TCS AI-based Alloy Database (TCAL11)

Technical Information

Available Starting with Thermo-Calc Version 2026b

Document created 12-Jun-26

Contents

About the TCS Al-based Alloys Database (TCAL)

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

- All industrial wrought aluminium alloys from 1000 series to 7000 series
- All industrial cast aluminium alloys from 1xx.x to 8xx.x
- Many of the 8000 and 9xx.x series, including Al-Li, Al-Sc, Al-Sn, Al-Ce, and Al-Er based alloys

It includes all major alloying elements and many minor alloying elements. It also includes nearly all stable phases in the assessed systems and most important metastable precipitates observed in industrial alloys.

In addition to thermodynamic data, the database has thermophysical and elastic properties data available for:

- Molar volume with thermal expansion coefficients
- Electrical resistivity
- Thermal conductivity
- Viscosity of metallic liquids
- Surface tension of metallic liquids
- Elastic moduli and elastic constants

TCAL11 Thermophysical Properties and TCAL11 Elastic Properties

Interconnectivity with Other Products

The database can be used with our entire suite of products: Thermo-Calc, the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Additive Manufacturing Modules, and all available SDKs.

The thermodynamic database is compatible with the corresponding mobility database TCS Al-alloys Mobility Database (MOBAL) that provides kinetic data for those working with the add-on kinetic modules – the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA) – as well as a few specific calculation types, such as Scheil with back diffusion. The current version of the mobility database is MOBAL8.

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 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.

Release History

- The current version of the database is TCAL11. To review the most recent changes, see TCAL11: Current Version Changes.
- To review additional older changes, see TCAL: Revision History.

TCS Al-based Alloys Database (TCAL) Resources

Database technical content and examples are available in different formats (html help files or PDFs).

Go to these locations to access the same content:

- **Locally Installed Help**: When in Thermo-Calc, press F1 to open the current version of the help in a local browser. You can also click **Online Help** from the **My Project** page to open the file. Then search or navigate to the **Databases** folder to browse the contents.
- **Web Help**: Go to the Documentation page to link to the most recent version of the web help. Then search or navigate to the **Databases** folder to browse the contents.
- **Website resources**: The individual database technical information and examples are also available in PDF format from the website. Download the *current version* of the PDFs for each database.

About the CALPHAD Method

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

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our website or our YouTube playlist.

Learn More

Go to the Aluminum-based Alloys Databases page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information* plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to aluminum including links to resources such as publications, webinars, videos, and more.

Read more on our website about applications for Sustainability. The webpage highlights several examples demonstrating how Thermo-Calc has been applied to address key sustainability challenges.

For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what properties can be calculated with Thermo-Calc and the Add-on Modules.

TCAL11 Elements, Systems, and Phases

This section summarizes the available elements, assessed systems, and total number of phases in the TCS Al-based Alloys Database (TCAL).

Included Elements

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

Included Elements									
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
Ta	Te	Ti	V	W	Y	Zn	Zr		

Assessed Systems and Phases

The most recent version of the database contains:

- 317 assessed binary systems, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 135 assessed ternary systems, mostly to their full range of composition. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 15 quaternaries are assessed within the Al-rich region.

- 723 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`.

Common Phases for Aluminum Alloys and TCAL11 Models for the Included Phases.

TCAL11 Properties Data

In this section:

TCAL11 Thermophysical Properties

This section summarizes the thermophysical properties available in this database.

Thermophysical Properties Parameters and Variables

Below is a summary of the available thermophysical parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode (CM) versus Graphical Mode (GM) as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property (Variable Name GM)	*Model Parameters*	*Variables to Show or Plot in CM or the SDKs*
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI
Electrical conductivity	ELQ**	ELCD for a system `ELCD(PHI)` for phase PHI
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI*	`SURF(LIQUID)` `SURF(ION)`**
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)`**
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)`**

* XI is not used in the TCOX database (all versions). As of 2023b it is also not used starting with the following versions of these databases: TCFE13, TCNI12.1, TCTI5.1, TCNOBL3, TCPMAG2, and TCCU6. As of 2024a, TCMG7, TCAL9, and TCHEA7. As of 2024b, TCSLD5. **`ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

The examples listed for the SDKs (TC-Python and TC-Toolbox for MATLAB) are using CM syntax. The quantities can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. See the various model descriptions or the SDK help for details.

Examples

In Thermo-Calc, press F1 and search or navigate to the relevant database to discover the Validation and Calculation Examples Collection, which is also available in PDF format on our website.

Go to the Aluminum-based Alloys Databases page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information* plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to aluminum including links to resources such as publications, webinars, videos, and more.

Learn More

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, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what properties can be calculated with Thermo-Calc and the Add-on Modules.

TCAL11 Elastic Properties

This section summarizes the elastic properties in this database.

Elastic Properties Parameters and Variables

Elastic properties are only available for cubic BCC (A2 and B2), cubic FCC (A1 and L12), and hexagonal HCP (A3) phases.

Graphical Mode

In the **Plot Renderer** in Graphical Mode, elastic constants and moduli can be selected from the drop-down list of axis variables.

The independent elastic constants are selected on the **Plot Renderer** as an axis variable **Elastic constant** and then choose an option (**C11**, **C12**, **C13**, **C33**, or **C44**) from the drop-down list.

The elastic moduli, **Bulk modulus**, **Shear modulus**, and **Young's modulus**, are directly available from the **Axis variable** list.

All can be tabulated and plotted using the quantity names, with options for a specific phase or all phases.

Console Mode

The quantities corresponding to the individual elastic constants and elastic moduli (derived from the elastic constants) can be can be calculated in Console Mode for individual phases or all phases. The results can be shown in the POLY module with the command SHOW_VALUE or shown as a plot in the POST module with the command PLOT_DIAGRAM using:

- `Cij(<phase name>)` or `Cij(*)`
- Bulk modulus: `BULKMOD(<phase name>)` or `BULKMOD(*)`
- Shear modulus: `SHEARMOD(<phase name>)` or `SHEARMOD(*)`
- Young's modulus: `YOUNGMOD(<phase name>)` or `YOUNGMOD(*)`

TC-Python and TC-Toolbox for MATLAB®

For the Software Development Kits (SDKs), i.e. TC-Python and TC-Toolbox, the quantities of elastic constants, bulk modulus, shear modulus, and Young's modulus can be retrieved for individual phases or all phases via `get_value_of()` or `get_values_of()` from any equilibrium calculation types using:

- `Cij(<phase name>)` or `Cij(ALL_PHASES/*)`
- `ThermodynamicQuantity.bulk_modulus(<phase name>)` or `ThermodynamicQuantity.bulk_modulus (ALL_PHASES/*)`
- `ThermodynamicQuantity.shear_modulus (<phase name>)` or `ThermodynamicQuantity.shear_modulus(ALL_PHASES/*)`
- `ThermodynamicQuantity.youngs_modulus(<phase name>)` or `ThermodynamicQuantity.youngs_modulus(ALL_PHASES/*)`

See the relevant SDK documentation for details.

Examples

In Thermo-Calc, press F1 and search or navigate to the relevant database to discover the Validation and Calculation Examples Collection, which is also available in PDF format on our website.

Go to the Aluminum-based Alloys Databases page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information* plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to aluminum including links to resources such as publications, webinars, videos, and more.

Learn More

The elastic properties (elastic moduli and elastic constants) are included with the database as of TCAL11 and are only available for cubic BCC (A2 and B2), cubic FCC (A1 and L12), and hexagonal HCP (A3) phases.

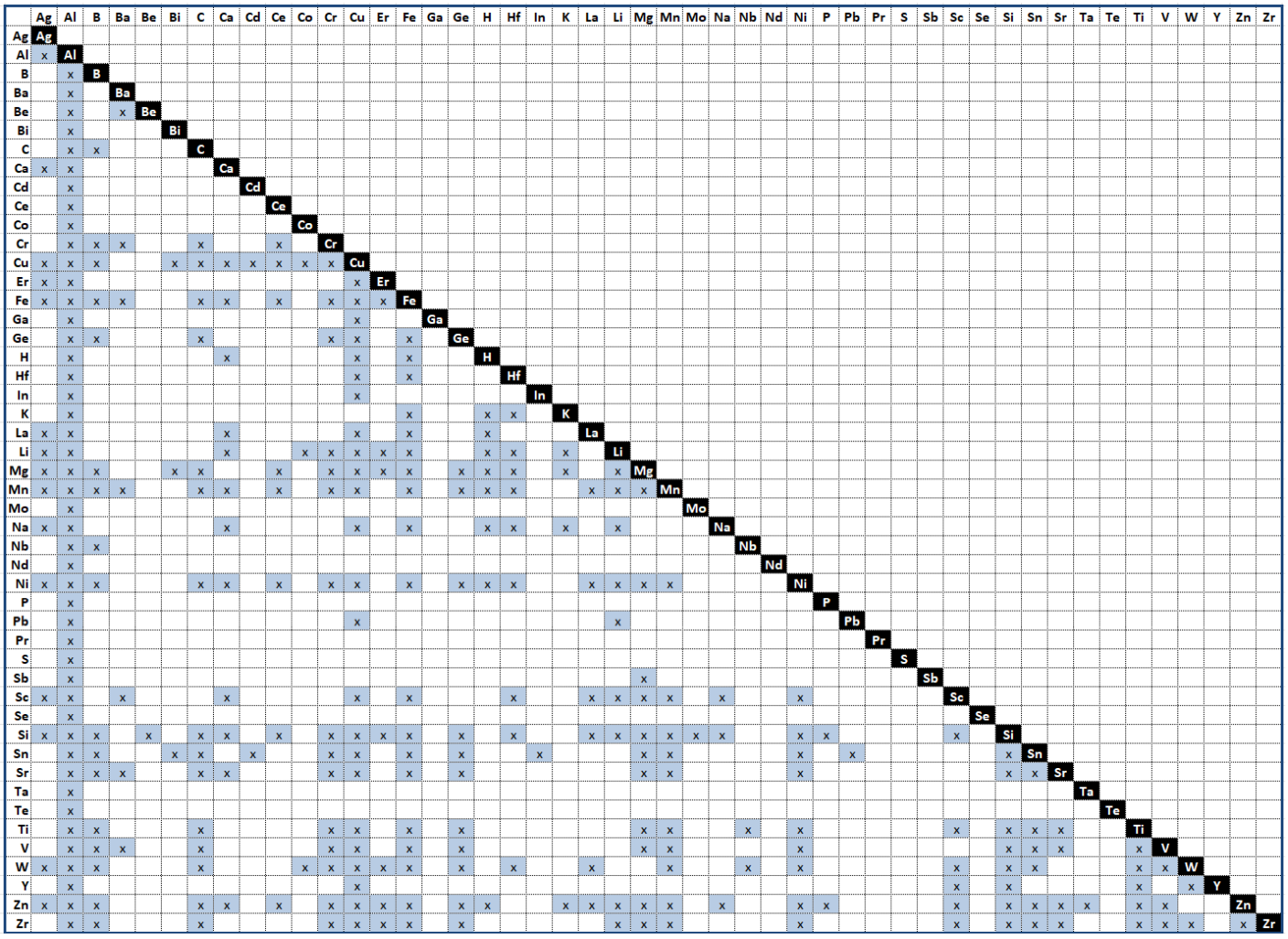
For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what properties can be calculated with Thermo-Calc and the Add-on Modules.

TCAL11 Systems

In this section:

TCAL11 Assessed Binary Systems

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



TCAL11 Assessed Ternary Systems

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

Assessed Ternary Systems							
Ag-Al-Cu	Al-B-Nb	Al-B-Ti	Al-B-Zr	Al-Be-Si	Al-Bi-Mg	Al-Bi-Sn	Al-C-Cr
Al-C-Mg	Al-C-Si	Al-C-Ti	Al-C-V	Al-Ca-Cu	Al-Ca-Fe	Al-Ca-Si	Al-Ca-Zn
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-Ce-Zn	Al-Cr-Cu	Al-Cr-Fe	Al-Cr-Mg	Al-Cr-Mn	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-Er-Si	Al-Er-Zn
Al-Er-Zr	Al-Fe-Mg	Al-Fe-Mn	Al-Fe-Ni	Al-Fe-Si	Al-Fe-Zn	Al-In-Sn	Al-La-Zn
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	Al-Ti-Zr
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	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	

TCAL11 Assessed Quaternary Systems

Assessed Quaternary Systems	
Al-Bi-Mg-Sn	Al-Ca-Fe-Si
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-Mg-Sc-Si	

TCAL11 Phases

In this section:

Common Phases for Aluminum Alloys

TCAL11 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, $Al_{15}Mn_3Si_2$, $Al_{16}Mn_4Si_3$ or $Al_{15}Mn_4Si_2$. 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 Al_3Fe.
AL2CU_C16	The so-called θ-Al_2Cu phase that forms in many Cu-containing aluminum alloys.
AL2CU_OMEGA	Ω-Al_2Cu, a metastable precipitate and the coherent version of the θ phase
THETA_PRIME	A semi-coherent precipitate with a stoichiometry of Al_2Cu in α-(Al).
THETA_DPRIME	Coherent metastable precipitates in α-(Al), also referred to as GPII zones. It has a stoichiometry close to Al_3Cu.
BETA_DPRIME	Metastable precipitate β'' related to Mg_2Si that forms in Al-Mg-Si based alloys. It may contain Al atoms ($Al_2Mg_5Si_4$) or be Al-free (Mg_5Si_6).
BETA_PRIME	Metastable precipitate β' related to Mg_2Si, aka Mg_9Si_5/$Mg_{1.8}Si$
U1_AL2MGSI2	An Al-containing pre-β Al-Mg-Si metastable precipitate, U1_Al_2MgSi_2
U2_AL4MG4SI4	An Al-containing pre-β Al-Mg-Si metastable precipitate, U2_$Al_4Mg_4Si_4$
AL18FE2MG7SI10	A quaternary phase, aka $Al_8FeMg_3Si_6$, 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.

Name in the Database	*Common Name and Description*
AL28CU4MN7	An Al-Cu-Mn intermetallic phase that forms in aluminum alloys.
Q_ALCUMGSI	A stable Al-Cu-Mg-Si quaternary phase, aka Q, $Al_5Cu_2Mg_8Si_6$, $Al_3Cu_2Mg_9Si_7$ and $Al_4Cu_2Mg_8Si_7$
QPRIME	The coherent / semi-coherent version of Q_ALCUMGSI
MG2SI_C1	Mg_2Si, which forms in Mg- and Si-containing aluminum alloys
AL9FE2SI2	A common Al-Fe-Si ternary phase in aluminum alloys, aka τ6, Al_5FeSi, 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 ($MgZn_2$) phase, eta and the M phase. This phase includes all $MgZn_2$-type phases.
ETA_PRIME	The metastable η' phase, which is related to the η-$MgZn_2$ phase
T_PHASE	A stable phase in Al-Mg-Zn, Al-Cu-Mg and Al-Cu-Mg-Zn. It is modeled as $(Al,Cu,Zn)_{49}Mg_{32}$ and is often designated as $Al_2Mg_3Zn_3$ in aluminum alloys.
T_PRIME	The metastable form of T phase, T’
S_PHASE	The S phase, Al_2CuMg
S_PRIME	The metastable S’ phase, precursor to the S phase
Q_AL7CU3MG6	An Al-Cu-Mg ternary phase, aka, $Al_7Cu_3Mg_6$ and the Q phase

TCAL11 Models for the Included Phases

The table lists all phases and the thermodynamic model used to describe the phase.

See the separate listing for Gas and Liquid Phases below.

Phase Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
ORTHORHOMBIC_S	alpha-S (A16)	A16	oF128	(70, Fddd)	-	1	(S)1
RED_P	Unknown Structure	-	-	-	-	1	(P)1
WHITE_P	Unknown Structure	-	-	-	-	1	(P)1
HEXAGONAL_A8	gamma-Se (A8)	A8	hP3	(152, P3_121)	Se, Te	1	(SE, TE)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	Metallic FCC_A1 solution, e.g. (Al), (Cu), and MC carbides	2	(AG, AL, 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(B, C, H, VA)1
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(AG, AL, CU, FE, ZR, MG, MN, NI, PR, TI, ZN)3
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	Metallic BCC_A2 solution	2	-
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, ZR, ZN)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, ZR, ZN)0.5(B, C, H, VA)3
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	2	(AL, CO, CU, FE, LI, MG, MN, NI, SI, ZN, CR, GE, SN, SR, TI, V, W, ZR)1(B, C, H, VA)1
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)	-	2	(AL, CE, CU, FE, HF, LI, MG, MN, NI, SI, ZN, CR, GE, SN, SR, TI, V,

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							W, ZR, AG)1(B, C, H, VA)1
DHCP	alpha-La (A3')	A3'	hP4	(194, P6_ 3/mmc)	-	1	(AL, CE, CU, LA, NI, ND, PR, SC)1
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(B, C, H, VA)0.5
BETA_RHOMBO_B	beta-B (R-105)	-	hR105	(166, R-3m)	-	2	(B)93(CU, NB, SI, B, C)12
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_ 3/mmc)	-	1	(B, C)1
RHOMBO_A7	alpha-As (A7)	A7	hR2	(166, R-3m)	Bi	1	(BI, IN, SB, SN)1
TETRA_A6	In (A6)	A6	tI2	(139, I4/mmm)	-	1	(IN, SN)1
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, CU, CR, FE, HF, LI, MG, MN, NI, TI, W, ZN, ZR)2(AL, CU, CR, ER, FE, HF, MG, MN, NI, SC, TI, W, ZN, ZR)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	Solution of Cu2Mg-type phases, cF24, Fd-3m, Al2Nd, Al2Pr	2	(AL, CA, CU, FE, LI, MG, ND, NI, SC, SI, ZN, CR, TI, ZR, LA, HF, W)2 (AL, CA, CE, CU, ER, FE, LI, MG, ND, NI, SC, SI, ZN, CR, TI, ZR, LA, HF, PR, W)1
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)	Solution of MgNi2-type phases, hP24, P63/mmc	2	(AL, CU, CR, FE, HF, MG, MN, NI, ZN, ZR)2(AL, CA, CU, CR, FE, HF, MG, NI, SC, ZN, ZR)1
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	Pure C, Ge, Si or solution phases based on them	1	(AL, SI, ZN, B, C, GA, GE, P, SR, SN, TI)1
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, ZN, PB, SN, TI)1
ORTHORHOMBIC_GA	alpha-Ga (A11)	A11	oS8	(64, Cmce)	-	1	(GA)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)	-	3	(FE, MN, NI)8(CR, V)4(FE, CR, MN, NI, V)18
AL45V7	Al45V7	-	mS104	(12, C2/m)	Al45Cr7, Al45V7	2	(AL, CU)45(CR, FE, MN, V)7
CUZR2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	AlCr2, CuTi2, CuZr2, Ti2Zn, ZnZr2	2	(AL, CR, CU, SI, ZN)1(AL, CR, TI, ZR)2
B2_BCC	CsCl (B2)	B2	cP2	(221, Pm-3m)	AlCo, CeZn, CuZr, ErZn, FeTi, TiZn, ZnZr, MgSc, MnZn(rt)	2	(AG, AL, CO, CU, FE, LI, MG, NI, PB, ZN)1(AG, CE, CO, ER, HF, LA, LI, MG, MN, PB, SC, TI, VA, ZR)1
MB2_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	AlB2, B2Cr, B2Mg, B2Mn, B2Ti, B2V, B2Zr	2	(MG, AL, MN, NB, CR, ZR, TI, V)1(B)2
FEB_B27	FeB (B27)	B27	oP8	(62, Pnma)	BFe, BMn, BTi, GeZr, SiTi, SrZn, SiZr	2	(FE, MN, TI, ZR, SR)1(B, SI, ZN, GE)1
AL3TI_D022	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	Al3Ti, Ni3V, GeMn3, Al3V	2	(AL, CU, MN, NB, NI, SI, TI)3(AL, GE, MN, NB, SC, TA, TI, V, ZR)1
ALZR2_B82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	SnTi2, GeMn2, AlZr2, AlSc2	2	(AL, GE, MN, SN, VA)1(ZR, MN, SC, TI, VA, Y)2
AL2ZR3_TP20	Zr3Al2	-	tP20	(136, P4_2/mnm)	Al2Zr3, Al2Hf3, ZN2Zr3	2	(AL, ZN)2(SC, HF, Y, ZR)3
CAZN13_CF112	NaZn13 (D23)	D23	cF112	(226, Fm-3c)	CaZn13, SrZn13	2	(CA, SR)1(AL, ZN)13
NI3SN_D019	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	Ni3Sn, SnTi3, SnMn3, AlLa3	2	(AL, SN, GE, VA)1(LA, MN, FE, NI, TI)3
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(AG, B, ER, GE, HF, SC, SI, SN, ZR)1
AL3ZR5_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	Al3Zr5, Cr3Si5, Ge3V5, Si3V5	2	(AL, SI, GE)3(ZR, CR, V)5
AL2SR_OI12	CeCu2	-	oI12	(74, Imma)	Al2Sr, SrZn2	2	(AL, MG, ZN)2(SR)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU5M_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	CaCu5, CeCu5, Cu5La, Cu5Sr, Al1Cu4Er1, AlCu5Y	2	(AL, CU)5(CA, CE, ER, LA, SR, Y)1
NI5M_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	CaNi5, LaNi5, ScNi5	2	(NI)5(CA, LA, SC)1
ZN5M_D2D	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	CaZn5, LaZn5, SrZn5	2	(AL, ZN)5(CA, CE, LA, SR)1
M3B4_D7B	Ta3B4 (D7b)	D7b	oI14	(71, Immm)	V3B4, Ti3B4, Mn3B4, Cr3B4	2	(B)4(AL, MN, NB, CR, TI, V)3
SI2ZR3_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	Si2Zr3, B2V3	2	(SI, B)2(NB, ZR, V)3
CO2SI_C23	Cotunnite (PbCl2, C23)	C23	oP12	(62, Pnma)	Ca2Si, Ni2Si, SiSr2, SnSr2, GeSr2	2	(CA, CU, FE, NI, SR)2(AL, SI, ZN, GE, SN)1
CR5B3_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	Ca5Si3, Sn3Sr5, Si4Sr5, Ge3Sr5, B3Cr5	2	(CA, CR, SR)0.625(AG, SI, B, GE, 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	(SI, GE)1(ZR, TI)3
SI4ZR5_TP36	Si4Zr5	-	tP36	(92, P4_12_12)	Si4Zr5, Si4Ti5, Ge4Zr5	2	(SI, GE)4(TI, ZR)5
SI2ZR_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	Si2Zr, Ge2Zr	2	(SI, GE)2(ZR)1
SI2TI_C54	TiSi2 (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	Ge2Ti, Si2Ti, Sn2Zr	2	(AL, GE, SI, SN)2(TI, ZR)1
ZRM5_C15B	AuBe5 (C15b)	C15b	cF24	(216, F-43m)	Cu5Zr, Ni5Zr	2	(CU, NI)5(ZR)1
FEM_B35	CoSn (B35)	B35	hP6	(191, P6/mmm)	FeSn, FeGe	2	(FE)1(SN, GE)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SN5TI6_OI44	Sn5Ti6-alpha	-	oI44	(71, Immm)	Sn5Ti6, Si5V6, Ge5Ti6	2	(GE, SN, SI)5(V, TI)6
M7C3_D101	C3Cr7 (D101)	D101	oP40	(62, Pnma)	Cr7C3, Mn7C3	2	(MN, CR)7(C)3
M23C6_D84	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)	Cr23C6, Mn23C6, Mn23SC6	2	(MN, CR)23(C, SC)6
V_PHASE	Mg2Zn11 (D8c)	D8c	cP39	(200, Pm-3)	solution of Mg2Zn11, Al5Cu6Mg2; aka Z	3	(AL, SI, ZN)5(CU, ZN)6(MG)2
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
AG2ER	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(AG)2(ER)1
AG51ER14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(AG)0.77(ER)0.23
AG2LA	KHg2	-	oI12	(74, Imma)	-	2	(LA)1(AG)2
AG51LA14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(LA)14(AG)51
AG5LA	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	-	2	(LA)1(AG)5
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(NA)1
AG4SC	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)	-	2	(AG)0.8(SC)0.2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AGZN3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	-	1	(AG, ZN)1
AGZN_HP9	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	-	2	(ZN)1(AG, ZN)2
AG5ZN8	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(AG, ZN)2(AG)2(AG, ZN)3(AG, ZN)6
ALB12	alpha-AlB12	-	tP216	(92, P4_12_ 12)	-	2	(AL, NB, TI)1(B)12
AL13BA7	Al13Ba7	-	hP20	(164, P-3m1)	-	2	(AL)13(BA)7
AL5BA3	Al5Ba3	-	hP16	(194, P6_ 3/mmc)	-	2	(AL)5(BA)3
AL5BA4	Al5Ba4	-	hP18	(194, P6_ 3/mmc)	-	2	(AL)5(BA)4
AL4C3	Al4C3 (D71)	D71	hR7	(166, R-3m)	-	3	(AL, SI)2(AL, MG, SI)2(C)3
AL14CA13	Al14Ca13	-	mS54	(12, C2/m)	-	2	(AL, MG, ZN)14(CA)13
AL3CA8	Ca8In3	-	aP22	(2, P-1)	-	2	(AL)3(CA, MG)8
AL11CE3	Al11La3	-	oI28	(71, Immm)	Al11Ce3, Al11La3(rt)	2	(AL, MG, ZN)0.7857(CE)0.2143
AL3CE_H	Unknown Structure	-	-	-	-	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

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALCE3_L	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	-	2	(AL)0.25(CE)0.75
AL13CO4	Orthorhombic Co4Al13 (Approximate Quasicrystal)	-	oP102	(31, Pmn2_1)	-	2	(AL)13(CO)4
AL3CO	Os4Al13	-	mS34	(12, C2/m)	-	2	(AL)3(CO)1
AL5CO2	Co2Al5 (D811)	D811	hP28	(194, P6_ 3/mmc)	-	2	(AL)5(CO)2
AL5CR	Al5Cr	-	mS732	(15, C2/c)	-	2	(AL, SI)5(CR, FE, MN)1
AL4CR	mu-Al4Mn	-	hP574	(194, P6_ 3/mmc)	-	2	(CR, FE)1(AL, SI, VA)4
ALCR_GAMMA1	Unknown Structure	-	-	-	-	4	(AL, CR, SI)2(CR)2(AL, CR)3(AL, SI)6
GAMMA_D810	Cr5Al8 (D810)	D810	hR26	(160, R3m)	-	3	(AL, SI)12(CR)5(AL, CR, FE, SI)9
ALCU_DEL	Al5Cu8	-	hR52	(160, R3m)	-	2	(AL, ZN)2(CU, FE)3
ALCU_EPS	InNi2 (B82)	B82	hP6	(194, P6_ 3/mmc)	-	2	(AL, CU, ZN, NI)1(CU, FE)1
ALCU_ETA	AlCu(r)	-	mS20	(12, C2/m)	-	2	(AL, CU)1(CU, FE, ZN, NI)1
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, SN, ZR, MN, NI, HF)2(AL, CU, FE, NI, B, MN, SI)1
AL2CU_OMEGA	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Al2Cu- OMEGA metastable precipitate	2	(AL)2(CU)1
THETA_PRIME	(Al2Cu)	-	tP*	(123, P4/mmm)	metal stable Al2Cu, theta prime	2	(AL)2(CU)1
THETA_DPRIME	(Al3Cu)	-	tP8	(123,	GII zones, theta double	2	(AL)3(CU)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				P4/mmm)	prime, Al3Cu, metastable		
ALCU_ZETA	Al9Cu11(h)	-	oF88	(42, Fmm2)	-	2	(AL)9(CU, FE)11
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	solution between Al8Cu5 (rt) and Cu5Zn8	3	(AL, FE, NI, SI, ZN)4(AL, CU, NI, SI, ZN)1(AG, CU, MN, FE, NI, ZN)8
GAMMA_H	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	Cu5Zn8-type Al8Cu5 (ht) phase	3	(AL, ZN)4(AL, CU, ZN)1(CU, MN, FE, NI)8
ALR_OP16	DyAl	-	oP16	(57, Pbcm)	AlEr, AlNd, AlPr(ht)	2	(AL, MG)1(ER, ND, PR, ZR)1
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(ER, ND, PR)2
AL2FE1	Al2Fe	-	aP18	(1, P1)	-	2	(AL, CU, SI, ZN)2(FE, MN, NI)1
AL5FE2	Al2.8Fe	-	oS24	(63, Cmcm)	-	2	(AL, CU, SI, ZN)5(FE, MN, NI)2
AL8FE5	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	aka Al5Fe4	1	(AL, CU, FE, MN)1
AL13FE4	Al13Fe4	-	mS102	(12, C2/m)	solution phases based on Al13Fe4, aka Al3Fe	3	(AL, CU)0.6275(CR, FE, MN, NI, ZN)0.235(AL, SI, VA, ZN)0.1375
AL4FE	AlmFe	-	tI110	(121, I-42m)	-	2	(AL)4.2(FE)1
AL3HF4	Al3Zr4	-	hP7	(191, P6/mmm)	-	2	(AL)3(HF)4
AL3LA	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	Al3La	2	(AL, ZN)3(LA)1
ALR_OS16	AlCe	-	oS16	(63, Cmcm)	AlLa, AlPr(rt)	2	(AL)1(LA, PR)1
AL53LA22	Hexagonal omega (C32)	C32	hP3	(191,	-	2	(AL)0.707(LA)0.293

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				P6/mmm)			
AL11R3_LT	Al11La3	-	oI28	(71, Immm)	Al11La3(rt), Al11Nd3 (rt), Al11Pr3(rt)	2	(AL, ZN)11(LA, ND, PR)3
AL11R3_HT	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	Al11La3(ht), Al11Nd3 (ht), Al11Pr3(ht)	2	(AL)11(LA, ND, PR)3
AL2LI3	Li3Al2	-	hr5	(166, R-3m)	-	2	(AL, MG, ZN)2(LI)3
AL1LI2	Li2Ga	-	oS12	(63, Cmcm)	-	2	(AL)1(LI)2
AL4LI9	Al4Li9	-	mS26	(12, C2/m)	-	2	(AL, ZN)4(LI)9
B32_ALLI	NaTl (B32)	B32	cF16	(227, Fd-3m)	-	2	(AL, LI, MG, ZN)1(LI, MG, VA)1
ALMG_BETA	Al45Mg28	-	cF1832	(227, Fd-3m)	-	2	(MG, LI)89(AL, ZN)140
ALMG_EPS	Al30Mg23	-	hR53	(148, R-3)	-	2	(MG)23(AL, ZN)30
ALMG_GAMMA	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	3	(LI, MG)5(AL, MG, ZN)12(AL, MG, ZN)12
ALMGZN_PHI	Mg21(Al, Zn)17	-	oP152	(57, Pbcm)	a Al-Mg-Zn ternary phase know as PHI	2	(MG)6(AL, ZN)5
AL12MN	Al12W	-	cI26	(204, Im-3)	-	2	(AL)12(CR, MN)1
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)	-	2	(AL, CU, ZN)6(CR, CU, FE, MN)1
AL4MN_R	lambda-Al4Mn	-	hP586	(176, P6_3/m)	AL461MN107	2	(AL)0.81162(CR, MN, FE)0.18838
AL4MN_U	mu-Al4Mn	-	hP574	(194, P6_ 3/mmc)	-	2	(AL, ZN)4(CR, MN)1
AL11MN4_LT	Al11Mn4	-	aP15	(2, P-1)	-	2	(AL, ZN)11(MN, FE)4
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25	-	oP156	(62, Pnma)	-	2	(AL, MN)29(MN)10

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL8MN5	Cr5Al8 (D810)	D810	hR26	(160, R3m)	-	3	(AL, TI, ZN)12(MN, TI)5(AL, MN, SI, TI, CU)9
AL12MO	Al12W	-	cI26	(204, Im-3)	-	2	(AL, SI)12(MO)1
AL5MO	Al5Mo	-	hR12	(167, R-3c)	-	2	(AL, SI)5(MO)1
AL22MO5	Al22Mo5	-	oF216	(43, Fdd2)	-	2	(AL, SI)22(MO)5
AL17MO4	Al17Mo4	-	mS84	(5, C2)	-	2	(AL, SI)17(MO)4
AL4MO	Al4W	-	mS30	(8, Cm)	-	2	(AL, SI)4(MO)1
AL3MO	MoAl3	-	mS32	(12, C2/m)	-	2	(AL, SI)3(MO)1
AL8MO3	Al8Mo3	-	mS22	(12, C2/m)	-	2	(AL, SI)8(MO)3
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(AL, MO, NB, TI)3
ALNB2	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)	-	3	(AL, NB, TI)10(NB, TI)4(AL, NB, TI)16
AL3ND	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	Al3Nd	2	(AL)3(ND)1
ALND3	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	AlNd3	2	(AL)1(ND)3
AL3NI_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(AL, MN, NI)0.75(FE, NI, B, C)0.25
AL3NI2	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)	-	3	(AL, SI, ZN)3(AL, CU, FE, MG, NI)2(NI, VA)1
AL3NI5	Ga3Pt5	-	oS16	(65, Cmmm)	-	2	(AL)0.375(NI)0.625
AL1P1	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)	-	2	(AL)1(P)1
AL3PR	Ni3Sn (D019)	D019	hP8	(194, P6_	Al3Pr	2	(AL)3(PR)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				3/mmc)			
ALPR3_L	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	AlPr3 (rt)	2	(AL)1(PR)3
MONOCLINIC	beta-S	-	mP48	(14, P2_1/c)	S (ht)	1	(S)1
AL1S1	Unknown Structure	-	-	-	AlS	2	(AL)1(S)1
AL2S3_L	Al2S3	-	hP30	(169, P6_1)	Al2S3 (rt)	2	(AL)2(S)3
AL2S3_H	Corundum (alpha-alumina, Al2O3, D51)	D51	hR10	(167, R-3c)	Al2S3 (ht)	2	(AL)2(S)3
AL1SB1	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)	-	2	(AL)1(SB)1
AL3X	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	Al3Sc (dissolving Ti, Zr), Al3Li	2	(ER, LI, SC, TI, Y, ZR)1(AL, MG, SI)3
AL2SC	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(SC, TI, Y, ZR)1(AL, MG)2
ALSC_OP	Unknown Structure	-	oP*	-	-	2	(SC, Y, ZR)1(AL, MG)1
AL2SE3	beta-Ga2Se3	-	mS20	(9, Cc)	Al2Se3	2	(AL)2(SE)3
AL7SR8	Ba8Ga7	-	cP60	(198, P2_13)	-	2	(AL)7(SR)8
AL4M_D13	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	Al4Ba, Al4Ca, Al4Ce, Al4Sr	2	(AL, MG, SI, ZN)4(BA, CA, CE, SR)1
ALTA2	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)	-	3	(AL, TA)10(TA)4(AL, TA)16
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(TE)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL2TE5	Al2Te5	-	mS14	(12, C2/m)	Al2Te5	2	(AL)2(TE)5
AL2TE3_L	Al2Te3(rt)	-	mP240	(4, P2_1)	Al2Te3 (rt)	2	(AL)2(TE)3
AL2TE3_H	Al2Te3 (ht)	-	mP40	(14, P2_1/c)	Al2Te3 (ht)	2	(AL)2(TE)3
AL2TI	Ga2Hf	-	tI24	(141, I4_ 1/amd)	-	2	(AL, NB, TI)2(AL, NB, SC, TI, ZR)1
AL5TI2	Al5Ti2	-	tP28	(123, P4/mmm)	-	2	(AL, NB, TI)5(AL, NB, TI, ZR)2
AL5TI3	Al5Ti3	-	tP32	(127, P4/mbm)	-	2	(AL)5(NB, TI)3
AL3TI_LT	Al3Ti-LT	-	tI32	(139, I4/mmm)	-	2	(AL, CU, NB, SI, TI)3(AL, MN, NB, SC, TI, ZR)1
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	-	2	(AL, CO, MN, NB, TI, W, ZR)3(AL, NB, SI, TI, W, C)1
AL21V2	Al10V	-	cF176	(227, Fd-3m)	-	2	(AL)21(V)2
AL23V4	Al23V4	-	hP54	(194, P6_ 3/mmc)	-	2	(AL)23(V)4
AL8V5	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(AL, V)2(V)2(AL, V)3(AL)6
AL77W23	Unknown Structure	-	-	-	-	2	(AL)77(W)23
AL4W	Al4W	-	mS30	(8, Cm)	also Al4Mo	2	(AL)4(W)1
AL7W3	Unknown Structure	-	-	-	-	2	(AL)7(W)3
AL2W	CrSi2 (C40)	C40	hP9	(180, P6_222)	-	2	(AL)2(W)1
AL5W	Al5W	-	hP12	(182, P6_322)	also AL5MO	2	(AL)5(W)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL12W	Al12W	-	cI26	(204, Im-3)	also AL12RE and AL12MO	2	(AL)12(W)1
ALY_B33	CrB (B33)	B33	oS8	(63, Cmcm)	-	2	(AL)1(SC, Y)1
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(AL, CU, SC, Y)1
AL4ZR5	Ti5Ga4	-	hP18	(193, P6_ 3/mcm)	-	2	(AL)4(SC, ZR)5
AL3ZR2_OF40	Zr2Al3	-	oF40	(43, Fdd2)	Al3Zr2, Al3Hf2	2	(AL, LI)3(ER, SC, HF, ZR)2
AL3ZR_D023	Al3Zr (D023)	D023	tI16	(139, I4/mmm)	Al3Zr, Al3Hf	2	(AL, MG, LI)3(ER, SC, HF, TI, ZR)1
B4C	B13C2 "B4C" (D1g)	D1g	hR15	(166, R-3m)	-	2	(B11C, B12)1(B2, C2B, CB2)1
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
MGB4	MgB4	-	oP20	(62, Pnma)	-	2	(MG)1(B)4
MGB7	MgB7	-	oI64	(74, Imma)	-	2	(MG)1(B)7
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(B)3
NI4B3_ORTH	o-Ni4B3	-	oP28	(62, Pnma)	-	2	(NI)0.586(B)0.414

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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(SI)2(B, SI)6
SIB6	SiB6	-	oP280	(58, Pnnm)	-	3	(B)210(SI)23(B, SI)48
SIBX	alpha-B (R-12)	-	hR12	(166, R-3m)	-	3	(B)61(SI)1(B, SI)8
SRB6	CaB6 (D21)	D21	cP7	(221, Pm-3m)	-	2	(SR)1(B)6
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(B)1
BW_BETA	CrB (B33)	B33	oS8	(63, Cmcm)	-	2	(B, VA)1(W)1
BW_ALPHA	MoB (Bg)	Bg	tI16	(141, I4_ 1/amd)	-	2	(B, VA)1(W)1
B5W2_X	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)	-	2	(B, VA)5(W)2
B9W2	W2B9	-	hP22	(147, P-3)	-	2	(B)9(W)2
ZRB12	UB12 (D2f)	D2f	cF52	(225, Fm-3m)	-	2	(B)12(ZR)1
BABE13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)	-	2	(BA)1(BE)13
BI2MG3_LT	La2O3 (D52)	D52	hP5	(164, P-3m1)	Bi2Mg3, P-3m1, La2O3-type (rt)	2	(BI, SN, VA)2(MG)3
BI2MG3_HT	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)	Bi2Mg3, Ia-3, Mn2O3-type (ht)	3	(BI, SN)1(BI, SN, VA)3(MG)6
CR3C2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)	-	2	(CR)3(C)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MG2C3	Mg2C3	-	oP10	(58, Pnnm)	-	2	(MG)2(C)3
MGC2	MgC2	-	tP6	(136, P4_2/mnm)	-	2	(MG)1(C)2
M5C2	Mn5C2 (Fe5C2 Hagg carbide)	-	mS28	(15, C2/c)	-	2	(MN)5(C)2
SIC	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)	-	2	(SI)1(C)1
V3C2	Sc2Te3	-	hR8	(166, R-3m)	-	2	(V)3(C)2
MC_SHP	Tungsten Carbide (WC, Bh)	Bh	hP2	(187, P-6m2)	-	2	(W)1(C)1
CA2CU	Ca2Cu	-	oP12	(62, Pnma)	-	2	(CA)2(CU)1
CA1CU1	alpha-CaCu	-	mP20	(11, P2_1/m)	alpha-CaCu (mP20, P2_1/m) & beta-CaCu (oP40, Pnma)	2	(CA)1(CU)1
HCP_CA	Mg	-	cP2	(194, P6_3/mmc)	-	2	(CA)1(H, VA)0.5
CAH2_LT	HgCl2 (C25)	C25	oP12	(62, Pnma)	-	2	(CA)1(H)2
CAH2_HT	Unknown Structure	-	-	-	-	2	(CA)1(H)2
CALI2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	-	2	(LI)2(CA)1
CA2NI7	Co7Gd2	-	hR18	(166, R-3m)	-	2	(CA)2(NI)7
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

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CASI2	CaSi2 (C12)	C12	hR6	(166, R-3m)	-	2	(CA)0.333333(SI)0.666667
CA3ZN	Re3B	-	oS16	(63, Cmcm)	-	2	(CA)3(ZN)1
CA5ZN3	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	-	2	(CA)5(ZN)3
CAZN_OC8	CrB (B33)	B33	oS8	(63, Cmcm)	-	2	(CA)1(ZN)1
MZN2	KHg2	-	oI12	(74, Imma)	CaZn2, CeZn2, ErZn2, LaZn2	2	(CA, CE, ER, LA)1(AL, ZN)2
CAZN3	CaZn3	-	hP32	(194, P6_ 3/mmc)	-	2	(CA)1(AL, ZN)3
CDCU2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	2	(CD)1(CU)2
CD3CU4	Cd3Cu4	-	cF1124	(216, F-43m)	-	2	-
CD8CU5	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(CU)2(CD, CU)3(CU)2(CU, CD)6
CD10CU3	Co2Al5 (D811)	D811	hP28	(194, P6_ 3/mmc)	-	2	-
SN_HP1	(Hg0.1Sn0.9)	-	hP1	(191, P6/mmm)	-	1	(CD, IN, SN)1
CU6CE	Copper (II) Azide [Cu (N3)2]	-	oP28	(62, Pnma)	-	2	-
CU4CE	Unknown Structure	-	oP20	-	-	2	(AL, CU)4(CE)1
CU2CE	KHg2	-	oI12	(74, Imma)	-	2	-
CUCE	FeB (B27)	B27	oP8	(62, Pnma)	-	2	-
MGCE	Unknown Structure	-	-	-	-	2	(AL, MG)1(CE)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MG3CE	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	2	(MG)3(MG, CE)1
MG41CE5	Ce5Mg41	-	tI92	(87, I4/m)	-	2	(MG)41(CE)5
MG17CE2	CeMg10	-	hP44	(194, P6_3/mmc)	-	2	(MG)17(CE)2
MG12CE	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)	-	2	(AL, MG)12(CE)1
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(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, NI)0.166667(AL, CE, NI)0.833333
CE5SI3	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	-	2	(SI)3(CE)5
CE3SI2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	-	2	(CE)3(SI)2
CE5SI4	Si4Zr5	-	tP36	(92, P4_12_12)	-	2	(CE)5(SI)4
CESI_OP8	FeB (B27)	B27	oP8	(62, Pnma)	-	2	(CE)1(SI)1
CE3SI4	Unknown Structure	-	-	-	-	2	(CE)1(SI)1.34
CE3SI5	GdSi1.4	-	oI12	(74, Imma)	-	2	(CE)0.37(SI)0.63

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RESI2	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_ 1/amd)	CeSi2, Si2Y (ht)	2	(CE, Y)1(AL, SI)2
CEZN3	CeZn3	-	oS16	(63, Cmcm)	-	2	(CE)0.25(AL, ZN)0.75
CO7W6	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	mu phase	4	(CO, W)4(CO, W)2(CO, W)1(CO, W)6
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(GE, CR)0.375
CR5GE3_LT	Unknown Structure	-	-	-	-	2	(CR, GE)0.625(GE, CR)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(MN)5
HIGH_SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)	-	3	(MN)8(CR)4(CR, MN)18
CR3SI_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(CR, SI)3(AL, CR, SI)1
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)	-	2	(CR, SI, V)1(AL, CR, SI)2
CRZN13	Unknown Structure	-	-	-	-	2	-
CRZN17	Unknown Structure	-	-	-	-	2	(CR)1(ZN)17
CU9ER2	Unknown Structure	-	-	-	-	2	(CU)9(ER)2
CU7ER2	Unknown Structure	-	-	-	-	2	(CU)7(ER)2
CU5ER_C15B	AuBe5 (C15b)	C15b	cF24	(216, F-43m)	-	2	(CU)5(ER)1
CU2ER	KHg2	-	oI12	(74, Imma)	-	2	(AL, CU)2(ER)1
CU9GA4_0	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	-	3	(CU)6(CU, GA)6(GA)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU9GA4_1	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	-	4	(CU)6(CU, GA)3(CU, GA)3(GA)1
CU9GA4_2	Cu8.2Ga4.8	-	cP52	-	-	4	(CU)3(CU, VA)3(CU, GA)3(GA)4
CU9GA4_3	Cu7.15Ga5.85	-	cP52	-	-	3	(CU, VA)6(CU, GA)3(GA)4
CUGA2	FeSi2-h	-	tP3	(123, P4/mmm)	-	2	(CU)1(GA)2
CUGA_THETA	Unknown Structure	-	-	-	-	2	(CU)0.778(GA)0.222
CU5HF	Unknown Structure	-	-	-	-	2	(CU)5(HF)1
CU51HF14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)51(HF)14
CU8HF3	Cu8Hf3	-	oP44	(62, Pnma)	-	2	(CU)8(HF)3
CU10HF7	Ni10Zr7	-	oS68	(64, Cmce)	-	2	(CU)10(HF)7
CU1HF2	CuZr2	-	tI6	(139, I4/mmm)	-	2	(CU)1(HF)2
CUIN_GAMMA	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	-	4	(CU)2(CU, IN)2(CU)3(CU, IN)6
CUIN_THETE	Cu7In3	-	aP40	(2, P-1)	-	2	(CU)0.7(IN)0.3
CU2IN_HT	InNi2 (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(LA)3
CU6LA1_LT	Cu6La	-	mP28	(14, P2_1/c)	-	2	(CU)6(LA)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU6LA1_HT	CeCu6	-	oP28	(62, Pnma)	-	2	(CU)6(LA)1
CU4LA1	Cu4La	-	tI90	(119, I-4m2)	-	2	(CU)4(LA)1
CU2LA1	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(CU)2(LA)1
CU1LA1	FeB (B27)	B27	oP8	(62, Pnma)	-	2	(CU)1(LA)1
CUMG2	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	-	2	(CU, NI)1(MG)2
CU4SC	Unknown Structure	-	t**	-	-	2	-
CU2SC_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	-
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	InNi2 (B82)	B82	hP6	(194, P6_ 3/mmc)	-	3	(CU)1(CU, SN)1(SN)1
CUSN_GAMMA	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	1	(CU, SN)1
CU10SN3	Cu10Sn3	-	hP26	(173, P6_3)	-	1	(CU, SN)1
CU3SN	Cu3Sn	-	oS80	(63, Cmcm)	-	2	(CU, SN)3(CU, SN)1
CU41SN11	Cu41Sn11	-	cF416	(216, F-43m)	-	2	(CU, SN)41(CU, SN)11
CU6SN5_LT	Cu6Sn5	-	mS44	(15, C2/c)	-	3	(CU)1(CU, SN)1(SN)1
CUSR	BaCu	-	hP8	(194, P6_	-	2	(SR)1(CU)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				3/mmc)			
CU2TI	Au2V	-	oS12	(63, Cmcm)	-	2	(CU)2(TI)1
CU3TI2	Cu3Ti2	-	tP10	(129, P4/nmm)	-	2	(CU)3(TI)2
CU4TI1	Au4Zr	-	oP20	(62, Pnma)	-	2	(AL, CU, TI)4(CU, TI)1
CU4TI3	Cu4Ti3	-	tI14	(139, I4/mmm)	-	2	(CU)4(TI)3
CUTI_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)	-	2	(CU, TI)1(CU, TI)1
CUTI3	CuTi3 (L60)	L60	tP4	(123, P4/mmm)	-	2	(CU, TI)1(TI)3
CU7Y1	Cu7Tb	-	hP8	(191, P6/mmm)	-	2	(CU2, Y)1(CU)5
CU4Y	Cu5Y1.25	-	mP16	(11, P2_1/m)	-	2	(CU)4(Y)1
CU7Y2	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)7(Y)2
CU2Y_H	Unknown Structure	-	hP*	-	-	2	(CU)2(Y)1
CU2Y_L	KHg2	-	oI12	(74, Imma)	-	2	(AL, CU)2(Y)1
EPSILON	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	-	1	(CU, MN, NI, ZN)1
CU10ZR7	Ni10Zr7	-	oS68	(64, Cmce)	-	2	(CU)10(ZR)7
CU51ZR14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)51(ZR)14
CU8ZR3	Cu8Hf3	-	oP44	(62, Pnma)	-	2	(CU)8(ZR)3
FE3ER	Ni3Pu	-	hR12	(166, R-3m)	-	2	(FE)3(ER)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FE23ER6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	2	(AL, FE)23(ER)6
FE17M2	Ni17Th2	-	hP38	(194, P6_ 3/mmc)	-	2	(AL, FE)17(CE, ER)2
MG24R5	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	2	(ER, MG)5(AL, MG)24
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
MZN3	Zn3Y	-	oP16	(62, Pnma)	ErZn3	2	(ER)1(ZN)3
MZN5	ErZn5	-	hP36	(194, P6_ 3/mmc)	ErZn5	2	(ER)1(AL, ZN)5
FE2GE1	InNi2 (B82)	B82	hP6	(194, P6_ 3/mmc)	-	3	(FE)1(FE, VA)1(GE)1
FEGE_ETA	Fe6.5Ge4	-	hP22	(194, P6_ 3/mmc)	-	2	(FE)13(GE)9
FE6GE5	Fe6Ge5	-	mS44	(12, C2/m)	-	2	(FE)6(GE)5
FE2GE3	Ru2Sn3	-	tP20	(116, P-4c2)	-	2	(FE)2(GE)3
C14_FE2HF	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	2	(FE)0.6667(HF, FE)0.3333
C36_FE2HF	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)	-	2	(FE)0.6667(HF)0.3333

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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(AL, SI)1
FESI2_H	FeSi2-h	-	tP3	(123, P4/mmm)	-	2	(FE, NI)3(AL, MG, SI)7
FESI2_L	FeSi2-l	-	oS48	(64, Cmce)	-	2	(FE, NI)1(AL, SI)2
FESI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	FeSi, MnSi, CrSi, CrGe	2	(FE, MN, NI, CR)1(AL, MG, SI, GE)1
MN5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	Mn5Si3, Cr3Si5, Fe5Si3, Ge3Mn5, Ge3Zr5, Si3Zr5, Sn3Ti5	2	(CU, FE, MN, NI, CR, ZR, TI)5(AL, CR, SI, GE, SN)3
FE5SN3_D82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(FE)5(SN)3
FE3SN2	Fe3Sn2	-	hR10	(166, R-3m)	-	2	(FE)3(SN)2
FE7W6	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	-	4	(FE, W)1(W)4(FE, W)2(FE, W)6
GAMMA_D82	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(FE, MN, ZN)2(FE, MN, NI, ZN)2(AL, CU, FE, MN, NI, SI, ZN)3(AL, ZN)6
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	-
FEZR3	Re3B	-	oS16	(63, Cmcm)	-	2	(FE)1(ZR)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GEMN3_HT	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	-	2	(GE, MN)1(MN)3
GE2MN3	Cr11Ge8	-	oP76	(62, Pnma)	-	2	(GE)2(MN)3
GE2MN5	Ge2Mn5-HT	-	hP42	(158, P3c1)	-	2	(GE, MN)2(MN)5
GE3MN7	Ga2Mg5 (D8g)	D8g	oI28	(72, Ibam)	Mn5Ge2	2	(GE)3(MN)7
GENI2	Co2Si (C37)	C37	oP12	(62, Pnma)	-	2	(NI)0.665(GE)0.335
GE3NI5_HT	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(GE, NI)0.625(GE, NI)0.375
GE2NI3	Nickeline (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
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(SR)1
GE3TI5	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	-	2	(TI)5(GE)3
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(H)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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
NIHF2	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	-	2	(NI, VA)1(HF)2
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

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
TET_A6P	In (A6)	A6	tI2	(139, I4/mmm)	-	1	(IN, SN)1
KNA2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	2	(K)1(NA)2
KZN13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)	-	2	(K)1(ZN)13
LA3NI	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(LA)3(NI)1
LA7NI3	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)	-	2	(LA)7(NI)3
LANI_OC8	CrB (B33)	B33	oS8	(63, Cmcm)	-	2	(LA)1(NI)1
LA2NI3	La2Ni3	-	oS20	(64, Cmce)	-	2	(LA)2(NI)3
LA7NI16	La7Ni16	-	tI46	(121, I-42m)	-	2	(LA)7(NI)16
LANI3	Ni3Pu	-	hR12	(166, R-3m)	-	2	(LA)1(NI)3
LA2NI7_LT	Ce2Ni7	-	hP36	(194, P6_ 3/mmc)	-	2	(LA)2(NI)7
LA2NI7_HT	Co7Gd2	-	hR18	(166, R-3m)	-	2	(LA)2(NI)7
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

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LAZN4	LaZn4	-	oS20	(63, Cmcm)	-	2	(LA)0.2(ZN)0.8
M3ZN22	Ce3Zn22	-	tI100	(141, I4_ 1/amd)	Ce3Zn22, La3Zn22	2	(CE, LA)0.12(ZN)0.88
MZN11	BaCd11	-	tI48	(141, I4_ 1/amd)	CaZn11, CeZn11, LaZn11	2	(CA, CE, LA)0.083(ZN)0.917
LAZN13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)	-	2	(LA)0.071(ZN)0.929
M2ZN17	Ni17Th2	-	hP38	(194, P6_ 3/mmc)	La2Zn17, Er2Zn17_L	2	(ER, LA)0.105(ZN)0.895
LI4PB	Li17Si4	-	cF420	(216, F-43m)	-	2	(LI)4(PB)1
LI7PB2	Li7Pb2	-	hP9	(164, P-3m1)	-	2	(LI)7(LI, PB)2
LI3PB	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	2	(LI)3(PB)1
LI5PB2	Li8Pb3	-	hR11	(166, R-3m)	-	2	(LI)5(PB)2
LIPB_LT	LiPb	-	hR2	(166, R-3m)	-	2	(LI, PB)1(LI, PB)1
LI22SI5	Li21Si5	-	cF416	(216, F-43m)	-	2	(LI)22(SI)5
LI13SI4	Li13Si4	-	oP34	(55, Pbam)	-	2	(LI)13(SI)4
LI7SI3	(Li7Si3)	-	hP60	(154, P3_221)	-	2	(LI)7(SI)3
LI12SI7	Li12Si7	-	oP152	(62, Pnma)	-	2	(LI)12(SI)7
LI2ZN3_L	Li(Li0.91Zn0.09)2Zn4	-	hR7	(166, R-3m)	-	2	(LI)2(LI, ZN)3
LI2ZN3_H	Li5Ga4	-	hP9	(164, P-3m1)	-	2	(LI, ZN)2(LI, ZN)3
LI2ZN5_L	Unknown Structure	-	-	-	-	2	(LI, ZN)2(ZN)5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LI2ZN5_H	Unknown Structure	-	-	-	-	2	(LI, ZN)2(ZN)5
LIZN4_L	Unknown Structure	-	-	-	-	2	(LI, ZN)1(LI, ZN)4
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(ZN)2
BCC_B32	NaTl (B32)	B32	cF16	(227, Fd-3m)	-	2	(LI, ZN)1(LI, ZN)1
MG2NI_HP18	Mg2Ni (Ca)	Ca	hP18	(180, P6_222)	-	2	(MG, ZN)2(CU, NI, ZN)1
MG3SB2_D53	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)	-	3	(AL, MG)6(AL, SB, VA)3(SB)1
MG3SB2_D52	La2O3 (D52)	D52	hP5	(164, P-3m1)	-	2	(AL, MG)3(AL, SB, VA)2
MG2SI_C1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	solution phase of Mg2Si, GeMg2, Mg2Sn	2	(BI, MG)2(BI, GE, SI, SN)1
MG2SR	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	2	(AL, MG)2(SR)1
MG38SR9	Mg38Sr9	-	hP94	(194, P6_ 3/mmc)	-	2	(AL, MG)38(SR)9
MG23SR6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	2	-
MG17SR2	Th2Zn17	-	hR19	(166, R-3m)	-	2	(AL, MG)17(SR)2
MG7ZN3	Mg51Zn20	-	oI158	(71, Immm)	-	2	(MG)51(ZN)20
MGZN	Zr21Re25	-	hR92	(167, R-3c)	-	2	(MG)12(AL, CU, ZN)13
MG2ZN3	Mg4Zn7	-	mS110	(12, C2/m)	-	2	(MG)2(AL, CU, ZN)3
L10_TETRA	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	-	2	(AL, CU, MN, NB, NI, TI, ZR)0.5(AL, CU, MN, NB, NI, TI, ZR, C)0.5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MNNI2	Unknown Structure	-	-	-	-	2	(MN, NI)1(NI)2
MNSC4	Unknown Structure	-	-	-	-	2	(MN)0.2(SC)0.8
MN11SI19	Mn11Si19	-	tP120	(118, P-4n2)	-	2	(MN)11(AL, SI)19
MN3SI	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	2	(FE, MN, NI)3(AL, SI)1
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	-	2	(AL, MN)17(SI, ZN)3
MN9SI2	Mn9Si2	-	oI186	(71, Immm)	-	2	(MN)33(SI)7
MN2SN	InNi2 (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(SN)2
MNTI_LT	Zr21Re25	-	hR92	(167, R-3c)	-	2	(AL, MN)1(TI)1
MNTI_HT	Unknown Structure	-	t**	-	-	2	(AL, MN)0.515(TI)0.485
MN3TI	Unknown Structure	-	-	-	-	2	(MN)3(TI)1
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(V)4(MN, V)16
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, W, SI)0.125(AL, MO, SI)0.375
MOSI2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(AL, SI)2(MO, W)1
NASI_LT	NaSi-lt	-	mS32	(15, C2/c)	-	2	(NA)1(SI)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NASI_HT	Unknown Structure	-	-	-	-	2	(NA)1(SI)1
NAZN13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)	-	2	(NA)1(ZN)13
NI7SC2	Ce2Ni7	-	hP36	(194, P6_3/mmc)	-	2	(SC)0.222222(NI)0.777778
NISC2	NiTi2	-	cF96	(227, Fd-3m)	-	2	(SC)0.72(NI)0.28
NI2SI_HT	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	3	(CU, NI)1(NI, VA)1(AL, SI)1
NI3SI2	Ni3Si2	-	oP80	(36, Cmc2_1)	-	2	(FE, NI)3(SI)2
NI3SI_HT	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(FE, NI)3(AL, SI)1
NI3SI_MT	Ge9Pd25	-	hP34	(147, P-3)	-	2	(SI)1(NI)3
NI5SI2	Ni31S12	-	hP42	(150, P321)	-	2	(CU, FE, NI)5(AL, SI)2
NISI_B31	MnP (B31)	B31	oP8	(62, Pnma)	GeNi, NiSi	2	(FE, NI)1(GE, SI, ZN)1
NISI2	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	-	2	(AL, CU, SI, ZN)2(CU, FE, MN, NI)1
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	InNi2 (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

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NITI2	NiTi2	-	cF96	(227, Fd-3m)	-	2	(NI, TI)1(NI, TI)2
NI2V7	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(NI)2(V)7
NI2V1	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	-	2	(NI)2(V)1
MONI4_BETA	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)	-	2	(W)1(NI)4
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(ZR)17
NI21ZR8	Hf8Ni21	-	aP29	(2, P-1)	-	2	(ZR)8(NI)21
NI11ZR9	Pt11Zr9	-	tI40	(87, I4/m)	-	2	(NI)11(ZR)9
NI7ZR2	Ni7Zr2	-	mS36	(12, C2/m)	-	2	(NI)7(ZR)2
SIP_OC48	(SiP)	-	oS48	(36, Cmc2_1)	-	2	(SI)1(P)1
SIP2	Pyrite (FeS2, C2)	C2	cP12	(205, Pa-3)	-	2	(SI)1(P)2
P2ZN3_LT	Zn3P2 (D59)	D59	tP40	(137, P4_2/nmc)	-	2	(P)2(ZN)3
P2ZN3_HT	Unknown Structure	-	-	-	-	2	(P)2(ZN)3
P2ZN_HT	Unknown Structure	-	-	-	-	2	(P)2(ZN)1
P2ZN_LT	ZnAs2	-	mP24	(14, P2_1/c)	-	2	(P)2(ZN)1
SC5SI3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	-	2	(SC)0.625(SI)0.375

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RESI_B33	CrB (B33)	B33	oS8	(63, Cmcm)	ScSi, YSi	2	(SC, Y)1(SI)1
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
SCZN2	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(SC)0.3333(ZN)0.6667
M13ZN58	Gd13Zn58	-	hP142	(194, P6_3/mmc)	Ce13Zn58, Er13Zn58, Sc13Zn58	2	(CE, ER, SC)0.1831(AL, ZN)0.8169
SC3ZN17	Be17Ru3	-	cI160	(204, Im-3)	-	2	(SC)0.15(ZN)0.85
MZN12	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)	ErZn12, ScZn12	2	(ER, SC)0.077(ZN)0.923
SI2SR_HT	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_1/amd)	-	2	(SI, VA)2(SR)1
SI2SR_LT	Si2Sr	-	cP12	(213, P4_132)	-	2	(SI)2(SR)1
SI3TI5_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	-	2	(SI)3(TI)5
V3SI	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(V, SI)0.75(SI, V)0.25
SI2Y_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	Si2Y (rt)	2	(SI)2(Y)1
SI5Y3_CC	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_1/amd)	Si5Y3 (ht)	2	(SI)5(Y)3
SI4Y5	Gd5Si4	-	oP36	(62, Pnma)	Si4Y5	2	(SI)4(Y)5
SI3Y5_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	Si3Y5	2	(SI)3(Y)5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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(TI)2
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(SN)3(SN, VA)1
SNZR3_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(SN, ZR)3(SN, ZR)1
SRZN5_LT	Pd5Pu3	-	oS32	(63, Cmcm)	-	2	(SR)1(ZN)5
TIZN2	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	2	(TI)1(ZN)2
TIZN5	Unknown Structure	-	-	-	-	2	(TI)1(ZN)5
TIZN10	Ti3Zn22	-	tP100	(135, P4_ 2/mbc)	-	2	(TI)1(ZN)10
TIZN15	TiZn16	-	oS68	(63, Cmcm)	-	2	(TI)1(ZN)15
V4ZN5	V4Zn5	-	tI18	(139, I4/mmm)	-	2	(V)4(ZN)5
V2ZR	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(V)2(ZR)1
ZN2ZR	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(ZN)2(ZR)1
ZN22ZR	Zn22Zr	-	cF184	(227, Fd-3m)	-	2	(ZN)22(ZR)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZN39ZR5	Zn39Zr5	-	mS88	(12, C2/m)	-	2	(ZN)39(ZR)5
ZN3ZR_LT	Unknown Structure	-	tI64	-	-	2	(ZN)3(ZR)1
ZN3ZR_HT	Unknown Structure	-	c**	-	-	2	(ZN)3(ZR)1
ALCCR2	AlCCr2	-	hP8	(194, P6_ 3/mmc)	-	3	(AL)1(C)1(CR, V)2
AL2MGC2	Ce2O2S	-	hP5	(164, P-3m1)	-	3	(AL)2(MG)1(C)2
AL4C4SI	Al5C3N (E94)	E94	hP18	(186, P6_3mc)	-	3	(AL)4(SI)1(C)4
AL8C7SI	Unknown Structure	-	-	-	-	3	(AL)8(SI)1(C)7
TI2ALC	AlCCr2	-	hP8	(194, P6_ 3/mmc)	H, Ti2AlC1-x	3	(TI)2(AL)1(C, VA)1
TI3ALC	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	P, Ti3AlC1-x	3	(TI)3(AL)1(C, VA)1
TI3AL1C2	CMo	-	hP12	(194, P6_ 3/mmc)	N, Ti3AlC2-x	3	(TI)3(AL, SI)1(C, VA)2
ALC3V4	AlN3Ti4	-	hP16	(194, P6_ 3/mmc)	-	4	(V)4(AL)1(C)2(C, VA)1
AL27CA3CU7	BaHg11 (D2e)	D2e	cP36	(221, Pm-3m)	-	3	(AL)27(CA)3(CU)7
CAAL2SI2	La2O2S	-	hP5	(164, P-3m1)	-	3	(CA)1(AL)2(SI)2
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, Al8CaCu4	3	(AL)0.6154(CA, CE, ER)0.0769(AL, CR, CU, FE, MN)0.3077
AL10CE2M7	Th2Zn17	-	hR19	(166, R-3m)	T2 in Al-Ce-Cu, Ce2Zn17	2	(AL, CR, CU, FE, MN, ZN)0.8947(CE, ER)0.1053

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3CECU	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	T3	2	(AL, CU)0.8(CE)0.2
ALCEM	Barringerite (Revised Fe2P, C22)	C22	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(CE)1
AL10REFE2	YbFe2Al10	-	oS52	(63, Cmcm)	-	3	(AL)10(CA, CE, ER)1(FE)2
AL8CEFE2	CeFe2Al8	-	oP44	(55, Pbam)	-	3	(AL)8(CE)1(FE)2
AL13CEMG6	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	3	(AL)0.667(CE)0.05(MG)0.283
AL2CENI	MgCuAl2 (E1a)	E1a	oS16	(63, Cmcm)	T2	3	(AL)2(CE)1(NI)1
AL5CE2NI5	Unknown Structure	-	-	-	T3, 13	3	(AL)0.35(CE)0.165(NI)0.485
AL4CENI	YNiAl4	-	oS24	(63, Cmcm)	T5	3	(AL)4(CE)1(NI)1
AL5CE1NI2	PrNi2Al5	-	oI16	(71, Immm)	T6	3	(AL)5(CE)1(NI)2
AL23CE4NI6	Y4Ni6Al23	-	mS66	(12, C2/m)	T8	3	(AL)23(CE)4(NI)6
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(CE)1
AL7CE5SI3	Unknown Structure	-	-	-	-	3	(AL)0.49(CE)0.333333(SI)0.176667
ALCESI2	CeAlSi2	-	hP8	(164, P-3m1)	-	3	(AL)1(CE)1(SI)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL4CE3SI6	Ce3Al4Si6	-	hP13	(164, P-3m1)	-	3	(AL)4(CE)3(SI)6
AL2MZN2	ThCr2Si2	-	tI10	(139, I4/mmm)	Al2CeZn2, Al2LaZn2	3	(AL, ZN)2(AL, ZN)2(CE, LA)1
ALCRFE_H	-	-	hR1512	(148, R-3)	-	2	(AL)0.81(CR, FE)0.19
ALCRFE_E	Al4Cr	-	oS584	(63, Cmcm)	-	3	(AL)0.77(CR)0.21(FE)0.02
ALCRFE_O1	(Al75Cr20Fe5)	-	oI366	(71, Immm)	-	3	(AL)0.76(CR)0.16(FE)0.08
ALCRFE_D3	Unknown Structure	-	-	-	-	3	(AL)0.71(CR)0.16(FE)0.13
AL13CR4SI4	Cr4Al13Si4	-	cF84	(216, F-43m)	Al-Cr-Si, tao 1	3	(AL)13(CR)4(SI)4
AL9CR3SI	Al9Mn3Si (E9c)	E9c	hP26	(194, P6_3/mmc)	Al-Cr-Si, tao 2	3	(AL)9(CR)3(SI)1
ALCRSI_T3	Al11Mn4	-	aP15	(2, P-1)	Al-Cr-Si, tao 3	2	(AL, SI)11(CR)4
ALCRSI_T4	Unknown Structure	-	-	-	Al-Cr-Si, tao 4, AL58CR32SI11	3	(AL)58(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(CU)2(AL)7
AL10CU10FE	(Al10Cu10Fe)	-	oF116	(42, Fmm2)	-	3	(FE)1(AL, CU)10(AL)10
AL2CULI	LiCuAl2	-	hP12	(191, P6/mmm)	Al-Cu-Li ternary phase, i.e. T1	3	(AL)0.5(CU)0.25(LI)0.25

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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(CU)3(MG)6
S_PHASE	MgCuAl2 (E1a)	E1a	oS16	(63, Cmcm)	aka Al2CuMg or S	3	(AL, SI)2(CU)1(MG)1
S_PRIME	MgCuAl2 (E1a)	E1a	oS16	(63, Cmcm)	slightly distorted S_ phase. Strain & interfacial energy need to added	3	(AL)2(CU)1(MG)1
S_DPRIME	Unknown Structure	-	mS*	-	metastable precipitate, related to S_PHASE	3	(AL)5(CU)5(MG)2
T_PHASE	Bergman [Mg32(Al, Zn)49]	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(AL, MG)6(AL, CU, MG, ZN)48(AL)1
AL28CU4MN7	Mn6Cu4Al29	-	oS156	(63, Cmcm)	Al20Cu2Mn3, Tau1	3	(AL)28(MN)7(CU)4
AL11CU5MN3	Unknown Structure	-	oP380	-	-	3	(AL)11(MN)3(CU)5
ALCU3MN2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	3	(AL)1(MN)2(CU)3
AL7CU4NI	(Cu0.8Ni0.2)2.53Al3.5	-	hR14	(166, R-3m)	-	2	(AL)1(FE, CU, NI, VA)1
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(CU)2(W)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL5CU1W2	Al5Cu1W2	-	tI8	(139, I4/mmm)	-	3	(AL)5(CU)1(W)2
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(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
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	Barringerite (Revised Fe2P, C22)	C22	hP9	(189, P-62m)	-	3	(AL)0.333334(CU)0.333333(Y)0.333333
AL6ER2FE11	Th2Zn17	-	hR19	(166, R-3m)	-	3	(AL)6(ER)2(FE)11
AL7ERMG2	Unknown Structure	-	-	-	-	3	(AL)0.66667(ER)0.1(MG)0.23333
T1_ALERSI	PuAl3	-	hP24	(194, P6_ 3/mmc)	-	3	(AL)0.7(SI)0.05(ER)0.25
T2_ALERSI	Y2Al3Si2	-	mS14	(12, C2/m)	-	3	(AL)0.4286(SI)0.2857(ER)0.2857
T3_ALERSI	YAlGe	-	oS12	(63, Cmcm)	-	3	(AL)0.33333(SI)0.33333(ER)0.33333
T4_ALERSI	Unknown Structure	-	-	-	-	3	(AL)0.4(SI)0.2667(ER)0.3333
T5_ALERSI	W2CoB2	-	oI10	(71, Immm)	-	3	(AL)0.2(SI)0.4(ER)0.4
T6_ALERSI	Mo2FeB2	-	tP10	(127, P4/mbm)	-	3	(AL)0.3(SI)0.3(ER)0.4
T7_ALERSI	Tb6Al3Si	-	tI80	(140, I4/mcm)	-	3	(AL)0.3(SI)0.1(ER)0.6

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ER3ZN4AL7	Al11La3	-	oI28	(71, Immm)	-	3	(ER)3(ZN)4(AL)7
ERZN5AL3	Unknown Structure	-	-	-	-	3	(ER)1(ZN)5(AL)3
AL9M2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)	aka Al9FeNi, metastable Al9Fe2	2	(AL)9(CO, FE, NI)2
AL10FE3NI	Co2Al5 (D811)	D811	hP28	(194, P6_ 3/mmc)	-	2	(AL)5(FE, NI)2
AL71FE5NI24	Unknown Structure	-	-	-	-	3	(AL)0.71(FE)0.05(NI)0.24
ALFESI_T9	Fe3Al2Si3	-	aP16	(2, P-1)	Al-Fe-Si ternary phase, tao 1 / tao 9	2	(AL, SI)5(FE)3
ALFESI_T2	Unknown Structure	-	-	-	Al-Fe-Si ternary phase, tao 2, gamma_AlFeSi	4	(AL)0.5(FE)0.2(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(FE)1
ALFESI_T8	Fe3Al2Si4	-	oS36	(63, Cmcm)	Al-Fe-Si ternary phase, AL2FE3SI4, tao 8	2	(AL, SI)2(FE)1
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

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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 (AgAsMg, 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
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(AL, ZN)2
T3_ALLIZN	Unknown Structure	-	-	-	ternary phase T3 in Al-Li-Zn	2	(ALLI, ZN)1(ZN)3
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(AL, CU, LI)2(TI, ZR)1
AL18MG3TM2	Mg3Cr2Al18	-	cF184	(227, Fd-3m)	-	3	(AL, MG)18(AL, MG)3(CR, MN, TI)2
ALMG3NI2	Mn3Ni2Si	-	cF96	(227, Fd-3m)	Ternary phase AlMg3Ni2, cF96, Fd-3m, Ti2Ni type	3	(AL)1(NI)2(MG)3
BETA_PRIME	Mg9Si5	-	hP14	(176, P6_3/m)	metastable precipitate, Mg9Si5/Mg1.8Si, related to Mg2Si	2	(MG)1.8(SI)1
B_PRIME	Unknown Structure	-	-	-	metastable precipitate, B_Prime, Al-containing	3	(AL)3(MG)9(SI)7

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
					Pre-beta phase		
U1_AL2MGSI2	Ce2O2S	-	hP5	(164, P-3m1)	metastable precipitate, U1_Al2MgSi2, Al-containing Pre-beta phase	3	(AL)2(MG)1(SI)2
U2_AL4MG4SI4	MnCuP	-	oP12	(62, Pnma)	metastable precipitate, U2_Al4Mg4Si4, Al-containing Pre-beta phase	3	(AL)1(MG)1(SI)1
BETA_DPRIME	Mg5Si6-a	-	mS22	(12, C2/m)	metastable beta double prime, related to Mg2Si, Mg5Si6, Al2Mg5Si4	3	(AL, SI)2(MG)5(SI)4
AL38MG58SR4	Unknown Structure	-	-	-	-	3	(AL)38(MG)58(SR)4
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(ZN)0.25
AL31MN6NI2	mu-Al4Mn	-	hP574	(194, P6_ 3/mmc)	Orthorhombic, ternary Al-Mn-Ni phase	3	(AL)31(MN)6(NI)2
AL2MN2SI3	(Al2Mn2Si3)	-	hP21	(174, P-6)	the Al-Mn-Si ternary phase, tao1	3	(AL)2(MN)2(SI)3
AL5MN6SI7	CrSi2 (C40)	C40	hP9	(180, P6_222)	the Al-Mn-Si ternary phase, tao2	3	(AL)5(MN)6(SI)7
AL1MN1SI1	TiSi2 (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	the Al-Mn-Si ternary phase, tao3	3	(AL)1(MN)1(SI)1
AL3MNSI2	(Al3MnSi2)	-	tP48	(85, P4/n)	the Al-Mn-Si ternary phase, tao4	3	(AL)3(MN)1(SI)2
AL3MN4SI2	Unknown Structure	-	-	-	the Al-Mn-Si ternary	3	(AL)3(MN)4(SI)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
					phase, tao5		
ALMNSI_T6	Unknown Structure	-	-	-	the Al-Mn-Si ternary phase, tao6	2	(AL, MN)4(SI)1
ALMNSI_T8	Mn3Al10	-	hP26	(194, P6_ 3/mmc)	the Al-Mn-Si ternary phase, tao 8	4	(AL)6(MN)3(AL, MN, SI)3(AL, SI)1
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(CR, FE, MN, MO)4(SI)1(AL, SI)2
AL2MNSI3	Ga5Pd	-	tI24	(140, I4/mcm)	the Al-Mn-Si ternary phase, tao10	3	(AL)2(MN)1(SI)3
AL24MN5ZN	Unknown Structure	-	-	-	-	3	(MN, ZN)5(ZN)1(AL)24
AL9MN2ZN	Unknown Structure	-	-	-	-	3	(MN)2(ZN)1(AL)9
AL11MN3ZN2	Unknown Structure	-	oS152	-	-	3	(MN)3(ZN)2(AL)11
C40_MOSI2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(AL, SI)2(MO)1
C54_MOSI2	TiSi2 (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	-	2	(AL, SI)2(MO)1
B82_OMEGA	InNi2 (B82)	B82	hP6	(194, P6_ 3/mmc)	-	3	(AL)1(NB, TI)1(TI)1
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(NI)1
AL6NI3SI	Ir3Ge7 (D8f)	D8f	cI40	(229, Im-3m)	-	3	(AL)6(NI)3(SI)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALNI16SI9	AlNi16Si9	-	oS104	(63, Cmcm)	-	3	(AL)1(NI)16(SI)9
TINI2AL5	ZrNi2Al5	-	tI16	(139, I4/mmm)	Tau5	3	(TI)14(NI)21(AL)65
G_PHASE	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	3	(AL, NI, TI)16(TI)6(NI)7
H_L21	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	-	3	(AL, NI, TI)0.5(AL, NI, TI)0.5(NI, VA)1
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
ALSC2SI2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	-	3	(AL)1(SC)2(SI)2
AL3Y5	Unknown Structure	-	-	-	stable in Al-Sc-Y	2	(AL)3(SC, Y)5
AL75SC17Y8	Unknown Structure	-	-	-	ternary compound in Al-Sc-Y	3	(AL)75(SC)17(Y)8
ALSISR	BaPtSb	-	hP3	(187, P-6m2)	-	2	(AL, SI)2(SR)1
AL2SI2SR	Ce2O2S	-	hP5	(164, P-3m1)	-	3	(AL)2(SI)2(SR)1
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(SI)1(Y)5
AL3SIY6	Tb6Al3Si	-	tI80	(140, I4/mcm)	Al3SiY6 (T2)	3	(AL)3(SI)1(Y)6
AL7SI3Y5	Unknown Structure	-	-	-	Al7Si3Y5 (T3)	3	(AL)7(SI)3(Y)5
AL2SIY	Unknown Structure	-	-	-	Al2SiY (T4)	3	(AL)2(SI)1(Y)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL11SI9Y10	Unknown Structure	-	-	-	Al11Si9Y10 (T5)	3	(AL)11(SI)9(Y)10
AL2SI2Y	Ce2O2S	-	hP5	(164, P-3m1)	Al2Si2Y (T6)	3	(AL)2(SI)2(Y)1
CULIMG_T	Mg2Ni (Ca)	Ca	hP18	(180, P6_222)	-	3	(CU)1(LI)0.08(MG)1.92
CU16MG6SI7	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	3	(CU)16(MG)6(SI)7
CU3MG2SI	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)	-	3	-
CU5MN4SI	Unknown Structure	-	-	-	-	3	(CU)0.5(MN)0.37(SI)0.13
CUMNZN	Unknown Structure	-	-	-	-	3	-
CU6NISI3	Unknown Structure	-	-	-	-	2	-
CU46NI25SI29	Unknown Structure	-	-	-	-	3	-
FE5NI3SI2	Unknown Structure	-	-	-	-	2	-
ZN13M2	Zn89(Fe0.5Ni0.5)13.8	-	cF432	(216, F-43m)	Fe-Ni-Zn ternary phase	2	-
MG3MNNI2	NiTi2	-	cF96	(227, Fd-3m)	-	3	(MG)3(MN)1(NI)2
MGNI6SI6	Unknown Structure	-	-	-	-	3	(MG)1(NI)6(SI)6
MG2NI3SI	Unknown Structure	-	-	-	-	3	(MG)2(NI)3(SI)1
MG10NI55SI35	Unknown Structure	-	-	-	-	3	(MG)2(NI)11(SI)7
MG2NI16SI11	MgNi8Si5.5	-	hP*	-	-	3	(MG)1(NI)8(SI)5.5
MG5NI9SI	Unknown Structure	-	-	-	-	3	(MG)1(NI)1.8(SI)0.2
MG9NI29SI16	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	3	(MG)9(NI)29(SI)16

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MGNI6ZN6	Unknown Structure	-	-	-	-	4	(MG, ZN)3(MG, NI, ZN)4(NI)1(ZN)2
MN15NI45SI40	Unknown Structure	-	-	-	Mn-Ni-Si ternary phase, T1 or N	3	-
MN15NI50SI35	Unknown Structure	-	-	-	Mn-Ni-Si ternary phase, T2 or PHI	3	-
MN6NI16SI7	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	Mn-Ni-Si ternary phase, T3 or G	3	-
MN1NI1SI1	MnCuP	-	oP12	(62, Pnma)	Mn-Ni-Si ternary phase, T4 or E	3	-
MNNISI_T5	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	Mn- Ni- Si ternary phase, T5 or "tao 1"	2	-
MNNISI_T6	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	Mn-Ni-Si ternary phase, T6 or "tao 2"	2	-
MN3NI2SI	Mn3Ni2Si	-	cF96	(227, Fd-3m)	Mn-Ni-Si ternary phase, T7 or Omega	3	-
MN2NISI	Unknown Structure	-	-	-	Mn-Ni-Si ternary phase, T8 or S	2	-
MN6NISI3	R-(Co, Cr, Mo)	-	hR53	(148, R-3)	Mn-Ni-Si ternary phase, T9 or R	3	-
MN66NI4SI30	Unknown Structure	-	-	-	Mn-Ni-Si ternary phase, T10 or U	3	-
MN52NI29SI19	Unknown Structure	-	-	-	Mn-Ni-Si ternary phase, T11 or W	3	-
MN7NI7ZN86	Unknown Structure	-	cF**	(216, F-43m)	-	3	(MN)0.07(NI)0.07(ZN)0.86
NI2SIZN_T1	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	-	3	-
NI9SI2ZN_T2	Al3Ti (D022)	D022	tI8	(139,	-	3	-

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				I4/mmm)			
NI2SIZN3_T3	Mn3Ni2Si	-	cF96	(227, Fd-3m)	-	3	-
NISIZN_T4	FeSi (B20)	B20	cP8	(198, P2_13)	Ni-Si-Zn tao 4, Ni3Si2Zn1	3	-
Q_ALCUMGSI	Q-(Al, Cu, Mg, Si)	-	hP21	(174, P-6)	Quaternary phase, aka Q, Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 & Al4Cu2Mg8Si7	4	(AL)5(CU)2(MG)8(SI)6
QPRIME	Q-(Al, Cu, Mg, Si)	-	hP21	(174, P-6)	Coherent / semi-coherent version of Q_ ALCUMGSI	4	(AL)5(CU)2(MG)8(SI)6
AL18FE2MG7SI10	Unknown Structure	-	-	-	Quaternary phase, aka Al8FeMg3Si6 and Q_ /PHI/H_PHASE	4	(AL)18(FE)2(MG)7(SI)10

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, C2H7P1S1, C2H7P1_1, C2H7P1_2, 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
LIQUID	Liquid	1	(AG, AL, ALSB, AL2S3, AL2TE3, B, BA, BE, BI, BI2MG3, C, CA, CD, CE, CO, CR, CU, ER, FE, GA, GE, H, HF, IN, K, LA, LI, LIH, LI4/5PB1/5, 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

TCAL11: Current Version Changes

Current Database Version	
Database name (acronym):	TCS Al-based Alloys Database (TCAL)
Database owner:	Thermo-Calc Software AB
Database version:	11.0
First release:	TCAL1 was released in 2011

For earlier changes, see TCAL: Revision History.

TCAL10 to TCAL11

Software release version: 2026b (June 2026)

New Systems

- 4 new binary systems are assessed: Be-Si, Ce-Zn, Er-Li, Er-Zn
- 12 new ternary systems are assessed: Al-Be-Si, Al-Ca-Cu, Al-Ca-Fe, Al-Ca-Si, Al-Ca-Zn, Al-Ce-Zn, Al-Cr-Cu, Al-Cr-Mn, Al-Er-Si, Al-Er-Zn, Al-Er-Zr, Al-La-Zn
- 1 new quaternary system is assessed: Al-Ca-Fe-Si

Other Improvements

- Al4Ba, Al4Ce are merged into Al4M_D13 phase
- CaZn2, LaZn2 are merged into MZn2 phase
- CaZn11, LaZn11 are merged into MZn11 phase
- Ce2Fe17, Fe17Er2 are merged into Fe17M2 phase
- AgEr, AgLa, AgSc, CuEr_B2, CuSc, LiPb_HT, NiHf_HT, NiSc_B2, Sc1Zn1 are merged into B2_BCC phase
- La2Zn17 is merged into M2Zn17 phase

- La3Zn22 is merged into M3Zn22 phase
- ScZn12 is merged into MZn12 phase
- Sc13Zn58 is merged into M13Zn58 phase
- CaCu5_D2D phase is split into Cu5M_D2D, Ni5M_D2D, Zn5M_D2D. Al1Cu4Er1, AlCu5Y, CeCu5, Cu5La1 are merged into Cu5M_D2D phase. LaNi5 is merged into Ni5M_D2D phase. LaZn5 is merged into Zn5M_D2D phase.
- Al11Ce3, Al3Ce_H: crystal structure information is corrected
- Al4Mn_R: crystal structure information for prototype lambda-Al4Mn is corrected
- Element Y: H298-H0, S298 are updated to be consistent with the Scientific Group Thermodata Europe (SGTE) PURE 5 database

Elastic Properties

- Added elastic properties for BCC (A2 and B2), FCC (A1 and L12), and HCP (A3) phases

Thermophysical Properties

- Added surface tensions of missing endmembers and interactions
- Added viscosities of Se-containing binary interactions
- Updated thermal conductivity and electrical resistivity of B
- Corrected volume of Al_5Fe_2

TCAL: Revision History

For the most recent changes, see TCAL11: Current Version Changes.

TCAL9.1 to TCAL10

Software release version: 2025b (June 2025).

Binary Systems

- Improvements make it possible to get reasonable calculation results of Sn solubility in (Al). The descriptions involving Sn are improved in these systems:
  - Al-Sn, B-Sn, Bi-Sn, Cd-Sn, Cu-Sn, Mg-Sn, Mn-Sn, Ni-Sn, Pb-Sn, Sn-Sr, and Sn-Ti.

Ternary Systems

- New assessments for 3 ternaries are added to have a better understanding of grain refiners in processing of aluminum alloys:
  - Al-B-Ti, Al-Ti-Zr, and Al-B-Zr.
- The new assessment of Al-Cr-Fe plus the improvements in Al-Fe-Mn and Al-Cu-Fe are incorporated to facilitate investigations on aluminum recycling.
- The updated assessments of Al-Bi-Sn, Al-Mg-Sn, Al-Pb-Sn, and Al-Si-Sn, enhance the accuracy of calculations on Sn-containing alloys.

Other Updates

- For unary tin, the descriptions of FCC_A1 and HCP_A3 are updated to be consistent with the Scientific Group Thermodata Europe (SGTE) PURE database.
- AlB2_C32 phase is renamed to MB2_C32.
- Al9CO2 phase is merged into Al9M2 phase.
- The description of Ag-La is refined by suppressing the inverse liquid miscibility gap and the stable high temperature BCC_A2 phase.

- The ternary assessment of Mg-Mn-Ni is improved to give more reliable calculation results on invariant reactions and the liquidus projection. The chemistry of the ternary phase is updated to be Mg_3MnNi_2.

Thermophysical Properties

- Added viscosity, surface tension and THCD/ELRS descriptions for the above newly added systems.
- For unary yttrium, molar volume descriptions of HCP_A3, BCC_A2, FCC_A1 are corrected.
- For unary hafnium, thermal conductivity description of liquid phase is corrected.

TCAL9.0 to TCAL9.1

Software release version: 2024b (June 2024)

- Thermal conductivity and electrical resistivity of liquid Al were re-assessed.
- Electrical resistivity of liquid phase in Al-Si system was re-assessed.
- Surface tension parameters were updated for the systems Ag-Cu, Bi-Sn, Cu-Sn, and Ag-Cu-Sn.
- Viscosity parameters were updated for the systems Ag-Cu, Al-Sb, Al-Te, B-Bi, B-Mg, B-Pb, B-Sn, B-Sr, B-Zn, Bi-C, Bi-Fe, Bi-Mo, Bi-Nd, C-Ca, C-Pb, C-Sn, Cr-Pb, Mg-Sb, Mg-Sn, Mo-Pb, Mo-Sn, Nb-Pb, Pb-Ti, Pb-V, and Cu-Ti-Zr
- The FCC_A1 parameters were corrected in the Cu-Hf system.

TCAL8.2 to TCAL9.0

Software release version: 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.

TCAL8.1 to TCAL8.2

Software release version: 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 version: 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 version: 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)

- 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.