TCHEA3: TCS High Entropy Alloy Database

Database name:	TCS High Entropy Alloy Database	*Database acronym:*	TCHEA
Database owner:	Thermo-Calc Software AB	*Database version:*	3.0
Database segment:	High entropy alloys (aka. multi-principal element alloys)		

TCHEA 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]. TCHEA 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.

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 are assessed to their full range of composition and temperature and can be calculated with the BINARY Module in Thermo-Calc. In total, more than 400 ternaries are assessed, and 136 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 included in the sections Assessed Binary Systems in Full Range of Composition and Temperature and Assessed Ternary Systems in Full Range of Composition and Temperature. Also see Tentatively 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.

TCHEA contains nearly all stable phases in all assessed binary systems and most ternary systems. In total, 438 solution and intermetallic phases are modelled. The section Phases Included in TCHEA lists all phases and the section Models for the Phases Included in TCHEA includes a detailed description of the models, e.g. number of sublattices and constituents on each sublattice.

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

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.

Assessed Binary Systems in 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
B	X																								
C	X	X																							
Co	X	X	X																						
Cr	X	X	X	X																					
Cu	X	X	X	X	X																				
Fe	X	X	X	X	X	X																			
Hf	X	X	X	X	X	X	X																		
Ir	X		X	X	X	X	X																		
Mn	X	X	X	X	X	X	X	X	X																
Mo	X	X	X	X	X	X	X	X		X															
N	X	X		X	X	X	X			X	X														
Nb	X	X	X	X	X	X	X	X		X	X	X													
Ni	X	X	X	X	X	X	X	X	X	X	X	X	X												
Re	X	X	X	X	X	X	X	X	X	X	X		X	X											
Rh	X		X	X	X	X	X		X	X				X	X										
Ru	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X									
Si	X	X	X	X	X	X	X	X		X	X	X	X	X	X		X								
Sn	X	X	X	X	X	X	X	X	X	X			X	X	X	X	X	X							
Ta	X	X	X	X	X	X	X	X		X	X	X	X	X	X		X	X	X						
Ti	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X					
V	X	X	X	X	X	X	X	X		X	X	X	X	X	X		X	X	X	X	X				
W	X	X	X	X	X	X	X	X			X	X	X	X	X		X	X	X	X	X	X			
Y	X	X	X	X	X	X	X	X		X	X		X	X	X		X	X	X	X	X	X	X		
Zn	X	X	X	X	X	X	X	X	X	X	X			X	X	X	X	X	X	X	X	X	X	X	
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

Critically assessed Ternary Systems in Full Range of Composition and Temperature

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

Tentatively Assessed Ternary Systems

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

Al-Co-Mo	Al-Si-Zr	Co-Mo-V	Cr-Nb-W	Fe-Nb-Ti	Mo-Ru-W
Al-Co-Nb	Al-Ta-Ti	Co-Nb-Ni	Cr-Nb-Zr	Fe-Nb-W	Mo-Si-Zr
Al-Co-Ru	Al-Ta-W	Co-Nb-Si	Cr-Ni-Ru	Fe-Nb-Zr	Nb-Ni-Re
Al-Co-Si	Al-Ti-V	Co-Nb-Ta	Cr-Ni-V	Fe-Ni-Ta	Nb-Ni-Si
Al-Co-Ta	Al-Ti-W	Co-Nb-Ti	Cr-N-Nb	Fe-Ni-V	Nb-Ni-Ta
Al-Cr-Fe	C-Co-Re	Co-Nb-W	Cr-N-V	Fe-Ni-Zr	Nb-Ni-V
Al-Cr-Mo	C-Co-V	Co-Ni-Ru	Cr-Re-Ru	Fe-Re-Ti	Nb-Ni-W
Al-Cr-Nb	C-Cr-Mn	Co-Ni-Ta	Cr-Re-Ta	Fe-Re-W	Nb-Ni-Zr
Al-Cr-Re	C-Cr-Mo	Co-Ni-Ti	Cr-Re-V	Fe-Re-Zr	Nb-Re-Ta
Al-Cr-Ru	C-Cr-N	Co-Ni-Zr	Cr-Re-W	Fe-Si-Ta	Nb-Re-Ti
Al-Cr-Si	C-Cr-Nb	Co-Re-Ta	Cr-Re-Zr	Fe-Si-Ti	Nb-Re-W
Al-Cr-Ta	C-Cr-Ni	Co-Re-W	Cr-Ru-Ta	Fe-Si-W	Nb-Re-Zr
Al-Cr-Ti	C-Cr-Re	Co-Ru-Ta	Cr-Ru-Ti	Fe-Si-Zr	Nb-Ru-SI
Al-Cr-W	C-Cr-Ta	Co-Ru-W	Cr-Ru-W	Fe-Ta-Ti	Nb-Si-Ti
Al-Cr-Zr	C-Cr-W	Co-Si-Ta	Cr-Si-Ta	Fe-Ta-W	Ni-Re-Ta
Al-C-Si	C-Fe-Nb	Co-Si-Ti	Cr-Si-W	Fe-Ta-Zr	Ni-Re-W
Al-Fe-Hf	C-Fe-Re	Co-Si-W	Cr-Si-Zr	Fe-Ti-W	NI-RE-ZR
Al-Fe-Mo	C-Fe-Ta	Co-Si-Zr	Cr-Ta-Ti	Fe-W-Zr	Ni-Ru-Ta
Al-Fe-Nb	C-Hf-Ta	Co-Ta-W	Cr-Ta-W	Hf-Mo-Ni	Ni-Ru-Ti
Al-Fe-Ni	C-Hf-Ti	Co-Ti-Zr	Cr-Ta-Zr	Hf-Mo-Si	Ni-Ru-W
Al-Fe-Re	C-Hf-W	Cr-Cu-Fe	Cr-Ti-V	Hf-Nb-Ni	Ni-Ru-Zr
Al-Fe-Ta	C-Mn-V	Cr-Cu-Ni	Cr-Ti-W	Hf-Nb-Re	Ni-Si-Ta
Al-Fe-W	C-Mo-N	C-Re-Ta	Cr-W-Zr	Hf-Ni-Re	Ni-Si-V
Al-Fe-Zr	C-Mo-Re	C-Re-V	C-Si-Ti	Hf-Ni-Ru	Ni-Si-W
Al-Hf-Ni	C-Mo-Si	C-Re-W	C-Ta-Ti	Hf-Ni-Si	Ni-Si-Zr
Al-Hf-Ru	C-Nb-V	Cr-Fe-Hf	C-Ti-Zr	Hf-Ni-Ta	Ni-Ta-Zr
Al-Hf-Si	C-Nb-Zr	Cr-Fe-Nb	Cu-Fe-Mo	Hf-Ni-W	Ni-W-Zr
Al-Hf-Ti	C-Ni-Ti	Cr-Fe-Re	Cu-Fe-Nb	Hf-Re-Ta	N-Ti-V
Al-Mo-Nb	C-Ni-V	Cr-Fe-Ta	Cu-Ni-Si	Hf-Re-W	Re-Ru-Ta
Al-Mo-Re	C-N-Nb	Cr-Fe-Ti	C-V-W	Hf-Ru-Ti	Re-Ru-Ti
Al-Mo-Ru	C-N-Ti	Cr-Fe-W	C-W-Zr	Hf-Ru-Zr	Re-Ru-W
Al-Mo-Si	Co-Cr-Hf	Cr-Fe-Zr	Fe-Hf-Mo	Hf-Si-Ta	Re-Ta-Ti

Al-Mo-Ti	Co-Cr-Mo	Cr-Hf-Mo	Fe-Hf-Nb	Hf-Si-Ti	Re-Ta-V
Al-Mo-W	Co-Cr-Nb	Cr-Hf-Nb	Fe-Hf-Ni	Hf-Si-W	Re-Ta-Zr
Al-Mo-Zr	Co-Cr-Re	Cr-Hf-Ni	Fe-Hf-Re	Mn-Ni-Si	Re-Ti-W
Al-Nb-Re	Co-Cr-Ru	Cr-Hf-Re	Fe-Hf-Si	Mn-Ni-V	Re-W-Zr
AL-Nb-Ru	Co-Cr-Si	Cr-Hf-Si	Fe-Hf-Ta	Mo-Nb-Ni	Ru-SI-TI
Al-Nb-Si	Co-Cr-Ta	Cr-Hf-Ta	Fe-Hf-Ti	Mo-Nb-Re	Ru-Ta-Ti
Al-Nb-Ta	Co-Cr-V	Cr-Hf-W	Fe-Hf-W	Mo-Ni-Re	Ru-Ta-W
Al-Nb-W	Co-Cu-Ti	Cr-Mo-N	Fe-Hf-Zr	Mo-Ni-Ru	Ru-Ti-Zr
Al-Ni-Re	Co-Fe-Hf	Cr-Mo-Nb	Fe-Mn-Ni	Mo-Ni-Si	Si-Ta-Zr
Al-Ni-V	Co-Fe-Nb	Cr-Mo-Re	Fe-Mo-N	Mo-Ni-W	Si-Ti-Zr
Al-Ni-Zr	Co-Fe-Ta	Cr-Mo-Ru	Fe-Mo-Nb	Mo-Ni-Zr	Si-W-Zr
Al-N-Ti	Co-Fe-Ti	Cr-Mo-Si	Fe-Mo-Re	Mo-N-V	Ta-W-Zr
Al-Re-Ru	Co-Fe-Zr	Cr-Mo-Ta	Fe-Mo-Si	Mo-Re-Ru	
Al-Re-Ta	Co-Hf-Ni	Cr-Mo-Ti	Fe-Mo-Ta	Mo-Re-Ta	
Al-Re-Ti	Co-Hf-Ti	Cr-Mo-W	Fe-Mo-Ti	Mo-Re-Ti	
Al-Re-W	Co-Mo-Nb	Cr-Mo-Zr	Fe-Mo-W	Mo-Re-V	

TCHEA Calculation Examples

FCC Forming Ternary Systems

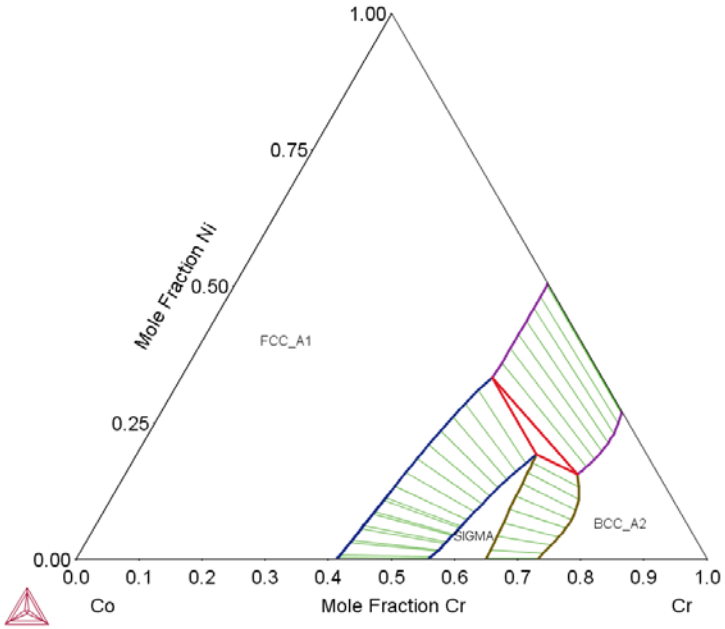

Figure 1. Calculated Co-Cr-Ni isothermal section at 1200 °C.

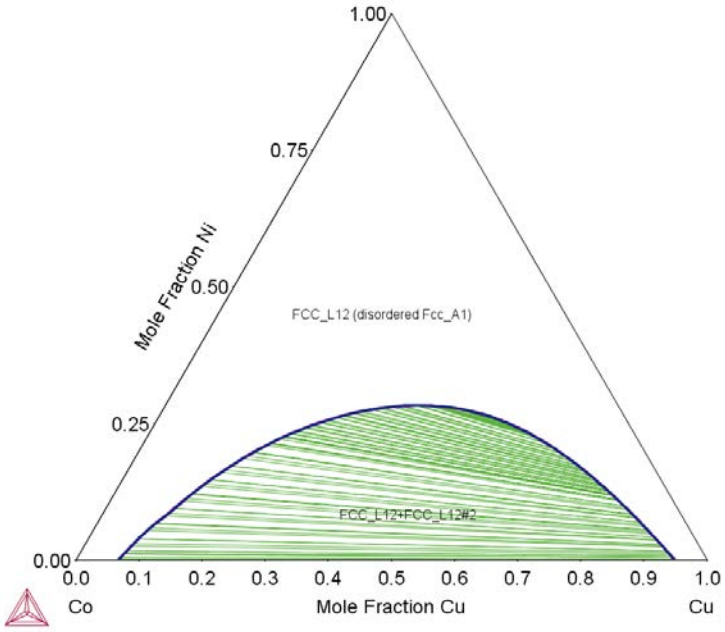

Figure 2: Calculated Co-Cu-Ni isothermal section at 1000 °C.

BCC Forming Ternary Systems

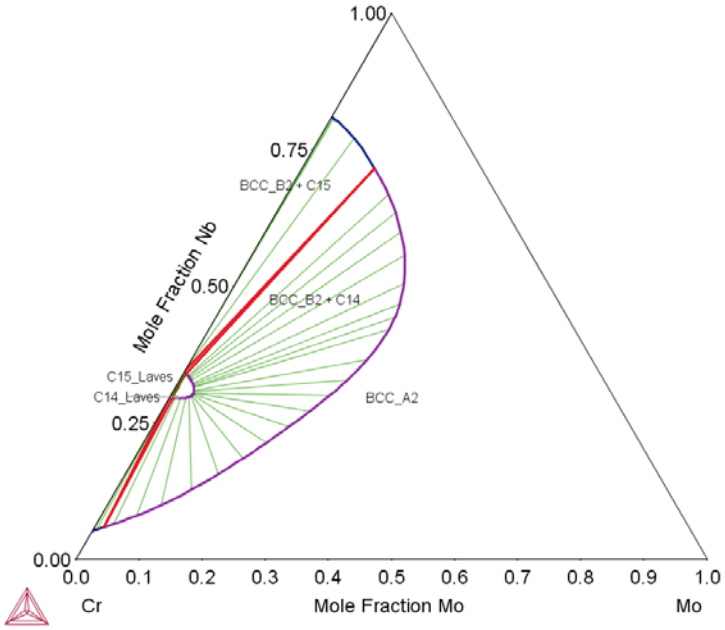

Figure 3. Calculated Cr-Mo-Nb isothermal section at 1500 °C.

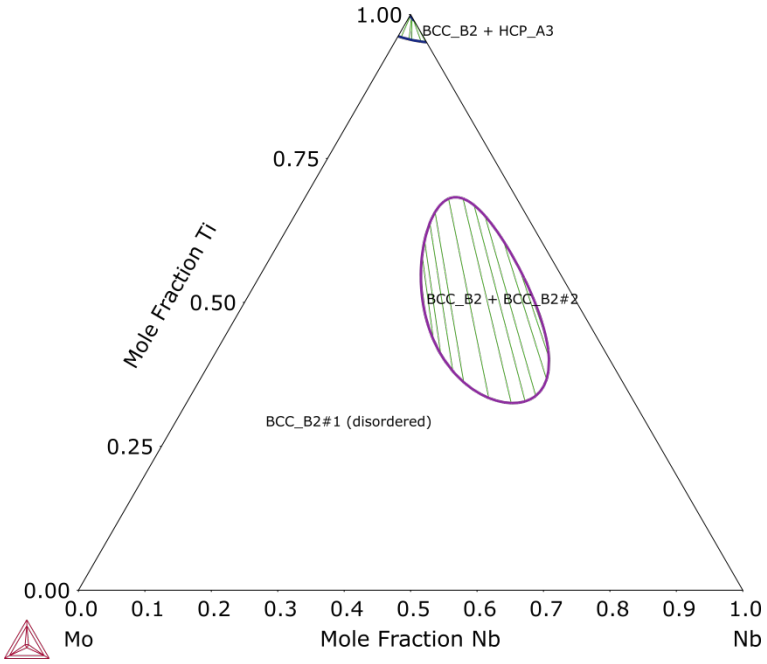

Figure 4. Calculated Mo-Nb-Ti isothermal section at 800 °C.

FCC/FCC+BCC Forming Ternary Systems

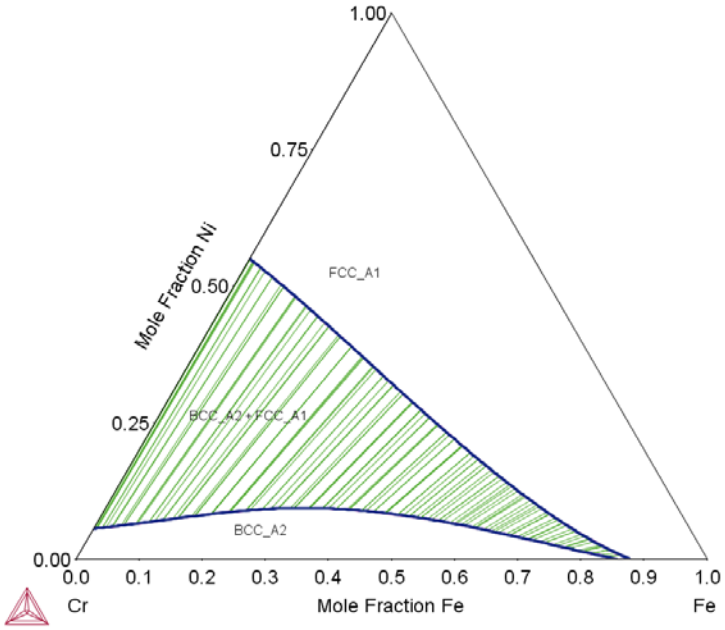

Figure 5. Calculated Cr-Fe-Ni isothermal section at 1000 °C.

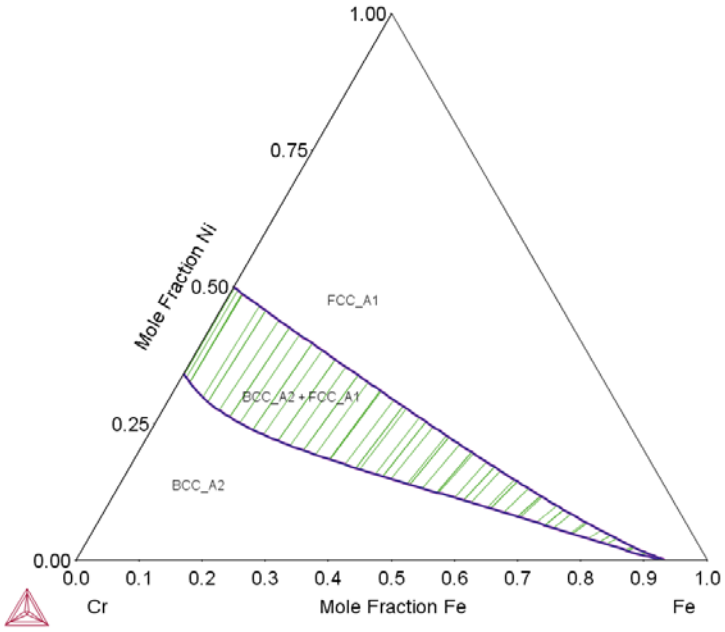

Figure 6. Calculated Cr-Fe-Ni isothermal section at 1300 °C.

FCC+BCC Forming Ternary Systems

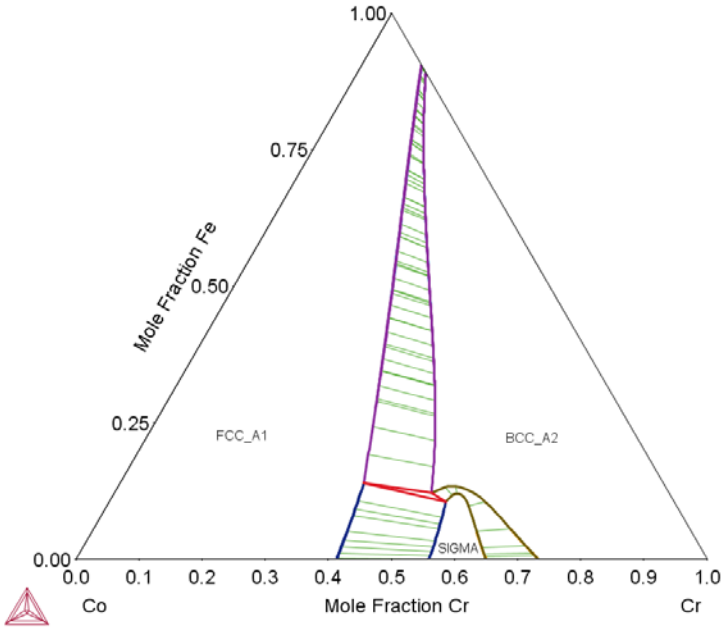

Figure 7. Calculated Co-Cr-Fe isothermal section at 1200 °C.

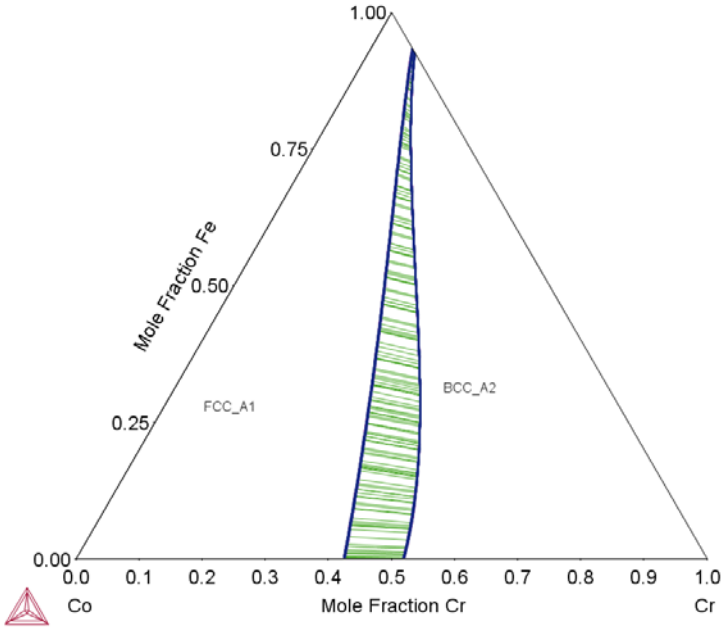

Figure 8. Calculated Co-Cr-Fe isothermal section at 1300 °C.

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].

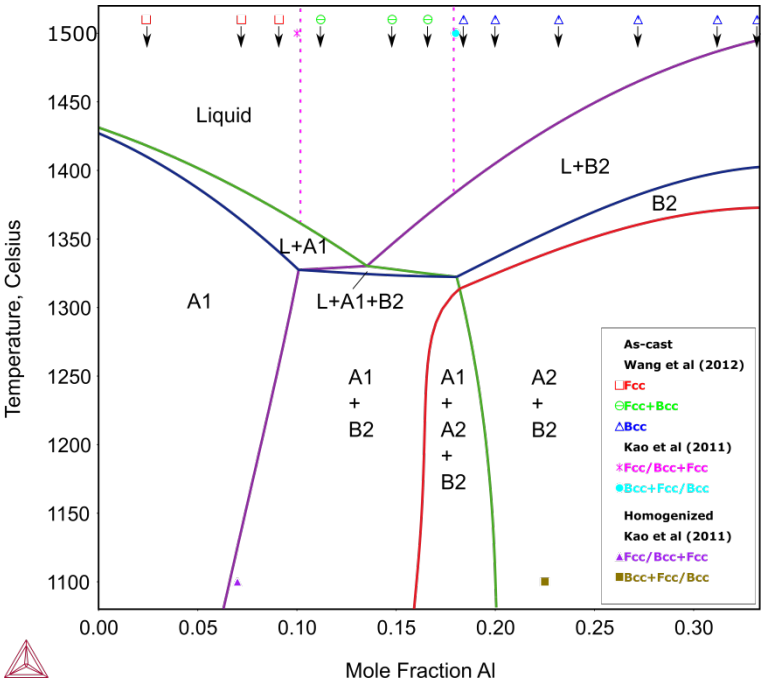

Figure 9. Calculated phase diagram along the composition line of CoCrFeNi-Al.

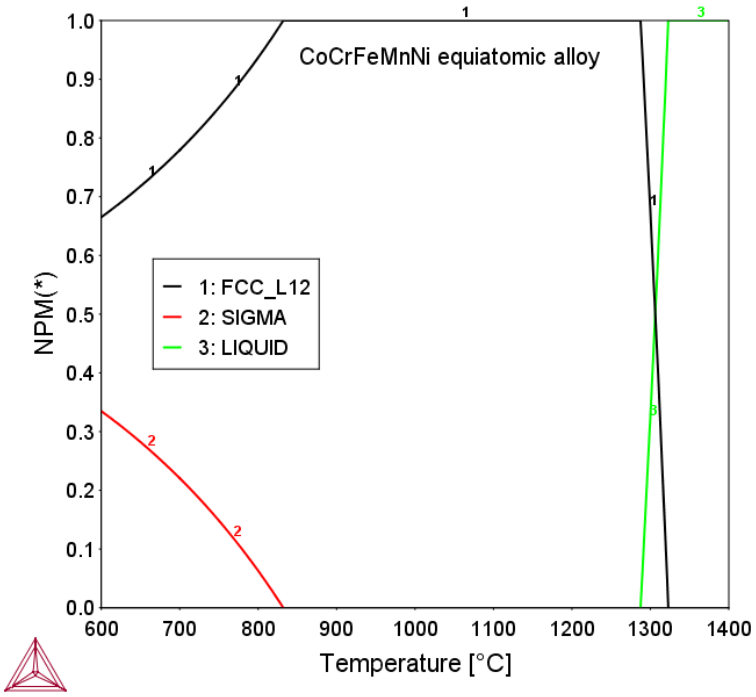

Figure 10. Equilibrium calculation of the phase formation in the Co-Cr-Fe-Mn-Ni equiatomic alloy.

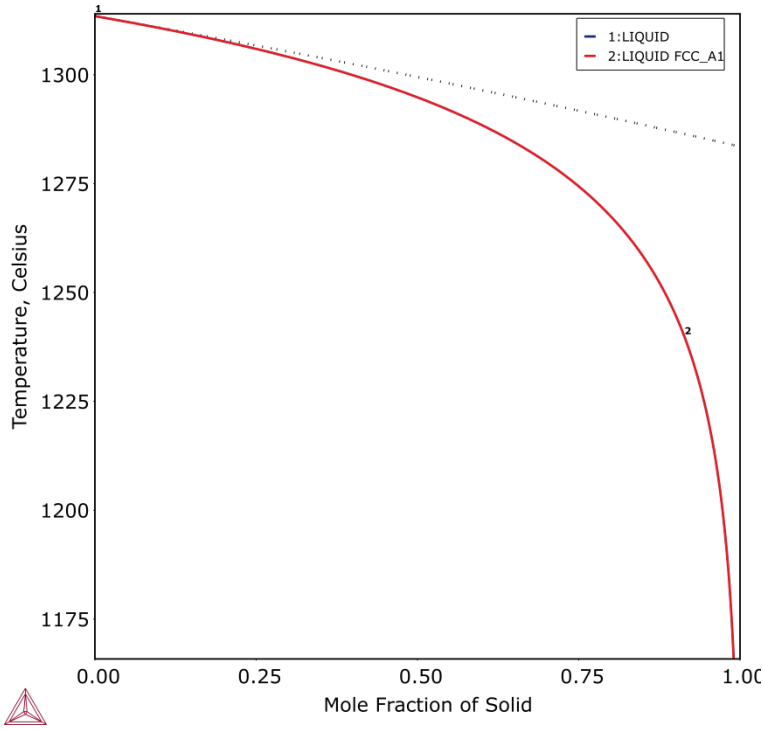

Figure 11. Scheil calculation of the phase formation in the Co-Cr-Fe-Mn-Ni equiatomic alloy.

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.

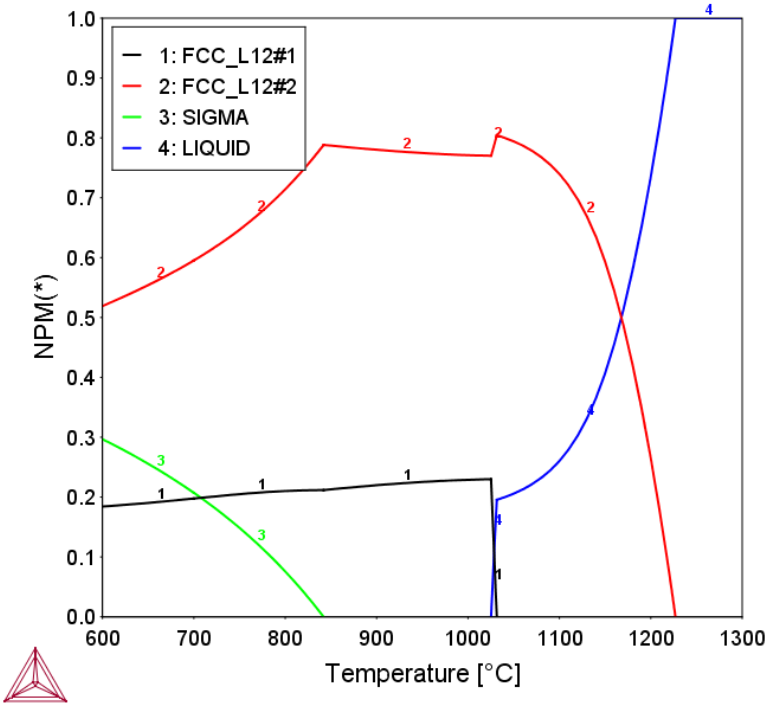

Figure 12. Equilibrium calculation of the phase formation in the Co-Cr-Cu-Fe-Mn-Ni equiatomic alloy.

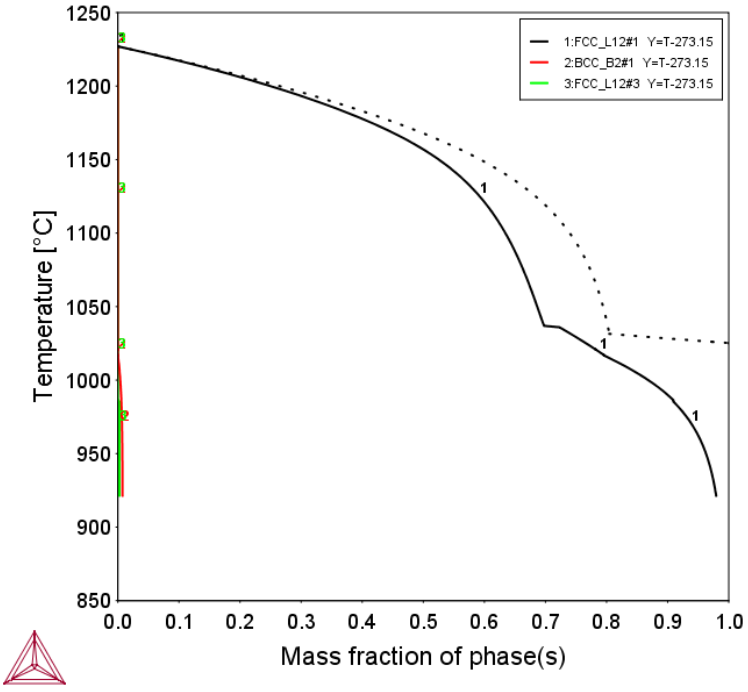

Figure 13. Scheil calculation of the phase formation in the Co-Cr-Cu-Fe-Mn-Ni equiatomic alloy.

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.

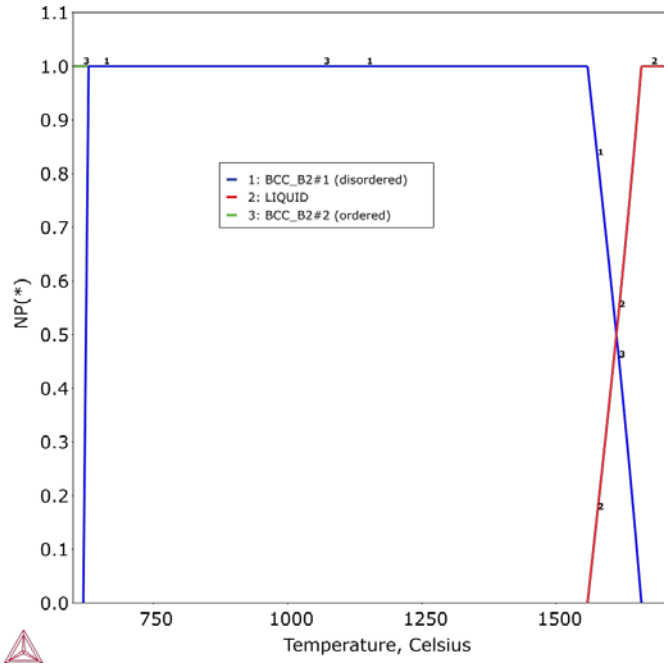

Figure 14. Equilibrium calculation of the phase formation in the Al-Cr-Mn-Ti-V equiatomic alloy.

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Suggested references for citing this database

[2017, Chen] H.-L. Chen, H. Mao, Q. Chen, Database development and Calphad calculations for high entropy alloys: Challenges, strategies, and tips. *Mater. Chem. Phys.* (2017). https://doi.org/10.1016/j.matchemphys.2017.07.082.

[2017, Mao] H. Mao, H.-L. Chen, Q. Chen, TCHEA1: A Thermodynamic Database Not Limited for "High Entropy" Alloys. *J. Phase Equilibria Diffus.* **38**, 353–368 (2017). https://doi.org/10.1007/s11669-017-0570-7.

Published research examples applying TCHEA database

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Phases Included in TCHEA

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 Graphic 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 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.

LIQUID:L
BCC_A2
BCC_B2
FCC_A1
FCC_L12
HCP_A3
AL10CU10FE
AL10FEMN2
AL10V
AL11CR2
AL11CU5MN3
AL11MN4_HT
AL11MN4_LT
AL11RE4
AL11TI5
AL12MN
AL12W
AL13CO4
AL13CR2
AL13FE2MN2
AL13FE4
AL13IR4
AL15SI2M4
AL16FEMN3
AL1MN1SI1
AL2_7IR
AL23CUFE4
AL23V4
AL28CU4MN7
AL28IR9
AL2FE
AL2MN2SI3
AL2MNSI3

AL2N2TI3
AL2TI
AL2W
AL2ZR3
AL31MN6NI2
AL3CO
AL3IR
AL3MN4SI2
AL3MNSI2
AL3NI1
AL3NI2_D513
AL3NI5
AL3RH_HT
AL3RH_LT
AL3Y_HT
AL3Y_LT
AL3ZR
AL3ZR2
AL3ZR4
AL3ZR5
AL45IR13
AL4C3
AL4CR
AL4MN_R
AL4MN_U
AL4RE
AL4SIC4
AL4W
AL4ZR5
AL5CO2_D811
AL5FE2
AL5FE4
AL5MN6SI7

AL5W
AL62CU25FE13
AL63MO37
AL6MN
AL77W23
AL7CU2FE
AL7CU4NI
AL7RH3
AL7V
AL7W3
AL8CR5_H
AL8CR5_L
AL8MN5
AL8MO3
AL8SIC7
AL8V5
AL9CO2
AL9CR4_H
AL9CR4_L
AL9IR2
ALB12_ALPHA
ALCCR2
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
ALN_B4
ALNTI2
ALNTI3
ALPHA_B19
ALRE
ALRE2
ALRH2
ALTI_L10
ALTI3_D019
ALZR
ALZR2
B11
B12ZR
B3SI
B4C
B4TA3_D7B
B5W2_X
B6SI
B9W2
BCT_A5
BCT_D022
BETA_RHOMBO_B
BM
BN_B4
BNSI
BW_ALPHA
BW_BETA
C14_LAVES

C15_LAVES
C16_THETA
C36_LAVES
CBCC_A12
CEMENTITE
CFC2_FENBZR
CHI_A12
CO10CU57TI33
CO11ZR2
CO17Y2
CO2SI_C23
CO3SI
CO3VV
CO3Y
CO3Y2
CO3Y4
CO5Y_D2D
CO5Y8
CO7HF
CO7M2
CO7Y6
COB
COSN_HP6
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
CRB4
CRNBSI
CRNI2_OP6
CRSI2_C40
CRZN13
CRZN17
CU10HF7
CU10SN3
CU10ZR7
CU15SI4_EPSILON
CU2TI
CU2TIZR
CU2Y_H
CU2Y_L
CU33SI7_DELTA
CU3SN
CU3TI2
CU41SN11
CU46NI25SI29
CU4TI1
CU4TI3
CU4Y
CU51HF14
CU51ZR14
CU56SI11_GAMMA
CU5MN4SI
CU6NISI3
CU6SN5_HT_NIAS
CU6SN5_LT
CU7Y1
CU7Y2

CU8HF3	HF8NI21	MN3SI
CU8ZR3	HFMN	MN3SN2
CUB_A13	HFNI_ALPHA	MN3TI
CUSI_ETA	HFNI3_ALPHA	MN4TI
CUTI3	HFNI3_BETA	MN6N4
D0I_MO2B5	HFRE	MN6N5
D5A_M3B2	HFSN2_C40	MN6SI
DIAMOND_A4	HIGH_SIGMA	MN9SI2
DIS_FCC_A1#1	IR3ZR5	MNB4
FCC_L10	IRZR_ALPHA	MNNI2
FE2SI	IRZR_B2	MNTA
FE3SN2	IRZR3	MNTI_HT
FE4N_LP1	L10_FCC	MNTI_LT
FE5SN3	M11SI8	MNZN9
FE8SI2C	M12C	MOB
FECN_CHI	M23C6	MOB4
FESI_B20	M2B_TETR	MOCOB
FESI2_H	M3B2	MONI_DELTA
FESI2_L	M3C2	MONI4_BETA
FEZN_DELTA	M3SI1	MOSI2_C11B
FEZN_GAMMA_D81	M3SI2_D5A	MOZN22
FEZN_GAMMA_D82	M4SI3	MOZN7
FEZN_ZETA	M5C2	MSI_B27
G_PHASE	M5SI3_D88	MSI2_C1
GAMMA_D03	M6C	MU_PHASE
GAMMA_D83	M6SI5	MZR3_E1A
GAMMA_H	M7C3	NB13NI75TI12
GAS	MB_B33	NB15NI56TI29
GRAPHITE	MB2_C32	NB15NI80TI5
H_L21	MC_ETA	NB3RU5
H_RZN5	MC_SHP	NB5NI75TI20
HCP_ZN	MN11SI19	NB8NI9TI3
HF3NI7	MN12Y	NBSN2
HF5SN4	MN2B_D1F	NI10ZR7

NI11ZR9
NI17Y2
NI2ALY2
NI2SI_TETA
NI2TA
NI2V
NI2Y
NI2Y3
NI31SI12
NI3ALY2
NI3B_D011
NI3SI_MONOCL
NI3SI_ORTHO
NI3SI2
NI3SN_D019
NI3SN4
NI3TA_D0A
NI3TI_D024
NI3Y
NI4B3
NI4Y
NI5ZR
NI6AL2Y3
NI7ZR2
NI8ALY3
NI8TA
NIAL2Y
NIALY
NISI_B31
NITI2
NIZN_TP2
NIZN8_DELTA
NIZR
P_PHASE

PI
R_PHASE
RE2SI
RE3B
RE7B3
REB2
RESI2_C11B
REZR2
RH2SN
RH3SN2
RH5TI3
RHSN
RHSN2_RT
RHSN4
RU25Y44
RU2B3
RU2SI_C37
RU2SI3
RU2SN3
RU2Y3
RU2Y5
RU3SN7
RU4SI3
RUB
RUB2
RUSI
RUY3
SI3N4
SI5V6
SIC
SIGMA
SN10Y11
SN2Y_C49
SN3TI5

SN3Y
SN4Y5
SN5TI6
SN5Y2
SNTI2
T1_CU2TI
T1CUNITI
T2_CU3TI2
T2CUNITI
T3_CU4TI3
T4CUFETI
T4CUNITI
T5CUFETI
T6CUNITI
TA3SN
TA5SI3_D8L
TAAL
TAAL2
TAN_EPS
TASN2
TAU
TI2N_C4
TI3N2
TI3SIC2
TI4N3
TISI2_C54
TIZN10
TIZN15
TIZN5
V2B3
V3C2
V3SN
V4ZN5
V5B6

VSN2
VZN3_L12
W2COB2
W3COC
W5SI3_D8M
Y13ZN58
Y15C19_H
Y15C19_R
Y2C3_H
Y2C3_R
Y2ZN17
Y3SI5_HT
Y3SI5_LT
YB4
YB6
YB66
YC_GAMMA
YC2_C11A
YSI2_HT
YZN2_A
YZN2_B
YZN3
Z_PHASE
ZN11Y3
ZN12Y
ZN22ZR
ZN2ZR_C15
ZN2ZR3
ZN39ZR5
ZN3ZR_HT
ZNZR_B2
ZR5SI4
ZRSI2_C49

Models for the Phases Included in TCHEA

LIQUID:L :AL AL1N1 B C CO CR CU FE HF IR MN MO N NB NI RH RE RU SI SN TA TI V W Y ZN ZR: > LIQUID mixture.
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 is 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.
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 is 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.
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
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: > This phase is rejected by default, used for Dictra simulation, it is a copy of FCC_A1
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 MN MO NB NI RE RU SI TA TI V W ZR:C VA:

BETA_RHOMBO_B 2 SUBL, SITES 93.00: 12.00: :B:B C CU SI:
DIAMOND_A4 :AL B C SI SN:
GRAPHITE :B C:
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: HCP_ZN :AL CO CR CU FE IR MN NI RE RH RU SN TI ZN:VA: > Disordered HCP_ZN solution phase; Also for pure Zn
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 AlNi6Ta
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 Ni3Mo, Ni3Nb
BCT_D022 2 SUBL, SITES 3.00: 1.00: :AL CR FE MO NB NI TI V:AL CR MO NB NI TA TI V SI: > gamma double prime
C14_LAVES 2 SUBL, SITES 2.00: 1.00: :AL CO CR CU FE HF MN MO NB NI SI RE RU TA TI W Y ZN ZR: AL CO CR CU FE HF MN MO NB NI SI RE RU TA TI W Y ZN ZR: > prototype CuZn2
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_MU contribution is introduced in the description of this phase

DIS_SIG :AL CO CR FE 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 MN MO NB NI RE RU SI TA TI V W: AL CO CR FE MN MO NB NI RE RU SI TA TI V W: AL CO CR FE MN MO NB NI RE RU SI TA TI V W: > DIS_SIG contribution is introduced in the description of this phase
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
P_PHASE 3 SUBL, SITES 24.00: 20.00: 12.00: :CR FE NI RE:CR FE MO NI RE:MO: > Prototype : Cr9Mo21Ni20
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:
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:
L10_FCC 2 SUBL, SITES 0.50: 0.50: :IR MN TI:IR MN TI:
NISI_B31 2 SUBL, SITES 1.00: 1.00: :NI:SI::
MC_ETA 2 SUBL, SITES 1.00: 1.00: :MO V W:C VA: > MoC, prototype TiAs
MC_SHP 2 SUBL, SITES 1.00: 1.00: :MO W:C N: > Prototype WC, also MoC low temperature
BM 2 SUBL, SITES 1.00: 1.00: :B:CR FE HF MN MO TI Y: > FeB, MnB, TiB, HfB etc., and YPt, StrukturBericht B27
COB 2 SUBL, SITES 1.00: 1.00: :CO RE:B:

MOB 2 SUBL, SITES 1.00: 1.00: :CR FE MO:B: > prototype CrB
BW_ALPHA 2 SUBL, SITES 1.00: 1.00: :B C VA:W:
BW_BETA 2 SUBL, SITES 1.00: 1.00: :B C VA:W:
CR2B_ORTH 2 SUBL, SITES 0.67: 0.33: :CR FE MO RE:B:
MN2B_D1F 2 SUBL, SITES 0.67: 0.33: :MN:B:
MNB4 2 SUBL, SITES 0.20: 0.80: :MN:B:
MOCOB 3 SUBL, SITES 1.00: 1.00: 1.00: :MO W:CO:B: > also WCoB
NI3B_D011 2 SUBL, SITES 3.00: 1.00: :CO CR FE MO NI:B: > Ni3B, Co3B
RE3B 2 SUBL, SITES 3.00: 1.00: :CR MO RE TA W:B:
B4TA3_D7B 2 SUBL, SITES 4.00: 3.00: :B:CR HF MN NB TA TI V: > Prototype:Ta3B4, also Cr3B4, Mn3B4, Nb3B4, Ti3B4, V3B4
B5W2_X 2 SUBL, SITES 5.00: 2.00: :B C VA:W:
RE7B3 3 SUBL, SITES 7.00: 3.00: 3.00: :CO CR MO NB RE RU TA W:B:B VA:
D5A_M3B2 2 SUBL, SITES 3.00: 2.00: :FE HF MO NB TA V:B: > TA3B2, NB3B2, V3B2, prototype U3SI2
W2COB2 3 SUBL, SITES 2.00: 1.00: 2.00: :MO W:CO NI:B: > also Mo2NiB2 and Mo2CoB2

CR5B3 2 SUBL, SITES 0.62: 0.38: :CR MO:B:
V5B6 2 SUBL, SITES 5.00: 6.00: :NB V:B:
TAU 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
MB_B33 2 SUBL, SITES 1.00: 1.00: :CR FE HF MO NB NI TA TI V:B: > CrB, NbB, NiB, TaB, VB
MB2_C32 2 SUBL, SITES 2.00: 1.00: :B:AL CR HF MN MO NB TA TI V Y ZR: > AlB2, CrB2, MnB2, MoB2, NbB2, TaB2, TiB2, VB2, YB2, ZrB2
M3B2 3 SUBL, SITES 0.40: 0.20: 0.40: :CR FE MO NI W:CR FE NI:B: > Mo2FeB2, Mo2CrB2
M2B_TETR 2 SUBL, SITES 2.00: 1.00: :AL CO CR FE MN MO NB NI RE TA W:B: > Co2B, Fe2B, Mn2B, Mo2B, Ni2B
YB4 2 SUBL, SITES 1.00: 4.00: :Y:B:
YB6 2 SUBL, SITES 1.00: 6.00: :Y:B:
YB66 2 SUBL, SITES 1.00: 66.00: :Y:B:
B12ZR 2 SUBL, SITES 12.00: 1.00: :B:Y ZR: > YB12, ZrB12
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: > Cr23C6
CEMENTITE 2 SUBL, SITES 3.00: 1.00: :CO CR FE MN MO NI V W:C N: > D011

M12C 3 SUBL, SITES 6.00: 6.00: 1.00: :CO NI:MO W:C: > Prototype Mo6Ni6C
M3C2 2 SUBL, SITES 3.00: 2.00: :CO CR MO V W:C: > Cr3C2
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
M7C3 2 SUBL, SITES 7.00: 3.00: :CO CR FE MN MO NI RE V W:C: > Cr7C3
M5C2 2 SUBL, SITES 5.00: 2.00: :FE MN:C: > Mn5C2
W3COC 3 SUBL, SITES 3.00: 1.00: 1.00: :W:CO NI:C: > also W3NiC
ALM3C_E21 3 SUBL, SITES 1.00: 3.00: 1.00: :AL:CO FE:C: ALM3C_E21 :AL:CO FE:C: > AlCo3C, AlFe3C, Perovskite
AL4C3 2 SUBL, SITES 4.00: 3.00: :AL SI:C:
YC2_C11A :C2Y1:
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:

YC_GAMMA 2 SUBL, SITES 1.00: 1.00: :Y:C C2 VA:
BN_B4 2 SUBL, SITES 1.00: 1.00: :B:N:
Z_PHASE 3 SUBL, SITES 1.00: 1.00: 1.00: :CR FE:MO NB V:N VA:
FE4N_LP1 2 SUBL, SITES 4.00: 1.00: :CO CR FE MN NI:C N:
FECN_CHI 2 SUBL, SITES 2.20: 1.00: :FE:C N:
PI 3 SUBL, SITES 12.80: 7.20: 4.00: :CR:FE NI:N:
ALN_B4 2 SUBL, SITES 1.00: 1.00: :AL:N:
SI3N4 2 SUBL, SITES 3.00: 4.00: :SI:N:
MN6N4 2 SUBL, SITES 6.00: 4.00: :MN:N:
MN6N5 2 SUBL, SITES 6.00: 5.00: :MN:N:
TI2N_C4 2 SUBL, SITES 2.00: 1.00: :TI:N:
TAN_EPS 2 SUBL, SITES 1.00: 1.00: :TA:N:
TI3N2 2 SUBL, SITES 0.71: 0.29: :TI:N:
TI4N3 2 SUBL, SITES 0.69: 0.32: :TI:N:
ALNTI2 3 SUBL, SITES 1.00: 1.00: 2.00: :AL:N:TI:
ALNTI3 3 SUBL, SITES 1.00: 1.00: 3.00: :AL:N:TI:
AL2N2TI3 3 SUBL, SITES 2.00: 2.00: 3.00: :AL:N:TI:

M5SI3_D88 4 SUBL, SITES 2.00: 3.00: 3.00: 1.00: :CR CU FE HF MN MO NI NB SI TI Y ZR: AL CR SI SN TI: CR CU FE HF MN MO NI NB TI Y ZR: C SN VA: > Fe5Si3, Ti5Si3, Zr5Si3, Y5Si3, Hf5Si3, Mo5Si3C, Cr5Si3C, Zr5Sn3, Zr5Sn4, Hf5Sn3, Y5Sn3, prototype Mn5Si3
W5SI3_D8M 3 SUBL, SITES 4.00: 1.00: 3.00: :CR FE MO NB V W:CR FE MO NB V W SI:AL SI: > Cr5Si3, Mo5Si3, W5Si3, protoype W5Si3
TA5SI3_D8L 2 SUBL, SITES 5.00: 3.00: :HF NB TA:AL SI:
ZR5SI4 2 SUBL, SITES 5.00: 4.00: :HF NB TI Y ZR:SI: > Hf5Si4, Ti5Si4, Y5Si4, Zr5Si4(alpha), prototype ZR5SI4
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
M3SI1 2 SUBL, SITES 3.00: 1.00: :HF NB TA TI ZR:SI: > Ti3Si, Ta3Si, Zr3Si
CO2SI_C23 2 SUBL, SITES 2.00: 1.00: :CO CR CU FE NI TI:SI: > Co2Si, Ni2Si(delta), Prototype Co2Si
MSI_B27 2 SUBL, SITES 1.00: 1.00: :HF NB TI Y ZR:SI: > TiSi, HfSi, YSi, ZrSi(alpha), Prototype FeB
FESI_B20 2 SUBL, SITES 1.00: 1.00: :CO CR FE MN NI RE:AL SI: > CoSi, CrSi, ReSi, Prototype FeSi
CRSI2_C40 2 SUBL, SITES 1.00: 2.00: :CR CU HF MO NB SI TA V:AL CR CU SI: > CrSi2, NbSi2, TaSi2, VSi2, Prototype CrSi2

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 MoSi2
ZRSI2_C49 2 SUBL, SITES 1.00: 2.00: :ZR Y HF NB:SI: > ZrSi2, YSi2, HfSi2, Prototype ZrSi2
YSI2_HT 2 SUBL, SITES 1.00: 2.00: :Y:SI:
Y3SI5_HT 2 SUBL, SITES 3.00: 5.00: :Y:SI:
Y3SI5_LT 2 SUBL, SITES 3.00: 5.00: :Y:SI:
TISI2_C54 2 SUBL, SITES 1.00: 2.00: :MO NB RU TI ZR:AL SI SN:
MSI2_C1 2 SUBL, SITES 1.00: 2.00: :CO CU NI:AL CU SI: > CoSi2, Prototype CaF2
M3SI2_D5A 2 SUBL, SITES 3.00: 2.00: :HF NB ZR:SI: > Hf3Si2, Zr3Si2
NI31SI12 2 SUBL, SITES 5.00: 2.00: :CO CR CU FE NI:SI:
CR3NI5SI2 4 SUBL, SITES 3.00: 5.00: 2.00: 1.00: :CR:NI:SI:C VA:
ALTI_L10 2 SUBL, SITES 1.00: 1.00: :AL CR MN MO TA TI W:AL CR MN MO TA TI W:
NIZR 2 SUBL, SITES 1.00: 1.00: :NI:TI Y ZR:
ALZR 2 SUBL, SITES 1.00: 1.00: :AL:HF Y ZR: >also AlHf, AlY
ALPHA_B19 2 SUBL, SITES 1.00: 1.00: :MO NB TI V ZR:MO NB TI V ZR:
B11 2 SUBL, SITES 1.00: 1.00: :CO CU NI TI:CU NI TA TI:

HFMN 2 SUBL, SITES 0.50: 0.50: :HF:MN:
FCC_L10 2 SUBL, SITES 0.50: 0.50: :CU MN NI:CU MN NI:
MNTA 2 SUBL, SITES 1.00: 1.00: :MN:TA:
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 ZR: AL CO CR CU FE HF MO NB NI SI RE RU TA TI V W Y ZR:
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:
NI2TA 2 SUBL, SITES 2.00: 1.00: :CO NI:TA TI:
NI2V 2 SUBL, SITES 2.00: 1.00: :MO NI:MO NB TA V:
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
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:
MNNI2 2 SUBL, SITES 1.00: 2.00: :MN NI:NI:
NITI2 2 SUBL, SITES 1.00: 2.00: :CO CR CU FE NI RE TI:AL CR CU HF NI TA TI ZR:
REZR2 2 SUBL, SITES 1.00: 2.00: :NI RE:ZR:
ALTI3_D019 2 SUBL, SITES 3.00: 1.00: :AL CO CR MN MO NI TA TI W:AL CR MO NB NI TA TI W:

AL3Y_HT 2 SUBL, SITES 0.75: 0.25: :AL:Y:
AL3Y_LT 2 SUBL, SITES 0.75: 0.25: :AL:Y:
AL3ZR 2 SUBL, SITES 3.00: 1.00: :AL ZN:HF ZR: > also Al3Hf, Zn3Zr
CUTI3 2 SUBL, SITES 1.00: 3.00: :CU TI:TI:
MZR3_E1A 2 SUBL, SITES 1.00: 3.00: :CO FE NI:Y ZR: > COZR3, FEZR3, NiY3, COY3
RUY3 2 SUBL, SITES 0.25: 0.75: :RU:Y:
H_L21 3 SUBL, SITES 0.50: 0.50: 1.00: :AL CR NI TI:AL HF NB NI TA TI ZR:CO FE NI RU VA: > The Heusler phase
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: > Th6Mn23 prototype
ALCU_DEL 2 SUBL, SITES 2.00: 3.00: :AL:CU FE:
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:
ALCU_PRIME 2 SUBL, SITES 2.00: 1.00: :AL:CU:
ALCU_ZETA 2 SUBL, SITES 9.00: 11.00: :AL:CU FE:
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:AL CU:CU FE MN NI: > Cu5Zn8-type Al8Cu5 (ht) phase
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:
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:
AL3IR 2 SUBL, SITES 0.75: 0.25: :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:
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:MN:AL CU MN SI TI:
ALMNTI_L12 3 SUBL, SITES 0.25: 0.08: 0.67: :AL MN TI:AL MN:AL MN TI: > TI25MN9AL66_L12
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:
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:
NIAL2Y 3 SUBL, SITES 1.00: 2.00: 1.00: :NI:AL:Y:
NIALY 3 SUBL, SITES 1.00: 1.00: 1.00: :NI:AL:Y:
NI2ALY2 3 SUBL, SITES 2.00: 1.00: 2.00: :NI:AL:Y:
NI6AL2Y3 3 SUBL, SITES 6.00: 2.00: 3.00: :NI:AL:Y:
NI3ALY2 3 SUBL, SITES 3.00: 1.00: 2.00: :NI:AL:Y:
NI8ALY3 3 SUBL, SITES 8.00: 1.00: 3.00: :NI:AL:Y:
AL6MN 2 SUBL, SITES 6.00: 1.00: :AL:FE MN RE RU:
ALRH2 2 SUBL, SITES 1.00: 2.00: :AL:RH:

AL3RH_LT 2 SUBL, SITES 3.00: 1.00: :AL:RH:
AL3RH_HT 2 SUBL, SITES 2.00: 1.00: :AL:RH VA:
AL7RH3 2 SUBL, SITES 7.00: 3.00: :AL:RH:
ALZR2 2 SUBL, SITES 1.00: 2.00: :AL:Y ZR: > also AlY2
AL2ZR3 2 SUBL, SITES 2.00: 3.00: :AL:HF Y ZR: > also Al2Hf3
AL3ZR4 2 SUBL, SITES 3.00: 4.00: :AL:HF ZR: > also Al3Hf4
AL3ZR2 2 SUBL, SITES 3.00: 2.00: :AL:HF ZR: > also Al3Hf2
AL3NI2 3 SUBL, SITES 3.00: 2.00: 1.00: :AL SI:AL CU NI RU:RU NI VA:
AL3NI2_D513 3 SUBL, SITES 3.00: 2.00: 1.00: :AL SI SN:AL CU NI RU:RU NI VA: > Al3Ni2, Al3Ru2
AL12W 2 SUBL, SITES 12.00: 1.00: :AL:MO RE W: > also AL12MO
AL4W 2 SUBL, SITES 4.00: 1.00: :AL:MO W: > also Al4Mo
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
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
AL2MNSI3 3 SUBL, SITES 2.00: 1.00: 3.00: :AL:MN:SI: > the Al-Mn-Si ternary phase, tao10
MONI4_BETA 2 SUBL, SITES 1.00: 4.00: :MO W:NI: > also WNi4
AL5W 2 SUBL, SITES 5.00: 1.00: :AL:MO W: > also AL5MO
CO10CU57TI33 3 SUBL, SITES 0.10: 0.57: 0.33: :CO:CU:TI:
RH3SN2 3 SUBL, SITES 0.12: 0.50: 0.38: :RH:RH:SN:
COSN_HP6 2 SUBL, SITES 0.50: 0.50: :CO FE NI:SN: > This is CoSn, FeSn
COSN3_OS32 2 SUBL, SITES 0.25: 0.75: :CO:SN:
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:

CO3Y 2 SUBL, SITES 3.00: 1.00: :CO:Y:
CO3Y2 2 SUBL, SITES 3.00: 2.00: :CO:Y:
CO7Y6 2 SUBL, SITES 7.00: 6.00: :CO:Y:
COY_BF 2 SUBL, SITES 1.00: 1.00: :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:
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:

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
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
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
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:
CUSI_ETA 2 SUBL, SITES 0.76: 0.24: :CU MN NI:SI:
GAMMA_D03 :CU MN NI SN ZN: > Cu3Sn Prototype BiF3 (cF16, Fm-3m)
CU3SN 2 SUBL, SITES 3.00: 1.00: :CU SN:CU SN:
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:
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:
MN11SI19 2 SUBL, SITES 11.00: 19.00: :MN:AL SI:
MN3SI 2 SUBL, SITES 3.00: 1.00: :MN FE:AL SI:
MN6SI 2 SUBL, SITES 17.00: 3.00: :AL MN:SI:
MN9SI2 2 SUBL, SITES 33.00: 7.00: :MN:SI:
MN3SN2 2 SUBL, SITES 3.00: 2.00: :MN:SN:
MN12Y 2 SUBL, SITES 12.00: 1.00: :MN:Y:
MNZN9 2 SUBL, SITES 1.00: 9.00: :MN:ZN:

NI3SN_D019 2 SUBL, SITES 0.75: 0.25: :CO CU MN NI SN TI:NI SN TI: > Ni3Sn_LT, Mn3Sn, Ti3Sn.
MOZN7 2 SUBL, SITES 1.00: 7.00: :MO:ZN:
MOZN22 2 SUBL, SITES 1.00: 22.00: :MO:ZN:
NI3SN4 3 SUBL, SITES 0.25: 0.25: 0.50: :CU NI:NI SN:SN:
NI2Y 2 SUBL, SITES 2.00: 1.00: :NI:Y:
NI2Y3 2 SUBL, SITES 2.00: 3.00: :NI:Y:
NI3Y 2 SUBL, SITES 3.00: 1.00: :FE NI:Y: > also Fe3Y
NI4Y 2 SUBL, SITES 4.00: 1.00: :NI:Y:
NIZN_TP2 2 SUBL, SITES 0.50: 0.50: :CU NI ZN:NI ZN:
NIZN8_DELTA 2 SUBL, SITES 1.00: 8.00: :NI:ZN:
NI7ZR2 2 SUBL, SITES 7.00: 2.00: :AL CO CR NI:HF Y ZR: > also NI7HF2, NI7Y2, CO7Y2 and CO7HF2
NI11ZR9 2 SUBL, SITES 11.00: 9.00: :NI:HF ZR:
NI10ZR7 2 SUBL, SITES 23.00: 17.00: :NI:HF ZR:
NI5ZR 2 SUBL, SITES 5.00: 1.00: :AL CU NI:HF Y ZR: > also Ni5Y, Ni5Hf, Cu5Hf and Cu5Zr
NI17Y2 2 SUBL, SITES 1.00: 0.12: :AL FE NI:Y: > also Fe17Y2

HF8NI21 2 SUBL, SITES 8.00: 21.00: :HF ZR:NI: > also ZR8NI21
AL13FE4 3 SUBL, SITES 0.63: 0.23: 0.14: :AL CU:FE MN RU:AL SI VA:
NI8TA 2 SUBL, SITES 8.00: 1.00: :NI:NB TA:
CO7M2 2 SUBL, SITES 7.00: 2.00: :CO:NB TA:
RHSN 2 SUBL, SITES 1.00: 1.00: :RH:SN:
RHSN4 2 SUBL, SITES 1.00: 4.00: :RH:SN:
RHSN2_RT 2 SUBL, SITES 0.33: 0.67: :RH:SN:
RH2SN 2 SUBL, SITES 2.00: 1.00: :RH:SN:
RH5TI3 2 SUBL, SITES 5.00: 3.00: :RH:TI:
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:
SNTI2 2 SUBL, SITES 1.00: 2.00: :SN:TI:
SN3TI5 2 SUBL, SITES 3.00: 5.00: :SN:TI:
SN5TI6 2 SUBL, SITES 5.00: 6.00: :SN:NB TI:

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:
ALB12_ALPHA 2 SUBL, SITES 1.00: 12.00: :AL:B:
W3COC 3 SUBL, SITES 3.00: 1.00: 1.00: :W:CO NI:C: > also W3NiC
ALM3C_E21 3 SUBL, SITES 1.00: 3.00: 1.00: :AL:CO FE:C: > AlCo3C, AlFe3C, Perovskite
AL4C3 2 SUBL, SITES 4.00: 3.00: :AL SI:C:
Z_PHASE 3 SUBL, SITES 1.00: 1.00: 1.00: :CR FE:MO NB V:N VA:
FE4N_LP1 2 SUBL, SITES 4.00: 1.00: :CO CR FE MN NI:C N:
FECN_CHI 2 SUBL, SITES 2.20: 1.00: :FE:C N:
PI 3 SUBL, SITES 12.80: 7.20: 4.00: :CR:FE NI:N:
ALN_B4 2 SUBL, SITES 1.00: 1.00: :AL:N:
SI3N4 2 SUBL, SITES 3.00: 4.00: :SI:N:
MN6N4 2 SUBL, SITES 6.00: 4.00: :MN:N:
MN6N5 2 SUBL, SITES 6.00: 5.00: :MN:N:
TI2N_C4 2 SUBL, SITES 2.00: 1.00: :TI:N:

TAN_EPS 2 SUBL, SITES 1.00: 1.00: :TA:N:
TI3N2 2 SUBL, SITES 0.71: 0.29: :TI:N:
TI4N3 2 SUBL, SITES 0.69: 0.32: :TI:N:
ALNTI2 3 SUBL, SITES 1.00: 1.00: 2.00: :AL:N:TI:
ALNTI3 3 SUBL, SITES 1.00: 1.00: 3.00: :AL:N:TI:
AL2N2TI3 3 SUBL, SITES 2.00: 2.00: 3.00: :AL:N:TI:
M5SI3_D88 4 SUBL, SITES 2.00: 3.00: 3.00: 1.00: :CR CU FE HF MN MO NI NB SI TI ZR:AL CR SI TI:CR CU FE HF MN MO NI NB TI ZR:C VA: > Fe5Si3, Ti5Si3, Zr5Si3, Hf5Si3, Mo5Si3C, Cr5Si3C prototype Mn5Si3
W5SI3_D8M 3 SUBL, SITES 4.00: 1.00: 3.00: :CR FE MO NB V W:CR FE MO NB V W SI:AL SI: > Cr5Si3, Mo5Si3, W5Si3, protoype W5Si3
TA5SI3_D8L 2 SUBL, SITES 5.00: 3.00: :HF NB TA:AL SI:
ZR5SI4 2 SUBL, SITES 5.00: 4.00: :HF NB TI ZR:SI: > Hf5Si4, Ti5Si4, Zr5Si4(alpha), prototype ZR5SI4
CR3SI_A15 3 SUBL, SITES 3.00: 1.00: 3.00: :CR FE MO NB NI RE SI TA TI V:AL CO CR MO NB NI RU SI TA TI V:C VA: > Cr3Ru, Cr3Si, Mo3Si, V3Si, Mo3Al, Nb3Al, V3Co, V3Ni
M3SI1 2 SUBL, SITES 3.00: 1.00: :HF NB TA TI ZR:SI: > Ti3Si, Ta3Si, Zr3Si
CO2SI_C23 2 SUBL, SITES 2.00: 1.00: :CO CR CU FE NI TI:SI: > Co2Si, Ni2Si(delta), Prototype Co2Si
MSI_B27 2 SUBL, SITES 1.00: 1.00: :HF NB TI ZR:SI: > TiSi, HfSi, ZrSi(alpha), Prototype FeB

FESI_B20 2 SUBL, SITES 1.00: 1.00: :CO CR FE MN NI RE:AL SI: > CoSi, CrSi, ReSi, Prototype FeSi
CRSI2_C40 2 SUBL, SITES 1.00: 2.00: :CR CU HF MO NB SI TA V:AL CR CU SI: > CrSi2, NbSi2, TaSi2, VSi2, Prototype CrSi2
MOSI2_C11B 2 SUBL, SITES 1.00: 2.00: :CO CU FE MO NI W:AL HF SI TI ZR: > also WSi2, CuHf2, CuTi2, CuZr2, Prototype MoSi2
ZRSI2_C49 2 SUBL, SITES 1.00: 2.00: :ZR HF NB:SI: > ZrSi2, HfSi2, Prototype ZrSi2
TISI2_C54 2 SUBL, SITES 1.00: 2.00: :MO NB RU TI:AL SI:
MSI2_C1 2 SUBL, SITES 1.00: 2.00: :CO CU NI:AL CU SI: > CoSi2, Prototype CaF2
M3SI2_D5A 2 SUBL, SITES 3.00: 2.00: :HF NB ZR:SI: > Hf3Si2, Zr3Si2
NI31SI12 2 SUBL, SITES 5.00: 2.00: :CO CR CU FE NI:SI:
CR3NI5SI2 4 SUBL, SITES 3.00: 5.00: 2.00: 1.00: :CR:NI:SI:C VA:
GAS:G :N2:
AL13CO4 2 SUBL, SITES 13.00: 4.00: :AL:CO:
AL3CO 2 SUBL, SITES 3.00: 1.00: :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:
AL9CR4_H 2 SUBL, SITES 9.00: 4.00: :AL:CR:
AL9CR4_L 2 SUBL, SITES 9.00: 4.00: :AL:CR:
ALCR2 2 SUBL, SITES 1.00: 2.00: :AL:CR:
AL2FE 2 SUBL, SITES 2.00: 1.00: :AL CU:FE MN:
AL5FE2 2 SUBL, SITES 5.00: 2.00: :AL CU:FE MN:
AL5FE4 :AL CU FE:
AL63MO37 2 SUBL, SITES 63.00: 37.00: :AL:MO:
AL8MO3 2 SUBL, SITES 8.00: 3.00: :AL:MO:
ALMO 2 SUBL, SITES 1.00: 1.00: :AL MO:AL MO:
AL3NI1 2 SUBL, SITES 0.75: 0.25: :AL:NI:
AL3NI5 2 SUBL, SITES 0.38: 0.62: :AL:NI:

AL11RE4 :AL:RE:	2 SUBL, SITES 11.00: 4.00:
AL4RE :AL:RE:	2 SUBL, SITES 4.00: 1.00:
ALRE2 :AL:RE:	2 SUBL, SITES 1.00: 2.00:
ALRE :AL:RE:	2 SUBL, SITES 1.00: 1.00:
TAAL :TA:AL:	2 SUBL, SITES 0.52: 0.48:
TAAL2 :TA:AL:	2 SUBL, SITES 0.35: 0.65:
AL11TI5 :AL:TI:	2 SUBL, SITES 17.00: 8.00:
AL2TI :AL:TI:	2 SUBL, SITES 2.00: 1.00:
AL10V :AL:V:	2 SUBL, SITES 10.00: 1.00:
AL7V :AL:V:	2 SUBL, SITES 7.00: 1.00:
AL23V4 :AL:V:	2 SUBL, SITES 23.00: 4.00:
AL8V5 :AL:V:	2 SUBL, SITES 8.00: 5.00:
AL77W23 :AL:W:	2 SUBL, SITES 77.00: 23.00:
AL7W3 :AL:W:	2 SUBL, SITES 7.00: 3.00:
AL2W :AL:W:	2 SUBL, SITES 2.00: 1.00:
AL3ZR5 :AL:ZR:	2 SUBL, SITES 3.00: 5.00:
AL4ZR5 :AL:ZR:	2 SUBL, SITES 4.00: 5.00:

B4C 2 SUBL, SITES 1.00: 1.00: :B11C B12:B2 C2B CB2:
CRB4 2 SUBL, SITES 0.20: 0.80: :CR:B:
D0I_MO2B5 2 SUBL, SITES 0.32: 0.68: :MO:B:
MOB4 2 SUBL, SITES 0.20: 0.80: :MO:B:
NI4B3 2 SUBL, SITES 0.57: 0.43: :NI:B:
REB2 3 SUBL, SITES 1.00: 2.00: 2.00: :RE:B:B VA:
RUB2 2 SUBL, SITES 1.00: 2.00: :RU:B:
RU2B3 2 SUBL, SITES 2.00: 3.00: :RU:B:
RUB 2 SUBL, SITES 1.00: 1.00: :RU:B:
B3SI 3 SUBL, SITES 6.00: 2.00: 6.00: :B:SI:B SI:
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:
V2B3 2 SUBL, SITES 0.40: 0.60: :V:B:
B9W2 2 SUBL, SITES 9.00: 2.00: :B:W:
SIC 2 SUBL, SITES 1.00: 1.00: :SI:C:
V3C2 2 SUBL, SITES 3.00: 2.00: :V:C:
CO7HF 2 SUBL, SITES 7.00: 1.00: :CO:HF:

CO3SI 2 SUBL, SITES 3.00: 1.00: :CO:SI:
CO3VV 2 SUBL, SITES 3.00: 1.00: :CO V:CO V:
CO11ZR2 2 SUBL, SITES 11.00: 2.00: :CO:ZR:
CR3MN5 2 SUBL, SITES 3.00: 5.00: :CR:MN:
HIGH_SIGMA 3 SUBL, SITES 8.00: 4.00: 18.00: :MN:CR:CR MN:
FE2SI 2 SUBL, SITES 0.67: 0.33: :FE:SI:
FESI2_H 2 SUBL, SITES 0.30: 0.70: :FE:SI:
FESI2_L 2 SUBL, SITES 0.33: 0.67: :FE:SI:
HFNI3_ALPHA 2 SUBL, SITES 0.25: 0.75: :HF:NI:
HFNI3_BETA 2 SUBL, SITES 0.25: 0.75: :HF:NI:
HF3NI7 2 SUBL, SITES 0.30: 0.70: :HF:NI:
HFNI_ALPHA 2 SUBL, SITES 0.50: 0.50: :HF:NI:
HFRE 2 SUBL, SITES 1.00: 1.00: :HF:RE:
HF5SN4 2 SUBL, SITES 5.00: 4.00: :HF:SN:
HFSN2_C40 2 SUBL, SITES 1.00: 2.00: :HF:SN:
IRZR_ALPHA 2 SUBL, SITES 1.00: 1.00: :IR ZR:ZR:
IR3ZR5 2 SUBL, SITES 3.00: 5.00: :IR:ZR:

IRZR3 2 SUBL, SITES 1.00: 3.00: :IR:ZR:
IRZR_B2 2 SUBL, SITES 1.00: 1.00: :IR ZR:IR ZR:
MNTI_LT 2 SUBL, SITES 1.00: 1.00: :MN:TI:
MNTI_HT 2 SUBL, SITES 0.52: 0.48: :MN:TI:
MN3TI 2 SUBL, SITES 3.00: 1.00: :MN:TI:
MN4TI 2 SUBL, SITES 0.81: 0.18: :MN:TI:
NB3RU5 2 SUBL, SITES 0.38: 0.62: :NB RU:RU:
NI3SI_MONOCL 2 SUBL, SITES 3.00: 1.00: :NI:SI:
NBSN2 2 SUBL, SITES 1.00: 2.00: :NB SN V:NB SN:
NI3SI_MONOCL 2 SUBL, SITES 3.00: 1.00: :NI:SI:
NI3SI_ORTHO 2 SUBL, SITES 3.00: 1.00: :NI:SI:
NI3SI2 2 SUBL, SITES 3.00: 2.00: :NI: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:
RESI2_C11B 2 SUBL, SITES 0.36: 0.64: :RE:SI:
RU2SI_C37 2 SUBL, SITES 2.00: 1.00: :RU:SI:
RU4SI3 2 SUBL, SITES 4.00: 3.00: :RU:SI:

RUSI :RU:SI:	2 SUBL, SITES 1.00: 1.00:
RU2SI3 :RU:SI:	2 SUBL, SITES 2.00: 3.00:
SI5V6 :SI:V:	2 SUBL, SITES 5.00: 6.00:
TA3SN :TA:SN:	2 SUBL, SITES 3.00: 1.00:
TASN2 :TA:SN:	2 SUBL, SITES 1.00: 2.00:
V3SN :SN:V:	2 SUBL, SITES 0.20: 0.80:
VSN2 :SN:V:	2 SUBL, SITES 0.60: 0.40:
SN3Y :SN:Y:	2 SUBL, SITES 3.00: 1.00:
SN5Y2 :SN:Y:	2 SUBL, SITES 5.00: 2.00:
SN2Y_C49 :SN:Y:	2 SUBL, SITES 2.00: 1.00:
SN10Y11 :SN:Y:	2 SUBL, SITES 10.00: 11.00:
SN4Y5 :SN:Y:	2 SUBL, SITES 4.00: 5.00:
V4ZN5 :V:ZN:	2 SUBL, SITES 4.00: 5.00:
VZN3_L12 :V:ZN:	2 SUBL, SITES 1.00: 3.00:
ZN12Y :ZN:Y:	2 SUBL, SITES 12.00: 1.00:
Y2ZN17 :Y:ZN:	2 SUBL, SITES 2.00: 17.00:
H_RZN5 :Y:ZN:	2 SUBL, SITES 1.00: 5.00:

Y13ZN58 2 SUBL, SITES 13.00: 58.00: :Y:ZN:
ZN11Y3 2 SUBL, SITES 11.00: 3.00: :ZN:Y:
YZN3 2 SUBL, SITES 1.00: 3.00: :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 22.00: 1.00: :ZN:ZR:
ZN39ZR5 2 SUBL, SITES 39.00: 5.00: :ZN:ZR:
ZN3ZR_HT 2 SUBL, SITES 3.00: 1.00: :ZN:ZR:
ZN2ZR_C15 2 SUBL, SITES 2.00: 1.00: :ZN:ZR:
ZN2ZR3 2 SUBL, SITES 2.00: 3.00: :ZN:ZR:
ZNZR_B2 2 SUBL, SITES 1.00: 1.00: :ZN:ZR:
ALCCR2 3 SUBL, SITES 1.00: 1.00: 2.00: :AL:C:CR:
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:
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:
AL31MN6NI2 3 SUBL, SITES 31.00: 6.00: 2.00: :AL:MN:NI: > Orthorhombic, ternary Al-Mn-Ni phase
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
FE8SI2C 3 SUBL, SITES 8.00: 2.00: 1.00: :FE:SI:C:
TI3SIC2 3 SUBL, SITES 3.00: 1.00: 2.00: :TI:SI:C:
CRNBSI 3 SUBL, SITES 1.00: 1.00: 1.00: :CR:NB:SI: > hP9 Fe2P
M11SI8 2 SUBL, SITES 11.00: 8.00: :CR NB:SI: > oP76 Cr11Ge8
M6SI5 2 SUBL, SITES 6.00: 5.00: :CR NB:SI: > oI44 V6Si5
CR2NI2SI 3 SUBL, SITES 5.00: 5.00: 3.00: :CR:NI:SI:
M4SI3 2 SUBL, SITES 4.00: 3.00: :CR NI:SI:
CFC2_FENBZR 3 SUBL, SITES 2.00: 1.00: 3.00: :FE NB ZR:NB ZR:NB ZR:

NB15NI56TI29 :NB:NI:TI:	3 SUBL, SITES 0.15: 0.56: 0.29:
NB8NI9TI3 :NB:NI:TI:	3 SUBL, SITES 0.40: 0.45: 0.15:
NB5NI75TI20 :NB:NI:TI:	3 SUBL, SITES 0.05: 0.75: 0.20:
NB13NI75TI12 :NB:NI:TI:	3 SUBL, SITES 0.13: 0.75: 0.12:
NB15NI80TI5 :NB:NI:TI:	3 SUBL, SITES 0.15: 0.80: 0.05: