TCMG5: TCS Mg-based Alloys Database

Database name:	TCS Mg-based Alloys Database	*Database acronym:*	TCMG
Database owner:	Thermo-Calc Software AB	*Database version:*	5.1

TCMG5 is a thermodynamic database for Mg-based alloys for use with the Thermo-Calc software package. TCMG5 can be used for a wide range of compositions from pure Mg to very complex Mg-based commercial magnesium alloys. It can be used not only 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 the 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 and Mg-RE-Zr alloys such as WE, as well as experimental magnesium alloys under development.

Included Elements (31)

The database has been developed in a 31-element framework:

Ag	Al	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									

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. In total, 195 binary systems and 91 ternary systems have been assessed. These assessed binary and ternary systems can be calculated with the BINARY module and the TERNARY module in Thermo-Calc, respectively.

TCMG5 Calculation Examples. Note that validation of such extrapolations should be always made by experiments. There are also TCMG5 Solidification Simulation Examples to demonstrate how to simulate solidification processes and how to appropriately interpret the simulated results.

In TCMG5, all the stable solution phases and intermetallic compounds that exist in each assessed system have been included. Note that in most cases phases having the same crystal structure had been merged as the same phase.

A full list of the phases and their models and constituents can be found in Phases Included in TCMG5 and Models for the Included Phases in TCMG5, respectively. For some phases with general names in the database, supplementary information is attached.

In Console Mode, you can list phases and constituents in the Database module and the GES module. For some phases, supplementary information is included in the definitions. In order to show the information, it is recommended to use “List-System” with the option of “Constituents” in the Database module.

The TCMG5 database enables predictions (such as multi-component phase equilibria calculation, equilibrium solidification simulation and Scheil solidification simulation) to be made for multicomponent systems and alloys of industrial importance. This means that TCMG5 may be utilized to extrapolate to higher-order systems by combining several critically assessed systems.

Limits

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

Database Revision History

If you are interested in the revision history for this database, the information is available in the online help (from Thermo-Calc go to **Help>Online Help**) or in the release notes on our website.

TCMG5 Assessed Binary Systems

These are the 195 assessed binary systems in the full range of composition and temperature.

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

TCMG5 Assessed Ternary Systems

These are the 91 assessed ternary systems.

Ag-Al-Cu
Ag-In-Sn
Al-Ca-Sr
Al-Cu-Si
Al-Fe-Mn
Ca-Sr-Zn
In-Sn-Zn
Mg-Ag-Cu
Mg-Ag-Gd
Mg-Ag-In
Mg-Ag-Sn
Mg-Al-Ca
Mg-Al-Ce
Mg-Al-Cu
Mg-Al-Fe
Mg-Al-Gd
Mg-Al-In
Mg-Al-Li
Mg-Al-Mn
Mg-Al-Na
Mg-Al-Nd
Mg-Al-Ni
Mg-Al-Si
Mg-Al-Sn
Mg-Al-Sr
Mg-Al-Y
Mg-Al-Zn
Mg-Al-Zr
Mg-Ca-Ce
Mg-Ca-Gd
Mg-Ca-Li
Mg-Ca-Nd
Mg-Ca-Ni
Mg-Ca-Si
Mg-Ca-Sn
Mg-Ca-Sr
Mg-Ca-Y
Mg-Ca-Zn
Mg-Ca-Zr
Mg-Ce-Gd
Mg-Ce-La
Mg-Ce-Mn
Mg-Ce-Nd
Mg-Ce-Si
Mg-Ce-Sr
Mg-Ce-Y
Mg-Ce-Zn
Mg-Ce-Zr
Mg-Cu-Fe
Mg-Cu-In
Mg-Cu-Li
Mg-Cu-Mn
Mg-Cu-Ni
Mg-Cu-Si
Mg-Cu-Y
Mg-Cu-Zn
Mg-Cu-Zr
Mg-Fe-Mn
Mg-Fe-Ni
Mg-Fe-Si
Mg-Fe-Zn
Mg-Gd-Li
Mg-Gd-Nd
Mg-Gd-Sm
Mg-Gd-Sr
Mg-Gd-Y
Mg-Gd-Zn
Mg-Gd-Zr

Mg-In-Li
Mg-In-Sn
Mg-In-Zn
Mg-La-Nd
Mg-La-Ni
Mg-La-Si
Mg-La-Y
Mg-Mn-Ni
Mg-Mn-Sc
Mg-Mn-Si
Mg-Mn-Y
Mg-Mn-Zn
Mg-Nd-Sr
Mg-Nd-Y
Mg-Nd-Zn
Mg-Ni-Zn
Mg-Pr-Y
Mg-Si-Sn
Mg-Si-Y
Mg-Si-Zn
Mg-Sn-Zn
Mg-Sr-Zn
Mg-Y-Zn

TCMG5 Assessed Quaternary Systems

These are the 5 assessed quaternary systems.

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

TCMG5 Calculation Examples

Some phase diagrams have been calculated with older versions of the TCMG database; small differences might be observed if these are recalculated with TCMG5. For the systems that have been considerably or significantly improved, the phase diagrams are recalculated with TCMG5.

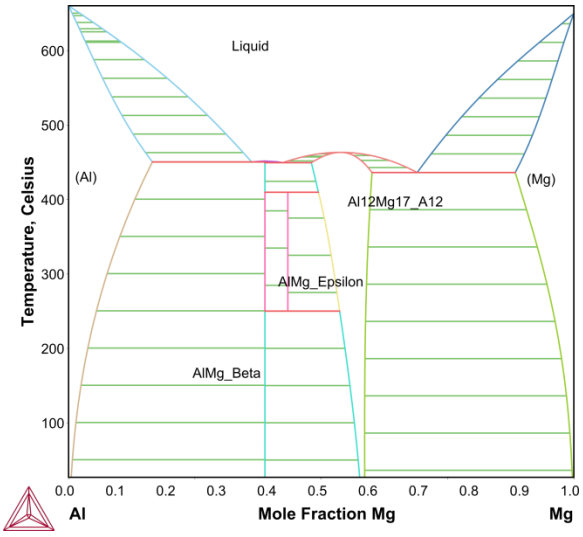

Figure 1: Calculated Al-Mg phase diagram [1998, Liang].

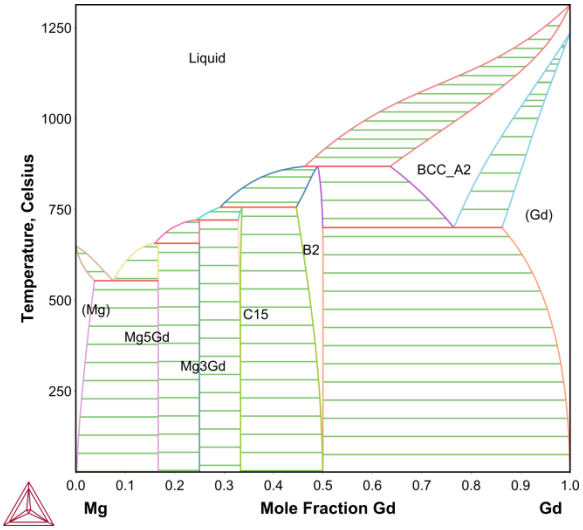

Figure 2: Calculated Gd-Mg phase diagram [2007, Guo].

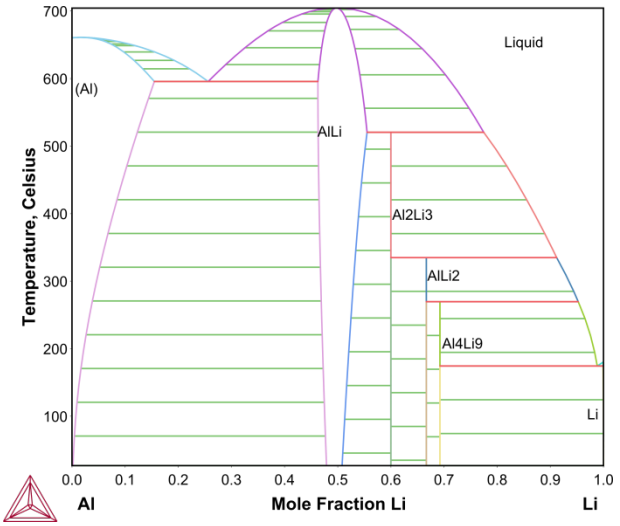

Figure 3: Calculated Al-Li phase diagram [1989, Saunders].

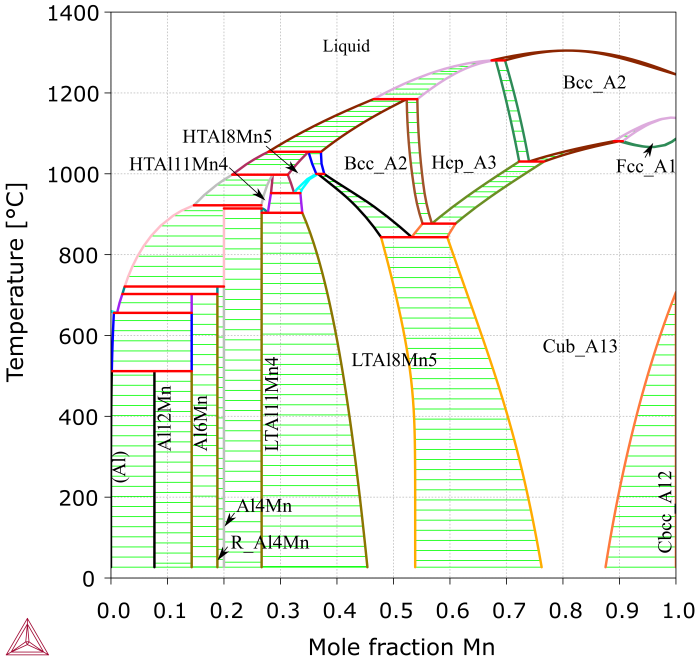

Figure 4: Calculated Al-Mn binary phase diagram [2018, Zheng].

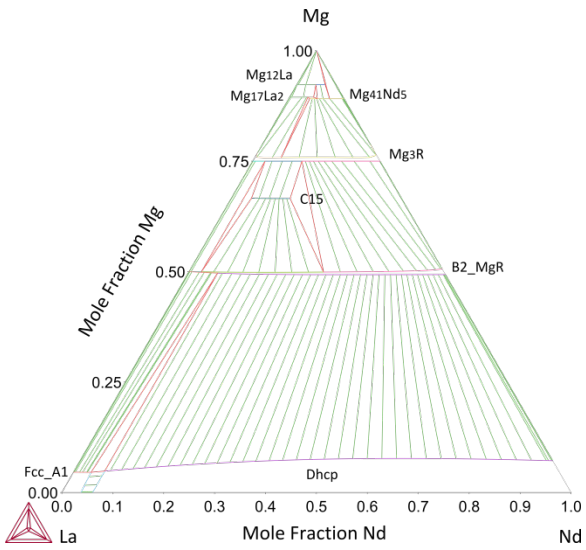

Figure 5: Calculated La-Mg-Nd isothermal section at 773 K, the assessment is based on the experimental work of Zhang [2014].

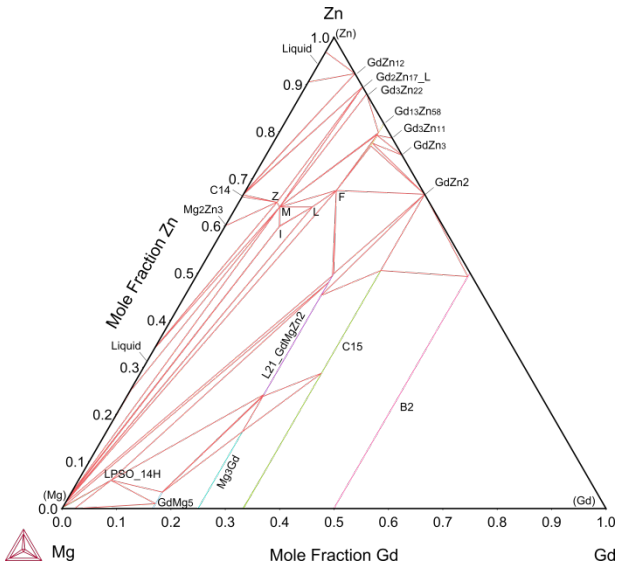

Figure 6: Calculated Mg-Gd-Zn phase equilibria at 673 K [2015a, Chen].

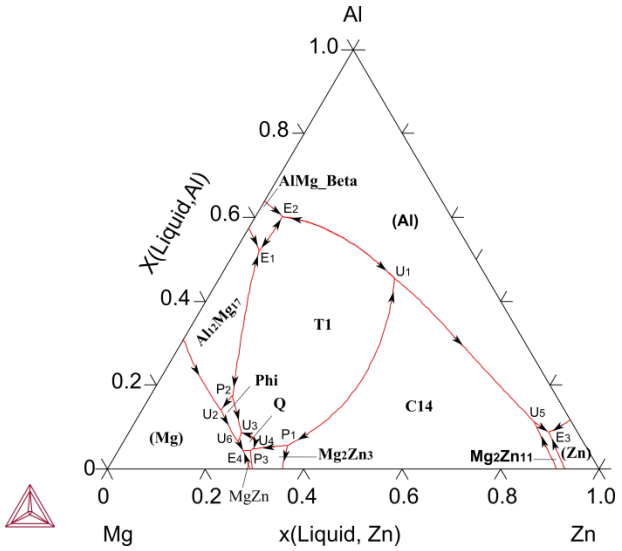

Figure 7: Calculated Al-Mg-Zn liquidus projection [1997, Liang; 2005, Petrov].

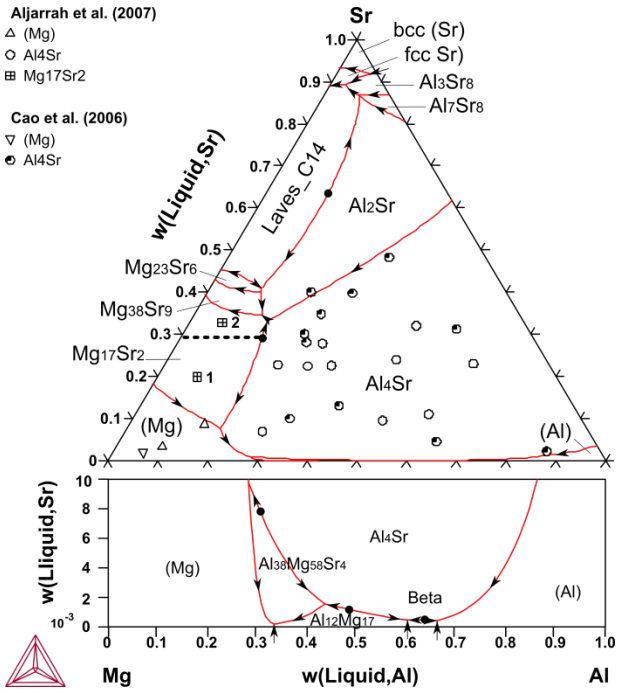

Figure 8: Calculated Al-Mg-Sr liquidus projection [2007, Janz], compared with the alloy compositions for which the primary phases were determined [2008, Cao; 2007, Aljarrah].

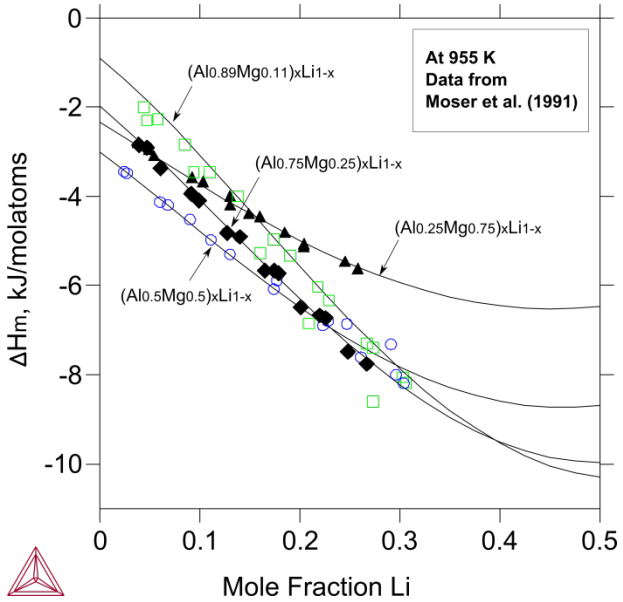

Figure 9: Calculated enthalpy of mixing of liquid at 955 K along several compositional lines in the Al-Li-Mg system [2011, Wang].

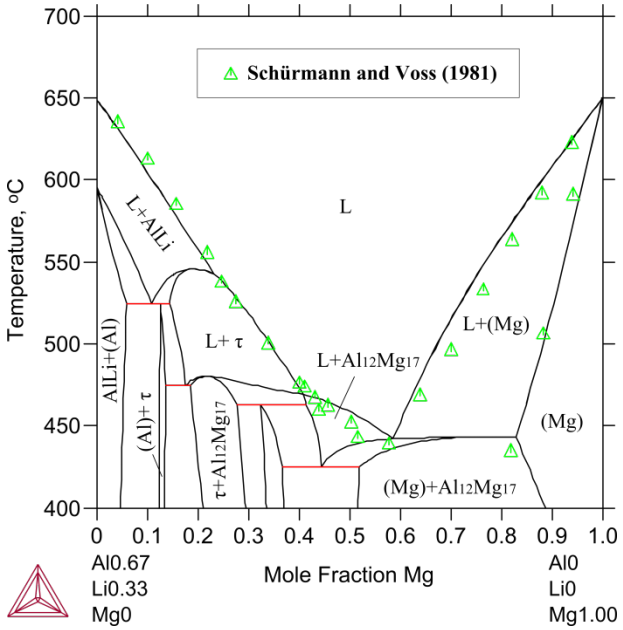

Figure 10: Calculated vertical section from Mg to $Al_{0.67}Li_{0.33}$ in the Al-Li-Mg system [2011, Wang].

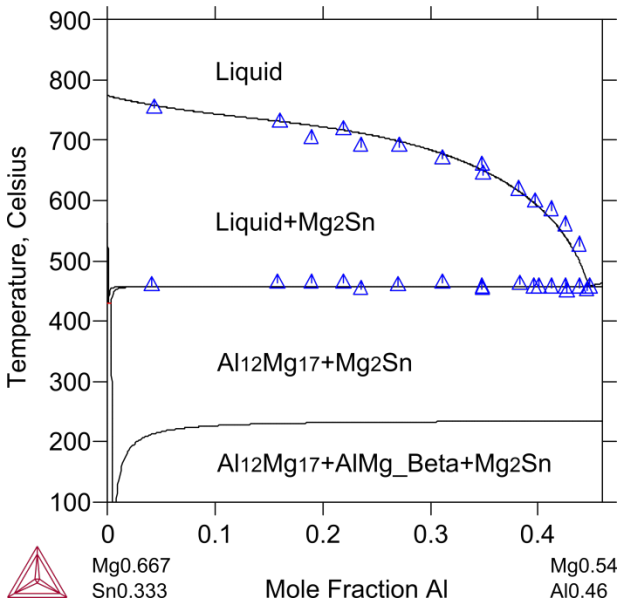

Figure 11: Calculated isothermal section from $Mg_{0.667}Sn_{0.333}$ to $Mg_{0.54}Al_{0.46}$ [2007, Doernberg].

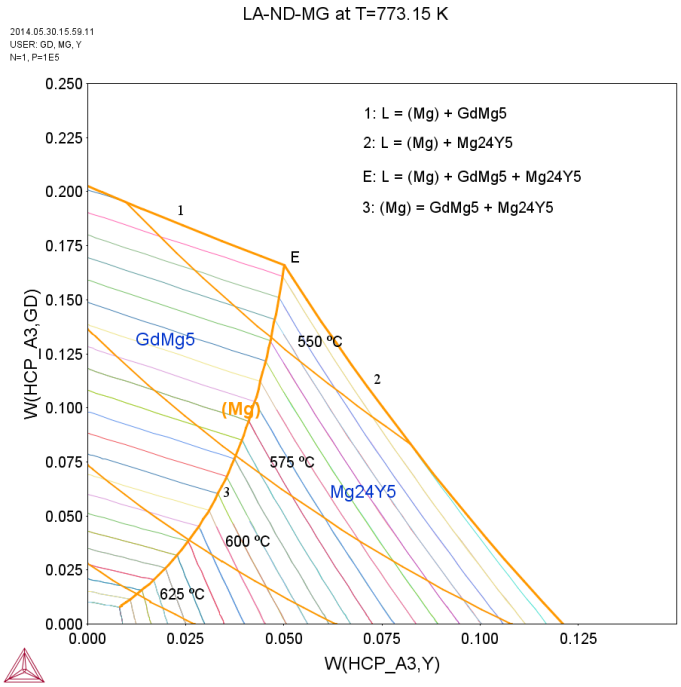

Figure 12: Calculated solidus and solvus of the (Mg) solution in the Gd-Mg-Y system [2007, Guo].

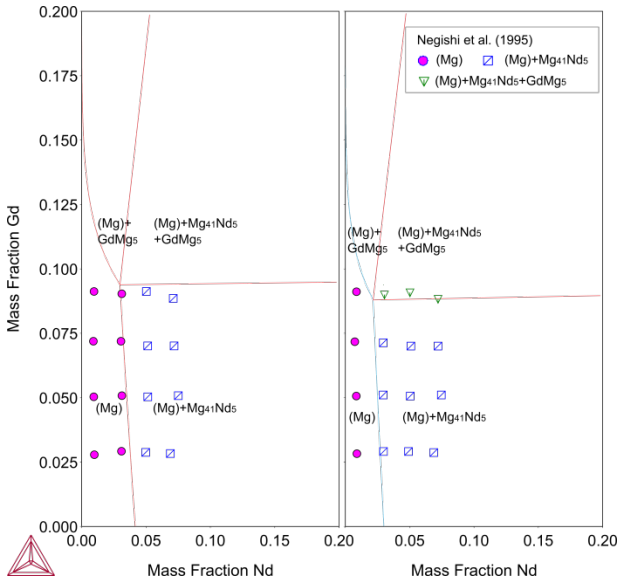

Figure 13: Calculated Mg-rich phase equilibria of the Gd-Mg-Nd system at 773 K and 808 K [2011, Qi].

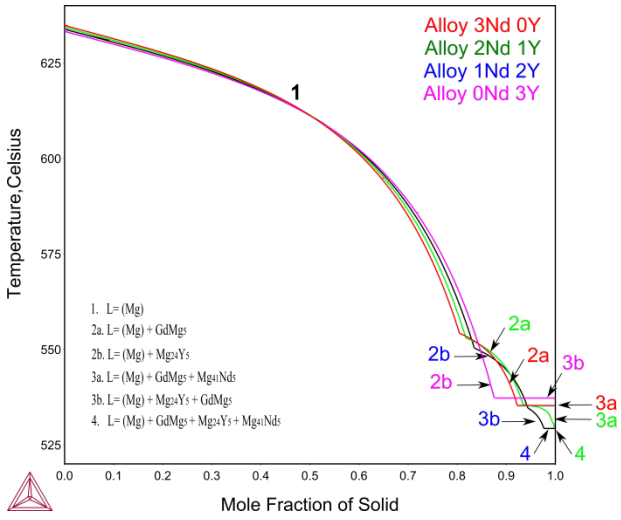

Figure 14: Scheil solidification calculations of the Mg-8Gd-0.6Zr-3(Nd, Y) alloys.

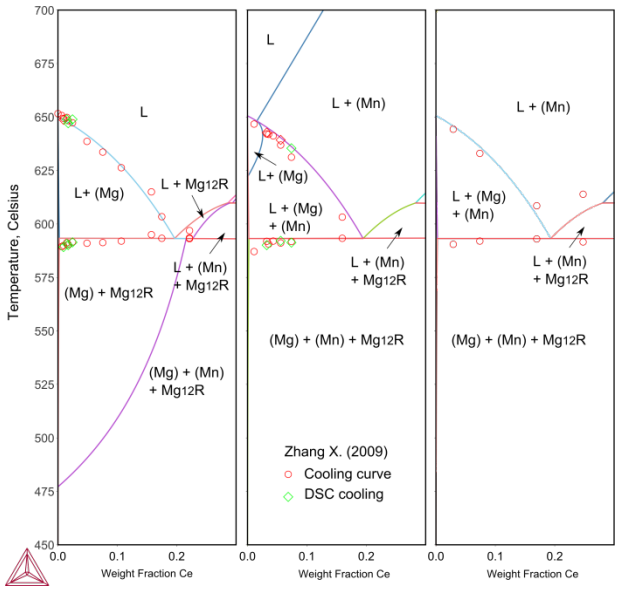

Figure 15: Calculated vertical sections in the Ce-Mg-Mn system, at 0.6 wt. % Mn, 1.8 wt. % Mn and 2.5 wt. % Mn, respectively, compared with experimental data from Zhang [2009].

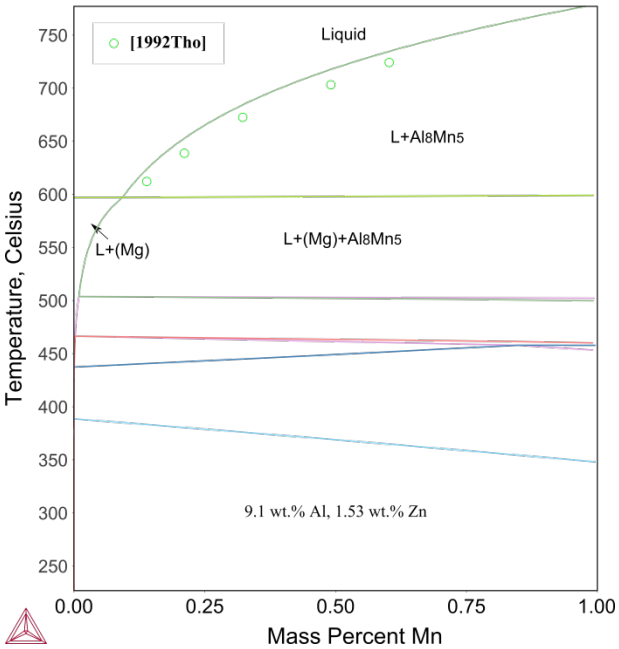

Figure 16: Calculated vertical section at 9.1 wt.% Al -1.53 wt.% Zn with Mn varying from 0 to 1 wt.% in the Mg-Al-Mn-Zn system. The experimental data are from Thorvaldsen and Aliravci [1992].

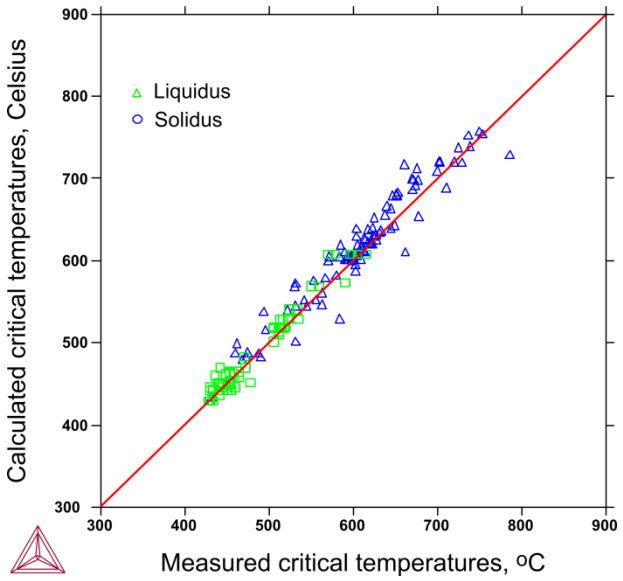

Figure 17: Comparison of calculated and measured liquidus temperatures and solidus temperatures of some ternary, quaternary, quinary and commercial Mg alloys.

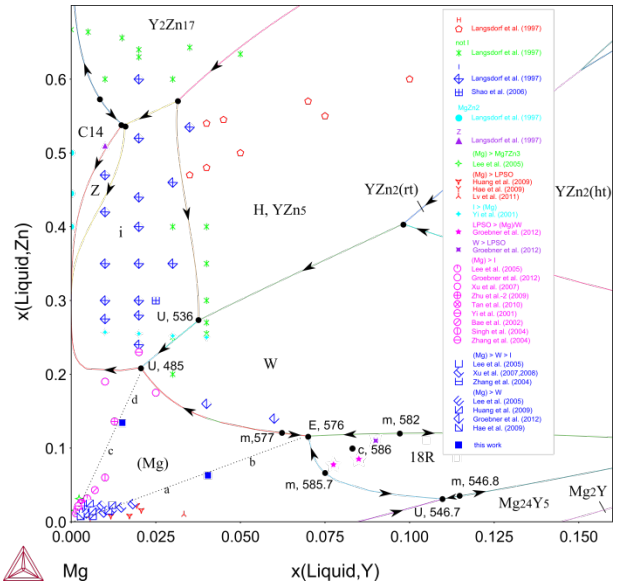

Figure 18: Calculated Mg-Y-Zn liquidus projection in the Mg-rich corner and the Mg-Zn vicinity [2015a, Chen].

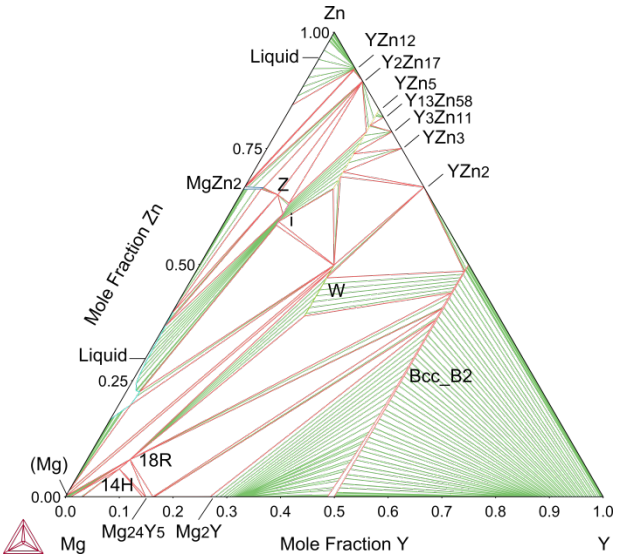

Figure 19: Calculated Mg-Y-Zn isothermal section at 773 K, showing the presence of 14H (LPSO), 18R (LPSO), W (Mg3R), I, Z and H (YZn5) [2015a, Chen].

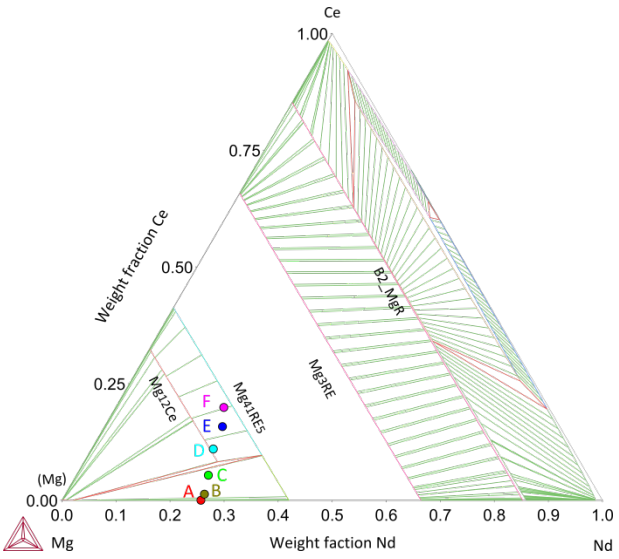

Figure 20: Calculated Ce-Mg-Nd isothermal section at 773 K. Heated alloys A, B and C: (Mg) and $Mg_{41}R_5$; D, E and F: $Mg_{41}R_5$ and $Mg_{12}R$.

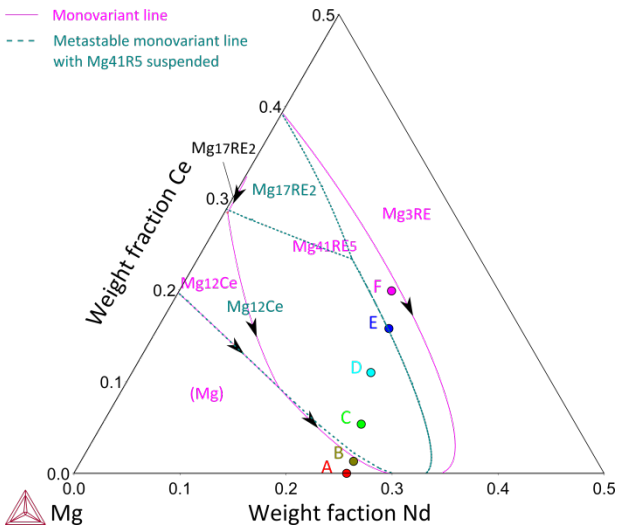

Figure 21: Calculated Ce-Mg-Nd liquidus projection. As-cast alloys A and B: (Mg) > $Mg_{12}R$; C: $Mg_{12}R$ > ?; D: $Mg_{12}R$ +(Mg) ?; E: Mg_3R > $Mg_{12}R$; F: $Mg_{41}R_5$ > $Mg_{12}R$. The phase formation in alloys C, D and E can be interpreted with the metastable calculation.

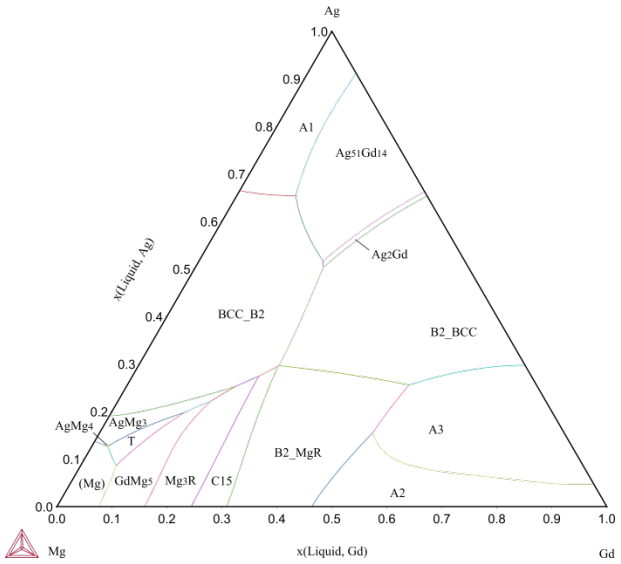

Figure 22: Calculated Ag-Gd-Mg liquidus projection [2015b, Chen].

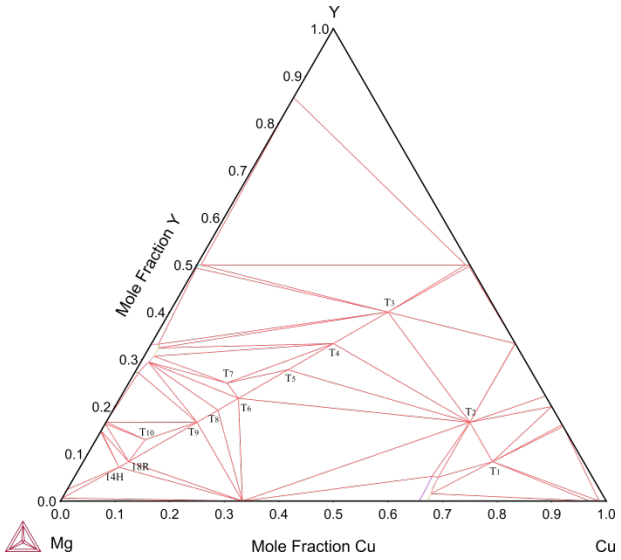

Figure 23: Calculated Cu-Mg-Y phase equilibria at 673 K [2015c, Chen].

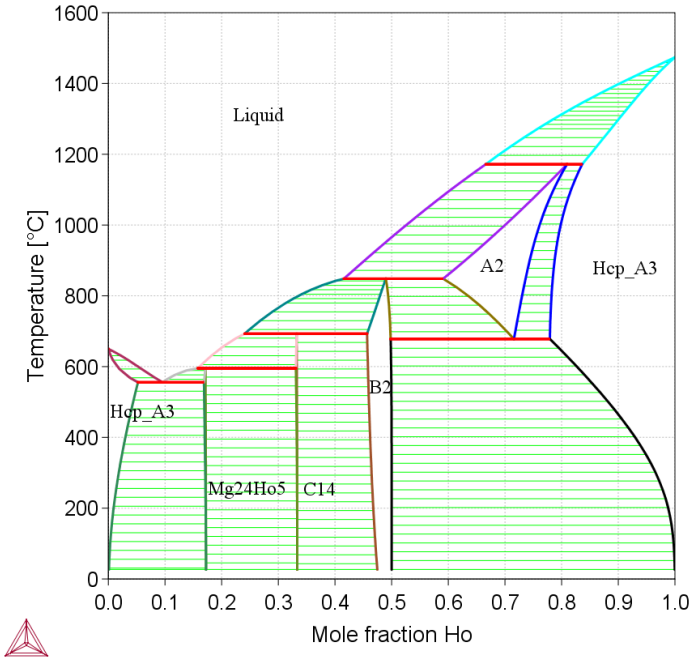

Figure 24: Calculated Ho-Mg phase diagram [2018a, Chen].

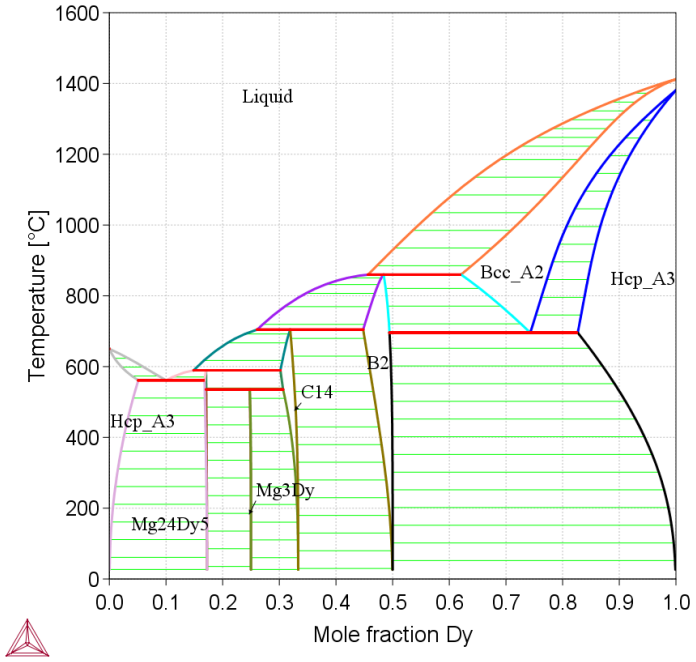

Figure 25: Calculated Dy-Mg phase diagram [2018a, Chen].

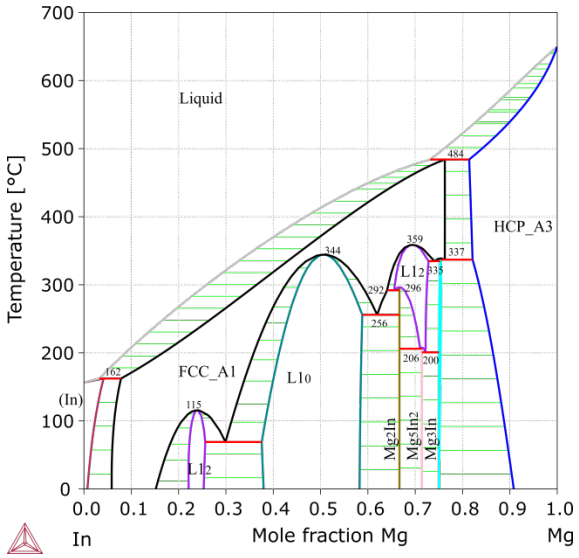

Figure 26: Calculated In-Mg phase diagram [2018a, Chen].

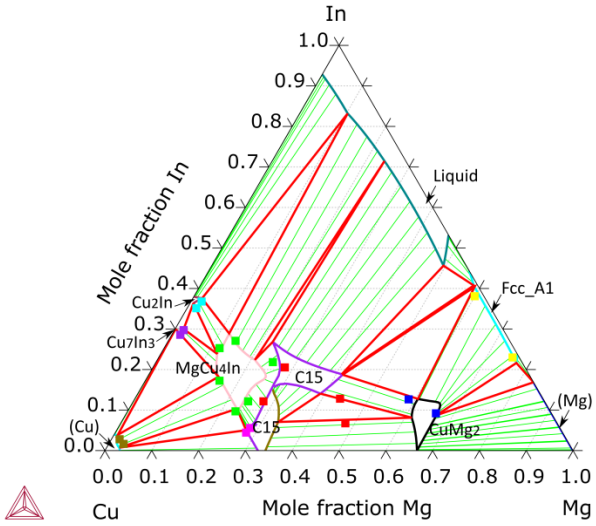

Figure 27: Calculated Cu-In-Mg phase equilibria at 673 K [2018b, Chen].

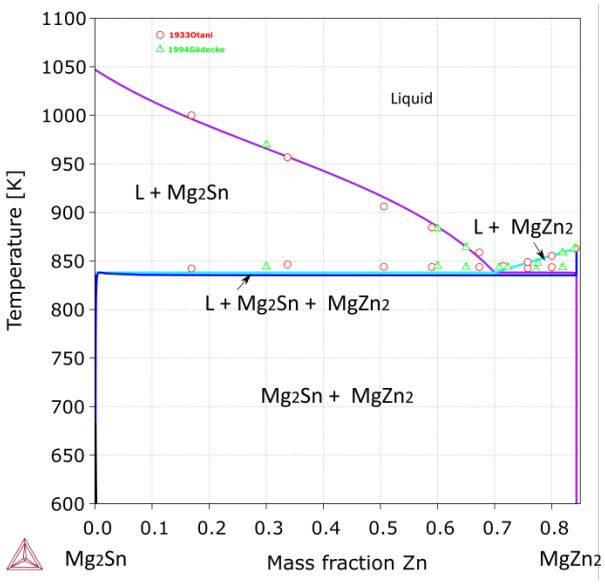

Figure 28: Calculated vertical section from Mg_2Sn to $MgZn_2$ [2010, Meng], compared with experimental data [1933, Otani].

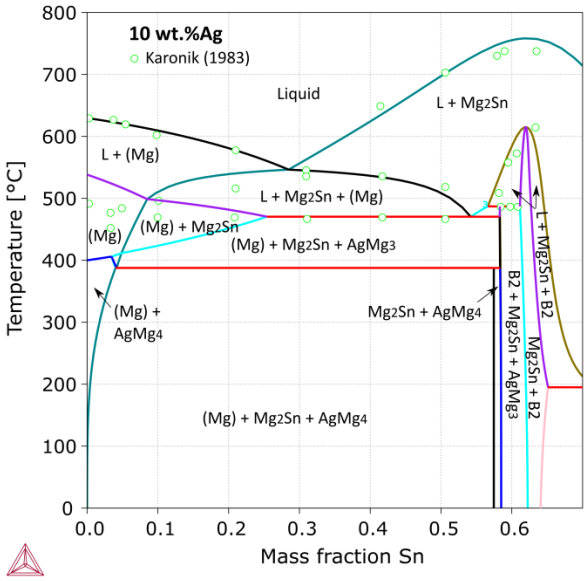

Figure 29: Calculated Ag-Mg-Sn vertical section at 10 wt.% Ag [2018c, Chen], compared with experimental data [1983, Karonik].

TCMG5 Solidification Simulation Examples

AZ91 is a series of the most important die casting Mg alloys. The typical microstructures of the solidified AZ91 alloys usually consist of (Mg) grains and mainly the $Al_{12}Mg_{17}$ phase at the grain boundaries [2009, Kabirian and 2006, Wang]. Similar microstructures are observed in other AZ series alloys [2011, Wu]. Using the TCMG5 database, you can simulate the solidification process of the AZ91 alloy with the Scheil module. It should be noted, however, that there are several aspects to pay attention to when you use the simulated results to interpret experimental observations.

It is recommended to always check the calculated phase fractions, before comparing the simulation with experimentally observed microstructures.

Figure 1 (left image) plots the total fraction of solid phases against temperature, from the solidification calculation of an AZ91 alloy (the solid line corresponds to the Scheil calculation and the dashed line to the equilibrium calculation). The calculation predicted the formation of three Al-Mn compounds, Al_8Mn_5, $Al_{11}Mn_4$ and Al_4Mn, in addition to the experimentally observed phases, hcp_A3-(Mg) and $Al_{12}Mg_{17}$. At a first glance, the prediction of phase formation is obviously different from the experimental observations. As can be seen in Figure 1 (right image), however, the amounts of the Al-Mn compounds are in negligible amounts. Of them, Al_8Mn_5 has the highest amount but less than 0.3% and the other two are less than 0.01%. They may be easily overlooked in experimental examination due to the small amounts. Especially, the Al_8Mn_5 phase forms in prior to (Al) and it would probably not appear at grain boundaries. That said, you can choose to neglect the discrepancies or plan to utilize more advanced techniques in further experimental investigations if the identification of these phases is important.

Mn is usually added as an alloying element in Mg-Al based alloys (including AZ, AM and AS series). This element is believed to be able to increase resistance against corrosion and prevent soldering in high-pressure die casting of magnesium alloys. Furthermore, Al_8Mn_5 usually forms at the beginning of the solidification of the AZ series Mg alloys and it had been reported that this phase might act as potent nucleation sites for (Mg). Although this ability of Al_8Mn_5 was doubted by the most recent work of Wang et al. [2010], this phase does precipitate in the solidified microstructures, which confirms the present simulation. It is not easy to experimentally identify the manganese aluminides in Al-Mg based alloys, especially $Al_{11}Mn_4$ [2004, Barber] and Al_4Mn [2004, Dhuka].

Not only does the Scheil simulation using TCMG5 agree with experimental observations, but also such theoretical calculations can predict the phases that have a minor or trace amount and are difficult to be identified by experiments. It is suggested to always check the phase fractions in simulated results.

Practically, during the simulation you can reject the phases that have negligible amounts.

You can feel it is distracting to include insignificant phases on diagrams. Practically, you can do a second-round simulation excluding those phases. This can be achieved using the Scheil module by first rejecting all phases and then restoring those of interest. Figure 2 presents the simulated Scheil solidification curve with

only liquid, Al_8Mn_5, hcp_A3 and $Al_{12}Mg_{17}$ included. The solidification curve is almost the same as that in Figure 1 (left) as is the phase formation of the major phases. However, with those minor phases excluded it is much easier to analyze the simulated results.

You can choose to exclude or include some of the minor alloying elements in a simulation.

Alternatively, instead of rejecting the minor phases and when doing the solidification simulation, you can exclude some of the minor alloying elements that have no significant effects on the solidification sequence. This is particularly useful when the alloy contains a large number of alloying elements and when many intermetallic phases may potentially form. In the case of the AZ91 alloy, you can consider excluding Mn in the simulation; this then gets rid of all the Mn-bearing compounds including Al_8Mn_5.

However, whether to include or exclude a minor alloying element depends on the purpose of the simulation. For example, sometimes it is important to know the impact of impurities on solidification and formation of the primary phase. Figure 3 presents a Scheil simulation of an AZ91D alloy by considering a small amount (about 0.15 wt.%) of Fe impurity. The solidification starts with the formation of B2-AlFe, followed by Al_8Mn_5. Recently it was experimentally observed by [2018, Zeng] that Al_8Mn_5 actually nucleated on the B2 phase. In this case, the impurity, Fe, as well as the minor alloying element, Mn, has to be considered in order to account for the experimental observations.

Interpretation of the thermal analysis data.

Al_8Mn_5 is the primary phase during the solidification of the AZ91 alloy. The liquidus temperature (i.e. the start of the solidification of Al_8Mn_5) is calculated to be 680 °C.

The first arrested thermal effect in some thermal analysis experiments, e.g., 600.6 °C [2014, Bakke] or 604 °C [2003, Riddle], does not correspond to the liquidus temperature, but is related to the start of the solidification of (Mg), which is 601.4 °C according to the Scheil calculation.

Since the amount of Al_8Mn_5 is low, the heat effect corresponding to the solidification of Al_8Mn_5 is too small to be readily detected. Precisely conducted thermal analysis, however, can still detect the thermal effect. Thorvaldsen and Aliravci [1992] successfully measured the Al_8Mn_5 liquidus in several AZ91 alloys with 9.1 wt. % Al, 1.53 wt. % Zn and Mn varying from 0 to 1 wt.%. It has been shown in Figure 16 (in calculation examples) that these data can be well accounted for by the phase diagram calculated using TCMG5.

It is suggested to make moderate use of Scheil solidification.

The Scheil solidification simulation can provide good approximations to real solidification processes and is widely used.

A real solidification is expected to be between a Scheil solidification simulation and an equilibrium solidification simulation.

Figure 4 shows the simulated equilibrium solidification profile and Scheil solidification profile in comparison with experimental thermal analysis [2003, Riddle]. As expected, the experimental profile is located between the two solidification simulations, while it can be better approximated with the Scheil simulation. The start temperature of the solidification of (Mg) and the eutectic temperature of L = (Mg) + $Al_{12}Mg_{17}$, together with the profile shape, are all accounted for by the Scheil simulation. However, the solid fractions from the Scheil simulation and the experiment do not agree well with each other in the region between 60% and 90%. This deviation indicates that the diffusion in the solid phases is not negligible (as assumed in the Scheil module) even though it is truly slow.

A real solidification process could much more approach to either of the two solidification simulations and deviate from the other, depending on the experimental conditions and the alloy systems. In order to account for the differences between the simulation and the experimental observation, you should consider the effect of back diffusion in a Scheil simulation.

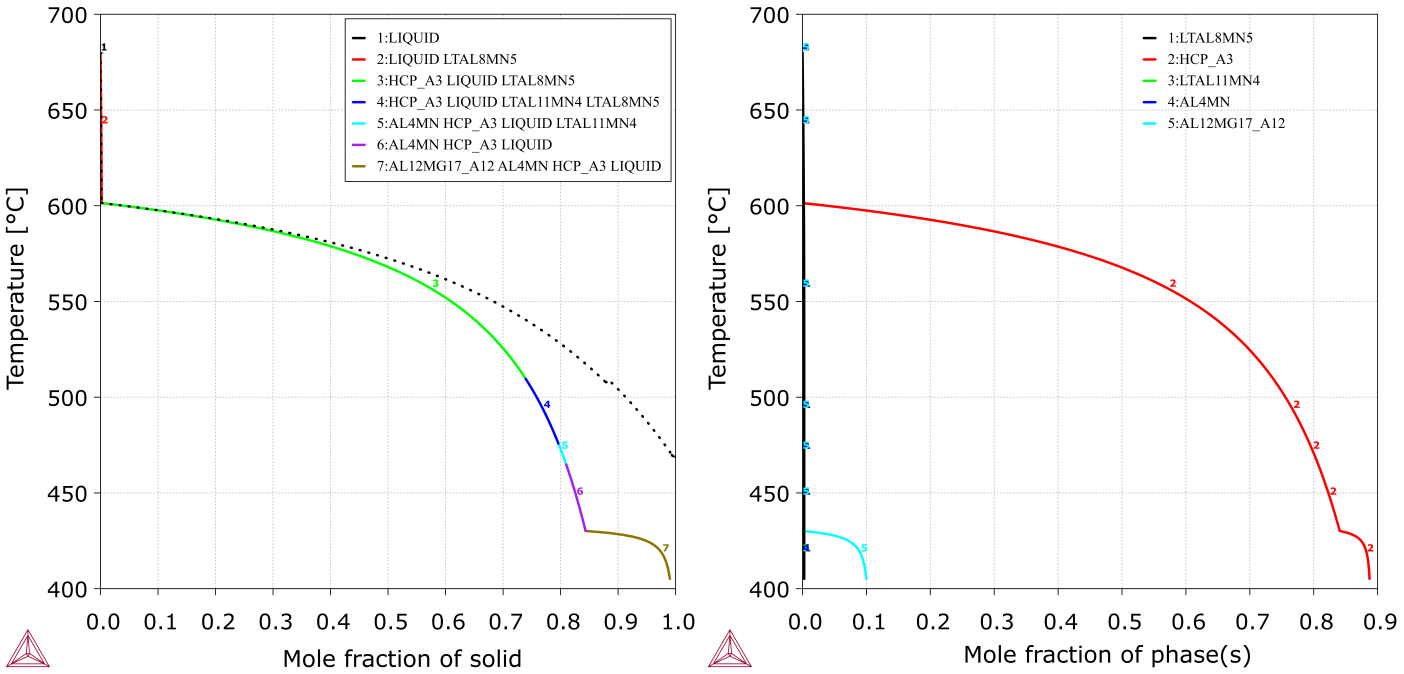

Figure 1: Scheil Solidification using TCMG5 with all the phases included. (The alloy composition used here is 8.82 wt. % Al, 0.91 wt. % Zn, 0.31 wt. % Mn, Mg balance).

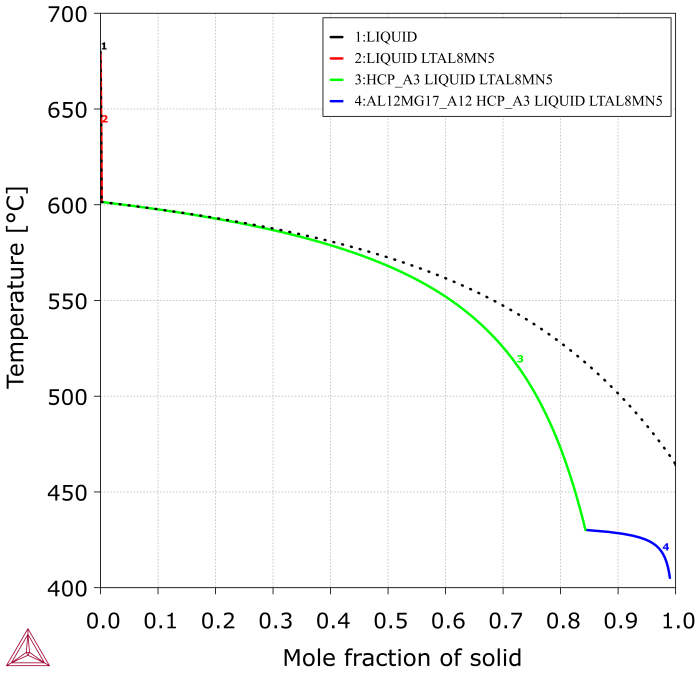

Figure 2: Scheil solidification of the AZ91 alloy with only Liquid, Al8Mn5, Hcp_A3 and Al12Mg17 included. (The alloy composition used here is 8.82 wt. % Al, 0.91 wt. % Zn, 0.31 wt. % Mn, Mg balance).

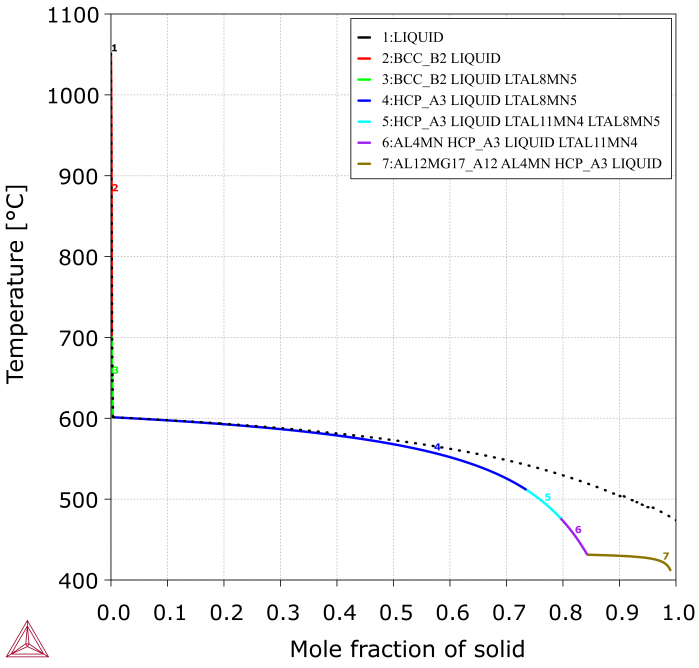

Figure 3: Scheil simulation of an AZ91D alloy (Mg-9Al-0.75Zn-0.30Mn) by considering Fe impurity of about 0.15 wt.%.

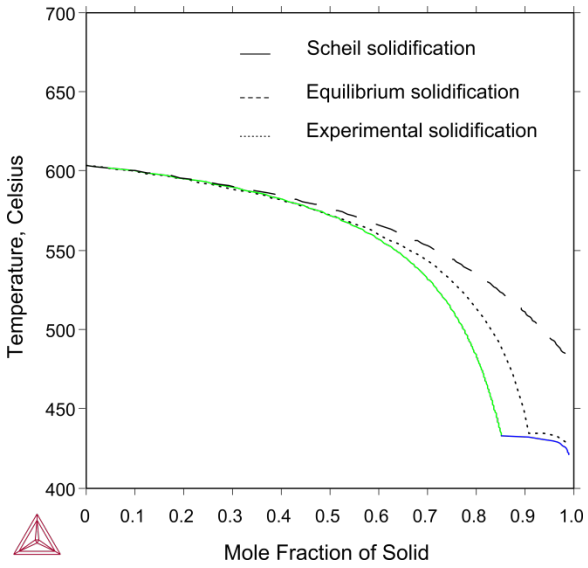

Figure 4: Comparison of the simulated equilibrium and Scheil solidification profiles with experimental thermal analysis [2003, Riddle] (The alloy composition used here is 8.7 wt. % Al, 0.5 wt. % Zn, 0.26 wt. % Mn, Mg balance).

TCMG5 References

[1989, Saunders] N. Saunders, Calculated stable and metastable phase equilibria in Al-Li-Zr alloys. Zeitschrift fur Met. 80, 894–903 (1989). Modified by H.-L. Chen in TCMG2.0 in order to implement the new compound $AlLi_2$.

[1992, Thorvaldsen] A. Thorvaldsen, C. A. Aliravci, Adv. Prod. Fabr. Light Met. Met. Matrix Comp., in Proceedings of the International Symposium, p. 277, (1992).

[1997, Liang] H. Liang, S. L. Chen, Y. A. Chang, A thermodynamic description of the Al-Mg-Zn system. Metall. Mater. Trans. A. 28, 1725–1734 (1997).

[1998, Liang] P. Liang et al., Experimental investigation and thermodynamic calculation of the central part of the Mg-Al phase diagram. Zeitschrift fur Met. 89, 536–540 (1998).

[2003, Riddle] Y. W. Riddle, M. M. Makhlouf, in Magnesium Technology 2003 (TMS (The Minerals, Metals & Materials Society), pp. 101–106 (2004).

[2004, Barber] L. P. Barber, Characterization of the solidification behavior and resultant microstructures of Magnesium-Aluminum alloys, Master's thesis, Worcester Polytechnic Institute, Worcester, MA (2004).

[2004, Dhuka] E. Dhuka, N. Lohja, H. Oettel, D. Heger, Precipitation in Mg alloy AZ61 in dependence of various heat treatments processes. Metalurgija. 10, 233–241 (2004).

[2005, Petrov] D. Petrov et al., Aluminium-Magnesium-Zinc, in Landolt-Boernstein New Series IV/11A3, pp. 191–209, (2005).

[2006, Wang] Y. Wang, G. Liu, Z. Fan, Microstructural evolution of rheo-diecast AZ91D magnesium alloy during heat treatment. Acta Mater. 54, 689–699 (2006).

[2007, Aljarrah] M. Aljarrah, M. A. Parvez, J. Li, E. Essadiqi, M. Medraj, Microstructural characterization of Mg–Al–Sr alloys. Sci. Technol. Adv. Mater. 8, 237–248 (2007).

[2007, Doernberg] E. Doernberg, A. Kozlov, R. Schmid-Fetzer, Experimental Investigation and Thermodynamic Calculation of Mg-Al-Sn Phase Equilibria and Solidification Microstructures. J. Phase Equilibria Diffus. 28, 523–535 (2007).

[2007, Guo] C. Guo, Z. Du, C. Li, A thermodynamic description of the Gd–Mg–Y system. Calphad. 31, 75–88 (2007).

[2007, Janz] A. Janz et al., Experimental study and thermodynamic calculation of Al–Mg–Sr phase equilibria. Intermetallics. 15, 506–519 (2007).

[2008, Cao] H. Cao et al., Experiments coupled with modeling to establish the Mg-rich phase equilibria of Mg–Al–Ca. Acta Mater. 56, 5245–5254 (2008).

[2009, Kabirian] F. Kabirian, R. Mahmudi, Effects of Zirconium Additions on the Microstructure of As-Cast and Aged AZ91 Magnesium Alloy. Adv. Eng. Mater. 11, 189–193 (2009).

[2009, Zhang] X. Zhang, D. Kevorkov, I.-H. Jung, M. O. Pekguleryuz, Phase equilibria on the ternary Mg–Mn–Ce system at the Mg-rich corner. J. Alloys Compd. 482, 420–428 (2009).

[2010, Wang] Y. Wang, M. Xia, Z. Fan, X. Zhou, G. E. Thompson, The effect of Al8Mn5 intermetallic particles on grain size of as-cast Mg–Al–Zn AZ91D alloy. Intermetallics. 18, 1683–1689 (2010).

[2011, Qi] H.Y. Qi, Thermodynamic assessment of the Gd-Mg-Nd system, unpublished work (with modifications).

[2011, Wang] P. Wang, Y. Du, S. Liu, Thermodynamic optimization of the Li–Mg and Al–Li–Mg systems. Calphad. 35, 523–532 (2011).

[2011, Wu] L. Wu, F. Pan, M. Yang, J. Wu, T. Liu, As-cast microstructure and Sr-containing phases of AZ31 magnesium alloys with high Sr contents. Trans. Nonferrous Met. Soc. China. 21, 784–789 (2011).

[2014, Bakke] D. P. Bakke, D. H. Westengen, in Essential Readings in Magnesium Technology (John Wiley & Sons, Inc., Hoboken, NJ, USA; pp. 313–318, (2014).

[2014, Zhang] F. Zhang, H. Xu, Y. Du, R. Schmid-Fetzer, T. Zhou, Phase equilibria of the Mg–La–Nd system at 500°C. J. Alloys Compd. 585, 384–392 (2014).

[2015a, Chen] H. Chen, “Thermodynamic assessment of the Gd-Mg-Zn and Mg-Y-Zn systems”, unpublished, (2015).

[2015b, Chen] H.-L. Chen, Thermodynamic assessment of the Ag-Gd-Mg system, unpublished work, (2015).

[2015c, Chen] H.-L. Chen, Thermodynamic assessment of the Cu-Mg-Y system, unpublished work, (2015).

[2018, Zheng] W. Zheng, H. Mao, X. Lu, Y. He, L. Li, M. Selleby, J. Ågren, Thermodynamic investigation of the Al-Fe-Mn system over the whole composition and wide temperature ranges, J ALLOY COMPD, 742, 1046-1057 (2018).

[2018, Zeng] G. Zeng, J. W. Xian, C. M. Gourlay, Nucleation and growth crystallography of Al8Mn5 on B2-Al (Mn,Fe) in AZ91 magnesium alloys, ACTA MATER, 153, 364-376 (2018).

Scientific Bibliography

See the Thermo-Calc Software scientific bibliography at: https://www.thermocalc.com/support/resources/.

Phases Included in TCMG5

LIQUID
BCC_A2
BCC_B2
B2_BCC
B2_MGR
BCT_A5
CBCC_A12
CUB_A13
DHCP
DIAMOND_A4
FCC_A1
L12_FCC
HCP_A3
FE2SI
FESI2_H
FESI2_L
C14_LAVES
C15_LAVES
C36_LAVES
MG2SI
MSI_B20

M5SI3_D88
AG51R14
MG41R5
XZN13
MG3R
L21_RMGZN2
ALR_OS16
CA5X3
RM5
CU6R
XZ2_C16
X3NI
MR_B27
M2R
M3R
MG17SR2
M23R6
XR
R3ZN22
RZN11
M5R
XZ2_C37
ALR_OP16
AL11R3

R7M3
MG12R
RSI2
RZN3
AL2R3
R5SI4
M10ZR7
R3SI2
R2NI7
AG9CA2
AG7CA2
AGCA3
AG4CE
AG2GD
AG51GD14
AG2IN_D83
AG5LA
AGMG4
AGMG3
AG51ND14
AG2ND_H
AG2PR
AG5PR
AG4SC

CU2SC_C11B
AGSC
AG3SN1
AG4SR
AGSR
AG2SR3
AGY
AG2Y
AG51Y4
AGZN
AGZN3
AG5ZN8
AGZR
AGZR2
AL4CA
AL14CA13
AL3CA8
AL4CE
AL3CE_H
AL3CE_L
ALCE2
ALRE3
ALCE3_L
ALCU_DEL

ALCU_EPS
ALCU_ETA
ALCU_PRIME
ALCU_ZETA
GAMMA_D83
GAMMA_H
AL13FE4
AL2FE
AL5FE2
D3_ALFE
Z_ALFEMN
PHI
AL2GD3
AL3GD
ALLA3
AL53LA22
AL3LA
AL11LA3_H
AL2LI3
ALLI2
AL4LI9
ALLI
ALMG_BETA
ALMG_EPSILON

AL12MG17_A12
LTAL11MN4
AL12MN
AL6MN
AL4MN
R_AL4MN HTAL8MN5 LTAL8MN5
AL8MN5_D810
HTAL11MN4
AL11ND3_H
AL3ND
ALND3
AL3NI2
AL3NI5
AL11PR3_H
AL3PR
ALPR3_L
AL3SC
AL2SC
ALSC
ALSC2
AL4SR
AL7SR8

AL3SR8
AL3Y_L
AL3Y_H
ALZR2
AL3ZR5
AL3ZR4
AL4ZR5
AL3ZR2
AL3ZR1
CACU5
CACU
CA2CU
CA8IN3
CA1IN2
CANI2
CA2NI7
CA3SI4
CA14SI19
CASI2
CA2SN_X
CA36SN23
CA31SN20
CA7SN6
CA3ZN

CAZN3
CU6CE
CU5CE
CU4CE
CU2CE
CE2IN
CE5IN4
CE9IN11
CE3IN5
CEGD3
CENI3
CENI2
CEZN2
CEZN3
CE3ZN11
CE13ZN58
CEZN5
CE2ZN17
CEZN11
CU9GD2
CU7GD2
CU9IN4_D83
CU7IN3
CU2IN_B82

CU2IN_LT
CU11IN9
CU37LA3
CU6LA_L
CU4LA
CU2LA
CUMG2
CU4ND
CU7ND2
CUND_H
CU6PR
CU5PR
CU4PR
CU2PR
CU4SC
CUSC
CU15SI4_EPSILON
CU56SI11_GAMMA
CUSI_ETA
CU33SI7_DELTA
CU3SN_H_GAMMA
CU10SN3
CU3SN_L
CU41SN11

ETA
CU6SN5
CUSR
CUTH2
CU2TH
CU6TH
CU51TH14
CU7Y1
CU4Y
CU7Y2
CU2Y_H
EPSILON
CUZN_GAMMA
CU51ZR14
CU8ZR3
CUZR2
MNI3_L12
FE17ND2
FE17ND5
FE17PR2
FE2SC_C14
FE2SC_C36
FE2SC_C15
FE6SC29

FE5SN3
FE3SN2
FESN
FE17TH2
FE5TH
FE7TH2_L
FE7TH2_H
FE17Y2
FE23Y6
GAMMA_FEZN
GAMMA1_FEZN
DELTA_FEZN
ZETA_FEZN
FEZR3
ORTHO_GA
MG5GA2
MG2GA
MGGA
MGGA2
MG2GA5
GD2IN
GD5IN3
GDIN
GD3IN5

GDIN3
GDMG5
GDND
GD3NI2
GD2NI7
GDNI4
GD5SI4
GD3SI5
GDSI2
GDZN2
GD3ZN11
GD13ZN58
GD2ZN17_L
GD2ZN17_H
GDZN12
KIN4
K17IN41
K39IN80
B2REIN
IN5RE3
IN3LA2
LIIN
LI5IN4
LI3IN2

LI2IN
LI13IN3
LI3IN
LI7IN
TETRA_A6
MG2IN
MG3IN
MN3IN
NI2IN_HT
NI13IN9
B2NIIN
NI3IN
NI2IN_LT
NIIN
NI2IN3
NI3IN7
NA6IN11
NA7IN12
NAIN
NA2IN
SCIN2
B2_SCIN
X2IN
SC3IN

PR3IN4
PR6IN5
INSN_AF
TET_ALPHA1_A6
IN3SR
IN5SR2
IN2SR
IN3SR2
INSR
IN3SR5
INSR3
THIN
TH2IN
ZRIN2
ZRIN
RE3IN
LANI5
LA2NI7_H
LA7NI16
LA2NI3
LASI2_A1
LA5SN3_L
LA5SN4
LA11SN10

LA2SN3
LA3SN5
LAY
LI22SI5
LI13SI4
LI7SI3
LI12SI7
LI13SN5
LI22SN5
LI2SN5
LI5SN2
LI7SN3
LI8SN3
LISN
LI7SN2
LI2ZN3_L
LI2ZN3_H
LI2ZN5_L
LI2ZN5_H
LIZN4_L
LIZN4_H
LIZN2
BCC_B32
MG2NI

MG5PR
RHOMBO_A7
MG3SB2_LT
MG3SB2_HT
MGSC
RHOMB_C19
MG38SR9
MG24R5
MG2ZN3
MGZN
MG51ZN20
MG2ZN11
MN17ND2
L10_TETRA
MNNI2
MN11SI19
MN3SI
MN6SI
MN9SI2
MN23SC6
MNSC4
MN19SN6
MN2SN
MNSN2

MN23Y6
MNZN9
ND2Y
NDZN2
ND3ZN11
ND13ZN58
ND2ZN17
NDZN11_H
NI5PR
NI7PR2
NI2PR
NI3SI_M
NI3SI_L
NI5SI2
THETA
NI3SI2
NISI
NI3SN_H
NI3SN_L
NI3SN2_H
NI3SN2_L
NI3SN4
NI17Y2
NI4Y

NI2Y1
NI2Y3
BETA_NIZN
GAMMA_NIZN
DELTA_NIZN
NI7ZR2
NI3ZR
NI21ZR8
NI11ZR9
PR2Y
PR13ZN58
PR2ZN17_H
SC5SI3
SCSI
SC3SI5_LT
SC3SI5_HT
SI2Y_H
SI4Y5
SI5Y3_H
SI5Y3_L
SI4ZR5_H
SI2ZR
SIZR3
ZR3SN_A15

ZR5SN3
ZRSN2
SRZN5_L
THZN2
THZN4
H_RZN5
Y13ZN58
YZN2_A
YZN2_B
ZN22ZR
ZN39ZR5
ZN3ZR_L
ZN3ZR_H
ZN2ZR1
ZN2ZR3
ZNZR2
AGGDMG_T
AL9CA31ZN10
AL2CAZN2
AL13CEMG6
ALCUMG_Q
ALCUMG_S
ALCUMG_T
ALCUMG_V

AL16FEMN3
AL13FE2MN2
AL10FEMN2
ALLIMG_T
ALMGMN_T
ALMGND_T
ALMG3NI2
AL38MG58SR4
AL4MGY
ALMGZN_PHI
ALMGZN_T1
ALMGZN_Q
ALMGZN_T2
CAMGSI_T1
CA7MG6SI14
CAMGSN_T1
CA2MG6ZN3
MG5CEY
T2_CEMGZN
T4_CEMGZN
T5_CEMGZN
T6_CEMGZN
T7_CEMGZN
MGCU4IN

CULIMG_T
CU16MG6SI7
CU3MG2SI
CUMGY_T1
CUMGY_T2
CUMGY_T3
CUMGY_T4
CUMGY_T5
CUMGY_T6
CUMGY_T7
CUMGY_T8
CUMGY_T9
CUMGY_T10
CUMGY_14H
CUMGY_18R
F_MGGDZN
Z_MGRZN
M_MGRZN
L_MGRZN
LI2MGIN
LAMGNI_T1
LAMGNI_T2
LAMGNI_T3
LAMGNI_T4

LAMGNI_T5
LAMGNI_T6
LAMGSI_T1
LAMGSI_T2
LAMGSI_T3
LAMGSI_T4
LAMGSI_T5
MG6MN3NI
MGNDZN_T1
MGNDZN_T2
MGNDZN_T3
MGNDZN_T4
LPSO_14H
LPSO_18R
I_MGRZN
AL3CU2MG9SI7

Models for the Included Phases in TCMG5

LIQUID :AG AL CA CA2SN CE CU DY ER FE GA GD HO IN K LA LASN LI MG MG3SB2 MG2SN MN NA ND NI PR SB SC SI SM SN SR TH Y ZN ZR ZZ:
BCC_A2 2 SUBL, SITES 1.00: 3.00: :AG AL 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:VA:
BCC_B2 3 SUBL, SITES 0.50: 0.50: 3.00: :AG AL 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:AG AL 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:VA:
B2_BCC 2 SUBL, SITES 0.50: 0.50: :AG CU NI ZN:CE GD ND Y PR ZR: > B2 phases modeled separately from A2
B2_MGR 2 SUBL, SITES 0.50: 0.50: :AG AL CU IN MG MN ND SN ZN:AG CA CE CU DY ER GD HO IN LA MG ND PR SM SN Y: > LaMg, MgNd, NdZn, CeMg, CeZn, MgY, YZn, GdMg, GdZn, MgSm, AgMg
BCT_A5 :AG AL IN SN ZN:
CBCC_A12 2 SUBL, SITES 1.00: 1.00: :AL CU FE IN MG MN NI SI SN ZN ZR:VA:
CUB_A13 2 SUBL, SITES 1.00: 1.00: :AG AL CA CE CU FE IN MG MN NI SI SN ZN ZR:VA:
DHCP

:AG AL CA CE CU GD IN LA MG MN ND NI PR SR Y:
DIAMOND_A4 :AL SI SN ZN:
FCC_A1 2 SUBL, SITES 1.00: 1.00: :AG AL CA CE CU FE GD IN K LA LI MG MN NA ND NI PR SC SI SN SR TH Y ZN ZR:VA:
L12_FCC 2 SUBL, SITES 1.00: 3.00: :AL CA CE IN LA MG ND PR SC TH Y:AG IN MG NI SN ZR: > L12 phases, CaSn3, LaSn3, Mg1.2In2.8, CeIn3, NdIn3, ScIn3, PrIn3, ThIn3
HCP_A3 2 SUBL, SITES 1.00: 0.50: :AG AL CA CE CU DY ER FE GA GD HO IN K LA LI MG MN NA ND NI PR SC SI SM SN SR TH Y ZN ZR:VA:
FE2SI 2 SUBL, SITES 2.00: 1.00: :FE NI:AL SI:
FESI2_H 2 SUBL, SITES 3.00: 7.00: :FE NI:MG SI:
FESI2_L 2 SUBL, SITES 1.00: 2.00: :FE NI:AL SI:
C14_LAVES 2 SUBL, SITES 2.00: 1.00: :AL CA CU GD LI MG MN NA NI SR Y ZN:AL CA CE CU DY ER GD HO K LA MG MN ND PR SC SR TH Y ZR ZN VA: > Al2Zr, CaLi2, CaMg2, Mg2Sr, Mg2Y, MgZn2, Mn2Zr, Na2K
C15_LAVES 2 SUBL, SITES 2.00: 1.00: :AL CA CU FE GD IN LA LI MG MN ND NI SI Y ZN ZR:AL CA CE CU FE GD IN LA LI MG ND NI PR SR SI SM TH Y ZN ZR:

> It includes 18 compounds, e.g. Al2Ca, Al2Ce, Cu2Mg, Fe2Gd, Mg2Gd
C36_LAVES 2 SUBL, SITES 2.00: 1.00: :AL CU FE GD MG MN NI ZN:AL CA CU GD MG NI TH ZN: > MgNi2 type phase, also includes MgNi2, (Cu,Zn)2Mg, (Al,Mg)2Ca
MG2SI 2 SUBL, SITES 2.00: 1.00: :MG SI:AL NI SI SN: > This is also Si2Ni & Mg2Sn
MSI_B20 2 SUBL, SITES 1.00: 1.00: :FE MN:MG SI: > FeSi & MnSi
M5SI3_D88 2 SUBL, SITES 5.00: 3.00: :FE GD LA MN Y ZR:IN SI SN: > Fe5Si3, Gd5Si3, Mn5Si3, Y5Si3, Zr5Si3, also LA5SN3(HT)
AG51R14 2 SUBL, SITES 51.00: 14.00: :AG:CE LA PR: > AG51PR14, AG51CE14, AG51LA14
MG41R5 2 SUBL, SITES 41.00: 5.00: :MG ZN:CA CE GD LA ND PR SM SR Y: > Mg41La5, Mg41Ce5, Mg41Nd5, Mg41Pr5, Mg41Sm5
XZN13 2 SUBL, SITES 1.00: 13.00: :CA NA SR:ZN: > CaZn13, NaZn13, SrZn13
MG3R 2 SUBL, SITES 3.00: 1.00: :LI MG ZN:CA CE DY ER GD LA MG ND PR SM SR Y: > MG3CE, GDMG3, MG3ND, MG3PR, MG3LA, Mg3Sm

L21_RMGZN2 3 SUBL, SITES 1.00: 1.00: 2.00: :CE GD Y:MG:MG ZN: > L21, isostructural to GdMg3: CeMgZn2, GdMgZn2, MgZn2Y, aka W
ALR_OS16 2 SUBL, SITES 1.00: 1.00: :AL:CE GD LA PR: > a phase based on ALCE, ALGD, ALLA, ALPR(rt)
CA5X3 2 SUBL, SITES 5.00: 3.00: :CA LA:AG SI SN ZN: > CA5SI3, CA5SN3, CA5AG3, CA5ZN3, also La5Si3
RM5 2 SUBL, SITES 1.00: 5.00: :CA CE GD LA ND SR Y:AG CU IN NI ZN: > Ag5Sr, Cu5La, SRZN5, GdNi5, Ni5Y, CaZn5, Cu5Nd, Cu5Sr, CeNi5, CaNi5, Cu5Gd
CU6R 2 SUBL, SITES 6.00: 1.00: :CU:CE ND GD LA: > Cu6Nd, Cu6Gd & Cu6La (HT)
XZ2_C16 2 SUBL, SITES 1.00: 2.00: :AG AL CU FE NI SI ZN ZR:AL FE IN SN TH ZR: > FeSn2, FeZr2, CuAl2, NiZr2, SiZr2, ZnTh2, AgIn2
X3NI 2 SUBL, SITES 3.00: 1.00: :AL GD LA NI PR Y:NI SI: > Gd3Ni, La3Ni, Pr3Ni, Y3Ni, also Al3Ni & NI3SI(ht)
MR_B27 2 SUBL, SITES 1.00: 1.00: :CU NI SI ZN:CE GD LA ND PR SR Y ZR: > CuCe, CuLa, CuNd(rt), NiY, ZnSr, SiLa, CuPr, SiGd & SiZr(rt)
M2R 2 SUBL, SITES 2.00: 1.00:

:AG AL CU MG ZN:CA CE GD LA ND PR SR Y: > This is also Ag2Ca, Ag2Sr, Al2Sr, CaZn2, SrZn2, etc.
M3R 2 SUBL, SITES 3.00: 1.00: :FE NI:CA GD LA MG PR Y TH: > Ni3Pr, Fe3Gd, Fe3Y, NI3Gd, NI3La, Ni3Y, NI3Ca, Fe3Th
MG17SR2 2 SUBL, SITES 2.00: 17.00: :CE GD LA ND PR SR TH Y:AL FE MG NI ZN: > also Ce2Mg17, La2Mg17, Ce2Fe17, Pr2Zn17, Y2Zn17, Gd2Fe17, Gd2Ni17, Th2Zn17
M23R6 2 SUBL, SITES 23.00: 6.00: :AL FE MG MN:CE GD ND PR SR TH Y ZR: > Fe23Gd6, Mn23Gd6, Mn23Nd6, Mn23Pr6, also Fe23Zr6, Mg23Sr6, Mg23Th6
XR 2 SUBL, SITES 1.00: 1.00: :AG AL NI SI SN ZN:CA CE GD LA PR Y ZR: > This is also NiZr, AgCa, SiCa, SnCa, SiZr_H, ZnCa
R3ZN22 2 SUBL, SITES 0.12: 0.88: :CE GD ND PR:ZN: > Ce3Zn22, Gd3Zn22, Nd3Zn22, Pr3Zn22
RZN11 2 SUBL, SITES 1.00: 11.00: :CA ND PR:ZN: > This is CaZn11, NdZn11_L, PrZn11
M5R 2 SUBL, SITES 5.00: 1.00: :CU NI ZR:GD ZR VA: > a phase based on Cu5Gd_L, Ni5Zr & Cu5Zr
XZ2_C37 2 SUBL, SITES 1.00: 2.00: :AL SI:CA GD ND NI PR Y:

> AlPr2, AlY2, AlNd2, AlGd2, SiNi2, SiCa2
ALR_OP16 2 SUBL, SITES 1.00: 1.00: :AL:ND PR: > a phase based on AlNd & AlPr(ht)
AL11R3 2 SUBL, SITES 11.00: 3.00: :AL ZN:CE LA ND PR Y: > Al11Ce3, Al11La3_L, Al11Nd3_L, Al11Pr3_L, Zn11Pr3, Zn11Y3
R7M3 2 SUBL, SITES 0.70: 0.30: :CE LA PR TH:FE NI: > Th7Fe3, Pr7Ni3, Ce7Ni3, La7Ni3
MG12R 2 SUBL, SITES 12.00: 1.00: :AL MG MN ZN:CE GD LA ND PR SR Y: > Mg12Ce, Mg12La, Mg12Pr, also Zn12Y, Mn12Gd, Mn12Y
RSI2 2 SUBL, SITES 1.00: 2.00: :LA Y:SI: > LASI2, SI2Y(rt)
RZN3 2 SUBL, SITES 1.00: 3.00: :GD ND PR Y:ZN: > GdZn3, NdZn3, PrZn3, YZn3
AL2R3 2 SUBL, SITES 0.40: 0.60: :AL:ZR Y: > a phase based on Al2Zr3 & Al2Y3
R5SI4 2 SUBL, SITES 5.00: 4.00: :LA MG ZR:SI: > La5Si4, Si4Zr5(rt)

M10ZR7 2 SUBL, SITES 10.00: 7.00: :CU NI:ZR: > Cu10Zr7, Ni10Zr7
R3SI2 2 SUBL, SITES 3.00: 2.00: :LA MG ZR:SI: > Si2Zr3, La3Si2
R2NI7 2 SUBL, SITES 2.00: 7.00: :CE LA MG Y:NI: > Ni7Y2, Ce2Ni7, La2Ni7(RT)
AG9CA2 2 SUBL, SITES 0.82: 0.18: :AG:CA:
AG7CA2 2 SUBL, SITES 0.78: 0.22: :AG:CA:
AGCA3 2 SUBL, SITES 0.25: 0.75: :AG:CA:
AG4CE 2 SUBL, SITES 4.00: 1.00: :AG:CE:
AG2GD 2 SUBL, SITES 0.67: 0.33: :AG:GD:
AG51GD14 2 SUBL, SITES 0.79: 0.21: :AG:GD:
AG2IN_D83 2 SUBL, SITES 0.68: 0.32: :AG:IN:
AG5LA 2 SUBL, SITES 5.00: 1.00: :AG:LA:

AGMG4 2 SUBL, SITES 0.20: 0.80: :AG:MG:
AGMG3 2 SUBL, SITES 0.23: 0.77: :AG CU SN:CU IN MG:
AG51ND14 2 SUBL, SITES 0.79: 0.21: :AG:ND:
AG2ND_H 2 SUBL, SITES 0.67: 0.33: :AG:ND:
AG2PR 2 SUBL, SITES 2.00: 1.00: :AG:PR:
AG5PR 2 SUBL, SITES 5.00: 1.00: :AG:PR:
AG4SC 2 SUBL, SITES 0.80: 0.20: :AG:SC:
CU2SC_C11B 2 SUBL, SITES 2.00: 1.00: :AG CU:SC:
AGSC 2 SUBL, SITES 0.50: 0.50: :AG:SC:
AG3SN1 2 SUBL, SITES 0.75: 0.25: :AG:AG SN:
AG4SR 2 SUBL, SITES 4.00: 1.00: :AG:SR:
AGSR 2 SUBL, SITES 1.00: 1.00: :AG:SR:
AG2SR3 2 SUBL, SITES 2.00: 3.00:

:AG:SR:
AGY 2 SUBL, SITES 0.50: 0.50: :AG:Y:
AG2Y 2 SUBL, SITES 0.67: 0.33: :AG:Y:
AG51Y4 2 SUBL, SITES 0.79: 0.21: :AG:Y:
AGZN 2 SUBL, SITES 1.00: 2.00: :ZN:AG ZN:
AGZN3 :AG ZN:
AG5ZN8 4 SUBL, SITES 2.00: 2.00: 3.00: 6.00: :AG ZN:AG:AG ZN:AG ZN:
AGZR 2 SUBL, SITES 0.50: 0.50: :AG:ZR:
AGZR2 2 SUBL, SITES 0.33: 0.67: :AG:ZR:
AL4CA 2 SUBL, SITES 4.00: 1.00: :AL MG:CA SR:
AL14CA13 2 SUBL, SITES 14.00: 13.00: :AL MG ZN:CA:
AL3CA8 2 SUBL, SITES 3.00: 8.00: :AL:CA MG:
AL4CE 2 SUBL, SITES 0.80: 0.20: :AL:CE:

AL3CE_H 2 SUBL, SITES 0.75: 0.25: :AL:CE:
AL3CE_L 2 SUBL, SITES 0.75: 0.25: :AL:CE:
ALCE2 2 SUBL, SITES 0.33: 0.67: :AL:CE:
ALRE3 2 SUBL, SITES 1.00: 3.00: :AL IN:CE PR: > L12-type, AlCe3_H, AlPr3_H, InCe3
ALCE3_L 2 SUBL, SITES 0.25: 0.75: :AL:CE:
ALCU_DEL 2 SUBL, SITES 2.00: 3.00: :AL ZN:CU FE:
ALCU_EPS 2 SUBL, SITES 1.00: 1.00: :AL CU ZN NI:CU FE:
ALCU_ETA 2 SUBL, SITES 1.00: 1.00: :AL CU:AG CU:
ALCU_PRIME 2 SUBL, SITES 2.00: 1.00: :AL:CU:
ALCU_ZETA 2 SUBL, SITES 9.00: 11.00: :AL:AG CU:
GAMMA_D83 3 SUBL, SITES 4.00: 1.00: 8.00: :AL SI:AL CU SI:AG CU:
GAMMA_H 3 SUBL, SITES 4.00: 1.00: 8.00: :AL:AL CU:AG CU:

AL13FE4 3 SUBL, SITES 0.63: 0.23: 0.14: :AL:FE MN:AL VA:
AL2FE 2 SUBL, SITES 2.00: 1.00: :AL:FE MN:
AL5FE2 2 SUBL, SITES 5.00: 2.00: :AL:FE MN:
D3_ALFE 3 SUBL, SITES 0.7 : 0.08 : 0.22 : : AL : AL,FE : FE,MN : Z_ALFEMN 2 SUBL, SITES 4 : 1 : : AL : FE,MN : PHI 3 SUBL, SITES 0.7 : 0.15 : 0.15 : : AL : AL,MN : FE,MN :
AL2GD3 2 SUBL, SITES 2.00: 3.00: :AL:GD:
AL3GD 2 SUBL, SITES 3.00: 1.00: :AL:GD:
ALLA3 2 SUBL, SITES 1.00: 3.00: :AL:LA:
AL53LA22 2 SUBL, SITES 0.71: 0.29: :AL:LA:
AL3LA 2 SUBL, SITES 3.00: 1.00: :AL:LA:
AL11LA3_H 2 SUBL, SITES 11.00: 3.00:

:AL:LA:
AL2LI3 2 SUBL, SITES 2.00: 3.00: :AL MG:LI:
ALLI2 2 SUBL, SITES 1.00: 2.00: :AL:LI:
AL4LI9 2 SUBL, SITES 4.00: 9.00: :AL:LI:
ALLI 2 SUBL, SITES 1.00: 1.00: :AL LI MG:LI MG VA:
ALMG_BETA 2 SUBL, SITES140.00: 89.00: :AL ZN:LI MG:
ALMG_EPSILON 2 SUBL, SITES 30.00: 23.00: :AL ZN:MG:
AL12MG17_A12 3 SUBL, SITES 10.00: 24.00: 24.00: :GD LI MG:AL CA MG ZN:AL MG NI ZN:
LTAL11MN4 2 SUBL, SITES 11.00: 4.00: :AL:MN FE:
AL12MN 2 SUBL, SITES 12.00: 1.00: :AL:MN:
AL6MN 2 SUBL, SITES 6.00: 1.00: :AL:MN FE:
AL4MN 2 SUBL, SITES 4.00: 1.00: :AL: FE MN:
R_AL4MN 2 SUBL, SITES 461.00 : 107.00 : :AL:MN FE:

HTAL8MN5 2 SUBL, SITES 8 : 5 : : AL,FE,MN : AL,FE,MN :
LTAL8MN5 3 SUBL, SITES 12.00: 5.00: 9.00: :AL : FE,MN : AL,FE,MN :
HTAL11MN4 2 SUBL, SITES 29.00: 10.00: : AL MN : FE MN :
AL11ND3_H 2 SUBL, SITES 11.00: 3.00: :AL:ND:
AL3ND 2 SUBL, SITES 3.00: 1.00: :AL:ND:
ALND3 2 SUBL, SITES 1.00: 3.00: :AL:ND:
AL3NI2 3 SUBL, SITES 3.00: 2.00: 1.00: :AL:AL MG NI:NI VA:
AL3NI5 2 SUBL, SITES 0.38: 0.62: :AL:NI:
AL11PR3_H 2 SUBL, SITES 11.00: 3.00: :AL:PR:
AL3PR 2 SUBL, SITES 3.00: 1.00: :AL:PR:
ALPR3_L 2 SUBL, SITES 1.00: 3.00: :AL:PR:
AL3SC 2 SUBL, SITES 1.00: 3.00: :SC:AL:

AL2SC 2 SUBL, SITES 1.00: 2.00: :SC:AL:
ALSC 2 SUBL, SITES 1.00: 1.00: :SC:AL:
ALSC2 2 SUBL, SITES 2.00: 1.00: :SC:AL:
AL4SR 2 SUBL, SITES 0.80: 0.20: :AL MG:CA SR:
AL7SR8 2 SUBL, SITES 0.47: 0.53: :AL:CA SR:
AL3SR8 2 SUBL, SITES 0.27: 0.73: :AL:SR:
AL3Y_L 2 SUBL, SITES 0.75: 0.25: :AL:Y:
AL3Y_H 2 SUBL, SITES 0.75: 0.25: :AL:Y:
ALZR2 2 SUBL, SITES 0.33: 0.67: :AL:ZR:
AL3ZR5 2 SUBL, SITES 0.38: 0.62: :AL:ZR:
AL3ZR4 2 SUBL, SITES 0.43: 0.57: :AL:ZR:
AL4ZR5 2 SUBL, SITES 0.44: 0.56: :AL:ZR:
AL3ZR2 2 SUBL, SITES 0.60: 0.40:

:AL:ZR:
AL3ZR1 2 SUBL, SITES 0.75: 0.25: :AL IN:ZR:
CACU5 2 SUBL, SITES 0.17: 0.83: :CA:CU:
CACU 2 SUBL, SITES 0.50: 0.50: :CA:CU:
CA2CU 2 SUBL, SITES 0.67: 0.33: :CA:CU:
CA8IN3 2 SUBL, SITES 8.00: 3.00: :CA:IN:
CA1IN2 2 SUBL, SITES 1.00: 2.00: :CA:IN:
CANI2 2 SUBL, SITES 0.33: 0.67: :CA:NI:
CA2NI7 2 SUBL, SITES 0.22: 0.78: :CA:NI:
CA3SI4 2 SUBL, SITES 0.43: 0.57: :CA:SI:
CA14SI19 2 SUBL, SITES 0.42: 0.58: :CA:SI:
CASI2 2 SUBL, SITES 0.33: 0.67: :CA:SI:
CA2SN_X 3 SUBL, SITES 1.00: 1.00: 1.00: :CA MG:CA:SN:

CA36SN23 2 SUBL, SITES 36.00: 23.00: :CA:SN:
CA31SN20 2 SUBL, SITES 31.00: 20.00: :CA:SN:
CA7SN6 2 SUBL, SITES 7.00: 6.00: :CA:SN:
CA3ZN 2 SUBL, SITES 3.00: 1.00: :CA:ZN:
CAZN3 2 SUBL, SITES 1.00: 3.00: :CA:ZN:
CU6CE 2 SUBL, SITES 0.86: 0.14: :CU:CE:
CU5CE 2 SUBL, SITES 0.83: 0.17: :CU:CE:
CU4CE 2 SUBL, SITES 0.80: 0.20: :CU:CE:
CU2CE 2 SUBL, SITES 0.67: 0.33: :CU IN:CE LA:
CE2IN 2 SUBL, SITES 2.00: 1.00: :CE:IN:
CE5IN4 2 SUBL, SITES 5.00: 4.00: :CE:IN:
CE9IN11 2 SUBL, SITES 9.00: 11.00: :CE:IN:
CE3IN5 2 SUBL, SITES 3.00: 5.00:

:CE:CE IN:
CEGD3 :GD CE:
CENI3 2 SUBL, SITES 0.25: 0.75: :CE:NI:
CENI2 2 SUBL, SITES 0.33: 0.67: :CE NI:CE NI:
CEZN2 2 SUBL, SITES 0.33: 0.67: :CE:MG ZN:
CEZN3 2 SUBL, SITES 0.25: 0.75: :CE:ZN:
CE3ZN11 2 SUBL, SITES 0.21: 0.79: :CE:MG ZN:
CE13ZN58 2 SUBL, SITES 0.18: 0.82: :CE:ZN:
CEZN5 2 SUBL, SITES 0.17: 0.83: :CE:MG ZN:
CE2ZN17 2 SUBL, SITES 0.10: 0.90: :CE:MG ZN:
CEZN11 2 SUBL, SITES 0.08: 0.92: :CE:MG ZN:
CU9GD2 2 SUBL, SITES 0.82: 0.18: :CU:GD:
CU7GD2 2 SUBL, SITES 0.78: 0.22: :CU:GD:

CU9IN4_D83 3 SUBL, SITES 0.65: 0.12: 0.23: :CU:CU IN:IN:
CU7IN3 2 SUBL, SITES 0.70: 0.30: :CU MG:IN:
CU2IN_B82 3 SUBL, SITES 1.00: 1.00: 1.00: :CU MG:CU VA:IN:
CU2IN_LT 2 SUBL, SITES 0.64: 0.36: :CU:IN:
CU11IN9 2 SUBL, SITES 0.55: 0.45: :CU:IN:
CU37LA3 :CU:LA:
CU6LA_L :CU:LA:
CU4LA :CU:LA:
CU2LA :CU:LA:
CUMG2 2 SUBL, SITES 1.00: 2.00: :AG CU IN NI:IN MG:
CU4ND 2 SUBL, SITES 0.80: 0.20: :CU:ND:
CU7ND2 2 SUBL, SITES 0.78: 0.22: :CU:ND:
CUND_H 2 SUBL, SITES 0.50: 0.50:

:CU:ND:
CU6PR 2 SUBL, SITES 0.86: 0.14: :CU:PR:
CU5PR 2 SUBL, SITES 0.83: 0.17: :CU:PR:
CU4PR 2 SUBL, SITES 0.80: 0.20: :CU:PR:
CU2PR 2 SUBL, SITES 0.67: 0.33: :CU:PR:
CU4SC 2 SUBL, SITES 4.00: 1.00: :CU:SC:
CUSC 2 SUBL, SITES 1.00: 1.00: :CU:SC:
CU15SI4_EPSILON 2 SUBL, SITES 15.00: 4.00: :CU MG:AL SI:
CU56SI11_GAMMA 2 SUBL, SITES 56.00: 11.00: :CU MG:SI:
CUSI_ETA 2 SUBL, SITES 0.76: 0.24: :CU:SI:
CU33SI7_DELTA 2 SUBL, SITES 0.82: 0.17: :CU:SI:
CU3SN_H_GAMMA :CU SN:
CU10SN3 :CU SN:

CU3SN_L 2 SUBL, SITES 3.00: 1.00: :CU SN:CU SN:
CU41SN11 2 SUBL, SITES 41.00: 11.00: :CU SN:CU SN:
ETA 3 SUBL, SITES 1.00: 1.00: 1.00: :CU:CU SN:SN:
CU6SN5 3 SUBL, SITES 1.00: 1.00: 1.00: :CU:CU SN:SN:
CUSR 2 SUBL, SITES 0.50: 0.50: :CU:SR:
CUTH2 :CU:TH:
CU2TH :CU:TH:
CU6TH :CU:TH:
CU51TH14 :CU:TH:
CU7Y1 2 SUBL, SITES 1.00: 5.00: :CU2 Y:CU:
CU4Y 2 SUBL, SITES 4.00: 1.00: :CU:Y:
CU7Y2 2 SUBL, SITES 7.00: 2.00: :CU:Y:
CU2Y_H 2 SUBL, SITES 2.00: 1.00:

:CU:Y:
EPSILON :CU MN ZN: > including CuZn_EPS, MnZn_EPS
CUZN_GAMMA 4 SUBL, SITES 2.00: 2.00: 3.00: 6.00: :CU ZN:CU ZN:CU:MG ZN:
CU51ZR14 2 SUBL, SITES 0.78: 0.22: :CU:ZR:
CU8ZR3 2 SUBL, SITES 0.73: 0.27: :CU:ZR:
CUZR2 2 SUBL, SITES 0.33: 0.67: :CU:ZR:
MNI3_L12 2 SUBL, SITES 1.00: 3.00: :FE MN NI:FE MN NI:
FE17ND2 2 SUBL, SITES 1.00: 0.12: :FE:ND:
FE17ND5 2 SUBL, SITES 1.00: 0.29: :FE:ND:
FE17PR2 2 SUBL, SITES 17.00: 2.00: :FE:PR:
FE2SC_C14 2 SUBL, SITES 0.67: 0.33: :FE:SC:
FE2SC_C36 2 SUBL, SITES 0.67: 0.33: :FE:SC:
FE2SC_C15 2 SUBL, SITES 0.64: 0.36:

:FE:SC:
FE6SC29 2 SUBL, SITES 0.17: 0.83: :FE:SC:
FE5SN3 2 SUBL, SITES 5.00: 3.00: :FE:SN:
FE3SN2 2 SUBL, SITES 3.00: 2.00: :FE:SN:
FESN 2 SUBL, SITES 1.00: 1.00: :FE:SN:
FE17TH2 :FE:TH:
FE5TH 2 SUBL, SITES 0.83: 0.17: :FE:TH:
FE7TH2_L 2 SUBL, SITES 0.78: 0.22: :FE:TH:
FE7TH2_H 2 SUBL, SITES 0.78: 0.22: :FE:TH:
FE17Y2 2 SUBL, SITES 1.00: 0.12: :FE:Y:
FE23Y6 2 SUBL, SITES 1.00: 0.26: :FE:Y:
GAMMA_FEZN 4 SUBL, SITES 0.15: 0.15: 0.23: 0.46: :FE ZN:FE ZN:FE ZN:ZN:
GAMMA1_FEZN 3 SUBL, SITES 0.14: 0.12: 0.74: :FE:FE ZN:ZN:

DELTA_FEZN 4 SUBL, SITES 0.06: 0.18: 0.53: 0.24: :FE:FE ZN:ZN:ZN:
ZETA_FEZN 3 SUBL, SITES 0.07: 0.86: 0.07: :FE VA:ZN:ZN VA:
FEZR3 2 SUBL, SITES 1.00: 3.00: :FE ZR:FE ZR:
ORTHO_GA :GA:
MG5GA2 2 SUBL, SITES 0.71: 0.29: :MG:GA IN:
MG2GA 2 SUBL, SITES 0.67: 0.33: :MG:GA:
MGGA 2 SUBL, SITES 0.50: 0.50: :MG:GA:
MGGA2 2 SUBL, SITES 0.33: 0.67: :MG:GA:
MG2GA5 2 SUBL, SITES 0.29: 0.71: :MG:GA:
GD2IN 2 SUBL, SITES 2.00: 1.00: :GD:IN:
GD5IN3 2 SUBL, SITES 5.00: 3.00: :GD:IN:
GDIN 2 SUBL, SITES 1.10: 1.00: :GD:IN:
GD3IN5 2 SUBL, SITES 3.00: 5.00:

:GD:IN:
GDIN3 2 SUBL, SITES 1.00: 3.00: :GD:IN:
GDMG5 2 SUBL, SITES 1.00: 5.00: :AG CA GD ND SM SR Y:MG ZN:
GDND 2 SUBL, SITES 0.50: 0.50: :GD ND:GD ND:
GD3NI2 2 SUBL, SITES 3.00: 2.00: :GD:NI:
GD2NI7 2 SUBL, SITES 2.00: 7.00: :GD:NI:
GDNI4 2 SUBL, SITES 1.00: 4.00: :GD:NI:
GD5SI4 2 SUBL, SITES 0.56: 0.44: :GD:SI:
GD3SI5 2 SUBL, SITES 0.38: 0.62: :GD:SI:
GDSI2 2 SUBL, SITES 0.33: 0.67: :GD:SI:
GDZN2 2 SUBL, SITES 0.33: 0.67: :GD SM:ZN:
GD3ZN11 2 SUBL, SITES 0.21: 0.79: :GD:ZN:
GD13ZN58 2 SUBL, SITES 0.18: 0.82: :GD:MG ZN:

GD2ZN17_L 2 SUBL, SITES 0.10: 0.90: :GD:ZN:
GD2ZN17_H 2 SUBL, SITES 0.10: 0.90: :GD SM:ZN:
GDZN12 2 SUBL, SITES 0.08: 0.92: :GD:ZN:
KIN4 2 SUBL, SITES 0.80: 0.20: :IN:K:
K17IN41 2 SUBL, SITES 0.69: 0.31: :IN:K:
K39IN80 2 SUBL, SITES 0.64: 0.36: :IN:K:
B2REIN 2 SUBL, SITES 1.00: 1.00: :LA ND Y:IN ND:
IN5RE3 2 SUBL, SITES 0.62: 0.38: :IN:LA ND PR TH Y: > IN5LA3, IN5ND3, IN5PR3
IN3LA2 2 SUBL, SITES 0.57: 0.43: :IN:LA:
LIIN 2 SUBL, SITES 1.00: 1.00: :IN LI:IN LI:
LI5IN4 2 SUBL, SITES 5.00: 4.00: :LI:IN:
LI3IN2 2 SUBL, SITES 3.00: 2.00: :LI:IN:

LI2IN 2 SUBL, SITES 2.00: 1.00: :LI:IN:
LI13IN3 2 SUBL, SITES 13.00: 3.00: :LI:IN:
LI3IN 2 SUBL, SITES 3.00: 1.00: :LI:IN:
LI7IN 2 SUBL, SITES 7.00: 1.00: :LI:IN:
TETRA_A6 :IN MG SN ZN:
MG2IN 2 SUBL, SITES 2.00: 1.00: :MG:IN:
MG3IN 2 SUBL, SITES 3.00: 1.00: :MG IN:MG IN:
MN3IN 2 SUBL, SITES 3.00: 1.00: :MN:IN:
NI2IN_HT 3 SUBL, SITES 1.00: 1.00: 1.00: :NI VA:NI:IN NI:
NI13IN9 3 SUBL, SITES 1.00: 1.00: 1.00: :NI VA:NI:IN:
B2NIIN 2 SUBL, SITES 1.00: 1.00: :NI VA:IN:
NI3IN 2 SUBL, SITES 3.00: 1.00: :NI:IN:
NI2IN_LT 2 SUBL, SITES 2.00: 1.00:

:NI LA:IN:
NIIN 2 SUBL, SITES 1.00: 1.00: :NI:IN:
NI2IN3 2 SUBL, SITES 2.00: 3.00: :NI:IN:
NI3IN7 2 SUBL, SITES 3.00: 7.00: :NI:IN:
NA6IN11 2 SUBL, SITES 0.35: 0.65: :NA:IN:
NA7IN12 2 SUBL, SITES 0.37: 0.63: :NA:IN:
NAIN 2 SUBL, SITES 1.00: 1.00: :NA:IN:
NA2IN 2 SUBL, SITES 2.00: 1.00: :NA:IN:
SCIN2 2 SUBL, SITES 1.00: 2.00: :SC:IN:
B2_SCIN 2 SUBL, SITES 1.10: 0.90: :SC:IN:
X2IN 2 SUBL, SITES 2.00: 1.00: :ND SC PR Y:IN: > ND2IN, SC2IN, PR2IN
SC3IN 2 SUBL, SITES 3.00: 1.00: :SC:IN:
PR3IN4 2 SUBL, SITES 3.00: 4.00:

:PR:IN:
PR6IN5 2 SUBL, SITES 6.00: 5.00: :PR:IN:
INSN_AF :IN SN:
TET_ALPHA1_A6 :IN SN:
IN3SR 2 SUBL, SITES 0.75: 0.25: :IN:SR:
IN5SR2 2 SUBL, SITES 0.71: 0.29: :IN:SR:
IN2SR 2 SUBL, SITES 0.67: 0.33: :IN:SR:
IN3SR2 2 SUBL, SITES 0.60: 0.40: :IN:SR:
INSR 2 SUBL, SITES 0.50: 0.50: :IN:SR:
IN3SR5 2 SUBL, SITES 0.38: 0.62: :IN:SR:
INSR3 2 SUBL, SITES 0.25: 0.75: :IN:SR:
THIN 2 SUBL, SITES 1.00: 1.00: :TH:IN: > oP24, ThTl type
TH2IN 2 SUBL, SITES 2.00: 1.00:

:TH:IN: > Al2Cu type
ZRIN2 2 SUBL, SITES 1.00: 2.00: :ZR:IN:
ZRIN 2 SUBL, SITES 1.00: 1.00: :ZR:IN:
RE3IN 2 SUBL, SITES 3.00: 1.00: :LA ND PR ZR:IN: > L12 type, Zr3In, La3In, Nd3In, Pr3In
LANI5 3 SUBL, SITES 0.17: 0.33: 0.50: :LA NI:NI LA:NI:
LA2NI7_H 2 SUBL, SITES 2.00: 7.00: :LA:NI:
LA7NI16 2 SUBL, SITES 0.30: 0.70: :LA:NI:
LA2NI3 2 SUBL, SITES 0.40: 0.60: :LA:NI:
LASI2_A1 2 SUBL, SITES 0.36: 0.64: :LA:SI:
LA5SN3_L 2 SUBL, SITES 0.62: 0.38: :LA:SN:
LA5SN4 2 SUBL, SITES 0.56: 0.45: :LA:SN:
LA11SN10 2 SUBL, SITES 0.52: 0.48: :LA:SN:

LA2SN3 2 SUBL, SITES 0.40: 0.60: :LA:SN:
LA3SN5 2 SUBL, SITES 0.38: 0.62: :LA:SN:
LAY 2 SUBL, SITES 1.00: 1.00: :LA Y:Y:
LI22SI5 2 SUBL, SITES 22.00: 5.00: :LI:SI:
LI13SI4 2 SUBL, SITES 13.00: 4.00: :LI:SI:
LI7SI3 2 SUBL, SITES 7.00: 3.00: :LI:SI:
LI12SI7 2 SUBL, SITES 12.00: 7.00: :LI:SI:
LI13SN5 2 SUBL, SITES 13.00: 5.00: :LI:SN:
LI22SN5 2 SUBL, SITES 22.00: 5.00: :LI:SN:
LI2SN5 2 SUBL, SITES 2.00: 5.00: :LI:SN:
LI5SN2 2 SUBL, SITES 5.00: 2.00: :LI:SN:
LI7SN3 2 SUBL, SITES 7.00: 3.00: :LI:SN:
LI8SN3 2 SUBL, SITES 8.00: 3.00:

:LI:SN:
LISN 2 SUBL, SITES 1.00: 1.00: :LI:LI SN:
LI7SN2 2 SUBL, SITES 7.00: 2.00: :LI SN:SN:
LI2ZN3_L 2 SUBL, SITES 2.00: 3.00: :LI:LI ZN:
LI2ZN3_H 2 SUBL, SITES 2.00: 3.00: :LI ZN:LI ZN:
LI2ZN5_L 2 SUBL, SITES 2.00: 5.00: :LI ZN:ZN:
LI2ZN5_H 2 SUBL, SITES 2.00: 5.00: :LI ZN:ZN:
LIZN4_L 2 SUBL, SITES 1.00: 4.00: :LI ZN:LI ZN:
LIZN4_H 2 SUBL, SITES 0.20: 0.80: :LI ZN:LI ZN:
LIZN2 2 SUBL, SITES 1.00: 2.00: :LI:ZN:
BCC_B32 2 SUBL, SITES 1.00: 1.00: :LI ZN:LI ZN:
MG2NI 2 SUBL, SITES 2.00: 1.00: :MG:CU NI ZN:
MG5PR 2 SUBL, SITES 5.00: 1.00: :MG:PR Y:

RHOMBO_A7 :SB:
MG3SB2_LT 2 SUBL, SITES 0.60: 0.40: :MG:SB:
MG3SB2_HT 2 SUBL, SITES 0.60: 0.40: :MG:SB:
MGSC 2 SUBL, SITES 1.00: 1.00: :MG:MG SC:
RHOMB_C19 :GD MG SM:
MG38SR9 2 SUBL, SITES 38.00: 9.00: :AL MG:CE ND SR:
MG24R5 3 SUBL, SITES 24.00: 4.00: 1.00: :MG:CA CE DY ER GD HO LA MG ND PR Y:DY ER HO Y:
MG2ZN3 2 SUBL, SITES 2.00: 3.00: :MG:AL CU ZN:
MGZN 2 SUBL, SITES 12.00: 13.00: :MG:AL CU ZN:
MG51ZN20 2 SUBL, SITES 51.00: 20.00: :MG:ZN:
MG2ZN11 2 SUBL, SITES 2.00: 11.00: :MG:AL CU SI ZN:
MN17ND2 2 SUBL, SITES 17.00: 2.00: :MN:ND:
L10_TETRA 2 SUBL, SITES 0.50: 0.50:

:MG MN IN NI SC:MG MN IN NI:
MNNI2 2 SUBL, SITES 1.00: 2.00: :MN NI:NI:
MN11SI19 2 SUBL, SITES 11.00: 19.00: :MN:SI:
MN3SI 2 SUBL, SITES 3.00: 1.00: :MN:SI:
MN6SI 2 SUBL, SITES 17.00: 3.00: :MN:SI:
MN9SI2 2 SUBL, SITES 33.00: 7.00: :MN:SI:
MN23SC6 2 SUBL, SITES 23.00: 6.00: :MN:SC:
MNSC4 2 SUBL, SITES 0.20: 0.80: :MN:SC:
MN19SN6 2 SUBL, SITES 0.76: 0.24: :MN:SN:
MN2SN 2 SUBL, SITES 0.67: 0.33: :MN:SN:
MNSN2 2 SUBL, SITES 0.33: 0.67: :MN:SN:
MN23Y6 2 SUBL, SITES 23.00: 6.00: :MG MN:Y:
MNZN9 2 SUBL, SITES 0.10: 0.90: :MN:ZN:

ND2Y 2 SUBL, SITES 2.00: 1.00: :ND Y:ND Y:
NDZN2 2 SUBL, SITES 0.33: 0.67: :ND:ZN:
ND3ZN11 2 SUBL, SITES 0.21: 0.79: :ND:ZN:
ND13ZN58 2 SUBL, SITES 0.18: 0.82: :ND:ZN:
ND2ZN17 2 SUBL, SITES 0.10: 0.90: :ND:ZN:
NDZN11_H 2 SUBL, SITES 0.08: 0.92: :ND:ZN:
NI5PR 2 SUBL, SITES 0.83: 0.17: :NI:PR:
NI7PR2 2 SUBL, SITES 0.78: 0.22: :NI:PR:
NI2PR 2 SUBL, SITES 0.67: 0.33: :NI:PR:
NI3SI_M 2 SUBL, SITES 0.75: 0.25: :NI:SI:
NI3SI_L 2 SUBL, SITES 0.76: 0.24: :NI:SI:
NI5SI2 2 SUBL, SITES 0.71: 0.29: :NI:SI:
THETA 3 SUBL, SITES 1.00: 1.00: 1.00:

:NI:NI VA:SI:
NI3SI2 2 SUBL, SITES 0.60: 0.40: :NI:SI:
NISI 2 SUBL, SITES 0.50: 0.50: :NI:SI:
NI3SN_H 3 SUBL, SITES 0.25: 0.25: 0.50: :NI SN:NI SN:NI:
NI3SN_L 2 SUBL, SITES 0.75: 0.25: :NI:SN:
NI3SN2_H 3 SUBL, SITES 0.33: 0.33: 0.33: :NI:NI SN:SN:
NI3SN2_L 3 SUBL, SITES 0.20: 0.40: 0.40: :SN:NI SN:NI:
NI3SN4 3 SUBL, SITES 0.25: 0.25: 0.50: :NI:NI SN:SN:
NI17Y2 2 SUBL, SITES 17.00: 2.00: :NI:Y:
NI4Y 2 SUBL, SITES 4.00: 1.00: :NI:Y:
NI2Y1 2 SUBL, SITES 2.00: 1.00: :NI:Y:
NI2Y3 2 SUBL, SITES 2.00: 3.00: :NI:Y:
BETA_NIZN :NI ZN:

GAMMA_NIZN :NI ZN:
DELTA_NIZN 2 SUBL, SITES 0.11: 0.89: :NI:ZN:
NI7ZR2 2 SUBL, SITES 7.00: 2.00: :NI:ZR:
NI3ZR 2 SUBL, SITES 3.00: 1.00: :NI:ZR:
NI21ZR8 2 SUBL, SITES 21.00: 8.00: :NI:ZR:
NI11ZR9 2 SUBL, SITES 11.00: 9.00: :NI:ZR:
PR2Y 2 SUBL, SITES 2.00: 1.00: :PR Y:PR Y:
PR13ZN58 2 SUBL, SITES 0.18: 0.82: :PR:ZN:
PR2ZN17_H 2 SUBL, SITES 2.00: 17.00: :PR:ZN:
SC5SI3 2 SUBL, SITES 0.62: 0.38: :SC:SI:
SCSI 2 SUBL, SITES 0.50: 0.50: :SC:SI:
SC3SI5_LT 2 SUBL, SITES 0.38: 0.62: :SC:SI:
SC3SI5_HT 2 SUBL, SITES 0.38: 0.62:

:SC:SI:
SI2Y_H 2 SUBL, SITES 2.00: 1.00: :SI:Y:
SI4Y5 2 SUBL, SITES 4.00: 5.00: :SI:Y:
SI5Y3_H 2 SUBL, SITES 5.00: 3.00: :SI:Y:
SI5Y3_L 2 SUBL, SITES 5.00: 3.00: :SI:Y:
SI4ZR5_H 2 SUBL, SITES 4.00: 5.00: :SI:ZR:
SI2ZR 2 SUBL, SITES 2.00: 1.00: :SI:ZR:
SIZR3 2 SUBL, SITES 1.00: 3.00: :SI:ZR:
ZR3SN_A15 2 SUBL, SITES 3.00: 1.00: :ZR SN:ZR SN:
ZR5SN3 3 SUBL, SITES 5.00: 3.00: 1.00: :ZR:SN:SN VA:
ZRSN2 2 SUBL, SITES 1.00: 2.00: :ZR:SN:
SRZN5_L 2 SUBL, SITES 1.00: 5.00: :SR:ZN:
THZN2 2 SUBL, SITES 1.00: 2.00: :TH:ZN:

THZN4 2 SUBL, SITES 1.00: 4.00: :TH:ZN:
H_RZN5 2 SUBL, SITES 1.00: 5.00: :GD Y:MG ZN:
Y13ZN58 2 SUBL, SITES 13.00: 58.00: :Y:ZN:
YZN2_A 2 SUBL, SITES 1.00: 2.00: :Y:ZN:
YZN2_B 2 SUBL, SITES 1.00: 2.00: :Y:ZN:
ZN22ZR 2 SUBL, SITES 0.96: 0.04: :ZN:ZR:
ZN39ZR5 2 SUBL, SITES 0.89: 0.11: :ZN:ZR:
ZN3ZR_L 2 SUBL, SITES 0.75: 0.25: :ZN:ZR:
ZN3ZR_H 2 SUBL, SITES 0.75: 0.25: :ZN:ZR:
ZN2ZR1 2 SUBL, SITES 0.67: 0.33: :ZN:ZR:
ZN2ZR3 2 SUBL, SITES 0.40: 0.60: :ZN:ZR:
ZNZR2 2 SUBL, SITES 0.33: 0.67: :ZN:ZR:
AGGDMG_T 2 SUBL, SITES 0.15: 0.85:

:AG GD:MG:
AL9CA31ZN10 3 SUBL, SITES 1.00: 1.00: 1.00:
:AL:CA:ZN:
AL2CAZN2 3 SUBL, SITES 2.00: 1.00: 2.00:
:AL:CA:ZN:
AL13CEMG6 3 SUBL, SITES 13.00: 1.00: 6.00:
:AL:CE:MG:
ALCUMG_Q 3 SUBL, SITES 7.00: 3.00: 6.00:
:AL:CU:MG:
ALCUMG_S 3 SUBL, SITES 2.00: 1.00: 1.00:
:AL SI:CU:MG:
ALCUMG_T 4 SUBL, SITES 26.00: 6.00: 48.00: 1.00:
:MG:AL MG:AL CU MG ZN:AL:
ALCUMG_V 3 SUBL, SITES 5.00: 6.00: 2.00:
:AL:CU:MG:
AL16FEMN3 2 SUBL, SITES 4.00: 1.00:
:AL:FE MN:
AL13FE2MN2 2 SUBL, SITES 4.00: 13.00:
:FE MN:AL:
AL10FEMN2 2 SUBL, SITES 3.00: 10.00:
:FE MN:AL:
ALLIMG_T 3 SUBL, SITES 0.53: 0.33: 0.14:
:AL:LI:MG:
ALMGMN_T 3 SUBL, SITES 18.00: 3.00: 2.00:
:AL:MG:MN:

ALMGND_T 3 SUBL, SITES 2.00: 0.88: 0.12: :AL:MG:ND:
ALMG3NI2 3 SUBL, SITES 1.00: 2.00: 3.00: :AL:NI:MG:
AL38MG58SR4 3 SUBL, SITES 38.00: 58.00: 4.00: :AL:MG:SR:
AL4MGY 3 SUBL, SITES 0.67: 0.17: 0.17: :AL MG Y:AL MG Y:MG Y:
ALMGZN_PHI 2 SUBL, SITES 21.00: 17.00: :MG:AL ZN:
ALMGZN_T1 4 SUBL, SITES 26.00: 6.00: 48.00: 1.00: :MG:MG AL:AL MG ZN:AL:
ALMGZN_Q 3 SUBL, SITES 0.15: 0.44: 0.41: :AL:MG:ZN:
ALMGZN_T2 3 SUBL, SITES 0.15: 0.43: 0.42: :AL:MG:ZN:
CAMGSI_T1 3 SUBL, SITES 0.33: 0.33: 0.33: :CA:CA MG:SI:
CA7MG6SI14 3 SUBL, SITES 0.26: 0.22: 0.52: :CA:MG:SI:
CAMGSN_T1 3 SUBL, SITES156.00: 94.00:175.00: :CA:MG:SN:
CA2MG6ZN3 3 SUBL, SITES 2.00: 6.00: 3.00: :CA:MG:ZN:
MG5CEY 2 SUBL, SITES 5.00: 1.00:

:MG:CE Y:
T2_CEMGZN 3 SUBL, SITES 0.02: 0.53: 0.45: :CE:MG:ZN: > Ce1Mg29Zn25, T2_Ce-Mg-Zn
T4_CEMGZN 3 SUBL, SITES 1.00: 2.50: 4.50: :CE:MG:ZN: > CeMg2.5Zn4.5, T4_Ce-Mg-Zn
T5_CEMGZN 3 SUBL, SITES 0.07: 0.28: 0.65: :CE:MG:ZN: > Ce3Mg13Zn30, T5_Ce-Mg-Zn
T6_CEMGZN 3 SUBL, SITES 0.06: 0.12: 0.81: :CE:MG:ZN: > CeMg2Zn13, T6_Ce-Mg-Zn
T7_CEMGZN 3 SUBL, SITES 0.17: 0.16: 0.68: :CE:MG:ZN: > Ce20Mg19Zn81, T7_Ce-Mg-Zn
MGCU4IN 3 SUBL, SITES 1.00: 4.00: 1.00: :IN MG:CU IN MG:IN MG:
CULIMG_T 3 SUBL, SITES 1.00: 0.08: 1.92: :CU:LI:MG:
CU16MG6SI7 3 SUBL, SITES 16.00: 6.00: 7.00: :CU:MG:SI:
CU3MG2SI 3 SUBL, SITES 2.74: 2.00: 1.26: :CU:MG:SI:
CUMGY_T1 3 SUBL, SITES 0.75: 0.17: 0.08:

:CU:MG:Y: > CU9MG2Y, T1_Cu-Mg-Y
CUMGY_T2 3 SUBL, SITES 4.00: 1.00: 1.00: :CU:MG:Y: > CU4MGY, T2_Cu-Mg-Y
CUMGY_T3 3 SUBL, SITES 2.00: 1.00: 2.00: :CU:MG:Y: > CU2MGY2, T3_Cu-Mg-Y
CUMGY_T4 3 SUBL, SITES 1.00: 1.00: 1.00: :CU:MG:Y: > CUMGY, T4_Cu-Mg-Y
CUMGY_T5 3 SUBL, SITES 0.28: 0.44: 0.28: :CU:MG:Y: > CU5MG8Y5, T5_Cu-Mg-Y
CUMGY_T6 3 SUBL, SITES 0.22: 0.57: 0.22: :CU:MG:Y: > CU5MG13Y5, T6_Cu-Mg-Y
CUMGY_T7 3 SUBL, SITES 0.18: 0.57: 0.25: :CU:MG:Y: > CU18MG57Y25, T7_Cu-Mg-Y
CUMGY_T8 3 SUBL, SITES 0.19: 0.62: 0.19: :CU:MG:Y: > CU5MG16Y5, T8_Cu-Mg-Y
CUMGY_T9 3 SUBL, SITES 1.00: 4.00: 1.00: :CU:MG:Y:

> CU9MG2Y, T9_Cu-Mg-Y
CUMGY_T10 3 SUBL, SITES 0.09: 0.78: 0.13: :CU:MG:Y: > CU9MG78Y13, T10_Cu-Mg-Y
CUMGY_14H 3 SUBL, SITES 0.86: 0.07: 0.07: :MG:Y:CU: > 14H-type Cu-Mg-Y LPSO phase
CUMGY_18R 3 SUBL, SITES 0.83: 0.08: 0.08: :MG:Y:CU: > 18R-type Cu-Mg-Y LPSO phase
F_MGGDZN 3 SUBL, SITES 0.17: 0.16: 0.68: :GD:MG:ZN: > Gd20Mg19Zn81,isostructural to Ce20Mg19Zn81, aka F
Z_MGRZN 3 SUBL, SITES 0.07: 0.28: 0.65: :GD Y:MG:ZN: > hexagonal Z phase, aka S, hP92
M_MGRZN 3 SUBL, SITES 0.08: 0.28: 0.64: :GD:MG:ZN: > hexagonal M phase, hP238, related to S/Z and L
L_MGRZN 3 SUBL, SITES 0.14: 0.22: 0.64: :GD:MG:ZN: > hexagonal L phase, hP480, related to S/Z and M
LI2MGIN 3 SUBL, SITES 2.00: 1.00: 1.00: :LI:MG:IN: > L21 type

LAMGNI_T1	3 SUBL, SITES 0.25: 0.25: 0.50:
:LA:NI:MG:	
LAMGNI_T2	3 SUBL, SITES 0.40: 0.40: 0.20:
:LA:NI:MG:	
LAMGNI_T3	2 SUBL, SITES 0.33: 0.67:
:LA MG:NI:	
LAMGNI_T4	3 SUBL, SITES 0.67: 0.17: 0.17:
:LA:NI:MG:	
LAMGNI_T5	3 SUBL, SITES 0.67: 0.22: 0.11:
:LA:NI:MG:	
LAMGNI_T6	2 SUBL, SITES 0.68: 0.33:
:LA:MG NI:	
LAMGSI_T1	2 SUBL, SITES 0.60: 0.40:
:LA MG:SI:	
LAMGSI_T2	3 SUBL, SITES 0.20: 0.40: 0.40:
:LA:SI:MG:	
LAMGSI_T3	3 SUBL, SITES 0.25: 0.50: 0.25:
:LA:SI:MG:	
LAMGSI_T4	3 SUBL, SITES 0.20: 0.03: 0.77:
:LA:SI:MG:	
LAMGSI_T5	3 SUBL, SITES 0.33: 0.00: 0.67:
:LA:SI:MG:	
MG6MN3NI	3 SUBL, SITES 3.00: 1.00: 2.00:
:MG:MN:NI:	
MGNDZN_T1	3 SUBL, SITES 0.35: 0.05: 0.60:

:MG:ND:ZN:
MGNDZN_T2 3 SUBL, SITES 0.35: 0.10: 0.55: :MG:ND:ZN:
MGNDZN_T3 3 SUBL, SITES 0.60: 0.10: 0.30: :MG:ND:ZN:
MGNDZN_T4 3 SUBL, SITES 0.30: 0.15: 0.55: :MG:ND:ZN:
LPSO_14H 3 SUBL, SITES 0.88: 0.06: 0.06: :MG:GD Y:ZN:
LPSO_18R 3 SUBL, SITES 0.84: 0.08: 0.08: :MG:Y:ZN:
I_MGRZN 3 SUBL, SITES 0.10: 0.30: 0.60: :GD Y:MG ZN:MG ZN:
AL3CU2MG9SI7 4 SUBL, SITES 3.00: 2.00: 9.00: 7.00: :AL:CU:MG:SI: