TCS Mg-based Alloys Database (TCMG7)

Technical Information

Available Starting with Thermo-Calc Version 2024a

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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

TCS Mg-based Alloys Database (TCMG) was developed to be used with our entire suite of products: Thermo-Calc, the Add-on Modules and all available SDKs.

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, and
- surface tension of liquid.

TCMG: TCS Magnesium-based Alloys Database Revision History. The current version of the database is TCMG7. See the link for any subversion release details.

The database is compatible with the TCS Mg-alloys Mobility Database (MOBMG). The current version is MOBMG2.

The CALPHAD Method

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

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

Use Case Examples

There are examples available to both demonstrate the *validation* of the database and to showcase the types of *calculations* that can be used for different materials or application areas such as process metallurgy, heat treatment, and more depending on the database. Sometimes an example is both a validation and a calculation example.

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.

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

TCMG7 Elements, Systems, Phases and Properties

Included Elements

There are 33 elements included in the most recent version of the database.

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:

- 223 assessed binary systems
- 124 assessed ternary systems
- 5 assessed quaternary systems
- 541 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`.

Properties Data

A variety of properties data is included with 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.

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

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

Below is a summary of the available parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use the TC-Python SDK. More details are described in the online help.

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Electrical conductivity	ELQ**	ELCD for a system `ELCD(PHI)` for phase PHI
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI*	`SURF(LIQUID)` `SURF(ION)` **
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)` **
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)` **

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

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

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

TCMG7 Systems

In this section:

TCMG7 Assessed Binary Systems

These are the 223 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		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		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

TCMG7 Assessed Ternary Systems

These are the 124 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	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-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-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-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-Sr	Mg-Nd-Y	Mg-Nd-Zn	Mg-Nd-Zr	Mg-Ni-Y	Mg-Ni-Zn
Mg-Pr-Y	Mg-Pr-Zn	Mg-Si-Sn	Mg-Si-Y	Mg-Si-Zn	Mg-Sn-Sr

Assessed Ternary Systems					
Mg-Sn-Zn	Mg-Sr-Zn	Mg-Y-Zn	Mg-Zn-Zr		

TCMG7 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

TCMG7 Phases

In this section:

Common Phases for Magnesium Alloys

TCMG7 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

TCMG7 Models for the Included Phases

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
GAS	Gas						1	[1.0]	(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	[1.0]	(AG, AL, AL2SM, BI, BI2MG3, BI3CA5_N, CA, CA2SN, CE, CU, DY, ER, FE, GA, GD, H, HO, IN, K, LA, LASN, 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	Im-3m	229		2	[1.0, 3.0]	(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	Pm-3m	221	A B2 phase described with the partitioning model and having a contribution from its disordered counterpart.	3	[0.5, 0.5, 3.0]	(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	Pm-3m	221	B2 phases modeled separately from A2	2	[0.5, 0.5]	(AG, CU, NI, ZN)0.5(CE, GD, ND, PR, Y, ZR)0.5

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
B2_MGR	CsCl (B2)	B2	cP2	Pm-3m	221	LaMg, MgNd, NdZn, CeMg, CeZn, MgY, YZn, GdMg, GdZn, MgSm, AgMg	2	[0.5, 0.5]	(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	I4_1/amd	141		1	[1.0]	(AG, AL, BI, IN, SN, SR, ZN)1
CBCC_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[1.0, 1.0]	(AL, CU, FE, IN, MG, MN, NI, SI, SN, ZN, ZR)1(VA)1
CUB_A13	beta-Mn (A13)	A13	cP20	P4_132	213		2	[1.0, 1.0]	(AG, AL, CA, CE, CU, FE, IN, MG, MN, NI, SI, SN, ZN, ZR)1(VA)1
DHCP	alpha-La (A3')	A3'	hP4	P6_3/mmc	194		2	[1.0, 2.0]	(AG, AL, CA, CE, CU, DY, GD, IN, LA, MG, MN, ND, NI, PR, SR, Y, ZR)1(H, VA)2
DIAMOND_A4	Diamond (A4)	A4	cF8	Fd-3m	227		1	[1.0]	(AL, SI, SN, ZN)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225		2	[1.0, 1.0]	(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	Pm-3m	221	L12 phases, CaSn3, LaSn3, Mg1.2In2.8, CeIn3, NdIn3, ScIn3, PrIn3, ThIn3	2	[1.0, 3.0]	(AL, CA, CE, IN, LA, MG, ND, PR, SC, TH, Y)1(AG, AL, IN, MG, NI, SN, ZR)3
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		2	[1.0, 0.5]	(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	P-3m1	164		2	[2.0, 1.0]	(FE)2(SI)1
FESI2_H	FeSi2-h		tP3	P4/mmm	123		2	[3.0, 7.0]	(FE)3(MG, SI)7
FESI2_L	FeSi2-l		oS48	Cmce	64		2	[1.0, 2.0]	(FE)1(SI)2

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194	> Al2Zr, CaLi2, CaMg2, Mg2Sr, Mg2Y, MgZn2, Mn2Zr, Na2K	2	[2.0, 1.0]	(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	Fd-3m	227	It includes 18 compounds, e.g. Al2Ca, Al2Ce, Cu2Mg, Fe2Gd, Mg2Gd	3	[2.0, 1.0, 2.0]	(AL, CA, CU, DY, ER, FE, GD, HO, IN, LA, LI, MG, MN, ND, NI, SI, Y, ZN, ZR)2(AL, CA, CE, CU, DY, ER, FE, GD, HO, IN, LA, LI, MG, ND, NI, PR, SC, SI, SM, SR, TH, Y, ZN, ZR)1(H, VA)2
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_3/mmc	194	> MgNi2 type phase, also includes MgNi2, (Cu,Zn)2Mg, (Al,Mg)2Ca	2	[2.0, 1.0]	(AL, CU, FE, GD, MG, MN, NI, ZN)2(AL, CA, CU, DY, ER, GD, HO, MG, NI, TH, ZN, ZR)1
MG2SI_C1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	This is also Si2Ni & Mg2Sn	2	[2.0, 1.0]	(BI, MG, SI)2(BI, MG, NI, SI, SN)1
MSI_B20	FeSi (B20)	B20	cP8	P2_13	198	FeSi & MnSi	2	[1.0, 1.0]	(FE, MN)1(MG, SI)1
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193	> Fe5Si3, Gd5Si3, Mn5Si3, Y5Si3, Zr5Si3, also LA5SN3(HT)	2	[5.0, 3.0]	(FE, GD, LA, MN, Y, ZR)5(IN, SI, SN)3
AG51R14	Ag51Gd14		hP68	P6/m	175	AG51PR14, AG51CE14, AG51LA14	2	[51.0, 14.0]	(AG)51(CE, LA, PR)14
MG41R5	Ce5Mg41		tI92	I4/m	87	Mg41La5, Mg41Ce5, Mg41Nd5, Mg41Pr5, Mg41Sm5	2	[41.0, 5.0]	(MG, ZN)41(CA, CE, DY, GD, LA, ND, PR, SM, SR, Y)5
XZN13	NaZn13 (D23)	D23	cF112	Fm-3c	226	CaZn13, LaZn13, NaZn13, SrZn13	2	[1.0, 13.0]	(CA, LA, NA, SR)1(ZN)13
AL3R	AL3HO		hR20	R-3m	166		2	[3.0, 1.0]	(AL)3(DY, ER, HO)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
MG3R_D03	BiF3 (D03)	D03	cF16	Fm-3m	225	MG3CE, GDMG3, MG3ND, MG3PR, MG3LA, Mg3Sm	2	[3.0, 1.0]	(LI, MG, ZN)3(CA, CE, DY, ER, GD, LA, MG, ND, PR, SM, SR, Y, ZR)1
L21_RMGZN2	Heusler (L21)	L21	cF16	Fm-3m	225	isostructural to GdMg3: CeMgZn2, GdMgZn2, MgZn2Y, aka W	3	[1.0, 1.0, 2.0]	(CE, GD, Y)1(MG)1(MG, ZN)2
ALR_OS16	AlCe		oS16	Cmcm	63	a phase based on ALCE, ALLA, ALPR (rt)	2	[1.0, 1.0]	(AL)1(CE, LA, PR)1
CA5X3	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140	CA5SI3, CA5SN3, CA5AG3, CA5ZN3, also La5Si3	2	[5.0, 3.0]	(CA, LA, SR)5(AG, SI, SN, ZN)3
RHOMBO_A7	alpha-As (A7)	A7	hR2	R-3m	166	based on Bi and Sb	1	[1.0]	(BI, SB, SN, ZN)1
RM5	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[1.0, 5.0]	(CA, CE, GD, LA, ND, SR, Y)1(AG, CU, IN, NI, ZN)5
CU6R	CeCu6		oP28	Pnma	62		2	[6.0, 1.0]	(CU)6(CE, GD, LA, ND)1
XZ2_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[1.0, 2.0]	(AG, AL, CU, FE, NI, SI, ZN, ZR)1(AL, FE, IN, SN, TH, ZR)2
X3NI	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(AL, GD, LA, NI, PR, Y)3(NI, SI)1
MR_B27	FeB (B27)	B27	oP8	Pnma	62		2	[1.0, 1.0]	(CU, NI, SI, ZN)1(CE, GD, LA, ND, PR, SR, Y, ZR)1
M2R	KHg2		oI12	Imma	74		2	[2.0, 1.0]	(AG, AL, CU, MG, ZN)2(CA, CE, DY, ER, GD, HO, LA, ND, PR, SR, Y)1
M3R	Ni3Pu		hR12	R-3m	166		2	[3.0, 1.0]	(FE, NI)3(CA, GD, LA, MG, PR, TH, Y)1
MG17SR2	Th2Zn17		hR19	R-3m	166		3	[2.0, 17.0, 14.0]	(CE, GD, LA, ND, PR, SR, TH, Y)2(AL, FE,

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
									MG, NI, ZN)17(H, VA)14
CE2ZN17	Th2Zn17		hR19	R-3m	166		2	[0.105, 0.895]	(CE)0.105(MG, ZN)0.895
FE17ND2	Th2Zn17		hR19	R-3m	166		2	[1.0, 0.1176]	(FE)1(ND)0.1176
FE17PR2	Th2Zn17		hR19	R-3m	166		2	[17.0, 2.0]	(FE)17(PR)2
FE17TH2	Th2Zn17		hR19	R-3m	166		2	[0.89, 0.11]	(FE)0.89(TH)0.11
MN17ND2	Th2Zn17		hR19	R-3m	166		2	[17.0, 2.0]	(MN)17(ND)2
NI7PR2	Th2Zn17		hR19	R-3m	166		2	[0.7778, 0.2222]	(NI)0.7778(PR)0.2222
M23R6	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		2	[23.0, 6.0]	(AL, FE, MG, MN)23(CE, GD, ND, PR, SR, TH, Y, ZR)6
XR	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(AG, AL, MG, NI, SI, SN, ZN)1(CA, CE, GD, LA, PR, SC, SR, Y, ZR)1
R3ZN22	Ce3Zn22		tI100	I4_1/amd	141		2	[0.12, 0.88]	(CE, GD, LA, ND, PR)0.12(ZN)0.88
RZN11	BaCd11		tI48	I4_1/amd	141		2	[1.0, 11.0]	(CA, LA, ND, PR)1(ZN)11
M5R	AuBe5 (C15b)	C15b	cF24	F-43m	216		2	[5.0, 1.0]	(CU, NI, ZR)5(GD, VA, ZR)1
XZ2_C37	Co2Si (C37)	C37	oP12	Pnma	62		2	[1.0, 2.0]	(AL, SI, SN)1(CA, DY, ER, GD, HO, MG, ND, NI, PR, SM, SR, Y)2
ALR_OP16	DyAl		oP16	Pbcm	57		2	[1.0, 1.0]	(AL)1(DY, ER, GD, HO, ND, PR, SM)1
AL11LA3_H	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[11.0, 3.0]	(AL)11(LA, SM)3
AL11ND3_H	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[11.0, 3.0]	(AL)11(ND)3
AL11PR3_H	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[11.0, 3.0]	(AL)11(PR)3

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AL11R3	Al11La3		oI28	Immm	71		2	[11.0, 3.0]	(AL, ZN)11(CE, LA, ND, PR, Y)3
GD3ZN11	Al11La3		oI28	Immm	71		2	[0.214, 0.786]	(DY, GD)0.214(ZN)0.786
CE3ZN11	Al11La3		oI28	Immm	71		2	[0.214, 0.786]	(CE)0.214(MG, ZN)0.786
R7M3	Fe3Th7 (D102)	D102	hP20	P6_3mc	186		2	[0.7, 0.3]	(CE, LA, PR, TH)0.7(FE, NI)0.3
MG12R	Mn12Th (D2b)	D2b	tI26	I4/mmm	139		2	[12.0, 1.0]	(AL, MG, MN, ZN)12(CE, DY, ER, GD, HO, LA, ND, PR, SR, Y)1
RSI2	GdSi1.4		oI12	Imma	74		2	[1.0, 2.0]	(LA, Y)1(SI)2
RZN3	Zn3Y		oP16	Pnma	62		2	[1.0, 3.0]	(DY, ER, GD, HO, ND, PR, Y)1(ZN)3
AL2R3	Zr3Al2		tP20	P4_2/mnm	136		2	[0.4, 0.6]	(AL, ZN)0.4(DY, ER, HO, Y, ZR)0.6
R5SI4	Si4Zr5		tP36	P4_12_12	92		2	[5.0, 4.0]	(LA, MG, ZR)5(SI)4
M10ZR7	Ni10Zr7		oS68	Cmce	64		2	[10.0, 7.0]	(CU, NI)10(ZR)7
R3SI2	Si2U3 (D5a)	D5a	tP10	P4/mbm	127		2	[3.0, 2.0]	(LA, MG, ZR)3(SI)2
R2NI7	Ce2Ni7		hP36	P6_3/mmc	194		2	[2.0, 7.0]	(CE, LA, MG, Y)2(NI)7
RZN5	ErZn5		hP36	P6_3/mmc	194		2	[1.0, 5.0]	(ER, HO)1(ZN)5
ALLA3	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[1.0, 3.0]	(AL)1(LA)3
ALND3	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[1.0, 3.0]	(AL)1(ND)3
AL3LA	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(AL)3(CE, GD, LA, ND, PR, SM, Y)1
MG3R_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(MG)3(GD, ND, Y, ZN)1
SC3IN	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(SC)3(IN)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
NI3IN1	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(NI)3(IN)1
IN3SR1	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[0.75, 0.25]	(IN)0.75(SR)0.25
NI3ZR	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(NI)3(ZR)1
AL4SR	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[0.8, 0.2]	(AL, MG)0.8(CA, SR)0.2
AL4CA	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[4.0, 1.0]	(AL, MG)4(CA, SM, SR)1
AL4CE	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[0.8, 0.2]	(AL)0.8(CE)0.2
KIN4	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[0.8, 0.2]	(IN)0.8(K)0.2
THZN4	Al4Ba (D13)	D13	tI10	I4/mmm	139		2	[1.0, 4.0]	(TH)1(ZN)4
AL4SM_D1B	Al4U (D1b)	D1b	oI20	Imma	74		2	[4.0, 1.0]	(AL)4(SM)1
RHOMB_C19	alpha-Sm (C19)	C19	hR3	R-3m	166		1	[1.0]	(AL, GD, MG, SM)1
NI2IN_HT	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[1.0, 1.0, 1.0]	(NI, VA)1(NI)1(IN, NI)1
NI2IN_LT	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[2.0, 1.0]	(LA, NI)2(IN)1
X2IN	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[2.0, 1.0]	(CE, GD, MN, ND, PR, SC, Y, ZR)2(AL, IN, SN)1
NI3SN2_H	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[0.33333, 0.33334, 0.33333]	(NI)0.33333(NI, SN)0.33334(SN)0.33333
ALCU_EPS	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[1.0, 1.0]	(AL, CU, NI, ZN)1(CU, FE)1
CU2IN_B82	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[1.0, 1.0, 1.0]	(CU, MG)1(CU, VA)1(IN)1
ETA	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[1.0, 1.0, 1.0]	(CU)1(CU, SN)1(SN)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
FE5SN3	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[5.0, 3.0]	(FE)5(SN)3
MG2NI9Y	LaMg2Ni9		hR36	R-3m	166		3	[2.0, 9.0, 1.0]	(MG)2(NI)9(Y)1
LPSO_14H	LPSO-14H		hP170	P6_3/mcm	193		4	[70.0, 8.0, 6.0, 1.0]	(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	C2/m	12		4	[58.0, 8.0, 6.0, 1.0]	(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	P6_3/mmc	194		2	[0.183, 0.817]	(CE)0.183(ZN)0.817
GD13ZN58	Gd13Zn58		hP142	P6_3/mmc	194		2	[0.183, 0.817]	(DY, ER, GD, HO)0.183(MG, ZN)0.817
PR13ZN58	Gd13Zn58		hP142	P6_3/mmc	194		2	[0.1831, 0.8169]	(PR)0.1831(ZN)0.8169
GD2ZN17_L	Ni17Th2		hP38	P6_3/mmc	194		2	[0.105, 0.895]	(DY, ER, GD, HO)0.105(AL, MN, ZN)0.895
GD2ZN17_H	Th2Zn17		hR19	R-3m	166		2	[0.105, 0.895]	(DY, ER, GD, HO, SM)0.105(ZN)0.895
I_MGRZN	Quasicrystal						3	[0.1, 0.3, 0.6]	(DY, ER, GD, HO, Y)0.1(MG, ZN)0.3(MG, ZN)0.6
LAMGZN_T1	Unkown Structure			Cmc21			2	[0.08, 0.92]	(LA)0.08(MG, ZN)0.92
LAMGZN_T2	Unknown Structure						3	[0.21, 0.57, 0.22]	(LA)0.21(ZN)0.57(MG, ZN)0.22
LAMGZN_T3	Cu2MnAl		cF16	Fm-3m	225		3	[1.0, 2.0, 1.0]	(DY, ER, HO, LA, PR)1(MG, ZN)2(MG)1
LI2MGIN	Cu2MnAl		cF16	Fm-3m	225		3	[2.0, 1.0, 1.0]	(LI)2(MG)1(IN)1
AG2Y	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[0.667, 0.333]	(AG)0.667(Y)0.333
CU2SC_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(AG, AL, CU)2(SC)1
CUZR2	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[0.333, 0.667]	(CU, ZN)0.333(ZR)0.667

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
Y13ZN58	Y13Zn58		hP146	P6_3/mmc	194		2	[13.0, 58.0]	(Y)13(ZN)58
ND13ZN58	Y13Zn58		hP146	P6_3/mmc	194		2	[0.183, 0.817]	(ND)0.183(ZN)0.817
T1_MGZNZR	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		3	[0.2633, 0.6667, 0.07]	(MG)0.2633(ZN)0.6667(ZR)0.07
T2_MGZNZR	Unknown Structure						3	[0.1633, 0.6667, 0.17]	(MG)0.1633(ZN)0.6667(ZR)0.17
T3_MGZNZR	Unknown Structure						3	[0.1133, 0.6667, 0.22]	(MG)0.1133(ZN)0.6667(ZR)0.22
T4_MGZNZR	Unknown Structure						3	[0.086, 0.84, 0.074]	(MG)0.086(ZN)0.84(ZR)0.074
AL3DY_D024	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194		2	[3.0, 1.0]	(AL)3(DY)1
AG9CA2	Unknown Structure						2	[0.818182, 0.181818]	(AG)0.818182(CA)0.181818
AG7CA2	Ag7Yb2		oS36	Cmcm	63		2	[0.777778, 0.222222]	(AG)0.777778(CA)0.222222
AGCA3	Unknown Structure						2	[0.25, 0.75]	(AG)0.25(CA)0.75
AG4CE	Unknown Structure						2	[4.0, 1.0]	(AG)4(CE)1
AG2GD	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[0.667, 0.333]	(AG)0.667(GD)0.333
AG51GD14	Ag51Gd14		hP68	P6/m	175		2	[0.785, 0.215]	(AG)0.785(GD)0.215
AG2IN_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215		2	[0.68, 0.32]	(AG)0.68(IN)0.32
AG5LA	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		2	[5.0, 1.0]	(AG)5(LA)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AGMG4	Ag9Mg37		hP116	P6_3/m	176		2	[0.2, 0.8]	(AG)0.2(MG)0.8
AGMG3	Hf54Os17		oI142	Immm	71		2	[0.23, 0.77]	(AG, CU, SN)0.23(CU, IN, MG)0.77
AG51ND14	Ag51Gd14		hP68	P6/m	175		2	[0.785, 0.215]	(AG)0.785(ND)0.215
AG2ND_H	Unknown Structure						2	[0.666667, 0.333333]	(AG)0.666667(ND)0.333333
AG2PR	Unknown Structure		hP*				2	[2.0, 1.0]	(AG)2(PR)1
AG5PR	Unknown Structure						2	[5.0, 1.0]	(AG)5(PR)1
AG4SC	Ni4Mo (D1a)	D1a	tI10	I4/m	87		2	[0.8, 0.2]	(AG, AL)0.8(SC)0.2
AG3SN1	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59		2	[0.75, 0.25]	(AG)0.75(AG, SN)0.25
AG4SR	Unknown Structure						2	[4.0, 1.0]	(AG)4(SR)1
AGSR	SrAg		oP16	Pnma	62		2	[1.0, 1.0]	(AG)1(SR)1
AG2SR3	Er3Ni2		hR15	R-3	148		2	[2.0, 3.0]	(AG)2(SR)3
AGY	CsCl (B2)	B2	cP2	Pm-3m	221		2	[0.5, 0.5]	(AG)0.5(Y)0.5
AG51Y4	Ag51Gd14		hP68	P6/m	175		2	[0.785, 0.215]	(AG)0.785(Y)0.215
AG1ZN1	zeta-AgZn (Bb)	Bb	hP9	P-3	147		2	[1.0, 2.0]	(ZN)1(AG, ZN)2
AGZN3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		1	[1.0]	(AG, ZN)1
AG5ZN8	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		4	[2.0, 2.0, 3.0, 6.0]	(AG, ZN)2(AG)2(AG, ZN)3(AG, ZN)6
AG1ZR1	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[0.5, 0.5]	(AG)0.5(ZR)0.5

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AGZR2	CuZr2		tI6	I4/mmm	139		2	[0.3333, 0.6667]	(AG)0.3333(ZR)0.6667
AL14CA13	Al14Ca13		mS54	C2/m	12		2	[14.0, 13.0]	(AL, MG, ZN)14(CA)13
AL3CA8	Ca8In3		aP22	P-1	2		2	[3.0, 8.0]	(AL)3(CA, MG)8
AL3CE_H	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[0.75, 0.25]	(AL)0.75(CE)0.25
ALCE2	Unknown Structure						2	[0.3333, 0.6667]	(AL)0.3333(CE)0.6667
ALRE3	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[1.0, 3.0]	(AL, IN)1(CE, PR)3
ALCE3_L	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[0.25, 0.75]	(AL)0.25(CE)0.75
ALCU_DEL	Al5Cu8		hR52	R3m	160		2	[2.0, 3.0]	(AL, ZN)2(CU, FE)3
ALCU_ETA	AlCu(r)		mS20	C2/m	12		2	[1.0, 1.0]	(AL, CU)1(AG, CU)1
ALCU_PRIME	Al9Cu11(h)		oF88	Fmm2	42		2	[2.0, 1.0]	(AL)2(CU)1
ALCU_ZETA	Al9Cu11(h)		oF88	Fmm2	42		2	[9.0, 11.0]	(AL)9(AG, CU)11
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215		3	[4.0, 1.0, 8.0]	(AL, SI)4(AL, CU, SI)1(AG, CU)8
GAMMA_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		3	[4.0, 1.0, 8.0]	(AL)4(AL, CU)1(AG, CU)8
AL13FE4	Al13Fe4		mS102	C2/m	12		3	[0.6275, 0.235, 0.1375]	(AL)0.6275(FE, MN)0.235(AL, VA)0.1375
AL2FE	Al2Fe		aP18	P1	1		2	[2.0, 1.0]	(AL)2(FE, MN)1
AL5FE2	Al2.8Fe		oS24	Cmcm	63		2	[5.0, 2.0]	(AL)5(FE, MN)2
AL2GD3	Gd3Al2		tP20	P4_2nm	102		2	[2.0, 3.0]	(AL)2(GD)3

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AL53LA22	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[0.707, 0.293]	(AL)0.707(LA)0.293
AL2LI3	Li3Al2		hr5	R-3m	166		2	[2.0, 3.0]	(AL, MG)2(LI)3
ALLI2	Li2Ga		oS12	Cmcm	63		2	[1.0, 2.0]	(AL)1(LI)2
AL4LI9	Al4Li9		mS26	C2/m	12		2	[4.0, 9.0]	(AL)4(LI)9
AL1LI1	NaTl (B32)	B32	cF16	Fd-3m	227		2	[1.0, 1.0]	(AL, LI, MG)1(LI, MG, VA)1
ALMG_BETA	Al45Mg28		cF1832	Fd-3m	227		2	[140.0, 89.0]	(AL, ZN)140(LI, MG)89
ALMG_EPSILON	Al30Mg23		hR53	R-3	148		2	[30.0, 23.0]	(AL, ZN)30(MG)23
AL12MG17_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[10.0, 24.0, 24.0]	(GD, LI, MG)10(AL, CA, MG, ZN)24(AL, MG, NI, ZN)24
LTAL11MN4	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(FE, MN)4
AL12MN	Al12W		cI26	Im-3	204		2	[12.0, 1.0]	(AL)12(MN)1
AL6MN	MnAl6 (D2h)	D2h	oS28	Cmcm	63		2	[6.0, 1.0]	(AL)6(FE, MN)1
AL4MN	mu-Al4Mn		hP574	P6_3/mmc	194		2	[4.0, 1.0]	(AL)4(FE, MN)1
R_AL4MN	lambda-Al4Mn		hP586	P6_3/m	176		2	[461.0, 107.0]	(AL)461(FE, MN)107
AL3NI2	Al3Ni2 (D513)	D513	hP5	P-3m1	164		3	[3.0, 2.0, 1.0]	(AL)3(AL, MG, NI)2(NI, VA)1
AL3NI5	Ga3Pt5		oS16	Cmmm	65		2	[0.375, 0.625]	(AL)0.375(NI)0.625
ALPR3_L	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[1.0, 3.0]	(AL)1(PR)3
AL7SR8	Ba8Ga7		cP60	P2_13	198		2	[0.46667, 0.53333]	(AL)0.46667(CA, SR)0.53333
AL3SR8	Unknown Structure						2	[0.27273, 0.72727]	(AL)0.27273(SR)0.72727

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
AL3Y_H	BaPb3		hR12	R-3m	166		2	[0.75, 0.25]	(AL)0.75(Y)0.25
AL3ZR5	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[0.375, 0.625]	(AL)0.375(ZR)0.625
AL3ZR4	Al3Zr4		hP7	P6/mmm	191		2	[0.42857, 0.57143]	(AL)0.42857(ZR)0.57143
AL4ZR5	Ti5Ga4		hP18	P6_3/mcm	193		2	[0.44444, 0.55556]	(AL)0.44444(ZR)0.55556
AL3ZR2	Zr2Al3		oF40	Fdd2	43		2	[0.6, 0.4]	(AL)0.6(ZR)0.4
AL3ZR1	Al3Zr (D023)	D023	tI16	I4/mmm	139		2	[0.75, 0.25]	(AL, IN, MG)0.75(ZR)0.25
BI2CA1	ZrSi2 (C49)	C49	oS12	Cmcm	63		2	[2.0, 1.0]	(BI)2(CA)1
BI10CA11	Ge10Ho11		tI84	I4/mmm	139		2	[10.0, 11.0]	(BI)10(CA)11
BI3CA5	beta-Yb5Sb3		oP32	Pnma	62		2	[3.0, 5.0]	(BI)3(CA)5
BICA2	La2Sb		tI12	I4/mmm	139		2	[1.0, 2.0]	(BI)1(CA)2
BI2MG3_LT	La2O3 (D52)	D52	hP5	P-3m1	164		2	[2.0, 3.0]	(BI, SN, VA)2(MG)3
BI2MG3_HT	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	206		3	[1.0, 3.0, 6.0]	(BI, SN)1(BI, SN, VA)3(MG)6
BIMN_LT	NiAs (B81)	B81	hP4	P6_3/mmc	194		2	[1.0, 1.0]	(BI)1(MN)1
BIMN_HT	Mn2.23Bi1.88		oP10	Pmma	51		2	[1.0, 1.08]	(BI)1(MN)1.08
CACU5	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[0.1667, 0.8333]	(CA)0.1667(CU)0.8333
CA1CU1	alpha-CaCu		mP20	P2_1/m	11		2	[0.5, 0.5]	(CA)0.5(CU)0.5
CA2CU	Ca2Cu		oP12	Pnma	62		2	[0.6667, 0.3333]	(CA)0.6667(CU)0.3333
CA8IN3	Ca8In3		aP22	P-1	2		2	[8.0, 3.0]	(CA)8(IN)3

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
CA1IN2	CaIn2		hP6	P6_3/mmc	194		2	[1.0, 2.0]	(CA)1(IN)2
CANI2	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[0.333, 0.667]	(CA)0.333(NI)0.667
CA2NI7	Co7Gd2		hR18	R-3m	166		2	[0.2222, 0.7778]	(CA)0.2222(NI)0.7778
CA3SI4	Ca3Si4		hP42	P6_3/m	176		2	[0.428571, 0.571429]	(CA)0.428571(SI)0.571429
CA14SI19	Ca14Si19		hR66	R-3c	167		2	[0.424242, 0.575758]	(CA)0.424242(SI)0.575758
CASI2	CaSi2 (C12)	C12	hR6	R-3m	166		2	[0.333333, 0.666667]	(CA)0.333333(SI)0.666667
CA2SN_X	CrB (B33)	B33	oS8	Cmcm	63		3	[1.0, 1.0, 1.0]	(CA, MG)1(CA)1(SN)1
CA36SN23	Sn23Yb36		tP118	P4/mbm	127		2	[36.0, 23.0]	(CA)36(SN)23
CA31SN20	Pu31Rh20		tI204	I4/mcm	140		2	[31.0, 20.0]	(CA)31(SN)20
CA7SN6	Ca7Sn6		oP52	Pnma	62		2	[7.0, 6.0]	(CA)7(SN)6
CA3ZN	Re3B		oS16	Cmcm	63		2	[3.0, 1.0]	(CA)3(ZN)1
CAZN3	CaZn3		hP32	P6_3/mmc	194		2	[1.0, 3.0]	(CA)1(ZN)3
CU6CE	Copper(II) Azide [Cu (N3)2]		oP28	Pnma	62		2	[0.857, 0.143]	(CU)0.857(CE)0.143
CU5CE	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[0.833, 0.167]	(CU)0.833(CE)0.167
CU4CE	Unknown Structure		oP20				2	[0.8, 0.2]	(CU)0.8(CE)0.2
CU2CE	KHg2		oI12	Imma	74		2	[0.667, 0.333]	(CU, IN)0.667(CE, LA)0.333
CE5IN4	Unknown Structure						2	[5.0, 4.0]	(CE)5(IN)4

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
CE9IN11	Unknown Structure						2	[9.0, 11.0]	(CE)9(IN)11
CE3IN5	Pd5Pu3		oS32	Cmcm	63		2	[3.0, 5.0]	(CE)3(CE, IN)5
CEGD3	alpha-Sm (C19)	C19	hR3	R-3m	166		1	[1.0]	(CE, GD)1
CENI3	CeNi3		hP24	P6_3/mmc	194		2	[0.25, 0.75]	(CE)0.25(NI)0.75
CENI2	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[0.333, 0.667]	(CE, NI)0.333(CE, NI)0.667
CEZN2	KHg2		oI12	Imma	74		2	[0.333, 0.667]	(CE)0.333(MG, ZN)0.667
CEZN3	CeZn3		oS16	Cmcm	63		2	[0.25, 0.75]	(CE)0.25(ZN)0.75
CEZN5	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[0.167, 0.833]	(CE)0.167(MG, ZN)0.833
CEZN11	BaCd11		tI48	I4_1/amd	141		2	[0.083, 0.917]	(CE)0.083(MG, ZN)0.917
CU9GD2	Unknown Structure		t**				2	[9.0, 2.0]	(CU)9(GD)2
CU7GD2	Unknown Structure						2	[7.0, 2.0]	(CU)7(GD)2
CUH_B3	Zincblende (ZnS, B3)	B3	cF8	F-43m	216		2	[1.0, 1.0]	(CU)1(H)1
CUH_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186		2	[1.0, 1.0]	(CU)1(H)1
CU9IN4_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215		3	[0.654, 0.115, 0.231]	(CU)0.654(CU, IN)0.115(IN)0.231
CU7IN3	Cu7In3		aP40	P-1	2		2	[0.7, 0.3]	(CU, MG)0.7(IN)0.3
CU2IN_LT	Unknown Structure						2	[0.64, 0.36]	(CU)0.64(IN)0.36
CU11IN9	AlCu(r)		mS20	C2/m	12		2	[0.55, 0.45]	(CU)0.55(IN)0.45
CU37LA3	NaZn13 (D23)	D23	cF112	Fm-3c	226		2	[37.0, 3.0]	(CU)37(LA)3

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
CU6LA_L	Cu6La		mP28	P2_1/c	14		2	[6.0, 1.0]	(CU)6(LA)1
CU4LA	Cu4La		tI90	I-4m2	119		2	[4.0, 1.0]	(CU)4(LA)1
CU2LA	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[2.0, 1.0]	(CU)2(LA)1
CUMG2	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[1.0, 2.0]	(AG, CU, IN, NI)1(IN, MG)2
CU4ND	Unknown Structure		o**				2	[0.8, 0.2]	(CU)0.8(ND)0.2
CU7ND2	Unknown Structure						2	[0.77777778, 0.22222222]	(CU)0.777778(ND)0.222222
CUND_H	Unknown Structure						2	[0.5, 0.5]	(CU)0.5(ND)0.5
CU6PR	Cu6La		mP28	P2_1/c	14		2	[0.857, 0.143]	(CU)0.857(PR)0.143
CU5PR	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[0.833, 0.167]	(CU)0.833(PR)0.167
CU4PR	Unknown Structure		o**				2	[0.8, 0.2]	(CU)0.8(PR)0.2
CU2PR	KHg2		oI12	Imma	74		2	[0.667, 0.333]	(CU)0.667(PR)0.333
CU4SC	Unknown Structure		t**				2	[4.0, 1.0]	(CU)4(SC)1
CUSC	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(CU)1(SC)1
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cI76	I-43d	220		2	[15.0, 4.0]	(CU, MG)15(AL, SI)4
CU56SI11_GAMMA	Mg3Ru2		cP20	P4_132	213		2	[56.0, 11.0]	(CU, MG)56(SI)11
CUSI_ETA	Cu3Si-h2		hR*	P-31m	162		2	[0.76, 0.24]	(CU)0.76(SI)0.24
CU33SI7_DELTA	Unknown Structure						2	[0.825, 0.175]	(CU)0.825(SI)0.175
CU3SN_H_GAMMA	BiF3 (D03)	D03	cF16	Fm-3m	225		1	[1.0]	(CU, SN)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
CU10SN3	Cu10Sn3		hP26	P6_3	173		1	[1.0]	(CU, SN)1
CU3SN_L	Cu3Sn		oS80	Cmcm	63		2	[3.0, 1.0]	(CU, SN)3(CU, SN)1
CU41SN11	Cu41Sn11		cF416	F-43m	216		2	[41.0, 11.0]	(CU, SN)41(CU, SN)11
CU6SN5	Cu6Sn5		mS44	C2/c	15		3	[1.0, 1.0, 1.0]	(CU)1(CU, SN)1(SN)1
CUSR	BaCu		hP8	P6_3/mmc	194		2	[0.5, 0.5]	(CU)0.5(SR)0.5
CUTH2	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[0.333, 0.667]	(CU)0.333(TH)0.667
CU2TH	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[0.667, 0.333]	(CU)0.667(TH)0.333
CU6TH	CeCu6		oP28	Pnma	62		2	[0.857, 0.143]	(CU)0.857(TH)0.143
CU51TH14	Ag51Gd14		hP68	P6/m	175		2	[0.7826, 0.2174]	(CU)0.7826(TH)0.2174
CU7Y1	Cu7Tb		hP8	P6/mmm	191		2	[1.0, 5.0]	(CU2, Y)1(CU)5
CU4Y	Cu5Y1.25		mP16	P2_1/m	11		2	[4.0, 1.0]	(CU)4(Y)1
CU7Y2	Ag51Gd14		hP68	P6/m	175		2	[7.0, 2.0]	(CU)7(Y)2
CU2Y_H	Unknown Structure		hP*				2	[2.0, 1.0]	(CU)2(Y)1
EPSILON	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		1	[1.0]	(CU, MN, ZN)1
CUZN_GAMMA	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		4	[2.0, 2.0, 3.0, 6.0]	(CU, ZN)2(CU, ZN)2(CU)3(MG, ZN)6
CU51ZR14	Ag51Gd14		hP68	P6/m	175		2	[0.7846, 0.2154]	(CU)0.7846(ZR)0.2154
CU8ZR3	Cu8Hf3		oP44	Pnma	62		2	[0.7273, 0.2727]	(CU)0.7273(ZR)0.2727
MNI3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[1.0, 3.0]	(FE, MN, NI)1(FE, MN, NI)3

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
FE17ND5	Fe17Nd5		hP264	P6_3/mcm	193		2	[1.0, 0.2941]	(FE)1(ND)0.2941
FE2SC_C14	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		2	[0.67, 0.33]	(FE)0.67(SC)0.33
FE2SC_C36	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_3/mmc	194		2	[0.67, 0.33]	(FE)0.67(SC)0.33
FE2SC_C15	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[0.64, 0.36]	(FE)0.64(SC)0.36
FE6SC29	Unknown Structure						2	[0.17, 0.83]	(FE)0.17(SC)0.83
FE3SN2	Fe3Sn2		hR10	R-3m	166		2	[3.0, 2.0]	(FE)3(SN)2
FESN	CoSn (B35)	B35	hP6	P6/mmm	191		2	[1.0, 1.0]	(FE)1(SN)1
FE5TH	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[0.83, 0.17]	(FE)0.83(TH)0.17
FE7TH2_L	Ce2Ni7		hP36	P6_3/mmc	194		2	[0.78, 0.22]	(FE)0.78(TH)0.22
FE7TH2_H	Th2Zn17		hR19	R-3m	166		2	[0.78, 0.22]	(FE)0.78(TH)0.22
FE17Y2	Fe17Lu2		hP80	P6_3/mmc	194		2	[1.0, 0.1176]	(FE)1(Y)0.1176
FE23Y6	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		2	[1.0, 0.2609]	(FE)1(Y)0.2609
GAMMA_FEZN	gamma-brass (Fe3Zn10, D81)	D81	cI52	Im-3m	229		4	[0.154, 0.154, 0.231, 0.461]	(FE, ZN)0.154(FE, ZN)0.154(FE, ZN)0.231 (ZN)0.461
GAMMA1_FEZN	Fe11Zn40		cF408	F-43m	216		3	[0.137, 0.118, 0.745]	(FE)0.137(FE, ZN)0.118(ZN)0.745
DELTA_FEZN	FeZn10		hP632	P6_3/mmc	194		4	[0.058, 0.18, 0.525, 0.237]	(FE)0.058(FE, ZN)0.18(ZN)0.525 (ZN)0.237
ZETA_FEZN	CoZn13		mS28	C2/m	12		3	[0.072, 0.856, 0.072]	(FE, VA)0.072(ZN)0.856(VA, ZN)0.072

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FEZR3	Re3B		oS16	Cmcm	63		2	[1.0, 3.0]	(FE, ZR)1(FE, ZR)3
ORTHO_GA	alpha-Ga (A11)	A11	oS8	Cmce	64		1	[1.0]	(GA)1
MG5GA2	Ga2Mg5 (D8g)	D8g	oI28	Ibam	72		2	[0.7143, 0.2857]	(MG)0.7143(GA, IN)0.2857
MG2GA1	Li2Sb		hP18	P-62c	190		2	[0.6667, 0.3333]	(MG)0.6667(GA)0.3333
MG1GA1	MgGa		tI32	I4_1/a	88		2	[0.5, 0.5]	(MG)0.5(GA)0.5
MGGA2	MgGa2		oP24	Pbam	55		2	[0.3333, 0.6667]	(MG)0.3333(GA)0.6667
MG2GA5	Ga5Mg2		tI28	I4/mmm	139		2	[0.2857, 0.7143]	(MG)0.2857(GA)0.7143
GD5IN3	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[5.0, 3.0]	(GD)5(IN)3
GD1IN1	Unknown Structure						2	[1.1, 1.0]	(GD)1.1(IN)1
GD3IN5	Pd5Pu3		oS32	Cmcm	63		2	[3.0, 5.0]	(GD)3(IN)5
GDIN3	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[1.0, 3.0]	(GD)1(IN)3
GDMG5	Unknown Structure						2	[1.0, 5.0]	(AG, CA, CE, GD, LA, ND, SM, SR, Y)1 (MG, ZN)5
MG7RE	Unknown Structure						2	[7.0, 1.0]	(MG)7(GD, ND, Y, ZN)1
GDND	alpha-Sm (C19)	C19	hR3	R-3m	166		2	[0.5, 0.5]	(GD, ND)0.5(GD, ND)0.5
GD3NI2	Unknown Structure						2	[3.0, 2.0]	(GD)3(NI)2
GD2NI7	Co7Gd2		hR18	R-3m	166		2	[2.0, 7.0]	(GD)2(NI)7
GDNI4	Unknown Structure						2	[1.0, 4.0]	(GD)1(NI)4
GD5SI4	Gd5Si4		oP36	Pnma	62		2	[0.5556, 0.4444]	(GD)0.5556(SI)0.4444

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GD3SI5	Unknown Structure						2	[0.375, 0.625]	(GD)0.375(SI)0.625
GDSI2	alpha-ThSi2 (Cc)	Cc	tI12	I4_1/amd	141		2	[0.3333, 0.6667]	(GD)0.3333(SI)0.6667
GDZN2	KHg2		oI12	Imma	74		2	[0.333, 0.667]	(GD, SM)0.333(ZN)0.667
GDZN12	Mn12Th (D2b)	D2b	tI26	I4/mmm	139		2	[0.077, 0.923]	(GD)0.077(ZN)0.923
K17IN41	K17In41		cF464	Fd-3m	227		2	[0.69, 0.31]	(IN)0.69(K)0.31
K39IN80	K39In80		hP238	P-3m1	164		2	[0.635, 0.365]	(IN)0.635(K)0.365
B2REIN	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(LA, ND, Y)1(IN, ND)1
IN5RE3	Pd5Pu3		oS32	Cmcm	63		2	[0.625, 0.375]	(IN)0.625(LA, ND, PR, TH, Y)0.375
IN3LA2	Unknown Structure						2	[0.57, 0.43]	(IN)0.57(LA)0.43
LIIN	NaTl (B32)	B32	cF16	Fd-3m	227		2	[1.0, 1.0]	(IN, LI)1(IN, LI)1
LI5IN4	Li5Ga4		hP9	P-3m1	164		2	[5.0, 4.0]	(LI)5(IN)4
LI3IN2	Li3Al2		hr5	R-3m	166		2	[3.0, 2.0]	(LI)3(IN)2
LI2IN	Li2Ga		oS12	Cmcm	63		2	[2.0, 1.0]	(LI)2(IN)1
LI13IN3	Li13In3		cF128	Fd-3m	227		2	[13.0, 3.0]	(LI)13(IN)3
LI3IN1	Unknown Structure						2	[3.0, 1.0]	(LI)3(IN)1
LI7IN	Unknown Structure						2	[7.0, 1.0]	(LI)7(IN)1
TETRA_A6	In (A6)	A6	tI2	I4/mmm	139		1	[1.0]	(IN, MG, SN, ZN)1
MG2IN	Mg2In		hP9	P-62m	189		2	[2.0, 1.0]	(MG)2(IN)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
MG3IN	Mg3In		hr16	R-3m	166		2	[3.0, 1.0]	(IN, MG, SN)3(IN, MG, SR)1
MN3IN	Unknown Structure						2	[3.0, 1.0]	(MN)3(IN)1
NI13IN9	Ga9Ni13		mS44	C2/m	12		3	[1.0, 1.0, 1.0]	(NI, VA)1(NI)1(IN)1
B2NIIN	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(NI, VA)1(IN)1
NIIN	CoSn (B35)	B35	hP6	P6/mmm	191		2	[1.0, 1.0]	(NI)1(IN)1
NI2IN3	Al3Ni2 (D513)	D513	hP5	P-3m1	164		2	[2.0, 3.0]	(NI)2(IN)3
NI3IN7	Ir3Ge7 (D8f)	D8f	cI40	Im-3m	229		2	[3.0, 7.0]	(NI)3(IN)7
NA6IN11	Na15In27.4		oS344	Cmcm	63		2	[0.3526, 0.6474]	(NA)0.3526(IN)0.6474
NA7IN12	In12Na7		tP228	P4_2/nmc	137		2	[0.3731, 0.6269]	(NA)0.3731(IN)0.6269
NAIN	NaTl (B32)	B32	cF16	Fd-3m	227		2	[1.0, 1.0]	(NA)1(IN)1
NA2IN	Na2Tl		oS48	C222_1	20		2	[2.0, 1.0]	(NA)2(IN)1
SCIN2	Li2Ga		oS12	Cmcm	63		2	[1.0, 2.0]	(SC)1(IN)2
B2_SCIN	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.1, 0.9]	(SC)1.1(IN)0.9
PR3IN4	Unknown Structure						2	[3.0, 4.0]	(PR)3(IN)4
PR6IN5	Unknown Structure						2	[6.0, 5.0]	(PR)6(IN)5
INSN_AF	Simple Hexagonal Lattice (Af)	Af	hP1	P6/mmm	191		1	[1.0]	(IN, SN)1
TET_ALPHA1_A6	In (A6)	A6	tI2	I4/mmm	139		1	[1.0]	(IN, SN)1
IN5SR2	Unknown Structure						2	[0.7143, 0.2857]	(IN)0.7143(SR)0.2857

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
IN2SR	CaIn2		hP6	P6_3/mmc	194		2	[0.6667, 0.3333]	(IN)0.6667(SR)0.3333
IN3SR2	Unknown Structure						2	[0.6, 0.4]	(IN)0.6(SR)0.4
IN1SR1	SrIn		oF64	Fdd2	43		2	[0.5, 0.5]	(IN)0.5(SR)0.5
IN3SR5	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140		2	[0.375, 0.625]	(IN)0.375(SR)0.625
INSR3	Unknown Structure						2	[0.25, 0.75]	(IN)0.25(SR)0.75
THIN	ThIn		oP24	Pbcm	57		2	[1.0, 1.0]	(TH)1(IN)1
TH2IN	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[2.0, 1.0]	(TH)2(IN)1
ZRIN2	Ga2Hf		tI24	I4_1/amd	141		2	[1.0, 2.0]	(ZR)1(IN)2
ZR1IN1	Unknown Structure						2	[1.0, 1.0]	(ZR)1(IN)1
RE3IN	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[3.0, 1.0]	(LA, ND, PR, ZR)3(IN)1
MGH2_C4	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136		2	[1.0, 2.0]	(MG)1(H)2
NDH_GAMMA	Unknown Structure						2	[1.0, 2.0]	(ND)1(H, VA)2
LANI5	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		3	[0.16667, 0.33333, 0.5]	(LA, NI)0.16667(LA, NI)0.33333(NI)0.5
LA2NI7_H	Co7Gd2		hR18	R-3m	166		2	[2.0, 7.0]	(LA)2(NI)7
LA7NI16	La7Ni16		tI46	I-42m	121		2	[0.3043, 0.6957]	(LA)0.3043(NI)0.6957
LA2NI3	La2Ni3		oS20	Cmce	64		2	[0.4, 0.6]	(LA)0.4(NI)0.6
LASI2_A1	GdSi1.4		oI12	Imma	74		2	[0.36, 0.64]	(LA)0.36(SI)0.64
LA5SN3_L	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[0.625, 0.375]	(LA)0.625(SN)0.375

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
LA5SN4	Sm5Ge4		oP36	Pnma	62		2	[0.555, 0.445]	(LA)0.555(SN)0.445
LA11SN10	Unknown Structure						2	[0.524, 0.476]	(LA)0.524(SN)0.476
LA2SN3	Nd2Sn3		aP20	P-1	2		2	[0.4, 0.6]	(LA)0.4(SN)0.6
LA3SN5	Pd5Pu3		oS32	Cmcm	63		2	[0.375, 0.625]	(LA, SR)0.375(SN)0.625
LAY	alpha-Sm (C19)	C19	hR3	R-3m	166		2	[1.0, 1.0]	(LA, Y)1(Y)1
LAZN4	LaZn4		oS20	Cmcm	63		2	[1.0, 4.0]	(LA, SR)1(SN, ZN)4
LI22SI5	Li21Si5		cF416	F-43m	216		2	[22.0, 5.0]	(LI)22(SI)5
LI13SI4	Li13Si4		oP34	Pbam	55		2	[13.0, 4.0]	(LI)13(SI)4
LI7SI3	(Li7Si3)		hP60	P3_221	154		2	[7.0, 3.0]	(LI)7(SI)3
LI12SI7	Li12Si7		oP152	Pnma	62		2	[12.0, 7.0]	(LI)12(SI)7
LI13SN5	Li13Sn5		hP18	P-3m1	164		2	[13.0, 5.0]	(LI)13(SN)5
LI22SN5	Li17Si4		cF420	F-43m	216		2	[22.0, 5.0]	(LI)22(SN)5
LI2SN5	Hg5Mn2		tP14	P4/mbm	127		2	[2.0, 5.0]	(LI)2(SN)5
LI5SN2	Mo2B5 (D8i)	D8i	hR7	R-3m	166		2	[5.0, 2.0]	(LI)5(SN)2
LI7SN3	Li7Sn3		mP20	P2_1/m	11		2	[7.0, 3.0]	(LI)7(SN)3
LI8SN3	Unknown Structure						2	[8.0, 3.0]	(LI)8(SN)3
LISN	LiSn		mP6	P2/m	10		2	[1.0, 1.0]	(LI)1(LI, SN)1
LI7SN2	Ge2Li7		oS36	Cmmm	65		2	[7.0, 2.0]	(LI, SN)7(SN)2

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
LI2ZN3_L	Li(Li0.91Zn0.09)2Zn4		hR7	R-3m	166		2	[2.0, 3.0]	(LI)2(LI, ZN)3
LI2ZN3_H	Li5Ga4		hP9	P-3m1	164		2	[2.0, 3.0]	(LI, ZN)2(LI, ZN)3
LI2ZN5_L	Unknown Structure						2	[2.0, 5.0]	(LI, ZN)2(ZN)5
LI2ZN5_H	Unknown Structure						2	[2.0, 5.0]	(LI, ZN)2(ZN)5
LIZN4_L	Unknown Structure						2	[1.0, 4.0]	(LI, ZN)1(LI, ZN)4
LIZN4_H	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194		2	[0.2, 0.8]	(LI, ZN)0.2(LI, ZN)0.8
LIZN2	Unknown Structure						2	[1.0, 2.0]	(LI)1(ZN)2
BCC_B32	NaTl (B32)	B32	cF16	Fd-3m	227		2	[1.0, 1.0]	(LI, ZN)1(LI, ZN)1
MG2NI1	Unknown Structure						3	[2.0, 1.0, 1.0]	(MG)2(CU, NI, ZN)1(H, VA)1
MG5PR	Unknown Structure						2	[5.0, 1.0]	(MG)5(PR, Y)1
MG3SB2_LT	La2O3 (D52)	D52	hP5	P-3m1	164		2	[0.6, 0.4]	(MG)0.6(SB)0.4
MG3SB2_HT	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	206		2	[0.601, 0.399]	(MG)0.601(SB)0.399
MG38SR9	Mg38Sr9		hP94	P6_3/mmc	194		2	[38.0, 9.0]	(AL, MG)38(CE, ND, SR)9
MG24R5	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[24.0, 4.0, 1.0]	(MG)24(CA, CE, DY, ER, GD, HO, LA, MG, ND, PR, Y)4(DY, ER, HO, Y)1
MG2ZN3	Mg4Zn7		mS110	C2/m	12		2	[2.0, 3.0]	(MG)2(AL, CU, ZN)3
MGZN	Zr21Re25		hR92	R-3c	167		2	[12.0, 13.0]	(MG)12(AL, CU, ZN)13
MG51ZN20	Mg51Zn20		oI158	Immm	71		2	[51.0, 20.0]	(MG)51(MN, ZN)20
MG2ZN11	Mg2Zn11 (D8c)	D8c	cP39	Pm-3	200		2	[2.0, 11.0]	(MG)2(AL, CU, SI, ZN)11

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
L10_TETRA	CuAu (L10)	L10	tP2	P4/mmm	123		2	[0.5, 0.5]	(IN, MG, MN, NI, SC)0.5(IN, MG, MN, NI)0.5
MNNI2	Unknown Structure						2	[1.0, 2.0]	(MN, NI)1(NI)2
MN11SI19	Mn11Si19		tP120	P-4n2	118		2	[11.0, 19.0]	(MN)11(SI)19
MN3SI	BiF3 (D03)	D03	cF16	Fm-3m	225		2	[3.0, 1.0]	(MN)3(SI)1
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166		2	[17.0, 3.0]	(MN)17(SI)3
MN9SI2	Mn9Si2		oI186	Immm	71		2	[33.0, 7.0]	(MN)33(SI)7
MN23SC6	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		2	[23.0, 6.0]	(MN)23(SC)6
MNSC4	Unknown Structure						2	[0.2, 0.8]	(MN)0.2(SC)0.8
MN19SN6	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[0.76, 0.24]	(MN)0.76(SN)0.24
MNSN2	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[0.333, 0.667]	(MN)0.333(SN)0.667
MN23Y6	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		2	[23.0, 6.0]	(MG, MN)23(Y)6
MNZN9_LT	Unkown Structure		hP*	P6_3/mmc	194		4	[58.0, 180.0, 525.0, 237.0]	(MN)58(MG, MN, ZN)180(ZN)525 (ZN)237
MNZN9_HT	Unknown Structure		hP*				2	[9.0, 1.0]	(MN, ZN)9(MN, ZN)1
ZETA_MNZN	CoZn13		mS28	P2/m	10		3	[9.0, 107.0, 9.0]	(MN, VA)9(ZN)107(MN)9
GAMMA_MNZN	Unknown Structure		cI52				4	[154.0, 154.0, 231.0, 461.0]	(MN, ZN)154(MN, ZN)154(MN, ZN)231 (ZN)461
ALPHA_MNZN	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[3.0, 1.0]	(MN, ZN)3(MN, ZN)1
BETA_MNZN	CsCl (B2)	B2	cP2	Pm-3m	221		2	[1.0, 1.0]	(MN)1(ZN)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
ND2Y	alpha-Sm (C19)	C19	hR3	R-3m	166		2	[2.0, 1.0]	(ND, Y)2(ND, Y)1
NDZN2	KHg2		oI12	Imma	74		2	[0.333, 0.667]	(ND)0.333(ZN)0.667
ND3ZN11	Al11La3		oI28	Immm	71		2	[0.214, 0.786]	(ND)0.214(MG, ZN)0.786
ND2ZN17	Ni17Th2		hP38	P6_3/mmc	194		2	[0.105, 0.895]	(ND)0.105(ZN)0.895
NDZN11_H	Unknown Structure						2	[0.0833, 0.9167]	(ND)0.0833(ZN)0.9167
NI5PR	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		2	[0.8333, 0.1667]	(NI)0.8333(PR)0.1667
NI2PR	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[0.6667, 0.3333]	(NI)0.6667(PR)0.3333
NI3SI_M	Ge9Pd25		hP34	P-3	147		2	[0.75, 0.25]	(NI)0.75(SI)0.25
NI3SI_L	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.76, 0.24]	(NI)0.76(SI)0.24
NI5SI2	Ni31S12		hP42	P321	150		2	[0.7143, 0.2857]	(NI)0.7143(SI)0.2857
THETA	K2UF6		hP9	P-62m	189		3	[1.0, 1.0, 1.0]	(NI)1(NI, VA)1(SI)1
NI3SI2	Ni3Si2		oP80	Cmc2_1	36		2	[0.6, 0.4]	(NI)0.6(SI)0.4
NISI	MnP (B31)	B31	oP8	Pnma	62		2	[0.5, 0.5]	(NI)0.5(SI)0.5
NI3SN_H	BiF3 (D03)	D03	cF16	Fm-3m	225		3	[0.25, 0.25, 0.5]	(NI, SN)0.25(NI, SN)0.25(NI)0.5
NI3SN_L	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[0.75, 0.25]	(NI)0.75(SN)0.25
NI3SN2_L	Ni3Sn2		oP20	Pnma	62		3	[0.2, 0.4, 0.4]	(SN)0.2(NI, SN)0.4(NI)0.4
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	C2/m	12		3	[0.25, 0.25, 0.5]	(NI)0.25(NI, SN)0.25(SN)0.5
NI17Y2	Fe17Lu2		hP80	P6_3/mmc	194		2	[17.0, 2.0]	(NI)17(Y)2

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
NI4Y	Unknown Structure		hR*				2	[4.0, 1.0]	(NI)4(Y)1
NI2Y1	Ni2Tm		cF192	F-43m	216		2	[2.0, 1.0]	(NI)2(MG, Y)1
NI2Y3	Ni2Y3		tP80	P4_12_12	92		2	[2.0, 3.0]	(NI)2(Y)3
BETA_NIZN	delta-CuTi (L2a)	L2a	tP2	P4/mmm	123		1	[1.0]	(NI, ZN)1
GAMMA_NIZN	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		1	[1.0]	(NI, ZN)1
DELTA_NIZN	Ni3Zn22		mS50	C2/m	12		2	[0.111, 0.889]	(NI)0.111(ZN)0.889
NI7ZR2	Ni7Zr2		mS36	C2/m	12		2	[7.0, 2.0]	(NI)7(ZR)2
NI21ZR8	Hf8Ni21		aP29	P-1	2		2	[21.0, 8.0]	(NI)21(ZR)8
NI11ZR9	Pt11Zr9		tI40	I4/m	87		2	[11.0, 9.0]	(NI)11(ZR)9
PR2Y	alpha-Sm (C19)	C19	hR3	R-3m	166		2	[2.0, 1.0]	(PR, Y)2(PR, Y)1
PR2ZN17_H	Ni17Th2		hP38	P6_3/mmc	194		2	[2.0, 17.0]	(PR)2(ZN)17
SC5SI3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193		2	[0.625, 0.375]	(SC)0.625(SI)0.375
SCSI	CrB (B33)	B33	oS8	Cmcm	63		2	[0.5, 0.5]	(SC)0.5(SI)0.5
SC3SI5_LT	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[0.375, 0.625]	(SC)0.375(SI)0.625
SC3SI5_HT	Unknown Structure		o**				2	[0.375, 0.625]	(SC)0.375(SI)0.625
SI2Y_H	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[2.0, 1.0]	(SI)2(Y)1
SI4Y5	Gd5Si4		oP36	Pnma	62		2	[4.0, 5.0]	(SI)4(Y)5
SI5Y3_H	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[5.0, 3.0]	(SI)5(Y)3

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SI5Y3_L	GdSi1.4		oI12	Imma	74		2	[5.0, 3.0]	(SI)5(Y)3
SI4ZR5_H	Unknown Structure						2	[4.0, 5.0]	(SI)4(ZR)5
SI2ZR	ZrSi2 (C49)	C49	oS12	Cmcm	63		2	[2.0, 1.0]	(SI)2(ZR)1
SIZR3	Ti3P		tP32	P4_2/n	86		2	[1.0, 3.0]	(SI)1(ZR)3
ZR3SN_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223		2	[3.0, 1.0]	(SN, ZR)3(SN, ZR)1
ZR5SN3	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193		3	[5.0, 3.0, 1.0]	(ZR)5(SN)3(SN, VA)1
ZRSN2	TiSi2 (C54)	C54	oF24	Fddd	70		2	[1.0, 2.0]	(ZR)1(SN)2
SRZN5_L	SrZn5		oP24	Pnma	62		2	[1.0, 5.0]	(SR)1(ZN)5
THZN2	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[1.0, 2.0]	(TH)1(ZN)2
H_RZN5	Unknown Structure						2	[1.0, 5.0]	(GD, Y)1(MG, ZN)5
YZN2_A	Unknown Structure						2	[1.0, 2.0]	(Y)1(ZN)2
YZN2_B	Unknown Structure						2	[1.0, 2.0]	(Y)1(ZN)2
ZN22ZR	Zn22Zr		cF184	Fd-3m	227		2	[0.9565, 0.0435]	(ZN)0.9565(ZR)0.0435
ZN39ZR5	Zn39Zr5		mS88	C2/m	12		2	[0.8864, 0.1136]	(ZN)0.8864(ZR)0.1136
ZN3ZR_L	Unknown Structure		tI64				2	[0.75, 0.25]	(ZN)0.75(ZR)0.25
ZN3ZR_H	Unknown Structure						2	[0.75, 0.25]	(ZN)0.75(ZR)0.25
T1_AGALSC	Heusler (L21)	L21	cF16	Fm-3m	225		3	[2.0, 1.0, 1.0]	(AG)2(AL)1(SC)1
T2_AGALSC	Unknown Structure						3	[0.28, 0.36, 0.36]	(AG)0.28(AL)0.36(SC)0.36

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
T3_AGALSC	Unknown Structure						3	[0.55, 0.27, 0.18]	(AG)0.55(AL)0.27(SC)0.18
AGGDMG_T	Unknown Structure						2	[0.15, 0.85]	(AG, GD)0.15(MG)0.85
AL9CA31ZN10	Unknown Structure						3	[1.0, 1.0, 1.0]	(AL)1(CA)1(ZN)1
AL2CAZN2	Al4Ba (D13)	D13	tI10	I4/mmm	139		3	[2.0, 1.0, 2.0]	(AL)2(CA)1(ZN)2
AL13CEMG6	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		3	[13.0, 1.0, 6.0]	(AL)13(CE)1(MG)6
AL8CEM4	Mn12Th (D2b)	D2b	tI26	I4/mmm	139		3	[0.6154, 0.0769, 0.3077]	(AL)0.6154(CE, GD, LA, Y)0.0769(AL, MN)0.3077
AL10CE2MN7	Zn17Th2		hR57	R-3m	166		2	[0.8947, 0.1053]	(AL, MN)0.8947(CE, GD, LA, Y)0.1053
ALCUMG_Q	Chalcopyrite (CuFeS2, E11)	E11	tI16	I-42d	122		3	[7.0, 3.0, 6.0]	(AL)7(CU)3(MG)6
ALCUMG_S	MgCuAl2 (E1a)		oS16	Cmcm	63		3	[2.0, 1.0, 1.0]	(AL, SI)2(CU)1(MG)1
ALCUMG_T	Bergman [Mg32 (Al,Zn)49, D8e]	D8e	cI162	Im-3	204		4	[26.0, 6.0, 48.0, 1.0]	(MG)26(AL, MG)6(AL, CU, MG, ZN)48 (AL)1
ALCUMG_V	Mg2Zn11 (D8c)	D8c	cP39	Pm-3	200		3	[5.0, 6.0, 2.0]	(AL)5(CU)6(MG)2
HTAL8MN5	Unknown Structure						2	[8.0, 5.0]	(AL, FE, MN)8(AL, FE, MN)5
LTAL8MN5	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		3	[12.0, 5.0, 9.0]	(AL)12(FE, MN)5(AL, FE, MN)9
HTAL11MN4	Mn6(Mn0.5Al0.5)8Al25		oP156	Pnma	62		2	[29.0, 10.0]	(AL, MN)29(FE, MN)10
D3_ALFE	Unknown Structure						3	[0.7, 0.08, 0.22]	(AL)0.7(AL, FE)0.08(FE, MN)0.22
Z_ALFEMN	Al14.4Cr3.4Ni1.1		hP227	P6_3/m	176		2	[4.0, 1.0]	(AL)4(FE, MN)1
PHI	Unknown Structure						3	[0.7, 0.15, 0.15]	(AL)0.7(AL, MN)0.15(FE, MN)0.15

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
ALLAMG_T1	Unknown Structure						3	[2.0, 0.15, 0.85]	(AL)2(LA)0.15(MG)0.85
AL8LAMN	Unknown Structure						3	[8.0, 1.0, 1.0]	(AL)8(LA)1(MN)1
ALLIMG_T	Unknown Structure						3	[0.53, 0.33, 0.14]	(AL)0.53(LI)0.33(MG)0.14
ALMGMN_T	Mg3Cr2Al18		cF184	Fd-3m	227		3	[18.0, 3.0, 2.0]	(AL)18(MG)3(MN)2
ALMGND_T	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		3	[2.0, 0.88, 0.12]	(AL)2(MG)0.88(ND)0.12
ALMG3NI2	Mn3Ni2Si		cF96	Fd-3m	227		3	[1.0, 2.0, 3.0]	(AL)1(NI)2(MG)3
AL38MG58SR4	Unknown Structure						3	[38.0, 58.0, 4.0]	(AL)38(MG)58(SR)4
AL4MGY	Unknown Structure						3	[0.6667, 0.1667, 0.1666]	(AL, MG, Y)0.6667(AL, MG, Y)0.1667 (MG, Y)0.1666
ALMGZN_PHI	Mg21(Al,Zn)17		oP152	Pbcm	57		2	[21.0, 17.0]	(MG)21(AL, ZN)17
ALMGZN_T1	Bergman [Mg32 (Al,Zn)49, D8e]	D8e	cI162	Im-3	204		4	[26.0, 6.0, 48.0, 1.0]	(MG)26(AL, MG)6(AL, MG, ZN)48(AL)1
ALMGZN_Q	Quasicrystal						3	[0.15, 0.44, 0.41]	(AL)0.15(MG)0.44(ZN)0.41
ALMGZN_T2	Mg46Zn37Al17		cP640	Pa-3	205		3	[0.15, 0.43, 0.42]	(AL)0.15(MG)0.43(ZN)0.42
BI2CAMG2	La2O3 (D52)	D52	hP5	P-3m1	164		3	[2.0, 1.0, 2.0]	(BI)2(CA)1(MG)2
CA7MG6SI14	Ca7Mg7.5Si14		hP42	P6/mmm	191		3	[0.2592593, 0.2222222, 0.5185185]	(CA)0.259259(MG)0.222222 (SI)0.518518
CAMGSN_T1	Co2Si (C37)	C37	oP12	Pnma	62		3	[156.0, 94.0, 175.0]	(CA)156(MG)94(SN)175
CA2MG6ZN3	Unknown Structure		h**				3	[2.0, 6.0, 3.0]	(CA)2(MG)6(ZN)3
REH_EPS	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		3	[1.0, 2.0, 1.0]	(CE, LA, ND)1(H, VA)2(H, VA)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
CEH2_35	Unknown Structure						2	[1.0, 2.35]	(CE)1(H)2.35
CEH2_9	CeH3		cF44	Fm-3m	225		2	[1.0, 2.9]	(CE)1(H)2.9
REMG2H7	Mg2LaH7		tP40	P4_12_12	92		3	[1.0, 2.0, 7.0]	(CE, LA)1(MG)2(H)7
MG5CEY	Sm11Cd45		cF448	F-43m	216		2	[5.0, 1.0]	(MG)5(CE, Y)1
T2_CEMGZN	Unknown Structure						3	[0.018182, 0.527273, 0.454545]	(CE)0.018182(MG)0.527273 (ZN)0.454545
T4_CEMGZN	Cu7Tb		hP8	P6/mmm	191		3	[1.0, 2.5, 4.5]	(CE, PR)1(MG)2.5(ZN)4.5
T5_CEMGZN	Mg13Zn30Sm3		hP92	P6_3/mmc	194		3	[0.065217, 0.282609, 0.652174]	(CE, PR)0.065217(MG)0.282609 (ZN)0.652174
T6_CEMGZN	Unknown Structure						3	[0.0625, 0.125, 0.8125]	(CE)0.0625(MG)0.125(ZN)0.8125
T7_CEMGZN	Mg19Zn81Ce20		cF480	F-43m	216		3	[0.166667, 0.158333, 0.675]	(CE)0.166667(MG)0.158333(ZN)0.675
MGCU4IN	MgCu4Sn		cF24	F-43m	216		3	[1.0, 4.0, 1.0]	(IN, MG)1(CU, IN, MG)4(IN, MG)1
CULIMG_T	Mg2Ni (Ca)	Ca	hP18	P6_222	180		3	[1.0, 0.08, 1.92]	(CU)1(LI)0.08(MG)1.92
CU16MG6SI7	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		3	[16.0, 6.0, 7.0]	(CU)16(MG)6(SI)7
CU3MG2SI_C1	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_3/mmc	194		3	[2.74, 2.0, 1.26]	(CU)2.74(MG)2(SI)1.26
CU9MG2Y	Cu9Mg2Tb		hP24	P6_3/mmc	194		3	[0.75, 0.166667, 0.083333]	(CU)0.75(MG)0.166667(Y)0.083333
CUMGY_T2	MgCu4Sn		cF24	F-43m	216		3	[4.0, 1.0, 1.0]	(CU, NI)4(MG)1(Y)1

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
CUMGY_T3	Mo2FeB2		tP10	P4/mbm	127		3	[2.0, 1.0, 2.0]	(CU, NI)2(MG)1(Y)2
CUMGY_T4	ZrNiAl		hP9	P-62m	189		3	[1.0, 1.0, 1.0]	(CU)1(MG)1(Y)1
CUMGY_T5	Cu5Mg8Y5		oP36	Pmma	51		3	[0.277778, 0.444444, 0.277778]	(CU)0.277778(MG)0.444444(Y)0.277778
CUMGY_T6	Cu5Mg13Y5		oS92	Cmcm	63		3	[0.2173913, 0.5652174, 0.2173913]	(CU)0.217391(MG)0.565217(Y)0.217391
CUMGY_T7	Unknown Structure						3	[0.18, 0.57, 0.25]	(CU)0.18(MG)0.57(Y)0.25
CUMGY_T8	Cu5Mg16Y5		oS104	Cmcm	63		3	[0.1923077, 0.6153846, 0.1923077]	(CU)0.192308(MG)0.615385(Y)0.192308
CUMGY_T9	CuMg4Tb		oS48	Cmcm	63		3	[1.0, 4.0, 1.0]	(CU)1(MG)4(Y)1
CUMGY_T10	Unknown Structure						3	[0.09, 0.78, 0.13]	(CU)0.09(MG)0.78(Y)0.13
F_MGGDZN	Mg19Zn81Ce20		cF480	F-43m	216		3	[0.166667, 0.158333, 0.675]	(GD)0.166667(MG)0.158333(ZN)0.675
Z_MGRZN	Unknown Structure						3	[0.07, 0.28, 0.65]	(GD, Y)0.07(MG)0.28(ZN)0.65
M_MGRZN	Unknown Structure						3	[0.08, 0.28, 0.64]	(GD)0.08(MG)0.28(ZN)0.64
L_MGRZN	Unknown Structure						3	[0.14, 0.22, 0.64]	(GD)0.14(MG)0.22(ZN)0.64
LAMGNI_T1	MgCuAl2 (E1a)		oS16	Cmcm	63		3	[0.25, 0.25, 0.5]	(LA)0.25(NI)0.25(MG)0.5
LAMGNI_T2	Mo2FeB2		tP10	P4/mbm	127		3	[0.4, 0.4, 0.2]	(LA)0.4(NI)0.4(MG)0.2
LAMGNI_T3	Unknown Structure						2	[0.333333, 0.666667]	(LA, MG)0.333333(NI)0.666667
LAMGNI_T4	Unknown Structure						3	[0.666666,	(LA)0.666666(NI)0.166667

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Info	Sublattices	Sites	Formula Unit
								0.166667, 0.166667]	(MG)0.166667
LAMGNI_T5	Unknown Structure						3	[0.666666, 0.22, 0.113334]	(LA)0.666666(NI)0.22(MG)0.113334
LAMGNI_T6	Unknown Structure						2	[0.675, 0.325]	(LA)0.675(MG, NI)0.325
LAMGSI_T1	Unknown Structure						2	[0.6, 0.4]	(LA, MG)0.6(SI)0.4
LAMGSI_T2	Unknown Structure						3	[0.2, 0.4, 0.4]	(LA)0.2(SI)0.4(MG)0.4
LAMGSI_T3	Unknown Structure						3	[0.25, 0.5, 0.25]	(LA)0.25(SI)0.5(MG)0.25
LAMGSI_T4	Unknown Structure						3	[0.2, 0.03333, 0.76667]	(LA)0.2(SI)0.03333(MG)0.76667
LAMGSI_T5	Unknown Structure						3	[0.3293, 0.004, 0.6667]	(LA)0.3293(SI)0.004(MG)0.6667
MG2NIH4	Mg2NiH4		mS56	C2/c	15		3	[2.0, 1.0, 4.0]	(MG)2(NI)1(H)4
MGSNSR_T1	Unknown Structure						3	[25.0, 24.0, 14.0]	(MG)25(SN)24(SR)14
MGSNSR_T2	Unknown Structure						3	[5.0, 3.0, 1.0]	(MG)5(SN)3(SR)1
MGSNSR_C37	Co2Si (C37)	C37	oP12	Pnma	62		3	[1.0, 1.0, 1.0]	(MG)1(SN)1(SR)1
MG6MN3NI	Unknown Structure						3	[3.0, 1.0, 2.0]	(MG)3(MN)1(NI)2
MGNDZN_T1	Unknown Structure						3	[0.35, 0.05, 0.6]	(MG)0.35(ND)0.05(ZN)0.6
MGNDZN_T2	Unknown Structure						3	[0.35, 0.1, 0.55]	(MG)0.35(ND)0.1(ZN)0.55
MG6REZN3	Unknown Structure						3	[0.6, 0.1, 0.3]	(MG)0.6(CE, LA, ND, PR)0.1(ZN)0.3
MGNDZN_T4	Unknown Structure						3	[0.3, 0.15, 0.55]	(MG)0.3(ND)0.15(ZN)0.55

Phase	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula Unit*
AL3CU2MG9SI7	Q-(Al,Cu,Mg,Si)		hP21	P-6	174		4	[3.0, 2.0, 9.0, 7.0]	(AL)3(CU)2(MG)9(SI)7

TCMG7 Properties Data

Model Descriptions

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

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

Examples

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

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:	**7.0**
First release	**TCMG1 was released in 2012**

Changes in the Most Recent Database Release

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.

Previous Releases

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 CuMg2 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 Mg12Ce, Mg41Sm5, Mg5Gd, Mg41Nd5, Al12Mg17, 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.