TCS Mg-based Alloys Database (TCMG6)

Technical Information

Available Starting with Thermo-Calc Version 2021a

Document created 6/3/2022

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 TCMG6. 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.

TCMG6 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:

- 208 assessed binary systems
- 102 assessed ternary systems
- 5 assessed quaternary systems
- 540 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 resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Electrical conductivity		ELCD for a system `ELCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI*	`SURF(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)`**
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)`**
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

* XI is not used in the TCS Metal Oxide Solutions Database (TCOX)
** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCMG6 Systems

In this section:

TCMG6 Assessed Binary Systems

These are the 208 assessed binary systems in the full range of composition and temperature.

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

TCMG6 Assessed Ternary Systems

These are the 102 assessed ternary systems.

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

TCMG6 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

TCMG6 Phases

In this section:

Common Phases for Magnesium Alloys

TCMG6 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 structure in Gd/Y-Mg-Zn, type 14H
LPSO_18R	Long Period Stacking Ordered structure in Mg-Y-Zn, 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

TCMG6 Models for the Included Phases

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AG1ZN1	Ag4.5Zn4.5	hP9	P -3		147	(Zn)1(Zn,Ag)2	
AG1ZR1	CuTi	tP4	P 4/n m m		129	(Ag)0.5(Zr)0.5	
AG2GD	MoSi2/CuZr2	tI6	I 4/m m m	C11b	139	(Ag)0.667(Gd)0.333	
AG2IN_D83	Cu9Al4	cP52	P -4 3 m		215	(Ag)0.68(In)0.32	
AG2ND_H	*	hP6	*			(Ag)0.666667(Nd)0.333333	
AG2PR	*	hP*	*			(Ag)2(Pr)1	
AG2SR3	Er3Ni2	hR45	R -3		148	(Ag)2(Sr)3	
AG2Y	MoSi2/CuZr2	tI6	I 4/m m m	C11b	139	(Ag)0.667(Y)0.333	
AG3SN1	Cu3Ti	oP8	P m m n			(Ag)0.75(Ag,Sn)0.25	
AG4CE	*	*	*			(Ag)4(Ce)1	
AG4SC	MoNi4	tI10	I 4/m	D1	87	(Ag)0.8(Sc)0.2	
AG4SR	*	*	*			(Ag)4(Sr)1	
AG51GD14	Ag51Gd14	hP68	P 6/m		175	(Ag)0.785(Gd)0.215	
AG51ND14	Ag51Gd14	hP68	P 6/m		175	(Ag)0.785(Nd)0.215	
AG51R14	Ag51Gd14	hP68	P 6/m		175	(Ag)51(La,Pr,Ce)14	> AG51PR14, AG51CE14, AG51LA14
AG51Y4	Ag51Gd14	hP68	P 6/m		175	(Ag)0.785(Y)0.215	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AG5LA	MgZn2	hP12	P 6_3/m m c	C14	194	(Ag)5(La)1	
AG5PR	*	*				(Ag)5(Pr)1	
AG5ZN8	Cu5Zn8	cI52	I -4 3 m	D82	217	(Zn,Ag)2(Ag)2(Zn,Ag)3(Ag,Zn)6	
AG7CA2	Ag7Yb2	oS36	C m c m		63	(Ag)0.777778(Ca)0.222222	
AG9CA2	*	*	*			(Ag)0.818182(Ca)0.181818	
AGCA3	*	*	*	*		(Ag)0.25(Ca)0.75	
AGGDMG_T	*	*	*			(Gd,Ag)0.15(Mg)0.85	
AGMG3	Hf54Os17	oI142	I m m m		71	(Sn,Cu,Ag)0.23(Cu,In,Mg)0.77	
AGMG4	Ag9Mg37	hP92	P 6_3/m		176	(Ag)0.2(Mg)0.8	
AGSC	CsCl	cP2	P m -3 m	B2	221	(Ag)0.5(Sc)0.5	
AGSR	AgSr	oP16	P n m a		62	(Ag)1(Sr)1	
AGY	CsCl	cP2	P m -3 m		221	(Ag)0.5(Y)0.5	
AGZN3	Mg	hP2	P 6_3/m m c		194	(Zn,Ag)1	
AGZR2	CuZr2	tI6	I 4/m m m		139	(Ag)0.3333(Zr)0.6667	
AL10CE2MN7	Th2Zn17	hR57	R -3 m		166	(Mn,Al)0.8947(Ce)0.1053	
AL11LA3_H	BaAl4	tI10	I 4/m m m		139	(Al)11(La)3	
AL11ND3_H	BaAl4	tI10	I 4/m m m		139	(Al)11(Nd)3	
AL11PR3_H	BaAl4	tI10	I 4/m m m		139	(Al)11(Pr)3	
AL11R3	La3Al11	oI28	I m m m		71	(Zn,Al)11(Pr,La,Nd,Y,Ce)3	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL12MG17_A12	Mg24Y5 / Al12Mg17	cI58	I -4 3 m		217	(Gd,Li,Mg)10(Zn,Ca,Al,Mg)24(Ni,Zn,Al,Mg)24	
AL12MN	Al12W	cI26	I m -3 m		229	(Al)12(Mn)1	
AL13CEMG6	MgNi2	hP24	P 6_3/m m c	C14	194	(Al)13(Ce)1(Mg)6	
AL13FE4	Al13Fe4	mS102	C 1 2/m 1		12	(Al)0.6275(Fe,Mn)0.235(Va,Al)0.1375	
AL14CA13	Al14Ca13	mS54	C 1 2/m 1		12	(Al,Mg,Zn)14(Ca)13	
AL1LI1	NaTl	cF16	F d -3 m		222	(Mg,Li,Al)1(Li,Va,Mg)1	
AL1SC1	CsCl	cP2	P m -3 m		221	(Sc)1(Al)1	
AL2CAZN2		tI10	I 4/m m m		139	(Al)2(Ca)1(Zn)2	
AL2FE	FeAl2	aP18	P 1		1	(Al)2(Mn,Fe)1	
AL2GD3	Gd3Al2	tP20	P 4_2 n m		102	(Al)2(Gd)3	
AL2LI3	Li3Al2	hP15	R -3 m		166	(Al,Mg)2(Li)3	
AL2R3	Zr3Al2	tP20	P 4_2/m n m		136	(Al)0.4(Y,Zr)0.6	
AL2SC	Cu2Mg	cF24	F d -3 m	C15	222	(Sc)1(Al)2	
AL38MG58SR4	*	*	*			(Al)38(Mg)58(Sr)4	
AL3CA8	Ca8In3	aP22	P -1		2	(Al)3(Mg,Ca)8	
AL3CE_H	Mg3Cd	hP8	P 6_3/m m c		194	(Al)0.75(Ce)0.25	
AL3CE_L	Mg3Cd	hP8	P 6_3/m m c		194	(Al)0.75(Ce)0.25	
AL3CU2MG9SI7		hP21	P -6		174	(Al)3(Cu)2(Mg)9(Si)7	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL3GD		hP36	R -3 m		166	(Al)3(Gd)1	
AL3LA	Mg3Cd	hP8	P 6_3/m m c	D019	194	(Al)3(La)1	
AL3ND	Mg3Cd	hP8	P 6_3/m m c		194	(Al)3(Nd)1	
AL3NI2	Ni2Al3	hP5	P -3 m 1		164	(Al)3(Mg,Ni,Al)2(Ni,Va)1	
AL3NI5	Pt5Ga3	oS16	C m m m		65	(Al)0.375(Ni)0.625	
AL3PR	Mg3Cd	hP8	P 6_3/m m c		194	(Al)3(Pr)1	
AL3SC	AuCu3	cP4	P m -3 m	L12	221	(Sc)1(Al)3	
AL3SR8	*	*	*			(Al)0.27273(Sr)0.72727	
AL3Y_H	BaPb3	hP36	R -3 m		166	(Al)0.75(Y)0.25	
AL3Y_L	Mg3Cd	hP8	P 6_3/m m c		194	(Al)0.75(Y)0.25	
AL3ZR1	Al3Zr	tI16	I 4/m m m		139	(Al,In,Mg)0.75(Zr)0.25	
AL3ZR2	Al3Zr2	oF40	F d d 2		43	(Al)0.6(Zr)0.4	
AL3ZR4	Al3Zr4	hP7	P 6/m m m		191	(Al)0.42857(Zr)0.57143	
AL3ZR5	W5Si3	tI32	I 4/m c m	D8m	140	(Al)0.375(Zr)0.625	
AL4CA	Al4Ba	tI10	I 4/m m m	D13	139	(Mg,Al)4(Sr,Ca)1	
AL4CE	Al4Ba	tI10	I 4/m m m	D13	139	(Al)0.8(Ce)0.2	
AL4LI9	Al4Li9	mS26	C 1 2/m 1		12	(Al)4(Li)9	
AL4MGY	*	*	*			(Mg,Al,Y)0.6667(Al,Y,Mg)0.1667(Mg,Y)0.1666	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
AL4MN	Mn55Al226.58	hP574	P 6_3/m m c		194	(Al)4(Fe,Mn)1	
AL4SR	BaAl4	tI10	I 4/m m m		139	(Al,Mg)0.8(Sr,Ca)0.2	
AL4ZR5	Ga4Ti5	hP18	P 6_3/m c m		193	(Al)0.44444(Zr)0.55556	
AL53LA22	AlB2	hP3	P 6/m m m	C32	191	(Al)0.707(La)0.293	
AL5FE2	FeAl2.8	oS14	C m c m		63	(Al)5(Mn,Fe)2	
AL6MN	Al6Mn	oS28	C m c m		63	(Al)6(Mn,Fe)1	
AL7SR8	Ba8Ga7	cP60	P 2_1 3		198	(Al)0.46667(Sr,Ca)0.53333	
AL8CEM4		tI26	I 4/m m m		139	(Al)0.6154(Ce)0.0769(Mn,Al)0.3077	
AL9CA31ZN10	*	*	*			(Al)1(Ca)1(Zn)1	
ALCE2	*	*	*			(Al)0.3333(Ce)0.6667	
ALCE3_L	Mg3Cd	hP8	P 6_3/m m c		194	(Al)0.25(Ce)0.75	
ALCUMG_Q	CuFeS2	cI96	I m -3 m		229	(Al)7(Cu)3(Mg)6	
ALCUMG_S	MgCuAl2	oS16	C m c m		63	(Al,Si)2(Cu)1(Mg)1	
ALCUMG_T	Mg32(Zn0.65Al0.35)49	cI162	I m -3 m		229	(Mg)26(Al,Mg)6(Mg,Zn,Al,Cu)48(Al)1	
ALCUMG_V	Mg2Zn11	cP39	P m -3		220	(Al)5(Cu)6(Mg)2	
ALCU_DEL	*	*	*			(Zn,Al)2(Fe,Cu)3	
ALCU_EPS	Co1.75Ge	hP6	P 6_3/m m c		194	(Al,Zn,Ni,Cu)1(Cu,Fe)1	
ALCU_ETA	*	*	*			(Cu,Al)1(Cu,Ag)1	
ALCU_PRIME	*	*	*			(Al)2(Cu)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
ALCU_ZETA	*	*	*			(Al)9(Ag,Cu)11	
ALLA3	Mg3Cd & Ni3Sn	hP8	P 6_3/m m c	D019	194	(Al)1(La)3	
ALLAMG_T1	*	*	*			(Al)2(La)0.15(Mg)0.85	
ALLI2	InLi2 / GaLi2	oS12	C m c m		63	(Al)1(Li)2	
ALLIMG_T		c*456	*			(Al)0.53(Li)0.33(Mg)0.14	
ALMG3NI2		cF96	F d -3 m		222	(Al)1(Ni)2(Mg)3	
ALMGMN_T	Al18Mg3Cr2	cF184	F d -3 m		222	(Al)18(Mg)3(Mn)2	
ALMGND_T	MgZn2	hP12	P 6_3/m m c		194	(Al)2(Mg)0.88(Nd)0.12	
ALMGZN_PHI	(Al,Zn)17Mg21	oP152	P b c m	orthorhombic	57	(Mg)21(Al,Zn)17	
ALMGZN_Q	*	cP676	P a -3	icosahedral	205	(Al)0.15(Mg)0.44(Zn)0.41	
ALMGZN_T1	(Al,Zn)49Mg32	cI162	I m -3	cubic	204	(Mg)26(Mg,Al)6(Al,Zn,Mg)48(Al)1	
ALMGZN_T2	Al17Mg46Zn37	cP640	P a -3	cubic	205	(Al)0.15(Mg)0.43(Zn)0.42	
ALMG_BETA	Mg28Al45	cF1168	F d -3 m		222	(Al,Zn)140(Li,Mg)89	
ALMG_EPSILON	Mg23Al30	hP159	R -3		148	(Zn,Al)30(Mg)23	
ALND3	Mg3Cd	hP8	P 6_3/m m c		194	(Al)1(Nd)3	
ALPR3_L	Mg3Cd	hP8	P 6_3/m m c		194	(Al)1(Pr)3	
ALRE3	AuCu3	cP4	P m -3 m	L12	221	(In,Al)1(Pr,Ce)3	
ALR_OP16	DyAl	oP16	P b c m		57	(Al)1(Nd,Pr)1	
ALR_OS16	CeAl	oS16	C m c m		63	(Al)1(Gd,La,Pr,Ce)1	> a phase based on ALCE,

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
							ALGD, ALLA, ALPR(rt)
ALSC2	Co1.75Ge	hP6	P 6_3/m m c		194	(Sc)2(Al)1	
ALZR2	Ni2In / C01.75Ge	hP6	P 6_3/m m c	B82	194	(Al)0.33333(Zr)0.66667	
B2NIIN	CsCl	cP2	P m -3 m		221	(Ni,Va)1(In)1	
B2REIN		cP2	P m -3 m		221	(Y,Nd,La)1(Nd,In)1	
B2_BCC	CsCl	cP2	P m -3 m		221	(Ag,Ni,Zn,Cu)0.5(Gd,Zr,Pr,Nd,Ce,Y)0.5	> B2 phases modeled separately from A2
B2_MGR	CsCl	cP2	P m -3 m		221	(Sn,Al,Mn,Nd,Ag,Mg,In,Cu,Zn)0.5(Ho,Y,Mg,Er,Ag,Ca,La,Gd,In,Ce,Nd,Dy,Cu,Sn,Pr,Sm)0.5	> LaMg, MgNd, NdZn, CeMg, CeZn, MgY, YZn, GdMg, GdZn, MgSm, AgMg
B2_SCIN	CsCl	cP2	P m -3 m		221	(Sc)1.1(In)0.9	
BCC_A2	W	cI2	I m -3 m	A2	229	(Nd,Bi,Er,Gd,Th,In,Sr,Sn,Sm,La,Ho,Sc,Ce,Cu,K,Ag,Al,Y,Na,Mg,Zr,Mn,Si,Ni,Fe,Li,Ca,Dy,Zn,Pr)1(Va)3	
BCC_B2	CsCl	cP2	P m -3 m	B2	221	(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	A B2 phase described with the partitioning model and having a contribution from its disordered counterpart.

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
BCC_B32	NaTl	cF16	F d -3 m		222	(Zn,Li)1(Li,Zn)1	
BCT_A5	Sn	tI4	I 4_1/a m d	A5	141	(Sn,In,Zn,Al,Ag)1	
BETA_NIZN	CuTi	tP2	P 4/m m m		123	(Ni,Zn)1	
BI10CA11	Ge10Ho11	tI84	I 4/m m m		139	(Bi)10(Ca)11	
BI2CA1	ZrSi2	oC12	C m c m		63	(Bi)2(Ca)1	
BI2CAMG2	La2O3	hP5	P -3 m 1		164	(Bi)2(Ca)1(Mg)2	
BI2MG3_HT	Mn2O3	cI80	I a -3	D5_3	206	(Bi)1(Va,Bi)3(Mg)6	
BI2MG3_LT	La2O3	hP5	P -3 m 1	D5_2	164	(Va,Bi)2(Mg)3	
BI3CA5	Yb5Sb3	oP32	P n m a		62	(Bi)3(Ca)5	
BICA2	La2Sb	tI12	I 4/m m m		139	(Bi)1(Ca)2	
BIMN_HT	Bi1.88Mn2.23	oP10	P m m a	B82	51	(Bi)1(Mn)1.08	
BIMN_LT	NiAs	hP4	P 6_3/m m c	B81	194	(Bi)1(Mn)1	
C14_LAVES	MgZn2	hP12	P 6_3/m m c	C14	194	(Ca, Gd, Al, Mg, Cu, Sr, Y, Ni, Na, Mn, Zn, Li)2(Nd, Cu, Ce, Mg, Va, Ho, Ca, K, Pr, Er, Gd, La, Y, Al, Mn, Sr, Zn, Th, Dy, Zr, Sc)1	> Al2Zr, CaLi2, CaMg2, Mg2Sr, Mg2Y, MgZn2, Mn2Zr, Na2K
C15_LAVES	Cu2Mg	cF24	F d -3 m	C15	222	(Zn, Si, Y, Fe, Nd, Ca, Ni, Gd, La, Mn, Zr, Al, Cu, In, Li, Mg)2(Zr, Zn, Sm, Ca, Y, Sr, Th, Pr, Gd, Mg, Si, Fe, Ni, In, Li, Cu, Ce, Al, La, Nd)1(Va)2	> It includes 18 compounds, e.g. Al2Ca, Al2Ce, Cu2Mg, Fe2Gd, Mg2Gd
C36_LAVES	MgNi2	hP24	P 6_3/m m c	C36	194	(Mn,Fe,Cu,Gd,Mg,Ni,Zn,Al)2(Mg,Zn,Cu,Al,Gd,Th,Ni,Ca)1	> MgNi2 type

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
							phase, also includes MgNi2, (Cu,Zn)2Mg, (Al,Mg)2Ca
CA14SI19	Ca14Si19	hP198	R -3 c		167	(Ca)0.424242(Si)0.575758	
CA1CU1	CaCu (h)	oP40	P n m a		62	(Ca)0.5(Cu)0.5	
CA1IN2		hP6	P 6_3/m m c		194	(Ca)1(In)2	
CA2CU	Ca2Cu	oP12	P n m a		62	(Ca)0.6667(Cu)0.3333	
CA2MG6ZN3		h**	*			(Ca)2(Mg)6(Zn)3	
CA2NI7	Gd2Co7	hP54	R -3 m		166	(Ca)0.2222(Ni)0.7778	
CA2SN_X	CrB / TlI	oS8	C m c m	B33 / Bf	63	(Ca,Mg)1(Ca)1(Sn)1	
CA31SN20	Pu31Pt20	tI204	I 4/m c m		140	(Ca)31(Sn)20	
CA36SN23	Yb36Sn23	tP118	P 4/m b m		127	(Ca)36(Sn)23	
CA3SI4	Ca3Si4	hP42	P 6_3/m		176	(Ca)0.428571(Si)0.571429	
CA3ZN	Re3B	oC16	C m c m	E1a	63	(Ca)3(Zn)1	
CA5X3	Cr5B3	tI32	I 4/m c m	D8l	140	(Ca,La)5(Si,Ag,Zn,Sn)3	> CA5SI3, CA5SN3, CA5AG3, CA5ZN3, also La5Si3
CA7MG6SI14	Ca7Mg6Si14	hP276				(Ca)0.2592593(Mg)0.2222222(Si)0.5185185	
CA7SN6	Ca7Sn6	oP52	P n m a		62	(Ca)7(Sn)6	
CA8IN3		aP22	P 1		1	(Ca)8(In)3	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CACU5	CaCu5	hP6	P 6/m m m	D2d	191	(Ca)0.1667(Cu)0.8333	
CAMGSI_T1	anti-PbCl2	oP12	*			(Ca)0.3333(Mg,Ca)0.3334(Si)0.3333	
CAMGSN_T1	anti-PbCl2	oP12	*			(Ca)156(Mg)94(Sn)175	
CANI2	Cu2Mg	cF24	F d -3 m		222	(Ca)0.333(Ni)0.667	
CASI2	CaSi2	hP9	R -3 m		166	(Ca)0.333333(Si)0.666667	
CAZN3	Ca3.33Zn10.11	hP32	P 6_3/m m c		194	(Ca)1(Zn)3	
CBCC_A12	Mn	cI58	I -4 3 m	A12	217	(Cu,In,Zn,Sn,Zr,Ni,Al,Fe,Mg,Mn,Si)1(Va)1	
CE13ZN58	Zn58Gd13	hP142	P 6_3/m m c		194	(Ce)0.183(Zn)0.817	
CEH2_35		tI30				(Ce)1(H)2.35	
CEH2_9	CeH3	cF44	F m -3 m		225	(Ce)1(H)2.9	
CE2IN	Co1.75Ge	hP6	P 6_3/m m c		194	(Ce)2(In)1	
CE2ZN17	Th2Ni17	hP57	R -3 m		166	(Ce)0.105(Mg,Zn)0.895	
CE3IN5	Pu3Pd5	oS32	C m c m		63	(Ce)3(In,Ce)5	
CE3ZN11	La3Al11	oI28	I m m m		71	(Ce)0.214(Mg,Zn)0.786	
CE5IN4	*	*	*			(Ce)5(In)4	
CE9IN11	*	*	*			(Ce)9(In)11	
CEGD3	Sm	hP9	R -3 m		166	(Ce,Gd)1	
CENI2	MgCu2	cF24	F d -3 m		222	(Ce,Ni)0.333(Ni,Ce)0.667	
CENI3	CeNi3	hP24	P 6_3/m m c		194	(Ce)0.25(Ni)0.75	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CEZN11	BaCd11	tI48	I 4_1/a m d		141	(Ce)0.083(Zn,Mg)0.917	
CEZN2	KHg2	oI12	I m m a		74	(Ce)0.333(Zn,Mg)0.667	
CEZN3	CeZn3	oS16	C m c m		63	(Ce)0.25(Zn)0.75	
CEZN5	CaCu5	hP6	P 6/m m m		191	(Ce)0.167(Mg,Zn)0.833	
CU10SN3	Cu10Sn3	hP26	P 6_3		173	(Cu,Sn)1	
CU11IN9	AlCu	mS20	C 2/m		12	(Cu)0.55(In)0.45	
CU15SI4_EPSILON	Cu15Si4	cI76	I -4 3 d		220	(Cu,Mg)15(Si,Al)4	
CU16MG6SI7	Mn23Th6	cF116	F m -3 m		225	(Cu)16(Mg)6(Si)7	
CU2CE	KHg2	oI12	I m m a		74	(Cu,In)0.667(La,Ce)0.333	
CU2IN_B82	Co1.75Ge	hP6	P 6_3/m m c		194	(Cu,Mg)1(Cu,Va)1(In)1	
CU2IN_LT	*	*	*			(Cu)0.64(In)0.36	
CU2LA	AlB2	hP3	P 6/m m m	C32	191	(Cu)2(La)1	
CU2PR	KHg2	oI12	I m m a		74	(Cu)0.667(Pr)0.333	
CU2SC_C11B	MoSi2/CuZr2	tI6	I 4/m m m	C11b	139	(Ag,Cu)2(Sc)1	
CU2TH	AlB2	hP3	P 6/m m m	C32	191	(Cu)0.667(Th)0.333	
CU2Y_H	*	*	*			(Cu)2(Y)1	
CU33SI7_DELTA	*	tP*	*			(Cu)0.825(Si)0.175	
CU37LA3	NaZn13	cF112	F m -3 c		226	(Cu)37(La)3	
CU3MG2SI_C1	MgNi2	hP24	P 6_3/m m c		194	(Cu)2.74(Mg)2(Si)1.26	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CU3SN_H_ GAMMA	BiF3	cF16	F m -3 m	L21	225	(Cu,Sn)1	
CU3SN_L	Cu3Sn	oS80	C m c m		63	(Cu,Sn)3(Cu,Sn)1	
CU41SN11	Cu41Sn11	cF416	F -4 3 m		216	(Cu,Sn)41(Cu,Sn)11	
CU4CE	*	oP20	*			(Cu)0.8(Ce)0.2	
CU4LA	Cu4La	tI90	I -4 m 2		119	(Cu)4(La)1	
CU4ND	*	o**	*			(Cu)0.8(Nd)0.2	
CU4PR	*	o**	*			(Cu)0.8(Pr)0.2	
CU4SC	Cu4Sc	tI*	*			(Cu)4(Sc)1	
CU4Y	*	*	*			(Cu)4(Y)1	
CU51TH14	Ag51Gd14	hP68	P 6/m		175	(Cu)0.7826(Th)0.2174	
CU51ZR14	Ag51Gd14	hP68	P 6/m		175	(Cu)0.7846(Zr)0.2154	
CU56SI11_ GAMMA	Mn	cP20	P 4_1 3 2		213	(Mg,Cu)56(Si)11	
CU5CE	CaCu5	hP6	P 6/m m m		191	(Cu)0.833(Ce)0.167	
CU5PR	CaCu5	hP6	P 6/m m m		191	(Cu)0.833(Pr)0.167	
CU6CE	Cu6Ce	oP28	P n m a		62	(Cu)0.857(Ce)0.143	
CU6LA_L	Cu6La	mP28	P 1 2_1/c 1		14	(Cu)6(La)1	
CU6PR	Cu6La	mP28	P 1 2_1/c 1		14	(Cu)0.857(Pr)0.143	
CU6R	Cu6Ce	oP28	P n m a		62	(Cu)6(Gd,Nd,Ce,La)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CU6SN5	Cu6Sn5	mS44	C 1 2/c 1		15	(Cu)1(Sn,Cu)1(Sn)1	
CU6TH	Cu6Ce	oP28	P n m a		62	(Cu)0.857(Th)0.143	
CU7GD2	*	*	*			(Cu)7(Gd)2	
CU7IN3	Cu7In3	cP40	P -1		2	(Mg,Cu)0.7(In)0.3	
CU7ND2	*	*	*			(Cu)0.77777778(Nd)0.22222222	
CU7Y1	Cu5.44Tb0.78	hP8	P 6/m m m		191	(Y,Cu2)1(Cu)5	
CU7Y2	*	*	*			(Cu)7(Y)2	
CU8ZR3	Cu8Hf3	oP44	P n m a		62	(Cu)0.7273(Zr)0.2727	
CU9GD2	*	t**	*			(Cu)9(Gd)2	
CUH_B3	ZnS	cF8	F -4 3 m		216	(Cu)1(H)1	
CUH_B4	ZnS	hP4	P 6_3/m c		186	(Cu)1(H)1	
CU9IN4_D83	Al4Cu9	cP52	P -4 3 m	D83	215	(Cu)0.654(In,Cu)0.115(In)0.231	
CU9MG2Y	Cu9Mg2Tb	hP24	P 6_3/m m c		194	(Cu)0.75(Mg)0.166667(Y)0.083333	
CUB_A13	Mn	cP20	P 4_1 3 2	A13	213	(In,Al,Zr,Mg,Ni,Ag,Cu,Ce,Fe,Zn,Si,Ca,Sn,Mn)1(Va)1	
CULIMG_T	Mg2Ni	hP18	P 6_2 2 2		180	(Cu)1(Li)0.08(Mg)1.92	
CUMG2	CuMg2	oF48	F d d d		70	(Ag,In,Ni,Cu)1(In,Mg)2	
CUMGY_14H			P 6_3/m c m		193	(Mg)0.85714286(Y)0.07142857(Cu)0.07142857	
CUMGY_18R	*	*	*			(Mg)0.833334(Y)0.083333(Cu)0.083333	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
CUMGY_T10	*	*	*			(Cu)0.09(Mg)0.78(Y)0.13	
CUMGY_T2	Cu4MgSn	cF24	F -4 3 m		216	(Cu)4(Mg)1(Y)1	
CUMGY_T3	Mo2FeB2	tP10	P 4/m b m		127	(Cu)2(Mg)1(Y)2	
CUMGY_T4	ZrNiAl	hP9	P -6 2 m		189	(Cu)1(Mg)1(Y)1	
CUMGY_T5	Cu5Mg8Y5	oP36	P m m a		51	(Cu)0.277778(Mg)0.444444(Y)0.277778	
CUMGY_T6	Cu5Mg13Y5	oS92	C m c m		63	(Cu)0.2173913(Mg)0.5652174(Y)0.2173913	
CUMGY_T7	*	*	*			(Cu)0.18(Mg)0.57(Y)0.25	
CUMGY_T8	Cu5Mg16Y5	oS104	C m c m		63	(Cu)0.1923077(Mg)0.6153846(Y)0.1923077	
CUMGY_T9	CuMg4Tb	oS48	C m c m		63	(Cu)1(Mg)4(Y)1	
CUND_H	*	*	*			(Cu)0.5(Nd)0.5	
CUSC	CsCl	cP2	P m -3 m	B2	221	(Cu)1(Sc)1	
CUSI_ETA	*	tP*	*			(Cu)0.76(Si)0.24	
CUSR	BaCu	hP8	P 6_3/m m c		194	(Cu)0.5(Sr)0.5	
CUTH2	CuAl2	tI12	I 4/m c m		140	(Cu)0.333(Th)0.667	
CUZN_GAMMA	Cu5Zn8	cI52	I -4 3 m	D82	217	(Zn,Cu)2(Cu,Zn)2(Cu)3(Zn,Mg)6	
CUZR2	MoSi2/CuZr2	tI6	I 4/m m m	C11b	139	(Cu)0.333(Zr)0.667	
D3_ALFE	*	*	P 10/m m c			(Al)0.7(Al,Fe)0.08(Mn,Fe)0.22	
DELTA_FEZN	FeZn10	hP 6_32	P 6_3/m m c		194	(Fe)0.058(Fe,Zn)0.18(Zn)0.525(Zn)0.237	
DELTA_NIZN	Zn22Ni3	mS50	C 1 2/m 1		12	(Ni)0.111(Zn)0.889	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
DHCP	Nd	hP4	P 6_3/m m c	A3'	194	(Ag,Ni,Y,In,Gd,Mn,Al,Nd,La,Sr,Cu,Ce,Mg,Pr,Ca)1(Va)2	
DIAMOND_A4	C	cF8	F d -3 m	A4	222	(Zn,Si,Sn,Al)1	
EPSILON	Mg	hP2	P 6_3/m m c		194	(Mn,Cu,Zn)1	
ETA	Co1.75Ge	hP6	P 6_3/m m c		194	(Cu)1(Sn,Cu)1(Sn)1	
FCC_A1	Cu	cF4	F m -3 m	A1	225	(Y, Sc, Pr, Sr, Gd, Zr, Na, Ca, In, Cu, Th, Sn, Zn, La, Si, Al, Bi, Nd, Ni, Ce, Li, Ag, Fe, Mg, Mn, K)1(Va)1	
FE17ND2	Zn17Th2	hP57	R -3 m		166	(Fe)1(Nd)0.1176	
FE17ND5	Fe17Nd5	hP264	P 6_3/m c m		193	(Fe)1(Nd)0.2941	
FE17PR2	Zn17Th2	hP57	R -3 m		166	(Fe)17(Pr)2	
FE17TH2	Zn17Th2	hP57	R -3 m		166	(Fe)0.89(Th)0.11	
FE17Y2	Lu1.82Fe17.35	hP38	P 6_3/m m c		194	(Fe)1(Y)0.1176	
FE23Y6	Mn23Th6	cF116	F m -3 m		225	(Fe)1(Y)0.2609	
FE2SC_C14	MgZn2	hP12	P 6_3/m m c	C14	194	(Fe)0.67(Sc)0.33	
FE2SC_C15	Cu2Mg	cF24	F d -3 m	C15	222	(Fe)0.64(Sc)0.36	
FE2SC_C36	MgNi2	hP24	P 6_3/m m c	C36	194	(Fe)0.67(Sc)0.33	
FE2SI	AlNi2	hP6	P -3 m 1		164	(Fe)2(Si)1	
FE3SN2	Fe3Sn2	hP30	R -3 m		166	(Fe)3(Sn)2	
FE5SN3	Co1.75Ge	hP6	P 6_3/m m c		194	(Fe)5(Sn)3	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
FE5TH	CaCu5	hP6	P 6/m m m		191	(Fe)0.83(Th)0.17	
FE6SC29	*	*	*	*		(Fe)0.17(Sc)0.83	
FE7TH2_H	Gd2Co7	hP54	R -3 m		166	(Fe)0.78(Th)0.22	
FE7TH2_L	Ce2Ni7	hP36	P 6_3/m m c		194	(Fe)0.78(Th)0.22	
FESI2_H	Fe0.92Si2	tP3	P 4/m m m		123	(Fe)3(Mg,Si)7	
FESI2_L	FeSi2	oS48	C m c e		64	(Fe)1(Si)2	
FESN	CoSn	hP6	P 6/m m m	B35	191	(Fe)1(Sn)1	
FEZR3	AuCu3	cP4	P m -3 m	L12	221	(Fe,Zr)1(Fe,Zr)3	
F_MGGDZN	Ce20Mg19Zn81	cF480	F -4 3 m		216	(Gd)0.166667(Mg)0.158333(Zn)0.675	
GAMMA1_FEZN		cF408	I -4 3 m		217	(Fe)0.137(Zn,Fe)0.118(Zn)0.745	
GAMMA_D83	Al4Cu9	cP52	P -4 3 m	D83	215	(Si,Al)4(Al,Cu,Si)1(Ag,Cu)8	
GAMMA_FEZN	Zn9(Zn0.5Fe0.5)2Fe2	cI52	I m -3 m / I -4 3 m	D81 / D82	229/217	(Fe,Zn)0.154(Fe,Zn)0.154(Zn,Fe)0.231(Zn)0.461	
GAMMA_H	Cu5Zn8	cI52	I -4 3 m	D82	217	(Al)4(Al,Cu)1(Ag,Cu)8	
GAMMA_NIZN	Cu5Zn8	cI52	I -4 3 m	D82	217	(Zn,Ni)1	
GAS						(Al,Mg2,Ni2,Al2,Ce,Ni,Cu,Cu2,La,Mg,Zn)1	
GD13ZN58	Zn58Gd13	hP142	P 6_3/m m c		194	(Gd)0.183(Zn,Mg)0.817	
GD1IN1						(Gd)1.1(In)1	
GD2IN		hP6	P 6_3/m m c		194	(Gd)2(In)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
GD2NI7	Gd2Co7	hP54	R -3 m		166	(Gd)2(Ni)7	
GD2ZN17_H	Th2Ni17	hP57	R -3 m		166	(Sm,Gd)0.105(Zn)0.895	
GD2ZN17_L	Zn17Th2	hP38	P 6_3/m m c		194	(Gd)0.105(Zn)0.895	
GD3IN5		cS32	C m c m		63	(Gd)3(In)5	
GD3NI2	*	t*20	*			(Gd)3(Ni)2	
GD3SI5	*	*	*			(Gd)0.375(Si)0.625	
GD3ZN11	La3Al11	oI28	I m m m		71	(Gd)0.214(Zn)0.786	
GD5IN3		tI32	I 4/m c m		140	(Gd)5(In)3	
GD5SI4	Gd5Si4	oP36	P n m a		62	(Gd)0.5556(Si)0.4444	
GDIN3		cP4	P m -3 m		221	(Gd)1(In)3	
GDMG5	Mg43 (Mg0.32Gd0.68)6Gd5	cF448	F -4 3 m	fcc	216	(Sm,Sr,Nd,Ca,Ag,Y,Gd)1(Mg,Zn)5	
GDND	Sm	hP9	R -3 m		166	(Nd,Gd)0.5(Nd,Gd)0.5	
GDNI4	*	hP10	*			(Gd)1(Ni)4	
GDSI2	ThSi2	tI12	I 4_1/a m d		141	(Gd)0.3333(Si)0.6667	
GDZN12	ThMn12	tI26	I 4/m m m		139	(Gd)0.077(Zn)0.923	
GDZN2	KHg2 & CeCu2	oI12	I m m a		74	(Sm,Gd)0.333(Zn)0.667	
HCP_A3	Mg	hP2	P 6_3/m m c	A3	194	(Bi, Ho, Pr, Ni, In, Gd, Li, Si, Dy, Ca, Fe, Sb, Sm, Nd, Ga, Mg, Sr, La, Zr, Mn, Ce, Zn, Th, Sn, Y, Ag, Sc, Al, Er, Cu, Na, K)1(Va)0.5	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
HTAL11MN4	Mn6(Mn0.5Al0.5)8Al25	oP156	P n m a		62	(Al,Mn)29(Mn,Fe)10	
HTAL8MN5	*	*	*			(Fe,Al,Mn)8(Fe,Mn,Al)5	
H_RZN5						(Y,Gd)1(Mg,Zn)5	
IN1SR1		oF64	F d d 2		43	(In)0.5(Sr)0.5	
IN2SR		hP6	P 6_3/m m c		194	(In)0.6667(Sr)0.3333	
IN3LA2	*	*	*			(In)0.57(La)0.43	
IN3SR1		hP8	P 6_3/m m c		194	(In)0.75(Sr)0.25	
IN3SR2		*	*			(In)0.6(Sr)0.4	
IN3SR5		tI32	I 4/m c m		140	(In)0.375(Sr)0.625	
IN5RE3		cS32	C m c m		63	(In)0.625(Y,Nd,Pr,La,Th)0.375	
IN5SR2		*	*			(In)0.7143(Sr)0.2857	
INSN_AF		hP1	P 6/m m m		191	(Sn,In)1	
INSR3		cF16	F m -3 m		225	(In)0.25(Sr)0.75	
I_MGRZN			F m 53			(Y,Gd)0.1(Zn,Mg)0.3(Mg,Zn)0.6	
K17IN41		cF464	F d -3 m		222	(In)0.69(K)0.31	
K39IN80		hP238	P -3 m 1		164	(In)0.635(K)0.365	
KIN4		tI10	I 4/m m m		139	(In)0.8(K)0.2	
L10_TETRA	CuAu	tP2	P 4/m m m	L10	123	(Sc,Mn,Ni,Mg,In)0.5(In,Mg,Mn,Ni)0.5	
L12_FCC	Cu3Au	cP4	P m -3 m		221	(Ca,Y,Th,In,Ce,Nd,Pr,Al,Mg,Sc,La)1(Ag,Sn,Mg,Ni,Zr,In)3	> L12 phases, CaSn3, LaSn3,

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
							Mg1.2In2.8, CeIn3, NdIn3, ScIn3, PrIn3, ThIn3
L21_RMGZN2	AlCu2Mn	cF16	F m -3 m	L21	225	(Y,Ce,Gd)1(Mg)1(Mg,Zn)2	> L21, isostructural to GdMg3: CeMgZn2, GdMgZn2, MgZn2Y, aka W
LA11SN10	*	*	*			(La)0.524(Sn)0.476	
LA2NI3	La2Ni3	oS20	C m c e		64	(La)0.4(Ni)0.6	
LA2NI7_H	Gd2Co7	hP54	R -3 m		166	(La)2(Ni)7	
LA2SN3	Nd2Sn3	aP20	P -1		2	(La)0.4(Sn)0.6	
LA3SN5	Pu3Pd5	oS32	C m c m		63	(La)0.375(Sn)0.625	
LA5SN3_L	W5Si3	tI32	I 4/m c m	D8m	140	(La)0.625(Sn)0.375	
LA5SN4	Sm5Ge4	oP36	P n m a		62	(La)0.555(Sn)0.445	
LA7NI16	La7Ni16	tI46	I -4 2 m		121	(La)0.3043(Ni)0.6957	
LAMGNI_T1	MgCuAl2	oS16	C m c m		63	(La)0.25(Ni)0.25(Mg)0.5	
LAMGNI_T2	Mo2FeB2	tP10	P 4/m b m		127	(La)0.4(Ni)0.4(Mg)0.2	
LAMGNI_T3	*	*	*			(Mg,La)0.333333(Ni)0.666667	
LAMGNI_T4	*	*	*			(La)0.666666(Ni)0.166667(Mg)0.166667	
LAMGNI_T5	*	*	*			(La)0.666666(Ni)0.22(Mg)0.113334	
LAMGNI_T6	*	*	*			(La)0.675(Mg,Ni)0.325	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
LAMGSI_T1	*	*	*			(Mg,La)0.6(Si)0.4	
LAMGSI_T2	*	*	*			(La)0.2(Si)0.4(Mg)0.4	
LAMGSI_T3	*	*	*			(La)0.25(Si)0.5(Mg)0.25	
LAMGSI_T4	*	*	*			(La)0.2(Si)0.03333(Mg)0.76667	
LAMGSI_T5	*	*	*			(La)0.3293(Si)0.004(Mg)0.6667	
LAMGZN_T	AlCu2Mn	cF16	F m -3 m	L2_1	225	(La)1(Mg,Zn)2(Mg)1	
LAMGZN_V	*	*	*			(La)0.05(Mg)0.42(Zn)0.53	
LANI5	CaCu5	hP6	P 6/m m m		191	(La,Ni)0.16667(Ni,La)0.33333(Ni)0.5	
LASI2_A1	ThSi2	tI12	I 4_1/a m d		141	(La)0.36(Si)0.64	
LAY		hP8	P 6_3/m m c		194	(La,Y)1(Y)1	
LAZN4		oS20	C m c m		63	(La)1(Zn,Mg)4	
LI12SI7	Li12Si7	oP152	P n m a		62	(Li)12(Si)7	
LI13IN3		cF128	F d -3 m		222	(Li)13(In)3	
LI13SI4	Li13Si4	oP34	P b a m		55	(Li)13(Si)4	
LI13SN5	Li13Sn5	hP18	P -3 m 1		164	(Li)13(Sn)5	
LI22SI5	Li21Si5	cF416	F -4 3 m		216	(Li)22(Si)5	
LI22SN5	Li17Pb4	cF432	F -4 3 m		216	(Li)22(Sn)5	
LI2IN		oS12	C m c m		63	(Li)2(In)1	
LI2MGIN		cF24	F m -3 m		225	(Li)2(Mg)1(In)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
LI2SN5	Hg5Mn2	tP14	P 4/m b m		127	(Li)2(Sn)5	
LI2ZN3_H	*	*	*			(Zn,Li)2(Zn,Li)3	
LI2ZN3_L	*	*	*			(Li)2(Zn,Li)3	
LI2ZN5_H	*	*	*			(Zn,Li)2(Zn)5	
LI2ZN5_L	*	*	*			(Zn,Li)2(Zn)5	
LI3IN1	*	*	*			(Li)3(In)1	
LI3IN2		hP15	R -3 m		166	(Li)3(In)2	
LI5IN4		hP9	P -3 m 1		164	(Li)5(In)4	
LI5SN2	Li5Sn2	hP21	R -3 m		166	(Li)5(Sn)2	
LI7IN	*	*	*			(Li)7(In)1	
LI7SI3	*	*	*			(Li)7(Si)3	
LI7SN2	Li7Ge2	oS36	C m m m		65	(Sn,Li)7(Sn)2	
LI7SN3	Li7Sn3	mP20	P 1 2_1/m 1		11	(Li)7(Sn)3	
LI8SN3	*	*	*			(Li)8(Sn)3	
LIIN		cF16	F d -3 m		222	(In,Li)1(Li,In)1	
LIQUID						(Gd, Na, Ce, Sn, Ga, K, Zn, Ni, Th, Mg2Sn, Bi, Er, Ag, Li, La, Pr, Mn, Sc, Lasn, Nd, Si, Dy, Fe, Cu, Zz, In, Zr, Bi3Ca5_N, Mg3Sb2, Ca2Sn, Sr, Bi2Mg3, Sb, Al, Mg, Ca, Sm, Ho, Y)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
LISN	LiSn	mP6	P 1 2/m 1		10	(Li)1(Sn,Li)1	
LIZN2	*	*	*			(Li)1(Zn)2	
LIZN4_H	*	*	*			(Li,Zn)0.2(Li,Zn)0.8	
LIZN4_L	*	*	*			(Li,Zn)1(Zn,Li)4	
LPSO_14H		hP168	P 6_3/m c m		193	(Mg)0.88(Y,Gd)0.06(Zn)0.06	
LPSO_18R		m*144	C 2/m		12	(Mg)0.84(Y)0.08(Zn)0.08	
LTAL11MN4	Mn4Al11	aP15	P -1		2	(Al)11(Fe,Mn)4	
LTAL8MN5	Cu5Zn8	cI52	I -4 3 m	D810	217	(Al)12(Mn,Fe)5(Al,Fe,Mn)9	
L_MGRZN		hP480	*			(Gd)0.14(Mg)0.22(Zn)0.64	
M10ZR7	Zr7Ni10	oS68	C m c e		64	(Ni,Cu)10(Zr)7	
M23R6	Mn23Th6	cF116	F m -3 m		225	(Mg,Mn,Al,Fe)23(Gd,Zr,Y,Sr,Th,Ce,Pr,Nd)6	
M2R	KHg2	oI12	I m m a		74	(Ag,Cu,Al,Mg,Zn)2(Pr,Gd,La,Ce,Nd,Ca,Y,Sr)1	
M3R	PuNi3	hP36	R -3 m		166	(Ni,Fe)3(Th,La,Gd,Pr,Mg,Y,Ca)1	
M5R	AuBe5	cF24	F -4 3 m		216	(Cu,Zr,Ni)5(Va,Zr,Gd)1	
M5SI3_D88	Mn5Si3	hP16	P 6_3/m c m	D88	193	(Fe,Gd,Y,La,Mn,Zr)5(Sn,Si,In)3	> Fe5Si3, Gd5Si3, Mn5Si3, Y5Si3, Zr5Si3, also LA5SN3(HT)
MG12R	ThMn12	tI26	I 4/m m m		139	(Zn,Mg,Al,Mn)12(La,Sr,Nd,Gd,Pr,Ce,Y)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
MG17SR2	Th2Ni17	hP57	R -3 m		166	(Ce,Gd,Nd,Sr,Th,La,Y,Pr)2(Ni,Al,Zn,Fe,Mg)17(Va)14	
MG1GA1		tI32	I 4_1/a		88	(Mg)0.5(Ga)0.5	
MG24R5	Mg24Y5 / Al12Mg17	cI58	I -4 3 m		217	(Mg)24(Y,Nd,Ce,Dy,La,Er,Mg,Ho,Pr,Gd,Ca)4(Dy,Er,Ho,Y)1	
MG2GA1	Mg2Ga	hP18	P -6 2 c		190	(Mg)0.6667(Ga)0.3333	
MG2GA5	Mg2Ga5	tI28	I 4/m m m		139	(Mg)0.2857(Ga)0.7143	
MG2IN	Mg2In	hP9	P -6 2 m		189	(Mg)2(In)1	
MG2NI1	Mg2Ni	hP18	P 6_2 2 2		180	(Mg)2(Zn,Cu,Ni)1(Va)1	
MG2NIH4		mS56	C 2/c		15	(Mg)2(Ni)1(H)4	
MG2SI_C1	CaF2	cF12	F m -3 m	C1	225	(Mg,Si)2(Si,Ni,Sn)1	> This is also Si2Ni & Mg2Sn
MG2ZN11	Mg2Zn11	cP39	P m -3		220	(Mg)2(Al,Cu,Zn,Si)11	
MG2ZN3	Mg4Zn7	mS110	C 1 2/m 1		12	(Mg)2(Zn,Al,Cu)3	
MG38SR9	Sr9Mg38	hP94	P 6_3/m m c		194	(Mg,Al)38(Nd,Sr,Ce)9	
MG3IN	Mg3In	hP48	R -3 m		166	(Mg,In)3(In,Mg)1	
MG3R_D019	*	hP8	P 6_3/m m c	D019	194	(Mg)3(Gd,Nd,Y,Zn)1	
MG3R_D03	BiF3	cF16	F m -3 m	D03	225	(Li,Zn,Mg)3(Gd,Sm,Mg,Er,La,Ca,Pr,Nd,Y,Dy,Ce,Sr)1	> MG3CE, GDMG3, MG3ND, MG3PR, MG3LA, Mg3Sm

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
MG3SB2_HT	β-Mn2O3	cI80	I a -3		206	(Mg)0.601(Sb)0.399	
MG3SB2_LT	La2O3 / Al3Ni2	hP5	P -3 m 1		164	(Mg)0.6(Sb)0.4	
MG41R5	Mg41Ce5	tI92	I 4/m		87	(Zn,Mg)41(La,Sr,Nd,Ca,Gd,Sm,Y,Pr,Ce)5	> Mg41La5, Mg41Ce5, Mg41Nd5, Mg41Pr5, Mg41Sm5
MG51ZN20	Mg51Zn20	oI158	I m m m		71	(Mg)51(Zn)20	
MG5CEY	Sm11Cd45	cF228	*			(Mg)5(Y,Ce)1	
MG5GA2	Mg5Ga2	oI28	I b a m		72	(Mg)0.7143(In,Ga)0.2857	
MG5PR	*	*	*			(Mg)5(Pr,Y)1	
MG6MN3NI	*	*	*			(Mg)3(Mn)1(Ni)2	
MG6REZN3	*	*	*			(Mg)0.6(Ce,Nd,La)0.1(Zn)0.3	
MG7RE	*	o*16		bct		(Mg)7(Nd,Zn,Y,Gd)1	
MGCU4IN	MgCu4Sn	cF24	F -4 3 m		216	(In,Mg)1(In,Cu,Mg)4(In,Mg)1	
MGGA2	MgGa2	oP24	P b a m		55	(Mg)0.3333(Ga)0.6667	
MGH2_C4	TiO2	tP6	P 4_2/m n m		136	(Mg)1(H)2	
MGNDZN_T1	*	*	*			(Mg)0.35(Nd)0.05(Zn)0.6	
MGNDZN_T2	*	*	*			(Mg)0.35(Nd)0.1(Zn)0.55	
MGNDZN_T4	*	*	*			(Mg)0.3(Nd)0.15(Zn)0.55	
MGSC	CsCl	cP2	P m -3 m	B2	221	(Mg)1(Mg,Sc)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
MGZN	Re25Zr21	hP276	R -3 c		167	(Mg)12(Zn,Cu,Al)13	
MN11SI19	Mn11Si9	tP20	P -4 n 2		118	(Mn)11(Si)19	
MN17ND2	Th2Ni17	hP57	R -3 m		166	(Mn)17(Nd)2	
MN19SN6	Ni3Sn / Mg3Cd	hP8	P 6_3/m m c	D019	194	(Mn)0.76(Sn)0.24	
MN23SC6	Mn23Th6	cF116	F m -3 m		225	(Mn)23(Sc)6	
MN23Y6	Mn4Y	tI60	I 4/m m m		139	(Mn,Mg)23(Y)6	
MN2SN	Co1.75Ge	hP6	P 6_3/m m c		194	(Mn)0.667(Sn)0.333	
MN3IN		cP56				(Mn)3(In)1	
MN3SI	AlFe3/BiF3	cF16	F m -3 m	D03_or_L21	225	(Mn)3(Si)1	
MN6SI	Cr0.16Mo0.38Co0.46	hP159	R -3		148	(Mn)17(Si)3	
MN9SI2	Mn19 (Mn0.62Si0.38)10Si2	oI186	I m m m		71	(Mn)33(Si)7	
MNI3_L12	AuCu3	cP4	P m -3 m	L12	221	(Mn,Fe,Ni)1(Fe,Mn,Ni)3	
MNNI2	*	*	*			(Ni,Mn)1(Ni)2	
MNSC4		*	*			(Mn)0.2(Sc)0.8	
MNSN2	Al2Cu	tI12	I 4/m c m	C16	140	(Mn)0.333(Sn)0.667	
MNZN9	*	*	*			(Mn)0.1(Zn)0.9	
MR_B27	FeB-b	oP8	P n m a		62	(Cu,Si,Ni,Zn)1(Nd,Zr,Pr,La,Sr,Y,Gd,Ce)1	
MSI_B20	FeSi	cP8	P 2_1 3	B20	198	(Mn,Fe)1(Si,Mg)1	> FeSi & MnSi

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
M_MGRZN	*	hP238	*			(Gd)0.08(Mg)0.28(Zn)0.64	
NA2IN	Na2Tl	oS48	C 2 2 2_1		20	(Na)2(In)1	
NA6IN11		oS344	C m c m		63	(Na)0.3526(In)0.6474	
NA7IN12		tP228	P 4_2/n m c		137	(Na)0.3731(In)0.6269	
NAIN	NaTl	cF16	F d -3 m		222	(Na)1(In)1	
ND13ZN58	Zn58Y13	hP146	P 6_3/m m c		194	(Nd)0.183(Zn)0.817	
ND2Y	Sm	hP9	R -3 m		166	(Y,Nd)2(Nd,Y)1	
ND2ZN17	Zn17Th2	hP38	P 6_3/m m c		194	(Nd)0.105(Zn)0.895	
ND3ZN11	La3Al11	oI28	I m m m		71	(Nd)0.214(Zn,Mg)0.786	
NDH_GAMMA	*	*	*			(Nd)1(Va)2	
NDZN11_H	*	*	*			(Nd)0.0833(Zn)0.9167	
NDZN2	KHg2	oI12	I m m a		74	(Nd)0.333(Zn)0.667	
NI11ZR9	Ni11Zr9	tI40	I 4/m		87	(Ni)11(Zr)9	
NI13IN9		mS44	C 1 2/m 1		12	(Ni,Va)1(Ni)1(In)1	
NI17Y2	Lu1.82Fe17.35	hP38	P 6_3/m m c		194	(Ni)17(Y)2	
NI21ZR8	Hf8Ni21	aP29	P -1		2	(Ni)21(Zr)8	
NI2IN3		hP5	P -3 m 1		164	(Ni)2(In)3	
NI2IN_HT		hP6	P 6_3/m m c		194	(Va,Ni)1(Ni)1(Ni,In)1	
NI2IN_LT		hP6	P 6_3/m m c		194	(La,Ni)2(In)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
NI2PR	MgCu2	cF24	F d -3 m		222	(Ni)0.6667(Pr)0.3333	
NI2Y1	Ni2Tm	cF192	F -4 3 m		216	(Ni)2(Y)1	
NI2Y3	Ni2Y3	tP80	P 4_1 2_1 2		92	(Ni)2(Y)3	
NI3IN1		hP8	P 6_3/m m c		194	(Ni)3(In)1	
NI3IN7		cI40	I m -3 m		229	(Ni)3(In)7	
NI3SI2	Ni3Si2	oS80	C m c 2_1		36	(Ni)0.6(Si)0.4	
NI3SI_L	AuCu3	cP4	P m -3 m	L12	221	(Ni)0.76(Si)0.24	
NI3SI_M	Pd25Ge9	hP34	P -3		147	(Ni)0.75(Si)0.25	
NI3SN2_H	Co1.75Ge	hP6	P 6_3/m m c		194	(Ni)0.33333(Sn,Ni)0.33334(Sn)0.33333	
NI3SN2_L	Ni3Sn2	oP20	P n m a		62	(Sn)0.2(Sn,Ni)0.4(Ni)0.4	
NI3SN4	Ni3Sn4	mS14	C 1 2/m 1		12	(Ni)0.25(Sn,Ni)0.25(Sn)0.5	
NI3SN_H	BiF3	cF16	F m -3 m	L21	225	(Ni,Sn)0.25(Ni,Sn)0.25(Ni)0.5	
NI3SN_L	Ni3Sn / Mg3Cd	hP8	P 6_3/m m c	D019	194	(Ni)0.75(Sn)0.25	
NI3ZR	Mg3Cd	hP8	P 6_3/m m c		194	(Ni)3(Zr)1	
NI4Y	*	hP*	*			(Ni)4(Y)1	
NI5PR	CaCu5	hP6	P 6/m m m		191	(Ni)0.8333(Pr)0.1667	
NI5SI2	Ni31Si12	hP43	P 3 2 1		150	(Ni)0.7143(Si)0.2857	
NI7PR2	Gd2Co7	hP54	R -3 m		166	(Ni)0.7778(Pr)0.2222	
NI7ZR2	Ni7Zr2	mS36	C 1 2/m 1		12	(Ni)7(Zr)2	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
NIIN		hP6	P 6/m m m		191	(Ni)1(In)1	
NISI	MnP / FeAs	oP8	P n m a	B31	62	(Ni)0.5(Si)0.5	
ORTHO_GA	Ga	oC8	C m c a	A11	64	(Ga)1	
PHI	*	*	P 6_3/m m c		194	(Al)0.7(Mn,Al)0.15(Fe,Mn)0.15	
PR13ZN58	Zn58Gd13	hP142	P 6_3/m m c		194	(Pr)0.1831(Zn)0.8169	
PR2Y	Sm	hP9	R -3 m		166	(Y,Pr)2(Y,Pr)1	
PR2ZN17_H	Zn17Th2	hP38	P 6_3/m m c		194	(Pr)2(Zn)17	
PR3IN4		*	*			(Pr)3(In)4	
PR6IN5		*	*			(Pr)6(In)5	
R2NI7	Ce2Ni7	hP36	P 6_3/m m c		194	(Y,Ce,Mg,La)2(Ni)7	
R3SI2	U3Si2	tP10	P 4/m b m		127	(Zr,La,Mg)3(Si)2	
R3ZN22	Zn22Ce3	tI100	I 4_1/a m d		141	(Gd,Pr,La,Nd,Ce)0.12(Zn)0.88	
R5SI4	Zr5Si4	tP36	P 4_1 2_1 2		92	(Mg,Zr,La)5(Si)4	
R7M3	Th7Fe3	hP20	P 6_3/m c		193	(La,Th,Pr,Ce)0.7(Fe,Ni)0.3	
RE3IN		cP4	P m -3 m		221	(La,Zr,Pr,Nd)3(In)1	
REH_EPS		cF12	F m -3 m		225	(Nd,La,Ce)1(Va)2(Va)1	
REMG2H7		tP40	P 4_1 2_1 2		92	(Ce,La)1(Mg)2(H)7	
RHOMBO_A7	As	hP6	R -3 m	A7	166	(Bi,Zn,Sb)1	> hR6, R -3 m, A7, based on Bi and Sb

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
RHOMB_C19		hP9	R -3 m		166	(Gd,Sm,Mg)1	
RM5	CaCu5	hP6	P 6/m m m		191	(Gd,Ce,Sr,Nd,Y,Ca,La)1(Zn,Ni,Ag,In,Cu)5	
RSI2	GdSi1.4	oI12	I m m a		74	(Y,La)1(Si)2	
RZN11	BaCd11	tI48	I 4_1/a m d		141	(Pr,La,Ca,Nd)1(Zn)11	
RZN3	Zn3Y	oP16	P n m a		62	(Gd,Pr,Y,Nd)1(Zn)3	
R_AL4MN	Mn53.3Al230.8	hP586	P 6_3/m		176	(Al)461(Mn,Fe)107	
SC3IN		hP8	P 6_3/m m c		194	(Sc)3(In)1	
SC3SI5_HT	*	o**	*	*		(Sc)0.375(Si)0.625	
SC3SI5_LT	AlB2	hP3	P 6/m m m	C32	191	(Sc)0.375(Si)0.625	
SC5SI3	Mn5Si3	hP16	P 6_3/m c m	D88	193	(Sc)0.625(Si)0.375	
SCIN2		oS12	C m c m		63	(Sc)1(In)2	
SCSI	CrB / TlI	oS8	C m c m	B33 / Bf	63	(Sc)0.5(Si)0.5	
SI2Y_H	*	hP3	P 6/m m m		191	(Si)2(Y)1	
SI2ZR	Si2Zr	oS12	C m c m		63	(Si)2(Zr)1	
SI4Y5	Gd5(Ce0.5Si0.5)4	mP36	P 1 2_1/c 1		14	(Si)4(Y)5	
SI4ZR5_H	*	*	*			(Si)4(Zr)5	
SI5Y3_H	AlB2	hP3	P 6/m m m	C32	191	(Si)5(Y)3	
SI5Y3_L	GdSi1.4	oI12	I m m a		74	(Si)5(Y)3	
SIZR3	PTi3	tP32	P 4_2/n		86	(Si)1(Zr)3	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
SRZN5_L	SrZn5	oP24	P n m a		62	(Sr)1(Zn)5	
T2_CEMGZN	*	*	*	*		(Ce)0.018182(Mg)0.527273(Zn)0.454545	
T4_CEMGZN	TbCu7	hP8	P 6/m m m		191	(Ce)1(Mg)2.5(Zn)4.5	
T5_CEMGZN	Sm3Mg13Zn30	hP92	P 6_3/m m c		194	(Ce)0.065217(Mg)0.282609(Zn)0.652174	
T6_CEMGZN	*	*	*	*		(Ce)0.0625(Mg)0.125(Zn)0.8125	
T7_CEMGZN	Ce20Mg19Zn81	cF480	F -4 3 m		216	(Ce)0.166667(Mg)0.158333(Zn)0.675	
TETRA_A6	In	tI2	I 4/m m m	A6	139	(Zn,Mg,In,Sn)1	
TET_ALPHA1_A6		tI2	I 4/m m m		139	(Sn,In)1	
TH2IN		tI12	I 4/m c m		140	(Th)2(In)1	
THETA	Co1.75Ge	hP6	P 6_3/m m c		194	(Ni)1(Ni,Va)1(Si)1	
THIN		oP24	P b c m		57	(Th)1(In)1	
THZN2	AlB2	hP3	P 6/m m m	C32	191	(Th)1(Zn)2	
THZN4	BaAl4	tI10	I 4/m m m		139	(Th)1(Zn)4	
X2IN		hP6	P 6_3/m m c		194	(Sc,Nd,Pr,Y)2(In)1	
X3NI	CFe3	oP16	P n m a	D011	62	(Pr,La,Al,Y,Ni,Gd)3(Si,Ni)1	
XR	CrB / TlI	oS8	C m c m	B33 / Bf	63	(Sn,Si,Zn,Al,Ag,Ni)1(Zr,Pr,Gd,Ca,Y,La,Ce)1	
XZ2_C16	CuAl2	tI12	I 4/m c m		140	(Ni,Al,Cu,Zn,Zr,Ag,Fe,Si)1(Al,Sn,Fe,In,Zr,Th)2	
XZ2_C37	Co2Si-b	oP12	P n m a		62	(Al,Si)1(Gd,Y,Ca,Nd,Ni,Pr)2	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
XZN13	NaZn13	cF112	F m -3 c		226	(Ca,La,Na,Sr)1(Zn)13	> CaZn13, LaZn13, NaZn13, SrZn13
Y13ZN58	Zn58.7Y12.65	hP146	P 6_3/m m c		194	(Y)13(Zn)58	
YZN2_A	*	*	*			(Y)1(Zn)2	
YZN2_B	*	*	*			(Y)1(Zn)2	
ZETA_FEZN	Zn13Co	mS28	C 1 2/m 1		12	(Fe,Va)0.072(Zn)0.856(Va,Zn)0.072	
ZN22ZR	Zn22Zr	cF184	F d -3 m		222	(Zn)0.9565(Zr)0.0435	
ZN2ZR1	Cu2Mg	cF24	F d -3 m	C15	222	(Zn)0.6667(Zr)0.3333	
ZN2ZR3	Al2Zr3	tP20	P 4_2/m n m		136	(Zn)0.4(Zr)0.6	
ZN39ZR5	Zn39Zr5	mS88	C 1 2/m 1		12	(Zn)0.8864(Zr)0.1136	
ZN3ZR_H	*	*	*			(Zn)0.75(Zr)0.25	
ZN3ZR_L	*	tI64	*			(Zn)0.75(Zr)0.25	
ZNZR2	MoSi2/CuZr2	tI6	I 4/m m m	C11b	139	(Zn)0.3333(Zr)0.6667	
ZR1IN1	*	*	*			(Zr)1(In)1	
ZR3SN_A15	Cr3Si	cP8	P m -3 n	A15	223	(Zr,Sn)3(Zr,Sn)1	
ZR5SN3	Mn5Si3	hP16	P 6_3/m c m	D88	193	(Zr)5(Sn)3(Va,Sn)1	
ZRIN2		tI24	I 4_1/a m d		141	(Zr)1(In)2	
ZRSN2	Si2Ti	oF24	F d d d	C54	70	(Zr)1(Sn)2	
Z_ALFEMN		hP227	P 6_3/m	*	176	(Al)4(Fe,Mn)1	

Name	Prototype	Pearson	Spacegroup	Strukturbericht	SG#	Sublattice	Notes
Z_MGRZN		h	P 6_3/m m c		194	(Gd,Y)0.07(Mg)0.28(Zn)0.65	

TCMG6 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:	**6.3**
First release	**TCMG1 was released in 2012**

Changes in the Most Recent Database Release

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.

Previous Releases

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.