TCS Mg-based Alloys Database (TCMG8)

Technical Information

Available Starting with Thermo-Calc Version 2025b

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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, it has thermophysical 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

TCMG8 Thermophysical 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.

Revision History

TCMG: TCS Magnesium-based Alloys Database Revision History. The current version of the database is TCMG8. See the link for any subversion release details.

TCS Mg-based Alloys Database (TCMG) Resources

Information about the database is available on our website and in the Thermo-Calc software online Help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online Help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCS Mg-based Alloys Database (TCMG) Technical Information* PDF document contains version specific information such as the binary, ternary, and higher-order assessed systems, phases and models. It also includes details about the properties data (e.g. viscosity, surface tension, etc.), a list of the included elements, and summaries of the database revision history by version.
- The *TCS Mg-based Alloys Database (TCMG) Validation and Calculation Examples Collection* PDF document contains a series of validation examples using experimental data, and a set of calculation examples showing some of the ways the database can be used.

Go to the 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.

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.

TCMG8 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 the most recent 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:

- 229 assessed binary systems
- 133 assessed ternary systems
- 5 assessed quaternary systems
- 575 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`.

TCMG8 Thermophysical Properties

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

- In total, 168 binary systems have viscosity parameters.
- 178 binary systems have surface tension parameters.
- 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.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

Model Descriptions

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

Thermophysical 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 versus Graphical Mode as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property (and Graphical Mode Variable Name)	*Model Parameters*	*Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)****
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

Property (and Graphical Mode Variable Name)	*Model Parameters*	*Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)****
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 are using Console Mode 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

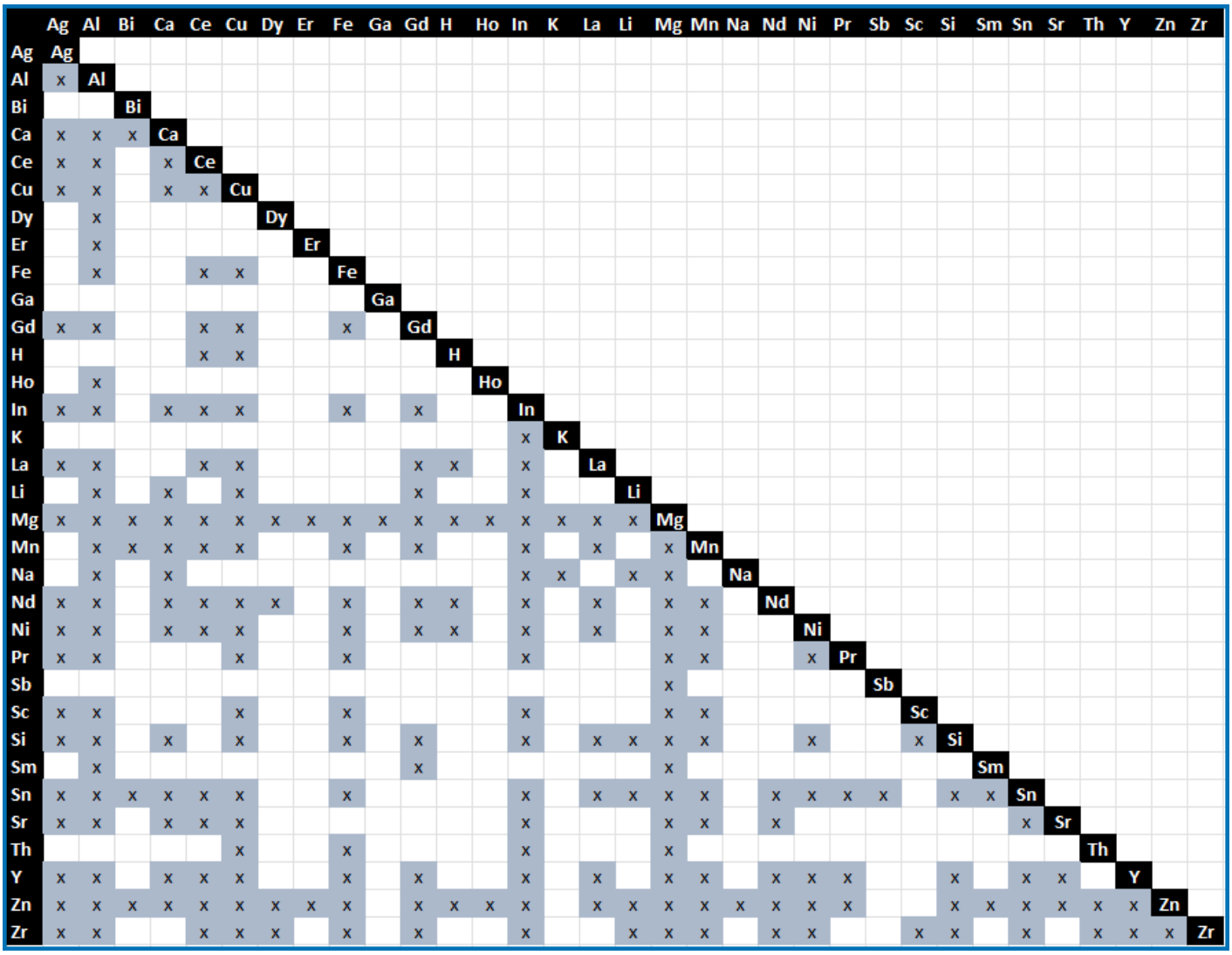
Go to the Magnesium-based Alloys Databases page on our website where you can access a Validation and Calculation Examples Collection and the Technical Information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to magnesium including links to resources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

TCMG8 Systems

In this section:

TCMG8 Assessed Binary Systems

These are the 229 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						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		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	Zn	
Zr	x	x			x	x	x		x		x			x			x	x	x		x	x			x	x		x		x	x	x	Zr

TCMG8 Assessed Ternary Systems

These are the 133 assessed ternary systems.

Assessed Ternary Systems					
Ag-Al-Cu	Ag-Al-Sc	Ag-Cu-Mg	Ag-Gd-Mg	Ag-In-Mg	Ag-In-Sn
Ag-Mg-Sn	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-Li-Mg	Al-Mg-Mn	Al-Mg-Na	Al-Mg-Nd	Al-Mg-Ni
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-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-Zn	Er-Mg-Zn	Fe-Mg-Mn	Fe-Mg-Ni	Fe-Mg-Si	Fe-Mg-Zn
Gd-La-Mg	Gd-Li-Mg	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-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

Assessed Ternary Systems					
Mg-Pr-Y	Mg-Pr-Zn	Mg-Sb-Sn	Mg-Si-Sn	Mg-Si-Y	Mg-Si-Zn
Mg-Sn-Sr	Mg-Sn-Y	Mg-Sn-Zn	Mg-Sr-Zn	Mg-Sr-Zr	Mg-Y-Zn
Mg-Zn-Zr					

TCMG8 Assessed Quaternary Systems

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

TCMG8 Phases

In this section:

Common Phases for Magnesium Alloys

TCMG8 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.
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.

Name in the Database	*Common Name and Description*
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

TCMG8 Models for the Included Phases

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
GAS	Gas					1	(AG, AG1AL1, AG1CU1, AG1H1, AG2, AL, AL1CU1, AL1H1, AL1H2, AL1H3, AL1SB1, AL2, BI, BI1H1, BI1H3, BI2, BI3, BI4, CA, CA1H1, CA2, CE, CU, CU2, CUH, DY, ER, FE, FE1H1, FE2, GA, GA1H1, GA1SB1, GA1SB2, GA2, GD, H, H1IN1, H1K1, H1LI1, H1MN1, H1NA1, H1NI1, H1SB1, H1SI1, H1SR1, H1ZN1, H1ZR1, H2, H2SI1, H3SB1, H3SI1, H4SI1, H4SN1, H6SI2, HMG, HO, IN, IN1SB1, IN1SB2, IN2, K, K1LI1, K1NA1, K2, LA, LI, LI1NA1, LI2, MG, MG2, MN, NA, NA2, ND, NI, NI2, PR, SB, SB2, SB3, SB4, SC, SI, SI2, SI3, SM, SN, SN2, SR, SR2, TH, Y, ZN, ZR, ZR2)1
LIQUID	Liquid					1	(AG, AL, AL2SM, BI, BI2MG3, BI3CA5_N, CA, CA2SN, CE, CU, DY, ER, FE, GA, GD, H, HO, IN, K, LA, LI, MG, MG2SN, MG3SB2, MN, NA, ND, NI, PR, SB, SC, SI, SM, SN, SNSR2, SR, TH, Y, ZN, ZR, ZZ)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, PR, Y, 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, 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

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(H, VA)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, 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	(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, VA, Y, ZN, ZR)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, CU, DY, 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,

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, PR, SM, Y, ZR)5(IN, SI, SN)3
AG51R14	Ag51Gd14		hP68	(175, P6/m)	AG51PR14, AG51CE14, AG51LA14	2	(AG)51(CE, LA, PR)14
MG41R5	Ce5Mg41		tI92	(87, I4/m)	Mg41La5, Mg41Ce5, Mg41Nd5, Mg41Pr5, Mg41Sm5	2	(MG, ZN)41(CA, CE, DY, 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(DY, ER, HO)1
MG3R_D03	BiF3 (D03)	D03	cF16	(225, Fm-3m)	MG3CE, GDMG3, MG3ND, MG3PR, MG3LA, Mg3Sm	2	(LI, MG, ZN)3(CA, CE, DY, ER, GD, LA, MG, ND, PR, SM, SR, Y, ZR)1
L21_RMGZN2	Heusler (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

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, SR, Y)1(AG, CU, IN, NI, ZN)5
CU6R	CeCu6		oP28	(62, Pnma)		2	(CU)6(CE, GD, LA, ND)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, TH, Y)1
MG17SR2	Th2Zn17		hR19	(166, R-3m)		3	(CE, GD, LA, ND, PR, SR, TH, Y)2(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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
M23R6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		2	(AL, FE, MG, MN)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(ZN)11
M5R	AuBe5 (C15b)	C15b	cF24	(216, F-43m)		2	(CU, NI, ZR)5(GD, VA, ZR)1
XZ2_C37	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(AL, SI, SN)1(CA, DY, ER, GD, HO, MG, 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	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(AL)11(LA, SM)3
AL11ND3_H	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(AL)11(ND)3
AL11PR3_H	Al4Ba (D13)	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	(AL, MG, MN, ZN)12(CE, DY, ER, GD, HO, LA, ND, PR, 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

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, Y, ZR)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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL4SR	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(AL, MG)0.8(CA, SR)0.2
AL4CA	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(AL, MG)4(CA, SM, SR)1
AL4CE	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(AL)0.8(CE)0.2
KIN4	Al4Ba (D13)	D13	tI10	(139, I4/mmm)		2	(IN)0.8(K)0.2
THZN4	Al4Ba (D13)	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)1
NI2IN_HT	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		3	(NI, VA)1(NI)1(IN, NI)1
NI2IN_LT	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(LA, NI)2(IN)1
X2IN	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(CE, GD, MN, ND, PR, SC, Y, ZR)2(AL, IN, SN)1
NI3SN2_H	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		3	(NI)0.33333(NI, SN)0.33334(SN)0.33333
ALCU_EPS	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(AL, CU, NI, ZN)1(CU, FE)1
CU2IN_B82	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		3	(CU, MG)1(CU, VA)1(IN)1
ETA	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		3	(CU)1(CU, SN)1(SN)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FE5SN3	Ni2In (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)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 (L21)	L21	cF16	(225, Fm-3m)		3	(DY, ER, HO, LA, PR)1(MG, ZN)2(MG)1
LI2MGIN	Heusler (L21)	L21	cF16	(225, Fm-3m)		3	(LI)2(MG)1(IN)1
AG2Y	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AG)0.667(Y)0.333
CU2SC_C11B	MoSi2 (C11b)	C11b	tI6	(139,		2	(AG, AL, CU)2(SC)1

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				I4/mmm)			
CUZR2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(CU, ZN)0.333(ZR)0.667
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

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(CE, LA)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

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
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, I4/mmm)		2	(AG)0.667(GD)0.333
AG51GD14	Ag51Gd14		hP68	(175, P6/m)		2	(AG)0.785(GD)0.215
AG2IN_D83	gamma-brass (Cu9Al4,	D83	cP52	(215, P-43m)		2	(AG)0.68(IN)0.32

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
	D83)						
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(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
AGY	CsCl (B2)	B2	cP2	(221, Pm-3m)		2	(AG)0.5(Y)0.5
AG51Y4	Ag51Gd14		hP68	(175, P6/m)		2	(AG)0.785(Y)0.215
AG1ZN1	zeta-AgZn (Bb)	Bb	hP9	(147, P-3)		2	(ZN)1(AG, ZN)2
AGZN3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)		1	(AG, ZN)1
AG5ZN8	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		4	(AG, ZN)2(AG)2(AG, ZN)3(AG, ZN)6

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AG1ZR1	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(AG)0.5(ZR)0.5
AGZR2	CuZr2		tI6	(139, I4/mmm)		2	(AG)0.3333(ZR)0.6667
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	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)		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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL5FE2	Al2.8Fe		oS24	(63, Cmcm)		2	(AL)5(FE, MN)2
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(AL, MG, NI, ZN)24
LTAL11MN4	Al11Mn4		aP15	(2, P-1)		2	(AL)11(FE, MN)4
AL12MN	Al12W		cI26	(204, Im-3)		2	(AL)12(MN)1
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)		2	(AL)6(FE, MN)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(FE, MN)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

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	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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CACU5	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CA)0.1667(CU)0.8333
CA1CU1	alpha-CaCu		mP20	(11, P2_1/m)		2	(CA)0.5(CU)0.5
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CU5CE	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CU)0.833(CE)0.167
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
CEGD3	alpha-Sm (C19)	C19	hR3	(166, R-3m)		1	(CE, GD)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
CEZN5	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CE)0.167(MG, ZN)0.833
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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
CU5PR	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(CU)0.833(PR)0.167
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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
FE5TH	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(FE)0.83(TH)0.17

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
ZETA_FEZN	CoZn13		mS28	(12, C2/m)		3	(FE, VA)0.072(ZN)0.856(VA, ZN)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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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, GD, LA, ND, SM, SR, Y)1(MG, ZN)5
MG7RE	Unknown Structure					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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
MG2IN	Mg2In		hP9	(189, P-62m)		2	(MG)2(IN)1
MG3IN	Mg3In		hr16	(166, R-3m)		2	(IN, MG, SN)3(IN, MG, 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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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 Lattice (Af)	Af	hP1	(191, P6/mmm)		1	(IN, SN)1
TET_ALPHA1_A6	In (A6)	A6	tI2	(139, I4/mmm)		1	(IN, SN)1
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
LANI5	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		3	(LA, NI)0.16667(LA, NI)0.33333(NI)0.5
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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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	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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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	(MG)24(CA, CE, DY, ER, GD, HO, LA, MG, ND, PR, 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, 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 (L10)	L10	tP2	(123, P4/mmm)		2	(IN, MG, MN, NI, SC)0.5(IN, MG, MN, NI)0.5
MNNI2	Unknown Structure					2	(MN, NI)1(NI)2
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN23Y6	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		2	(MG, MN)23(Y)6
MNZN9_LT	unknown 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
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
NI5PR	CaCu5 (D2d)	D2d	hP6	(191, P6/mmm)		2	(NI)0.8333(PR)0.1667
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
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	(SN, ZR)3(SN, ZR)1
ZR5SN3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)		3	(ZR)5(SN)3(SN, VA)1
ZRSN2	TiSi2 (C54)	C54	oF24	(70, Fddd)		2	(ZR)1(SN)2
SRZN5_L	SrZn5		oP24	(62, Pnma)		2	(SR)1(ZN)5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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
T1_AGALSC	Heusler (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
AGGDMG_T	Unknown Structure					2	(AG, GD)0.15(MG)0.85
AL9CA31ZN10	Unknown Structure					3	(AL)1(CA)1(ZN)1
AL2CAZN2	Al4Ba (D13)	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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALCUMG_Q	Chalcopyrite (CuFeS2, E11)	E11	tI16	(122, I-42d)		3	(AL)7(CU)3(MG)6
ALCUMG_S	MgCuAl2 (E1a)		oS16	(63, Cmcm)		3	(AL, SI)2(CU)1(MG)1
ALCUMG_T	Bergman [Mg32 (Al,Zn)49, D8e]	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
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
AL38MG58SR4	Unknown Structure					3	(AL)38(MG)58(SR)4

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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]	D8e	cI162	(204, Im-3)		4	(MG)26(AL, MG)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
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
CA2MG6ZN3	Unknown Structure		h**			3	(CA)2(MG)6(ZN)3
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
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

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	(CU)2.74(MG)2(SI)1.26
CU4MGSN_T1	Half-Heusler (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

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)		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
MG2NIH4	Mg2NiH4		mS56	(15, C2/c)		3	(MG)2(NI)1(H)4
MGSNSR_T1	Unknown Structure					3	(MG)25(SN)24(SR)14

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
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	Unknown Structure					3	(MG)0.35(ND)0.05(ZN)0.6
MGNDZN_T2	Unknown Structure					3	(MG)0.35(ND)0.1(ZN)0.55
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
AL3CU2MG9SI7	Q-(Al,Cu,Mg,Si)		hP21	(174, P-6)		4	(AL)3(CU)2(MG)9(SI)7

TCMG: TCS Magnesium-based Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS Mg-based Alloys Database (TCMG)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**8.0**
First release	**TCMG1 was released in 2012**

Changes in the Most Recent Database Release

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)

Previous Releases

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.