TCS Al-based Alloy Database (TCAL7)

Technical Information

Available Starting with Thermo-Calc Version 2020b

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Contents

About the TCS Al-based Alloy Database (TCAL)

TCAL: TCS Aluminium-based Alloys Database Revision History

TCS Al-based Alloy Database (TCAL) is a thermodynamic database developed for aluminum-based alloys, including but not limited to, the industrial grades. The current version of the database is TCAL7.

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, and
- surface tension of metallic liquids.

Molar volume with thermal expansion coefficients properties data have been available since TCAL2. Electrical resistivity, thermal conductivity, viscosity of metallic liquids, and surface tension of metallic liquids properties data are available starting with TCAL7.

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.
- Intetegrate 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 *TCAL: TCS Al-based Alloy Database 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 *TCAL: TCS Al-based Alloy Database 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 the technical information and 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.

TCAL7 Elements, Systems, Phases and Properties

Included Elements

There are 39 elements included in the most recent version of the database.

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

Assessed Systems and Phases

The most recent version of the database contains:

- 267 assessed binary systems, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 99 assessed ternary systems, mostly to their full range of composition. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- Some quaternaries are assessed within the Al-rich region.
- More than 600 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 rejected by default and has to be manually restored if required for a calculation.

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

A variety of properties data is included with the TCS Al-based Alloy Database (TCAL).

You can find information on our website about the thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources will also be made available on our website in the near future so keep checking back or subscribe to our newsletter.

Molar volume with thermal expansion coefficients properties data have been available since TCAL2. Electrical resistivity, thermal conductivity, viscosity of metallic liquids, and surface tension of metallic liquids properties data are available starting with TCAL7.

Below is a summary of the available parameters and variables for this database 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.

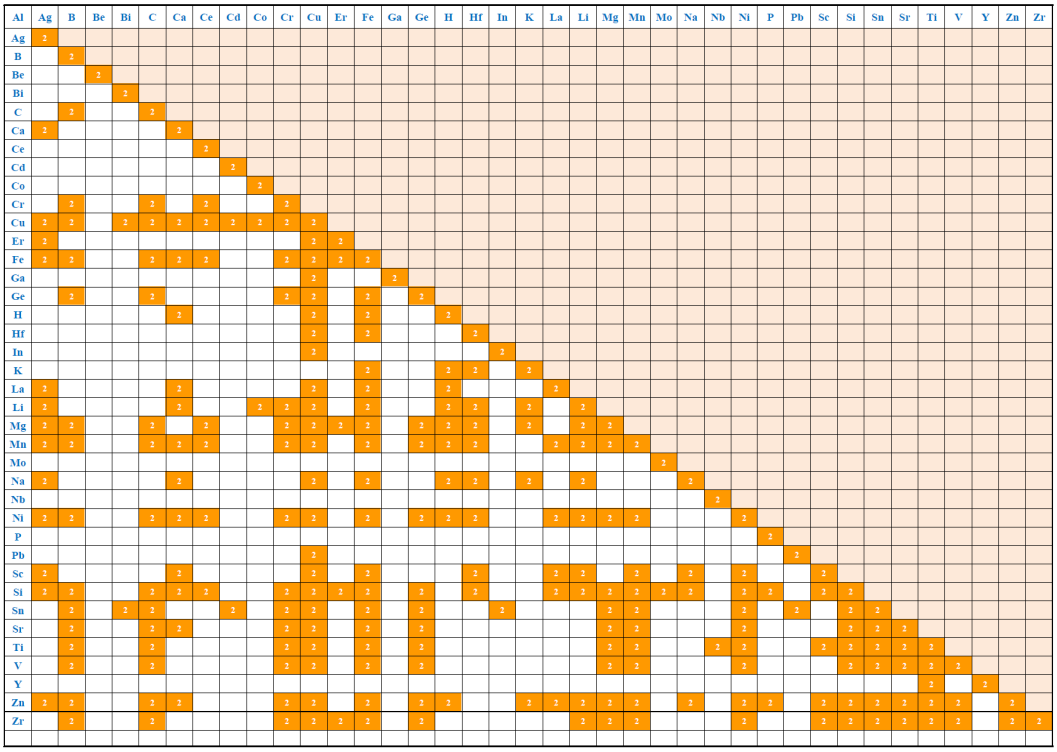
Property	Model Parameters in TDB File	Variables to Show or Plot in Console Mode and TC-Python
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Electrical conductivity		ELCD for a system `ELCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI	`SURF(LIQUID)`
Dynamic viscosity	VICS	`DVIS(LIQUID)`
Kinematic viscosity		`KVIS(LIQUID)`
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

TCAL7 Systems

In this section:

TCAL7 Assessed Binary Systems

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



TCAL7 Assessed Ternary Systems

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

Assessed Ternary Systems			
Ag-Al-Cu	Al-Bi-Sn	Al-C-Cr	Al-C-Mg
Al-C-Si	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-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-Si	Al-Li-Zr	Al-Mg-Mn	Al-Mg-Ni
Al-Mg-Si	Al-Mg-Ti	Al-Mg-Zn	Al-Mn-Ni
Al-Mn-Si	Al-Mn-Zn	Al-Mo-Si	Al-Nb-Ti
Al-Ni-Si	Al-Ni-Zn	Al-P-Si	Al-P-Zn
Al-Pb-Sn	Al-Sc-Si	Al-Si-Sn	Al-Si-Sr
Al-Sc-Ti	Al-Sc-Zr	Al-Si-Ti	Al-Si-Zn
Al-Sn-Zn	Al-Ti-Y	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	Fe-Mg-Zn	Fe-Mn-Ni	Fe-Mn-Si

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

TCAL7 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

TCAL7 Phases

In this section:

Common Phases for Aluminum Alloys

TCAL7 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
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
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

Name in the Database	Common Name and Description
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

TCAL7 Models for the Included Phases

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AG2CA	KHg2	oI12	I m m a		74	(Ag)0.666667(Ca)0.333333	
AG2ER	MoSi2	tI6	I 4/m m m	C11_b	139	(Ag)2(Er)1	
AG2LA	KHg2	oI12	I m m a		74	(La)1(Ag)2	
AG2NA	Cu2Mg	cF24	F d -3 m	C15	227	(Ag)2(Na)1	
AG4SC	MoNi4	tI10	I 4/m	D1	87	(Ag)0.8(Sc)0.2	
AG51ER14	Ag51Gd14	hP68	P 6/m		175	(Ag)0.77(Er)0.23	
AG51LA14	Ag51Gd14	hP68	P 6/m		175	(La)14(Ag)51	
AG5LA	MgZn2	hP12	P 6_3/m m c	C14	194	(La)1(Ag)5	
AG5ZN8	Cu5Zn8	cI52	I -4 3 m	D82	217	(Ag,Zn)2(Ag)2(Zn,Ag)3(Zn,Ag)6	
AG7CA2	Ag7Yb2	oS36	C m c m		63	(Ag)0.777778(Ca)0.222222	
AG9CA2						(Ag)0.818182(Ca)0.181818	
AGCA3						(Ag)0.25(Ca)0.75	
AGER	CsCl	cP2	P m -3 m	B2	221	(Ag)1(Er)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AGLA	CsCl	cP2	P m -3 m		221	(La)1(Ag)1	
AGMG3	Hf54Os17	oI142	I m m m		71	(Ag)0.23(Mg)0.77	Ag17Mg54
AGMG4	Ag9Mg37	hP116	P 6 3/m		176	(Ag)0.2(Mg)0.8	Ag9Mg37
AGSC	CsCl	cP2	P m -3 m	B2	221	(Ag)0.5(Sc)0.5	
AGZN3	Mg	hP24	P 6_3/m m c		194	(Ag,Zn)1	
AGZN_HP9	W	cI2	I m -3 m		229	(Zn)1(Ag,Zn)2	
AL10CE2M7	Th2Zn17	hR57	R -3 m		166	(Fe,Al,Mn,Cr,Cu)0.8947(Er,Ce)0.1053	T2
AL10CEFE2	YbFe2Al10	oC52	C m c m		63	(Al)10(Er,Ce)1(Fe)2	
AL10CU10FE		oF*	F m m 2		42	(Fe)1(Cu,Al)10(Al)10	
AL10FE3NI	Co2Al5	hP28	P 6_3/m m c		194	(Al)5(Ni,Fe)2	
AL11CE3	La3Al11	oI28	I m m m		71	(Al,Mg)0.7857(Ce)0.2143	
AL11CU5MN3		oP380				(Al)11(Mn)3(Cu)5	
AL11LA3_HT	BaAl4	tI10	I 4/m m m		139	(Al)11(La)3	
AL11LA3_LT	La3Al11	oI28	I m m m		71	(Al)11(La)3	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL11MN3ZN2		oC152				(Mn)3(Zn)2(Al)11	
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25	oP156	P n m a		62	(Al,Mn)29(Mn)10	
AL11MN4_LT	Mn4Al11	aP15	P -1		2	(Zn,Al)11(Fe,Mn)4	
AL12MN	Al12W	cI26	I m -3 m		229	(Al)12(Mn)1	
AL12MO	Al12W	cI26	I m -3		204	(Si,Al)12(Mo)1	
AL13CEMG6	MgZn2	hP12	P 6_3/m m c		194	(Al)0.667(Ce)0.05(Mg)0.283	
AL13CO4	Al19Co6	mS100	C 2/m		12	(Al)13(Co)4	
AL13CR4SI4		cF84	F -4 3 m		216	(Al)13(Cr)4(Si)4	Al-Cr-Si, tao 1
AL13FE4	Al13Fe4	mS102	C 2/m		12	(Al,Cu)0.6275(Ni,Mn,Zn,Fe)0.235(Va,Al,Zn,Si)0.1375	solution phases based on Al13Fe4, aka Al3Fe
AL13NI38ZN49						(Al)0.13(Ni)0.38(Zn)0.49	Al-Ni-Zn ternary phase
AL14CA13	Al14Ca13	mS54	C 2/m		12	(Al,Zn,Mg)14(Ca)13	
AL15SI2M4		cP168	P m -3		200	(Al)16(Mn,Mo,Cr,Fe)4(Si)1(Si,Al)2	Solution of Al-Mn-Si ternary phase, tao 9, Al15(Mn,Fe)3Si2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL17MO4	Al17Mo4	mC84	C 2		5	(Si,Al)17(Mo)4	
AL18FE2MG7SI10			hexagonal			(Al)18(Fe)2(Mg)7(Si)10	Quaternary phase, aka Al8FeMg3Si6 and Q_/PHI/H_PHASE
AL18MG3TM2	Mg3Cr2Al18	cF184	F d -3 m		227	(Mg,Al)18(Mg,Al)3(Mn,Cr,Ti)2	
AL1CE1SI1	Ce(Al,Si)2	tI12	I 4_1 m d		109	(Al,Si)2(Ce)1	
AL1CE2	*	*	*			(Al)0.3333(Ce)0.6667	
AL1LI2	InLi2 / GaLi2	oS12	C m c m		63	(Al)1(Li)2	
AL1MN1SI1						(Al)1(Mn)1(Si)1	the Al-Mn-Si ternary phase, tao3
AL20CECR2		cF184	F d -3 m		227	(Al)0.869565(Ce)0.043478(Cr)0.086957	
AL21V2		cF184	F d -3 m		227	(Al)21(V)2	
AL22MO5		oF216	F d d 2		43	(Al,Si)22(Mo)5	
AL23CE4NI6		mS66	C 2/m		12	(Al)23(Ce)4(Ni)6	T8
AL23V4		hP54	P 6_3/m m c		194	(Al)23(V)4	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL24MN5ZN		o**				(Zn,Mn)5(Zn)1(Al)24	
AL28CU4MN7	Mn6Cu4Al29	oC156	C m c m		63	(Al)28(Mn)7(Cu)4	
AL2CENI		oS16	C m c m		63	(Al)2(Ce)1(Ni)1	T2
AL2CULI	LiCuAl2	hP12	P 6/m m m		191	(Al)0.5(Cu)0.25(Li)0.25	Al-Cu-Li ternary phase, i.e. T1
AL2CU_C16	Al2Cu	tI12	I 4/m c m	C16	140	(Ge,Hf,Zr,Fe,Al,Mn,Ni,Sn)2 (B,Ni,Cu,Fe,Al,Mn,Si)1	Al2Cu,AlHf2,Fe2B,FeGe2,FeZr2,FeSn2,Mn2B,MnSn2,NiB2,NiZr2,SiZr2
AL2CU_OMEGA	Al2Cu	*tI12	*I 4/m c m	*C16	140	(Al)2(Cu)1	Al2Cu-OMEGA metastable precipitate
AL2ER3		tP20	P 4_2/m n m		136	(Al,Mg)0.4(Er)0.6	
AL2FE1	FeAl2	aP18	P 1		1	(Si,Cu,Al,Zn)2(Ni,Mn,Fe)1	
AL2LI3	Li3Al2	hR15	R -3 m		166	(Al,Mg)2(Li)3	
AL2MGC2	MgAl2C2	hP5	P -3 m 1		164	(Al)2(Mg)1(C)2	
AL2MN2SI3		hP*	P -6		174	(Al)2(Mn)2(Si)3	the Al-Mn-Si ternary phase, tao1
AL2MNSI3						(Al)2(Mn)1(Si)3	the Al-Mn-Si ternary phase, tao10
AL2SC	Cu2Mg	cF24	F d -3 m	C15	227	(Ti,Zr,Sc)1(Al)2	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL2SI2SR	MgAl2C2	hP5	P -3 m 1		164	(Al)2(Si)2(Sr)1	
AL2SR_OI12	CeCu2 / KHg2	oI12	I m m a		74	(Zn,Al)2(Sr)1	Al2Sr, SrZn2
AL2TI	Gd2Hf	tI24	I 4_1/a m d		141	(Nb,Al,Ti)2(Sc,Nb,Ti,Al)1	
AL2Y_C15	Cu2Mg	cF24	F d -3 m	C15	227	(Al,Y)2(Y,Al)1	
AL2ZR3_TP20	Al2Zr3	tP20	P 4_2/m n m		136	(Al,Zn)2(Sc,Y,Zr,Hf)3	Al2Zr3, Al2Hf3, ZN2Zr3
AL31MN6NI2						(Al)31(Mn)6(Ni)2	Orthorhombic, ternary Al-Mn-Ni phase
AL3CA8	Ca8In3	aP22	P -1		2	(Al)3(Mg,Ca)8	
AL3CECU	BaAl4	tI10	I 4/m m m		139	(Cu,Al)0.8(Ce)0.2	T3
AL3CE_H	Mg3Cd	hP8	P 6_3/m m c		194	(Al)0.75(Ce)0.25	
AL3CE_L	Mg3Cd	hP8	P 6_3/m m c		194	(Si,Al)0.75(Ce)0.25	
AL3CO				cub		(Al)3(Co)1	
AL3CU1ER1		oI10	I m m m		71	(Al)0.6(Cu)0.2(Er)0.2	
AL3HF4	Al3Zr4	hP7	P 6/m m m		191	(Al)3(Hf)4	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL3LA	Mg3Cd	hP8	P 6_3/m m c	D019	194	(Al)3(La)1	
AL3LI8SI5		cP16	P -4 3 m		215	(Li)0.5(Al)0.1875(Si)0.3125	
AL3MN4SI2	FeSi	cP8	P 2_1 3		198	(Al)3(Mn)4(Si)2	the Al-Mn-Si ternary phase, tao5
AL3MNSI2						(Al)3(Mn)1(Si)2	the Al-Mn-Si ternary phase, tao4
AL3MO	Al3Mo	mC32	C 2/m		12	(Si,Al)3(Mo)1	
AL3NI2	Ni2Al3	hP5	P -3 m 1		164	(Zn,Al,Si)3(Al,Fe,Cu,Ni,Mg)2(Va,Ni)1	
AL3NI5	Pt5Ga3	oS16	C m m m		65	(Al)0.375(Ni)0.625	
AL3NI_D011	CFe3	oP16	P n m a	D011	62	(Ni,Al,Mn)0.75(Ni,B,C,Fe)0.25	
AL3TI_D022	Al3Ti	tI8	I 4/m m m	D022	139	(Mn,Ni,Al,Si,Ti,Nb)3 (V,Zr,Sc,Al,Nb,Mn,Ge,Ti)1	Al3Ti, Ni3V, GeMn3, Al3V
AL3TI_LT	Al3Ti	tI32	I 4/m m m		139	(Si,Nb,Ti,Al)3(Ti,Nb,Sc,Al)1	
AL3X	AuCu3	cP4	P m -3 m	L12	221	(Sc,Li,Ti,Zr,Er)1(Si,Mg,Al)3	Al3Sc (dissolving Ti, Zr), Al3Li
AL3Y_HT	BaPb3	hR36	P 6_3/m m c		194	(Al)0.75(Y)0.25	
AL3Y_LT	Mg3Cd	hP8	P 6_3/m m c		194	(Al)0.75(Y)0.25	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL3ZR2_OF40	Al3Zr2	oF40	F d d 2		43	(Li,Al)3(Zr,Sc,Hf)2	Al3Zr2, Al3Hf2
AL3ZR5_D8M	W5Si3	tI32	I 4/m c m	D8m	140	(Ge,Si,Al)3(Cr,V,Zr)5	Al3Zr5, Cr3Si5, Ge3V5, Si3V5
AL3ZR_D023	Al3Zr	tI16	I 4/m m m		139	(Li,Al)3(Zr,Hf,Sc,Ti)1	Al3Zr, Al3Hf
AL40CE30NI30						(Al)0.403(Ce)0.304(Ni)0.293	T12
AL45V7	Al45V7	mC104	C 2/m		12	(Al)45(V,Cr)7	Al45Cr7, Al45V7
AL4C3	Al4C3	hR21	R -3 m		166	(Al,Si)2(Al,Si,Mg)2(C)3	
AL4C4SI		hP18	P 6_3 m c		186	(Al)4(Si)1(C)4	
AL4CE1	Al4Ba	tI10	I 4/m m m	D13	139	(Al)0.8(Ce)0.2	
AL4CE3SI6	Al4Ce3Si6	hP13	P -3 m 1		164	(Al)4(Ce)3(Si)6	
AL4CENI		oC24	C m c m		63	(Al)4(Ce)1(Ni)1	T5
AL4CR	Al4Mn	hP574	P 6_3/m m c		194	(Cr)1(Va,Al,Si)4	
AL4FE	AlmFe	tI110	I -4 2 m		121	(Al)4.2(Fe)1	
AL4LI9	Al4Li9	mS26	C 2/m		12	(Al)4(Li)9	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL4MN_R	Al230.8Mn53.3	hP586	P 6 3/m		176	(Al)0.81162(Fe,Mn)0.18838	AL461MN107
AL4MN_U	Mn55Al226.58	hP574	P 6_3/m m c		194	(Al,Zn)4(Mn)1	
AL4MO	Al4W	mC30	C m		8	(Al,Si)4(Mo)1	
AL4M_D13	Al4Ba	tI10	I 4/m m m	D13	139	(Al,Si)4(Sr,Ca)1	Al4Ca, Al4Sr
AL4ZR5	Ga4Ti5	hP18	P 6_3/m c m		193	(Al)4(Zr,Sc)5	
AL53LA22	AlB2	hP3	P 6/m m m	C32	191	(Al)0.707(La)0.293	
AL5CE1NI2		oI16	I m m m		71	(Al)5(Ce)1(Ni)2	T6
AL5CE2NI5						(Al)0.35(Ce)0.165(Ni)0.485	T3, 13
AL5CO2	Al5Co2	hP28	P 6_3/m m c		194	(Al)5(Co)2	
AL5CR	Al11Cr2	mS*	C 2/c	orth	15	(Si,Al)5(Cr)1	
AL5CU3ER2						(Al)0.5(Cu)0.3(Er)0.2	
AL5FE2	FeAl2.8	oS24	C m c m		63	(Si,Cu,Zn,Al)5(Mn,Fe,Ni)2	
AL5FE4						(Al,Fe,Cu,Mn)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL5MN6SI7						(Al)5(Mn)6(Si)7	the Al-Mn-Si ternary phase, tao2
AL5MO	Al5Mo	hP36	R -3 c		167	(Si,Al)5(Mo)1	
AL5TI2	Al5Ti2	tP28	P 4/m m m		123	(Al,Nb,Ti)5(Ti,Al,Nb)2	
AL5TI3		tP*	P 4/m b m		127	(Al)5(Ti,Nb)3	
AL60CE12NI28						(Al)0.6(Ce)0.12(Ni)0.28	T11
AL62CU25FE13						(Fe)0.125(Cu,Al)0.255(Al)0.62	
AL63MO37	*	*	*			(Al,Si)0.63(Mo)0.37	
AL6ER2FE11	Th2Zn17	hR57	R -3 m		166	(Al)6(Er)2(Fe)11	
AL6MN	Al6Mn	oS28	C m c m		63	(Zn,Cu,Al)6(Mn,Cu,Fe)1	
AL6NI3SI	Ir3Ge7	cI40	I m -3 m		229	(Al)6(Ni)3(Si)1	
AL71FE5NI24						(Al)0.71(Fe)0.05(Ni)0.24	
AL7CE5SI3						(Al)0.49(Ce)0.333333(Si)0.176667	
AL7CU2FE		tP40	P 4/m n c		128	(Ni,Fe)1(Cu)2(Al)7	Solution phase of the ternary compound Al7Cu2Fe

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL7CU4NI		hP*/ hR*				(Al)1(Va,Cu,Ni,Fe)1	
AL7ERMG2						(Al)0.66667(Er)0.1(Mg)0.23333	
AL7SR8	Ba8Ga7	cP60	P 2_1 3		198	(Al)7(Sr)8	
AL8C7SI						(Al)8(Si)1(C)7	
AL8CEFE2	CeFe2Al8	oP44				(Al)8(Ce)1(Fe)2	
AL8CEM4	ThMn12	tI26	I 4/m m m		139	(Al)0.6154(Ce,Er)0.0769 (Al,Fe,Cu,Mn,Cr)0.3077	T1
AL8FE2SI	Fe3Al7.4Si	hP24 5	P 6_3/m m c		194	(Al)0.6612(Mn,Fe)0.19(Si)0.0496 (Si,Al)0.0992	solution of the Al-Fe-Si ternary phase, tao 5, alpha_AlFeSi
AL8MN5	Cr4.5 (Cr0.56Al0.44)9 Al12	hR26 / hR78	R 3 m	D810	160	(Zn,Al)12(Mn)5(Si,Al,Mn,Cu)9	
AL8MO3	Al8Mo3	mC22	C 2/m		12	(Si,Al)8(Mo)3	
AL8V5	Cu5Zn8	cI52	I -4 3 m	D82	217	(V,Al)2(V)2(Al,V)3(Al)6	
AL9CO2	Al9Co2	mP22	P 2_1/c		14	(Al)9(Co)2	
AL9CR3SI	Mn3Al9Si		P 6_3/m m c		194	(Al)9(Cr)3(Si)1	Al-Cr-Si, tao 2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
AL9CU6ER5						(Al)0.45(Cu)0.3(Er)0.25	
AL9FE2SI2	Fe2Al9Si2	mC52	C 2/c		15	(Al)0.598(Mn,Fe)0.152(Si)0.1(Al,Si)0.15	Al-Fe-Si ternary phase, tao 6, aka Al5FeSi, beta_AlFeSi
AL9FENI	Co2Al9	mP22	P 2_1/c		14	(Al)9(Ni,Fe)2	
AL9MN2ZN						(Mn)2(Zn)1(Al)9	
ALB12		tP208	P 4_1 2_12		92	(Al)1(B)12	
ALB2_C32	AlB2	hP3	P 6/m m m	C32	191	(Mn,Mg,Ti,Al,Zr,V,Cr)1(B)2	AlB2, B2Cr, B2Mg, B2Mn, B2Ti, B2V, B2Zr
ALC3V4		hP16	P 6_3/m m c		194	(V)4(Al)1(C)2(Va,C)1	
ALCCR2		hP8	P 6_3/m m c		194	(Al)1(C)1(V,Cr)2	Prototype AlCCr2 (hP8)
ALCE2CU2						(Al)0.2(Ce)0.4(Cu)0.4	T5
ALCE3_H	AuCu3	cP4	P m -3 m	L12	221	(Al)0.25(Ce)0.75	
ALCE3_L	Mg3Cd	hP8	P 6_3/m m c		194	(Al)0.25(Ce)0.75	
ALCEFE		o**				(Fe,Al)2(Ce)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
ALCEM	Fe2P	hP9	P -6 2 m		189	(Al)0.3333(Ce,Er)0.3333(Ni,Cu)0.3334	T4
ALCESI2		hP8	P -3 m 1		164	(Al)1(Ce)1(Si)2	
ALCE_OC16	CeAl	oS16	C m c m		63	(Al)0.5(Ce)0.5	
ALCRSI_T3	Mn4Al11	aP15	P -1		2	(Si,Al)11(Cr)4	Al-Cr-Si, tao 3
ALCRSI_T4						(Al)58(Cr)31.5(Si)10.5	Al-Cr-Si, tao 4, AL58CR32SI11
ALCR_GAMMA1						(Si,Cr,Al)2(Cr)2(Cr,Al)3(Si,Al)6	
ALCU3MN2						(Al)1(Mn)2(Cu)3	
ALCULI_B	CaF2	cF12	F m -3 m		225	(Al)0.6(Cu)0.32(Li)0.08	Al-Cu-Li ternary phase, TB
ALCULI_R	Mg32(Zn,Al)49	cI162	I m -3 m		229	(Al)0.55(Cu)0.117(Li)0.333	Al-Cu-Li ternary phase, R
ALCULI_T2			quasicrystalline			(Al)0.57(Cu)0.11(Li)0.32	Al-Cu-Li ternary phase, T2
ALCUSC_TAU	ThMn12	tI26	I 4/m m m		139	(Cu,Al)0.6154(Al,Cu)0.3077(Sc)0.0769	
ALCU_DEL						(Zn,Al)2(Fe,Cu)3	
ALCU_EPS	Co1.75Ge	hP6	P 6_3/m m c		194	(Ni,Cu,Al,Zn)1(Fe,Cu)1	
ALCU_ETA	CuAl	mS20	C 2/m		12	(Cu,Al)1(Ni,Cu,Zn,Fe)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
ALCU_ZETA						(Al)9(Cu,Fe)11	
ALER2		oP12	P n m a		62	(Mg,Al)0.33333(Er)0.66667	
ALER_OP16		oP16	P b c m		57	(Mg,Al)0.5(Er)0.5	
ALFESI_T10	Al10Mn3 / Al5Co2	hP26 / hP28	P 6_3/m m c		194	(Al)0.6(Fe)0.25(Si)0.15	Al-Fe-Si ternary phase, AL60FE25SI15, tao 10
ALFESI_T11	Co2Al5	hP28	P 6_3/m m c		194	(Al)0.65(Fe)0.25(Si)0.1	Al-Fe-Si ternary phase, AL85FE30SI15, tao 11
ALFESI_T2				mono		(Al)0.5(Fe)0.2(Si)0.1(Si,Al)0.2	Al-Fe-Si ternary phase, tao 2, gamma_AlFeSi
ALFESI_T3	Al2FeSi	oC12 8	C m m a	orthorhombic	67	(Al)0.56(Fe)0.24(Si)0.2	Al-Fe-Si ternary phase, AL56FE24SI10, tao 3
ALFESI_T4	Ga5Pd	tI24	I 4/m c m	tetragonal	140	(Al)0.4166(Fe)0.1667(Si)0.25(Al,Si)0.1667	Al-Fe-Si ternary phase, tao 4, delta_AlFeSi
ALFESI_T7	Fe2Al3Si3	mP6 4	P 2_1/c		14	(Al,Si)3(Fe)1	Al-Fe-Si ternary phase, AL9FE5SI6, tao 7
ALFESI_T8	Fe3Al2Si4	oC36	C m c m		63	(Si,Al)2(Fe)1	Al-Fe-Si ternary phase, AL2FE3SI4, tao 8
ALFESI_T9	Fe2Al2Si3	aP16	P -1		2	(Si,Al)5(Fe)3	Al-Fe-Si ternary phase, tao 1 / tao 9
ALFEZN_GAMMA	*	*	*			(Fe,Zn,Al)0.255(Zn)0.745	Al-Fe-Zn ternary phase, aka gamma 2, no detailed structure
ALLA	CeAl	oS16	C m c m		63	(Al)1(La)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
ALLI2ZR	Li2ZrAl	cF16	F -4 3 m		216	(Al)1(Li)2(Zr)1	
ALLI5SI2	Li5.3Al0.7Si2	hP8	P6_3/mmc		194	(Li)0.6625(Al)0.0875(Si)0.25	
ALLIMG_T		c*456				(Al)0.53(Li)0.33(Mg)0.14	
ALLISI		cF12	F -4 3 m		216	(Li)0.333333(Al)0.333333(Si)0.333334	
ALM3_A15	Cr3Si	cP8	P m -3 n	A15	223	(Al,Ti,Nb,Mo,Si)1(Ti,Mo,Nb,Al)3	A15
ALMG3NI2		cF96	F d -3 m		227	(Al)1(Ni)2(Mg)3	Ternary phase AlMg3Ni2, cF96, F d -3 m, Ti2Ni type
ALMGZN_PHI	Mg21(Zn,Al)17	oP152	P b c m		57	(Mg)6(Zn,Al)5	a Al-Mg-Zn ternary phase know as PHI
ALMG_BETA	Mg28Al45	cF1832	F d -3 m		227	(Li,Mg)89(Zn,Al)140	
ALMG_EPS	Mg23Al30	hR159	R -3		148	(Mg)23(Zn,Al)30	
ALMG_GAMMA	Mg24Y5 / Al12Mg17	cI58	I -4 3 m		217	(Li,Mg)5(Zn,Al,Mg)12(Zn,Mg,Al)12	
ALMNSI_T6				*		(Mn,Al)4(Si)1	the Al-Mn-Si ternary phase, tao6
ALMNSI_T8	Al10Mn3	hP26	P 6_3/m m c	hexagonal	194	(Al)6(Mn)3(Mn,Al,Si)3(Si,Al)1	the Al-Mn-Si ternary phase, tao 8

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
ALNB2		tP30	P 4_2/m n m		136	(Al,Ti,Nb)10(Nb,Ti)4(Ti,Nb,Al)16	
ALNI16SI9	Ni61Al4Si35	oC104	C m c m		63	(Al)1(Ni)16(Si)9	
ALNI2SI	FeSi	cP8	P 2_1 3		198	(Si,Va,Al)1(Ni)1	
ALNI2ZN	BiF3	cF16	F m -3 m	L21	225	(Al)0.25(Ni)0.5(Zn)0.25	
ALP		cF8	F m -3 m		225	(Al)1(P)1	
ALSC2SI2		tP10	P 4/m b m		127	(Al)1(Sc)2(Si)2	
ALSC_OP		oP*				(Zr,Sc)1(Al)1	
ALSI3TI2	Zr3Al4Si5	tI24	I 4_1/a m d		141	(Si,Al)0.2(Si)0.466667(Ti)0.333333	Al-Si-Ti Tao 2
ALSI7TI4	ZrSi2	oC128	C m c m		63	(Si,Al)0.1(Si)0.566667(Ti)0.333333	Al-Si-Ti Tao 1
ALSISR		hP3	P -6 m 2		187	(Si,Al)2(Sr)1	
ALTI3_D019	CdMg3	hP8	P 6_3/m m c		194	(Nb,Ti,Al)3(Al,Nb,Ti,Si)1	
ALY_B33	CrB / TlI	oC8 / oS8	C m c m	B33 / Bf	63	(Al)1(Y)1	
ALZR2_B82	Ni2In /	hP6	P 6_3/m	B82	194	(Mn,Ge,Va,Sn,Al)1(Zr,Ti,Mn,Sc,Va,Y)2	SnTi2, GeMn2, AlZr2, AlSc2

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
	C01.75Ge		m c				
B2_BCC	CsCl	cP2	P m -3 m	B2	221	(Fe,Al,Cu,Co,Zn)1(Ti,Va,Mn,Zr,Co)1	CuZr, FeTi, TiZn, ZnZr, MnZn(rt), AlCo
B32_ALLI	NaTl	cF16	F d -3 m	B32	227	(Mg,Al,Li)1(Mg,Li,Va)1	
B4C		hP45	R -3 m		166	(B12,B11C)1(Cb2,C2B,B2)1	
B82_ OMEGA		hP6	P 6_3/m m c	B82	194	(Al)1(Ti,Nb)1(Ti)1	
BCC_A2	W	cI2	I m -3 m	BCC_A2	229	(Li, Ce, Nb, Ga, Ti, K, Er, Cu, Co, Mg, Cr, V, Hf, Mo, Va, Ca, Sr, Zr, Al, Bi, Fe, Ge, Mn, Si, Ni, Zn, Ag, Na, Pb, Y, In, Cd, Sc, Be, Sn, P, La)1(H, B, Va, C)3	Metallic BCC_A2 solution
BCC_B32	NaTl	cF16	F d -3 m		227	(Li,Zn)1(Zn,Li)1	
BCT_A5	C	cF8	F d -3 m	A4	227	(Cd,B,Al,In,Cu,Ge,Ga,Ti,Bi,Zn,Sn,Pb)1	Pure Sn or its solution
BETA_ DPRIME		mS22	C 2/m		12	(Si,Al)2(Mg)5(Si)4	metastable beta double prime, related to Mg2Si, Mg5Si6, Al2Mg5Si4
BETA_ PRIME		hP14	P 6_3/m		176	(Mg)1.8(Si)1	metastable precipitate, Mg9Si5/Mg1.8Si, related to Mg2Si
BETA_ RHOMBO_B	B	hR423	R -3 m		166	(B)93(Si,C,B,Cu)12	
B_PRIME						(Al)3(Mg)9(Si)7	metastable precipitate, B_Prime, Al-containing Pre-beta phase

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
C14_FE2HF	MgZn2	hP12	P 6_3/m m c	C14	194	(Fe)0.6667(Hf,Fe)0.3333	
C14_LAVES	MgZn2	hP12	P 6_3/m m c	C14	194	(Zr, Mg, Li, Ti, Mn, Cu, Cr, Ni, Hf, Al, Zn, Fe)2(Er, Al, Mn, Fe, Ti, Mg, Hf, Cu, Sc, Zr, Cr, Zn)1	Solution of MgZn2-type phases, including MgZn2 (Eta, aka M or sigma)
C15_FE2HF	Cu2Mg	cF24	F d -3 m	C15	227	(Fe)0.6667(Hf)0.3333	
C15_LAVES	Cu2Mg	cF24	F d -3 m	C15	227	(Sc, Cr, Zr, Si, Li, Fe, Mg, Cu, Ti, Ca, Ni, Al, Hf, Zn, La)2(Fe, Cu, Ni, Er, Cr, Ce, Sc, Mg, La, Al, Si, Hf, Ca, Zr, Zn, Li, Ti)1	Solution of Cu2Mg-type phases, cF24, F d -3 m
C36_FE2HF	MgNi2	hP24	P 6_3/m m c	C36	194	(Fe)0.6667(Hf)0.3333	
C36_LAVES	MgNi2	hP24	P 6_3/m m c	C36	194	(Mn, Ni, Zr, Mg, Hf, Fe, Cu, Cr, Zn, Al)2 (Sc, Cu, Zr, Hf, Al, Fe, Ni, Zn, Cr, Mg)1	Solution of MgNi2-type phases
C40_MOSI2	MoSi2 / CuZr2	tI6	I 4/m m m	C11b	139	(Al,Si)2(Mo)1	
C54_MOSI2	Si2Ti	oF24	F d d d	C54	70	(Si,Al)2(Mo)1	
CA14SI19	Ca14Si19	hR198	R -3 c		167	(Ca)0.424242(Si)0.575758	
CA1CU1	CaCu (h)	oP40	P n m a		62	(Ca)1(Cu)1	
CA2CU	Ca2Cu	oP12	P n m a		62	(Ca)2(Cu)1	
CA2NI7	Gd2Co7	hR54	R -3 m		166	(Ca)2(Ni)7	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CA3SI4	Ca3Si4	hP42	P 6 3/m		176	(Ca)0.428571(Si)0.571429	
CA3ZN	Re3B	oC16	C m c m	E1a	63	(Ca)3(Zn)1	
CA5ZN3	Cr5B3	tI32	I 4/m c m	D8l	140	(Ca)5(Zn)3	
CACU5_D2D	CaCu5	hP6	P 6/m m m	D2d	191	(Sr,Sc,Ca)1(Ni,Cu,Zn)5	CaCu5, CaNi5, CaZn5, Cu5Sr, ScNi5, SrZn5
CAH2_HT	*	*	*	*		(Ca)1(H)2	
CAH2_LT	PbCl2	oP12	P n m a		62	(Ca)1(H)2	
CALI2	MgZn2	hP12	P 6_3/m m c	C14	194	(Li)2(Ca)1	
CANI3	PuNi3	hR36	R -3 m		166	(Ca)0.25(Ni)0.75	
CASI2	CaSi2	hR18	R -3 m		166	(Ca)0.333333(Si)0.666667	
CAZN11	BaCd11	tI48	I 4_1/a m d		141	(Ca)1(Zn)11	
CAZN13_CF112	NaZn13	cF112	F m -3 c		226	(Ca,Sr)1(Zn)13	CaZn13, SrZn13
CAZN2	KHg2	oI12	I m m a		74	(Ca)1(Zn)2	
CAZN3	Ca3.33Zn10.11	hP32	P 6_3/m m c		194	(Ca)1(Zn)3	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CAZN_OC8	CrB / Tll	oC8 / oS8	C m c m	B33 / Bf	63	(Ca)1(Zn)1	
CBCC_A12	Mn	cI58	I -4 3 m	A12	217	(Sr, Cr, Al, Mn, Zr, Sn, Li, Si, Ti, Ni, Mg, Ge, V, Fe, Cu, Co, Zn)1(Va, C, H, B)1	
CD10CU3	Al5Co2	hP28	P 6_3/m m c		194	(Cd)0.7692(Cu)0.2308	
CD3CU4	Cd121Cu160	cF1124	F -4 3 m		216	(Cd)0.4286(Cu)0.5714	
CD8CU5	Cu5Zn8	cI52	I -4 3 m	D82	217	(Cu)2(Cd,Cu)3(Cu)2(Cu,Cd)6	
CDCU2	MgZn2	hP12	P 6_3/m m c	C14	194	(Cd)1(Cu)2	
CE2FE17	Th2Ni17	hR57	R -3 m		166	(Ce)2(Fe,Al)17	
CE2NI7	Ce2Ni7	hP36	P 6_3/m m c		194	(Ce)0.222222(Ni,Al)0.777778	
CE3SI2	U3Si2	tP10	P 4/m b m		127	(Ce)3(Si)2	
CE3SI4						(Ce)1(Si)1.34	
CE3SI5	GdSi1.4	oI12	I m m a		74	(Ce)0.37(Si)0.63	
CE5SI3	Cr5B3	tI32	I 4/m c m		140	(Si)3(Ce)5	
CE5SI4	Zr5Si4	tP36	P 4_1 2_1		92	(Ce)5(Si)4	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
			2				
CE7NI3	Th7Fe3	hP20	P 6_3 m c		186	(Ce)0.7(Ni)0.3	
CENI2	MgCu2	cF24	F d -3 m		227	(Ni,Ce)0.333333(Ni,Ce)0.666667	
CENI3	CeNi3	hP24	P 6_3/m m c		194	(Ce)0.25(Ni,Al)0.75	
CENI5	CaCu5	hP6	P 6/m m m		191	(Er,Ce,Ni)0.166667(Cu,Ce,Ni,Al)0.833333	
CENI_OC8	TlI	oS8	C m c m		63	(Ce)0.5(Ni)0.5	
CESI2	ThSi2	tI12	I 4_1/a m d		141	(Ce)1(Al,Si)2	
CESI_OP8	FeB-b	oP8	P n m a		62	(Ce)1(Si)1	
CO2SI_C23	Co2Si-b	oP12	P n m a		62	(Ca,Ni,Cu,Fe,Sr)2(Zn,Sn,Ge,Si,Al)1	Ca2Si, Ni2Si, SiSr2, SnSr2, GeSr2
CR11GE19	Mn11Si19	tP120	P -4 n 2		118	(Cr)0.367(Ge)0.633	
CR2B_ORTH	CuMg2	oF48	F d d d		70	(Cr)0.666667(B)0.333333	
CR3C2	Cr3C2-b	oP20	P n m a		62	(Cr)3(C)2	
CR3GE	Cr3Si	cP8	P m -3 n	A15	223	(Ge,Cr)0.75(Ge,Cr)0.25	
CR3MN5						(Cr)3(Mn)5	Cr2Mn3 ht

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CR3SI_A15	Cr3Si	cP8	P m -3 n	A15	223	(Si,Cr)3(Si,Cr,Al)1	
CR5B3_D81	Cr5B3	tI32	I 4/m c m	D8l	140	(Ca,Sr,Cr)0.625(B,Sn,Ge,Ag,Si)0.375	Ca5Si3, Sn3Sr5, Si4Sr5, Ge3Sr5, B3Cr5
CR5GE3_HT	W5Si3	hP16	I 4/m c m	D8m	140	(Ge,Cr)0.625(Ge,Cr)0.375	
CR5GE3_LT						(Ge,Cr)0.625(Cr,Ge)0.375	
CRB4	B4Cr	oI10	I m m m		71	(Cr)0.2(B)0.8	
CRB_B33	CrB / TlI	oC8 / oS8	C m c m	B33 / Bf	63	(V,Ca,Al,Sr,Cr,Ni)1 (Sc,B,Ag,Ge,Si,Sn,Zr,Hf)1	AgCa, AlHf, AlZr, BNi, BV, GeSr, NiZr, SiSr, SnSr
CRSI2_C40	CrSi2	hP9	P 6_2 2 2	C40	180	(V,Si,Cr)1(Cr,Al,Si)2	
CRZN13						(Cr)1(Zn)13	
CRZN17		hP*	*			(Cr)1(Zn)17	
CU10HF7	Zr7Ni10	oS68	C m c a		64	(Cu)10(Hf)7	
CU10SN3	Cu10Sn3	hP26	P 6_3		173	(Sn,Cu)1	
CU10ZR7	Zr7Ni10	oS68	C m c a		64	(Cu)10(Zr)7	
CU11IN9	AlCu	mS20	C 2/m		12	(Cu)0.55(In)0.45	
CU15SI4_EPSILON	Cu15Si4	cI76	I -4 3 d		220	(Mn,Cu,Mg,Zn)0.789474(Si,Al)0.210526	
CU16MG6SI	*Cu2Mg	cP24	P 4_1 3 2		213	(Cu)16(Mg)6(Si)7	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
7			P 4_3 3 2		212		
CU1HF2	CuZr2	tI6	I 4/m m m		139	(Cu)1(Hf)2	
CU1LA1	FeB-b	oP8	P n m a		62	(Cu)1(La)1	
CU2CE	KHg2	oI12	I m m a		74	(Cu)2(Ce)1	
CU2ER	KHg2	oI12	I m m a		74	(Al,Cu)2(Er)1	
CU2IN_HT	Co1.75Ge	hP6	P 6_3/m m c		194	(Cu)0.545(In,Cu)0.122(In)0.333	
CU2IN_LT	*	*	*			(Cu)0.64(In)0.36	
CU2LA1	AlB2	hP3	P 6/m m m	C32	191	(Cu)2(La)1	
CU2SC_C11B	MoSi2 / CuZr2	tI6	I 4/m m m	C11b	139	(Ag,Cu)2(Sc)1	
CU2TI		oS12	C m c m		63	(Cu)2(Ti)1	
CU33SI7_DELTA	*	tP*	*			(Cu,Zn)0.825(Si)0.175	
CU37LA3	NaZn13	cF112	F m -3 c		226	(Cu)37(La)3	
CU3MG2SI	MgNi2	hP24	P 6_3/m m c		194	(Cu)2.74(Mg)2(Si)1.26	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CU3SN	Cu3Sn	oS80	C m c m		63	(Sn,Cu)3(Sn,Cu)1	
CU3TI2	Cu3Ti2	tP10	P 4/n m m		129	(Cu)3(Ti)2	
CU41SN11	Cu41Sn11	cF416	F -4 3 m		216	(Cu,Sn)41(Cu,Sn)11	
CU46NI25SI29						(Cu)0.458(Ni)0.25(Si)0.292	
CU4CE	*	oP20	*			(Cu,Al)4(Ce)1	
CU4LA1	Cu4La	tI90	I -4 m 2		119	(Cu)4(La)1	
CU4SC		t**				(Cu)4(Sc)1	
CU4TI1		oP20	P n m a		62	(Ti,Cu)4(Ti,Cu)1	
CU4TI3		tI14	I 4/m m m		139	(Cu)4(Ti)3	
CU51HF14		hP65	P 6/m		175	(Cu)51(Hf)14	
CU51ZR14		hP65	P 6/m		175	(Cu)51(Zr)14	
CU56SI11_GAMMA	Mg3Ru2	cP20	P 4_1 3 2		213	(Zn,Cu,Si,Mn,Mg,Ni)0.835821 (Si)0.164179	
CU5CE		hP6	P 6/m m m		191	(Al,Cu)5(Ce)1	
CU5ER_	Be5Au	cF24	F -4 3 m		216	(Cu)5(Er)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
C15B							
CU5HF	*	*	*	*		(Cu)5(Hf)1	
CU5LA1	CaCu5	hP6	P 6/m m m		191	(Cu)5(La)1	
CU5MN4SI						(Cu)0.5(Mn)0.37(Si)0.13	
CU6CE	Cu6Ce	oP28	P n m a		62	(Cu)6(Ce)1	
CU6LA1_HT	Cu6Ce	oP28	P n m a		62	(Cu)6(La)1	
CU6LA1_LT	Cu6La	mP28	P 2_1/c		14	(Cu)6(La)1	
CU6NISI3						(Cu,Ni)0.732(Si)0.268	
CU6SN5_HT	Co1.75Ge	hP6	P 6_3/m m c		194	(Cu)1(Sn,Cu)1(Sn)1	
CU6SN5_LT	Cu6Sn5	mS44	C 2/c		15	(Cu)1(Sn,Cu)1(Sn)1	
CU7ER2						(Cu)7(Er)2	
CU8HF3	Cu8Hf3	oP44	P n m a		62	(Cu)8(Hf)3	
CU8ZR3	Cu8Hf3	oP44	P n m a		62	(Cu)8(Zr)3	
CU9ER2						(Cu)9(Er)2	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CU9GA4_0	Cu9Al4	cP52	P -4 3 m	D83	215	(Cu)6(Cu,Ga)6(Ga)1	
CU9GA4_1	Cu9Al4	cP52	P -4 3 m	D83	215	(Cu)6(Cu,Ga)3(Ga,Cu)3(Ga)1	
CU9GA4_2	Cu8.2Ga4.8	cP52	*			(Cu)3(Va,Cu)3(Ga,Cu)3(Ga)4	
CU9GA4_3	Cu7.15Ga5.85	cP52	*			(Cu,Va)6(Ga,Cu)3(Ga)4	
CUB_A13	Mn	cP20	P 4_1 3 2	A13	213	(Mg,Si,Hf,Ce,Ag,Ti,Mn,Sr,Fe,Al,Sn,Cr,Cu,V,Zn,Li,Ni,Ge,Zr)1(H,B,C,Va)1	
CUCE	FeB-b	oP8	P n m a		62	(Cu)1(Ce)1	
CUER_B2	CsCl	cI2	I m 3 m	B2	229	(Cu,Al)1(Er)1	
CUGA2	Fe0.92Si2	tP3	P 4/m m m		123	(Cu)1(Ga)2	
CUGA_THETA	*	*	*	distorted D019		(Cu)0.778(Ga)0.222	
CUIN_GAMMA	Al4Cu9	cP52	P -4 3 m	D83	215	(Cu)2(In,Cu)2(Cu)3(Cu,In)6	
CUIN_THETE	Cu7In3	cP40	P -1		2	(Cu)0.7(In)0.3	
CULIMG_T	Mg2Ni	hP18	P 6_2 2 2		180	(Cu)1(Li)0.08(Mg)1.92	
CUMG2	CuMg2	oF48	F d d d		70	(Cu,Ni)1(Mg)2	
CUMNZN						(Cu)0.334(Mn)0.333(Zn)0.333	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
CUSC	CsCl	cP2	P m -3 m	B2	221	(Cu)1(Sc)1	
CUSI_ETA	*	tP*	*			(Zn,Cu,Ni,Mn)0.76(Si)0.24	
CUSN_GAMMA	BiF3	cF16	F m -3 m	L21	225	(Cu,Sn)1	
CUSR	BaCu	hP8	P 6_3/m m c		194	(Sr)1(Cu)1	
CUTI3	CuTi3	tP4	P 4/m m m		123	(Ti,Cu)1(Ti)3	
CUTI_B11	CuTi	tP4	P 4/n m m		129	(Ti,Cu)1(Cu,Ti)1	
CUZR2_C11B	MoSi2 / CuZr2	tI6	I 4/m m m	C11b	139	(Cr,Cu,Zn,Si,Al)1(Zr,Ti,Cr,Al)2	AlCr2, CuTi2, CuZr2, Ti2Zn, ZnZr2
DHCP	Nd	hP4	P 6_3/m m c	A3'	194	(Cu,Ni,La,Ce,Sc)1	
DIAMOND_A4	C	cF8	F d -3 m	A4	227	(Ga,Sr,B,C,Sn,Zn,Si,Ge,Ti,P,Al)1	Pure C, Ge, Si or solution phases based on them
EPSILON	Mg	hP2	P 6_3/m m c		194	(Cu,Mn,Zn)1	
ER5SI3	Mn5Si3	hP16	P 6_3/m c m		193	(Er)0.625(Si)0.375	
ER5SI4	Gd5Si4	oP36	P n m a		62	(Er)0.555556(Si)0.444444	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
ERSI2	AlB2 ErSi1.67	hP3 oP6	P 6/m m m P m m m		19147	(Er)0.37(Si)0.63	
ERSI_OC8	TlI	oS8	C m c m		63	(Er)0.51(Si)0.49	
ERSI_OP8	FeB-b	oP8	P n m a		62	(Er)0.5(Si)0.5	
ETA_PRIME						(Al)0.21(Mg)0.28(Zn,Cu)0.51	metastable precipitate, related to MgZn2-based Eta phase
FCC_A1	Cu	cF4	F m -3 m	A1	225	(La, Er, Sn, Ga, Mn, Al, Cu, Ti, Cd, V, Si, Ag, Zn, P, Mo, Fe, Be, Pb, Sr, Ca, Nb, Li, Bi, K, Ce, Ni, Hf, Sc, Mg, Ge, Zr, Co, Na, Cr, In)1(H, B, Va, C)1	Metallic FCC_A1 solution, e.g. (Al), (Cu), and MC carbides
FE17ER2	Th2Ni17	hP38	P 6_3/m m c		194	(Al,Fe)17(Er)2	
FE1HF2						(Fe)0.3333(Hf)0.6667	
FE23ER6	Th6Mn23	cF116	F m -3 m		225	(Fe,Al)23(Er)6	
FE2GE1	C01.75Ge	hP6	P 6_3/m m c		194	(Fe)1(Va,Fe)1(Ge)1	
FE2GE3	Ru2Sn3	tP20	P -4 c 2		116	(Fe)2(Ge)3	
FE2SC_C15	Cu2Mg	cF24	F d -3 m	C15	227	(Fe)0.64(Sc)0.36	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
FE2SI	AlNi2	hP6	P -3 m 1		164	(Fe,Ni)2(Si,Al)1	
FE3ER	PuNi3	hR36	R -3 m		166	(Fe)3(Er)1	
FE3SN2	Fe3Sn2	hR30	R -3 m		166	(Fe)3(Sn)2	
FE5NI3SI2						(Ni,Fe)4(Si)1	
FE5SN3_D82	Co1.75Ge	hP6	P 6_3/m m c		194	(Fe)5(Sn)3	
FE6GE5	Fe6Ge5	mS44	C 2/m		12	(Fe)6(Ge)5	
FE6SC29						(Fe)0.17(Sc)0.83	
FEB_B27	FeB	oP8	P n m a	B27	62	(Fe,Ti,Sr,Zr,Mn)1(Zn,Ge,B,Si)1	BFe, BMn, BTi, GeZr, SiTi, SrZn, SiZr
FEGE_ETA	Fe6.5Ge4	hP22	P 6_3/m m c		194	(Fe)13(Ge)9	
FEM_B35	CoSn	hP6	P 6/m m m	B35	191	(Fe)1(Ge,Sn)1	FeSn, FeGe
FESI2_H	Fe0.92Si2	tP36	P 4/m m m		123	(Fe,Ni)3(Al,Si,Mg)7	
FESI2_L	FeSi2	oS48	C m c a		64	(Fe,Ni)1(Si,Al)2	
FESI_B20	FeSi	cP16	P 2_1 3	B20	198	(Ni,Mn,Cr,Fe)1(Al,Mg,Si,Ge)1	FeSi, MnSi, CrSi, CrGe
FEZN_DELTA	FeZn10	hP63	P 6_3/m		194	(Fe)0.058(Zn, Al, Mn, Cu, Ni, Fe, Si)0.18	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
		2	m c			(Zn)0.525 (Zn) 0.237	
FEZN_GAMMA1						(Fe)0.137(Ni,Si,Fe,Cu,Zn,Al)0.118 (Mn,Zn)0.745	
FEZN_ZETA	Zn13Co	mS28	C 2/m		12	(Va,Mn,Fe,Ni)0.072(Zn,Al)0.856 (Si,Zn,Va,Al,Cu)0.072	
FEZR3	Re3B	oC16 / oS16	C m c m	E1a	63	(Fe)1(Zr)3	
GAMMA_D810	Cr4.5 (Cr0.56Al0.44)9 Al12	hR26 / hR78	R 3 m	D810	160	(Si,Al)12(Cr)5(Al,Cr,Si)9	
GAMMA_D82	Cu5Zn8	cI52	I -4 3 m	D82	217	(Zn,Fe,Mn)2(Ni,Mn,Zn,Fe)2 (Cu,Mn,Si,Ni,Zn,Al,Fe)3(Al,Zn)6	
GAMMA_D83	*	cP52	*	D83		(Al,Ni,Si,Zn,Fe)4(Zn,Si,Ni,Al,Cu)1 (Ni,Zn,Ag,Cu,Mn,Fe)8	solution between Al8Cu5 (rt) and Cu5Zn8
GAMMA_H	Cu5Zn8	*	*	D82		(Zn,Al)4(Zn,Al,Cu)1(Ni,Cu,Fe,Mn)8	Cu5Zn8-type Al8Cu5 (ht) phase
GAS						(C2, Cr2, Ge2, Sn, Si4, Cu2, P, Cu, C, Fe2, Cu1H1, C5, B2, Si3, Mg2, Ti, P2, C3, K2, Ca1H1, Al1H1, B, Sn2, Co2, Li, Cr, Al2, Al1C1, Ti2, H, P4, C4, Mn, H1Na1, Al1H3, Ni2, Na2, Na, K1Li1, Ge, Co, Ca, V, Si2, Li2, Ca2, Sr, Ni, Mg, H1Li1, K, Sr2, Si, Sc, Fe, H2, C60, Al1H2, Al, Zn)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
GE12NI19		mC62	C 2		5	(Ge,Ni)0.613(Ge,Ni)0.387	
GE2MN3	Cr11Ge8	oP76	P n m a		62	(Ge)2(Mn)3	
GE2MN5	Ge2Mn5	hP42	P 3 c 1		158	(Mn,Ge)2(Mn)5	
GE2NI3	AsNi	hP4	P 6_3/m m c		194	(Ni,Ge)0.6(Ge)0.4	
GE2NI5	Pd5Sb2	hP84	P 6_3/m m c		194	(Ni)0.72(Ge)0.28	
GE2SR	Co2Si-b	oP12	P n m a	C23	62	(Ge)2(Sr)1	
GE3MN7	Mg5Ga2	oI28	I b a m		72	(Ge)3(Mn)7	Mn5Ge2
GE3NI5_HT	Co1.75Ge	hP6	P 6_3/m m c		194	(Ge,Ni)0.625(Ni,Ge)0.375	
GE3NI5_LT	Ni5Ge3	mS32	C 2		5	(Ni)0.63(Ge)0.37	
GE3TI5	Mn5Si3	hP16	P 6_3/m c m	D88	193	(Ti)5(Ge)3	
GEMN3_HT	Al3Ti	tI8	I 4/m m m	D022	139	(Ge,Mn)1(Mn)3	
GENI2	Co2Si-b	oP12	P n m a	C23	62	(Ni)0.665(Ge)0.335	
GENI3_GAMMA	NaTl	cF16	F d -3 m		227	(Ni)0.744(Ge)0.256	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
GRAPHITE	C (graphite)	hP4	P 6_3/m m c	A9	194	(B,C)1	
HCP_A3	Mg	hP2	P 6_3/m m c	A3	194	(Mn, V, Li, Ga, Bi, Si, Co, Zn, Cd, Ca, Cr, Ti, Na, Mg, Be, Ce, Zr, Y, Pb, La, Nb, Hf, Ge, Sc, Mo, Er, Ni, Sr, Sn, Al, Ag, K, Fe, Cu, In)1(Va, B, C, H)0.5	Metallic HCP_A3 solution, alpha_ Mg/Hf/Sc/Ti/Zr, epsilon_CuZn, etc.
HCP_CA	Mg	cP2	P 6_3/m m c	A3	194	(Ca)1(Va,H)0.5	
HF2SI	CuAl2	tI12	I 4/m c m		140	(Hf)0.6666667(Si)0.3333333	
HF3SI2	U3Si2	tP10	P 4/m b m		127	(Hf)0.6(Si)0.4	
HF5SI3	Mn5Si3	hP16	P 6_3/m c m		193	(Hf)0.625(Si)0.375	
HF5SI4	Zr5Si4	tP36	P 4_1 2_1 2		92	(Hf)0.555556(Si)0.444444	
HFMN	NiTi2	cF96	F d -3 m		227	(Hf)0.5(Mn)0.5	
HFSI2	ZrSi2	oS12	C m c m		63	(Hf)0.333333(Si)0.666667	
HFSI_OP8	FeB-b	oP8	P n m a		62	(Hf)0.5(Si)0.5	
HIGH_ SIGMA						(Mn)8(Cr)4(Mn,Cr)18	
KNA2	MgZn2	hP12	P 6_3/m m c	C14	194	(K)1(Na)2	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
KZN13	NaZn13	cF112	F m -3 c		226	(K)1(Zn)13	
L10_TETRA	CuAu	tP2	P 4/m m m	L10	123	(Ni,Ti,Cu,Al,Nb,Mn)0.5 (Nb,Mn,Cu,Ni,Ti,Al)0.5	
L12_FCC	AuCu3	cP4	P m -3 m	L12	221	(Ni,Al,Ti,Ge,V)1(Al,Ni,Zn,Fe,Zr)3	L12 phase, Ni3Si_rt, AlZr3, GeNi3, TiZn3, VZn3
LA2NI3	La2Ni3	oS20	C m c a		64	(La)2(Ni)3	
LA2NI7_HT	Gd2Co7	hR54	R -3 m		166	(La)2(Ni)7	
LA2NI7_LT	Ce2Ni7	hP36	P 6_3/m m c		194	(La)2(Ni)7	
LA2ZN17	Th2Ni17	hP38	P 6_3/m m c		194	(La)0.105(Zn)0.895	
LA3NI	Fe3C	oP16	P n m a		62	(La)3(Ni)1	
LA3SI2	U3Si2	tP10	P 4/m b m		127	(La)0.6(Si)0.4	
LA3ZN22	Zn22Ce3	tI100	I 4_1/a m d		141	(La)0.12(Zn)0.88	
LA5SI3	Cr5B3	tI32	I 4/m c m	D8l	140	(La)0.625(Si)0.375	
LA5SI4	Zr5Si4	tP36	P 4_1 2_1 2		92	(La)0.5556(Si)0.4444	
LA7NI16	La7Ni16	tI46	I -4 2 m		121	(La)7(Ni)16	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
LA7NI3	Th7Fe3	hP20	P 6_3 m c		186	(La)7(Ni)3	
LAH3	CeH3	cF44	F m -3 m		225	(La)0.25(Va,H)0.5(H,Va)0.25	
LANI3	PuNi3	hR36	R -3 m		166	(La)1(Ni)3	
LANI5	CaCu5	hP6	P 6/m m m		191	(La)1(Ni)5	
LANI_OC8	CrB / TlI	oC8 / oS8	C m c m	B33 / Bf	63	(La)1(Ni)1	
LASI2_A1	GdSi1.4	oI12	I m m a		74	(La)0.36(Si)0.64	
LASI2_A2	ThSi2	tI12	I 4_1/a m d		141	(La)0.3333(Si)0.6667	
LASI_OP8	FeB-b	oP8	P n m a		62	(La)0.5(Si)0.5	
LAZN11	BaCd11	tI48	I 4_1/a m d		141	(La)0.083(Zn)0.917	
LAZN13	NaZn13	cF112	F m -3 c		226	(La)0.071(Zn)0.929	
LAZN2	KHg2	oI12	I m m a		74	(La)0.333(Zn)0.667	
LAZN4	Zn4La	oS20	C m c m		63	(La)0.2(Zn)0.8	
LAZN5	CaCu5	hP6	P 6/m m m		191	(La)0.1667(Zn)0.8333	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
LI12SI7	Li12Si7	oP152	P n m a		62	(Li)12(Si)7	
LI13SI4	Li13Si4	oP34	P b a m		55	(Li)13(Si)4	
LI22SI5	Li21Si5	cF416	F -4 3 m		216	(Li)22(Si)5	
LI2ZN3_H	Li5Ga4	hP94	P -3 m 1		164	(Zn,Li)2(Zn,Li)3	
LI2ZN3_L	Li (Li0.91Zn0.09)2 Zn4	hR21	R -3 m		66	(Li)2(Zn,Li)3	
LI2ZN5_H						(Zn,Li)2(Zn)5	
LI2ZN5_L						(Zn,Li)2(Zn)5	
LI7SI3		hP60	P 3_2 2 1		154	(Li)7(Si)3	
LIQUID						(Zn, Sn, B, Mg2Ge, Cu, Ca, Nb, K, Co, Cd, Mg2Sn1, Lih, Ga, Ce, Ag, Pb, Cr, Mg, Ge, Be, Al, Sr, Bi, Na, Sc, V, P, Si, Mo, Mn, In, Ti, Li, Fe, Zn2Zr, Er, Ni, Y, La, C, Hf, H, Zr)1	
LIZN2						(Li)1(Zn)2	
LIZN4_H	Mg	hP2	P 6_3/m m c		194	(Li,Zn)0.2(Zn,Li)0.8	
LIZN4_L						(Li,Zn)1(Li,Zn)4	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
M11GE8_OP76	Ge18Mn11	oP76	P n m a		62	(V,Cr)0.579(Ge)0.421	Cr11Ge8, V11Ge8
M23C6_D84	Cr23C6	cF116	F m -3 m	D84	225	(Mn,Cr)23(Sc,C)6	Cr23C6, Mn23C6, Mn23SC6
M3B4_D7B	Ta3B4	oI14	I m m m	D7b	71	(B)4(V,Cr,Ti,Mn)3	V3B4, Ti3B4, Mn3B4, Cr3B4
M5C2	Mn5C2	mS28	C 2/c		15	(Mn)5(C)2	
M7C3_D101	Cr7C3	oP40	P n m a	D101	62	(Mn,Cr)7(C)3	Cr7C3, Mn7C3
MG10NI55SI35	Mg3Ni11Si6					(Mg)2(Ni)11(Si)7	
MG12CE	ThMn12	tI26	I 4/m m m		139	(Mg,Al)12(Ce)1	
MG17CE2	Ce1.71Mg17.58	hP44	P 6_3/m m c		194	(Mg)17(Ce)2	
MG17SR2	Th2Ni17	hR57	R -3 m		166	(Mg)17(Sr)2	
MG23SR6	Mn23Th6	cF116	F m -3 m		225	(Mg)23(Sr)6	
MG24R5	Mg24Y5 / Al12Mg17	cI58	I -4 3 m		217	(Mg,Er)5(Mg,Al)24	
MG2C3	Mg2C3	oP10	P n n m		58	(Mg)2(C)3	
MG2NI16SI1	MgNi8Si5.5	hP*				(Mg)1(Ni)8(Si)5.5	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
1							
MG2NI3SI						(Mg)2(Ni)3(Si)1	
MG2NI_HP18	Mg2Ni	hP18	P 6_2 2 2	Ca	180	(Mg,Zn)2(Zn,Ni,Cu)1	
MG2SI_C1	CaF2	cF12	F m -3 m	C1	225	(Mg)2(Si,Ge,Sn)1	solution phase of Mg2Si, GeMg2, Mg2Sn
MG2SR	MgZn2	hP12	P 6_3/m m c	C14	194	(Mg)2(Sr)1	
MG2ZN3	Mg4Zn7	mS110	C 2/m		12	(Mg)2(Cu,Al,Zn)3	
MG38SR9	Sr9Mg38	hP94	P 6_3/m m c		194	(Mg)38(Sr)9	
MG3CE	BiF3	cF16	F m -3 m	D03	225	(Mg)3(Mg,Ce)1	
MG41CE5	Mg41Ce5	tI92	I 4/m		87	(Mg)41(Ce)5	
MG5NI9SI						(Mg)1(Ni)1.8(Si)0.2	
MG6MN3NI						(Mg)0.5(Mn)0.1666667(Ni)0.33333333	
MG7ZN3	Mg51Zn20	oI158	I m m m		71	(Mg)51(Zn)20	
MG9NI29SI16	Mg6Ni16Si7	cF116	F m -3 m		225	(Mg)9(Ni)29(Si)16	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
MGB4	MgB4	oP20	P n m a		62	(Mg)1(B)4	
MGB7	MgB7	oI64	I m m a		74	(Mg)1(B)7	
MGC2	MgC2	tP6	P 4_2/m n m		136	(Mg)1(C)2	
MGCE						(Mg,Al)1(Ce)1	
MGH2	TiO2	tP6	P 4_2/m n m		136	(Mg)1(H)2	
MGNI6SI6						(Mg)1(Ni)6(Si)6	
MGNI6ZN6						(Zn,Mg)3(Mg,Zn,Ni)4(Ni)1(Zn)2	
MGZN	Re25Zr21	hR276	R -3 c		167	(Mg)12(Cu,Al,Zn)13	
MN11SI19	Mn11Si9	tP20	P -4 n 2		118	(Mn)11(Al,Si)19	
MN15NI45SI40	Mn3Ni9Si8					(Mn)0.15(Ni)0.45(Si)0.4	Mn-Ni-Si ternary phase, T1 or N
MN15NI50SI35	Mn3Ni10Si7					(Mn)0.15(Ni)0.5(Si)0.35	Mn-Ni-Si ternary phase, T2 or PHI
MN1NI1SI1	TiNiSi	oP12	P n m a		62	(Mn)1(Ni)1(Si)1	Mn-Ni-Si ternary phase, T4 or E
MN2B_D1F	CuMg2	oF48	F d d d	D1F	70	(Mn)0.6707(B)0.3293	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
MN2NISI						(Ni,Mn)3(Si)1	Mn-Ni-Si ternary phase, T8 or S
MN2SN	Co1.75Ge	hP6	P 6_3/m m c		194	(Mn)0.643(Sn)0.357	Mn(2-x)Sn
MN3NI2SI	Mn3Ni2Si	cF96	F d -3 m		227	(Mn)3(Ni)2(Si)1	Mn-Ni-Si ternary phase, T7 or Omega
MN3SI	AlFe3 or BiF3	cF16	F m -3 m	D03 or L21	225	(Mn,Ni,Fe)3(Si,Al)1	
MN3SN2	Ni3Sn	oP20	P n m a		62	(Mn)3(Sn)2	
MN3TI						(Mn)3(Ti)1	
MN4TI	Cr0.16Mo0.38Co0.46	hR159	R -3		148	(Mn)0.815(Ti)0.185	
MN52NI29SI19						(Mn)0.52(Ni)0.29(Si)0.19	Mn-Ni-Si ternary phase, T11 or W
MN5SI3_D88	Mn5Si3	hP16	P 6_3/m c m	D88	193	(Cu,Fe,Zr,Cr,Ni,Mn,Ti)5(Ge,Sn,Si,Cr,Al)3	Mn5Si3, Cr3Si5, Fe5Si3, Ge3Mn5, Ge3Zr5, Si3Zr5, Sn3Ti5
MN66NI4SI30						(Mn)0.66(Ni)0.04(Si)0.3	Mn-Ni-Si ternary phase, T10 or U
MN6NI16SI7	Mg6Cu16Si7	cF116	F m -3 m		225	(Mn)0.206897(Ni)0.551724(Si)0.241379	Mn-Ni-Si ternary phase, T3 or G
MN6NISI3	*(Cr0.16Mo0.38Co0.46)	*hR159	*R -3		148	(Mn)0.61(Ni)0.12(Si)0.27	Mn-Ni-Si ternary phase, T9 or R

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
MN6SI	(Cr0.16Mo0.38Co0.46)	hR159	R -3		148	(Al,Mn)17(Si,Zn)3	
MN7NI7ZN86		cF**	F -4 3 m		216	(Mn)0.07(Ni)0.07(Zn)0.86	
MN9SI2	Mn19(Mn0.62Si0.38)10Si2	oI186	I m m m		71	(Mn)33(Si)7	
MNB4	MnB4	mS10	C 2/m		12	(Mn)0.2(B)0.8	
MNNI2	CuAu	tP20	P 4/m m m	L10	123	(Ni,Mn)1(Ni)2	
MNNISI_T5	MgZn2	hP12	P 6_3/m m c		194	(Mn)1(Ni,Si)2	Mn-Ni-Si ternary phase, T5 or "tao 1"
MNNISI_T6	MgCu2	cF24	F d -3 m		227	(Mn)1(Ni,Si)2	Mn-Ni-Si ternary phase, T6 or "tao 2"
MNSC4						(Mn)0.2(Sc)0.8	
MNTI_HT		t**				(Mn)0.515(Ti)0.485	
MNTI_LT	Zr21Re25	hR276	R -3 c		167	(Mn)1(Ti)1	
MNV_SIGMA	CrFe	tP30	P 4_2/m n m	D8b	136	(V,Mn)10(V)4(V,Mn)16	
MNZN9						(Mn)0.1(Zn)0.9	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG number	Sublattice	Notes
MO5SI3		tI32	I 4/m c m		140	(Mo)0.5(Mo,Si)0.125(Si,Mo,Al)0.375	
MOSI2		tI6	I 4/m m m		139	(Si,Al)2(Mo)1	
NASI_HT						(Na)1(Si)1	
NASI_LT	NaSi	mS32	C 2/c		15	(Na)1(Si)1	
NAZN13	NaZn13	cF112	F m -3 c		226	(Na)1(Zn)13	
NI10HF7	Zr7Ni10	oS68	C m c a		64	(Ni)0.588(Hf)0.412	
NI10ZR7	Ni10Zr7	oS68	C m c a		64	(Ni)23(Zr)17	
NI11HF9	Zr9Pt11	tI40	I 4/m		87	(Ni)0.55(Hf)0.45	
NI11ZR9	Ni11Zr9	tI40	I 4/m		87	(Ni)11(Zr)9	
NI21HF8	Hf8Ni21	aP29	P -1		2	(Ni)0.724(Hf)0.276	
NI21ZR8	Hf8Ni21	aP29	P -1		2	(Zr)8(Ni)21	
NI2SIZN3_T3	Mn3Ni2Si	cF96	F d -3 m		227	(Ni)2(Si)1(Zn)3	
NI2SIZN_T1	Cu2MnAl	cF16	F m -3 m		225	(Ni)0.5(Si)0.25(Zn)0.25	
NI2SI_HT	Co1.75Ge	hP6	P 6_3/m m c		194	(Cu,Ni)1(Ni,Va)1(Si,Al)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
NI2V1	Al3Ti	tI8	I 4/m m m	D022	139	(Ni)2(V)1	
NI2V7	Cr3Si	cP8	P m -3 n		223	(Ni)2(V)7	
NI3HF_HT	BaPb3	hR36	R -3 m		166	(Ni)0.75(Hf)0.25	
NI3HF_LT	Ta (Rh0.33Pd0.67) 3	hP40	P 6_3/m m c		194	(Ni)0.75(Hf)0.25	
NI3SI2	Ni3Si2	oS80	C m c 2_1		36	(Ni,Fe)3(Si)2	
NI3SI_HT	Fe3C	oP16	P n m a		62	(Ni,Fe)3(Al,Si)1	
NI3SI_MT	Pd25Ge9	hP34	P -3		147	(Si)1(Ni)3	
NI3SN2_HT	Co1.75Ge	hP6	P 6_3/m m c		194	(Ni)0.33333(Sn,Ni)0.33334(Sn)0.33333	
NI3SN2_LT	Ni3Sn2	oP20	P n m a		62	(Sn)0.2(Sn,Ni)0.4(Ni)0.4	
NI3SN4	Ni3Sn4	mS14	C 2/m		12	(Ni)0.25(Ni,Sn)0.25(Sn)0.5	
NI3SN_D019	Ni3Sn / Mg3Cd	hP8	P 6_3/m m c	D019	194	(Ge,Sn,Va,Al)1(Ni,Fe,La,Ti,Mn)3	Ni3Sn, SnTi3, SnMn3, AlLa3
NI3SN_HT	BiF3	cF16	F m -3 m	L21	225	(Sn,Ni)0.25(Ni,Sn)0.25(Ni)0.5	
NI3TI_D024	Ni3Ti	hP16	P 6_3/m m c	D024	194	(Ni,Ti)0.75(Ni,Ti)0.25	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
NI4B3_MONO		mS28	C 2/c		15	(Ni)0.564(B)0.436	
NI4B3_ORTH		oP28	P n m a		62	(Ni)0.586(B)0.414	
NI5HF	Be5Au	cF24	F -4 3 m		216	(Ni)0.833(Hf)0.167	
NI5SI2	Ni31Si12	hP43	P 3 2 1		150	(Ni,Cu,Fe)5(Al,Si)2	
NI7HF2	Zr2Ni7	mS36	C 2/m		12	(Ni)0.778(Ni,Hf)0.222	
NI7HF3	Hf3Ni7	aP20	P -1		2	(Ni)0.7(Hf)0.3	
NI7SC2	Ce2Ni7	hP36	P 6_3/m m c		194	(Sc)0.222222(Ni)0.777778	
NI7ZR2	Ni7Zr2	mS36	C 2/m		12	(Ni)7(Zr)2	
NI9SI2ZN_T2	TiAl3	tI8	I 4/m m m		139	(Ni)0.75(Si)0.1675(Zn)0.0825	
NIHF2	CuAl2	tI12	I 4/m c m		140	(Va,Ni)1(Hf)2	
NIHF_HT	CsCl	cP2	P m -3 m		221	(Ni)0.5(Hf)0.5	
NIHF_LT	TlI	oS8	C m c m		63	(Ni)0.5(Hf)0.5	
NISC2	NiTi2	cF96	F d -3 m		227	(Sc)0.72(Ni)0.28	
NISC_B2	CsCl	cP2	P m -3 m	B2	221	(Sc)1(Ni)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
NISI2	CaF2	cF12	F m -3 m	C1	225	(Cu,Zn,Al,Si)2(Ni,Fe,Cu,Mn)1	
NISIZN_T4	FeSi	cP8	P 2_1 3		198	(Ni)3(Si)2(Zn)1	Ni-Si-Zn tao 4, Ni3Si2Zn1
NISI_B31	MnP / FeAs	oP8	P n m a	B31	62	(Fe,Ni)1(Zn,Si,Ge)1	GeNi, NiSi
NISR	*	hP*	*			(Ni)0.5(Sr)0.5	
NITI2	NiTi2	cF96	F d -3 m		227	(Ti,Ni)1(Ni,Ti)2	
NIZN8	Zn22Ni3	mS50	C 2/m		12	(Ni)0.1111111(Zn,Al,Mn)0.8888889	
NIZN_LT	CuTi	tP2	P 4/m m m		123	(Fe,Si,Mn,Al,Ni,Zn)0.5 (Mg,Ni,Si,Zn,Mn,Fe,Al)0.5	
O1_DIS		*oS28	*C m c m		63	(Ti,Nb,Al)0.75(Al,Ti,Nb)0.25	The disordered O phase
ORD_L12	Al3Cu	tP8	P 4/m m m	L12	123	(Mn, Cu, Co, Sn, Si, Li, Sc, Be, Fe, Ni, Ga, Bi, K, Mo, Na, Ge, Er, Ce, Zn, In, Ca, Sr, Hf, Zr, Cr, Pb, Ti, Cd, Mg, Al, Ag, V, La)0.75(Sc, Er, Bi, Ti, Co, Sr, La, In, Zn, Sn, Cu, Ag, Zr, V, K, Pb, Cd, Li, Fe, Ce, Mn, Mo, Mg, Na, Ni, Ga, Be, Al, Ge, Cr, Si, Ca, Hf)0.25(Va)1	Ordered L12, having Gibbs energy contribution from DISO_A1
ORTHORHOMBIC_GA	Ga	oC8	C m c a	A11	64	(Ga)1	
O_PHASE	AlNbTi2	oS28	C m c m		63	(Nb,Ti)0.5(Al,Nb,Ti)0.25(Nb,Ti)0.25	The O phase

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
P2ZN3_HT						(P)2(Zn)3	
P2ZN3_LT	Zn3P2	tP40	P 4_2/n m c		137	(P)2(Zn)3	
P2ZN_HT						(P)2(Zn)1	
P2ZN_LT	ZnAs2	mP24	P 2_1/c		14	(P)2(Zn)1	
QPRIME		*hP21	*P -6		174	(Al)5(Cu)2(Mg)8(Si)6	Coherent / semi-coherent version of Q_ALCUMGSI
Q_AL7CU3MG6	CuFeS2	cI96	I m -3 m		229	(Al)7(Cu)3(Mg)6	Al7Cu3Mg6, Al-Cu-Mg ternary phase, aka. Q_AL7CU3MG6
Q_ALCUMGSI		hP21	P -6		174	(Al)5(Cu)2(Mg)8(Si)6	Quaternary phase, aka Q, Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 & Al4Cu2Mg8Si7
RED_P	P	mP84	P 2/c		13	(P)1	
RHOMBO_A7	As	hR6	R -3 m	A7	166	(In,Sn,Bi)1	
SC13ZN58		hP142	P 6_3/m m c		194	(Sc)0.1831(Zn)0.8169	
SC1ZN1	CsCl	cP2	P m -3 m	B2	221	(Sc)0.5(Zn)0.5	
SC3SI5_HT	*	o**	*	*		(Sc)0.375(Si)0.625	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
SC3SI5_LT	AlB2	hP3	P 6/m m m	C32	191	(Sc)0.375(Si)0.625	
SC3ZN17		cI160	I m -3		204	(Sc)0.15(Zn)0.85	
SC5SI3	Mn5Si3	hP16	P 6_3/m c m	D88	193	(Sc)0.625(Si)0.375	
SCSI	CrB / TlI	oC8 / oS8	C m c m	B33 / Bf	63	(Sc)0.5(Si)0.5	
SCZN12	ThMn12	tI26	I 4/m m m		139	(Sc)0.077(Zn)0.923	
SCZN2	Hg2U	hP3	P 6_3/m m c		194	(Sc)0.3333(Zn)0.6667	
SI2SR_HT	ThSi2	tI12	I 4_1/a m d		141	(Va,Si)2(Sr)1	
SI2SR_LT	Si2Sr	cP12	P 4_1 3 2		213	(Si)2(Sr)1	
SI2TI_C54	Si2Ti	oF24	F d d d	C54	70	(Al,Sn,Ge,Si)2(Zr,Ti)1	Ge2Ti, Si2Ti, Sn2Zr
SI2ZR3_D5A	U3Si2	tP10	P 4/m b m	D5a	127	(Si,B)2(V,Zr)3	Si2Zr3, B2V3
SI2ZR_C49	Si2Zr	oC12	C m c m		63	(Si,Ge)2(Zr)1	Si2Zr, Ge2Zr
SI3TI5_D88	Mn5Si3	hP16	P 6_3/m c m	D88	193	(Si)3(Ti)5	
SI4ZR5_	Cr5B3	tI32	I 4/m c m	D8l	140	(Si,Ge)4(Ti,Zr)5	Si4Zr5, Si4Ti5, Ge4Zr5

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
TP36							
SIB3	B4C	hR42 or hR15	R -3 m	D1g	166	(B)6(Si)2(Si,B)6	
SIB6	SiB6	oP280	P n n m		58	(B)210(Si)23(Si,B)48	
SIBX		hR12	R -3 m		166	(B)61(Si)1(Si,B)8	
SIC	ZnS	cF8	F -4 3 m		216	(C)1(Si)1	
SIGMA	Cr0.49Fe0.51	tP30	P 4_2/m n m	D8b	136	(Fe,Ni,Mn)8(V,Cr)4(Fe,Cr,Ni,Mn,V)18	
SIP2	FeS2 GeAs2	cP12 oP24	P a -3 P b a m		20555	(Si)1(P)2	
SIP_OC48	SiP	oS48	C m c 2_1		36	(Si)1(P)1	
SIZR3_TP32	Ti3P	tP32	P 4_2/n		86	(Ge,Si)1(Ti,Zr)3	SiZr3, SiTi3, GeZr3
SN3TI2	Ti2Sn3	oS40	C m c a		64	(Sn)3(Ti)2	
SN3ZR5	Mn5Si3	hP16	P 6_3/m c m	D88	193	(Zr)5(Sn)3(Va,Sn)1	aka eta
SN5TI6_OI44	Nb6Sn5 / Sn5Ti6	oI44	I m m m		71	(Ge,Sn,Si)5(V,Ti)6	Sn5Ti6, Si5V6, Ge5Ti6

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
SNZR3_A15	Cr3Si	cP8	P m -3 n	A15	223	(Sn,Zr)3(Zr,Sn)1	
SN_HP1	(Hg0.1Sn0.9)	hP1	P 6/m m m		191	(In,Cd,Sn)1	
SR3SN5	Pu3Pd5	oS32	C m c m		63	(Sr)0.375(Sn)0.625	
SRB6	CaB6	cP7	P m -3 m		221	(Sr)1(B)6	
SRSN3	Mg3In	hR48	R -3 m		166	(Sr)0.25(Sn)0.75	
SRSN4	SrSn4	oS20	C m c m		63	(Sr)0.2(Sn)0.8	
SRZN5_LT	Pu3Pd5	oS32	C m c m		63	(Sr)1(Zn)5	
S_DPRIME		mS* / mP*	monoclinic			(Al)5(Cu)5(Mg)2	metastable precipitate, related to S_PHASE
S_PHASE	MgCuAl2	oS16	C m c m		63	(Al,Si)2(Cu)1(Mg)1	aka Al2CuMg or S
S_PRIME	*MgCuAl2	*oS16	*C m c m		63	(Al)2(Cu)1(Mg)1	slightly distorted S_phase. Strain & interfacial energy need to added
TETRA_A6	In	tI2	I 4/m m m	A6	139	(Sn,In)1	
TET_A6P	(In,Sn)	tI2	I 4/m m m	A6	139	(Sn,In)1	
THETA_DPRIME	Al3Cu	tP8	P 4/m m m	L12	123	(Al)3(Cu)1	GII zones, theta double prime, Al3Cu, metastable

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
THETA_PRIME	Al2Cu	tP*	P 4/m m m		123	(Al)2(Cu)1	metal stable Al2Cu, theta prime
TIZN10	Ti3Zn22	tP100	P 42/m b c		135	(Ti)1(Zn)10	
TIZN15	TiZn16	oS68	C m c m		63	(Ti)1(Zn)15	
TIZN2	MgZn2	hP12	P 6_3/m m c	C14	194	(Ti)1(Zn)2	
TIZN5						(Ti)1(Zn)5	
T_PHASE	(Al,Zn)49Mg32	cI162 or cI160	I m -3		204	(Mg)26(Al,Mg)6(Zn,Al,Mg,Cu)48(Al)1	Solution (Al,Cu,Zn)49Mg32, stable in Al-Mg-Zn, Al-Cu-Mg, Al-Cu-Mg-Zn
T_PRIME	~ (Al,Zn)49Mg32	~cI162 or cI160	~I m -3		204	(Al)0.3(Mg)0.45(Zn)0.25	metastable precipitate, related to T_PHASE
U1_AL2MGSI2		hP5	P -3 m 1		164	(Al)2(Mg)1(Si)2	metastable precipitate, U1_Al2MgSi2, Al-containing Pre-beta phase
U2_AL4MG4SI4		oP12	P n m a		62	(Al)1(Mg)1(Si)1	metastable precipitate, U2_Al4Mg4Si4, Al-containing Pre-beta phase
V17GE31	V17Ge31	tP192	P -4 n 2		118	(V)0.354(Ge)0.646	
V2B3	V2B3	oS20	C m c m		63	(V)0.4(B)0.6	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
V2ZR	Cu2Mg	cF24	F d -3 m		227	(V)2(Zr)1	
V3C2	Sc0.67Te	hR24	R -3 m		166	(V)3(C)2	
V3GE	Cr3Si	cP8	P m -3 n	A15	223	(V)0.75(Ge)0.25	
V3SI	Cr3Si	cP8	P m -3 n	A15	223	(Si,V)0.75(V,Si)0.25	
V3SN	Cr3Si	oP8	P m -3 n	A15	223	(Sn)0.205(V)0.795	
V4ZN5	V4Zn5	tI18	I 4/m m m		139	(V)4(Zn)5	
V5B6	V5B6	oS22	C m m m		65	(V)0.454545(B)0.545455	
VSN2	CuMg2	oF48	F d d d	C15	70	(Sn)0.6(V)0.4	
V_PHASE	Mg2Zn11	cP39	P m -3		220	(Si,Al,Zn)5(Cu,Zn)6(Mg)2	solution of Mg2Zn11, Al5Cu6Mg2; aka Z
WHITE_P	P	aP24	P -1		2	(P)1	
ZN13M2	Zn89(Fe0.5Ni0.5)13.8	cF432	F -4 3 m		216	(Ni,Fe)1(Zn)6.5	Fe-Ni-Zn ternary phase
ZN22ZR	Zn22Zr	cF184	F d -3 m		227	(Zn)22(Zr)1	
ZN2ZR	Cu2Mg	cF24	F d -3 m	C15	222	(Zn)2(Zr)1	
ZN39ZR5	Zn39Zr5	mS88	C 2/m		12	(Zn)39(Zr)5	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Strukturbericht*	*SG number*	*Sublattice*	*Notes*
ZN3ZR_HT					223	(Zn)3(Zr)1	
ZN3ZR_LT		tI64			223	(Zn)3(Zr)1	
ZRB12	UB12	cF52	F m -3 m	D2F	225	(B)12(Zr)1	
ZRM5_C15B	Be5Au	cF24	F -4 3 m		216	(Cu,Ni)5(Zr)1	Cu5Zr, Ni5Zr

TCAL7 Properties Data

For more information about the models, and when in Thermo-Calc, press F1 to search the online help.

You can find information on our website about the thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources will also be made available on our website in the near future so keep checking back or subscribe to our newsletter.

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:	**7.1**
First release:	**TCAL1 was released in 2011**

Changes in the Most Recent Database Release

TCAL7.0 to TCAL7.1

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

Previous Releases

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 aluminium 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.