn)17		oP152	(57, Pbcm)	a Al-Mg-Zn ternary phase know as PHI	2	(MG)6.0(AL, ZN)5.0
AL12MN	Al12W		cI26	(204, Im-3)		2	(AL)12.0(MN)1.0
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)		2	(AL, CU, ZN)6.0(CU, FE, MN)1.0
AL4MN_R	lambda-Al4Mn		hP586	(194, P6_ 3/mmc)	AL461MN107	2	(AL)0.81162(FE, MN)0.18838
AL4MN_U	mu-Al4Mn		hP574	(194, P6_ 3/mmc)		2	(AL, ZN)4.0(MN)1.0
AL11MN4_LT	Al11Mn4		aP15	(2, P-1)		2	(AL, ZN)11.0(FE, MN)4.0
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25		oP156	(62, Pnma)		2	(AL, MN)29.0 (MN)10.0
AL8MN5	Cr5Al8 (D810)	D810	hR26	(160, R3m)		3	(AL, TI, ZN)12.0 (MN, TI)5.0(AL, CU,

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							MN, SI, TI)9.0
AL12MO	Al12W		cI26	(204, Im-3)		2	(AL, SI)12.0(MO)1.0
AL5MO	Al5Mo		hR12	(167, R-3c)		2	(AL, SI)5.0(MO)1.0
AL22MO5	Al22Mo5		oF216	(43, Fdd2)		2	(AL, SI)22.0(MO)5.0
AL17MO4	Al17Mo4		mS84	(5, C2)		2	(AL, SI)17.0(MO)4.0
AL4MO	Al4W		mS30	(8, Cm)		2	(AL, SI)4.0(MO)1.0
AL3MO	MoAl3		mS32	(12, C2/m)		2	(AL, SI)3.0(MO)1.0
AL8MO3	Al8Mo3		mS22	(12, C2/m)		2	(AL, SI)8.0(MO)3.0
AL63MO37	Unknown Structure					2	(AL, SI)0.63 (MO)0.37
ALM3_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(AL, MO, NB, SI, TI)1.0(AL, MO, NB, TI)3.0
ALNB2	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		3	(AL, NB, TI)10.0(NB, TI)4.0(AL, NB, TI)16.0
AL3ND	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	Al3Nd	2	(AL)3.0(ND)1.0
ALND3	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	AlNd3	2	(AL)1.0(ND)3.0
AL3NI_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(AL, MN, NI)0.75(B, C, FE, NI)0.25
AL3NI2	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)		3	(AL, SI, ZN)3.0(AL, CU, FE, MG, NI)2.0 (NI, VA)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3NI5	Ga3Pt5		oS16	(65, Cmmm)		2	(AL)0.375(NI)0.625
AL1P1	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(AL)1.0(P)1.0
AL3PR	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	Al3Pr	2	(AL)3.0(PR)1.0
ALPR3_L	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	AlPr3 (rt)	2	(AL)1.0(PR)3.0
MONOCLINIC	beta-S		mP48	(14, P2_1/c)	S (ht)	1	(S)1.0
AL1S1	Unknown Structure				AlS	2	(AL)1.0(S)1.0
AL2S3_L	alpha-Al2S3		hP30	(169, P6_1)	Al2S3 (rt)	2	(AL)2.0(S)3.0
AL2S3_H	Corundum (Al2O3, D51)	D51	hR10	(167, R-3c)	Al2S3 (ht)	2	(AL)2.0(S)3.0
AL1SB1	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(AL)1.0(SB)1.0
AL3X	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	Al3Sc (dissolving Ti, Zr), Al3Li	2	(ER, LI, SC, TI, Y, ZR)1.0(AL, MG, SI)3.0
AL2SC	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(SC, TI, Y, ZR)1.0(AL, MG)2.0
ALSC_OP	Unknown Structure		oP*			2	(SC, Y, ZR)1.0(AL, MG)1.0
AL2SE3	beta-Ga2Se3		mS20	(9, Cc)	Al2Se3	2	(AL)2.0(SE)3.0
AL7SR8	Ba8Ga7		cP60	(198, P2_13)		2	(AL)7.0(SR)8.0
AL4M_D13	Al4Ba (D13)	D13	tI10	(139, I4/mmm)	Al4Ca, Al4Sr	2	(AL, MG, SI)4.0(CA, SR)1.0
ALTA2	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)		3	(AL, TA)10.0(TA)4.0 (AL, TA)16.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
TA1AL2	Al69Ta39		cF444	(216, F-43m)		2	(AL, TA)0.6389(AL, TA)0.3611
TAAL	Al38Ta48		mP86	(14, P2_1/c)		2	(AL, TA)0.8837(AL, TA)1.1163
ALTE	Unknown Structure				AlTe	2	(AL)1.0(TE)1.0
AL2TE5	Al2Te5		mS14	(12, C2/m)	Al2Te5	2	(AL)2.0(TE)5.0
AL2TE3_L	Al2Te3(rt)		mP240	(4, P2_1)	Al2Te3 (rt)	2	(AL)2.0(TE)3.0
AL2TE3_H	Al2Te3 (ht)		mP40	(14, P2_1/c)	Al2Te3 (ht)	2	(AL)2.0(TE)3.0
AL2TI	Ga2Hf		tI24	(141, I4_1/amd)		2	(AL, NB, TI)2.0(AL, NB, SC, TI)1.0
AL5TI2	Al5Ti2		tP28	(123, P4/mmm)		2	(AL, NB, TI)5.0(AL, NB, TI)2.0
AL5TI3	Al5Ti3		tP32	(127, P4/mbm)		2	(AL)5.0(NB, TI)3.0
AL3TI_LT	Al3Ti-LT		tI32	(139, I4/mmm)		2	(AL, CU, NB, SI, TI)3.0(AL, MN, NB, SC, TI)1.0
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)		2	(AL, CO, MN, NB, TI, W)3.0(AL, C, NB, SI, TI, W)1.0
AL21V2	Al10V		cF176	(227, Fd-3m)		2	(AL)21.0(V)2.0
AL23V4	Al23V4		hP54	(194, P6_3/mmc)		2	(AL)23.0(V)4.0
AL8V5	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		4	(AL, V)2.0(V)2.0(AL, V)3.0(AL)6.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL77W23	Unknown Structure					2	(AL)77.0(W)23.0
AL4W	Al4W		mS30	(8, Cm)	also Al4Mo	2	(AL)4.0(W)1.0
AL7W3	Unknown Structure					2	(AL)7.0(W)3.0
AL2W	CrSi2 (C40)	C40	hP9	(180, P6_222)		2	(AL)2.0(W)1.0
AL5W	Al5W		hP12	(182, P6_322)	also AL5MO	2	(AL)5.0(W)1.0
AL12W	Al12W		cI26	(204, Im-3)	also AL12RE and AL12MO	2	(AL)12.0(W)1.0
ALY_B33	CrB (B33)	B33	oS8	(63, Cmcm)		2	(AL)1.0(SC, Y)1.0
AL3Y_HT	BaPb3		hR12	(166, R-3m)		2	(AL)0.75(SC, Y)0.25
AL3Y_LT	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)		2	(AL, CU)0.75(SC, Y)0.25
AL2Y_C15	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(AL, CU, SC, Y)2.0 (AL, CU, SC, Y)1.0
AL4ZR5	Ti5Ga4		hP18	(193, P6_ 3/mcm)		2	(AL)4.0(SC, ZR)5.0
AL3ZR2_OF40	Zr2Al3		oF40	(43, Fdd2)	Al3Zr2, Al3Hf2	2	(AL, LI)3.0(HF, SC, ZR)2.0
AL3ZR_D023	Al3Zr (D023)	D023	tI16	(139, I4/mmm)	Al3Zr, Al3Hf	2	(AL, LI, MG)3.0(HF, SC, TI, ZR)1.0
B4C	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		2	(B11C, B12)1.0(B2, C2B, CB2)1.0
CR2B_ORTH	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(CR)0.666667 (B)0.333333
CRB4	CrB4		oI10	(71, Immm)		2	(CR)0.2(B)0.8

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MGB4	MgB4		oP20	(62, Pnma)		2	(MG)1.0(B)4.0
MGB7	MgB7		oI64	(74, Imma)		2	(MG)1.0(B)7.0
MN2B_D1F	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(MN)0.6707 (B)0.3293
MNB4	MnB4		mS10	(12, C2/m)		2	(MN)0.2(B)0.8
NB2B3	V2B3		oS20	(63, Cmcm)		2	(AL, NB)2.0(B)3.0
NI4B3_ORTH	o-Ni4B3		oP28	(62, Pnma)		2	(NI)0.586(B)0.414
NI4B3_MONO	m-Ni4B3		mS28	(15, C2/c)		2	(NI)0.564(B)0.436
SIB3	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		3	(B)6.0(SI)2.0(B, SI)6.0
SIB6	SiB6		oP280	(58, Pnnm)		3	(B)210.0(SI)23.0(B, SI)48.0
SIBX	alpha-B (hR12)		hR12	(166, R-3m)		3	(B)61.0(SI)1.0(B, SI)8.0
SRB6	CaB6 (D21)	D21	cP7	(221, Pm-3m)		2	(SR)1.0(B)6.0
V2B3	V2B3		oS20	(63, Cmcm)		2	(V)0.4(B)0.6
V5B6	V5B6		oS22	(65, Cmmm)		2	(AL, NB, V)0.454545 (B)0.545455
M2B_TETR	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(W)2.0(B)1.0
BW_BETA	CrB (B33)	B33	oS8	(63, Cmcm)		2	(B, VA)1.0(W)1.0
BW_ALPHA	MoB (Bg)	Bg	tI16	(141, I4_ 1/amd)		2	(B, VA)1.0(W)1.0
B5W2_X	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)		2	(B, VA)5.0(W)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
B9W2	W2B9		hP22	(147, P-3)		2	(B)9.0(W)2.0
ZRB12	UB12 (D2f)	D2f	cF52	(225, Fm-3m)		2	(B)12.0(ZR)1.0
BABE13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)		2	(BA)1.0(BE)13.0
BI2MG3_LT	La2O3 (D52)	D52	hP5	(164, P-3m1)	Bi2Mg3, P-3m1, La2O3-type (rt)	2	(BI, SN, VA)2.0 (MG)3.0
BI2MG3_HT	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)	Bi2Mg3, Ia-3, Mn2O3-type (ht)	3	(BI, SN)1.0(BI, SN, VA)3.0(MG)6.0
CR3C2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(CR)3.0(C)2.0
MG2C3	Mg2C3		oP10	(58, Pnnm)		2	(MG)2.0(C)3.0
MGC2	MgC2		tP6	(136, P4_2/mnm)		2	(MG)1.0(C)2.0
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(MN)5.0(C)2.0
SIC	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(C)1.0(SI)1.0
V3C2	Sc2Te3		hR8	(166, R-3m)		2	(V)3.0(C)2.0
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	(187, P-6m2)		2	(W)1.0(C)1.0
CA2CU	Ca2Cu		oP12	(62, Pnma)		2	(CA)2.0(CU)1.0
CA1CU1	alpha-CaCu		mP20	(11, P2_1/m)	alpha-CaCu (mP20, P2_1/m) & beta-CaCu (oP40, Pnma)	2	(CA)1.0(CU)1.0
HCP_CA	Mg		cP2	(194, P6_3/mmc)		2	(CA)1.0(H, VA)0.5
CAH2_LT	HgCl2 (C25)	C25	oP12	(62, Pnma)		2	(CA)1.0(H)2.0
CAH2_HT	Unknown Structure					2	(CA)1.0(H)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CALI2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(LI)2.0(CA)1.0
CA2NI7	Co7Gd2		hR18	(166, R-3m)		2	(CA)2.0(NI)7.0
CANI3	Ni3Pu		hR12	(166, R-3m)		2	(CA)0.25(NI)0.75
CA3SI4	Ca3Si4		hP42	(176, P6_3/m)		2	(CA)0.428571 (SI)0.571429
CA14SI19	Ca14Si19		hR66	(167, R-3c)		2	(CA)0.424242 (SI)0.575758
CASI2	CaSi2 (C12)	C12	hR6	(166, R-3m)		2	(CA)0.333333 (SI)0.666667
CA3ZN	Re3B		oS16	(63, Cmcm)		2	(CA)3.0(ZN)1.0
CA5ZN3	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)		2	(CA)5.0(ZN)3.0
CAZN_OC8	CrB (B33)	B33	oS8	(63, Cmcm)		2	(CA)1.0(ZN)1.0
CAZN2	KHg2		oI12	(74, Imma)		2	(CA)1.0(ZN)2.0
CAZN3	CaZn3		hP32	(194, P6_ 3/mmc)		2	(CA)1.0(ZN)3.0
CAZN11	BaCd11		tI48	(141, I4_ 1/amd)		2	(CA)1.0(ZN)11.0
CDCU2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(CD)1.0(CU)2.0
CD3CU4	Cd3Cu4		cF1124	(216, F-43m)		2	(CD)0.4286 (CU)0.5714
CD8CU5	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		4	(CU)2.0(CD, CU)3.0 (CU)2.0(CD, CU)6.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CD10CU3	Co2Al5 (D811)	D811	hP28	(194, P6_ 3/mmc)		2	(CD)0.7692 (CU)0.2308
SN_HP1	(Hg0.1Sn0.9)		hP1	(191, P6/mmm)		1	(CD, IN, SN)1.0
CU6CE	Copper(II) Azide [Cu (N3)2]		oP28	(62, Pnma)		2	(CU)6.0(CE)1.0
CU5CE	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(AL, CU)5.0(CE)1.0
CU4CE	Unknown Structure		oP20			2	(AL, CU)4.0(CE)1.0
CU2CE	KHg2		oI12	(74, Imma)		2	(CU)2.0(CE)1.0
CUCE	FeB (B27)	B27	oP8	(62, Pnma)		2	(CU)1.0(CE)1.0
CE2FE17	Ni17Th2		hP38	(194, P6_ 3/mmc)		2	(CE)2.0(AL, FE)17.0
MGCE	Unknown Structure					2	(AL, MG)1.0(CE)1.0
MG3CE	BiF3 (D03)	D03	cF16	(225, Fm-3m)		2	(MG)3.0(CE, MG)1.0
MG41CE5	Ce5Mg41		tI92	(87, I4/m)		2	(MG)41.0(CE)5.0
MG17CE2	CeMg10		hP44	(194, P6_ 3/mmc)		2	(MG)17.0(CE)2.0
MG12CE	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)		2	(AL, MG)12.0 (CE)1.0
CE7NI3	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)		2	(CE)0.7(NI)0.3
CENI_OC8	CrB (B33)	B33	oS8	(63, Cmcm)		2	(CE)0.5(NI)0.5
CENI2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(CE, NI)0.333333

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							(CE, NI)0.666667
CENI3	CeNi3		hP24	(194, P6_ 3/mmc)		2	(CE)0.25(AL, NI)0.75
CE2NI7	Ce2Ni7		hP36	(194, P6_ 3/mmc)		2	(CE)0.222222(AL, NI)0.777778
CENI5	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CE, ER, NI)0.166667(AL, CE, CU, NI)0.833333
CE5SI3	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)		2	(SI)3.0(CE)5.0
CE3SI2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		2	(CE)3.0(SI)2.0
CE5SI4	Si4Zr5		tP36	(92, P4_12_ 12)		2	(CE)5.0(SI)4.0
CESI_OP8	FeB (B27)	B27	oP8	(62, Pnma)		2	(CE)1.0(SI)1.0
CE3SI4	Unknown Structure					2	(CE)1.0(SI)1.34
CE3SI5	GdSi1.4		oI12	(74, Imma)		2	(CE)0.37(SI)0.63
RESI2	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_ 1/amd)	CeSi2, Si2Y (ht)	2	(CE, Y)1.0(AL, SI)2.0
CO7W6	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	mu phase	4	(CO, W)4.0(CO, W)2.0(CO, W)1.0 (CO, W)6.0
CR3GE	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(CR, GE)0.75(CR, GE)0.25
CR5GE3_HT	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)		2	(CR, GE)0.625(CR, GE)0.375
CR5GE3_LT	Unknown Structure					2	(CR, GE)0.625(CR,

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							GE)0.375
CR11GE19	Mn11Si19		tP120	(118, P-4n2)		2	(CR)0.367(GE)0.633
CR3MN5	alpha-Mn (A12)	A12	cI58	(217, I-43m)	Cr2Mn3 ht	2	(CR)3.0(MN)5.0
HIGH_SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		3	(MN)8.0(CR)4.0(CR, MN)18.0
CR3SI_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(CR, SI)3.0(AL, CR, SI)1.0
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)		2	(CR, SI, V)1.0(AL, CR, SI)2.0
CRZN13	Unknown Structure					2	(CR)1.0(ZN)13.0
CRZN17	Unknown Structure					2	(CR)1.0(ZN)17.0
CU9ER2	Unknown Structure					2	(CU)9.0(ER)2.0
CU7ER2	Unknown Structure					2	(CU)7.0(ER)2.0
CU5ER_C15B	AuBe5 (C15b)	C15b	cF24	(216, F-43m)		2	(CU)5.0(ER)1.0
CU2ER	KHg2		oI12	(74, Imma)		2	(AL, CU)2.0(ER)1.0
CUER_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(AL, CU)1.0(ER)1.0
CU9GA4_0	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)		3	(CU)6.0(CU, GA)6.0 (GA)1.0
CU9GA4_1	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)		4	(CU)6.0(CU, GA)3.0 (CU, GA)3.0(GA)1.0
CU9GA4_2	Cu8.2Ga4.8		cP52			4	(CU)3.0(CU, VA)3.0 (CU, GA)3.0(GA)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU9GA4_3	Cu7.15Ga5.85		cP52			3	(CU, VA)6.0(CU, GA)3.0(GA)4.0
CUGA2	FeSi2-h		tP3	(123, P4/mmm)		2	(CU)1.0(GA)2.0
CUGA_THETA	Unknown Structure					2	(CU)0.778(GA)0.222
CU5HF	Unknown Structure					2	(CU)5.0(HF)1.0
CU51HF14	Ag51Gd14		hP68	(175, P6/m)		2	(CU)51.0(HF)14.0
CU8HF3	Cu8Hf3		oP44	(62, Pnma)		2	(CU)8.0(HF)3.0
CU10HF7	Ni10Zr7		oS68	(64, Cmce)		2	(CU)10.0(HF)7.0
CU1HF2	CuZr2		tI6	(139, I4/mmm)		2	(CU)1.0(HF)2.0
CUIN_GAMMA	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)		4	(CU)2.0(CU, IN)2.0 (CU)3.0(CU, IN)6.0
CUIN_THETE	Cu7In3		aP40	(2, P-1)		2	(CU)0.7(IN)0.3
CU2IN_HT	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		3	(CU)0.545(CU, IN)0.122(IN)0.333
CU2IN_LT	Unknown Structure					2	(CU)0.64(IN)0.36
CU11IN9	AlCu(r)		mS20	(12, C2/m)		2	(CU)0.55(IN)0.45
CU37LA3	NaZn13 (D23)	D23	cF112	(226, Fm-3c)		2	(CU)37.0(LA)3.0
CU6LA1_LT	Cu6La		mP28	(14, P2_1/c)		2	(CU)6.0(LA)1.0
CU6LA1_HT	CeCu6		oP28	(62, Pnma)		2	(CU)6.0(LA)1.0
CU5LA1	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CU)5.0(LA)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU4LA1	Cu4La		tI90	(119, I-4m2)		2	(CU)4.0(LA)1.0
CU2LA1	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(CU)2.0(LA)1.0
CU1LA1	FeB (B27)	B27	oP8	(62, Pnma)		2	(CU)1.0(LA)1.0
CUMG2	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(CU, NI)1.0(MG)2.0
CU4SC	Unknown Structure		t**			2	(CU)4.0(SC)1.0
CU2SC_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AG, CU)2.0(SC)1.0
CUSC	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(CU)1.0(SC)1.0
CU33SI7_DELTA	Unknown Structure					2	(CU, ZN)0.825 (SI)0.175
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cI76	(220, I-43d)		2	(CU, MG, MN, ZN)0.789474(AL, SI)0.210526
CU56SI11_GAMMA	Mg3Ru2		cP20	(213, P4_132)		2	(CU, MG, MN, NI, SI, ZN)0.835821 (SI)0.164179
CUSI_ETA	Cu3Si-h2		hR*	(162, P-31m)		2	(CU, MN, NI, ZN)0.76(SI)0.24
CU6SN5_HT	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		3	(CU)1.0(CU, SN)1.0 (SN)1.0
CUSN_GAMMA	BiF3 (D03)	D03	cF16	(225, Fm-3m)		1	(CU, SN)1.0
CU10SN3	Cu10Sn3		hP26	(173, P6_3)		1	(CU, SN)1.0
CU3SN	Cu3Sn		oS80	(63, Cmcm)		2	(CU, SN)3.0(CU, SN)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU41SN11	Cu41Sn11		cF416	(216, F-43m)		2	(CU, SN)41.0(CU, SN)11.0
CU6SN5_LT	Cu6Sn5		mS44	(15, C2/c)		3	(CU)1.0(CU, SN)1.0 (SN)1.0
CUSR	BaCu		hP8	(194, P6_ 3/mmc)		2	(SR)1.0(CU)1.0
CU2TI	Au2V		oS12	(63, Cmcm)		2	(CU)2.0(TI)1.0
CU3TI2	Cu3Ti2		tP10	(129, P4/nmm)		2	(CU)3.0(TI)2.0
CU4TI1	Au4Zr		oP20	(62, Pnma)		2	(AL, CU, TI)4.0(CU, TI)1.0
CU4TI3	Cu4Ti3		tI14	(139, I4/mmm)		2	(CU)4.0(TI)3.0
CUTI_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(CU, TI)1.0(CU, TI)1.0
CUTI3	CuTi3 (L60)	L60	tP4	(123, P4/mmm)		2	(CU, TI)1.0(TI)3.0
CU7Y1	Cu7Tb		hP8	(191, P6/mmm)		2	(CU2, Y)1.0(CU)5.0
CU4Y	Cu5Y1.25		mP16	(11, P2_1/m)		2	(CU)4.0(Y)1.0
CU7Y2	Ag51Gd14		hP68	(175, P6/m)		2	(CU)7.0(Y)2.0
CU2Y_H	Unknown Structure		hP*			2	(CU)2.0(Y)1.0
CU2Y_L	KHg2		oI12	(74, Imma)		2	(AL, CU)2.0(Y)1.0
EPSILON	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)		1	(CU, MN, NI, ZN)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU10ZR7	Ni10Zr7		oS68	(64, Cmce)		2	(CU)10.0(ZR)7.0
CU51ZR14	Ag51Gd14		hP68	(175, P6/m)		2	(CU)51.0(ZR)14.0
CU8ZR3	Cu8Hf3		oP44	(62, Pnma)		2	(CU)8.0(ZR)3.0
FE3ER	Ni3Pu		hR12	(166, R-3m)		2	(FE)3.0(ER)1.0
FE23ER6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		2	(AL, FE)23.0(ER)6.0
FE17ER2	Ni17Th2		hP38	(194, P6_ 3/mmc)		2	(AL, FE)17.0(ER)2.0
MG24R5	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(ER, MG)5.0(AL, MG)24.0
ER5SI3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)		2	(ER)0.625(SI)0.375
ER5SI4	Gd5Si4		oP36	(62, Pnma)		2	(ER)0.555556 (SI)0.444444
ERSI_OC8	CrB (B33)	B33	oS8	(63, Cmcm)		2	(ER)0.51(SI)0.49
ERSI_OP8	FeB (B27)	B27	oP8	(62, Pnma)		2	(ER)0.5(SI)0.5
ERSI2	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(ER)0.37(SI)0.63
FE2GE1	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		3	(FE)1.0(FE, VA)1.0 (GE)1.0
FEGE_ETA	Fe6.5Ge4		hP22	(194, P6_ 3/mmc)		2	(FE)13.0(GE)9.0
FE6GE5	Fe6Ge5		mS44	(12, C2/m)		2	(FE)6.0(GE)5.0
FE2GE3	Ru2Sn3		tP20	(116, P-4c2)		2	(FE)2.0(GE)3.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
C14_FE2HF	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(FE)0.6667(FE, HF)0.3333
C36_FE2HF	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)		2	(FE)0.6667 (HF)0.3333
C15_FE2HF	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(FE)0.6667 (HF)0.3333
FE1HF2	Unknown Structure					2	(FE)0.3333 (HF)0.6667
FE2SC_C15	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(FE)0.64(SC)0.36
FE6SC29	Unknown Structure					2	(FE)0.17(SC)0.83
FE2SI	AlNi2		hP6	(164, P-3m1)		2	(FE, NI)2.0(AL, SI)1.0
FESI2_H	FeSi2-h		tP3	(123, P4/mmm)		2	(FE, NI)3.0(AL, MG, SI)7.0
FESI2_L	FeSi2-l		oS48	(64, Cmce)		2	(FE, NI)1.0(AL, SI)2.0
FESI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	FeSi, MnSi, CrSi, CrGe	2	(CR, FE, MN, NI)1.0 (AL, GE, MG, SI)1.0
MN5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)	Mn5Si3, Cr3Si5, Fe5Si3, Ge3Mn5, Ge3Zr5, Si3Zr5, Sn3Ti5	2	(CR, CU, FE, MN, NI, TI, ZR)5.0(AL, CR, GE, SI, SN)3.0
FE5SN3_D82	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(FE)5.0(SN)3.0
FE3SN2	Fe3Sn2		hR10	(166, R-3m)		2	(FE)3.0(SN)2.0
FE7W6	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		4	(FE, W)1.0(W)4.0 (FE, W)2.0(FE, W)6.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GAMMA_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		4	(FE, MN, ZN)2.0(FE, MN, NI, ZN)2.0(AL, CU, FE, MN, NI, SI, ZN)3.0(AL, ZN)6.0
FEZN_GAMMA1	Unknown Structure					3	(FE)0.137(AL, CU, FE, NI, SI, ZN)0.118 (MN, ZN)0.745
FEZN_DELTA	FeZn10		hP632	(194, P6_ 3/mmc)		4	(FE)0.058(AL, CU, FE, MN, NI, SI, ZN)0.18(ZN)0.525 (ZN)0.237
FEZN_ZETA	CoZn13		mS28	(12, C2/m)		3	(FE, MN, NI, VA)0.072(AL, ZN)0.856(AL, CU, SI, VA, ZN)0.072
FEZR3	Re3B		oS16	(63, Cmcm)		2	(FE)1.0(ZR)3.0
GEMN3_HT	Al3Ti (D022)	D022	tI8	(139, I4/mmm)		2	(GE, MN)1.0 (MN)3.0
GE2MN3	Cr11Ge8		oP76	(62, Pnma)		2	(GE)2.0(MN)3.0
GE2MN5	Ge2Mn5-HT		hP42	(158, P3c1)		2	(GE, MN)2.0 (MN)5.0
GE3MN7	Ga2Mg5 (D8g)	D8g	oI28	(72, Ibam)	Mn5Ge2	2	(GE)3.0(MN)7.0
GENI2	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(NI)0.665(GE)0.335
GE3NI5_HT	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(GE, NI)0.625(GE, NI)0.375
GE2NI3	NiAs (B81)	B81	hP4	(194, P6_ 3/mmc)		2	(GE, NI)0.6(GE)0.4
GENI3_GAMMA	NaTl (B32)	B32	cF16	(227, Fd-3m)		2	(NI)0.744(GE)0.256

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GE2NI5	Pd5Sb2		hP42	(185, P6_3cm)		2	(NI)0.72(GE)0.28
GE3NI5_LT	Ge3Ni5		mS32	(5, C2)		2	(NI)0.63(GE)0.37
GE12NI19	Ni19Ge12		mS62	(5, C2)		2	(GE, NI)0.613(GE, NI)0.387
GE2SR	BaSi2		oP24	(62, Pnma)		2	(GE)2.0(SR)1.0
GE3TI5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)		2	(TI)5.0(GE)3.0
V3GE	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(V)0.75(GE)0.25
V17GE31	Ge31V17		tP192	(118, P-4n2)		2	(V)0.354(GE)0.646
LAH3	CeH3		cF44	(225, Fm-3m)		3	(LA)0.25(H, VA)0.5 (H, VA)0.25
MGH2	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)		2	(MG)1.0(H)2.0
HFMN	NiTi2		cF96	(227, Fd-3m)		2	(HF)0.5(MN)0.5
NI5HF	AuBe5 (C15b)	C15b	cF24	(216, F-43m)		2	(NI)0.833(HF)0.167
NI7HF2	Ni7Zr2		mS36	(12, C2/m)		2	(NI)0.778(HF, NI)0.222
NI3HF_LT	PdRh2Ta		hP40	(194, P6_ 3/mmc)		2	(NI)0.75(HF)0.25
NI3HF_HT	BaPb3		hR12	(166, R-3m)		2	(NI)0.75(HF)0.25
NI21HF8	Hf8Ni21		aP29	(2, P-1)		2	(NI)0.724(HF)0.276
NI7HF3	Hf3Ni7		aP20	(2, P-1)		2	(NI)0.7(HF)0.3
NI10HF7	Ni10Zr7		oS68	(64, Cmce)		2	(NI)0.588(HF)0.412

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI11HF9	Pt11Zr9		tI40	(87, I4/m)		2	(NI)0.55(HF)0.45
NIHF_LT	CrB (B33)	B33	oS8	(63, Cmcm)		2	(NI)0.5(HF)0.5
NIHF_HT	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(NI)0.5(HF)0.5
NIHF2	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(NI, VA)1.0(HF)2.0
HF2SI	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(HF)0.6666667 (SI)0.3333333
HF3SI2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		2	(HF)0.6(SI)0.4
HF5SI3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)		2	(HF)0.625(SI)0.375
HFSI_OP8	FeB (B27)	B27	oP8	(62, Pnma)		2	(HF)0.5(SI)0.5
HF5SI4	Si4Zr5		tP36	(92, P4_12_12)		2	(HF)0.555556 (SI)0.444444
HFSI2	ZrSi2 (C49)	C49	oS12	(63, Cmcm)		2	(HF)0.333333 (SI)0.666667
TET_A6P	In (A6)	A6	tI2	(139, I4/mmm)		1	(IN, SN)1.0
KNA2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)		2	(K)1.0(NA)2.0
KZN13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)		2	(K)1.0(ZN)13.0
LA3NI	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(LA)3.0(NI)1.0
LA7NI3	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)		2	(LA)7.0(NI)3.0
LANI_OC8	CrB (B33)	B33	oS8	(63, Cmcm)		2	(LA)1.0(NI)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LA2NI3	La2Ni3		oS20	(64, Cmce)		2	(LA)2.0(NI)3.0
LA7NI16	La7Ni16		tI46	(121, I-42m)		2	(LA)7.0(NI)16.0
LANI3	Ni3Pu		hR12	(166, R-3m)		2	(LA)1.0(NI)3.0
LA2NI7_LT	Ce2Ni7		hP36	(194, P6_ 3/mmc)		2	(LA)2.0(NI)7.0
LA2NI7_HT	Co7Gd2		hR18	(166, R-3m)		2	(LA)2.0(NI)7.0
LANI5	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(LA)1.0(NI)5.0
LA3SI2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		2	(LA)0.6(SI)0.4
LA5SI3	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)		2	(LA)0.625(SI)0.375
LA5SI4	Si4Zr5		tP36	(92, P4_12_ 12)		2	(LA)0.5556 (SI)0.4444
LASI_OP8	FeB (B27)	B27	oP8	(62, Pnma)		2	(LA)0.5(SI)0.5
LASI2_A1	GdSi1.4		oI12	(74, Imma)		2	(LA)0.36(SI)0.64
LASI2_A2	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_ 1/amd)		2	(LA)0.3333 (SI)0.6667
LAZN2	KHg2		oI12	(74, Imma)		2	(LA)0.333(ZN)0.667
LAZN4	LaZn4		oS20	(63, Cmcm)		2	(LA)0.2(ZN)0.8
LAZN5	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(LA)0.1667 (ZN)0.8333
LA3ZN22	Ce3Zn22		tI100	(141, I4_ 1/amd)		2	(LA)0.12(ZN)0.88

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LAZN11	BaCd11		tI48	(141, I4_ 1/amd)		2	(LA)0.083(ZN)0.917
LAZN13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)		2	(LA)0.071(ZN)0.929
LA2ZN17	Ni17Th2		hP38	(194, P6_ 3/mmc)		2	(LA)0.105(ZN)0.895
LI4PB	Li17Si4		cF420	(216, F-43m)		2	(LI)4.0(PB)1.0
LI7PB2	Li7Pb2		hP9	(164, P-3m1)		2	(LI)7.0(LI, PB)2.0
LI3PB	BiF3 (D03)	D03	cF16	(225, Fm-3m)		2	(LI)3.0(PB)1.0
LI5PB2	Li8Pb3		hR11	(166, R-3m)		2	(LI)5.0(PB)2.0
LIPB_LT	LiPb		hR2	(166, R-3m)		2	(LI, PB)1.0(LI, PB)1.0
LIPB_HT	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(LI, PB)1.0(LI, PB)1.0
LI22SI5	Li21Si5		cF416	(216, F-43m)		2	(LI)22.0(SI)5.0
LI13SI4	Li13Si4		oP34	(55, Pbam)		2	(LI)13.0(SI)4.0
LI7SI3	(Li7Si3)		hP60	(154, P3_221)		2	(LI)7.0(SI)3.0
LI12SI7	Li12Si7		oP152	(62, Pnma)		2	(LI)12.0(SI)7.0
LI2ZN3_L	Li(Li0.91Zn0.09)2Zn4		hR7	(166, R-3m)		2	(LI)2.0(LI, ZN)3.0
LI2ZN3_H	Li5Ga4		hP9	(164, P-3m1)		2	(LI, ZN)2.0(LI, ZN)3.0
LI2ZN5_L	Unknown Structure					2	(LI, ZN)2.0(ZN)5.0
LI2ZN5_H	Unknown Structure					2	(LI, ZN)2.0(ZN)5.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LIZN4_L	Unknown Structure					2	(LI, ZN)1.0(LI, ZN)4.0
LIZN4_H	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)		2	(LI, ZN)0.2(LI, ZN)0.8
LIZN2	Unknown Structure					2	(LI)1.0(ZN)2.0
BCC_B32	NaTl (B32)	B32	cF16	(227, Fd-3m)		2	(LI, ZN)1.0(LI, ZN)1.0
MG2NI_HP18	Mg2Ni (Ca)	Ca	hP18	(180, P6_222)		2	(MG, ZN)2.0(CU, NI, ZN)1.0
MG3SB2_D53	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)		3	(AL, MG)6.0(AL, SB, VA)3.0(SB)1.0
MG3SB2_D52	La2O3 (D52)	D52	hP5	(164, P-3m1)		2	(AL, MG)3.0(AL, SB, VA)2.0
MG2SI_C1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	solution phase of Mg2Si, GeMg2, Mg2Sn	2	(BI, MG)2.0(BI, GE, SI, SN)1.0
MG2SR	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(AL, MG)2.0(SR)1.0
MG38SR9	Mg38Sr9		hP94	(194, P6_ 3/mmc)		2	(AL, MG)38.0 (SR)9.0
MG23SR6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		2	(AL, MG)23.0 (SR)6.0
MG17SR2	Th2Zn17		hR19	(166, R-3m)		2	(AL, MG)17.0 (SR)2.0
MG7ZN3	Mg51Zn20		oI158	(71, Immm)		2	(MG)51.0(ZN)20.0
MGZN	Zr21Re25		hR92	(167, R-3c)		2	(MG)12.0(AL, CU, ZN)13.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MG2ZN3	Mg4Zn7		mS110	(12, C2/m)		2	(MG)2.0(AL, CU, ZN)3.0
L10_TETRA	CuAu (L10)	L10	tP2	(123, P4/mmm)		2	(AL, CU, MN, NB, NI, TI)0.5(AL, C, CU, MN, NB, NI, TI)0.5
MNNI2	Unknown Structure					2	(MN, NI)1.0(NI)2.0
MNSC4	Unknown Structure					2	(MN)0.2(SC)0.8
MN11SI19	Mn11Si19		tP120	(118, P-4n2)		2	(MN)11.0(AL, SI)19.0
MN3SI	BiF3 (D03)	D03	cF16	(225, Fm-3m)		2	(FE, MN, NI)3.0(AL, SI)1.0
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		2	(AL, MN)17.0(SI, ZN)3.0
MN9SI2	Mn9Si2		oI186	(71, Immm)		2	(MN)33.0(SI)7.0
MN2SN	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)	Mn(2-x)Sn	2	(MN)0.643 (SN)0.357
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(MN)3.0(SN)2.0
MNTI_LT	Zr21Re25		hR92	(167, R-3c)		2	(AL, MN)1.0(TI)1.0
MNTI_HT	Unknown Structure		t**			2	(AL, MN)0.515 (TI)0.485
MN3TI	Unknown Structure					2	(MN)3.0(TI)1.0
MN4TI	R-(Co,Cr,Mo)		hR53	(148, R-3)		2	(AL, MN)0.815 (TI)0.185
MNV_SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)		3	(MN, V)10.0(V)4.0 (MN, V)16.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MNZN9	Unknown Structure		h**			2	(MN)0.1(ZN)0.9
MO5SI3	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)		3	(MO, W)0.5(MO, SI, W)0.125(AL, MO, SI)0.375
MOSI2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AL, SI)2.0(MO, W)1.0
NASI_LT	NaSi-lt		mS32	(15, C2/c)		2	(NA)1.0(SI)1.0
NASI_HT	Unknown Structure					2	(NA)1.0(SI)1.0
NAZN13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)		2	(NA)1.0(ZN)13.0
NI7SC2	Ce2Ni7		hP36	(194, P6_3/mmc)		2	(SC)0.222222 (NI)0.777778
NISC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(SC)1.0(NI)1.0
NISC2	NiTi2		cF96	(227, Fd-3m)		2	(SC)0.72(NI)0.28
NI2SI_HT	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		3	(CU, NI)1.0(NI, VA)1.0(AL, SI)1.0
NI3SI2	Ni3Si2		oP80	(36, Cmc2_1)		2	(FE, NI)3.0(SI)2.0
NI3SI_HT	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(FE, NI)3.0(AL, SI)1.0
NI3SI_MT	Ge9Pd25		hP34	(147, P-3)		2	(SI)1.0(NI)3.0
NI5SI2	Ni31S12		hP42	(150, P321)		2	(CU, FE, NI)5.0(AL, SI)2.0
NISI_B31	MnP (B31)	B31	oP8	(62, Pnma)	GeNi, NiSi	2	(FE, NI)1.0(GE, SI, ZN)1.0
NISI2	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(AL, CU, SI, ZN)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							(CU, FE, MN, NI)1.0
NI3SN2_LT	Ni3Sn2		oP20	(62, Pnma)		3	(SN)0.2(NI, SN)0.4 (NI)0.4
NI3SN_HT	BiF3 (D03)	D03	cF16	(225, Fm-3m)		3	(NI, SN)0.25(NI, SN)0.25(NI)0.5
NI3SN2_HT	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		3	(NI)0.33333(NI, SN)0.33334 (SN)0.33333
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	(12, C2/m)		3	(NI)0.25(NI, SN)0.25 (SN)0.5
NISR	Unknown Structure		hP*			2	(NI)0.5(SR)0.5
NI3TI_D024	Ni3Ti (D024)	D024	hP16	(194, P6_ 3/mmc)		2	(NI, TI)0.75(NI, TI)0.25
NITI2	NiTi2		cF96	(227, Fd-3m)		2	(NI, TI)1.0(NI, TI)2.0
NI2V7	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(NI)2.0(V)7.0
NI2V1	Al3Ti (D022)	D022	tI8	(139, I4/mmm)		2	(NI)2.0(V)1.0
MONI4_BETA	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)		2	(W)1.0(NI)4.0
NIZN_LT	delta-CuTi (L2a)	L2a	tP2	(123, P4/mmm)		2	(AL, FE, MN, NI, SI, ZN)0.5(AL, FE, MG, MN, NI, SI, ZN)0.5
NIZN8	Ni3Zn22		mS50	(12, C2/m)		2	(NI)0.1111111(AL, MN, ZN)0.8888889
NI10ZR7	Ni10Zr7		oS68	(64, Cmce)		2	(NI)23.0(ZR)17.0
NI21ZR8	Hf8Ni21		aP29	(2, P-1)		2	(ZR)8.0(NI)21.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI11ZR9	Pt11Zr9		tI40	(87, I4/m)		2	(NI)11.0(ZR)9.0
NI7ZR2	Ni7Zr2		mS36	(12, C2/m)		2	(NI)7.0(ZR)2.0
SIP_OC48	(SiP)		oS48	(36, Cmc2_1)		2	(SI)1.0(P)1.0
SIP2	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)		2	(SI)1.0(P)2.0
P2ZN3_LT	Zn3P2 (D59)	D59	tP40	(137, P4_ 2/nmc)		2	(P)2.0(ZN)3.0
P2ZN3_HT	Unknown Structure					2	(P)2.0(ZN)3.0
P2ZN_HT	Unknown Structure					2	(P)2.0(ZN)1.0
P2ZN_LT	ZnAs2		mP24	(14, P2_1/c)		2	(P)2.0(ZN)1.0
SC5SI3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)		2	(SC)0.625(SI)0.375
RESI_B33	CrB (B33)	B33	oS8	(63, Cmcm)	ScSi, YSi	2	(SC, Y)1.0(SI)1.0
SC3SI5_LT	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(SC)0.375(SI)0.625
RE3SI5_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	Si5Y3 (rt)	2	(SC, Y)0.375 (SI)0.625
SC1ZN1	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(SC)0.5(ZN)0.5
SCZN2	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(SC)0.3333 (ZN)0.6667
SC13ZN58	Gd13Zn58		hP142	(194, P6_ 3/mmc)		2	(SC)0.1831 (ZN)0.8169
SC3ZN17	Be17Ru3		cI160	(204, Im-3)		2	(SC)0.15(ZN)0.85

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SCZN12	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)		2	(SC)0.077(ZN)0.923
SI2SR_HT	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_ 1/amd)		2	(SI, VA)2.0(SR)1.0
SI2SR_LT	Si2Sr		cP12	(213, P4_132)		2	(SI)2.0(SR)1.0
SI3TI5_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)		2	(SI)3.0(TI)5.0
V3SI	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(SI, V)0.75(SI, V)0.25
SI2Y_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	Si2Y (rt)	2	(SI)2.0(Y)1.0
SI5Y3_CC	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_ 1/amd)	Si5Y3 (ht)	2	(SI)5.0(Y)3.0
SI4Y5	Gd5Si4		oP36	(62, Pnma)	Si4Y5	2	(SI)4.0(Y)5.0
SI3Y5_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)	Si3Y5	2	(SI)3.0(Y)5.0
SR3SN5	Pd5Pu3		oS32	(63, Cmcm)		2	(SR)0.375(SN)0.625
SRSN3	Mg3In		hr16	(166, R-3m)		2	(SR)0.25(SN)0.75
SRSN4	SrSn4		oS20	(63, Cmcm)		2	(SR)0.2(SN)0.8
SN3TI2	Unknown Structure					2	(SN)3.0(TI)2.0
V3SN	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(SN)0.205(V)0.795
VSN2	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(SN)0.6(V)0.4
SN3ZR5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)	aka eta	3	(ZR)5.0(SN)3.0(SN, VA)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SNZR3_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)		2	(SN, ZR)3.0(SN, ZR)1.0
SRZN5_LT	Pd5Pu3		oS32	(63, Cmcm)		2	(SR)1.0(ZN)5.0
TIZN2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		2	(TI)1.0(ZN)2.0
TIZN5	Unknown Structure					2	(TI)1.0(ZN)5.0
TIZN10	Ti3Zn22		tP100	(135, P4_ 2/mbc)		2	(TI)1.0(ZN)10.0
TIZN15	TiZn16		oS68	(63, Cmcm)		2	(TI)1.0(ZN)15.0
V4ZN5	V4Zn5		tI18	(139, I4/mmm)		2	(V)4.0(ZN)5.0
V2ZR	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(V)2.0(ZR)1.0
ZN2ZR	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(ZN)2.0(ZR)1.0
ZN22ZR	Zn22Zr		cF184	(227, Fd-3m)		2	(ZN)22.0(ZR)1.0
ZN39ZR5	Zn39Zr5		mS88	(12, C2/m)		2	(ZN)39.0(ZR)5.0
ZN3ZR_LT	Unknown Structure		tI64			2	(ZN)3.0(ZR)1.0
ZN3ZR_HT	Unknown Structure		c**			2	(ZN)3.0(ZR)1.0
ALCCR2	AlCCr2		hP8	(194, P6_ 3/mmc)		3	(AL)1.0(C)1.0(CR, V)2.0
AL2MGC2	Ce2O2S		hP5	(164, P-3m1)		3	(AL)2.0(MG)1.0 (C)2.0
AL4C4SI	Al5C3N (E94)	E94	hP18	(186, P6_3mc)		3	(AL)4.0(SI)1.0(C)4.0
AL8C7SI	Unknown Structure					3	(AL)8.0(SI)1.0(C)7.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
TI2ALC	AlCCr2		hP8	(194, P6_ 3/mmc)	H, Ti2AlC1-x	3	(TI)2.0(AL)1.0(C, VA)1.0
TI3ALC	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	P, Ti3AlC1-x	3	(TI)3.0(AL)1.0(C, VA)1.0
TI3AL1C2	CMo		hP12	(194, P6_ 3/mmc)	N, Ti3AlC2-x	3	(TI)3.0(AL, SI)1.0(C, VA)2.0
ALC3V4	AlN3Ti4		hP16	(194, P6_ 3/mmc)		4	(V)4.0(AL)1.0(C)2.0 (C, VA)1.0
AL20CECR2	CeCr2Al20		cF184	(227, Fd-3m)		3	(AL)0.869565 (CE)0.043478 (CR)0.086957
AL8CEM4	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)	T1	3	(AL)0.6154(CE, ER)0.0769(AL, CR, CU, FE, MN)0.3077
AL10CE2M7	Th2Zn17		hR19	(166, R-3m)	T2	2	(AL, CR, CU, FE, MN)0.8947(CE, ER)0.1053
AL3CECU	Al4Ba (D13)	D13	tI10	(139, I4/mmm)	T3	2	(AL, CU)0.8(CE)0.2
ALCEM	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)	T4	3	(AL)0.3333(CE, ER)0.3333(CU, NI)0.3334
ALCE2CU2	Unknown Structure				T5	3	(AL)0.2(CE)0.4 (CU)0.4
ALCEFE	Unknown Structure					2	(AL, FE)2.0(CE)1.0
AL10CEFE2	YbFe2Al10		oS52	(63, Cmcm)		3	(AL)10.0(CE, ER)1.0 (FE)2.0
AL8CEFE2	CeFe2Al8		oP44	(55, Pbam)		3	(AL)8.0(CE)1.0 (FE)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL13CEMG6	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)		3	(AL)0.667(CE)0.05 (MG)0.283
AL2CENI	MgCuAl2 (E1a)		oS16	(63, Cmcm)	T2	3	(AL)2.0(CE)1.0 (NI)1.0
AL5CE2NI5	Unknown Structure				T3, 13	3	(AL)0.35(CE)0.165 (NI)0.485
AL4CENI	YNiAl4		oS24	(63, Cmcm)	T5	3	(AL)4.0(CE)1.0 (NI)1.0
AL5CE1NI2	PrNi2Al5		oI16	(71, Immm)	T6	3	(AL)5.0(CE)1.0 (NI)2.0
AL23CE4NI6	Y4Ni6Al23		mS66	(12, C2/m)	T8	3	(AL)23.0(CE)4.0 (NI)6.0
AL60CE12NI28	Unknown Structure				T11	3	(AL)0.6(CE)0.12 (NI)0.28
AL40CE30NI30	Unknown Structure				T12	3	(AL)0.403(CE)0.304 (NI)0.293
AL1CE1SI1	LaPtSi		tI12	(109, I4_1md)		2	(AL, SI)2.0(CE)1.0
AL7CE5SI3	Unknown Structure					3	(AL)0.49 (CE)0.333333 (SI)0.176667
ALCESI2	CeAlSi2		hP8	(164, P-3m1)		3	(AL)1.0(CE)1.0 (SI)2.0
AL4CE3SI6	Ce3Al4Si6		hP13	(164, P-3m1)		3	(AL)4.0(CE)3.0 (SI)6.0
AL13CR4SI4	Cr4Al13Si4		cF84	(216, F-43m)	Al-Cr-Si, tao 1	3	(AL)13.0(CR)4.0 (SI)4.0
AL9CR3SI	Al9Mn3Si (E9c)	E9c	hP26	(194, P6_	Al-Cr-Si, tao 2	3	(AL)9.0(CR)3.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				3/mmc)			(SI)1.0
ALCRSI_T3	Al11Mn4		aP15	(2, P-1)	Al-Cr-Si, tao 3	2	(AL, SI)11.0(CR)4.0
ALCRSI_T4	Unknown Structure				Al-Cr-Si, tao 4, AL58CR32SI11	3	(AL)58.0(CR)31.5 (SI)10.5
AL9CU6ER5	Unknown Structure					3	(AL)0.45(CU)0.3 (ER)0.25
AL5CU3ER2	Unknown Structure					3	(AL)0.5(CU)0.3 (ER)0.2
AL3CU1ER1	Ce(Ni0.59Sb0.41)4		oI10	(71, Immm)		3	(AL)0.6(CU)0.2 (ER)0.2
AL62CU25FE13	Quasicrystal					3	(FE)0.125(AL, CU)0.255(AL)0.62
AL7CU2FE	FeCu2Al7 (E9a)	E9a	tP40	(128, P4/mnc)	Solution phase of the ternary compound Al7Cu2Fe	3	(FE, NI)1.0(CU)2.0 (AL)7.0
AL10CU10FE	(Al10Cu10Fe)		oF116	(42, Fmm2)		3	(FE)1.0(AL, CU)10.0 (AL)10.0
AL2CULI	LiCuAl2		hP12	(191, P6/mmm)	Al-Cu-Li ternary phase, i.e. T1	3	(AL)0.5(CU)0.25 (LI)0.25
ALCULI_T2	Quasicrystal				Al-Cu-Li ternary phase, T2	3	(AL)0.57(CU)0.11 (LI)0.32
ALCULI_R	Li13(Cu0.53Si0.47)27		cI160	(204, Im-3)	Al- Cu-Li ternary phase, R	3	(AL)0.55(CU)0.117 (LI)0.333
ALCULI_B	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	Al-Cu- Li ternary phase, TB	3	(AL)0.6(CU)0.32 (LI)0.08
Q_AL7CU3MG6	Mg11Cu6Al12		cF464	(227, Fd-3m)	Al7Cu3Mg6, Al-Cu-Mg ternary phase, aka. Q_AL7CU3MG6	3	(AL)7.0(CU)3.0 (MG)6.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
S_PHASE	MgCuAl2 (E1a)		oS16	(63, Cmcm)	aka Al2CuMg or S	3	(AL, SI)2.0(CU)1.0 (MG)1.0
S_PRIME	MgCuAl2 (E1a)		oS16	(63, Cmcm)	slightly distorted S_phase. Strain & interfacial energy need to added	3	(AL)2.0(CU)1.0 (MG)1.0
S_DPRIME	Unknown Structure		mS*		metastable precipitate, related to S_PHASE	3	(AL)5.0(CU)5.0 (MG)2.0
T_PHASE	Bergman [Mg32(Al,Zn)49, D8e]	D8e	cI162	(204, Im-3)	Solution (Al,Cu,Zn)49Mg32, stable in Al-Mg-Zn, Al-Cu-Mg, Al-Cu-Mg-Zn	4	(MG)26.0(AL, MG)6.0(AL, CU, MG, ZN)48.0(AL)1.0
AL28CU4MN7	Unknown Structure					3	(AL)28.0(MN)7.0 (CU)4.0
AL11CU5MN3	Unknown Structure		oP380			3	(AL)11.0(MN)3.0 (CU)5.0
ALCU3MN2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		3	(AL)1.0(MN)2.0 (CU)3.0
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5		hR14	(166, R-3m)		2	(AL)1.0(CU, FE, NI, VA)1.0
ALCUSC_TAU	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)		3	(AL, CU)0.6154(AL, CU)0.3077 (SC)0.0769
AL7CU2W	Unknown Structure					3	(AL)7.0(CU)2.0 (W)1.0
AL5CU1W2	Al5Cu1W2		tI8	(139, I4/mmm)		3	(AL)5.0(CU)1.0 (W)2.0
AL8CU4Y	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)		3	(AL)0.615385 (CU)0.307692 (Y)0.076923
AL45CU65Y10	BaCd11		tI48	(141, I4_ 1/amd)		3	(AL)0.375 (CU)0.541667

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							(Y)0.083333
AL42CU68Y10	(Al,Cu)11Tb		oF96	(70, Fddd)		3	(AL)0.35 (CU)0.566667 (Y)0.083333
ALCU17Y2	Zn17Th2		hR57	(166, R-3m)		2	(AL, CU)0.894737 (Y)0.105263
ALCU5Y	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(AL, CU)0.833333 (Y)0.166667
ALCU11Y3	Al11La3		oI28	(71, Immm)		2	(AL, CU)0.785714 (Y)0.214286
AL7CU2Y3	Ni3Pu		hR12	(166, R-3m)		3	(AL)0.583333 (CU)0.166667 (Y)0.25
ALCUY	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		3	(AL)0.333334 (CU)0.333333 (Y)0.333333
AL6ER2FE11	Th2Zn17		hR19	(166, R-3m)		3	(AL)6.0(ER)2.0 (FE)11.0
AL7ERMG2	Unknown Structure					3	(AL)0.66667(ER)0.1 (MG)0.23333
AL9M2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)	aka Al9FeNi, metastable Al9Fe2	2	(AL)9.0(FE, NI)2.0
AL10FE3NI	Co2Al5 (D811)	D811	hP28	(194, P6_3/mmc)		2	(AL)5.0(FE, NI)2.0
AL71FE5NI24	Unknown Structure					3	(AL)0.71(FE)0.05 (NI)0.24
ALFESI_T9	Fe2Al2Si3		aP16	(2, P-1)	Al-Fe-Si ternary phase, tao 1 / tao 9	2	(AL, SI)5.0(FE)3.0
ALFESI_T2	Unknown Structure				Al-Fe-Si ternary phase, tao 2, gamma_AlFeSi	4	(AL)0.5(FE)0.2

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							(SI)0.1(AL, SI)0.2
ALFESI_T3	Fe(Al0.67Si0.33)3		oS128	(67, Cmme)	Al-Fe-Si ternary phase, AL56FE24SI10, tao 3	3	(AL)0.56(FE)0.24 (SI)0.2
ALFESI_T4	Ga5Pd		tI24	(140, I4/mcm)	Al-Fe-Si ternary phase, tao 4, delta_AlFeSi	4	(AL)0.4166 (FE)0.1667(SI)0.25 (AL, SI)0.1667
AL8FE2SI	Fe23Al81Si15		hP246	(194, P6_ 3/mmc)	solution of the Al-Fe-Si ternary phase, tao 5, alpha_AlFeSi	4	(AL)0.6612(FE, MN)0.19(SI)0.0496 (AL, SI)0.0992
AL9FE2SI2	Fe2Al9Si2		mS52	(15, C2/c)	Al-Fe-Si ternary phase, tao 6, aka Al5FeSi, beta_AlFeSi	4	(AL)0.598(FE, MN)0.152(SI)0.1 (AL, SI)0.15
ALFESI_T7	Fe2Al3Si3		mP64	(14, P2_1/c)	Al-Fe-Si ternary phase, AL9FE5SI6, tao 7	2	(AL, SI)3.0(FE)1.0
ALFESI_T8	Fe3Al2Si4		oS36	(63, Cmcm)	Al-Fe-Si ternary phase, AL2FE3SI4, tao 8	2	(AL, SI)2.0(FE)1.0
ALFESI_T10	Mn3Al10		hP26	(194, P6_ 3/mmc)	Al-Fe-Si ternary phase, AL60FE25SI15, tao 10	3	(AL)0.6(FE)0.25 (SI)0.15
ALFESI_T11	Co2Al5 (D811)	D811	hP28	(194, P6_ 3/mmc)	Al-Fe-Si ternary phase, AL85FE30SI15, tao 11	3	(AL)0.65(FE)0.25 (SI)0.1
ALFEZN_GAMMA	Unknown Structure				Al-Fe-Zn ternary phase, aka gamma 2, no detailed structure	2	(AL, FE, ZN)0.255 (ZN)0.745
ALLIMG_T	Unknown Structure					3	(AL)0.53(LI)0.33 (MG)0.14
ALLISI	Half-Heusler (C1b)	C1b	cF12	(216, F-43m)		3	(LI)0.333333 (AL)0.333333 (SI)0.333334
AL3LI8SI5	Li8Al3Si5		cP16	(215, P-43m)	T3	3	(LI)0.5(AL)0.1875 (SI)0.3125

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALLI5SI2	Li5.3Al0.7Si2		hP8	(194, P6_ 3/mmc)		3	(LI)0.6625 (AL)0.0875(SI)0.25
T1_ALLIZN	Li13Cu6Ga21		cI160	(204, Im-3)	ternary phase T1 in Al-Li-Zn	2	(LI)1.0(AL, ZN)2.0
T3_ALLIZN	Unknown Structure				ternary phase T3 in Al- Li-Zn	2	(ALLI, ZN)1.0(ZN)3.0
T2_ALLIZN	NaTl (B32)	B32	cF16	(227, Fd-3m)	ternary phase T2 in Al-Li-Zn	2	(LI)0.5(AL, ZN)0.5
ALM2M1_L21	Hg2TiCu Inverse Heusler		cF16	(216, F-43m)	AlLi2Zr, AlCu2Ti	3	(AL, CU)1.0(AL, CU, LI)2.0(TI, ZR)1.0
AL18MG3TM2	Mg3Cr2Al18		cF184	(227, Fd-3m)		3	(AL, MG)18.0(AL, MG)3.0(CR, MN, TI)2.0
ALMG3NI2	Mn3Ni2Si		cF96	(227, Fd-3m)	Ternary phase AlMg3Ni2, cF96, Fd-3m, Ti2Ni type	3	(AL)1.0(NI)2.0 (MG)3.0
BETA_PRIME	Mg9Si5		hP14	(176, P6_3/m)	metastable precipitate, Mg9Si5/Mg1.8Si, related to Mg2Si	2	(MG)1.8(SI)1.0
B_PRIME	Unknown Structure				metastable precipitate, B_Prime, Al-containing Pre-beta phase	3	(AL)3.0(MG)9.0 (SI)7.0
U1_AL2MGSI2	Ce2O2S		hP5	(164, P-3m1)	metastable precipitate, U1_Al2MgSi2, Al- containing Pre-beta phase	3	(AL)2.0(MG)1.0 (SI)2.0
U2_AL4MG4SI4	MnCuP		oP12	(62, Pnma)	metastable precipitate, U2_Al4Mg4Si4, Al- containing Pre-beta phase	3	(AL)1.0(MG)1.0 (SI)1.0
BETA_DPRIME	Mg5Si6-a		mS22	(12, C2/m)	metastable beta double prime, related to Mg2Si, Mg5Si6, Al2Mg5Si4	3	(AL, SI)2.0(MG)5.0 (SI)4.0
AL38MG58SR4	Unknown Structure					3	(AL)38.0(MG)58.0 (SR)4.0
ETA_PRIME	Unknown Structure				metastable precipitate, related to MgZn2-based Eta phase	3	(AL)0.21(MG)0.28 (CU, ZN)0.51
T_PRIME	Bergman [Mg32(Al,Zn)49,	D8e	cI162	(204, Im-3)	metastable precipitate, related to T_PHASE	3	(AL)0.3(MG)0.45

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
	D8e]						(ZN)0.25
AL31MN6NI2	mu-Al4Mn		hP574	(194, P6_ 3/mmc)	Orthorhombic, ternary Al-Mn-Ni phase	3	(AL)31.0(MN)6.0 (NI)2.0
AL2MN2SI3	(Al2Mn2Si3)		hP21	(174, P-6)	the Al-Mn-Si ternary phase, tao1	3	(AL)2.0(MN)2.0 (SI)3.0
AL5MN6SI7	CrSi2 (C40)	C40	hP9	(180, P6_222)	the Al-Mn-Si ternary phase, tao2	3	(AL)5.0(MN)6.0 (SI)7.0
AL1MN1SI1	TiSi2 (C54)	C54	oF24	(70, Fddd)	the Al-Mn-Si ternary phase, tao3	3	(AL)1.0(MN)1.0 (SI)1.0
AL3MNSI2	(Al3MnSi2)		tP48	(85, P4/n)	the Al-Mn-Si ternary phase, tao4	3	(AL)3.0(MN)1.0 (SI)2.0
AL3MN4SI2	Unknown Structure				the Al-Mn-Si ternary phase, tao5	3	(AL)3.0(MN)4.0 (SI)2.0
ALMNSI_T6	Unknown Structure				the Al-Mn-Si ternary phase, tao6	2	(AL, MN)4.0(SI)1.0
ALMNSI_T8	Mn3Al10		hP26	(194, P6_ 3/mmc)	the Al-Mn-Si ternary phase, tao 8	4	(AL)6.0(MN)3.0(AL, MN, SI)3.0(AL, SI)1.0
AL15SI2M4	Al15(Mn,Fe)3Si2		cI168	(204, Im-3)	Solution of Al- Mn-Si ternary phase, tao 9, Al15(Mn,Fe)3Si2	4	(AL)16.0(CR, FE, MN, MO)4.0(SI)1.0 (AL, SI)2.0
AL2MNSI3	Ga5Pd		tI24	(140, I4/mcm)	the Al-Mn-Si ternary phase, tao10	3	(AL)2.0(MN)1.0 (SI)3.0
AL24MN5ZN	Unknown Structure					3	(MN, ZN)5.0(ZN)1.0 (AL)24.0
AL9MN2ZN	Unknown Structure					3	(MN)2.0(ZN)1.0 (AL)9.0
AL11MN3ZN2	Unknown Structure		oS152			3	(MN)3.0(ZN)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							(AL)11.0
C40_MOSI2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AL, SI)2.0(MO)1.0
C54_MOSI2	TiSi2 (C54)	C54	oF24	(70, Fddd)		2	(AL, SI)2.0(MO)1.0
B82_OMEGA	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		3	(AL)1.0(NB, TI)1.0 (TI)1.0
O_PHASE	NaHg		oS16	(63, Cmcm)	The O phase	3	(NB, TI)0.5(AL, NB, TI)0.25(NB, TI)0.25
O1_DIS	NaHg		oS16	(63, Cmcm)	The disordered O phase	2	(AL, NB, TI)0.75(AL, NB, TI)0.25
ALNI2SI	FeSi (B20)	B20	cP8	(198, P2_13)		2	(AL, SI, VA)1.0 (NI)1.0
AL6NI3SI	Ir3Ge7 (D8f)	D8f	cI40	(229, Im-3m)		3	(AL)6.0(NI)3.0 (SI)1.0
ALNI16SI9	AlNi16Si9		oS104	(63, Cmcm)		3	(AL)1.0(NI)16.0 (SI)9.0
TINI2AL5	ZrNi2Al5		tI16	(139, I4/mmm)	Tau5	3	(TI)14.0(NI)21.0 (AL)65.0
G_PHASE	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		3	(AL, NI, TI)16.0 (TI)6.0(NI)7.0
H_L21	Heusler (L21)	L21	cF16	(225, Fm-3m)		3	(AL, NI, TI)0.5(AL, NI, TI)0.5(NI, VA)1.0
ALNI2ZN	Unknown Structure					3	(AL)0.25(NI)0.5 (ZN)0.25
AL13NI38ZN49	Unknown Structure				Al-Ni-Zn ternary phase	3	(AL)0.13(NI)0.38 (ZN)0.49

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALSC2SI2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)		3	(AL)1.0(SC)2.0 (SI)2.0
AL3Y5	Unknown Structure				stable in Al-Sc-Y	2	(AL)3.0(SC, Y)5.0
AL75SC17Y8	Unknown Structure				ternary compound in Al- Sc-Y	3	(AL)75.0(SC)17.0 (Y)8.0
ALSISR	BaPtSb		hP3	(187, P-6m2)		2	(AL, SI)2.0(SR)1.0
AL2SI2SR	Ce2O2S		hP5	(164, P-3m1)		3	(AL)2.0(SI)2.0 (SR)1.0
ALSI3TI2	Zr3Al4Si5		tI24	(141, I4_ 1/amd)	Al-Si- Ti Tao 2	3	(AL, SI)0.2 (SI)0.466667 (TI)0.333333
ALSI7TI4	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	Al-Si-Ti Tao 1	3	(AL, SI)0.1 (SI)0.566667 (TI)0.333333
AL14SIY5	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	Al14SiY5 (T1)	3	(AL)14.0(SI)1.0 (Y)5.0
AL3SIY6	Tb6Al3Si		tI80	(140, I4/mcm)	Al3SiY6 (T2)	3	(AL)3.0(SI)1.0(Y)6.0
AL7SI3Y5	Unknown Structure				Al7Si3Y5 (T3)	3	(AL)7.0(SI)3.0(Y)5.0
AL2SIY	Unknown Structure				Al2SiY (T4)	3	(AL)2.0(SI)1.0(Y)1.0
AL11SI9Y10	Unknown Structure				Al11Si9Y10 (T5)	3	(AL)11.0(SI)9.0 (Y)10.0
AL2SI2Y	Ce2O2S		hP5	(164, P-3m1)	Al2Si2Y (T6)	3	(AL)2.0(SI)2.0(Y)1.0
CULIMG_T	Mg2Ni (Ca)	Ca	hP18	(180, P6_222)		3	(CU)1.0(LI)0.08 (MG)1.92
CU16MG6SI7	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		3	(CU)16.0(MG)6.0 (SI)7.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU3MG2SI	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)		3	(CU)2.74(MG)2.0 (SI)1.26
CU5MN4SI	Unknown Structure					3	(CU)0.5(MN)0.37 (SI)0.13
CUMNZN	Unknown Structure					3	(CU)0.334 (MN)0.333 (ZN)0.333
CU6NISI3	Unknown Structure					2	(CU, NI)0.732 (SI)0.268
CU46NI25SI29	Unknown Structure					3	(CU)0.458(NI)0.25 (SI)0.292
FE5NI3SI2	Unknown Structure					2	(FE, NI)4.0(SI)1.0
ZN13M2	Zn89(Fe0.5Ni0.5)13.8		cF432	(216, F-43m)	Fe-Ni-Zn ternary phase	2	(FE, NI)1.0(ZN)6.5
MG6MN3NI	Unknown Structure					3	(MG)0.5 (MN)0.1666667 (NI)0.33333333
MGNI6SI6	Unknown Structure					3	(MG)1.0(NI)6.0 (SI)6.0
MG2NI3SI	Unknown Structure					3	(MG)2.0(NI)3.0 (SI)1.0
MG10NI55SI35	Unknown Structure					3	(MG)2.0(NI)11.0 (SI)7.0
MG2NI16SI11	MgNi8Si5.5		hP*			3	(MG)1.0(NI)8.0 (SI)5.5
MG5NI9SI	Unknown Structure					3	(MG)1.0(NI)1.8 (SI)0.2
MG9NI29SI16	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		3	(MG)9.0(NI)29.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							(SI)16.0
MGNI6ZN6	Unknown Structure					4	(MG, ZN)3.0(MG, NI, ZN)4.0(NI)1.0 (ZN)2.0
MN15NI45SI40	Unknown Structure				Mn-Ni-Si ternary phase, T1 or N	3	(MN)0.15(NI)0.45 (SI)0.4
MN15NI50SI35	Unknown Structure				Mn-Ni-Si ternary phase, T2 or PHI	3	(MN)0.15(NI)0.5 (SI)0.35
MN6NI16SI7	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	Mn-Ni-Si ternary phase, T3 or G	3	(MN)0.206897 (NI)0.551724 (SI)0.241379
MN1NI1SI1	MnCuP		oP12	(62, Pnma)	Mn-Ni-Si ternary phase, T4 or E	3	(MN)1.0(NI)1.0 (SI)1.0
MNNISI_T5	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	Mn-Ni- Si ternary phase, T5 or "tao 1"	2	(MN)1.0(NI, SI)2.0
MNNISI_T6	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	Mn-Ni-Si ternary phase, T6 or "tao 2"	2	(MN)1.0(NI, SI)2.0
MN3NI2SI	Mn3Ni2Si		cF96	(227, Fd-3m)	Mn-Ni-Si ternary phase, T7 or Omega	3	(MN)3.0(NI)2.0 (SI)1.0
MN2NISI	Unknown Structure				Mn-Ni-Si ternary phase, T8 or S	2	(MN, NI)3.0(SI)1.0
MN6NISI3	R-(Co,Cr,Mo)		hR53	(148, R-3)	Mn-Ni-Si ternary phase, T9 or R	3	(MN)0.61(NI)0.12 (SI)0.27
MN66NI4SI30	Unknown Structure				Mn-Ni-Si ternary phase, T10 or U	3	(MN)0.66(NI)0.04 (SI)0.3
MN52NI29SI19	Unknown Structure				Mn-Ni-Si ternary phase, T11 or W	3	(MN)0.52(NI)0.29 (SI)0.19
MN7NI7ZN86	Unknown Structure		cF**	(216, F-43m)		3	(MN)0.07(NI)0.07 (ZN)0.86

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
NI2SIZN_T1	Heusler (L21)	L21	cF16	(225, Fm-3m)		3	(NI)0.5(SI)0.25 (ZN)0.25
NI9SI2ZN_T2	Al3Ti (D022)	D022	tI8	(139, I4/mmm)		3	(NI)0.75(SI)0.1675 (ZN)0.0825
NI2SIZN3_T3	Mn3Ni2Si		cF96	(227, Fd-3m)		3	(NI)2.0(SI)1.0 (ZN)3.0
NISIZN_T4	FeSi (B20)	B20	cP8	(198, P2_13)	Ni-Si-Zn tao 4, Ni3Si2Zn1	3	(NI)3.0(SI)2.0 (ZN)1.0
Q_ALCUMGSI	Q-(Al,Cu,Mg,Si)		hP21	(174, P-6)	Quaternary phase, aka Q, Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 & Al4Cu2Mg8Si7	4	(AL)5.0(CU)2.0 (MG)8.0(SI)6.0
QPRIME	Q-(Al,Cu,Mg,Si)		hP21	(174, P-6)	Coherent / semi- coherent version of Q_ALCUMGSI	4	(AL)5.0(CU)2.0 (MG)8.0(SI)6.0
AL18FE2MG7SI10	Unknown Structure				Quaternary phase, aka Al8FeMg3Si6 and Q_/PHI/H_PHASE	4	(AL)18.0(FE)2.0 (MG)7.0(SI)10.0

Gas and Liquid Phases

Name	*Prototype*	*Sublattices*	*Formula Unit*
GAS	Gas	1	(AG, AG1AL1, AG1CU1, AG1H1, AG1S1, AG1SE1, AG1TE1, AG2, AG2S1, AG2SE1, AG2TE1, AL, AL1B3H12, AL1C1, AL1C2, AL1CU1, AL1CU1S1, AL1CU1S2, AL1H1, AL1H2, AL1H3, AL1P1, AL1P2, AL1S1, AL1S2, AL1SB1, AL1SE1, AL1TE1, AL2, AL2C2, AL2C6H18, AL2S1, AL2S2, AL2SE1, AL2SE2, AL2TE1, AL2TE2, B, B10H14, B1C1, B1C2, B1C3H9, B1C6H15, B1H1, B1H1S1, B1H2, B1H3, B1S1, B1S2, B1SE1, B1TE1, B2, B2C1, B2H6, B2S1, B2S2, B2S3, B4S6, B5H9, BA, BA1H1, BA1S1, BA2, BE, BE1C2, BE1H1, BE1H2, BE1S1, BE2, BI, BI1H1, BI1H3, BI1S1, BI1SE1, BI1TE1, BI2, BI3, BI4, C, C1H1, C1H1P1, C1H1SI1_1, C1H1SI1_2, C1H2, C1H2SI1_1, C1H2SI1_2, C1H3, C1H3P1, C1H3SI1_1, C1H3SI1_2, C1H3SI1_3, C1H3SI1_4, C1H4, C1H4S1, C1H4SI1_1, C1H4SI1_2, C1H4SI1_3, C1H5P1, C1H5P1S1, C1H5SI1_1, C1H5SI1_2, C1H6P2, C1H6SI1, C1P1, C1P1SI1, C1P1SI2, C1P2, C1S1, C1S2, C1SE1, C1SE2, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2H1, C2H10SI2, C2H1SI1, C2H2, C2H2SI1, C2H3, C2H3SI1_1, C2H3SI1_2, C2H4, C2H4SI1_1, C2H4SI1_2, C2H5, C2H5SI1, C2H6, C2H6SI1_1, C2H6SI1_2, C2H6SI1_3, C2H7P1_1, C2H7P1_2, C2H7P1S1, C2H7SI1_1, C2H7SI1_2, C2H8SI1, C2H8SI1_2, C2P1, C2P2, C2SI1, C2SI2, C2SI3, C3, C3H1, C3H10SI1, C3H4_1, C3H4_2, C3H6_1, C3H6_2, C3H8, C3H8SI1, C3H9SI1_1, C3H9SI1_2, C4, C4H1, C4H10_1, C4H10_2, C4H11SI1, C4H12SI1_1, C4H12SI1_2, C4H2_1, C4H2_2, C4H4_1, C4H4_2, C4H6_1, C4H6_2, C4H6_3, C4H6_4, C4H6_5, C4H8_1, C4H8_2, C4H8_3, C4H8_4, C4H8_5, C4H8_6, C5, C60, C6H6, CA, CA1H1, CA1S1, CA2, CD, CD1H1, CD1S1, CD1SE1, CD1TE1, CE, CE1S1, CE1SE1, CE1TE1, CO, CO1H1, CO1S1, CO1SE1, CO1TE1, CO2, CR, CR1H1, CR1S1, CR1S2, CR1SE1, CR1TE1, CR2, CU, CU1H1, CU1S1, CU1SE1, CU1TE1, CU2, CU2S1, CU2SE1, ER, ER1S1, ER1SE1, ER1TE1, FE, FE1H1, FE1S1, FE1SE1, FE1TE1, FE2, GA, GA1H1, GA1P1, GA1SB1, GA1SB2, GA1TE1, GA1TE2, GA2, GA2S1, GA2SE1, GA2TE1, GE, GE1H4, GE1S1, GE1S2, GE1SE1, GE1TE1, GE1TE2, GE2, H, H1IN1, H1K1, H1LI1, H1MG1, H1MN1, H1MO3, H1NA1, H1NI1, H1P1, H1PB1, H1S1, H1SB1, H1SE1, H1SI1, H1SR1, H1TE1, H1ZN1, H1ZR1, H2, H2P1, H2S1, H2S2, H2SE1, H2SI1, H2TE1, H3P1, H3SB1, H3SI1, H4SI1, H4SN1, H6SI2, HF, IN, IN1P1, IN1S1, IN1SB1, IN1SB2, IN1SE1, IN1TE1, IN1TE2, IN2, IN2S1, IN2SE1, IN2TE1, K, K1LI1, K1NA1, K1S1, K2, K2S1, LA, LA1S1, LA1SE1, LA1TE1, LI, LI1NA1, LI2, MG, MG1S1, MG2, MN, MN1S1, MN1SE1, MN1TE1, MO, MO1S1, MO1S2, MO2, NA, NA2, NB, NB1S1, NB1SE1, NB1SE2, ND, ND1S1, ND1SE1, ND1TE1, NI, NI1S1, NI1TE1, NI2, P, P1S1, P1SB1, P1SE1, P1SI1, P1SI2, P1TE1, P2, P2SI2, P3, P3SB1, P4, P4S3, PB, PB1S1, PB1S2, PB1SE1, PB1TE1, PB2, PB2S2, S, S1SB1, S1SC1, S1SE1, S1SI1, S1SN1, S1SR1, S1TA1, S1TE1, S1TI1, S1V1, S1W1, S1Y1, S1ZN1, S1ZR1, S2, S2SB3, S2SI1, S2SN1, S2SN2, S2TI1, S2W1, S2ZR1, S3, S3SB2, S3SB4, S4, S4SB2, S5, S6, S7, S8, SB, SB1SE1, SB1TE1, SB2, SB3, SB4, SC, SC1SE1, SC1TE1, SE, SE1SI1, SE1SN1, SE1SR1, SE1TE1, SE1TI1, SE1V1, SE1Y1, SE1ZN1, SE2, SE3, SE4, SE5, SE6, SE7, SE8, SI, SI1TE1, SI2, SI3, SI4, SN, SN1TE1, SN1TE2, SN2, SN2TE2, SR, SR2, TA, TE, TE1TI1, TE1V1, TE1Y1, TE1ZN1, TE2, TE3, TE4, TE5, TE6, TE7, TI, TI2, V, W, Y, ZN, ZR, ZR2)1.0
LIQUID	Liquid	1	(AG, AL, AL2S3, AL2TE3, ALSB, B, BA, BE, BI, BI2MG3, C, CA, CD, CE, CO, CR, CU, ER, FE, GA, GE, H, HF, IN, K, LA, LI, LI4/5PB1/5, LIH, MG, MG2GE, MG2SN1, MG3SB2, MN, MO, NA, NB, ND, NI, P, PB, PR, S, SB, SC, SE, SI, SN, SR, TA, TE, TI, V, W, Y, ZN, ZN2ZR, ZR)1.0

TCAL9 Properties Data

Model Descriptions

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

You can find information on our website about the 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 Aluminum-based Alloys Databases page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to aluminum including links to resources such as publications, webinars, videos, and more.

TCAL: TCS Aluminium-based Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS Al-based Alloy Database (TCAL)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**9.0**
First release:	**TCAL1 was released in 2011**

Changes in the Most Recent Database Release

TCAL8.2 to TCAL9.0

Software release 2024a (December 2023/January 2024)

New Elements

- Four (4) new elements: Ba, Sb, Ta, and W (for a total of 48 elements).

New Systems

- 38 new binary systems are assessed: Ag-W, Al-Ba, Al-Sb, Al-Ta, Al-W, B-Nb, B-W, Ba-Be, Ba-Cr, Ba-Fe, Ba-Mn, Ba-Sc, Ba-Sr, Ba-V, C-W, Co-W, Cr-W, Cu-W, Cu-Y, Er-W, Fe-W, Ge-W, Hf-W, La-W, Li-Pb, Mg-Sb, Mn-W, Nb-W, Ni-W, Sc-W, Sc-Y, Si-W, Sn-W, Ta-Zn, Ti-W, V-W, W-Y, and W-Zr.

- 11 new ternary systems are assessed: Al-B-Nb, Al-C-Ti, Al-Cu-W, Al-Cu-Y, Al-Li-Pb, Al-Li-Zn, Al-Mg-Sb, Al-Mg-Sr, Al-Ni-Ti, Al-Sc-Y, and Al-Ta-Zn.

Other Updates

- Full Gas descriptions are added. There is a change to default settings. From this release, the GAS phase is restored by default when retrieving the data from the database. In order to reject it when it is not required for a calculation, you now have to manually reject it.

- Mn-Ni-Zn: descriptions of BCC_B2, EPSILON are updated in order to better account for the experimental data.

Surface Tension Re-assessed

- The surface tension was re-assessed based on the Redlich-Kister-Muggianu (R-K-M) sub-regular solution model.

Previous Releases

TCAL8.1 to TCAL8.2

Software release 2023a (December 2022/January 2023)

- Corrected an error in the molar volume of the B2 phase in the Al-Fe-Ni system.

TCAL8.0 to TCAL8.1

Software release 2022a (December 2021/January 2022)

- Updates to the surface tension, viscosity, and volume data for liquid.
- All assessed binary systems now have the SURF/VISC parameters.
- Updates to electrical resistivity and thermal conductivity of several solid phases (Al_2Cu, Al_6Mn, $Al_9Fe_2Si_2$ and Si) and liquid in several binaries (Ag-Al, Ag-Cu, Al-Cu, Al-Si, and Al-Zn), as well as molar volume and thermal expansivity of Pr.
- Modeling of the Y solubility in (Al).

TCAL7.1 to TCAL8.0

Software release 2021b (June 2021)

New elements and systems:

- 5 new elements: Nd, Pr, S, Se and Te
- 8 new assessed binaries: Al-Nd, Al-Pr, Al-S, Al-Se, Al-Te, Bi-Mg, Mg-Sc and Si-Y
- 9 new assessed ternaries: Al-Bi-Mg, Al-Cu-Ti, Al-Mg-Sc, Al-Mg-Sn, Al-Mg-Zr, Al-Mn-Ti, Al-Si-Y, Bi-Mg-Sn and Mg-Sc-Si
- 2 new assessed quaternaries: Al-Bi-Mg-Sn and Al-Mg-Sc-Si
- Surface tension, viscosity and volume of liquid, and electrical resistivity and thermal conductivity of some previously unassessed systems and some of the new systems have been modeled.

Other updates:

- Al-V and Al-Sc: the (Al) solvus is better described.
- Mg-Sn and H-Zn: new thermodynamic descriptions.
- Al-Li-Si: the ternary phases are refined to better account for their melting.
- Al-Ni-Si: the B2 description is refined.
- Al-Cr-Mg: Al18Mg3Cr2 (AL18MG3TM2) is refined.

- The partitioning ORD_L12 is removed. The compounds that it describes are merged into L12_FCC. This causes negligible changes in Al-Ce-Ni and Al-Mg-Ni, and triggers minor adjustments of Ag-Mg, Al-Ni, Fe-Ni, Ge-Ni, Mn-Ni, Ni-Si, Al-Cu-Ni, Al-Fe-Ni, Al-Mn-Ni, Al-Ni-Si, Al-Ni-Zn, Cu-Fe-Ni, Cu-Mn-Ni, Cu-Ni-Si, Fe-Mg-Ni, Fe-Mn-Ni, Mg-Mn-Ni, Fe-Ni-Si, Fe-Ni-Zn, Mg-Ni-Si, Mn-Ni-Si, Mn-Ni-Zn, and Ni-Si-Zn.
- ETA_PRIME, which is an important aging hardening precipitate, is refined in Al-Mg-Zn and Al-Cu-Mg-Zn.
- AL9FENI is identified as the metastable Al9Fe2 phase being stabilized by the Ni addition and thus renamed as Al9M2. The family of Al-Fe metastable phases is almost completely described.
- Thermophysical properties descriptions of many systems and for many phases are improved. These properties include viscosity and surface tension of liquid, molar volume, electrical resistivity, and thermal conductivity.

TCAL7.0 to TCAL7.1

Software release 2021a (January 2021)

- Modeling of Mg-Si-Sn
- Update of Al-Mo
- Update of molar volume data
- Update of electrical resistivity and thermal conductivity data

TCAL6.0 to TCAL7.0

Software release 2020b (June 2020)

New Thermophysical Properties

- Electrical resistivity is modeled for crystalline phases and liquid. The descriptions can be used for deriving electrical conductivity.
- Thermal conductivity is modeled for crystalline phases and liquid. The descriptions can be used for deriving thermal resistivity as well as thermal diffusivity (by combining with our density and heat capacity data).
- Viscosity and surface tension of liquid are modeled.

New Elements and Systems

- Added new minor-alloying elements: Nb, P and Y.
- Al-P, P-Si, P-Zn, Al-P-Si, and Al-P-Zn are modeled. The systems help to predict the formation of the ALP phase in aluminum alloys and to interpret its impacts on the microstructure modification.

- Al-Nb, as well as Nb-Ti and Al-Nb-Ti, is modeled for the minor-alloying element Nb.
- Al-Y, as well as Ti-Y and Al-Ti-Y, is modeled for the minor-alloying element Y.
- Six more Al-containing ternary systems are modeled, Al-C-Cr, Al-C-Mg, Al-C-V, Al-Cr-Mg, Al-Mg-Ti, and Al-Si-Sr, to make the Al-rich multi-component description more complete.

New Metastable Phase

- The semi-coherent version of the quaternary Q_ALCUMGSI phase is modeled as a metastable phase, QPRIME. It is expected to be used in precipitation simulations.

Updated Systems and Phases

- Al-C is updated taking into account the most recent modeling work.
- Si-Sr is updated and now reproduces the most recent modeling work.
- Al-C-Si is updated with the improved Al-C binary description.
- Al-Sc-Si is updated by modeling the Si solubility in the AL3X (Al3Sc-based) phase, which is a strengthening precipitate in some aluminum alloys
- Al-Fe-Mg-Si: the quaternary phase π-AL18FE2MG7SI10 is refined to make better predictions for solidification and lower-temperature heat treatments of related aluminum alloys.
- Al-Fe-Mn-Si is updated by modeling the Mn solubility in AL8FE2SI.
- Cr and Mo are introduced to the Al15Si2M4 (M = Cr, Fe, Mn and Mo) phase, which is of industrial importance in Al-Mn-Si and Al-Fe-Mn-Si based alloys.

TCAL5.1 to TCAL6.0

Software release 2019a (December 2018).

- Added a new element Mo, the Al-Mo and Mo-Si binary systems, and the Al-Mo-Si ternary system
- FCC_A1 is now independently modeled and no longer coupled with FCC_L12. The FCC_L12 phase modeled with the partitioning model is now separated and named as ORD_L12.
- Updated the Al-Cu-Mg-Zn metastable precipitates of industrial importance: S_prime and T_prime are remodeled; S_DPrime is newly modeled; especially, the Eta_prime phase is remodeled by considering the Cu solubility.

TCAL5.0 to TCAL5.1

Software release version: 2018b (June 2018)

Updates to the following systems:

- $Al_6(Cu, Fe, Mn)$ remodeled in Al-Cu-Fe-Mn and treated as a metastable phase in Al-Cu-Fe
- Improved description of Al_7Cu_2Fe
- Updated Si-Ti and Al-Si-Ti
- Improved volume description

TCAL4.0 to TCAL5.0

Software release version: 2017b (October 2017)

This update highlights the assessment of 18 binary systems and 25 ternary systems relevant to the 8xxx and 8xx.x series of industrial aluminum alloys, including but not limited to Al-Ce, Al-Er, Al-Li, Al-Sc, and Al-Sn based alloys.

The rare earth element Er, which may form the L12-type Al3Er stable precipitate in aluminum alloys, was newly added to the database. The Ag-Er, Al-Er, Cu-Er, Er-Fe, Er-Mg, Er-Si and Er-Zr binary systems and the Al-Cu-Er, Al-Er-Fe and Al-Er-Mg ternary systems were assessed.

The Ce-Cr, Ce-Fe, Ce-Mg, Ce-Mn, Ce-Ni and Ce-Si binary systems and the Al-Ce-Cr, Al-Ce-Cu, Al-Ce-Fe, Al-Ce-Mg, Al-Ce-Mn, Al-Ce-Ni and Al-Ce-Si ternary systems were assessed.

The L12 type metastable Al3Li (δ') phase, which is an important strengthening precipitate in some Li-containing aluminum alloys, was modeled. The Al-Li-Zr and Cu-Li-Mg systems were assessed.

The Bi-Sn, Cd-Sn, In-Sn and Sn-Pb binary systems and the Al-Bi-Sn, Al-Cd-Sn, Al-Cr-Sn, Al-Cu-Sn, Al-In-Sn, Al-Sn-Pb, Al-Sn-Si and Al-Sn-Zn ternary systems were assessed.

Sc-Ti, Al-Sc-Si, Al-Sc-Ti, Al-Sc-Zr and Al-Si-Ti were assessed. Ag-Cu was replaced and Ag-Al-Cu was assessed.

TCAL3.0 to TCAL4.0

Software release version: 2015a (June 2015)

The metastable Al-Cu precipitate Ω was modeled as the Al2Cu_OMEGA phase. In the Al-Cu-Mg-Zn system, the descriptions of the metastable precipitates ETA_PRIME (η') and T_PRIME (T') were refined. In the Al-Mg-Si system, the BETA_AL_DPRIME (Al-containing β'') phase was merged into BETA_DPRIME (β'') and treated as the same phase.

53 Ag-, H-, Hf-, K-, La-, Li-, Na- and/or Sc-containing binary systems were added, Ag-Cu, Ag-Fe, Ag-La, Ag-Li, Ag-Mg, Ag-Mn, Ag-Na, Ag-Ni, Ag-Si, Ag-Zn, Cu-H, Cu-Hf, Cu-La, Cu-Na, Fe-H, Fe-Hf, Fe-K, Fe-La, Fe-Li, Fe-Na, H-K, H-La, H-Li, H-Mg, H-Mn, H-Na, H-Ni, H-Zn, Hf-K, Hf-Li, Hf-Mg, Hf-Mn, Hf-Na, Hf-Ni, Hf-Sc, Hf-Si, K-Li, K-Mg, K-Na, K-Zn, La-Mn, La-Ni, La-Sc, La-Si, La-Zn, Li-Mn, Li-Na, Li-Sc, Li-Zn, Na-Sc, Na-Si, Na-Zn, and Sc-Zn. The previous Ag-Al binary description was replaced.

HCP_ZN was merged into HCP_A3. Necessary adjustments were made for the descriptions of Zn-containing systems in order to reproduce the phase equilibria.

Zr was introduced to Al3Ti_D022 and Ti to Al3Zr_D023. Al-Ti was updated in the Al-rich region. A preliminary assessment of the Al-Ti-Zr system was conducted. The description of Al4Mn_R in the Al-Fe-Mn system was refined.

Molar volumes and thermal expansivities were evaluated for all the newly added phases and end-members. Some existing volume data were updated as well.

TCAL2.1.1 to TCAL3.0

Software release version: 4.0 (June 2014)

19 binary systems were added, Ag-Ca, Ca-Cu, Ca-Fe, Ca-H, Ca-La, Ca-Li, Ca-Mn, Ca-Na, Ca-Ni, Ca-Sc, Ca-Si, Ca-Sr, Ca-Zn, Ag-Sc, Fe-Sc, Mn-Sc, Ni-Sc, Sc-Si and Sc-Zr.

Modeling of Al-Cu metastable precipitates: GPI Zones (described as the miscibility gap of fcc_A1), θ''-Al_3Cu (i.e. GPII Zones) and θ'-Al_2Cu.

Modeling of Al-Cu-Mg-Zn metastable phases: S'-Al_2CuMg, T'-$Al_{0.3}Mg_{0.4}Zn_{0.3}$ and η'-$Al_3Mg_{2.5}Zn_{3.5}$.

Modeling of Al-Mg-Si metastable precipitates: β''-Mg_5Si_6 (GPII zones), Al-containing β''-$Al_2Mg_5Si_4$, β'-Mg_9Si_5, U1-Al_2MgSi_2, U2-$Al_4Mg_4Si_4$ and B'-$Al_3Mg_9Si_7$.

Modeling of the metastable Al_mFe phase (modeled as Al_4Fe), which has been observed in some as-cast aluminum alloys such as AA1xxx, AA5128 and A206.

Necessary volume data were assessed for the new phases and newly introduced end-members. The Sn-Zn and Cu-Fe-Ni descriptions were updated. Some known issues were solved.

TCAL2.0 to TCAL2.1.1

Software release version: 3.1 (December 2013)

The Al-Fe-Mn-Si quaternary description had been systematically refined, including a deep revision of the Al-Fe-Si description and adjustments of the Al-Fe-Mn and Al-Mn-Si descriptions. It has been validated that this refinement improved the phase formation in a wide range of casting and wrought aluminum alloys, since Fe, Mn and Si are the most common additives and/or impurities in aluminum alloys.

A new Al-Ni description had been adopted and adjustments were subsequently made on the Al-Ni-based ternary systems.

The BCC_B2 description in the Ni-Zn binary system was reassessed. The Al-Ni-Zn ternary was reassessed. The Al-Mn-Ni description was improved by solving some known issues.

Both the Al-Cr and Al-V binary systems were improved in the Al-Rich corner. The Al-Si molar volume data were refined.

TCAL1.2 to TCAL2.0

Software release version: 3.0 (2013).

Since TCAL2, all necessary volume data (including molar volume and thermal expansion) had been added for most of the solution phases and intermetallic phases. This allows for the calculation of volume fraction of phases, as well as density, thermal expansivity and lattice parameters using Thermo-Calc. However, it should be noted that the molar volume data incorporated has no pressure dependence.

21 more binary systems have been implemented: Al-Be, Al-Bi, Al-Cd, Al-Ce, Al-Co, Al-Ga, Al-In, Al-Pb, Bi-Cu, Cd-Cu, Ce-Cu, Co-Li, Cr-Li, Cu-Co, Cu-Ga, Cu-In, Cu-Pb, Cu-Sc, Li-Ni, Li-Si and Li-Zr. Some of them were reassessed in this project. Additionally, the Al-Ca and Al-Sc descriptions have been updated. The $AlLi_2$ phase was considered in Al-Li.

The three ternary systems, Al-C-Si, Al-Cu-Sc, and Al-Li-Si, have been newly implemented. The previous provisional description of the Al-Cr-Si system has been replaced by a much more reliable description, which is derived from a thorough thermodynamic modeling over the entire compositional range and a wide temperature range. The Mn-Ni-Si description is also updated.

TCAL1.1 to TCAL1.2

TCAL1.2 was updated in 2012.

The Cu-Li, Li-Mg, Al-Cu-Li and Al-Li-Mg systems have been assessed and/or implemented in order to be able to predict the phase formation in Al-Cu-Li-Mg(-Zn) alloys (i.e. some of the 2xxx and 8xxx series alloys). The descriptions of the Al-Cu-Mg-Si and Al-Fe-Mn-Si core systems have been refined and validated, in order to give more accurate predictions for commercial Al-based alloys, including wrought alloys from series 2xxx to series 7xxx and foundry alloys series 3xx.x. The Al-Cr-Si system was tentatively assessed to include the Cr-bearing phase $Al_{13}Cr_4Si_4$.

The two compounds, AL8FEMNSI2 and AL5CU2MN3, were removed from the database since their existences were disputed. The VSI2 phase was merged into CRSI2_C40, and the AB3_L12 phase into L12_FCC. Thermodynamic models were reviewed for most phases, and many un-assessed parameters were reasonably estimated. Some phases were renamed to use their conventional names.

Additionally, the C-Mg binary description was reassessed. Now the two Mg carbides, MgC_2 and Mg_2C_3, are metastable and the C solubility in liquid Mg is greatly reduced to accord with the mostly published experimental data.

TCAL1.0 to TCAL1.1

TCAL1 was released in 2011 and TCAL1.1 was updated in 2012.

The description of the Al-Zn-Mg-Cu-Fe core system has been systematically refined and validated in order to give more accurate predictions for commercial Al-based alloys, especially the 7xxx series alloys. More specifically, crucial corrections or modifications have been made for the following related ternary systems, Al-Cu-Fe, Al-Cu-Mg, Al-Cu-Zn, and Al-Mg-Zn.

Another major enhancement is that users can now get the conventional phase names in Al-based alloys for a general name used in the database by using the command LIST_SYSTEM CONSTITUENT in the TDB module.