TCHEA4: TCS High Entropy Alloy Database

Database name:	TCS High Entropy Alloy Database	*Database acronym:*	TCHEA
Database owner:	Thermo-Calc Software AB	*Database version:*	4

TCHEA4 is a thermodynamic database for high entropy alloys (HEA) [2004 and 2006, Yeh], which are also known as multi-principal element alloys (MPEA) [2013, Wang; 2015, Senkov]. TCHEA4 is developed in a CALPHAD spirit based on the critical evaluation of all the binary systems and many ternary systems. A hybrid approach of experiments, first-principal calculations and CALPHAD modeling has been used to obtain reliable thermodynamic descriptions of the BCC, FCC and HCP solutions. That enables predictions to be made for multi-component alloy systems, especially for HEAs.

Included Elements (26)

The database has been developed in a 26-element framework:

Al	B	C	Co	Cr	Cu	Fe	Hf	Ir	Mn	Mo	N	Nb	Ni	Re
Rh	Ru	Si	Sn	Ta	Ti	V	W	Y	Zn	Zr				

Almost all binary systems in this 26-element framework (307 in total) are assessed to their full range of composition and temperature and can be calculated with the BINARY Module in Thermo-Calc. In total, 493 ternaries are assessed, and 192 of them to the full range of composition and temperature. These can be calculated with the TERNARY Module in Thermo-Calc.

The database can be used to calculate various phase diagrams and property diagrams in the assessed systems and higher-order systems.

- TCHEA4 Assessed Binary Systems
- TCHEA4 Critically Assessed Ternary Systems

The extrapolation to higher-order systems helps to understand the phase equilibria in HEAs, so as to predict the phase formation, phase fractions and phase compositions or to calculate the driving force of forming a phase. The database can also be used to predict solidification behaviour of HEAs with the SCHEIL_GULLIVER module in Thermo-Calc. All necessary molar volume data and thermal expansion data have been assessed or estimated for most of the phases.

TCHEA4 contains nearly all stable phases in all assessed binary systems and most ternary systems. In total, 500 solution and intermetallic phases are modeled.

Phases Included in TCHEA4 lists all phases and Models for the Phases Included in TCHEA4 includes a detailed description of the models, e.g. number of sublattices and constituents on each sublattice.

Also see TCHEA4 Calculation Examples for a variety of validation information.

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 or other databases, the information is available in the online help (from Thermo-Calc go to **Help>Online Help**) or in the release notes on our website. For the TCFE (TCS Steel and Fe-alloys) database there is a dedicated page with the history of its development.

TCHEA4 Assessed Binary Systems

These are the assessed binary systems (307 in total) in the full range of composition and temperature.

	Al	B	C	Co	Cr	Cu	Fe	Hf	Ir	Mn	Mo	N	Nb	Ni	Re	Rh	Ru	Si	Sn	Ta	Ti	V	W	Y	Zn	Zr
B	x	B																								
C	x	x	C																							
Co	x	x	x	Co																						
Cr	x	x	x	x	Cr																					
Cu	x	x	x	x	x	Cu																				
Fe	x	x	x	x	x	x	Fe																			
Hf	x	x	x	x	x	x	x	Hf																		
Ir	x	x	x	x	x	x	x	x	Ir																	
Mn	x	x	x	x	x	x	x	x	x	Mn																
Mo	x	x	x	x	x	x	x	x	x	x	Mo															
N	x	x		x	x	x	x	x		x	x	N														
Nb	x	x	x	x	x	x	x	x	x	x	x	x	Nb													
Ni	x	x	x	x	x	x	x	x	x	x	x	x	x	Ni												
Re	x	x	x	x	x	x	x	x	x	x	x		x	x	Re											
Rh	x	x	x	x	x	x	x	x	x	x				x	x	Rh										
Ru	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	Ru									
Si	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	Si								
Sn	x	x	x	x	x	x	x	x	x	x			x	x	x	x	x	x	Sn							
Ta	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	Ta						
Ti	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	Ti					
V	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	V				
W	x	x	x	x	x	x	x	x		x	x	x	x	x	x		x	x	x	x	x	x	W			
Y	x	x	x	x	x	x	x	x		x	x		x	x	x		x	x	x	x	x	x	x	Y		
Zn	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	Zn	
Zr	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	Zr
	Al	B	C	Co	Cr	Cu	Fe	Hf	Ir	Mn	Mo	N	Nb	Ni	Re	Rh	Ru	Si	Sn	Ta	Ti	V	W	Y	Zn	

updated added

TCHEA4 Critically Assessed Ternary Systems

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

Al-B-Ti
Al-C-Co
Al-C-Fe
Al-Co-Ni
Al-Co-Ti
Al-Co-W
Al-Co-Zr
Al-Cr-Ni
Al-Cr-Sn
Al-Cr-Ti
Al-C-Ti
Al-Cu-Fe
Al-Cu-Mn
Al-Cu-Ni
Al-Cu-Si
Al-Cu-Sn
Al-Cu-Zn
Al-Fe-Mn
Al-Fe-N
Al-Fe-Si
Al-Fe-Ti
Al-Mn-Ni
Al-Mn-Si
Al-Mn-Ti
Al-Mn-Zn
Al-Mo-Ni
Al-Mo-Ti

Al-Nb-Ni
Al-Nb-Ti
Al-Ni-Ru
Al-Ni-Si
Al-Ni-Ta
Al-Ni-Ti
Al-Ni-W
Al-Ni-Zn
Al-N-Ti
Al-Ru-Ti
Al-Si-Sn
Al-Si-Ti
Al-Si-Zn
Al-Sn-Ti
Al-Sn-Zn
Al-Ta-Ti
Al-Ti-V
Al-Ti-W
Al-Ti-Y
Al-Ti-Zr
C-Co-Cr
C-Co-Fe
C-Co-Mo
C-Co-Nb
C-Co-Ni
C-Co-Ta
C-Co-Ti

C-Co-W
C-Cr-Fe
C-Cr-Hf
C-Cr-Si
C-Cr-Ti
C-Cr-V
C-Cr-Zr
C-Cu-Fe
C-Fe-Mn
C-Fe-Mo
C-Fe-N
C-Fe-Ni
C-Fe-Si
C-Fe-Ti
C-Fe-V
C-Fe-W
C-Hf-Mo
C-Hf-Ni
C-Mn-Si
C-Mo-Ni
C-Mo-Ta
C-Mo-Ti
C-Mo-V
C-Mo-W
C-Mo-Zr
C-Nb-Ni
C-Nb-Re

C-Nb-Ti
C-Nb-W
C-Ni-Ta
C-Ni-Ti
C-Ni-W
C-Ni-Zr
Co-Cr-Cu
Co-Cr-Fe
Co-Cr-Ni
Co-Cr-Ti
Co-Cr-W
Co-Cu-Fe
Co-Cu-Mn
Co-Cu-Nb
Co-Cu-Ni
Co-Fe-Mo
Co-Fe-N
Co-Fe-Ni
Co-Fe-W
Co-Mo-Ti
Co-Ni-Si
Co-Ni-V
Co-Ni-W
Co-Sn-Ti
Co-Ta-Ti
Co-W-Zr
Cr-Cu-Mo

Cr-Cu-Nb
Cr-Cu-Si
Cr-Cu-Sn
Cr-Cu-Zr
Cr-Fe-Mn
Cr-Fe-Mo
Cr-Fe-N
Cr-Fe-Ni
Cr-Fe-Si
Cr-Fe-V
Cr-Mn-N
Cr-Mn-Ti
Cr-Mo-Ni
Cr-Nb-Ni
Cr-Ni-Re
Cr-Ni-Si
Cr-Ni-Ta
Cr-Ni-Ti
Cr-Ni-W
Cr-Ni-Zr
Cr-N-Ni
Cr-Si-Ti
Cr-Ti-Zr
C-Ta-W
C-Ti-W
Cu-Fe-Mn
Cu-Fe-N

Cu-Fe-Ni
Cu-Fe-Si
Cu-Fe-Sn
Cu-Fe-Ti
Cu-Fe-V
Cu-Mn-Ni
Cu-Mn-Si
Cu-Mn-Sn
Cu-Mn-Zn
Cu-Mo-Ni
Cu-Ni-Ti
Cu-Ni-Zn
Cu-Ti-Zr
Fe-Mn-N
Fe-Mn-Si
Fe-Mo-Ni
Fe-Nb-Ni
Fe-Ni-Ru
Fe-Ni-Si
Fe-Ni-Ti
Fe-Ni-W
Fe-N-Nb
Fe-N-Ni
Fe-N-Ti
Fe-N-V
Fe-Ti-V
Hf-Nb-Si

Hf-Ni-Ti
Ir-Rh-Ru
Mn-Si-Zn
Mo-Nb-Ti
Mo-Ni-Ta
Mo-N-Ni
Mo-Ta-Ti
Mo-Ti-V
Mo-Ti-W
Mo-Ti-Zr
Nb-Ni-Ti
Nb-Sn-Ti
Nb-Ta-Ti
Nb-Ti-V
Nb-Ti-W
Nb-Ti-Zr
Ni-Si-Ti
Ni-Ta-Ti
Ni-Ta-W
Ni-Ti-W
Ni-Ti-Zr
N-Ni-Ti
Re-Ta-W
Si-Ti-W
Ta-Ti-V
Ta-Ti-W
Ta-Ti-Zr
Ti-V-W
Ti-V-Zr
Ti-W-Zr

TCHEA4 Tentatively Assessed Ternary Systems

Al-C-Cr
Al-C-Ni
Al-Co-Cr
Al-Co-Hf
Al-Co-Mo
Al-Co-Nb
Al-Co-Ru
Al-Co-Si
Al-Co-Ta
Al-Cr-Fe
Al-Cr-Mo
Al-Cr-Nb
Al-Cr-Re
Al-Cr-Ru
Al-Cr-Si
Al-Cr-Ta
Al-Cr-W
Al-Cr-Zr
Al-C-Si
Al-Fe-Hf
Al-Fe-Mo
Al-Fe-Nb
Al-Fe-Ni
Al-Fe-Re
Al-Fe-Ta
Al-Fe-W
Al-Fe-Zr
Al-Hf-Ni

Al-Hf-Ru
Al-Hf-Si
Al-Hf-Ti
Al-Mo-Nb
Al-Mo-Re
Al-Mo-Ru
Al-Mo-Si
Al-Mo-W
Al-Mo-Zr
Al-Nb-Re
AL-Nb-Ru
Al-Nb-Si
Al-Nb-Ta
Al-Nb-W
Al-Ni-Re
Al-Ni-V
Al-Ni-Zr
Al-Re-Ru
Al-Re-Ta
Al-Re-Ti
Al-Re-W
Al-Ru-Ta
Al-Ru-W
Al-Ru-Zr
Al-Si-Zr
Al-Ta-W
C-Co-Re
C-Co-V

C-Cr-Mn
C-Cr-Mo
C-Cr-N
C-Cr-Nb
C-Cr-Ni
C-Cr-Re
C-Cr-Ta
C-Cr-W
C-Fe-Nb
C-Fe-Re
C-Fe-Ta
C-Hf-Ta
C-Hf-Ti
C-Hf-W
C-Mn-V
C-Mo-N
C-Mo-Re
C-Mo-Si
C-Nb-V
C-Nb-Zr
C-Ni-Ti
C-Ni-V
C-N-Nb
C-N-Ti
Co-Cr-Hf
Co-Cr-Mo
Co-Cr-Nb
Co-Cr-Re

Co-Cr-Ru
Co-Cr-Si
Co-Cr-Ta
Co-Cr-V
Co-Cu-Ti
Co-Fe-Hf
Co-Fe-Nb
Co-Fe-Ta
Co-Fe-Ti
Co-Fe-Zr
Co-Hf-Ni
Co-Hf-Ti
Co-Mo-Nb
Co-Mo-Ni
Co-Mo-Re
Co-Mo-Ru
Co-Mo-Ta
Co-Mo-V
Co-Nb-Ni
Co-Nb-Si
Co-Nb-Ta
Co-Nb-Ti
Co-Nb-W
Co-Ni-Ru
Co-Ni-Ta
Co-Ni-Ti
Co-Ni-Zr
Co-Re-Ta

Co-Re-W
Co-Ru-Ta
Co-Ru-W
Co-Si-Ta
Co-Si-Ti
Co-Si-W
Co-Si-Zr
Co-Ta-W
Co-Ti-Zr
Cr-Cu-Fe
Cr-Cu-Ni
C-Re-Ta
C-Re-V
C-Re-W
Cr-Fe-Hf
Cr-Fe-Nb
Cr-Fe-Re
Cr-Fe-Ta
Cr-Fe-Ti
Cr-Fe-W
Cr-Fe-Zr
Cr-Hf-Mo
Cr-Hf-Nb
Cr-Hf-Ni
Cr-Hf-Re
Cr-Hf-Si
Cr-Hf-Ta
Cr-Hf-W

Cr-Mo-N
Cr-Mo-Nb
Cr-Mo-Re
Cr-Mo-Ru
Cr-Mo-Si
Cr-Mo-Ta
Cr-Mo-Ti
Cr-Mo-W
Cr-Mo-Zr
Cr-Nb-Re
Cr-Nb-Si
Cr-Nb-Ta
Cr-Nb-Ti
Cr-Nb-W
Cr-Nb-Zr
Cr-Ni-Ru
Cr-Ni-V
Cr-N-Nb
Cr-N-V
Cr-Re-Ru
Cr-Re-Ta
Cr-Re-V
Cr-Re-W
Cr-Re-Zr
Cr-Ru-Ta
Cr-Ru-Ti
Cr-Ru-W
Cr-Si-Ta

Cr-Si-W
Cr-Si-Zr
Cr-Ta-Ti
Cr-Ta-W
Cr-Ta-Zr
Cr-Ti-V
Cr-Ti-W
Cr-W-Zr
C-Si-Ti
C-Ta-Ti
C-Ti-Zr
Cu-Fe-Mo
Cu-Fe-Nb
Cu-Ni-Si
C-V-W
C-W-Zr
Fe-Hf-Mo
Fe-Hf-Nb
Fe-Hf-Ni
Fe-Hf-Re
Fe-Hf-Si
Fe-Hf-Ta
Fe-Hf-Ti
Fe-Hf-W
Fe-Hf-Zr
Fe-Mn-Ni
Fe-Mo-N
Fe-Mo-Nb
Fe-Mo-Re
Fe-Mo-Si
Fe-Mo-Ta

Fe-Mo-Ti
Fe-Mo-W
Fe-Mo-Zr
Fe-Nb-Re
Fe-Nb-Si
Fe-Nb-Ta
Fe-Nb-Ti
Fe-Nb-W
Fe-Nb-Zr
Fe-Ni-Ta
Fe-Ni-V
Fe-Ni-Zr
Fe-Re-Ti
Fe-Re-W
Fe-Re-Zr
Fe-Si-Ta
Fe-Si-Ti
Fe-Si-W
Fe-Si-Zr
Fe-Ta-Ti
Fe-Ta-W
Fe-Ta-Zr
Fe-Ti-W
Fe-W-Zr
Hf-Mo-Ni
Hf-Mo-Si
Hf-Nb-Ni
Hf-Nb-Re
Hf-Ni-Re
Hf-Ni-Ru
Hf-Ni-Si

Hf-Ni-Ta
Hf-Ni-W
Hf-Re-Ta
Hf-Re-W
Hf-Ru-Ti
Hf-Ru-Zr
Hf-Si-Ta
Hf-Si-Ti
Hf-Si-W
Mn-Ni-Si
Mn-Ni-V
Mo-Nb-Ni
Mo-Nb-Re
Mo-Ni-Re
Mo-Ni-Ru
Mo-Ni-Si
Mo-Ni-W
Mo-Ni-Zr
Mo-N-V
Mo-Re-Ru
Mo-Re-Ta
Mo-Re-Ti
Mo-Re-V
Mo-Re-W
Mo-Re-Zr
Mo-Ru-SI
Mo-Ru-Ta
Mo-Ru-W
Mo-Si-Zr
Nb-Ni-Re
Nb-Ni-Si

Nb-Ni-Ta
Nb-Ni-V
Nb-Ni-W
Nb-Ni-Zr
Nb-Re-Ta
Nb-Re-Ti
Nb-Re-W
Nb-Re-Zr
Nb-Ru-SI
Nb-Si-Ti
Ni-Re-Ta
Ni-Re-W
NI-RE-ZR
Ni-Ru-Ta
Ni-Ru-Ti
Ni-Ru-W
Ni-Ru-Zr
Ni-Si-Ta
Ni-Si-V
Ni-Si-W
Ni-Si-Zr
Ni-Ta-Zr
Ni-W-Zr
N-Ti-V
Re-Ru-Ta
Re-Ru-Ti
Re-Ru-W
Re-Ta-Ti
Re-Ta-V
Re-Ta-Zr
Re-Ti-W

Re-W-Zr
Ru-SI-TI
Ru-Ta-Ti
Ru-Ta-W
Ru-Ti-Zr
Si-Ta-Zr
Si-Ti-Zr
Si-W-Zr
Ta-W-Zr

TCHEA4 Calculation Examples

FCC Forming Ternary Systems

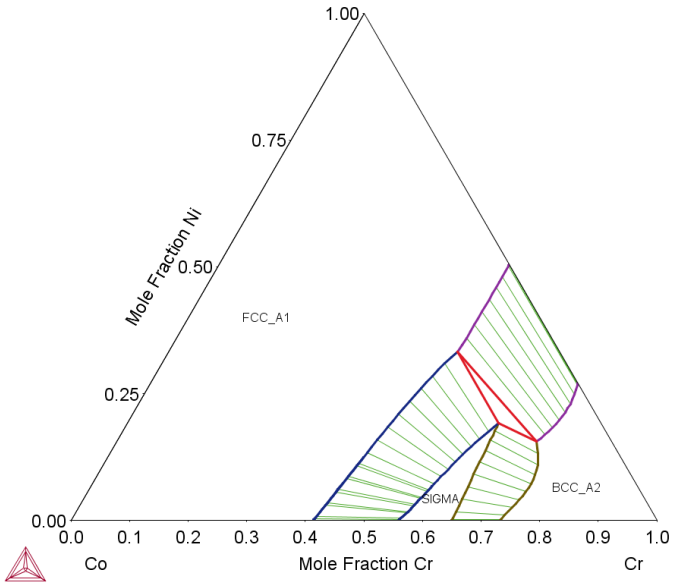

Figure 1: Calculated Co-Cr-Ni isothermal section at 1200 °C.

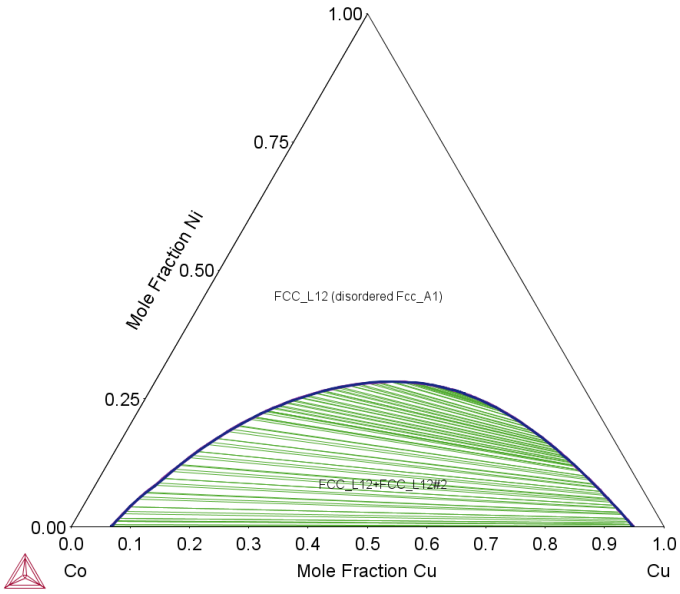

Figure 2: Calculated Co-Cu-Ni isothermal section at 1000 °C.

BCC Forming Ternary Systems

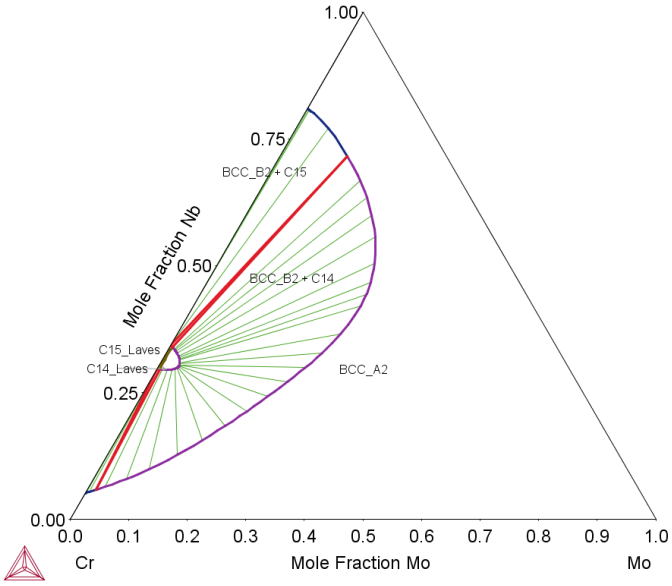

Figure 3: Calculated Cr-Mo-Nb isothermal section at 1500 °C.

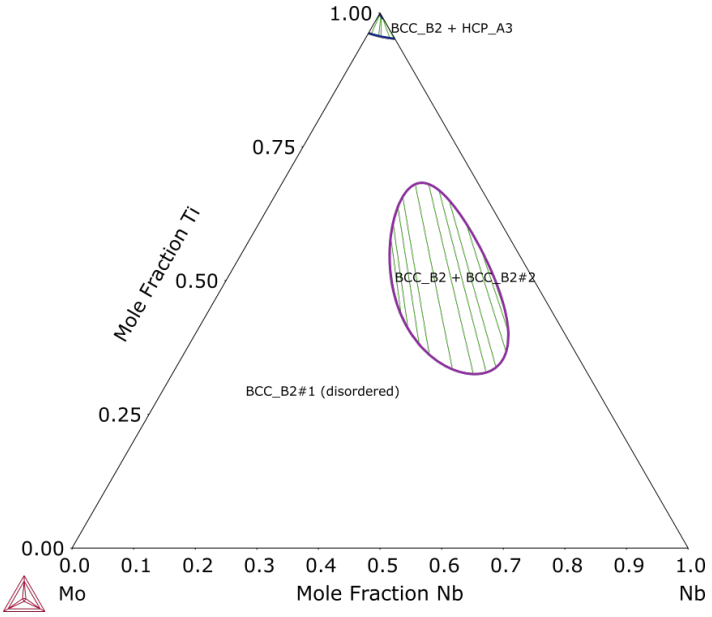

Figure 4: Calculated Mo-Nb-Ti isothermal section at 800 °C.

FCC/FCC+BCC Forming Ternary Systems

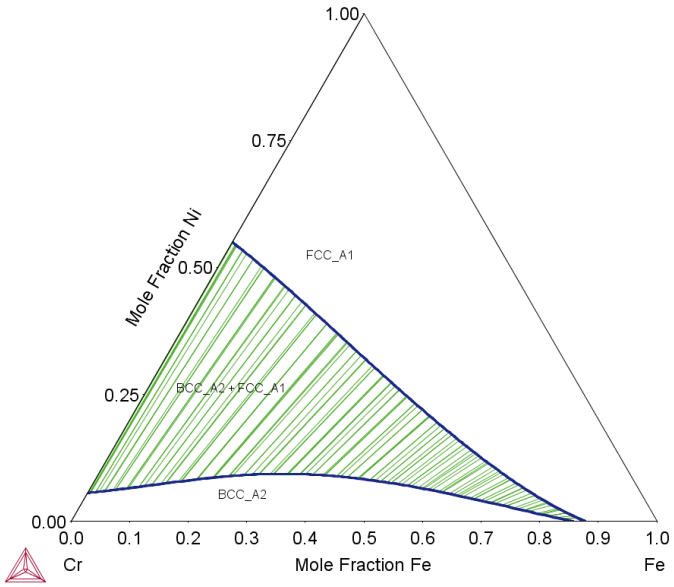

Figure 5: Calculated Cr-Fe-Ni isothermal section at 1000 °C.

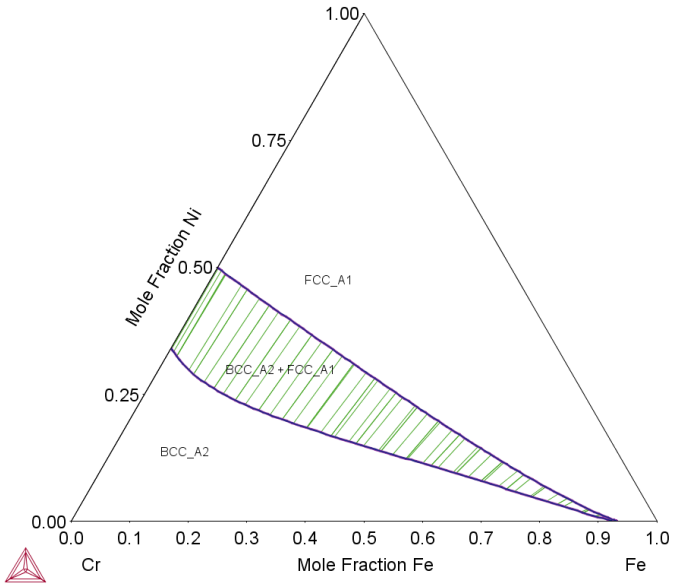

Figure 6: Calculated Cr-Fe-Ni isothermal section at 1300 °C.

FCC+BCC Forming Ternary Systems

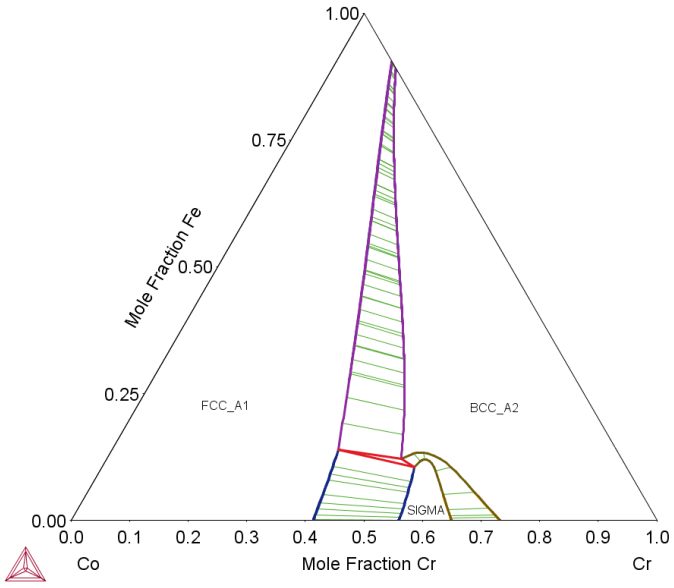

Figure 7: Calculated Co-Cr-Fe isothermal section at 1200 °C.

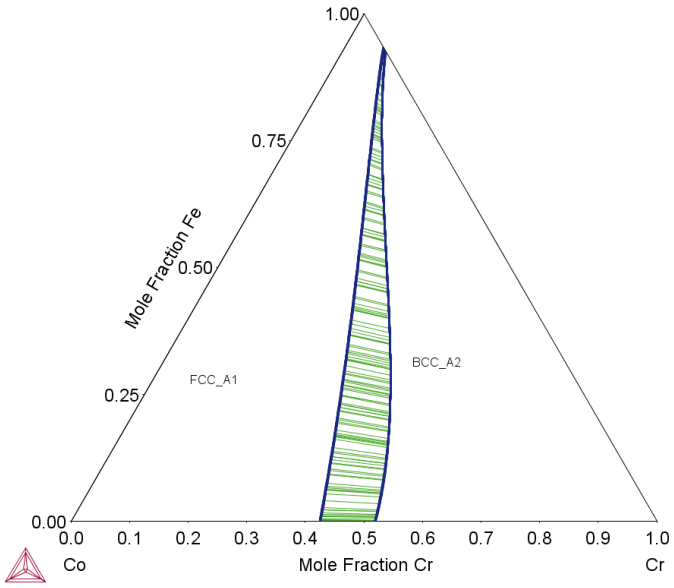

Figure 8: Calculated Co-Cr-Fe isothermal section at 1300 °C.

Multi-Component Alloy Systems

Figure 9 shows the effect of the Al addition on the phase formation in the CoCrFeNi-bases high entropy alloy. With a small amount of Al addition (<10 at.% Al), only FCC forms in as-cast alloys. The region roughly from 10 to 18 at.% Al is near the eutectic reaction, where both FCC and BCC can form in as-cast alloys. With an Al addition above 18 at.%, only BCC forms. It should be noted, however, that the phase formation also depends on the actual experimental conditions, especially the cooling rate and the heat treatment. The data from Wang [2012] indicate the compositions of the investigated as-cast alloys and the observed phases. The data from Kao et al. [2011] are the composition limits for forming BCC, FCC and BCC+FCC in as-cast alloys or alloys homogenized at 1000 °C.

Figure 10 and Figure 11 show the phase formation in the Co-Cr-Fe-Mn-Ni equiatomic alloy from the equilibrium calculation and the Scheil calculation, respectively. They indicate that a single FCC solid solution can be obtained during solidification at different cooling rates (from equilibrium solidification to extremely non-equilibrium solidification). The single FCC state remains during a wide temperature ranged down to 600 °C. Cantor et al [2004] and Otto et al. [2013] observed only FCC in as-cast alloys. The single phase state remained after the alloy had been annealed at 1000 °C or 850 °C for three days [2013, Otto].

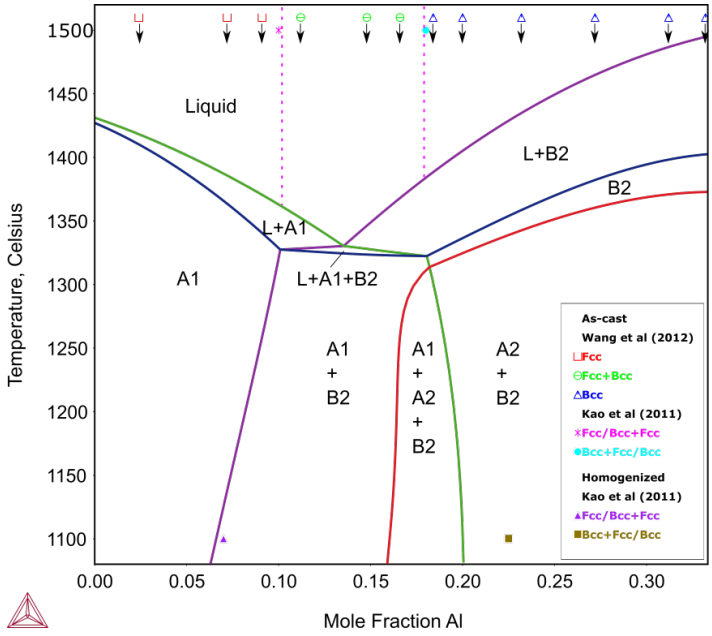

Figure 9: Calculated phase diagram along the composition line of CoCrFeNi-Al.

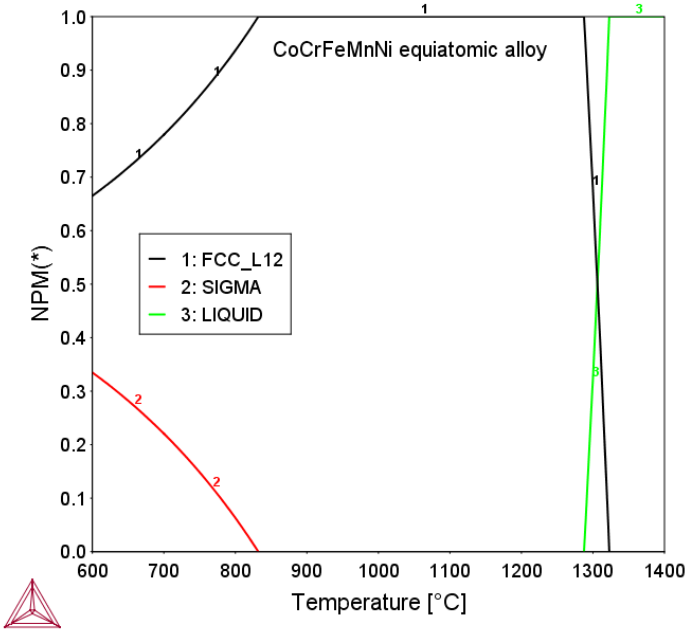

Figure 10: Equilibrium calculation of the phase formation in the Co-Cr-Fe-Mn-Ni equiatomic alloy.

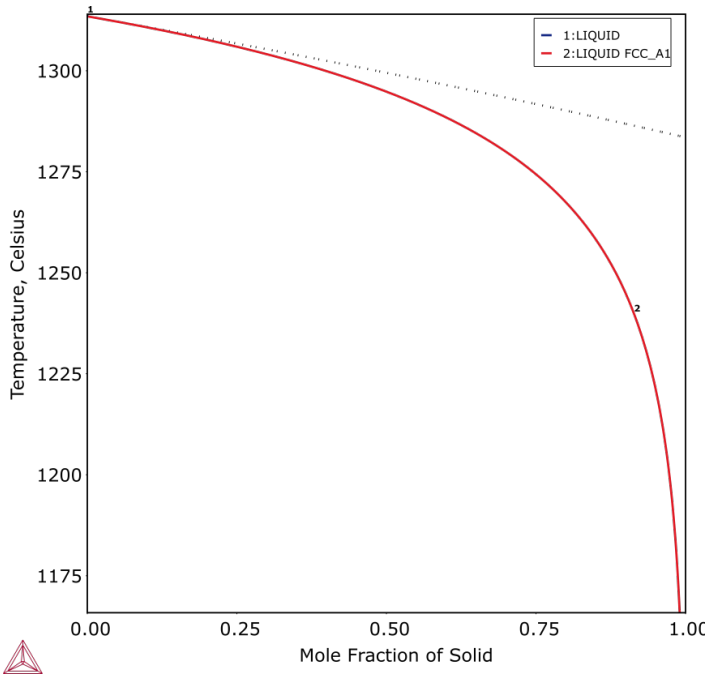

Figure 11: Scheil calculation of the phase formation in the Co-Cr-Fe-Mn-Ni equiatomic alloy.

Cantor et al. [2004] had investigated as-cast alloys prepared by melting spinning and reported that adding Cu into the Co-Cr-Fe-Mn-Ni alloy destabilized FCC dendrites and caused an interdendritic segregation with no second phase. According to the present calculation, as shown in Figure 12, however, the interdendritic region actually corresponds to a Cu-rich secondary FCC phase. In other words, there is a miscibility gap of FCC. Note that the conclusion of no second phase by Cantor et al. [2004] had been drawn merely based on the poor XRD pattern, which was not sufficient to identify two sets of FCC phases. Figure 12 suggested a peritectic type transformation from the primary FCC and liquid to the secondary FCC, but the amount of liquid involved in the transition is much more than that of the pimary FCC. The phase formation was dramatically affected by the composition segregation during the fast cooling, the accumulation of Cr in the residual liquid caused the BCC phase to form. The amount of BCC was calculated to be less than 1 %, so it might be overlooked during the microstructure examination. Moreover, the formation of BCC might be suspended during melting spinning, due to insufficient diffusion in both liquid and FCC and/or inefficient nucleation of BCC.

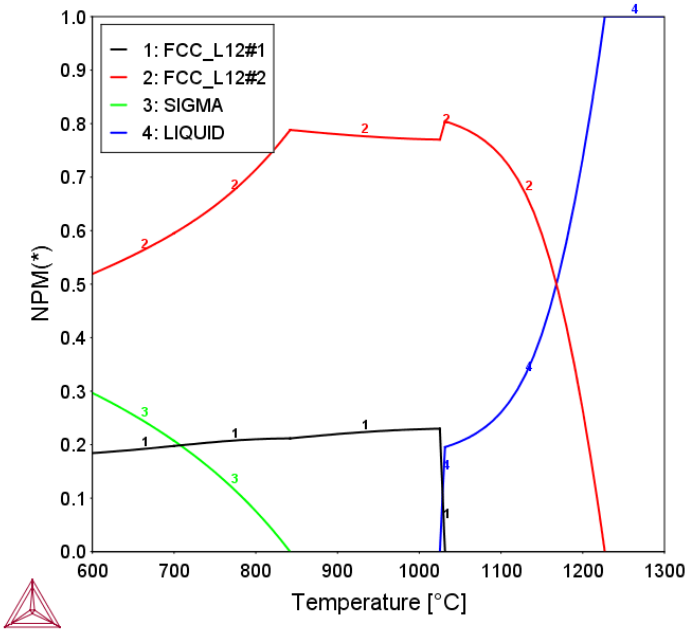

Figure 12: Equilibrium calculation of the phase formation in the Co-Cr-Cu-Fe-Mn-Ni equiatomic alloy.

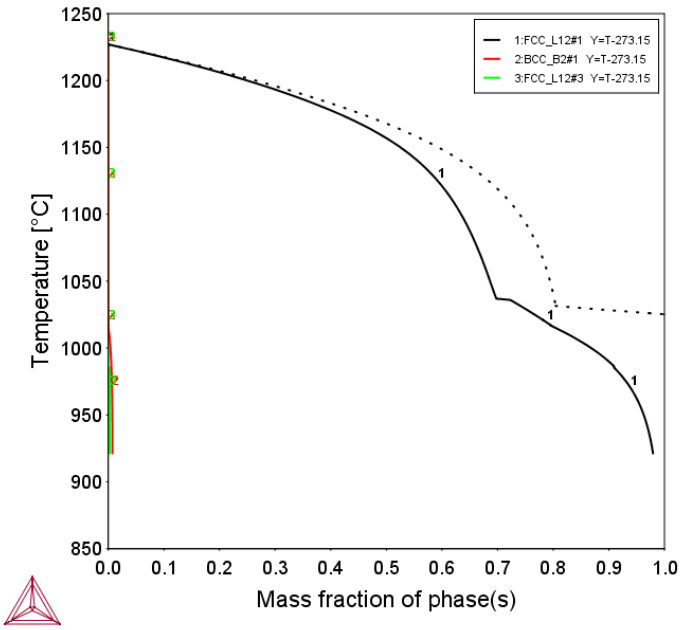

Figure 13: Scheil calculation of the phase formation in the Co-Cr-Cu-Fe-Mn-Ni equiatomic alloy.

Figure 14 shows that single BCC_A2 solid solution can be obtained in as-cast equiatomic Al-Cr-Mn-Ti-V alloys. The BCC single phase remains in a wide temperature range down to 629 °C, where it starts to order to form the B2 phase.

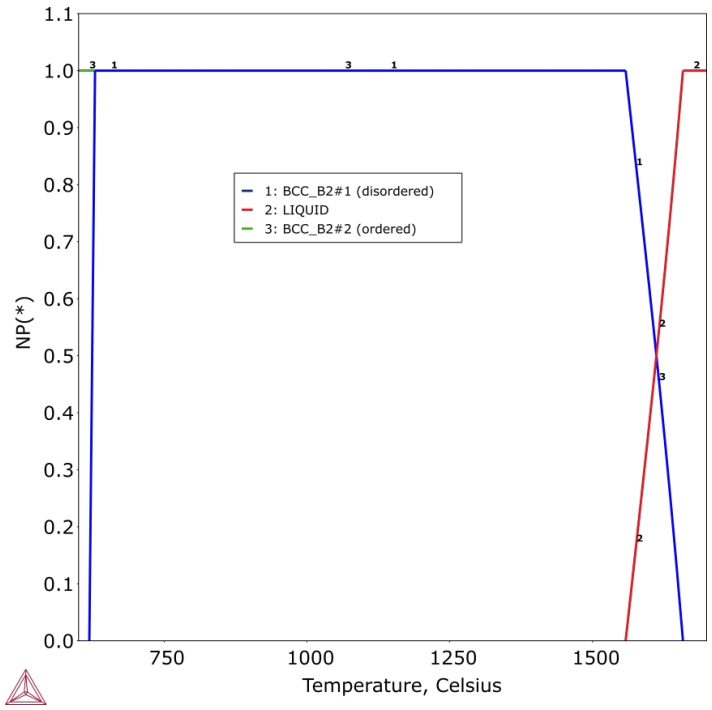

Figure 14: Equilibrium calculation of the phase formation in the Al-Cr-Mn-Ti-V equiatomic alloy.

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About the Included Phases

TCHEA4 contains nearly all stable phases in all assessed binary systems and most ternary systems. In total, 500 solution and intermetallic phases are modeled.

Phases Included in TCHEA4 lists all phases and Models for the Phases Included in TCHEA4 includes a detailed description of the models, e.g. number of sublattices and constituents on each sublattice.

The ordered B2 and $L1_2$ phases, together with bcc_A2 and fcc_A1, respectively, have been modeled with the so-called partitioning model, which describes an ordered phase and its disordered counterpart using a single Gibbs energy curve. This type of description is of particular importance to be able to predict second order transformations between a disordered phase and its ordered structures. Also note that there may be several possible composition sets for the phases named FCC_L12 and BCC_B2 designated by #1, #2, and so on (e.g. FCC_L12#1 and FCC_L12#2), due to the co-existence of disordered and ordered structures or the presence of miscibility gap. The #n suffix (where n is an integer) is generated dynamically by Thermo-Calc when using global minimization and therefore the identification of the phases should be determined from their site occupations. It can be found by LIST_EQUILIBRIUM with the VXNS option in the Console Mode or showing the site fraction in moles of the constituent elements in the Graphical Mode. When the site occupancies of the first and second sublattices are equal the phase is disordered.

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. In order to show the information, it is recommended to use the command LIST_SYSTEM with the option of `Constituents` in the Database (TDB) module.

Phases Included in TCHEA4

LIQUID
BCC_A2
BCC_B2
FCC_A1
FCC_L12
HCP_A3
AL10CU10FE
AL10FEMN2
AL10V
AL11CR2
AL11CU5MN3
AL11MN3ZN2
AL11MN4_HT
AL11MN4_LT
AL11RE4
AL12MN
AL12W
AL13CO4
AL13CR2
AL13FE2MN2
AL13FE4
AL13IR4
AL13NI38ZN49
AL15SI2M4
AL16FEMN3
AL1MN1SI1
AL2_7IR
AL23CUFE4

AL23V4
AL24MN5ZN
AL28CU4MN7
AL28IR9
AL2FE
AL2MN2SI3
AL2MNSI3
AL2TI_LT
AL2TI3N2
AL2W
AL2ZR3
AL31MN6NI2
AL3CO
AL3IR
AL3MN4SI2
AL3MNSI2
AL3NI_D011
AL3NI2_D513
AL3NI5
AL3RH_HT
AL3RH_LT
AL3TI_D022
AL3TI_LT
AL3Y_HT
AL3Y_LT
AL3ZR_D023
AL3ZR2
AL3ZR4

AL3ZR5
AL45IR13
AL4C3
AL4CR
AL4MN_R
AL4MN_U
AL4RE
AL4SIC4
AL4W
AL4ZR5
AL5CO2_D811
AL5CU4ZN
AL5FE2
AL5FE4
AL5MN6SI7
AL5TI2_HT
AL5TI3
AL5W
AL62CU25FE13
AL63MO37
AL6MN
AL77W23
AL7CU2FE
AL7CU4NI
AL7RH3
AL7V
AL7W3
AL8CR5_H

AL8CR5_L
AL8MN5
AL8MO3
AL8SIC7
AL8V5
AL9CO2
AL9CR4_H
AL9CR4_L
AL9IR2
AL9MN2ZN
ALB12_ALPHA
ALCR2C
ALCU_DEL
ALCU_EPS
ALCU_ETA
ALCU_PRIME
ALCU_ZETA
ALCU3MN2
ALFESI_ALPHA
ALFESI_BETA
ALFESI_DELTA
ALFESI_ GAMMA
ALFESI_TAU1
ALFESI_TAU3
ALM3C_E21
ALMNSI_T6
ALMNSI_T8
ALMNTI_L12

ALMO_A2
ALN_B4
ALNI2ZN
ALPHA_B19
ALRE
ALRE2
ALRH2
ALSI3TI2
ALTI_L10
ALTI2N
ALTI3_D019
ALTI3N
ALZR
ALZR2_B82
B3SI
B4C
B6SI
B82_OMEGA
BCT_A5
BETA_ RHOMBO_B
BN_B4
BNSI
C14_LAVES
C15_LAVES
C16_THETA
C36_LAVES
CBCC_A12
CEMENTITE

CHI_A12
CO10CU57TI33
CO11ZR2
CO17Y2
CO2SI_C23
CO3SI
CO3V
CO3Y
CO3Y2
CO3Y4
CO5Y_D2D
CO5Y8
CO7HF
CO7M2
CO7Y6
COSN_B35
COSN3_OS32
COY_BF
COZN_DELTA
COZN_ GAMMA_D82
COZN_ GAMMA1
COZN_ GAMMA2
COZN_HT
COZN_LT
CR2B_ORTH
CR2NI2SI

CR3MN5
CR3NI5SI2
CR3SI_A15
CR5B3_D81
CRMN3_HT_ SIGMA
CRNBSI
CRNI2_OP6
CRSI2_C40
CRZN13
CRZN17
CU10HF7
CU10SN3
CU10ZR7
CU15SI4_ EPSILON
CU2TI
CU2TIZR
CU2Y_H
CU2Y_L
CU33SI7_ DELTA
CU3SN
CU3TI2
CU41SN11
CU46NI25SI29
CU4MNSN
CU4TI1
CU4TI3
CU4Y
CU51HF14
CU51ZR14
CU56SI11_

GAMMA
CU5MN4SI
CU6NISI3
CU6SN5_HT_ NIAS
CU6SN5_LT
CU7Y1
CU7Y2
CU8HF3
CU8ZR3
CUB_A13
CUMNZN
CUSI_ETA
CUTI_B11
CUTI3
DIAMOND_A4
DIS_MU
DIS_SIG
FE2SI
FE3SN2
FE4N_LP1
FE5SN3
FE8SI2C
FECN_CHI
FENBZR_CFC2
FESI_B20
FESI2_H
FESI2_L
FEZN_DELTA
FEZN_ GAMMA_D81
FEZN_ GAMMA_D82

FEZN_ZETA
G_PHASE
GAMMA_D03
GAMMA_D83
GAMMA_H
GAS:G
GPHASE_ ALCOTI
GRAPHITE
HEUSLER_L21
HF2M
HF3N2
HF3NI7
HF3RH4
HF3RH5
HF4N3
HF5IR3
HF5SN4
HF8NI21
HFIR
HFIR3
HFMN
HFN
HFNI_ALPHA
HFNI3_ALPHA
HFNI3_BETA
HFRE
HFRH
HFSN2_C40
IR2Y3
IR2Y5
IR3SI

IR3SI2
IR3SI4
IR3SI5
IR3Y
IR3Y5
IR3ZR5
IR4B3
IR4B5
IR4SI5
IR5B4
IRMN_L10
IRNB_L10
IRSI
IRSI3_HT
IRSI3_LT
IRV_L10
IRV_RT
IRY3
IRZR_ALPHA
IRZR_B2
IRZR3
M11SI8
M12C
M23C6
M2B_TETR
M3B2_D5A
M3B2_T
M3B4_D7B
M3C2
M3SI
M3SI2_D5A

M4SI3
M5B6
M5C2
M5SI3_D88
M6C
M6SI5
M7C3
MB_B27
MB_B33
MB2_C32
MB4
MC_ETA
MC_SHP
MN11SI19
MN12Y
MN15NI45SI40
MN15NI50SI35
MN1NI1SI1
MN2B_D1F
MN2NISI
MN3NI2SI
MN3SI
MN3SN2
MN3TI
MN4TI
MN52NI29SI19
MN66NI4SI30
MN6N4
MN6N5
MN6NI16SI7
MN6NISI3

MN6SI
MN9SI2
MNNI_L10
MNNI2
MNNISI_T5
MNNISI_T6
MNTA
MNTI_HT
MNTI_LT
MNZN9
MO2B5_D8I
MO3IR
MO7IR3
MOB_BG
MOIR_HT
MOIR_LT
MOIR3
MONI_DELTA
MONI4_BETA
MOSI2_C11B
MOZN22
MOZN7
MSI_B27
MSI2_C1
MU_PHASE
MZR3_E1A
NB13NI75TI12
NB15NI56TI29
NB15NI80TI5
NB2ZN3
NB3RU5

NB5NI75TI20
NB8NI9TI3
NBSN2
NBZN
NBZN15
NBZN2
NBZN3
NBZN7
NI10ZR7
NI11ZR9
NI17Y2
NI2SI_TETA
NI2TA_C11B
NI2V
NI2Y
NI2Y3
NI31SI12
NI3B_D011
NI3SI_ MONOCL
NI3SI_ORTHO
NI3SI2
NI3SN4
NI3TA_D0A
NI3TI_D024
NI3Y
NI4B3
NI4Y
NI5ZR_C15B
NI7ZR2
NI8M
NISI_B31

NITI2
NIZN_TP2
NIZN8_DELTA
NIZR
O_PHASE
O1_DIS
P_PHASE
PI_A13
R_PHASE
RE2SI
RE3B_E1A
RE7B3_D102
REB2
RESI2_C11B
REZR2
RH2SN
RH3SN2
RH3ZR
RH4ZR3_HT
RH4ZR3_LT
RH5TI3
RH5ZR3
RH7B3
RHB
RHSN
RHSN2_RT
RHSN4
RHZR_HT
RHZR_LT
RHZR2
RU25Y44

RU2B3
RU2SI_C37
RU2SI3
RU2SN3
RU2Y3
RU2Y5
RU3SN7
RUB
RUSI
RUY3
SI3N4
SIC
SIGMA
SN10Y11
SN2Y_C49
SN3Y
SN4Y5
SN5TI6
SN5Y2
SNTI2
T_M23B6_D84
T1_CU2TI
T1CUNITI
T2_CU3TI2
T2CUNITI
T3_CU4TI3
T4CUFETI
T4CUNITI
T5CUFETI
T6CUNITI
TA3SN

TA41IR59
TA43IR57
TA5SI3_D8L
TAAL
TAAL2
TAN_EPS
TASN2
TAU_COSNTI
TI2ALC
TI2N_C4
TI3ALC
TI3ALC2
TI3N2
TI3SIC2
TI4N3
TISI2_C54
TIZN10
TIZN15
TIZN5
V2B3
V3SN
V4ZN5
VSN2
VZN3_L12
W2B5_D8I
W2B9
W3MC
W5SI3_D8M
WB_ALPHA
WB_BETA
Y13ZN58

Y15C19_H
Y15C19_R
Y2C3_H
Y2C3_R
Y2ZN17
Y3SI5_HT
Y3SI5_LT
YB6
YB66
YC_GAMMA
YC2_C11A
YSI2_HT
YZN2_A
YZN2_B
YZN3
YZN5
Z_PHASE
ZN11Y3
ZN12Y
ZN22ZR
ZN2ZR3
ZN39ZR5
ZN3ZR_HT
ZNZR_B2
ZR5SI4_TP36
ZRB12_D2F
ZRSI2_C49

Models for the Phases Included in TCHEA4

LIQUID:L :AL AL1N1 B C CO CR CU FE HF HF1N1 IR MN MO N NB NI RH RE RU SI SN TA TI V W Y ZN ZR: > LIQUID mixture.
FCC_A1 2 SUBL, SITES 1.00: 1.00: :AL CO CR CU FE HF IR MN MO NB NI RE RH RU SI SN TA TI V W Y ZN ZR:B C N VA: > If FCC_L12 is defined, this phase will be combined to it.
FCC_L12 3 SUBL, SITES 0.75: 0.25: 1.00: :AL CO CR CU FE HF IR MN MO NB NI RE RH RU SI SN TA TI V W Y ZN ZR:AL CO CR CU FE HF IR MN MO NB NI RE RH RU SI SN TA TI V W Y ZN ZR:B C N VA: > This phase has some contribution from FCC_A1.
BCC_A2 2 SUBL, SITES 1.00: 3.00: :AL CO CR CU FE HF IR MN MO NB NI RE RH RU SI SN TA TI V W Y ZN ZR VA:B C N VA: > If BCC_B2 is defined, this phase will be combined to it.
BCC_B2 3 SUBL, SITES 0.50: 0.50: 3.00: :AL CO CR CU FE HF IR MN MO NB NI RE RH RU SI SN TA TI V W Y ZN ZR VA:AL CO CR CU FE HF IR MN MO NB NI RE RH RU SI SN TA TI V W Y ZN ZR VA:B C N VA: > This phase has some contribution from BCC_A2.
HCP_A3 2 SUBL, SITES 1.00: 0.50: :AL CO CR CU FE HF IR MN MO NB NI RE RH RU SI SN TA TI V W Y ZN ZR:B C N VA: > Disordered HCP_A3 solution phase; Also for pure Co, Re, Ru, Ti
CBCC_A12 2 SUBL, SITES 1.00: 1.00: :AL CO CR CU FE IR MN MO NB NI RE RU SI SN TA TI V W Y ZN ZR:B C VA:
CUB_A13 2 SUBL, SITES 1.00: 1.00: :AL CO CR CU FE HF IR MN MO NB NI RE RU SI SN TA TI V W Y ZN ZR:B C VA:
DIS_FCC_A1 2 SUBL, SITES 1.00: 1.00:

:AL CO CR CU FE HF IR MN MO NB NI RE RH RU SI SN TA TI V W Y ZN ZR:B C N VA:
DIAMOND_A4 :AL B C SI SN: > Pure C, Si or solution phases based on them
BETA_RHOMBO_B 2 SUBL, SITES 93.00: 12.00: :B:B C CU SI:
GRAPHITE :B C: > Strukturbericht A9
BCT_A5 :AL CU NI SN ZN: > Disordered BCT solution phase; Also for pure Sn
HCP_ZN 2 SUBL, SITES 1.00: 0.50: :AL CO CR CU FE IR MN NI RE RH RU SN TI ZN:VA:
T_M23B6_D84 4 SUBL, SITES 20.00: 6.00: 6.00: 3.00: :CO HF NI RE:B:B VA:AL CR HF MO RE TA TI V W ZR: > ternary borides, Prototype CR23C6, Strukturbericht D84
NI3B_D011 2 SUBL, SITES 3.00: 1.00: :CO CR FE MO NI:B: > also Co3B
RE3B_E1A 2 SUBL, SITES 3.00: 1.00: :CR MO RE TA W:B:
RE7B3_D102 3 SUBL, SITES 7.00: 3.00: 3.00: :CO CR MO NB RE RU TA W:B:B VA:
RH7B3 2 SUBL, SITES 0.70: 0.30: :RH:B:
M2B_TETR 2 SUBL, SITES 2.00: 1.00: :AL CO CR FE MN MO NB NI RE TA W:B: > also Co2B, Fe2B, Mn2B, Mo2B, Ni2B, Ta2B, W2B, Strukturbericht C16
CR2B_ORTH 2 SUBL, SITES 0.67: 0.33:

:CR FE MO RE:B: > Strukturbericht D1f
MN2B_D1F 2 SUBL, SITES 0.67: 0.33: :MN:B:
CR5B3_D81 2 SUBL, SITES 0.62: 0.38: :CR MO:B: > also Mo5B3
M3B2_D5A 2 SUBL, SITES 3.00: 2.00: :FE HF MO NB TA V:B: > also TA3B2, NB3B2, V3B2, prototype U3SI2, Strukturbericht D5a
M3B2_T 3 SUBL, SITES 0.40: 0.20: 0.40: :CR FE MO NI W:CR FE NI:B: > ternary borides, Mo2FeB2, Mo2CrB2
IR4B3 2 SUBL, SITES 4.00: 3.00: :IR:B:
NI4B3 2 SUBL, SITES 0.57: 0.43: :NI:B:
IR5B4 2 SUBL, SITES 5.00: 4.00: :IR:B:
MB_B27 2 SUBL, SITES 1.00: 1.00: :B:CO CR FE HF MN MO RE TI Y: > prototype FeB(beta), StrukturBericht B27, also CoB, HfB, MnB, TiB
MB_B33 2 SUBL, SITES 1.00: 1.00: :CR FE HF MO NB NI TA TI V:B: > CrB, NbB, NiB, TaB, VB
MOB_BG 2 SUBL, SITES 1.00: 1.00: :CR FE MO:B: > MoB, Strukturbericht Bg
WB_ALPHA 2 SUBL, SITES 1.00: 1.00: :B C VA:W: > Strukturbericht Bg

RUB 2 SUBL, SITES 1.00: 1.00: :RU:B:
WB_BETA 2 SUBL, SITES 1.00: 1.00: :B C VA:W: > Strukturbericht B33, prototype CrB
RHB 2 SUBL, SITES 1.00: 1.10: :RH:B: > Strukturbericht B81
M5B6 2 SUBL, SITES 5.00: 6.00: :NB V:B: > proptotype V5B6, also Nb5B6
IR4B5 2 SUBL, SITES 4.00: 5.00: :IR:B:
M3B4_D7B 2 SUBL, SITES 4.00: 3.00: :B:AL CR HF MN NB TA TI V: > Prototype: Ta3B4, also Cr3B4, Mn3B4, Nb3B4, Ti3B4, V3B4 and ternary
RU2B3 2 SUBL, SITES 2.00: 3.00: :RU:B:
V2B3 2 SUBL, SITES 0.40: 0.60: :V:B:
MB2_C32 2 SUBL, SITES 2.00: 1.00: :B:AL CR HF MN MO NB RU TA TI V Y ZR: > AlB2,CrB2,HfB2,MnB2,MoB2,NbB2,RuB2,TaB2,TiB2,VB2,YB2,ZrB2
REB2 3 SUBL, SITES 1.00: 2.00: 2.00: :RE:B:B VA:
MO2B5_D8I 2 SUBL, SITES 0.32: 0.68: :MO:B: > Strukturbericht D8i
W2B5_D8I 2 SUBL, SITES 5.00: 2.00: :B C VA:W:
MB4 2 SUBL, SITES 0.20: 0.80:

:CR MN MO Y:B:
W2B9 2 SUBL, SITES 9.00: 2.00: :B:W:
YB6 2 SUBL, SITES 1.00: 6.00: :Y:B:
ZRB12_D2F 2 SUBL, SITES 12.00: 1.00: :B:Y ZR: > also YB12, Strukturbericht D2f
ALB12_ALPHA 2 SUBL, SITES 1.00: 12.00: :AL TI:B:
YB66 2 SUBL, SITES 1.00: 66.00: :Y:B:
M12C 3 SUBL, SITES 6.00: 6.00: 1.00: :CO NI:MO W:C: > Prototype Mo6Ni6C
M6C 4 SUBL, SITES 2.00: 2.00: 2.00: 1.00: :CO FE NI:MO NB TA W:CO CR FE MO NB NI TA V W:C: > Prototype W3Fe3C, Strukturbericht E93
ALM3C_E21 3 SUBL, SITES 1.00: 3.00: 1.00: :AL:CO FE:C: > AlCo3C, AlFe3C, Perovskite
TI3ALC 3 SUBL, SITES 3.00: 1.00: 1.00: :TI:AL:C VA:
W3MC 3 SUBL, SITES 3.00: 1.00: 1.00: :W:CO NI:C: > W3CoC, W3NiC
M23C6 3 SUBL, SITES 20.00: 3.00: 6.00: :CO CR FE MN NI RE V:CO CR FE MN MO NI RE V W:C: > prototype Cr23C6, Strukturbericht D84
ALCR2C 3 SUBL, SITES 1.00: 1.00: 2.00: :AL:C:CR:

CEMENTITE 2 SUBL, SITES 3.00: 1.00: :CO CR FE MN MO NI V W:C N: > Strukturbericht D011
TI2ALC 3 SUBL, SITES 2.00: 1.00: 1.00: :TI:AL:C VA:
M5C2 2 SUBL, SITES 5.00: 2.00: :FE MN:C: > Mn5C2
M7C3 2 SUBL, SITES 7.00: 3.00: :CO CR FE MN MO NI RE V W:C: > proptotype Cr7C3, Strukturbericht D101
TI3ALC2 3 SUBL, SITES 3.00: 1.00: 2.00: :TI:AL SI:C VA:
M3C2 2 SUBL, SITES 3.00: 2.00: :CO CR MO V W:C: > prototype Cr3C2(beta), Strukturbericht D510
AL4C3 2 SUBL, SITES 4.00: 3.00: :AL SI:C: > Strukturbericht D71
MC_ETA 2 SUBL, SITES 1.00: 1.00: :MO V W:C VA: > MoC, prototype TiAs, Strukturbericht Bi
MC_SHP 2 SUBL, SITES 1.00: 1.00: :MO W:C N: > Prototype WC, also MoC low temperature,
YC_GAMMA 2 SUBL, SITES 1.00: 1.00: :Y:C C2 VA:
Y15C19_H 2 SUBL, SITES 19.00: 15.00: :C:Y:
Y15C19_R 2 SUBL, SITES 19.00: 15.00: :C:Y:

Y2C3_H 3 SUBL, SITES 2.00: 2.00: 1.00: :Y:C:C VA:
Y2C3_R 3 SUBL, SITES 2.00: 2.00: 1.00: :Y:C:C VA:
YC2_C11A :C2Y1:
PI_A13 3 SUBL, SITES 12.80: 7.20: 4.00: :CR:FE NI:N: > Cr-(Fe,Ni)-nitrides
FE4N_LP1 2 SUBL, SITES 4.00: 1.00: :CO CR FE MN NI:C N: > Only stable in Co-N, Fe-N and Cr-Fe-N when gas suspended
ALTI3N 3 SUBL, SITES 1.00: 3.00: 1.00: :AL:TI:N: > Strukturbericht E21
ALTI2N 3 SUBL, SITES 1.00: 2.00: 1.00: :AL:TI:N:
AL2TI3N2 3 SUBL, SITES 2.00: 3.00: 2.00: :AL:TI:N:
FECN_CHI 2 SUBL, SITES 2.20: 1.00: :FE:C N: > Only stable in C-Fe-N when gas suspended
TI4N3 2 SUBL, SITES 0.69: 0.32: :TI:N:
TI2N_C4 2 SUBL, SITES 2.00: 1.00: :TI:N:
Z_PHASE 3 SUBL, SITES 1.00: 1.00: 1.00: :CR FE:MO NB V:N VA:
HF3N2 2 SUBL, SITES 3.00: 2.00: :HF:N:
MN6N4 2 SUBL, SITES 6.00: 4.00:

:MN:N:
TI3N2 2 SUBL, SITES 0.71: 0.29: :TI:N:
HF4N3 2 SUBL, SITES 4.00: 3.00: :HF:N:
MN6N5 2 SUBL, SITES 6.00: 5.00: :MN:N:
ALN_B4 2 SUBL, SITES 1.00: 1.00: :AL:N:
TAN_EPS 2 SUBL, SITES 1.00: 1.00: :TA:N:
HFN 2 SUBL, SITES 1.00: 1.00: :HF:N VA:
MN6SI 2 SUBL, SITES 17.00: 3.00: :AL MN:SI ZN:
MN9SI2 2 SUBL, SITES 33.00: 7.00: :MN:SI:
CR3NI5SI2 4 SUBL, SITES 3.00: 5.00: 2.00: 1.00: :CR:NI:SI:C VA:
CR2NI2SI 3 SUBL, SITES 5.00: 5.00: 3.00: :CR:NI:SI:
CR3SI_A15 3 SUBL, SITES 3.00: 1.00: 3.00: :CR FE IR MO NB NI RE SI SN TA TI V ZR:AL CO CR IR MO NB NI RH RU SI SN TA TI V ZR:C VA: > also Cr3Ir, Cr3Rh, Cr3Ru, Mo3Al, Mo3Si, Nb3Al, Nb3Sn, Ti3Ir, V3Co, V3Ir, V3Ni, V3Si. Prototype Cr3Si.
CO3SI 2 SUBL, SITES 3.00: 1.00: :CO:SI:
IR3SI 2 SUBL, SITES 3.00: 1.00: :IR:SI:
M3SI 2 SUBL, SITES 3.00: 1.00:

:HF NB TA TI ZR:SI: > also Nb3Si, Ta3Si, Ti3Si, Zr3Si
MN3SI 2 SUBL, SITES 3.00: 1.00: :MN FE:AL SI:
NI3SI_ORTHO 2 SUBL, SITES 3.00: 1.00: :NI:SI: > Strukturbericht D011
NI31SI12 2 SUBL, SITES 5.00: 2.00: :CO CR CU FE NI:SI: > Ni5Si2 and its solution
CO2SI_C23 2 SUBL, SITES 2.00: 1.00: :CO CR CU FE IR NI TI:SI: > Prototype Co2Si (alpha), also Ni2Si (delta)
CRNBSI 3 SUBL, SITES 1.00: 1.00: 1.00: :CR:NB:SI: > hP9 Fe2P
FE2SI 2 SUBL, SITES 0.67: 0.33: :FE:SI:
NI2SI_TETA 3 SUBL, SITES 1.00: 1.00: 1.00: :CU NI:NI VA:AL SI:
RE2SI 2 SUBL, SITES 2.00: 1.00: :RE:SI:
RU2SI_C37 2 SUBL, SITES 2.00: 1.00: :RU:SI:
M5SI3_D88 4 SUBL, SITES 2.00: 3.00: 3.00: 1.00: :CR CU FE HF MN MO NI NB SI TI W Y ZR:AL CR SI SN TI:CR CU FE HF MN MO NI NB TI Y ZR:C SN VA: > Fe5Si3, Hf5Si3, Mn5Si3, Ti5Cr3, Ti5Si3, Ti5Sn3, Y5Si3, Zr5Si3, Hf5Sn3, Y5Sn3, Zr5Sn3, Zr5Sn4, Mo5Si3C, Cr5Si3C, prototype Mn5Si3
TA5SI3_D8L 2 SUBL, SITES 5.00: 3.00: :HF NB TA:AL SI:

> also Nb5Si3, protoype Cr5B3, Strukturbericht D8l
W5SI3_D8M 3 SUBL, SITES 4.00: 1.00: 3.00: :CR FE MO NB TI V W:CR FE MO NB TI V W SI:AL SI SN: > also Cr5Si3, Mo5Si3, Nb5Si3, V5Si3
IR3SI2 2 SUBL, SITES 3.00: 2.00: :IR:SI:
M3SI2_D5A 2 SUBL, SITES 3.00: 2.00: :HF NB ZR:SI: > Hf3Si2, Zr3Si2
NI3SI2 2 SUBL, SITES 3.00: 2.00: :NI:SI:
M11SI8 2 SUBL, SITES 11.00: 8.00: :CR NB:SI: > Cr11Si8, Nb11Si8
M4SI3 2 SUBL, SITES 4.00: 3.00: :CR NI RU:SI: > Cr4Si3, Nb4Si3, Ru4Si3
ZR5SI4_TP36 2 SUBL, SITES 5.00: 4.00: :HF NB TI Y ZR:AL SI: > Hf5Si4, Ti5Si4, Y5Si4, Zr5Si4(alpha), prototype Zr5Si4
M6SI5 2 SUBL, SITES 6.00: 5.00: :CR NB TI V:SI: > Cr6Si5, Nb6Si5, V6Si5
FESI_B20 2 SUBL, SITES 1.00: 1.00: :CO CR FE MN NI RE:AL SI: > also CoSi, CrSi, Mn Si, ReSi, Prototype FeSi
IRSI 2 SUBL, SITES 1.00: 1.00: :IR:SI:
MSI_B27 2 SUBL, SITES 1.00: 1.00: :HF NB TI Y ZR:AL SI: > TiSi, HfSi, YSi, ZrSi(alpha), Prototype FeB

NISI_B31 2 SUBL, SITES 1.00: 1.00: :NI:SI:
RUSI 2 SUBL, SITES 1.00: 1.00: :RU:SI:
IR4SI5 2 SUBL, SITES 4.00: 5.00: :IR:SI:
IR3SI4 2 SUBL, SITES 3.00: 4.00: :IR:SI:
RU2SI3 2 SUBL, SITES 2.00: 3.00: :RU:SI:
IR3SI5 2 SUBL, SITES 3.00: 5.00: :IR:SI:
Y3SI5_HT 2 SUBL, SITES 3.00: 5.00: :Y:SI:
Y3SI5_LT 2 SUBL, SITES 3.00: 5.00: :Y:SI:
MN11SI19 2 SUBL, SITES 11.00: 19.00: :MN:AL SI:
CRSI2_C40 2 SUBL, SITES 1.00: 2.00: :CR CU HF MO NB SI TA TI V W:AL CR CU SI: > CrSi2, NbSi2, TaSi2, VSi2, Prototype CrSi2
FESI2_H 2 SUBL, SITES 0.30: 0.70: :FE:SI:
FESI2_L 2 SUBL, SITES 0.33: 0.67: :FE:SI:
MSI2_C1 2 SUBL, SITES 1.00: 2.00: :CO CU MN NI:AL CU SI: > CoSi2, Prototype CaF2
MOSI2_C11B 2 SUBL, SITES 1.00: 2.00: :AL CO CU FE MO NI RH W ZN:AL CR HF SI TI ZR: > also AlCr2,CuHf2,CuTi2,CuZr2,PdTi2,RhTi2,Ti2Zn,WSi2,ZnZr2, Prototype

RESI2_C11B 2 SUBL, SITES 0.36: 0.64: :RE:SI:
TISI2_C54 2 SUBL, SITES 1.00: 2.00: :MO NB RU TI ZR:AL SI SN: > also ZrSn2
YSI2_HT 2 SUBL, SITES 1.00: 2.00: :Y:SI:
ZRSI2_C49 2 SUBL, SITES 1.00: 2.00: :ZR Y HF NB:SI: > ZrSi2, YSi2, HfSi2, Prototype ZrSi2
IRSI3_LT 2 SUBL, SITES 1.00: 3.00: :IR:SI:
IRSI3_HT 2 SUBL, SITES 1.00: 3.00: :IR:SI:
ALFESI_ALPHA 4 SUBL, SITES 0.66: 0.19: 0.05: 0.10: :AL:FE:SI:AL SI:
ALFESI_BETA 3 SUBL, SITES 14.00: 3.00: 3.00: :AL:FE:SI:
ALFESI_GAMMA 3 SUBL, SITES 3.00: 1.00: 1.00: :AL:FE:SI:
ALFESI_DELTA 3 SUBL, SITES 0.55: 0.15: 0.30: :AL:FE:SI:
ALFESI_TAU1 3 SUBL, SITES 2.00: 2.00: 1.00: :AL:FE:SI:
ALFESI_TAU3 3 SUBL, SITES 2.00: 1.00: 1.00: :AL:FE:SI:
AL2MN2SI3 3 SUBL, SITES 2.00: 2.00: 3.00: :AL:MN:SI: > the Al-Mn-Si ternary phase, tao1
AL5MN6SI7 3 SUBL, SITES 5.00: 6.00: 7.00: :AL:MN:SI:

> the Al-Mn-Si ternary phase, tao2
AL1MN1SI1 3 SUBL, SITES 1.00: 1.00: 1.00: :AL:MN:SI: > the Al-Mn-Si ternary phase, tao3
AL3MNSI2 3 SUBL, SITES 3.00: 1.00: 2.00: :AL:MN:SI: > the Al-Mn-Si ternary phase, tao4
AL3MN4SI2 3 SUBL, SITES 3.00: 4.00: 2.00: :AL:MN:SI: > the Al-Mn-Si ternary phase, tao5
ALMNSI_T6 2 SUBL, SITES 4.00: 1.00: :AL MN:SI: > the Al-Mn-Si ternary phase, tao6
ALMNSI_T8 5 SUBL, SITES 6.00: 2.00: 12.00: 6.00: 2.00: :MN VA:MN VA:AL:AL SI:AL SI: > the Al-Mn-Si ternary phase, tao8
AL2MNSI3 3 SUBL, SITES 2.00: 1.00: 3.00: :AL:MN:SI: > the Al-Mn-Si ternary phase, tao10
MN15NI45SI40 3 SUBL, SITES 0.15: 0.45: 0.40: :MN:NI:SI: > Mn-Ni-Si ternary phase, T1 or N
MN15NI50SI35 3 SUBL, SITES 0.15: 0.50: 0.35: :MN:NI:SI: > Mn-Ni-Si ternary phase, T2 or PHI
MN6NI16SI7 3 SUBL, SITES 0.21: 0.55: 0.24: :MN:NI:SI: > Mn-Ni-Si ternary phase, T3 or G
MN1NI1SI1 3 SUBL, SITES 1.00: 1.00: 1.00: :MN:NI:SI: > Mn-Ni-Si ternary phase, T4 or E

MNNISI_T5 2 SUBL, SITES 1.00: 2.00: :MN:NI SI: > Mn-Ni-Si ternary phase, T5 or "tao 1"
MNNISI_T6 2 SUBL, SITES 1.00: 2.00: :MN:NI SI: > Mn-Ni-Si ternary phase, T6 or "tao 2"
MN3NI2SI 3 SUBL, SITES 3.00: 2.00: 1.00: :MN:NI:SI: > Mn-Ni-Si ternary phase, T7 or Omega
MN2NISI 2 SUBL, SITES 3.00: 1.00: :MN NI:SI: > Mn-Ni-Si ternary phase, T8 or S
MN6NISI3 3 SUBL, SITES 0.61: 0.12: 0.27: :MN:NI:SI: > Mn-Ni-Si ternary phase, T9 or R
MN66NI4SI30 3 SUBL, SITES 0.66: 0.04: 0.30: :MN:NI:SI: > Mn-Ni-Si ternary phase, T10 or U
MN52NI29SI19 3 SUBL, SITES 0.52: 0.29: 0.19: :MN:NI:SI: > Mn-Ni-Si ternary phase, T11 or W
B4C 2 SUBL, SITES 1.00: 1.00: :B11C B12:B2 C2B CB2: > Strukturbericht D1g
BN_B4 2 SUBL, SITES 1.00: 1.00: :B:N:
B3SI 3 SUBL, SITES 6.00: 2.00: 6.00: :B:SI:B SI: > Strukturbericht D1g
B6SI 3 SUBL, SITES210.00: 23.00: 48.00: :B:SI:B SI:

BNSI 3 SUBL, SITES 61.00: 1.00: 8.00: :B:SI:B SI:
SIC 2 SUBL, SITES 1.00: 1.00: :SI:C: > Strukturbericht B3
SI3N4 2 SUBL, SITES 3.00: 4.00: :SI:N:
AL4SIC4 3 SUBL, SITES 4.00: 1.00: 4.00: :AL:SI:C:
AL8SIC7 3 SUBL, SITES 8.00: 1.00: 7.00: :AL:SI:C:
FE8SI2C 3 SUBL, SITES 8.00: 2.00: 1.00: :FE:SI:C: > Prototype Mn8Si2C
TI3SIC2 3 SUBL, SITES 3.00: 1.00: 2.00: :TI:SI:C:
DIS_MU :AL CO CR CU FE MN MO NB NI RE TA TI W: > Part of the description of MU_PHASE.
MU_PHASE 4 SUBL, SITES 1.00: 2.00: 6.00: 4.00: :AL CO CR CU FE MN MO NB NI RE TA TI W:AL CO CR CU FE MN MO NB NI RE TA TI W:AL CO CR CU FE MN MO NB NI RE TI TA W:AL CO CR CU FE MN MO NB NI RE TA TI W:
DIS_SIG :AL CO CR FE IR MN MO NB NI RE RU SI TA TI V W: > Part of the description of SIGMA phase.
SIGMA 3 SUBL, SITES 10.00: 4.00: 16.00: :AL CO CR FE IR MN MO NB NI RE RU SI TA TI V W:AL CO CR FE IR MN MO NB NI RE RU SI TA TI V W:AL CO CR FE IR MN MO NB NI RE RU SI TA TI V W: > DIS_SIG contribution is introduced in the description of this phase
CHI_A12 3 SUBL, SITES 24.00: 10.00: 24.00:

:CR FE NI RE:AL CR HF MO NB TA TI W ZR:CR FE MO NB NI RE TA W:
> also Hf5Re24, Mo2Re8, Ta3Re7, Ti5Re24, WRe3, Zr5Re24
G_PHASE 3 SUBL, SITES 16.00: 6.00: 7.00:
:AL CO FE MN NI TI:HF NB TI Y ZR:CO FE MN NI SI:
> prototype Th6Mn23, Strukturbericht D8a, also Al16Ni7Ti6(Mu)
GAMMA_D83 3 SUBL, SITES 4.00: 1.00: 8.00:
:AL NI SI ZN:AL CU NI SI ZN:CU FE MN NI ZN:
> Cu5Zn8, Ni5Zn8, Al5Cu8 (rt), Prototype Cu9Al4 (cP52, P-43m)
GAMMA_H 3 SUBL, SITES 4.00: 1.00: 8.00:
:AL ZN:AL CU ZN:CU FE MN NI:
> Cu5Zn8-type Al8Cu5 (ht) phase
HEUSLER_L21 3 SUBL, SITES 0.50: 0.50: 1.00:
:AL CR NI SN TI:AL HF NB NI TA TI ZR:CO FE NI RU VA:
> Heusler phase, Strukturbericht L21
P_PHASE 3 SUBL, SITES 24.00: 20.00: 12.00:
:CR FE NI RE:CR FE MO NI RE:MO:
> Prototype : Cr9Mo21Ni20
R_PHASE 3 SUBL, SITES 27.00: 14.00: 12.00:
:CO CR FE NI RE:MO W:CO CR FE MO NI RE W:
> Prototype : Co5Cr2Mo3
MNNI_L10 2 SUBL, SITES 0.50: 0.50:
:CU MN NI:CU MN NI:
IRMN_L10 2 SUBL, SITES 0.50: 0.50:
:IR MN TI:IR MN TI:
> also IrTi
ALTI_L10 2 SUBL, SITES 1.00: 1.00:
:AL CO CR MN MO NB SN TA TI V W ZR:AL CO CR MN MO NB SN TA TI V W ZR:
> Solution of ordered L10.
ALCU_EPS 2 SUBL, SITES 1.00: 1.00:
:AL CU NI:CU FE:
ALCU_ETA 2 SUBL, SITES 1.00: 1.00:

:AL CU:CU FE NI ZN:
ALPHA_B19 2 SUBL, SITES 1.00: 1.00: :MO NB TI V ZR:MO NB TI V ZR: > ordered HCP, prototype AuCd
ALRE 2 SUBL, SITES 1.00: 1.00: :AL:RE:
ALZR 2 SUBL, SITES 1.00: 1.00: :AL:HF Y ZR: > also AlHf, AlY
COSN_B35 2 SUBL, SITES 0.50: 0.50: :CO FE NI:SN: > This is CoSn, FeSn
COY_BF 2 SUBL, SITES 1.00: 1.00: :CO:Y:
CUTI_B11 2 SUBL, SITES 1.00: 1.00: :CO CU NI TI:CU NI TA TI:
HFIR 2 SUBL, SITES 1.00: 1.00: :HF:IR:
HFMN 2 SUBL, SITES 0.50: 0.50: :HF:MN:
HFNI_ALPHA 2 SUBL, SITES 0.50: 0.50: :HF:NI:
HFRE 2 SUBL, SITES 1.00: 1.00: :HF:RE:
HFRH 2 SUBL, SITES 1.00: 1.00: :HF RH:RH:
IRV_L10 2 SUBL, SITES 0.50: 0.50: :IR:IR V:
IRV_RT 2 SUBL, SITES 1.00: 1.00: :IR:V:
IRZR_B2 2 SUBL, SITES 1.00: 1.00:

:IR ZR:IR ZR:
IRZR_ALPHA 2 SUBL, SITES 1.00: 1.00: :IR ZR:ZR:
MNTA 2 SUBL, SITES 1.00: 1.00: :MN:TA:
MNTI_LT 2 SUBL, SITES 1.00: 1.00: :MN:TI:
MOIR_HT 2 SUBL, SITES 1.00: 1.00: :IR MO:IR MO:
MOIR_LT 2 SUBL, SITES 1.00: 1.00: :MO:IR:
NBZN 2 SUBL, SITES 0.50: 0.50: :NB:ZN:
NIZN_TP2 2 SUBL, SITES 0.50: 0.50: :AL CU NI ZN:AL NI ZN:
NIZR 2 SUBL, SITES 1.00: 1.00: :NI:TI Y ZR:
RHSN 2 SUBL, SITES 1.00: 1.00: :RH:SN:
RHZR_LT 2 SUBL, SITES 1.00: 1.00: :RH:RH ZR: > i.e. alpha_RhZr
RHZR_HT 2 SUBL, SITES 1.00: 1.00: :RH:RH ZR: > i.e. beta_RhZr
ZNZR_B2 2 SUBL, SITES 1.00: 1.00: :ZN:ZR:
ALCU_PRIME 2 SUBL, SITES 2.00: 1.00: :AL:CU:
AL2FE 2 SUBL, SITES 2.00: 1.00: :AL CU:FE MN:

ALRE2 2 SUBL, SITES 1.00: 2.00: :AL:RE:
ALRH2 2 SUBL, SITES 1.00: 2.00: :AL:RH:
AL2TI_LT 2 SUBL, SITES 2.00: 1.00: :AL NB TI:AL CO NB TA TI V ZR:
AL2W 2 SUBL, SITES 2.00: 1.00: :AL:W:
ALZR2_B82 2 SUBL, SITES 1.00: 2.00: :AL:TI Y ZR: > also AlY2
C14_LAVES 2 SUBL, SITES 2.00: 1.00: :AL CO CR CU FE HF MN MO NB NI SI RE RU TA TI V W Y ZN ZR:AL CO CR CU FE HF MN MO NB NI SI RE RU TA TI V W Y ZN ZR: > prototype CuZn2
C15_LAVES 2 SUBL, SITES 2.00: 1.00: :AL CO CR CU FE HF IR MN MO NB NI SI RE RU TA TI V W Y ZN ZR:AL CO CR CU FE HF MO NB NI SI RE RU TA TI V W Y ZR:
C16_THETA 2 SUBL, SITES 2.00: 1.00: :AL HF MN MO NB SN TA TI W ZR:AL CO CR CU FE IR MN NI RH SI: > Al2Cu,Hf2Al,Hf2Ni,Sn2Co,Sn2Fe,Sn2Rh,Sn2Mn,Ta2Co,Ta2Ni,Zr2Co,Zr2Ni,Zr2Ir
C36_LAVES 2 SUBL, SITES 2.00: 1.00: :AL CO CR CU FE HF MO NB NI TA TI W ZR:AL CO CR CU FE HF MO NB NI TA TI W ZR:
CRNI2_OP6 2 SUBL, SITES 1.00: 2.00: :CR MO W:MO NI W:
CU2TI 2 SUBL, SITES 2.00: 1.00: :CO CU NI:TI:
CU2Y_H 2 SUBL, SITES 2.00: 1.00: :CU:Y:
CU2Y_L 2 SUBL, SITES 2.00: 1.00:

:CU:Y:
HF2M 2 SUBL, SITES 2.00: 1.00: :HF:IR RH:
HFSN2_C40 2 SUBL, SITES 1.00: 2.00: :HF:SN:
MNNI2 2 SUBL, SITES 1.00: 2.00: :MN NI:NI:
NBZN2 2 SUBL, SITES 0.33: 0.67: :NB:ZN:
NI2V 2 SUBL, SITES 2.00: 1.00: :MO NI:MO NB TA V: > Ni2V and its solutions
NI2TA_C11B 2 SUBL, SITES 2.00: 1.00: :CO NI:TA TI:
NITI2 2 SUBL, SITES 1.00: 2.00: :CO CR CU FE NI RE TI:AL CR CU HF NI TA TI ZR:
NI2Y 2 SUBL, SITES 2.00: 1.00: :NI:Y:
REZR2 2 SUBL, SITES 1.00: 2.00: :NI RE:ZR:
RHSN2_RT 2 SUBL, SITES 0.33: 0.67: :RH:SN:
RH2SN 2 SUBL, SITES 2.00: 1.00: :RH:SN:
SNTI2 2 SUBL, SITES 1.00: 2.00: :SN:TI:
SN2Y_C49 2 SUBL, SITES 2.00: 1.00: :SN:Y:
RHZR2 2 SUBL, SITES 1.00: 2.00: :RH:ZR:
TASN2 2 SUBL, SITES 1.00: 2.00:

:TA:SN:
VSN2 2 SUBL, SITES 0.60: 0.40: :SN:V:
YZN2_A 2 SUBL, SITES 1.00: 2.00: :Y:ZN:
YZN2_B 2 SUBL, SITES 1.00: 2.00: :Y:ZN:
AL3CO 2 SUBL, SITES 3.00: 1.00: :AL:CO:
ALCU_DEL 2 SUBL, SITES 2.00: 3.00: :AL:CU FE:
AL3IR 2 SUBL, SITES 0.75: 0.25: :AL:IR:
AL3NI_D011 2 SUBL, SITES 0.75: 0.25: :AL:NI:
AL3RH_LT 2 SUBL, SITES 3.00: 1.00: :AL:RH:
ALTI3_D019 2 SUBL, SITES 3.00: 1.00: :AL CO CR CU MN MO NB NI SN TA TI V W ZR:AL C CR MO NB NI SI SN TA TI V W: > Ni3Sn_LT, Mn3Sn, Ti3Sn.
AL3TI_D022 2 SUBL, SITES 3.00: 1.00: :AL CO CR FE MO NB NI SI TI V:AL CO CR MO NB NI SI TA TI V ZR: > gamma double prime, prototype Al3Ti, also Al3Nb, Al3Ta, Al3V, Ni3V
AL3Y_HT 2 SUBL, SITES 0.75: 0.25: :AL:Y:
AL3Y_LT 2 SUBL, SITES 0.75: 0.25: :AL:Y:
AL3ZR_D023 2 SUBL, SITES 3.00: 1.00: :AL ZN:HF TI ZR: > also Al3Hf, Zn3Zr
COSN3_OS32 2 SUBL, SITES 0.25: 0.75:

:CO:SN:
CO3V 2 SUBL, SITES 3.00: 1.00: :CO NI V:CO V:
CO3Y 2 SUBL, SITES 3.00: 1.00: :CO:Y:
CU3SN 2 SUBL, SITES 3.00: 1.00: :CU SN:CU SN:
CUTI3 2 SUBL, SITES 1.00: 3.00: :CU TI:TI:
HFIR3 2 SUBL, SITES 1.00: 3.00: :HF:IR:
HFNI3_ALPHA 2 SUBL, SITES 0.25: 0.75: :HF:NI:
HFNI3_BETA 2 SUBL, SITES 0.25: 0.75: :HF:NI:
IRY3 2 SUBL, SITES 1.00: 3.00: :IR:Y:
IR3Y 2 SUBL, SITES 3.00: 1.00: :IR:Y:
IRZR3 2 SUBL, SITES 1.00: 3.00: :IR:ZR:
MZR3_E1A 2 SUBL, SITES 1.00: 3.00: :CO FE NI:Y ZR: > COZR3, FEZR3, NiY3, COY3
MN3TI 2 SUBL, SITES 3.00: 1.00: :MN:TI:
MOIR3 2 SUBL, SITES 1.00: 3.00: :MO:IR MO:
MO3IR 2 SUBL, SITES 3.06: 0.94: :MO:IR:
NBZN3 2 SUBL, SITES 0.25: 0.75:

:NB:ZN:
NI3TA_D0A 2 SUBL, SITES 3.00: 1.00: :AL CO CR FE NI NB:AL FE MO NB NI TA TI V W: > also delta, Ni3Mo, Ni3Nb, Strukturbericht D0a, prototype Cu3Ti
NI3TI_D024 2 SUBL, SITES 0.75: 0.25: :AL CO CR CU FE HF NI TA TI W ZR:AL CR CU HF MO NB NI SI TA TI W ZR: > also Eta, AlNi6Ta
NI3Y 2 SUBL, SITES 3.00: 1.00: :FE NI:Y: > also Fe3Y
RH3ZR 2 SUBL, SITES 3.00: 1.00: :RH ZR:RH ZR:
RUY3 2 SUBL, SITES 0.25: 0.75: :RU:Y:
SN3Y 2 SUBL, SITES 3.00: 1.00: :SN:Y:
TA3SN 2 SUBL, SITES 3.00: 1.00: :TA:SN:
V3SN 2 SUBL, SITES 0.20: 0.80: :SN:V:
VZN3_L12 2 SUBL, SITES 1.00: 3.00: :V:ZN:
YZN3 2 SUBL, SITES 1.00: 3.00: :Y:ZN:
ZN3ZR_HT 2 SUBL, SITES 3.00: 1.00: :ZN:ZR:
AL13CO4 2 SUBL, SITES 13.00: 4.00: :AL:CO:
AL5CO2_D811 2 SUBL, SITES 5.00: 2.00: :AL:CO RH: > also Al5Rh2

AL9CO2 2 SUBL, SITES 9.00: 2.00: :AL:CO RH: > also Al9Rh2
AL11CR2 3 SUBL, SITES 10.00: 1.00: 2.00: :AL:AL:CR:
AL13CR2 2 SUBL, SITES 13.00: 2.00: :AL:CR:
AL4CR 2 SUBL, SITES 4.00: 1.00: :AL:CR:
AL8CR5_H 2 SUBL, SITES 8.00: 5.00: :AL:CR:
AL8CR5_L 2 SUBL, SITES 8.00: 5.00: :AL:CR: > Strukturbericht D810
AL9CR4_H 2 SUBL, SITES 9.00: 4.00: :AL:CR:
AL9CR4_L 2 SUBL, SITES 9.00: 4.00: :AL:CR:
ALCU_ZETA 2 SUBL, SITES 9.00: 11.00: :AL:CU FE:
AL23CUFE4 3 SUBL, SITES 23.00: 1.00: 4.00: :AL:CU:FE:
AL62CU25FE13 3 SUBL, SITES 0.12: 0.26: 0.62: :FE:AL CU:AL:
AL7CU2FE 3 SUBL, SITES 1.00: 2.00: 7.00: :FE NI:CU:AL: > Solution phase of the ternary compound Al7Cu2Fe
AL10CU10FE 3 SUBL, SITES 1.00: 10.00: 10.00: :FE:AL CU:AL:
AL7CU4NI 2 SUBL, SITES 1.00: 1.00: :AL:FE CU NI VA:

AL28CU4MN7 3 SUBL, SITES 28.00: 7.00: 4.00: :AL:MN:CU:
AL11CU5MN3 3 SUBL, SITES 11.00: 3.00: 5.00: :AL:MN:CU:
ALCU3MN2 3 SUBL, SITES 1.00: 2.00: 3.00: :AL:MN:CU:
AL13FE4 3 SUBL, SITES 0.63: 0.23: 0.14: :AL CU:FE MN RU:AL SI VA: > solution phases based on Al13Fe4 (aka Al3Fe) and Al13Ru4
AL5FE2 2 SUBL, SITES 5.00: 2.00: :AL CU:FE MN:
AL5FE4 :AL CU FE:
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:
AL9IR2 2 SUBL, SITES 0.82: 0.18: :AL:IR:
AL45IR13 2 SUBL, SITES 0.78: 0.22: :AL:IR:
AL13IR4 2 SUBL, SITES 0.77: 0.23: :AL:IR:
AL28IR9 2 SUBL, SITES 0.76: 0.24: :AL:IR:
AL2_7IR 2 SUBL, SITES 0.73: 0.27: :AL:IR:
AL12MN 2 SUBL, SITES 12.00: 1.00: :AL:MN:

AL4MN_R 2 SUBL, SITES461.00:107.00: :AL:MN FE: > AL461MN107
AL4MN_U 2 SUBL, SITES 4.00: 1.00: :AL:MN:
AL11MN4_LT 2 SUBL, SITES 11.00: 4.00: :AL:MN FE:
AL11MN4_HT 2 SUBL, SITES 29.00: 10.00: :AL MN:MN:
AL8MN5 3 SUBL, SITES 12.00: 5.00: 9.00: :AL TI ZN:MN:AL CU MN SI TI:
AL6MN 2 SUBL, SITES 6.00: 1.00: :AL:FE MN RE RU: > also Al6Re, Al6Ru
AL31MN6NI2 3 SUBL, SITES 31.00: 6.00: 2.00: :AL:MN:NI: > Orthorhombic, ternary Al-Mn-Ni phase
ALMNTI_L12 3 SUBL, SITES 0.25: 0.08: 0.67: :AL MN TI:AL MN:AL MN TI: > TI25MN9AL66_L12
AL63MO37 2 SUBL, SITES 63.00: 37.00: :AL:MO:
AL8MO3 2 SUBL, SITES 8.00: 3.00: :AL:MO:
ALMO_A2 2 SUBL, SITES 1.00: 1.00: :AL MO:AL MO: > Strukturbericht A2, it was badly described
AL3NI5 2 SUBL, SITES 0.38: 0.62: :AL:NI:
AL3NI2_D513 3 SUBL, SITES 3.00: 2.00: 1.00: :AL SI SN ZN:AL CU NI RU:RU NI VA:

> Al3Ni2, Al3Ru2
AL11RE4 2 SUBL, SITES 11.00: 4.00: :AL:RE:
AL4RE 2 SUBL, SITES 4.00: 1.00: :AL:RE:
AL3RH_HT 2 SUBL, SITES 2.00: 1.00: :AL:RH VA:
AL7RH3 2 SUBL, SITES 7.00: 3.00: :AL:RH:
AL15SI2M4 3 SUBL, SITES 14.00: 4.00: 5.00: :AL:FE MN:AL SI: > Solution of Al-Mn-Si ternary phase, tao 9, Al15(Mn,Fe)3Si2
AL3TI_LT 2 SUBL, SITES 3.00: 1.00: :AL TI:AL TI ZR:
AL5TI2_HT 2 SUBL, SITES 5.00: 2.00: :AL TI:AL NB TA TI V ZR:
AL5TI3 2 SUBL, SITES 5.00: 3.00: :AL:TA TI:
AL10V 2 SUBL, SITES 10.00: 1.00: :AL:V:
AL7V 2 SUBL, SITES 7.00: 1.00: :AL:V:
AL23V4 2 SUBL, SITES 23.00: 4.00: :AL:V:
AL8V5 2 SUBL, SITES 8.00: 5.00: :AL:V:
AL77W23 2 SUBL, SITES 77.00: 23.00: :AL:W:
AL7W3 2 SUBL, SITES 7.00: 3.00: :AL:W:
AL12W 2 SUBL, SITES 12.00: 1.00:

:AL:MO RE W: > also Al12Mo, Al12Re
AL4W 2 SUBL, SITES 4.00: 1.00: :AL:MO W: > also Al4Mo
AL5W 2 SUBL, SITES 5.00: 1.00: :AL:MO W: > also AL5MO
AL2ZR3 2 SUBL, SITES 2.00: 3.00: :AL:HF TI Y ZR: > also Al2Hf3, Al2Y3
AL3ZR4 2 SUBL, SITES 3.00: 4.00: :AL:HF TI ZR: > also Al3Hf4
AL3ZR2 2 SUBL, SITES 3.00: 2.00: :AL:HF ZR: > also Al3Hf2
AL3ZR5 2 SUBL, SITES 3.00: 5.00: :AL:TI ZR: > Strukturbericht D8m, prototype Si3W5
AL4ZR5 2 SUBL, SITES 4.00: 5.00: :AL:ZR:
CO7HF 2 SUBL, SITES 7.00: 1.00: :CO:HF:
CO10CU57TI33 3 SUBL, SITES 0.10: 0.57: 0.33: :CO:CU:TI:
CO7M2 2 SUBL, SITES 7.00: 2.00: :CO:NB TA: > Co7Nb2, Co7Ta2
CO17Y2 3 SUBL, SITES 1.00: 2.00: 15.00: :CO2 Y:CO2 Y:CO:

CO5Y_D2D 3 SUBL, SITES 1.00: 4.00: 1.00: :CO2 Y:CO:CO VA:
CO3Y2 2 SUBL, SITES 3.00: 2.00: :CO:Y:
CO7Y6 2 SUBL, SITES 7.00: 6.00: :CO:Y:
CO3Y4 2 SUBL, SITES 3.00: 4.00: :CO:Y:
CO5Y8 2 SUBL, SITES 5.00: 8.00: :CO:Y:
COZN_LT 2 SUBL, SITES 1.00: 1.00: :CO ZN:VA:
COZN_HT 2 SUBL, SITES 1.00: 1.00: :CO ZN:VA:
COZN_GAMMA_D82 2 SUBL, SITES 1.00: 1.00: :CO ZN:VA: > Zn11Co2 Prototype Zn9(Zn0.5Fe0.5)2Fe2 (cI52, I-43m)
COZN_DELTA 2 SUBL, SITES 0.12: 0.88: :CO:ZN:
COZN_GAMMA1 2 SUBL, SITES 0.12: 0.88: :CO:ZN:
COZN_GAMMA2 2 SUBL, SITES 0.07: 0.93: :CO:ZN:
CO11ZR2 2 SUBL, SITES 11.00: 2.00: :CO:ZR:
CRMN3_HT_SIGMA 3 SUBL, SITES 8.00: 4.00: 18.00: :MN:CR:CR MN:
CR3MN5 2 SUBL, SITES 3.00: 5.00: :CR:MN:
CRZN13 2 SUBL, SITES 1.00: 13.00: :CR:ZN:

CRZN17 2 SUBL, SITES 1.00: 17.00: :CR:ZN:
CU51HF14 2 SUBL, SITES 51.00: 14.00: :CU:HF:
CU8HF3 2 SUBL, SITES 8.00: 3.00: :CU:HF:
CU10HF7 2 SUBL, SITES 10.00: 7.00: :CU:HF:
CU5MN4SI 3 SUBL, SITES 0.50: 0.37: 0.13: :CU:MN:SI:
CU6NISI3 2 SUBL, SITES 0.73: 0.27: :CU NI:SI:
CU46NI25SI29 3 SUBL, SITES 0.46: 0.25: 0.29: :CU:NI:SI:
CU6SN5_HT_NIAS 3 SUBL, SITES 1.00: 1.00: 1.00: :CO CU MN NI VA:AL CU NI SN:CO CU MN NI VA: > Cu6Sn5_HT, Co3Sn2, Mn(2-x)Sn, Ni3Sn2
CU33SI7_DELTA 2 SUBL, SITES 0.82: 0.17: :CU:SI:
CU15SI4_EPSILON 2 SUBL, SITES 0.79: 0.21: :CU MN:AL SI:
CU56SI11_GAMMA 2 SUBL, SITES 0.84: 0.16: :CU MN NI SI:SI:
CU56SI11_GAMMA 2 SUBL, SITES 0.84: 0.16: :CU MN NI SI:SI:
CUSI_ETA 2 SUBL, SITES 0.76: 0.24: :CU MN NI:SI:
CU6SN5_LT 3 SUBL, SITES 1.00: 1.00: 1.00: :CU:CU SN:SN:
CU10SN3 2 SUBL, SITES 0.77: 0.23: :CU NI:SN:

CU41SN11 2 SUBL, SITES 41.00: 11.00: :CU SN ZN:CU SN ZN: > Cu41Sn11 with solubility of Zn.
CU3TI2 2 SUBL, SITES 3.00: 2.00: :CU NI FE:CO TI:
CU4TI1 2 SUBL, SITES 4.00: 1.00: :CU TI:CU TI:
CU4TI3 2 SUBL, SITES 4.00: 3.00: :CO CU NI:TI:
CU2TIZR 3 SUBL, SITES 0.50: 0.25: 0.25: :CU:TI:ZR:
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:
CU10ZR7 2 SUBL, SITES 10.00: 7.00: :CU:ZR:
CU51ZR14 2 SUBL, SITES 51.00: 14.00: :CU:ZR:
CU8ZR3 2 SUBL, SITES 8.00: 3.00: :CU:ZR:
FENBZR_CFC2 3 SUBL, SITES 2.00: 1.00: 3.00: :FE NB ZR:NB ZR:NB ZR:
FE3SN2 2 SUBL, SITES 3.00: 2.00: :FE:SN:
FE5SN3 2 SUBL, SITES 5.00: 3.00: :FE:SN:
FEZN_GAMMA_D82 4 SUBL, SITES 0.15: 0.15: 0.23: 0.46: :FE ZN:FE ZN:FE ZN:ZN:

FEZN_GAMMA_D81 3 SUBL, SITES 0.14: 0.12: 0.74: :FE:FE ZN:ZN:
FEZN_DELTA 4 SUBL, SITES 0.06: 0.18: 0.53: 0.24: :FE:FE ZN:ZN:ZN:
FEZN_ZETA 3 SUBL, SITES 0.07: 0.86: 0.07: :FE VA:ZN:VA ZN:
GAMMA_D03 :CU MN NI SN ZN: > Cu3Sn solution, Prototype BiF3 (cF16, Fm-3m)
HF5IR3 2 SUBL, SITES 5.00: 3.00: :HF:IR:
HF3NI7 2 SUBL, SITES 0.30: 0.70: :HF:NI:
HF8NI21 2 SUBL, SITES 8.00: 21.00: :HF ZR:NI: > also ZR8NI21, prototype Hf8Ni21
HF3RH4 2 SUBL, SITES 3.00: 4.00: :HF:RH:
HF3RH5 2 SUBL, SITES 3.00: 5.00: :HF:RH:
HF5SN4 2 SUBL, SITES 5.00: 4.00: :HF:SN:
IR2Y3 2 SUBL, SITES 2.00: 3.00: :IR:Y:
IR2Y5 2 SUBL, SITES 2.00: 5.00: :IR:Y:
IR3Y5 2 SUBL, SITES 3.00: 5.00: :IR:Y:
IR3ZR5 2 SUBL, SITES 3.00: 5.00: :IR:ZR:
MN3SN2 2 SUBL, SITES 3.00: 2.00:

:MN:SN:
MNTI_HT 2 SUBL, SITES 0.52: 0.48: :MN:TI:
MN4TI 2 SUBL, SITES 0.81: 0.18: :MN:TI:
MN12Y 2 SUBL, SITES 12.00: 1.00: :MN:Y:
MNZN9 2 SUBL, SITES 1.00: 9.00: :MN:ZN:
MO7IR3 2 SUBL, SITES 0.70: 0.30: :MO:IR:
MONI4_BETA 2 SUBL, SITES 1.00: 4.00: :MO W:NI: > also WNi4, Strukturbericht D1a
MONI_DELTA 3 SUBL, SITES 24.00: 20.00: 12.00: :CO CR FE NI RE:CO CR FE MO NI RE W:CU MO W:
MOZN7 2 SUBL, SITES 1.00: 7.00: :MO:ZN:
MOZN22 2 SUBL, SITES 1.00: 22.00: :MO:ZN:
NB15NI56TI29 3 SUBL, SITES 0.15: 0.56: 0.29: :NB:NI:TI:
NB8NI9TI3 3 SUBL, SITES 0.40: 0.45: 0.15: :NB:NI:TI:
NB5NI75TI20 3 SUBL, SITES 0.05: 0.75: 0.20: :NB:NI:TI:
NB13NI75TI12 3 SUBL, SITES 0.13: 0.75: 0.12: :NB:NI:TI:
NB15NI80TI5 3 SUBL, SITES 0.15: 0.80: 0.05: :NB:NI:TI:
NB3RU5 2 SUBL, SITES 0.38: 0.62:

:NB RU:RU:
NBSN2 2 SUBL, SITES 1.00: 2.00: :NB SN V:NB SN:
NBZN7 2 SUBL, SITES 0.12: 0.88: :NB:ZN:
NBZN15 2 SUBL, SITES 0.06: 0.94: :NB:ZN:
NB2ZN3 2 SUBL, SITES 0.40: 0.60: :NB:ZN:
NI8M 2 SUBL, SITES 8.00: 1.00: :NI:NB TA: > Ni8Ta, Ni8Nb
NI7ZR2 2 SUBL, SITES 7.00: 2.00: :AL CO CR NI:HF Y ZR: > also NI7HF2, NI7Y2, CO7HF2 and CO7Y2
NI3SN4 3 SUBL, SITES 0.25: 0.25: 0.50: :CU NI:NI SN:SN:
NI2Y3 2 SUBL, SITES 2.00: 3.00: :NI:Y:
NI4Y 2 SUBL, SITES 4.00: 1.00: :NI:Y:
NI17Y2 2 SUBL, SITES 1.00: 0.12: :AL FE NI:Y: > also Fe17Y2
NIZN8_DELTA 2 SUBL, SITES 0.11: 0.89: :NI:AL ZN:
NI11ZR9 2 SUBL, SITES 11.00: 9.00: :NI:HF ZR: > also Ni11Hf9
NI10ZR7 2 SUBL, SITES 23.00: 17.00: :NI:HF ZR:

> also Ni10Hf7
NI5ZR_C15B 2 SUBL, SITES 5.00: 1.00: :AL CU NI:HF Y ZR: > also Ni5Y, Ni5Hf, Cu5Hf and Cu5Zr, Strukturbericht C15b
RHSN4 2 SUBL, SITES 1.00: 4.00: :RH:SN:
RH3SN2 3 SUBL, SITES 0.12: 0.50: 0.38: :RH:RH:SN:
RH5TI3 2 SUBL, SITES 5.00: 3.00: :RH:TI:
RH4ZR3_LT 2 SUBL, SITES 4.00: 3.00: :RH ZR:ZR: > alpha_Rh4Zr3
RH4ZR3_HT 2 SUBL, SITES 4.00: 3.00: :RH ZR:ZR: > beta_Rh4Zr3
RH5ZR3 2 SUBL, SITES 5.00: 3.00: :RH:RH ZR:
RU3SN7 2 SUBL, SITES 0.30: 0.70: :RU:SN:
RU2SN3 2 SUBL, SITES 0.40: 0.60: :RU:SN:
RU2Y3 2 SUBL, SITES 0.40: 0.60: :RU:Y:
RU25Y44 2 SUBL, SITES 0.36: 0.64: :RU:Y:
RU2Y5 2 SUBL, SITES 0.29: 0.71: :RU:Y:
SN5TI6 2 SUBL, SITES 5.00: 6.00: :AL SN:NB TI: > also Sn5Nb6

SN5Y2 2 SUBL, SITES 5.00: 2.00: :SN:Y:
SN10Y11 2 SUBL, SITES 10.00: 11.00: :SN:Y:
SN4Y5 2 SUBL, SITES 4.00: 5.00: :SN:Y:
TAAL 2 SUBL, SITES 0.52: 0.48: :TA:AL:
TAAL2 2 SUBL, SITES 0.35: 0.65: :TA:AL:
TA41IR59 2 SUBL, SITES 0.41: 0.59: :TA:IR:
TA43IR57 2 SUBL, SITES 0.43: 0.57: :TA:IR TA:
T1CUNITI 2 SUBL, SITES 2.00: 1.00: :CU NI:TI: > the Cu-Ni-Ti ternary phase, Tau1
T2CUNITI 3 SUBL, SITES 0.17: 2.83: 2.00: :CU:NI:TI: > the Cu-Ni-Ti ternary phase, Tau2
T4CUNITI 3 SUBL, SITES 0.05: 0.70: 0.25: :CU:NI:TI: > the Cu-Ni-Ti ternary phase, Tau4
T6CUNITI 3 SUBL, SITES 0.25: 0.50: 0.25: :CU:NI:TI: > the Cu-Ni-Ti ternary phase, Tau6
T1_CU2TI 2 SUBL, SITES 2.00: 1.00: :CU FE:TI: > the Cu-Fe-Ti ternary phase, Tau1
T2_CU3TI2 2 SUBL, SITES 3.00: 2.00: :CU FE:TI:

> the Cu-Fe-Ti ternary phase, Tau2
T3_CU4TI3 2 SUBL, SITES 4.00: 3.00: :CU FE:TI: > the Cu-Fe-Ti ternary phase, Tau3
T4CUFETI 2 SUBL, SITES 0.63: 0.37: :CU FE:TI: > the Cu-Fe-Ti ternary phase, Tau4
T5CUFETI 2 SUBL, SITES 0.55: 0.45: :CU FE:TI: > the Cu-Fe-Ti ternary phase, Tau5
TIZN5 2 SUBL, SITES 1.00: 5.00: :TI:ZN:
TIZN10 2 SUBL, SITES 1.00: 10.00: :TI:ZN:
TIZN15 2 SUBL, SITES 1.00: 15.00: :TI:ZN:
V4ZN5 2 SUBL, SITES 4.00: 5.00: :V:ZN:
Y2ZN17 2 SUBL, SITES 2.00: 17.00: :Y:ZN:
Y13ZN58 2 SUBL, SITES 13.00: 58.00: :Y:ZN:
YZN5 2 SUBL, SITES 1.00: 5.00: :Y:ZN:
ZN12Y 2 SUBL, SITES 12.00: 1.00: :ZN:Y:
ZN11Y3 2 SUBL, SITES 11.00: 3.00: :ZN:Y:
ZN22ZR 2 SUBL, SITES 22.00: 1.00: :ZN:ZR:
ZN39ZR5 2 SUBL, SITES 39.00: 5.00:

:ZN:ZR:
ZN2ZR3 2 SUBL, SITES 2.00: 3.00: :ZN:ZR:
GAS:G :N2:
IRNB_L10 2 SUBL, SITES 1.00: 1.00: :IR NB:IR NB:
NI3SI_MONOCL 2 SUBL, SITES 3.00: 1.00: :NI:SI:
GPHASE_ALCOTI 4 SUBL, SITES 1.00: 16.00: 7.00: 6.00: :AL CO:AL TI:CO:TI:
AL5CU4ZN 4 SUBL, SITES 1.00: 4.00: 4.00: 1.00: :AL CU:AL:CU:ZN:
AL24MN5ZN 3 SUBL, SITES 5.00: 1.00: 24.00: :MN ZN:ZN:AL:
AL9MN2ZN 3 SUBL, SITES 2.00: 1.00: 9.00: :MN:ZN:AL:
AL11MN3ZN2 3 SUBL, SITES 3.00: 2.00: 11.00: :MN:ZN:AL:
O_PHASE 3 SUBL, SITES 0.50: 0.25: 0.25: :NB TA TI:AL NB TA TI:NB TA TI: > The O phase
O1_DIS 2 SUBL, SITES 0.75: 0.25: :AL NB TI:AL NB TI: > The disordered O phase
ALNI2ZN 3 SUBL, SITES 0.25: 0.50: 0.25: :AL:NI:ZN:
AL13NI38ZN49 3 SUBL, SITES 0.13: 0.38: 0.49: :AL:NI:ZN: > Al-Ni-Zn ternary phase
ALSI3TI2 3 SUBL, SITES 0.17: 0.50: 0.33:

:AL:SI:TI:
B82_OMEGA 3 SUBL, SITES 1.00: 1.00: 1.00: :AL SN:CO NB SN TA TI:TI:
TAU_COSNTI 3 SUBL, SITES 1.00: 1.00: 1.00: :CO NI:SN:TI:
CU4MNSN 3 SUBL, SITES 0.67: 0.17: 0.17: :CU:SN:MN:
CUMNZN 3 SUBL, SITES 0.33: 0.33: 0.33: :CU:MN:ZN: