TCS Mg-based Alloys Database (TCMG9)

Technical Information

Available Starting with Thermo-Calc Version 2026b

Document created 12-Jun-26

Contents

About the TCS Mg-based Alloys Database (TCMG)

TCS Mg-based Alloys Database (TCMG) is a thermodynamic and properties database for magnesium-based alloys. It can be used for a wide range of compositions from pure magnesium to very complex magnesium-based commercial magnesium alloys. It can be used for calculating phase diagrams and thermodynamic properties of assessed systems, but also for predicting phase equilibria and simulating solidification processes for a wide range of magnesium alloys of industrial relevance, including:

- Mg-Al based alloys such as AZ, AE, AJ, AM, AS, and AX
- Mg-Zn-Zr alloys such as ZK60
- Mg-RE (rare earth)-Zn (EZ) alloys
- Mg-RE-Zr alloys such as WE
- Experimental magnesium alloys under development

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

- Electrical resistivity of all solid phases and liquid
- Thermal conductivity of all solid phases and liquid
- Molar volume and thermal expansivity of all solid phases and liquid
- Viscosity of liquid
- Surface tension of liquid
- Elastic moduli and elastic constants

TCMG9 Thermophysical Properties and TCMG9 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 Mg-alloys Mobility Database (MOBMG) 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 is MOBMG2.

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.

The TCS Mg-based Alloys Database (TCMG) enables predictions (such as multi-component phase equilibria calculations, equilibrium solidification simulation and Scheil solidification simulation) to be made for multicomponent systems and alloys of industrial importance. This means that the database can be utilized to extrapolate to higher-order systems by combining several critically assessed systems.

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 TCMG9. To review the most recent changes, see TCMG9: Current Version Changes.
- To review additional older changes, see TCMG: Revision History.

TCS Mg-based Alloys Database (TCMG) 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 Magnesium-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 magnesium including links to resources such as examples, publications, and more.

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.

TCMG9 Elements, Systems, and Phases

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

Included Elements

There are 33 elements included in this version of the database.

Included Elements									
Ag	Al	Bi	Ca	Ce	Cu	Dy	Er	Fe	Ga
Gd	H	Ho	In	K	La	Li	Mg	Mn	Na
Nd	Ni	Pr	Sb	Sc	Si	Sm	Sn	Sr	Th
Y	Zn	Zr							

Assessed Systems and Phases

A hybrid approach of experiments, first-principles calculations and CALPHAD modeling have been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges.

All the stable solution phases and intermetallic compounds that exist in each assessed system are included. Note that in most cases phases having the same crystal structure had been merged as the same phase.

The most recent version of the database contains:

- 232 assessed binary systems
- 147 assessed ternary systems
- 5 assessed quaternary systems
- 602 phases

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`.

TCMG9 Properties Data

In this section:

TCMG9 Thermophysical Properties

This section summarizes the thermophysical properties available in the TCS Mg-based Alloys Database (TCMG).

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 Magnesium-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 magnesium including links to resources such as examples, publications, and more.

Learn More

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.

TCMG9 Elastic Properties

This section summarizes the elastic properties in the TCS Mg-based Alloys Database (TCMG).

Interactions have been either assessed or estimated for every binary combination in the common solution phases, including liquid, FCC_A1, BCC_A2, and HCP_A3.

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 Magnesium-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 magnesium including links to resources such as examples, publications, and more.

Learn More

The elastic properties (elastic moduli and elastic constants) are included with the database as of TCMG9 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.

TCMG9 Systems

In this section:

TCMG9 Assessed Binary Systems

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

	Ag	Al	Bi	Ca	Ce	Cu	Dy	Er	Fe	Ga	Gd	H	Ho	In	K	La	Li	Mg	Mn	Na	Nd	Ni	Pr	Sb	Sc	Si	Sm	Sn	Sr	Th	Y	Zn	Zr
Ag	Ag																																
Al	x	Al																															
Bi			Bi																														
Ca	x	x	x	Ca																													
Ce	x	x		x	Ce																												
Cu	x	x		x	x	Cu																											
Dy		x					Dy																										
Er	x	x						Er																									
Fe		x			x	x			Fe																								
Ga										Ga																							
Gd	x	x			x	x			x		Gd																						
H					x	x						H																					
Ho		x											Ho																				
In	x	x		x	x	x			x		x			In																			
K														x	K																		
La	x	x			x	x					x	x		x		La																	
Li		x		x		x					x			x			Li																
Mg	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	Mg															
Mn		x	x	x	x	x			x		x			x		x		x	Mn														
Na		x		x										x	x		x	x		Na													
Nd	x	x		x	x	x	x		x		x	x		x		x		x	x		Nd												
Ni	x	x		x	x	x			x		x	x		x		x		x	x			Ni											
Pr	x	x				x			x					x				x	x			x	Pr										
Sb																		x						Sb									
Sc	x	x				x			x					x				x	x						Sc								
Si	x	x		x		x			x		x			x		x	x	x	x			x			x	Si							
Sm		x									x							x									Sm						
Sn	x	x	x	x	x	x			x					x		x	x	x	x		x	x	x	x		x	x	Sn					
Sr	x	x		x	x	x								x				x	x		x							x	Sr				
Th						x			x					x				x											Th				
Y	x	x		x	x	x			x		x			x		x		x	x		x	x	x			x	x	x	x	Y			
Zn	x	x	x	x	x	x	x	x	x		x	x	x	x		x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	Zn	
Zr	x	x			x	x	x		x		x			x			x	x	x		x	x			x	x		x		x	x	x	Zr

TCMG9 Assessed Ternary Systems

These are the assessed ternary systems in this version of the database.

Assessed Ternary Systems							
Ag-Al-Cu	Ag-Al-Mg	Ag-Al-Sc	Ag-Cu-Mg	Ag-Er-Mg	Ag-Gd-Mg	Ag-In-Mg	Ag-In-Sn
Ag-La-Mg	Ag-Mg-Sn	Ag-Mg-Y	Ag-Pr-Sn	Al-Ca-Mg	Al-Ca-Sr	Al-Ca-Zn	Al-Ce-Mg
Al-Ce-Mn	Al-Cu-Mg	Al-Cu-Si	Al-Dy-Mg	Al-Er-Mg	Al-Fe-Mg	Al-Fe-Mn	Al-Gd-Mg
Al-Gd-Mn	Al-Ho-Mg	Al-In-Mg	Al-La-Mg	Al-La-Mn	Al-La-Y	Al-Li-Mg	Al-Mg-Mn
Al-Mg-Na	Al-Mg-Nd	Al-Mg-Ni	Al-Mg-Pr	Al-Mg-Sc	Al-Mg-Si	Al-Mg-Sm	Al-Mg-Sn
Al-Mg-Sr	Al-Mg-Y	Al-Mg-Zn	Al-Mg-Zr	Al-Mn-Y	Al-Y-Zn	Bi-Ca-Mg	Bi-Mg-Mn
Bi-Mg-Sn	Bi-Mg-Zn	Ca-Ce-Mg	Ca-Cu-Mg	Ca-Gd-Mg	Ca-Li-Mg	Ca-Mg-Nd	Ca-Mg-Ni
Ca-Mg-Si	Ca-Mg-Sn	Ca-Mg-Sr	Ca-Mg-Y	Ca-Mg-Zn	Ca-Mg-Zr	Ca-Sr-Zn	Ce-Gd-Mg
Ce-H-Mg	Ce-La-Mg	Ce-Mg-Mn	Ce-Mg-Nd	Ce-Mg-Si	Ce-Mg-Sn	Ce-Mg-Sr	Ce-Mg-Y
Ce-Mg-Zn	Ce-Mg-Zr	Cu-Fe-Mg	Cu-H-Mg	Cu-In-Mg	Cu-Li-Mg	Cu-Mg-Mn	Cu-Mg-Ni
Cu-Mg-Si	Cu-Mg-Sn	Cu-Mg-Y	Cu-Mg-Zn	Cu-Mg-Zr	Dy-Mg-Sm	Dy-Mg-Zn	Er-Gd-Mg
Er-Mg-Zn	Fe-Mg-Mn	Fe-Mg-Ni	Fe-Mg-Si	Fe-Mg-Zn	Gd-La-Mg	Gd-Li-Mg	Gd-Mg-Mn
Gd-Mg-Nd	Gd-Mg-Sm	Gd-Mg-Sr	Gd-Mg-Y	Gd-Mg-Zn	Gd-Mg-Zr	H-La-Mg	H-Mg-Nd
H-Mg-Ni	Ho-Mg-Zn	In-Li-Mg	In-Mg-Sn	In-Sn-Zn	La-Mg-Nd	La-Mg-Ni	La-Mg-Si
La-Mg-Sn	La-Mg-Y	La-Mg-Zn	Mg-Mn-Nd	Mg-Mn-Ni	Mg-Mn-Sc	Mg-Mn-Si	Mg-Mn-Sn
Mg-Mn-Sr	Mg-Mn-Y	Mg-Mn-Zn	Mg-Nd-Sn	Mg-Nd-Sr	Mg-Nd-Y	Mg-Nd-Zn	Mg-Nd-Zr
Mg-Ni-Y	Mg-Ni-Zn	Mg-Pr-Sn	Mg-Pr-Y	Mg-Pr-Zn	Mg-Sb-Sn	Mg-Sc-Zn	Mg-Si-Sn
Mg-Si-Y	Mg-Si-Zn	Mg-Sm-Y	Mg-Sn-Sr	Mg-Sn-Y	Mg-Sn-Zn	Mg-Sr-Zn	Mg-Sr-Zr
Mg-Y-Zn	Mg-Y-Zr	Mg-Zn-Zr					

TCMG9 Assessed Quaternary Systems

These are the assessed quaternary systems in this version of the database.

Quaternary Systems
Mg-Al-Ca-Zn
Mg-Al-Ca-Sr
Mg-Al-Cu-Si
Mg-Al-Mn-Zn
Mg-Gd-Nd-Y

TCMG9 Phases

In this section:

Common Phases for Magnesium Alloys

TCMG9 Models for the Included Phases

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

Name in the Database	*Common Name and Description*
LIQUID	Liquid phase, which covers the melt of Mg alloys
HCP_A3	HCP_A3 type solid solution phase, which covers the (Mg) matrix phase
GDMG5	GdMg5-based Mg-rich phase, dissolving other elements, especially rare earth elements
MG24R5	Mg-rich phase, including $Mg_{24}Y_5$, $Mg_{24}Ho_5$, $Mg_{24}Dy_5$ and $Mg_{24}Er_5$
AL12MG17_A12	Al-Mg compound that forms in Mg-Al based alloys
AL13CEMG6	Laves_C36-type ternary phase in Al-Ce-Mg
ALCUMG_Q	Al-Cu-Mg ternary compound
ALLIMG_T	Al-Li-Mg ternary compound
LPSO_14H	Long-period stacking-ordered (LPSO) structure, type 14H
LPSO_18R	Long-period stacking-ordered (LPSO) structure, type 18R
I_MGRZN	Icosahedral quasi-crystalline phase in Gd/Y-Mg-Zn system
Z_MGRZN	Hexagonal Z phase in Gd-Mg-Zn. Also known as the S-phase, hP92
M_MGRZN	Hexagonal M phase in Gd-Mg-Zn, hP238, related to the S/Z- and L-phase
L_MGRZN	Hexagonal L phase in Gd-Mg-Zn, hP480, related to the S/Z- and M-phase
F_MGGDZN	$Gd_{20}Mg_{19}Zn_{81}$ and $Ce_{20}Mg_{19}Zn_{81}$. Also known as the F-phase
L21_RMGZN2	Heusler phase in Mg-alloys, including $CeMgZn_2$, $GdMgZn_2$ and $MgZn_2Y$. Also known as the W-phase. Related to MG3R_D03
C15_LAVES	Laves_C15 phase, which covers some Mg-compounds, Al_2Ca, Al_2Ce, Cu_2Mg, Fe_2Gd and Mg_2Gd etc.

Name in the Database	*Common Name and Description*
C36_LAVES	Laves_C36 phase, which covers $MgNi_2$, $(Cu,Zn)_2Mg$ and $(Al,Mg)_2Ca$
C14_LAVES	Laves_C14 phase, which covers some Mg-compounds, Al_2Zr, $CaLi_2$, $CaMg_2$, Mg_2Sr, Mg_2Y, $MgZn_2$, Mn_2Zr and Na_2K etc.
MG17SR2	$Mg_{17}Sr_2$ and Ce_2Mg_{17}, also Ce_2Fe_{17}, Gd_2Fe_{17}, Gd_2Ni_{17}, La_2Mg_{17}, La_2Zn_{17}, Pr_2Zn_{17}, Th_2Zn_{17} and Y_2Zn_{17}
MG3R_D03	Stable or metastable phase in Mg-RE (rare earth) alloys, Mg_3Ce, Mg_3Gd, Mg_3Nd, Mg_3Pr, Mg_3La and Mg_3Sm
AL11R3	$Al_{11}Ce_3$, $Al_{11}La_3$_L, $Al_{11}Nd_3$_L, $Al_{11}Pr_3$_L, $Zn_{11}Pr_3$ and $Zn_{11}Y_3$
MG12R	Mg-rich phase, may form in $Mg_{12}Ce$, $Mg_{12}La$, $Mg_{12}Pr$, also $Zn_{12}Y$, $Mn_{12}Gd$ and $Mn_{12}Y$ and more systems
MG41R5	Mg-rich phase, may form in $Mg_{41}La_5$, $Mg_{41}Ce_5$, $Mg_{41}Nd_5$, $Mg_{41}Pr_5$ and $Mg_{41}Sm_5$ and more systems
MG2SI_C1	Mg_2Si, also Si_2Ni, Mg_2Sn
MG7RE	Metastable precipitate in Mg-RE(rare earth), including Mg_7Gd, Mg_7Y and Mg_7Nd, as well as dissolving Zn
MG3R_D019	Metastable precipitate in Mg-RE(rare earth), including Mg_3Gd, Mg_3Y and Mg_3Nd, as well as dissolving Zn
MG2NIH4	High-pressure phase in the Mg-Ni-H system, important to hydrogen storage
MGH2_C4	MgH_2, important to hydrogen storage

TCMG9 Models for the Included Phases

Phase Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
GAS	Gas	-	-	-	-	1	(AL, AL2, CE, CU, CU2, CUH, H, H2, MG, MG2, HMG, LA, NI, NI2, ZN, AG, AG1AL1, AG1CU1, AG1H1, AG2, AL1CU1, AL1H1, AL1H2, AL1H3, AL1SB1, BI, BI1H1, BI1H3, BI2, BI3, BI4, CA, CA1H1, CA2, DY, ER, FE, FE1H1, FE2, GA, GA1H1, GA1SB1, GA1SB2, GA2, GD, H1IN1, H1K1, H1LI1, H1MN1, H1NA1, H1NI1, H1SB1, H1SI1, H1SR1, H1ZN1, H1ZR1, H2SI1, H3SB1, H3SI1, H4SI1, H4SN1, H6SI2, HO, IN, IN1SB1, IN1SB2, IN2, K, K1LI1, K1NA1, K2, LI, LI1NA1, LI2, MN, NA, NA2, ND, PR, SB, SB2, SB3, SB4, SC, SI, SI2, SI3, SM, SN, SN2, SR, SR2, TH, Y, ZR, ZR2)1
LIQUID	Liquid	-	-	-	-	1	(AG, AL, AL2SM, BI, BI3CA5_N, BI2MG3, CA, CA2SN, CE, CU, DY, ER, FE, GA, GD, H, HO, IN, K, LA, LI, MG, MG3SB2, MG2SN, MN, NA, ND, NI, PR, SB, SC, SI, SM, SN, SNSR2, SR, TH, Y, ZN, ZR)1
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	-	2	(AG, AL, BI, CA, CE, CU, DY, ER, FE, GD, HO, IN, K, LA, LI, MG, MN, NA, ND, NI, PR, SC, SI, SM, SN, SR, TH, Y, ZN, ZR)1(H, VA)3
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	A B2 phase described with the partitioning model and having a contribution from its disordered counterpart.	3	(AG, AL, BI, CA, CE, CU, DY, ER, FE, GD, HO, IN, K, LA, LI, MG, MN, NA, ND, NI, PR, SC, SI, SM, SN, SR, TH, Y, ZN, ZR)0.5(AG, AL, BI, CA, CE, CU, DY, ER, FE, GD, HO, IN, K, LA, LI, MG, MN, NA, ND, NI, PR, SC, SI, SM, SN, SR, TH, Y, ZN, ZR)0.5(H, VA)3
B2_BCC	CsCl (B2)	B2	cP2	(221, Pm-3m)	B2 phases modeled separately from A2	2	(AG, CU, NI, ZN)0.5(CE, GD, ND, Y, PR, ZR)0.5
B2_MGR	CsCl (B2)	B2	cP2	(221, Pm-3m)	LaMg, MgNd, NdZn, CeMg, CeZn, MgY, YZn, GdMg, GdZn, MgSm, AgMg	2	(AG, AL, CU, IN, LI, MG, MN, ND, SN, ZN)0.5(AG, CA, CE, CU, DY, ER, GD, HO, IN, LA, MG, ND, PR, SC, SM, SN, Y, ZR)0.5
BCT_A5	beta-Sn (A5)	A5	tI4	(141, I4_1/amd)	-	1	(AG, AL, BI, IN, SB, SN, SR, ZN)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	2	(AL, CU, FE, IN, MG, MN, NI, SI, SN, ZN, ZR)1(VA)1
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)	-	2	(AG, AL, CA, CE, CU, FE, IN, MG, MN, NI, SI, SN, ZN, ZR)1(VA)1
DHCP	alpha-La (A3')	A3'	hP4	(194, P6_ 3/mmc)	-	2	(AG, AL, CA, CE, CU, DY, GD, IN, LA, MG, MN, ND, NI, PR, SN, SR, Y, ZR)1(VA, H)2
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	-	1	(AL, SI, SN, ZN)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	-	2	(AG, AL, BI, CA, CE, CU, ER, FE, GD, IN, K, LA, LI, MG, MN, NA, ND, NI, PR, SC, SI, SM, SN, SR, TH, Y, ZN, ZR)1(H, VA)1
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	L12 phases, CaSn3, LaSn3, Mg1.2In2.8, CeIn3, NdIn3, ScIn3, PrIn3, ThIn3	2	(AL, CA, CE, IN, LA, MG, ND, PR, SC, SM, SN, TH, Y)1(AG, AL, CE, IN, MG, ND, NI, PR, SN, ZR)3
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	-	2	(AG, AL, BI, CA, CE, CU, DY, ER, FE, GA, GD, HO, IN, K, LA, LI, MG, MN, NA, ND, NI, PR, SB, SC, SI, SM, SN, SR, TH, Y, ZN, ZR)1(H, VA)0.5
FE2SI	AlNi2	-	hP6	(164, P-3m1)	-	2	(FE)2(SI)1
FESI2_H	FeSi2-h	-	tP3	(123, P4/mmm)	-	2	(FE)3(MG, SI)7
FESI2_L	FeSi2-l	-	oS48	(64, Cmce)	-	2	(FE)1(SI)2
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	Al2Zr, CaLi2, CaMg2, Mg2Sr, Mg2Y, MgZn2, Mn2Zr, Na2K	2	(AG, AL, CA, CU, GD, LI, MG, MN, NA, NI, SR, Y, ZN)2(AL, CA, CE, CU, DY, ER, GD, HO, K, LA, MG, MN, ND, PR, SC, SR, TH, Y, ZR, ZN, VA)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	It includes 18 compounds, e.g. Al2Ca, Al2Ce, Cu2Mg, Fe2Gd, Mg2Gd	3	(AL, CA, DY, CU, ER, FE, GD, HO, IN, LA, LI, MG, MN, ND, NI, SI, SN, Y, ZN, ZR)2(AL, CA, CE, CU, DY, ER, FE, GD, HO, IN, LA, LI, MG, ND, NI, PR, SC, SI, SM, SN, SR, TH, Y, ZN, ZR)1(H, VA)2
C36_LAVES	MgNi2 Hexagonal Laves	C36	hP24	(194, P6_	MgNi2 type	2	(AL, CU, FE, GD, MG, MN, NI, ZN)2(AL, CA, CU, DY, ER, GD, HO, MG, NI, TH,

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
	(C36)			3/mmc)	phase, also includes MgNi2, (Cu, Zn)2Mg, (Al, Mg)2Ca		ZN, ZR)1
MG2SI_C1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is also Si2Ni & Mg2Sn	2	(BI, MG, SI)2(BI, MG, NI, SI, SN)1
MSI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	FeSi & MnSi	2	(FE, MN)1(MG, SI)1
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)	Fe5Si3, Gd5Si3, Mn5Si3, Y5Si3, Zr5Si3, also LA5SN3(HT)	2	(CE, FE, GD, LA, MN, ND, Y, PR, SM, ZR)5(IN, SI, SN)3
AG51R14	Ag51Gd14	-	hP68	(175, P6/m)	AG51PR14, AG51CE14, AG51LA14	2	(AG, MG)51(CE, ER, LA, PR)14
MG41R5	Ce5Mg41	-	tI92	(87, I4/m)	Mg41La5, Mg41Ce5, Mg41Nd5, Mg41Pr5, Mg41Sm5	2	(MG, ZN)41(DY, CA, CE, GD, LA, ND, PR, SM, SR, Y)5
XZN13	NaZn13 (D23)	D23	cF112	(226, Fm-3c)	CaZn13, LaZn13, NaZn13, SrZn13	2	(CA, LA, NA, SR)1(ZN)13
AL3R	AL3HO	-	hR20	(166, R-3m)	-	2	(AL)3(ER, DY, HO)1
MG3R_D03	BiF3 (D03)	D03	cF16	(225, Fm-3m)	MG3CE, GDMG3, MG3ND, MG3PR, MG3LA, Mg3Sm	2	(AG, LI, MG, ZN)3(CA, CE, DY, ER, GD, LA, MG, MN, ND, PR, SM, SR, Y, ZR)1
L21_RMGZN2	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	isostructural to GdMg3: CeMgZn2, GdMgZn2, MgZn2Y, aka W	3	(CE, GD, Y)1(MG)1(MG, ZN)2
ALR_OS16	AlCe	-	oS16	(63, Cmcm)	a phase based on ALCE, ALLA, ALPR	2	(AL)1(CE, LA, PR)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
					(rt)		
CA5X3	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	CA5SI3, CA5SN3, CA5AG3, CA5ZN3, also La5Si3	2	(CA, LA, SR)5(AG, SI, SN, ZN)3
RHOMBO_A7	alpha-As (A7)	A7	hR2	(166, R-3m)	based on Bi and Sb	1	(BI, SB, SN, ZN)1
RM5	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)	-	2	(CA, CE, GD, LA, ND, PR, SR, TH, Y)1(AG, CU, FE, IN, MG, NI, ZN)5
CU6R	CeCu6	-	oP28	(62, Pnma)	-	2	(CU)6(CE, ND, GD, LA)1
XZ2_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	-	2	(AG, AL, CU, FE, NI, SI, ZN, ZR)1(AL, FE, IN, SN, TH, ZR)2
X3NI	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	-	2	(AL, GD, LA, NI, PR, Y)3(NI, SI)1
MR_B27	FeB (B27)	B27	oP8	(62, Pnma)	-	2	(CU, NI, SI, ZN)1(CE, GD, LA, ND, PR, SR, Y, ZR)1
M2R	KHg2	-	oI12	(74, Imma)	-	2	(AG, AL, CU, MG, ZN)2(CA, CE, DY, ER, GD, HO, LA, ND, PR, SR, Y)1
M3R	Ni3Pu	-	hR12	(166, R-3m)	-	2	(FE, NI)3(CA, GD, LA, MG, PR, Y, TH)1
MG17SR2	Th2Zn17	-	hR19	(166, R-3m)	-	3	(CE, GD, LA, ND, PR, SR, TH, Y)2(AG, AL, FE, MG, NI, ZN)17(H, VA)14
CE2ZN17	Th2Zn17	-	hR19	(166, R-3m)	-	2	(CE)0.105(MG, ZN)0.895
FE17ND2	Th2Zn17	-	hR19	(166, R-3m)	-	2	(FE)1(ND)0.1176
FE17PR2	Th2Zn17	-	hR19	(166, R-3m)	-	2	(FE)17(PR)2
FE17TH2	Th2Zn17	-	hR19	(166, R-3m)	-	2	(FE)0.89(TH)0.11
MN17ND2	Th2Zn17	-	hR19	(166, R-3m)	-	2	(MN)17(ND)2
NI7PR2	Th2Zn17	-	hR19	(166, R-3m)	-	2	(NI)0.7778(PR)0.2222

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
M23R6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	2	(AL, FE, MG, MN, ZN)23(CE, GD, ND, PR, SR, TH, Y, ZR)6
XR	CrB (B33)	B33	oS8	(63, Cmcm)	-	2	(AG, AL, MG, NI, SI, SN, ZN)1(CA, CE, GD, LA, ND, PR, SC, SR, Y, ZR)1
R3ZN22	Ce3Zn22	-	tI100	(141, I4_ 1/amd)	-	2	(CE, GD, LA, ND, PR)0.12(ZN)0.88
RZN11	BaCd11	-	tI48	(141, I4_ 1/amd)	-	2	(CA, LA, ND, PR)1(MG, ZN)11
M5R	AuBe5 (C15b)	C15b	cF24	(216, F-43m)	-	2	(CU, NI, ZR)5(GD, ZR, VA)1
XZ2_C37	Co2Si (C37)	C37	oP12	(62, Pnma)	-	2	(AL, SI, SN)1(CA, MG, DY, ER, GD, HO, ND, NI, PR, SM, SR, Y)2
ALR_OP16	DyAl	-	oP16	(57, Pbcm)	-	2	(AL)1(DY, ER, GD, HO, ND, PR, SM)1
AL11LA3_H	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	2	(AL)11(LA, SM)3
AL11ND3_H	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	2	(AL)11(ND)3
AL11PR3_H	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	2	(AL)11(PR)3
AL11R3	Al11La3	-	oI28	(71, Immm)	-	2	(AL, ZN)11(CE, LA, ND, PR, Y)3
GD3ZN11	Al11La3	-	oI28	(71, Immm)	-	2	(DY, GD)0.214(ZN)0.786
CE3ZN11	Al11La3	-	oI28	(71, Immm)	-	2	(CE)0.214(MG, ZN)0.786
R7M3	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)	-	2	(CE, LA, PR, TH)0.7(FE, NI)0.3
MG12R	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)	-	2	(AG, AL, MG, MN, ZN)12(CE, DY, ER, GD, HO, LA, ND, PR, SC, SR, Y)1
RSI2	GdSi1.4	-	oI12	(74, Imma)	-	2	(LA, Y)1(SI)2
RZN3	Zn3Y	-	oP16	(62, Pnma)	-	2	(DY, ER, GD, HO, ND, PR, Y)1(ZN)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL2R3	Zr3Al2	-	tP20	(136, P4_2/mnm)	-	2	(AL, ZN)0.4(DY, ER, HO, ZR, Y)0.6
R5SI4	Si4Zr5	-	tP36	(92, P4_12_12)	-	2	(LA, MG, ZR)5(SI)4
M10ZR7	Ni10Zr7	-	oS68	(64, Cmce)	-	2	(CU, NI)10(ZR)7
R3SI2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	-	2	(LA, MG, ZR)3(SI)2
R2NI7	Ce2Ni7	-	hP36	(194, P6_3/mmc)	-	2	(CE, LA, MG, Y)2(NI)7
RZN5	ErZn5	-	hP36	(194, P6_3/mmc)	-	2	(ER, HO)1(ZN)5
ALLA3	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(AL)1(LA)3
ALND3	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(AL)1(ND)3
AL3LA	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(AL)3(CE, GD, LA, ND, PR, SM, Y)1
MG3R_D019	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(MG)3(GD, ND, Y, ZN)1
SC3IN	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(SC)3(IN)1
NI3IN1	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(NI)3(IN)1
IN3SR1	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(IN)0.75(SR)0.25
NI3ZR	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)	-	2	(NI)3(ZR)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL4SR	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	2	(AL, MG)0.8(CA, SR)0.2
AL4CA	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	2	(AL, MG)4(CA, SM, SR)1
AL4CE	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	2	(AL)0.8(CE)0.2
KIN4	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	2	(IN)0.8(K)0.2
THZN4	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	2	(TH)1(ZN)4
AL4SM_D1B	Al4U (D1b)	D1b	oI20	(74, Imma)	-	2	(AL)4(SM)1
RHOMB_C19	alpha-Sm (C19)	C19	hR3	(166, R-3m)	-	1	(AL, GD, MG, SM, Y)1
NI2IN_HT	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	3	(NI, VA)1(NI)1(IN, NI)1
NI2IN_LT	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(NI, LA)2(IN)1
X2IN	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(CE, GD, MN, ND, SC, PR, Y, ZR)2(AL, IN, SN)1
NI3SN2_H	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	3	(NI)0.33333(NI, SN)0.33334(SN)0.33333
ALCU_EPS	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	2	(AL, CU, ZN, NI)1(CU, FE)1
CU2IN_B82	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	3	(CU, MG)1(CU, VA)1(IN)1
ETA	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	-	3	(CU)1(CU, SN)1(SN)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FE5SN3	InNi2 (B82)	B82	hP6	(194, P6_ 3/mmc)	-	2	(FE)5(SN)3
MG2NI9Y	LaMg2Ni9	-	hR36	(166, R-3m)	-	3	(MG)2(NI)9(Y)1
LPSO_14H	LPSO-14H	-	hP170	(193, P6_ 3/mcm)	-	4	(MG)70(CE, DY, ER, GD, HO, LA, MG, ND, PR, SC, SM, Y)8(AL, CU, MG, NI, ZN)6(MG)1
LPSO_18R	LPSO-18R	-	mS146	(12, C2/m)	-	4	(MG)58(CE, DY, ER, GD, HO, LA, MG, ND, PR, SC, SM, Y)8(AL, CU, MG, NI, ZN)6(MG)1
CE13ZN58	Gd13Zn58	-	hP142	(194, P6_ 3/mmc)	-	2	(CE)0.183(ZN)0.817
GD13ZN58	Gd13Zn58	-	hP142	(194, P6_ 3/mmc)	-	2	(DY, ER, GD, HO, SC)0.183(MG, ZN)0.817
PR13ZN58	Gd13Zn58	-	hP142	(194, P6_ 3/mmc)	-	2	(PR)0.1831(ZN)0.8169
GD2ZN17_L	Ni17Th2	-	hP38	(194, P6_ 3/mmc)	-	2	(DY, ER, GD, HO)0.105(AL, MN, ZN)0.895
GD2ZN17_H	Th2Zn17	-	hR19	(166, R-3m)	-	2	(DY, ER, GD, HO, SM)0.105(ZN)0.895
I_MGRZN	Quasicrystal	-	-	-	-	3	(DY, ER, GD, HO, Y)0.1(MG, ZN)0.3(MG, ZN)0.6
LAMGZN_T1	Unknown Structure	-	-	-	-	2	(LA)0.08(MG, ZN)0.92
LAMGZN_T2	Unknown Structure	-	-	-	-	3	(LA)0.21(ZN)0.57(MG, ZN)0.22
LAMGZN_T3	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	-	3	(DY, ER, HO, LA, PR)1(MG, ZN)2(MG)1
LI2MGIN	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	-	3	(LI)2(MG)1(IN)1
AG2R_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(AG)2(Y, ER)1
CU2SC_C11B	MoSi2 (C11b)	C11b	tI6	(139,	-	2	(AL, AG, CU)2(SC)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				I4/mmm)			
CUZR2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(AG, CU, ZN)1(ZR)2
Y13ZN58	Y13Zn58	-	hP146	(194, P6_3/mmc)	-	2	(Y)13(ZN)58
ND13ZN58	Y13Zn58	-	hP146	(194, P6_3/mmc)	-	2	(ND)0.183(ZN)0.817
T1_MGZNZR	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	-	3	(MG)0.2633(ZN)0.6667(ZR)0.07
T2_MGZNZR	Unknown Structure	-	-	-	-	3	(MG)0.1633(ZN)0.6667(ZR)0.17
T3_MGZNZR	Unknown Structure	-	-	-	-	3	(MG)0.1133(ZN)0.6667(ZR)0.22
T4_MGZNZR	Unknown Structure	-	-	-	-	3	(MG)0.086(ZN)0.84(ZR)0.074
AL3DY_D024	Ni3Ti (D024)	D024	hP16	(194, P6_3/mmc)	-	2	(AL)3(DY)1
R5SN3_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	-	2	(LA, PR, Y)5(SN)3
R4SN3_D73	Th3P4 (D73)	D73	cI28	(220, I-43d)	-	2	(SM)4(SN)3
R5SN4_OP36	Sm5Ge4	-	oP36	(62, Pnma)	-	2	(CE, LA, ND, PR, SM, Y)5(SN)4
ND4SN5	Unknown Structure	-	-	-	-	2	(ND)4(SN)5
PR5SN4_HT	Unknown Structure	-	-	-	-	2	(PR)5(SN)4
R11SN10	Ge10Ho11	-	tI84	(139, I4/mmm)	-	2	(CE, LA, ND, SM, Y)11(SN)10
R3SN5_OS32	Pd5Pu3	-	oS32	(63, Cmcm)	-	2	(CE, LA, ND, PR, SR)3(SN)5
PR3SN5_HT	Unknown Structure	-	-	-	-	2	(PR)3(SN)5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
R2SN3	Nd2Sn3	-	aP20	(2, P-1)	-	2	(CE, LA, ND, PR, SM)2(SN)3
RSN2	Ga2Zr	-	oS12	(65, Cmmm)	-	2	(ND, PR, SM, Y)1(SN)2
R2SN5	Ce2Sn5	-	oS28	(65, Cmmm)	-	2	(CE, ND, PR, Y)2(SN)5
R3SN7	Ce3Sn7	-	oS20	(65, Cmmm)	-	2	(CE, ND, PR)3(SN)7
MGRESN_TI12	CeMgSn	-	tI12	(139, I4/mmm)	-	3	(MG)1(ND, PR, Y)1(SN)1
MGRESN_OP12	TiNiSi	-	oP12	(62, Pnma)	-	3	(MG)1(LA, CE)1(SN)1
MGRESN2	LaMgSn2	-	tI32	(121, I-42m)	-	3	(MG)1(CE, LA, ND, PR)1(SN)2
MG23RE6SN	SiZn23Zr6	-	cF120	(225, Fm-3m)	-	3	(MG)23(CE, LA, ND, PR)6(SN)1
MGPRSN_T4	Unknown Structure	-	-	-	-	3	(MG)0.56(PR)0.17(SN)0.27
MGPRSN_T5	Unknown Structure	-	-	-	-	3	(MG)0.42(PR)0.335(SN)0.245
MGPRSN_T6	Unknown Structure	-	-	-	-	3	(MG)0.38(PR)0.25(SN)0.37
MGPRSN_T7	Unknown Structure	-	-	-	-	3	(MG)0.2(PR)0.35(SN)0.45
LAMGSN_T2	Cu4Si2Zr3	-	hP9	(189, P-62m)	-	3	(LA)3(MG)4(SN)2
LAMGSN_T3	Unknown Structure	-	-	-	-	3	(LA)25(MG)40(SN)35
LAMGSN_T4	LaMg3Ge2	-	hP34	(163, P-31c)	-	3	(LA)1(MG)2.65(SN)2
LAMGSN_T6	Unknown Structure	-	-	-	-	3	(LA)25(MG)35(SN)40
LAMGSN_T7	Unknown Structure	-	-	-	-	3	(LA)35(MG)20(SN)45
MGNDSN_T4	Unknown Structure	-	-	-	-	3	(MG)40(ND)33.3(SN)26.7

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MGNDSN_T5	Unknown Structure	-	-	-	-	3	(MG)44(ND)22(SN)34
MGNDSN_T6	Unknown Structure	-	-	-	-	3	(MG)40(ND)24(SN)36
MGNDSN_T7	Unknown Structure	-	-	-	-	3	(MG)16(ND)39(SN)45
CEMGSN_T4	Cu4Si2Zr3	-	hP9	(189, P-62m)	-	3	(CE)3(MG)4(SN)2
CEMGSN_T5	Unknown Structure	-	-	-	-	3	(CE)22(MG)44(SN)34
CEMGSN_T6	Unknown Structure	-	-	-	-	3	(CE)24(MG)40(SN)36
AGPRSN_T1	GaGeLi	-	hP6	(194, P6_ 3/mmc)	-	3	(AG)1(PR)1(SN)1
AGPRSN_T2	CuHf5Sn3	-	hP18	(193, P6_ 3/mcm)	-	3	(AG)1(PR)5(SN)3
AGPRSN_T3	Cu4Gd3Ge4	-	oI22	(71, Immm)	-	3	(AG)4(PR)3(SN)4
SBSN	SbSn	-	hR8	(166, R-3m)	-	2	(SB, SN, VA)4(SB)3
SB3SN4	Sn4As3	-	hR7	(166, R-3m)	-	2	(SB)3(SN)4
SCZN2	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(SC)1(ZN)2
SC3ZN17	Be17Ru3	-	cI160	(204, Im-3)	-	2	(SC)3(ZN)17
AG9CA2	Unknown Structure	-	-	-	-	2	(AG)0.818182(CA)0.181818
AG7CA2	Ag7Yb2	-	oS36	(63, Cmcm)	-	2	(AG)0.777778(CA)0.222222
AGCA3	Unknown Structure	-	-	-	-	2	(AG)0.25(CA)0.75
AG4CE	Unknown Structure	-	-	-	-	2	(AG)4(CE)1
AG2GD	MoSi2 (C11b)	C11b	tI6	(139,	-	2	(AG)0.667(GD)0.333

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				I4/mmm)			
AG51GD14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(AG)0.785(GD)0.215
AG2IN_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	-	2	(AG)0.68(IN)0.32
AG5LA	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	2	(AG)5(LA)1
AGMG4	Ag9Mg37	-	hP116	(176, P6_3/m)	-	2	(AG)0.2(AL, MG)0.8
AGMG3	Hf54Os17	-	oI142	(71, Immm)	-	2	(AG, CU, SN)0.23(CU, IN, MG)0.77
AG51ND14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(AG)0.785(ND)0.215
AG2ND_H	Unknown Structure	-	-	-	-	2	(AG)0.666667(ND)0.333333
AG2PR	Unknown Structure	-	hP*	-	-	2	(AG)2(PR)1
AG5PR	Unknown Structure	-	-	-	-	2	(AG)5(PR)1
AG4SC	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)	-	2	(AG, AL)0.8(SC)0.2
AG3SN1	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)	-	2	(AG)0.75(AG, SN)0.25
AG4SR	Unknown Structure	-	-	-	-	2	(AG)4(SR)1
AGSR	SrAg	-	oP16	(62, Pnma)	-	2	(AG)1(SR)1
AG2SR3	Er3Ni2	-	hR15	(148, R-3)	-	2	(AG)2(SR)3
AG51Y4	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(AG)0.785(Y)0.215
AG1ZN1	gamma-AgZn (Bb)	Bb	hP9	(147, P-3)	-	2	-
AGZN3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	-	1	-

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AG5ZN8	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	-
AGZR_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)	-	2	(AG)1(ZR)1
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
AL3CE_H	Unknown Structure	-	-	-	-	2	(AL)0.75(CE)0.25
ALCE2	Unknown Structure	-	-	-	-	2	(AL)0.3333(CE)0.6667
ALRE3	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(AL, IN)1(CE, PR)3
ALCE3_L	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	-	2	(AL)0.25(CE)0.75
ALCU_DEL	Al5Cu8	-	hR52	(160, R3m)	-	2	(AL, ZN)2(CU, FE)3
ALCU_ETA	AlCu(r)	-	mS20	(12, C2/m)	-	2	(AL, CU)1(AG, CU)1
ALCU_PRIME	Al9Cu11(h)	-	oF88	(42, Fmm2)	-	2	(AL)2(CU)1
ALCU_ZETA	Al9Cu11(h)	-	oF88	(42, Fmm2)	-	2	(AL)9(AG, CU)11
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	-	3	(AL, SI)4(AL, CU, SI)1(AG, CU)8
GAMMA_H	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	3	(AL)4(AL, CU)1(AG, CU)8
AL13FE4	Al13Fe4	-	mS102	(12, C2/m)	-	3	(AL)0.6275(FE, MN)0.235(AL, VA)0.1375
AL2FE	Al2Fe	-	aP18	(1, P1)	-	2	(AL)2(FE, MN)1
AL5FE2	Al2.8Fe	-	oS24	(63, Cmcm)	-	2	(AL)5(FE, MN)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL2GD3	Gd3Al2	-	tP20	(102, P4_2nm)	-	2	(AL)2(GD)3
AL53LA22	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(AL)0.707(LA)0.293
AL2LI3	Li3Al2	-	hr5	(166, R-3m)	-	2	(AL, MG)2(LI)3
ALLI2	Li2Ga	-	oS12	(63, Cmcm)	-	2	(AL)1(LI)2
AL4LI9	Al4Li9	-	mS26	(12, C2/m)	-	2	(AL)4(LI)9
AL1LI1	NaTl (B32)	B32	cF16	(227, Fd-3m)	-	2	(AL, LI, MG)1(LI, MG, VA)1
ALMG_BETA	Al45Mg28	-	cF1832	(227, Fd-3m)	-	2	(AL, ZN)140(LI, MG)89
ALMG_EPSILON	Al30Mg23	-	hR53	(148, R-3)	-	2	(AL, ZN)30(MG)23
AL12MG17_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	3	(GD, LI, MG)10(AL, CA, MG, ZN)24(AG, AL, MG, NI, ZN)24
LTAL11MN4	Al11Mn4	-	aP15	(2, P-1)	-	2	(AL)11(MN, FE)4
AL12MN	Al12W	-	cI26	(204, Im-3)	-	2	(AL)12(MN)1
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)	-	2	(AL)6(MN, FE)1
AL4MN	mu-Al4Mn	-	hP574	(194, P6_ 3/mmc)	-	2	(AL)4(FE, MN)1
R_AL4MN	lambda-Al4Mn	-	hP586	(176, P6_3/m)	-	2	(AL)461(MN, FE)107
AL3NI2	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)	-	3	(AL)3(AL, MG, NI)2(NI, VA)1
AL3NI5	Ga3Pt5	-	oS16	(65, Cmmm)	-	2	(AL)0.375(NI)0.625
ALPR3_L	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	-	2	(AL)1(PR)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL7SR8	Ba8Ga7	-	cP60	(198, P2_13)	-	2	(AL)0.46667(CA, SR)0.53333
AL3SR8	Unknown Structure	-	-	-	-	2	(AL)0.27273(SR)0.72727
AL3Y_H	BaPb3	-	hR12	(166, R-3m)	-	2	(AL)0.75(Y)0.25
AL3ZR5	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	-	2	(AL)0.375(ZR)0.625
AL3ZR4	Al3Zr4	-	hP7	(191, P6/mmm)	-	2	(AL)0.42857(ZR)0.57143
AL4ZR5	Ti5Ga4	-	hP18	(193, P6_3/mcm)	-	2	(AL)0.44444(ZR)0.55556
AL3ZR2	Zr2Al3	-	oF40	(43, Fdd2)	-	2	(AL)0.6(ZR)0.4
AL3ZR1	Al3Zr (D023)	D023	tI16	(139, I4/mmm)	-	2	(AL, IN, MG)0.75(ZR)0.25
BI2CA1	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	-	2	(BI)2(CA)1
BI10CA11	Ge10Ho11	-	tI84	(139, I4/mmm)	-	2	(BI)10(CA)11
BI3CA5	beta-Yb5Sb3	-	oP32	(62, Pnma)	-	2	(BI)3(CA)5
BICA2	La2Sb	-	tI12	(139, I4/mmm)	-	2	(BI)1(CA)2
BI2MG3_LT	La2O3 (D52)	D52	hP5	(164, P-3m1)	-	2	(BI, SN, VA)2(MG)3
BI2MG3_HT	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)	-	3	(BI, SN)1(BI, SN, VA)3(MG)6
BIMN_LT	Nickeline (NiAs, B81)	B81	hP4	(194, P6_3/mmc)	-	2	(BI)1(MN)1
BIMN_HT	Mn2.23Bi1.88	-	oP10	(51, Pmma)	-	2	(BI)1(MN)1.08
CA1CU1	alpha-CaCu	-	mP20	(11, P2_1/m)	-	2	(CA)0.5(CU)0.5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CA2CU	Ca2Cu	-	oP12	(62, Pnma)	-	2	(CA)0.6667(CU)0.3333
CA8IN3	Ca8In3	-	aP22	(2, P-1)	-	2	(CA)8(IN)3
CA1IN2	CaIn2	-	hP6	(194, P6_ 3/mmc)	-	2	(CA)1(IN)2
CANI2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(CA)0.333(NI)0.667
CA2NI7	Co7Gd2	-	hR18	(166, R-3m)	-	2	(CA)0.2222(NI)0.7778
CA3SI4	Ca3Si4	-	hP42	(176, P6_3/m)	-	2	(CA)0.428571(SI)0.571429
CA14SI19	Ca14Si19	-	hR66	(167, R-3c)	-	2	(CA)0.424242(SI)0.575758
CASI2	CaSi2 (C12)	C12	hR6	(166, R-3m)	-	2	(CA)0.333333(SI)0.666667
CA2SN_X	CrB (B33)	B33	oS8	(63, Cmcm)	-	3	(CA, MG)1(CA)1(SN)1
CA36SN23	Sn23Yb36	-	tP118	(127, P4/mbm)	-	2	(CA)36(SN)23
CA31SN20	Pu31Rh20	-	tI204	(140, I4/mcm)	-	2	(CA)31(SN)20
CA7SN6	Ca7Sn6	-	oP52	(62, Pnma)	-	2	(CA)7(SN)6
CA3ZN	Re3B	-	oS16	(63, Cmcm)	-	2	(CA)3(ZN)1
CAZN3	CaZn3	-	hP32	(194, P6_ 3/mmc)	-	2	(CA)1(ZN)3
CU6CE	Copper (II) Azide [Cu (N3)2]	-	oP28	(62, Pnma)	-	2	(CU)0.857(CE)0.143
CU4CE	Unknown Structure	-	oP20	-	-	2	(CU)0.8(CE)0.2
CU2CE	KHg2	-	oI12	(74, Imma)	-	2	(CU, IN)0.667(CE, LA)0.333

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CEGD3	alpha-Sm (C19)	C19	hR3	(166, R-3m)	-	1	(GD, CE)1
CE5IN4	Unknown Structure	-	-	-	-	2	(CE)5(IN)4
CE9IN11	Unknown Structure	-	-	-	-	2	(CE)9(IN)11
CE3IN5	Pd5Pu3	-	oS32	(63, Cmcm)	-	2	(CE)3(CE, IN)5
CENI3	CeNi3	-	hP24	(194, P6_ 3/mmc)	-	2	(CE)0.25(NI)0.75
CENI2	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(CE, NI)0.333(CE, NI)0.667
CEZN2	KHg2	-	oI12	(74, Imma)	-	2	(CE)0.333(MG, ZN)0.667
CEZN3	CeZn3	-	oS16	(63, Cmcm)	-	2	(CE)0.25(ZN)0.75
CEZN11	BaCd11	-	tI48	(141, I4_ 1/amd)	-	2	(CE)0.083(MG, ZN)0.917
CU9GD2	Unknown Structure	-	t**	-	-	2	(CU)9(GD)2
CU7GD2	Unknown Structure	-	-	-	-	2	(CU)7(GD)2
CUH_B3	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)	-	2	(CU)1(H)1
CUH_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	-	2	(CU)1(H)1
CU9IN4_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)	-	3	(CU)0.654(CU, IN)0.115(IN)0.231
CU7IN3	Cu7In3	-	aP40	(2, P-1)	-	2	(CU, MG)0.7(IN)0.3
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

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU37LA3	NaZn13 (D23)	D23	cF112	(226, Fm-3c)	-	2	(CU)37(LA)3
CU6LA_L	Cu6La	-	mP28	(14, P2_1/c)	-	2	(CU)6(LA)1
CU4LA	Cu4La	-	tI90	(119, I-4m2)	-	2	(CU)4(LA)1
CU2LA	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(CU)2(LA)1
CUMG2	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	-	2	(AG, CU, IN, NI)1(IN, MG)2
CU4ND	Unknown Structure	-	o**	-	-	2	(CU)0.8(ND)0.2
CU7ND2	Unknown Structure	-	-	-	-	2	(CU)0.77777778(ND)0.22222222
CUND_H	Unknown Structure	-	-	-	-	2	(CU)0.5(ND)0.5
CU6PR	Cu6La	-	mP28	(14, P2_1/c)	-	2	(CU)0.857(PR)0.143
CU4PR	Unknown Structure	-	o**	-	-	2	(CU)0.8(PR)0.2
CU2PR	KHg2	-	oI12	(74, Imma)	-	2	(CU)0.667(PR)0.333
CU4SC	Unknown Structure	-	t**	-	-	2	(CU)4(SC)1
CUSC	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	2	(CU)1(SC)1
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cI76	(220, I-43d)	-	2	(CU, MG)15(AL, SI)4
CU56SI11_GAMMA	Mg3Ru2	-	cP20	(213, P4_132)	-	2	(CU, MG)56(SI)11
CUSI_ETA	Cu3Si-h2	-	hR*	(162, P-31m)	-	2	(CU)0.76(SI)0.24
CU33SI7_DELTA	Unknown Structure	-	-	-	-	2	(CU)0.825(SI)0.175
CU3SN_H_GAMMA	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	1	(CU, SN)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU10SN3	Cu10Sn3	-	hP26	(173, P6_3)	-	1	(CU, SN)1
CU3SN_L	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	Cu6Sn5	-	mS44	(15, C2/c)	-	3	(CU)1(CU, SN)1(SN)1
CUSR	BaCu	-	hP8	(194, P6_ 3/mmc)	-	2	(CU)0.5(SR)0.5
CUTH2	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	-	2	(CU)0.333(TH)0.667
CU2TH	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(CU)0.667(TH)0.333
CU6TH	CeCu6	-	oP28	(62, Pnma)	-	2	(CU)0.857(TH)0.143
CU51TH14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)0.7826(TH)0.2174
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
EPSILON	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	-	1	(CU, MN, ZN)1
CUZN_GAMMA	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	4	(CU, ZN)2(CU, ZN)2(CU)3(MG, ZN)6
CU51ZR14	Ag51Gd14	-	hP68	(175, P6/m)	-	2	(CU)0.7846(ZR)0.2154
CU8ZR3	Cu8Hf3	-	oP44	(62, Pnma)	-	2	(CU)0.7273(ZR)0.2727

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MNI3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(FE, MN, NI)1(FE, MN, NI)3
FE17ND5	Fe17Nd5	-	hP264	(193, P6_3/mcm)	-	2	(FE)1(ND)0.2941
FE2SC_C14	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)	-	2	(FE)0.67(SC)0.33
FE2SC_C36	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_3/mmc)	-	2	(FE)0.67(SC)0.33
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
FE3SN2	Fe3Sn2	-	hR10	(166, R-3m)	-	2	(FE)3(SN)2
FESN	CoSn (B35)	B35	hP6	(191, P6/mmm)	-	2	(FE)1(SN)1
FE7TH2_L	Ce2Ni7	-	hP36	(194, P6_3/mmc)	-	2	(FE)0.78(TH)0.22
FE7TH2_H	Th2Zn17	-	hR19	(166, R-3m)	-	2	(FE)0.78(TH)0.22
FE17Y2	Fe17Lu2	-	hP80	(194, P6_3/mmc)	-	2	(FE)1(Y)0.1176
FE23Y6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	2	(FE)1(Y)0.2609
GAMMA_FEZN	gamma-brass (Fe3Zn10, D81)	D81	cI52	(229, Im-3m)	-	4	(FE, ZN)0.154(FE, ZN)0.154(FE, ZN)0.231(ZN)0.461
GAMMA1_FEZN	Fe11Zn40	-	cF408	(216, F-43m)	-	3	(FE)0.137(FE, ZN)0.118(ZN)0.745
DELTA_FEZN	FeZn10	-	hP632	(194, P6_3/mmc)	-	4	(FE)0.058(FE, ZN)0.18(ZN)0.525(ZN)0.237

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZETA_FEZN	CoZn13	-	mS28	(12, C2/m)	-	3	(FE, VA)0.072(ZN)0.856(ZN, VA)0.072
FEZR3	Re3B	-	oS16	(63, Cmcm)	-	2	(FE, ZR)1(FE, ZR)3
ORTHO_GA	alpha-Ga (A11)	A11	oS8	(64, Cmce)	-	1	(GA)1
MG5GA2	Ga2Mg5 (D8g)	D8g	oI28	(72, Ibam)	-	2	(MG)0.7143(GA, IN)0.2857
MG2GA1	Li2Sb	-	hP18	(190, P-62c)	-	2	(MG)0.6667(GA)0.3333
MG1GA1	MgGa	-	tI32	(88, I4_1/a)	-	2	(MG)0.5(GA)0.5
MGGA2	MgGa2	-	oP24	(55, Pbam)	-	2	(MG)0.3333(GA)0.6667
MG2GA5	Ga5Mg2	-	tI28	(139, I4/mmm)	-	2	(MG)0.2857(GA)0.7143
GD5IN3	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	-	2	(GD)5(IN)3
GD1IN1	Unknown Structure	-	-	-	-	2	(GD)1.1(IN)1
GD3IN5	Pd5Pu3	-	oS32	(63, Cmcm)	-	2	(GD)3(IN)5
GDIN3	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(GD)1(IN)3
GDMG5	Sm11Cd45	-	cF448	(216, F-43m)	-	2	(AG, CA, CE, ER, GD, LA, ND, SM, SR, Y)1(MG, ZN)5
MG7RE	Unkown Strcture	-	c-bco	(63, Cmcm)	-	2	(MG)7(GD, ND, Y, ZN)1
GDND	alpha-Sm (C19)	C19	hR3	(166, R-3m)	-	2	(GD, ND)0.5(GD, ND)0.5
GD3NI2	Unknown Structure	-	-	-	-	2	(GD)3(NI)2
GD2NI7	Co7Gd2	-	hR18	(166, R-3m)	-	2	(GD)2(NI)7
GDNI4	Unknown Structure	-	-	-	-	2	(GD)1(NI)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GD5SI4	Gd5Si4	-	oP36	(62, Pnma)	-	2	(GD)0.5556(SI)0.4444
GD3SI5	Unknown Structure	-	-	-	-	2	(GD)0.375(SI)0.625
GDSI2	alpha-ThSi2 (Cc)	Cc	tI12	(141, I4_ 1/amd)	-	2	(GD)0.3333(SI)0.6667
GDZN2	KHg2	-	oI12	(74, Imma)	-	2	(GD, SM)0.333(ZN)0.667
GDZN12	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)	-	2	(GD)0.077(ZN)0.923
K17IN41	K17In41	-	cF464	(227, Fd-3m)	-	2	(IN)0.69(K)0.31
K39IN80	K39In80	-	hP238	(164, P-3m1)	-	2	(IN)0.635(K)0.365
B2REIN	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	2	(LA, ND, Y)1(IN, ND)1
IN5RE3	Pd5Pu3	-	oS32	(63, Cmcm)	-	2	(IN)0.625(LA, ND, PR, TH, Y)0.375
IN3LA2	Unknown Structure	-	-	-	-	2	(IN)0.57(LA)0.43
LIIN	NaTl (B32)	B32	cF16	(227, Fd-3m)	-	2	(IN, LI)1(IN, LI)1
LI5IN4	Li5Ga4	-	hP9	(164, P-3m1)	-	2	(LI)5(IN)4
LI3IN2	Li3Al2	-	hr5	(166, R-3m)	-	2	(LI)3(IN)2
LI2IN	Li2Ga	-	oS12	(63, Cmcm)	-	2	(LI)2(IN)1
LI13IN3	Li13In3	-	cF128	(227, Fd-3m)	-	2	(LI)13(IN)3
LI3IN1	Unknown Structure	-	-	-	-	2	(LI)3(IN)1
LI7IN	Unknown Structure	-	-	-	-	2	(LI)7(IN)1
TETRA_A6	In (A6)	A6	tI2	(139, I4/mmm)	-	1	(IN, MG, SN, ZN)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MG2IN	Mg2In	-	hP9	(189, P-62m)	-	2	(MG)2(IN)1
MG3IN	Mg3In	-	hr16	(166, R-3m)	-	2	(MG, IN, SN)3(MG, IN, SR)1
MN3IN	Unknown Structure	-	-	-	-	2	(MN)3(IN)1
NI13IN9	Ga9Ni13	-	mS44	(12, C2/m)	-	3	(NI, VA)1(NI)1(IN)1
B2NIIN	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	2	(NI, VA)1(IN)1
NIIN	CoSn (B35)	B35	hP6	(191, P6/mmm)	-	2	(NI)1(IN)1
NI2IN3	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)	-	2	(NI)2(IN)3
NI3IN7	Ir3Ge7 (D8f)	D8f	cI40	(229, Im-3m)	-	2	(NI)3(IN)7
NA6IN11	Na15In27.4	-	oS344	(63, Cmcm)	-	2	(NA)0.3526(IN)0.6474
NA7IN12	In12Na7	-	tP228	(137, P4_2/nmc)	-	2	(NA)0.3731(IN)0.6269
NAIN	NaTl (B32)	B32	cF16	(227, Fd-3m)	-	2	(NA)1(IN)1
NA2IN	Na2Tl	-	oS48	(20, C222_1)	-	2	(NA)2(IN)1
SCIN2	Li2Ga	-	oS12	(63, Cmcm)	-	2	(SC)1(IN)2
B2_SCIN	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	2	(SC)1.1(IN)0.9
PR3IN4	Unknown Structure	-	-	-	-	2	(PR)3(IN)4
PR6IN5	Unknown Structure	-	-	-	-	2	(PR)6(IN)5
INSN_AF	Simple Hexagonal (HgSn6-10 Af)	Af	hP1	(191, P6/mmm)	-	1	(IN, SN)1
TET_ALPHA1_A6	In (A6)	A6	tI2	(139,	-	1	(IN, SN)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				I4/mmm)			
IN5SR2	Unknown Structure	-	-	-	-	2	(IN)0.7143(SR)0.2857
IN2SR	CaIn2	-	hP6	(194, P6_ 3/mmc)	-	2	(IN)0.6667(SR)0.3333
IN3SR2	Unknown Structure	-	-	-	-	2	(IN)0.6(SR)0.4
IN1SR1	SrIn	-	oF64	(43, Fdd2)	-	2	(IN)0.5(SR)0.5
IN3SR5	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	-	2	(IN)0.375(SR)0.625
INSR3	Unknown Structure	-	-	-	-	2	(IN)0.25(SR)0.75
THIN	ThIn	-	oP24	(57, Pbcm)	-	2	(TH)1(IN)1
TH2IN	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	-	2	(TH)2(IN)1
ZRIN2	Ga2Hf	-	tI24	(141, I4_ 1/amd)	-	2	(ZR)1(IN)2
ZR1IN1	Unknown Structure	-	-	-	-	2	(ZR)1(IN)1
RE3IN	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(LA, ND, PR, ZR)3(IN)1
MGH2_C4	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)	-	2	(MG)1(H)2
NDH_GAMMA	Unknown Structure	-	-	-	-	2	(ND)1(H, VA)2
LA2NI7_H	Co7Gd2	-	hR18	(166, R-3m)	-	2	(LA)2(NI)7
LA7NI16	La7Ni16	-	tI46	(121, I-42m)	-	2	(LA)0.3043(NI)0.6957
LA2NI3	La2Ni3	-	oS20	(64, Cmce)	-	2	(LA)0.4(NI)0.6

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
LASI2_A1	GdSi1.4	-	oI12	(74, Imma)	-	2	(LA)0.36(SI)0.64
LAY	alpha-Sm (C19)	C19	hR3	(166, R-3m)	-	2	(LA, Y)1(Y)1
LAZN4	LaZn4	-	oS20	(63, Cmcm)	-	2	(LA, SR)1(SN, ZN)4
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
LI13SN5	Li13Sn5	-	hP18	(164, P-3m1)	-	2	(LI)13(SN)5
LI22SN5	Li17Si4	-	cF420	(216, F-43m)	-	2	(LI)22(SN)5
LI2SN5	Hg5Mn2	-	tP14	(127, P4/mbm)	-	2	(LI)2(SN)5
LI5SN2	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)	-	2	(LI)5(SN)2
LI7SN3	Li7Sn3	-	mP20	(11, P2_1/m)	-	2	(LI)7(SN)3
LI8SN3	Unknown Structure	-	-	-	-	2	(LI)8(SN)3
LISN	alpha-LiSn	-	mP6	(10, P2/m)	-	2	(LI)1(LI, SN)1
LI7SN2	Ge2Li7	-	oS36	(65, Cmmm)	-	2	(LI, SN)7(SN)2
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
MG2NI1	Unknown Structure	-	-	-	-	3	(MG)2(CU, NI, ZN)1(H, VA)1
MG5PR	Unknown Structure	-	-	-	-	2	(MG)5(PR, Y)1
MG3SB2_LT	La2O3 (D52)	D52	hP5	(164, P-3m1)	-	2	(MG)0.6(SB)0.4
MG3SB2_HT	Bixbyite (Mn2O3, D53)	D53	cI80	(206, Ia-3)	-	2	(MG)0.601(SB)0.399
MG38SR9	Mg38Sr9	-	hP94	(194, P6_ 3/mmc)	-	2	(AL, MG)38(CE, ND, SR)9
MG24R5	alpha-Mn (A12)	A12	cI58	(217, I-43m)	-	3	(AG, MG)24(CA, CE, DY, ER, GD, HO, LA, MG, ND, PR, SM, Y)4(DY, ER, HO, Y)1
MG2ZN3	Mg4Zn7	-	mS110	(12, C2/m)	-	2	(MG)2(AL, CU, ZN)3
MGZN	Zr21Re25	-	hR92	(167, R-3c)	-	2	(MG)12(AL, CU, SR, ZN)13
MG51ZN20	Mg51Zn20	-	oI158	(71, Immm)	-	2	(MG)51(MN, ZN)20
MG2ZN11	Mg2Zn11 (D8c)	D8c	cP39	(200, Pm-3)	-	2	(MG)2(AL, CU, SI, ZN)11
L10_TETRA	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	-	2	(MG, MN, IN, NI, SC)0.5(MG, MN, IN, NI)0.5
MNNI2	Unknown Structure	-	-	-	-	2	(MN, NI)1(NI)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN11SI19	Mn11Si19	-	tP120	(118, P-4n2)	-	2	(MN)11(SI)19
MN3SI	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	2	(MN)3(SI)1
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	-	2	(MN)17(SI)3
MN9SI2	Mn9Si2	-	oI186	(71, Immm)	-	2	(MN)33(SI)7
MN23SC6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	2	(MN)23(SC)6
MNSC4	Unknown Structure	-	-	-	-	2	(MN)0.2(SC)0.8
MN19SN6	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	-	2	(MN)0.76(SN)0.24
MNSN2	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	-	2	(MN)0.333(SN)0.667
MN23Y6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)	-	2	(MG, MN)23(Y)6
MNZN9_LT	Unkown Structure	-	hP*	(194, P6_ 3/mmc)	-	4	(MN)58(MG, MN, ZN)180(ZN)525(ZN)237
MNZN9_HT	Unknown Structure	-	hP*	-	-	2	(MN, ZN)9(MN, ZN)1
ZETA_MNZN	CoZn13	-	mS28	(10, P2/m)	-	3	(MN, VA)9(ZN)107(MN)9
GAMMA_MNZN	Unknown Structure	-	cI52	-	-	4	(MN, ZN)154(MN, ZN)154(MN, ZN)231(ZN)461
ALPHA_MNZN	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(MN, ZN)3(MN, ZN)1
BETA_MNZN	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	2	(MN)1(ZN)1
ND2Y	alpha-Sm (C19)	C19	hR3	(166, R-3m)	-	2	(ND, Y)2(ND, Y)1
NDZN2	KHg2	-	oI12	(74, Imma)	-	2	(ND)0.333(ZN)0.667

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ND3ZN11	Al11La3	-	oI28	(71, Immm)	-	2	(ND)0.214(MG, ZN)0.786
ND2ZN17	Ni17Th2	-	hP38	(194, P6_ 3/mmc)	-	2	(ND)0.105(ZN)0.895
NDZN11_H	Unknown Structure	-	-	-	-	2	(ND)0.0833(ZN)0.9167
NI2PR	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(NI)0.6667(PR)0.3333
NI3SI_M	Ge9Pd25	-	hP34	(147, P-3)	-	2	(NI)0.75(SI)0.25
NI3SI_L	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(NI)0.76(SI)0.24
NI5SI2	Ni31S12	-	hP42	(150, P321)	-	2	(NI)0.7143(SI)0.2857
THETA	K2UF6	-	hP9	(189, P-62m)	-	3	(NI)1(NI, VA)1(SI)1
NI3SI2	Ni3Si2	-	oP80	(36, Cmc2_1)	-	2	(NI)0.6(SI)0.4
NISI	MnP (B31)	B31	oP8	(62, Pnma)	-	2	(NI)0.5(SI)0.5
NI3SN_H	BiF3 (D03)	D03	cF16	(225, Fm-3m)	-	3	(NI, SN)0.25(NI, SN)0.25(NI)0.5
NI3SN_L	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	-	2	(NI)0.75(SN)0.25
NI3SN2_L	Ni3Sn2	-	oP20	(62, Pnma)	-	3	(SN)0.2(NI, SN)0.4(NI)0.4
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	(12, C2/m)	-	3	(NI)0.25(NI, SN)0.25(SN)0.5
NI17Y2	Fe17Lu2	-	hP80	(194, P6_ 3/mmc)	-	2	(NI)17(Y)2
NI4Y	Unknown Structure	-	hR*	-	-	2	(NI)4(Y)1
NI2Y1	Ni2Tm	-	cF192	(216, F-43m)	-	2	(NI)2(MG, Y)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI2Y3	Ni2Y3	-	tP80	(92, P4_12_12)	-	2	(NI)2(Y)3
BETA_NIZN	delta-CuTi (L2a)	L2a	tP2	(123, P4/mmm)	-	1	(NI, ZN)1
GAMMA_NIZN	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	1	(NI, ZN)1
DELTA_NIZN	Ni3Zn22	-	mS50	(12, C2/m)	-	2	(NI)0.111(ZN)0.889
NI7ZR2	Ni7Zr2	-	mS36	(12, C2/m)	-	2	(NI)7(ZR)2
NI21ZR8	Hf8Ni21	-	aP29	(2, P-1)	-	2	(NI)21(ZR)8
NI11ZR9	Pt11Zr9	-	tI40	(87, I4/m)	-	2	(NI)11(ZR)9
PR2Y	alpha-Sm (C19)	C19	hR3	(166, R-3m)	-	2	(PR, Y)2(PR, Y)1
PR2ZN17_H	Ni17Th2	-	hP38	(194, P6_3/mmc)	-	2	(PR)2(ZN)17
SC5SI3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	-	2	(SC)0.625(SI)0.375
SCSI	CrB (B33)	B33	oS8	(63, Cmcm)	-	2	(SC)0.5(SI)0.5
SC3SI5_LT	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(SC)0.375(SI)0.625
SC3SI5_HT	Unknown Structure	-	o**	-	-	2	(SC)0.375(SI)0.625
SI2Y_H	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(SI)2(Y)1
SI4Y5	Gd5Si4	-	oP36	(62, Pnma)	-	2	(SI)4(Y)5
SI5Y3_H	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(SI)5(Y)3

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SI5Y3_L	GdSi1.4	-	oI12	(74, Imma)	-	2	(SI)5(Y)3
SI4ZR5_H	Unknown Structure	-	-	-	-	2	(SI)4(ZR)5
SI2ZR	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	-	2	(SI)2(ZR)1
SIZR3	Ti3P	-	tP32	(86, P4_2/n)	-	2	(SI)1(ZR)3
ZR3SN_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	-	2	(ZR, SN)3(ZR, SN)1
ZR5SN3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	-	3	(ZR)5(SN)3(SN, VA)1
ZRSN2	TiSi2 (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	-	2	(ZR)1(SN)2
SRZN5_L	SrZn5	-	oP24	(62, Pnma)	-	2	(SR)1(ZN)5
THZN2	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	-	2	(TH)1(ZN)2
H_RZN5	Unknown Structure	-	-	-	-	2	(GD, Y)1(MG, ZN)5
YZN2_A	Unknown Structure	-	-	-	-	2	(Y)1(ZN)2
YZN2_B	Unknown Structure	-	-	-	-	2	(Y)1(ZN)2
ZN22ZR	Zn22Zr	-	cF184	(227, Fd-3m)	-	2	(ZN)0.9565(ZR)0.0435
ZN39ZR5	Zn39Zr5	-	mS88	(12, C2/m)	-	2	(ZN)0.8864(ZR)0.1136
ZN3ZR_L	Unknown Structure	-	tI64	-	-	2	(ZN)0.75(ZR)0.25
ZN3ZR_H	Unknown Structure	-	-	-	-	2	(ZN)0.75(ZR)0.25
AGALMG_T1	ZrNiAl	-	hP12	(194, P6_3/mmc)	-	3	(AG)1(AL)1(MG)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
T1_AGALSC	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	-	3	(AG)2(AL)1(SC)1
T2_AGALSC	Unknown Structure	-	-	-	-	3	(AG)0.28(AL)0.36(SC)0.36
T3_AGALSC	Unknown Structure	-	-	-	-	3	(AG)0.55(AL)0.27(SC)0.18
AGERMG_T1	Unknown Strcuture	-	-	(227, Fd-3m)	-	3	(AG)0.1(MG)0.84(ER)0.06
AGERMG_T2	Unknown Structure	-	-	-	-	3	(AG)0.1358(MG)0.6969(ER)0.1673
AGERMG_T3	Unknown Structure	-	-	-	-	3	(AG)0.3223(MG)0.5015(ER)0.1762
AGERMG_T4	ZrNiAl	-	hP9	(189, P-62m)	-	3	(AG)1(MG)1(ER)1
AGERMG_T5	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	-	3	(AG)2(MG)1(ER)1
AGGDMG_T	Unknown Structure	-	-	-	-	2	(AG, GD)0.15(MG)0.85
AGLAMG_T1	ZrNiAl	-	hP9	(189, P-62m)	-	3	(AG)1(LA)1(MG)1
AGLAMG_T2	Unknown Structure	-	-	-	-	3	(AG)10(LA)4(MG)3
AGLAMG_T3	Unknown Structure	-	-	-	-	2	(LA)1(AG, MG)4
AGLAMG_T4	Unknown Structure	-	-	-	-	2	(LA)1(AG, MG)6
AGLAMG_T5	Unknown Structure	-	-	-	-	3	(AG)10.3(LA)4(MG)12
AGLAMG_T6	Unknown Structure	-	-	-	-	2	(LA)3(AG, MG)16
AGLAMG_T7	Unknown Structure	-	-	-	-	2	(LA)1(AG, MG)12
AGMGY_T1	-	-	cF280	(227, Fd-3m)	-	3	(AG)0.1(MG)0.84(Y)0.06
AGMGY_T2	Unknown Structure	-	-	-	-	3	(AG)0.1661(MG)0.6739(Y)0.16

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AGMGY_T3	Unknown Structure	-	-	-	-	3	(AG)0.3(MG)0.52(Y)0.18
AGMGY_T4	Unknown Structure	-	-	-	-	3	(AG)0.178(MG)0.5857(Y)0.2364
AGMGY_T5	ZrNiAl	-	hP9	(189, P-62m)	-	3	(AG)1(MG)1(Y)1
AGMGY_T6	Heusler (Cu2AlMn, L21)	L21	cF16	(225, Fm-3m)	-	3	(AG)2(MG)1(Y)1
AGMGY_T7	Al10Ca4In3	-	oS68	(64, Cmce)	-	3	(AG)10(MG)3(Y)4
AL9CA31ZN10	Unknown Structure	-	-	-	-	3	(AL)1(CA)1(ZN)1
AL2CAZN2	D13 (BaAl4)	D13	tI10	(139, I4/mmm)	-	3	(AL)2(CA)1(ZN)2
AL13CEMG6	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	3	(AL)13(CE)1(MG)6
AL8CEM4	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)	-	3	(AL)0.6154(CE, GD, LA, Y)0.0769(AL, MN)0.3077
AL10CE2MN7	Zn17Th2	-	hR57	(166, R-3m)	-	2	(AL, MN)0.8947(CE, GD, LA, Y)0.1053
ALCUMG_Q	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)	-	3	(AL)7(CU)3(MG)6
ALCUMG_S	MgCuAl2 (E1a)	E1a	oS16	(63, Cmcm)	-	3	(AL, SI)2(CU)1(MG)1
ALCUMG_T	Bergman [Mg32(Al, Zn)49]	D8e	cI162	(204, Im-3)	-	4	(MG)26(AL, MG)6(AL, CU, MG, ZN)48(AL)1
ALCUMG_V	Mg2Zn11 (D8c)	D8c	cP39	(200, Pm-3)	-	3	(AL)5(CU)6(MG)2
HTAL8MN5	Unknown Structure	-	-	-	-	2	(AL, FE, MN)8(AL, FE, MN)5
LTAL8MN5	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	3	(AL)12(FE, MN)5(AL, FE, MN)9
HTAL11MN4	Mn6(Mn0.5Al0.5)8Al25	-	oP156	(62, Pnma)	-	2	(AL, MN)29(FE, MN)10

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
D3_ALFE	Unknown Structure	-	-	-	-	3	(AL)0.7(AL, FE)0.08(FE, MN)0.22
Z_ALFEMN	Al14.4Cr3.4Ni1.1	-	hP227	(176, P6_3/m)	-	2	(AL)4(FE, MN)1
PHI	Unknown Structure	-	-	-	-	3	(AL)0.7(AL, MN)0.15(FE, MN)0.15
ALLAMG_T1	Unknown Structure	-	-	-	-	3	(AL)2(LA)0.15(MG)0.85
AL8LAMN	Unknown Structure	-	-	-	-	3	(AL)8(LA)1(MN)1
ALLIMG_T	Unknown Structure	-	-	-	-	3	(AL)0.53(LI)0.33(MG)0.14
ALMGMN_T	Mg3Cr2Al18	-	cF184	(227, Fd-3m)	-	3	(AL)18(MG)3(MN)2
ALMGND_T	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	3	(AL)2(MG)0.88(ND)0.12
ALMG3NI2	Mn3Ni2Si	-	cF96	(227, Fd-3m)	-	3	(AL)1(NI)2(MG)3
ALMGPR_T1	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	3	(AL)50(MG)22(PR)3
AL38MG58SR4	Unknown Structure	-	-	-	-	3	(AL)38(MG)58(SR)4
AL4MGY	Unknown Structure	-	-	-	-	3	(AL, MG, Y)0.6667(AL, MG, Y)0.1667(MG, Y)0.1666
ALMGZN_PHI	Mg21(Al, Zn)17	-	oP152	(57, Pbcm)	-	2	(MG)21(AL, ZN)17
ALMGZN_T1	Bergman [Mg32(Al, Zn)49]	D8e	cI162	(204, Im-3)	-	4	(MG)26(MG, AL)6(AL, MG, ZN)48(AL)1
ALMGZN_Q	Quasicrystal	-	-	-	-	3	(AL)0.15(MG)0.44(ZN)0.41
ALMGZN_T2	Mg46Zn37Al17	-	cP640	(205, Pa-3)	-	3	(AL)0.15(MG)0.43(ZN)0.42
BI2CAMG2	La2O3 (D52)	D52	hP5	(164, P-3m1)	-	3	(BI)2(CA)1(MG)2

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CACUMG_T1	Unknown Structure	-	-	-	-	2	(CA)2(CU, MG)3
CACUMG_T2	Unknown Structure	-	-	-	-	2	(CU)3(CA, MG)1
CA7MG6SI14	Ca7Mg7.5Si14	-	hP42	(191, P6/mmm)	-	3	(CA)0.2592593(MG)0.2222222(SI)0.5185185
CAMGSN_T1	Co2Si (C37)	C37	oP12	(62, Pnma)	-	3	(CA)156(MG)94(SN)175
CAMGZN_T1	Unknown Structure	-	hP36	(194, P6_3/mmc)	-	3	(CA)1(ZN)1(MG, ZN)4
CAMGZN_T2	Unknown Structure	-	-	-	-	3	(CA)7(MG)8(ZN)35
CAMGZN_T3	Unknown Structure	-	hP92	(194, P6_3/mmc)	-	3	(CA)3(MG)13(ZN)30
CAMGZN_T4	Unknown Structure	-	-	-	-	3	(CA)2(MG)55(ZN)43
REH_EPS	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	-	3	(CE, LA, ND)1(H, VA)2(H, VA)1
CEH2_35	Unknown Structure	-	-	-	-	2	(CE)1(H)2.35
CEH2_9	CeH3	-	cF44	(225, Fm-3m)	-	2	(CE)1(H)2.9
REMG2H7	Mg2LaH7	-	tP40	(92, P4_12_12)	-	3	(CE, LA)1(MG)2(H)7
MG5CEY	Sm11Cd45	-	cF448	(216, F-43m)	-	2	(MG)5(CE, Y)1
T1_CEMGZN	Unknown Structure	-	-	-	-	2	(MG, ZN)12(CE)1
T2_CEMGZN	Unknown Structure	-	-	-	-	3	(CE)0.018182(MG)0.527273(ZN)0.454545
T4_CEMGZN	Cu7Tb	-	hP8	(191, P6/mmm)	-	3	(CE, PR)1(MG)2.5(ZN)4.5
T5_CEMGZN	Mg13Zn30Sm3	-	hP92	(194, P6_3/mmc)	-	3	(CE, PR)0.065217(MG)0.282609(ZN)0.652174

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
T6_CEMGZN	Unknown Structure	-	-	-	-	3	(CE)0.0625(MG)0.125(ZN)0.8125
T7_CEMGZN	Mg19Zn81Ce20	-	cF480	(216, F-43m)	-	3	(CE)0.166667(MG)0.158333(ZN)0.675
MGCU4IN	MgCu4Sn	-	cF24	(216, F-43m)	-	3	(IN, MG)1(CU, IN, MG)4(IN, MG)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_C1	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)	-	3	-
CU4MGSN_T1	Half-Heusler (AgAsMg, C1b)	C1b	cF12	(216, F-43m)	-	3	(CU)0.666(SN)0.167(MG)0.167
CUMGSN_T2	Unknown Structure	-	-	-	-	3	(CU)0.334(SN)0.333(MG)0.333
CU9MG2Y	Cu9Mg2Tb	-	hP24	(194, P6_ 3/mmc)	-	3	(CU)0.75(MG)0.166667(Y)0.083333
CUMGY_T2	MgCu4Sn	-	cF24	(216, F-43m)	-	3	(CU, NI)4(MG)1(Y)1
CUMGY_T3	Mo2FeB2	-	tP10	(127, P4/mbm)	-	3	(CU, NI)2(MG)1(Y)2
CUMGY_T4	ZrNiAl	-	hP9	(189, P-62m)	-	3	(CU)1(MG)1(Y)1
CUMGY_T5	Cu5Mg8Y5	-	oP36	(51, Pmma)	-	3	(CU)0.277778(MG)0.444444(Y)0.277778
CUMGY_T6	Cu5Mg13Y5	-	oS92	(63, Cmcm)	-	3	(CU)0.2173913(MG)0.5652174(Y)0.2173913
CUMGY_T7	Unknown Structure	-	-	-	-	3	(CU)0.18(MG)0.57(Y)0.25
CUMGY_T8	Cu5Mg16Y5	-	oS104	(63, Cmcm)	-	3	(CU)0.1923077(MG)0.6153846(Y)0.1923077
CUMGY_T9	CuMg4Tb	-	oS48	(63, Cmcm)	-	3	(CU)1(MG)4(Y)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CUMGY_T10	Unknown Structure	-	-	-	-	3	(CU)0.09(MG)0.78(Y)0.13
F_MGGDZN	Mg19Zn81Ce20	-	cF480	(216, F-43m)	-	3	(GD)0.166667(MG)0.158333(ZN)0.675
Z_MGRZN	Unknown Structure	-	-	-	-	3	(GD, Y)0.07(MG)0.28(ZN)0.65
M_MGRZN	Unknown Structure	-	-	-	-	3	(GD)0.08(MG)0.28(ZN)0.64
L_MGRZN	Unknown Structure	-	-	-	-	3	(GD)0.14(MG)0.22(ZN)0.64
LAMGNI_T1	MgCuAl2 (E1a)	E1a	oS16	(63, Cmcm)	-	3	(LA)0.25(NI)0.25(MG)0.5
LAMGNI_T2	Mo2FeB2	-	tP10	(127, P4/mbm)	-	3	(LA)0.4(NI)0.4(MG)0.2
LAMGNI_T3	Unknown Structure	-	-	-	-	2	(LA, MG)0.333333(NI)0.666667
LAMGNI_T4	Unknown Structure	-	-	-	-	3	(LA)0.666666(NI)0.166667(MG)0.166667
LAMGNI_T5	Unknown Structure	-	-	-	-	3	(LA)0.666666(NI)0.22(MG)0.113334
LAMGNI_T6	Unknown Structure	-	-	-	-	2	(LA)0.675(MG, NI)0.325
LAMGSI_T1	Unknown Structure	-	-	-	-	2	(LA, MG)0.6(SI)0.4
LAMGSI_T2	Unknown Structure	-	-	-	-	3	(LA)0.2(SI)0.4(MG)0.4
LAMGSI_T3	Unknown Structure	-	-	-	-	3	(LA)0.25(SI)0.5(MG)0.25
LAMGSI_T4	Unknown Structure	-	-	-	-	3	(LA)0.2(SI)0.03333(MG)0.76667
LAMGSI_T5	Unknown Structure	-	-	-	-	3	(LA)0.3293(SI)0.004(MG)0.6667
LAMGZN_T9	Unknown Structure	-	-	-	-	3	(LA)0.014(MG)0.5245(ZN)0.4615
LAMGZN_T10	Unknown Structure	-	-	-	-	3	(LA)0.008(MG)0.4495(ZN)0.5425

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MG2NIH4	Mg2NiH4	-	mS56	(15, C2/c)	-	3	(MG)2(NI)1(H)4
MGSNSR_T1	Unknown Structure	-	-	-	-	3	(MG)25(SN)24(SR)14
MGSNSR_T2	Unknown Structure	-	-	-	-	3	(MG)5(SN)3(SR)1
MGSNSR_C37	Co2Si (C37)	C37	oP12	(62, Pnma)	-	3	(MG)1(SN)1(SR)1
MG3MNNI2	NiTi2	-	cF96	(227, Fd-3m)	-	3	(MG)3(MN)1(NI)2
MGNDZN_T1	Mg13Zn30Sm3	-	hP92	(194, P6_ 3/mmc)	-	3	(MG)0.283(ND)0.065(ZN)0.652
MGNDZN_T2	Quasicrystal	-	-	-	-	3	(MG)0.25(ND)0.1(ZN)0.65
MG6REZN3	Unknown Structure	-	-	-	-	3	(MG)0.6(CE, LA, ND, PR)0.1(ZN)0.3
MGNDZN_T4	Unknown Structure	-	-	-	-	3	(MG)0.3(ND)0.15(ZN)0.55
MGSRZN_T1	Ni11Sc3Si4	-	-	(194, P6_ 3/mmc)	-	2	(MG, ZN)15(SR)3
MGSRZN_T2	Unknown Structure	-	-	-	-	2	(MG, ZN)11(SR)1
MGSRZN_T3	Unknown Structure	-	-	-	-	3	(MG)20(SR)18(ZN)62
MGSRZN_T4	Unknown Structure	-	-	-	-	3	(MG)55(SR)2(ZN)43
MGSRZN_T5	Unknown Structure	-	-	-	-	3	(MG)44(SR)35(ZN)21
AL3CU2MG9SI7	Q-(Al, Cu, Mg, Si)	-	hP21	(174, P-6)	-	4	(AL)3(CU)2(MG)9(SI)7

TCMG9: Current Version Changes

Current Database Version	
Database name (acronym):	TCS Mg-based Alloys Database (TCMG)
Database owner:	Thermo-Calc Software AB
Database version:	9.0
First release:	TCMG1 was released in 2012

For earlier changes, see TCMG: Revision History.

TCMG8.0 to TCMG9.0

Software release version: 2026b (June 2026)

New Phases

- 27 new phases (total 602)

Binary Systems

- 3 new binary systems (total 232): Ag-Er, Sc-Zn, Sm-Y
- 5 binary systems reassessed: Ag-Mg, Ag-Zr, Ca-Cu, Gd-Mg, Mn-Nd

Ternary Systems

- 14 new ternary systems (total 147): Ag-(Al, Er, La, Y)-Mg, Al-La-Y, Al-Mg-Pr, Ca-Cu-Mg, Dy-Mg-Sm, Er-Gd-Mg, Gd-Mg-Mn, Mg-Mn-Nd, Mg-Sc-Zn, Mg-Sm-Y, Mg-Y-Zr
- 12 ternary systems reassessed: Ca-Mg-Zn, Mg-Nd-Zn, Ce-Mg-Y, Mg-Nd-Sr, Ce-Mg-Zn, La-Mg-Zn, Mg-Sr-Zn, Al-Ca-Mg, Al-Gd-Mg, Gd-Mg-Sr, Al-Mg-Y, Gd-La-Mg

Metastable Phases

- Stability of β series metastable phases in Gd-Mg binary system is modified.

Elastic Properties

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

Thermophysical Properties

- Molar volumes, surface tensions, viscosities and resistivities/conductivities are updated with the additions of new phases.
- Corrected molar volume parameters of BCC_B2 phase in Al-Fe-Ni system.

TCMG8.0 to TCMG8.1

Software release version: 2026b (June 2026)

Note that this update is in parallel with the full TCMG9 release in order to provide the bug fix to existing TCMG8 users.

- Thermophysical Properties: Corrected molar volume of BCC_B2 phase in Al-Fe-Ni system.

TCMG: Revision History

For the most recent changes, see TCMG9: Current Version Changes.

TCMG7.0 to TCMG8.0

Software release version: 2025b (June 2025)

Binary Systems

- Six (6) newly assessed binary systems (total 229): (Ce, Nd, Pr, Sb, Sm, Y)-Sn
- One (1) reassessed system: La-Sn

Ternary Systems

- Nine (9) newly assessed ternary systems (total 133): (Ce, La, Nd, Pr, Sb, Y)-Mg-Sn, Ag-Pr-Sn, Cu-Mg-Sn, Mg-Sr-Zr,
- Three (3) reassessed systems: Al-Fe-Mg, Mg-Mn-Ni, and Mg-Nd-Zn

Phases

- 34 new phases (575 phases in total)

TCMG6.3 to TCMG7.0

Software release 2024a (December 2023/January 2024)

Molar Volume

- Modeled molar volume of the BCC phase in the Li-Mg, Al-Fe, and Fe-Si systems.

Surface Tension Re-assessed

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

Binary Systems

A total of 223 assessed binary systems:

- 15 new systems: Al-Dy, Al-Er, Al-Ho, Al-Sm, Bi-Sn, Dy-Nd, Dy-Zn, Dy-Zr, Er-Zn, Gd-La, Ho-Zn, La-Mn, Mn-Sr, Nd-Zr, and Sn-Sr.
- 5 updated systems: Al-Sc, Cu-Sr, Mg-Sc, Mn-Zn, and Ni-Si.

Ternary Systems

A total of 124 assessed ternary systems:

- 22 new systems: Ag-Al-Sc, Al-Dy-Mg, Al-Er-Mg, Al-Gd-Mn, Al-Ho-Mg, Al-La-Mn, Al-Mg-Sc, Al-Mg-Sm, Al-Mn-Y, Al-Y-Zn, Bi-Mg-Sn, Dy-Mg-Zn, Er-Mg-Zn, Gd-La-Mg, Ho-Mg-Zn, Mg-Mn-Sn, Mg-Mn-Sr, Mg-Nd-Zr, Mg-Ni-Y, Mg-Pr-Zn, Mg-Sn-Sr, and Mg-Zn-Zr.
- 11 updated systems: Al-Gd-Mg, Al-Mg-Nd, Ce-Gd-Mg, Ce-La-Mg, Cu-Mg-Y, Gd-Mg-Nd, Gd-Mg-Zn, La-Mg-Zn, Mg-Ni-Zn, Mg-Si-Sn, Mg-Mn-Zn.

Long-Period Stacking-Ordered (LPSO) Phases

A variety of work is done to improve the LPSO phases.

- A new model for the following phases are used, where RE is rare earth elements that are included in the current database:
  - For LPSO-14H phase: $(Mg)_{70}(RE)_8(Al,Cu,Ni,Zn)_6(Mg)_1$.
  - For LPSO-18R phase: $(Mg)_{58}(RE)_8(Al,Cu,Ni,Zn)_6(Mg)_1$.
- Five (5) updated binaries related to the LPSO phases:
  - Cu-Sr: The DHCP phase that appeared on the Cu-rich side is destabilized.
  - Ni-Si: The Mg2Si_C1 phase at the Si-rich side had a wide homogeneity range, which was not experimentally confirmed. In the new version, this homogeneity range is negligible.
  - Mg-Sc: It is remodeled as a subsystem for modeling of Al-Mg-Sc. B2 had a large solubility range in the previous version. In this version, the B2 solubility range is smaller.
  - Mn-Zn: It is remodeled using new experimental data.
  - Al-Sc: B2 was a ground state in the previous version. In this version, XR is modeled as a stable phase.

- Eleven (11) updated ternary systems related to the LPSO phases:
    - These systems are updated to include the LPSO phases: Al-Gd-Mg, Al-Mg-Nd, Cu-Mg-Y, and Gd-Mg-Zn.
    - These systems are remodeled based on the recent experimental data: Ce-(Gd,La)-Mg, (La,Mn)-Mg-Zn, Gd-Mg-Nd, Mg-Ni-Zn, and Mg-Si-Sn.

TCMG6.2 to TCMG6.3

Software release version: 2022b (June 2022)

- Remodeled Ag-Mg over the entire composition range, with a focus on the Mg-rich corner.
- Refined Al-Mg-Y description via stabilizing the Al2Y phase.
- The GAS phase now has a complete thermodynamic description within the framework of the database.

TCMG6.1 to TCMG6.2

Software release version: 2022a (December 2021/January 2022)

- Electrical resistivity (ELRS) and thermal conductivity (THCD) descriptions for hcp_A3 Mg-Ca/Mn/Sn/Zr are derived based on experimental data.
- The Mg-Y hcp_A3 THCD description is refined.
- Mg-Cu hcp_A3 ELRS and THCD are re-estimated. ELRS and thermal conductivity (THCD) of $CuMg_2$ are tentatively estimated with experimental data from (Mg)+CuMg2 two-phase alloys.
- Mg-Dy and Mg-La ELRS and THCD are re-estimated.
- Molar volume and thermal expansion coefficient of DHCP and liquid Pr are updated

TCMG6.0 to TCMG6.1

Software release version: 2021b (June 2021).

New Assessments

- The interaction parameters for liquid viscosity of 30 binary systems and 1 ternary system.
- The interaction parameters for surface tension of the liquid of 12 binary systems.

Other Updates

- Viscosity parameters of Al-Mg and Al-Ga systems were re-assessed.
- Surface tension parameters of the Al-Ga system were re-assessed.
- Improved thermal conductivity for systems including but not limited to:
  - HCP_A3 Mg-Al, Mg-Ce, Mg-Gd, Mg-Nd, Mg-Sm, Mg-Y, Mg-Zn, and Mg-Gd-Y.
  - FCC_A1 Al-Mg, Cu-Zn, Fe-Ni, Fe-Si, Mn-Ni, Ni-Si, and Ni-Zr
  - BCC_A2 Al-Fe, Fe-Ni, Fe-Si, and Ni-Zr
  - liquid Fe-Ni and more
- Improved electrical resistivity for systems including but not limited to:
  - HCP_A3 Mg-Sm, Mg-Nd, Mg-Gd, and Mg-Y
  - fcc_A1 Cu-Fe, Fe-Si, Mn-Ni, Ni-Si, and Ni-Zr
  - bcc_A2 Al-Fe, Cu-Fe, Fe-Mn, Fe-Ni, Fe-Si, and Ni-Zr
- Electrical resistivity and thermal conductivity were reassessed for $Mg_{12}Ce$, $Mg_{41}Sm_5$, Mg_5Gd, $Mg_{41}Nd_5$, $Al_{12}Mg_{17}$, MgZn and AlFe.
- Phase equilibria of Ce-La was extrapolated.

TCMG5.1 to TCMG6.0

Software release version: 2021a (January 2021).

Newly Modeled Thermophysical Properties

- Electrical resistivity assessed or estimated for all the phases (except for GAS)
- Thermal conductivity assessed or estimated for all the phases (except for GAS)
- Viscosity assessed for liquid
- Surface tension assessed for liquid
- Molar volume and thermal expansivity assessed for all the phases

New Elements

- Bi and H

Newly Modeled Thermodynamic Systems

11 ternaries and 12 binaries were updated.

4 binaries and 3 ternaries are within the scope of Mg-Bi-based alloys:

- Bi-Ca, Bi-Mg, Bi-Mn, Bi-Zn,
- Bi-Ca-Mg, Bi-Mg-Mn, Bi-Mg-Zn

8 binaries and 5 ternaries are among the core systems of hydrogen storage Mg alloys:

- Ce-H, Cu-H, La-Zn, H-La,
- H-Mg, H-Nd, H-Ni, H-Zn,
- Ce-H-Mg, Cu-H-Mg, H-La-Mg,
- H-Mg-Nd, Mg-H-Ni

3 important ternary systems:

- Al-Ce-Mn, Al-La-Mg, La-Mg-Zn

Newly Modeled Metastable Precipitates

The metastable precipitates Mg_7R, Mg_3R ($D0_3$), Mg_3R ($D0_{19}$) that form during aging of Mg-RE (rare earth) alloys have been modeled in the following systems:

- Mg-Gd
- Mg-Nd
- Mg-Y

Updated Phase Equilibria

- Cu-Gd: thermodynamic descriptions are improved for several compounds
- Mg-Nd-Zn: remodeled based on the recent experimental data
- Mg-Al-Ce: remodeling of the Mg-rich $Mg_{12}Ce$ phase and the ternary C15 and $Al_{13}CeMg_6$ phases

TCMG5.0 to TCMG5.1

Software release version: 2019a (December 2018).

The Al-Mn, Al-Fe and Al-Fe-Mn systems were updated.

TCMG4 to TCMG5

Software release version: 2018b (June 2018)

- 7 new elements added: Dy, Er, Ga, Ho, In, Sb and Sm.
- 9 Mg-containing binary systems are assessed: Mg-Dy, Mg-Er, Mg-Ga, Mg-Ho, Mg-In, Mg-K, Mg-Sb, Mg-Sm and Mg-Th. Ag-Mg is remodeled.
- 25 non-Mg binary systems are assessed: Ag-In, Al-In, Ca-In, Ce-In, Cu-In, Fe-In, Gd-In, Gd-Sm, In-K, In-La, In-Li, In-Mn, In-Na, In-Nd, In-Ni, In-Pr, In-Sc, In-Si, In-Sn, In-Sr, In-Th, In-Y, In-Zn, In-Zr and Sm-Zn. Most of these are In-containing.
- 11 ternary systems are modeled: Mg-Ag-In, Mg-Ag-Sn, Mg-Al-In, Mg-Cu-In, Mg-Gd-Sm, Mg-In-Li, Mg-In-Sn, Mg-In-Zn, Mg-Sn-Zn, Ag-In-Sn and In-Sn-Zn. Ag-Gd-Mg is remodeled.
- These systems are also updated: Al-Mg-Zr, Mg-Si-Sn, Cu-Li and Cu-Li-Mg.

TCMG3 TO TCMG4

Software release version: 2015a (June 2015)

- Seven Mg-containing ternary systems were assessed and added to the database: Ag-Cu-Mg, Ag-Gd-Mg, Ca-Gd-Mg, Ca-Mg-Nd, Ce-Mg-Sr, Cu-Li-Mg and Cu-Mg-Y. As a subsystem of Ce-Mg-Sr, the Ce-Sr binary system was assessed.
- Gd-Mg-Zn was deeply refined and Mg-Y-Zn was updated as well.
- The binary Ca-Y and Cu-Li systems and the Mg-containing ternary Al-Ca-Mg, Ca-Mg-Y, Ce-Mg-Zn and Mg-Nd-Sr systems were reassessed.
- The ternary Ca-Sr-Zn system was extrapolated.
- 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.

TCMG2 TO TCMG3

Software release version: 4.0 (June 2014)

- Sc was included in the database, resulting in a total number of 24 elements. Sc-containing systems, Ag-Sc, Al-Sc, Mg-Sc, Mn-Sc, Cu-Sc, Fe-Sc, Sc-Si, Sc-Zr, and Mg-Mn-Sc, were added. Of them, Fe-Sc, Mg-Sc, and Mn-Sc were reassessed.
- The Mn-Nd, Sr-Y, La-Nd, Ce-La-Mg, Ce-Mg-Nd, and La-Mg-Nd systems were assessed and added.

- The La-Mg, Ce-Mg, Mg-Nd and Mg-Y-Zn systems were deeply revised and the La-Nd, Ca-Mn, Mg-Nd-Sr, and Gd-Mg-Sr systems were updated.
- Some known issues were solved.

TCMG1.1 TO TCMG2.0

TCMG2 was released in 2012.

Three binary systems are refined, Ag-Mg, Ce-Mg, and Al-Li. For Ag-Mg, the description of L12 was updated. For Ce-Mg, the Mg-rich description was refined to better account for the Mg-rich binary eutectic reaction, as well as the ternary eutectic reaction in the Ce-Mg-Mn system. In the Al-Li system, the AlLi2 phase was implemented.

Ten ternary systems are assessed or extrapolated, Ca-Ce-Mg, Cu-Mg-Mn, Fe-Mg-Ni, Fe-Mg-Zn, Mg-Mn-Ni, Mg-Mn-Si, Mg-Mn-Zn, Mg-Ni-Zn, and Mg-Si-Zn, together with a non-Mg containing ternary system Ag-Al-Cu.

TCMG1.0 TO TCMG1.1

TCMG1 released in January 2012 and TCMG1.1 in August 2012.

The Gd-Mg-Zn ternary system are reassessed and validated against the experimental information on the phase formation in as-cast and heat treated Gd-Mg-Zn-(Zr) alloys. Consequently, the H and Z phases had been removed from the database, and the W phase was treated as the solution based on GdMg3. The following systems have been assessed, Ca-Nd, Ca-Mn, Ce-Gd, Nd-Sr, Ca-Mg-Zr, Gd-Mg-Zr, Ce-Gd-Mg and Gd-Mg-Sr.