TCNI5 - TCS Ni-based Superalloys Database, Version 5.0

Thermo-Calc Software is pleased to announce the release of TCNI5, a thermodynamic database for different kinds of Ni-based superalloys for use with the Thermo-Calc and DICTRA software packages. Developed using the CALPHAD approach with industry input and support, TCNI5 is based on the critical evaluation of binary, ternary and in some cases higher order systems which enables predictions to be made for multicomponent systems and alloys of industrial importance. The database has also been validated where possible against higher order systems as well. In version 5 (TCNI5), all necessary volume data (including molar volume and thermal expansion) for various alloy phases were incorporated, which allows for the calculation of volume fraction of phases, as well as density, thermal expansivity and lattice parameters, e.g. misfits between γ and γ', using Thermo-Calc. However, it should be noted that the molar volume data incorporated has no pressure dependence.

The TCNI5 database contains an extensive GAS mixture phase (Al, Ar and different species in the C-H-N-O system) for the main purpose of considering oxygen/nitrogen-gas controls in alloy making processes, and different gas atmospheres under e.g. heat treatments. Note that argon, Ar, hydrogen, H, and oxygen, O, are included in the gas phase only, and there is no solid solubility or condensed phase compounds with these elements included in the TCNI5 database.

In total, TCNI5 includes critically assessed thermodynamic descriptions for 23 elements and 292 phases. Most of the binary systems in this database have been assessed and can be calculated with the BINARY Module in Thermo-Calc. TCNI5 also contains many assessed ternary systems, at least those being in equilibrium with γ and γ' phase, and can be calculated with the TERNARY Module in Thermo-Calc.

- Elements included: Al. Ar, B, C, Co, Cr, Fe, H, Hf, Mo, N, Nb, Ni, O, Pd, Pt, Re, Si, Ta, Ti, V, W, Zr
- Ordered and disordered bcc (A2 and B2/beta) and fcc (A1 and L12/γ′) phases are modeled with a two sub-lattice model using a single Gibbs energy curve which enables order/disorder transformations to be modeled.
- All possible binary systems and most Ni-containing ternary systems have been assessed to the full range of composition.
- Molar volume data critically assessed for most phases of importance to Ni-based Superalloys.

Only the phases of interest for superalloys are defined by default, which means that when retrieving the data from the database other phases will automatically be rejected and would need to be manually restored by the user if these are required for a calculation. The complete description of all the binary systems and many ternary systems are available using the BINARY and TERNARY modules. Note that there are several possible composition sets for the phases named FCC_L12 and BCC_B2; they are either disordered (A1/carbonitride and A2) or ordered (L12 (γ') and B2 (beta)).

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Assessed binary systems in full range of composition and temperature.

	Al	B	C	Co	Cr	Fe	Hf	Mo	N	Nb	Ni	Pd	Pt	Re	Si	Ta	Ti	V	W
B	x																		
C	x	x																	
Co	x	x	x																
Cr	x	x	x	x															
Fe	x	x	x	x	x														
Hf	x	x	x	x	x	x													
Mo	x	x	x	x	x	x	x												
N	x	x		x	x	x		x											
Nb	x	x	x	x	x	x	x	x	x										
Ni	x	x	x	x	x	x	x	x	x	x									
Pd	x	x	x	x	x	x	x	x		x	x								
Pt	x	x	x	x	x	x	x			x	x	x							
Re	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					
Ta	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			
V	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	
Zr	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

Assessed ternary systems in full range of composition and temperature.

Al-B-Co Al-B-Cr Al-B-Hf Al-B-Mo Al-B-Ni Al-B-Re Al-B-Ti Al-B-Zr Al-C-Cr Al-C-Hf Al-C-Mo Al-C-Ni Al-C-Ta Al-C-Ti Al-C-W Al-C-Zr Al-Co-Cr Al-Co-Fe Al-Co-Hf Al-Co-Mo Al-Co-Ni Al-Co-Ta Al-Co-Ti Al-Co-W Al-Co-Zr Al-Cr-Hf Al-Cr-Ni Al-Cr-Pt Al-Cr-Ta Al-Cr-Ti Al-Cr-Zr Al-Fe-Mo Al-Fe-Ni Al-Fe-Ti Al-Hf-Mo Al-Hf-Ni Al-Hf-Re Al-Hf-Ta Al-Hf-Ti Al-Hf-W Al-Hf-Zr Al-Mo-Ni Al-Mo-Re Al-Nb-Ni Al-Nb-Si Al-Ni-Pd Al-Ni-Pt Al-Ni-Re Al-Ni-Si Al-Ni-Ta Al-Ni-Ti Al-Ni-V Al-Ni-W Al-Ni-Zr Al-Ta-Ti B-Co-Cr B-Co-Hf B-Co-Mo B-Co-Ni B-Co-Re B-Co-Ta B-Co-Ti B-Co-W B-Cr-Ni B-Cr-Re B-Fe-Nb B-Hf-Nb B-Hf-Ni B-Hf-Re B-Hf-Ta B-Mo-Nb B-Mo-Ni B-Mo-Re B-Nb-Re B-Ni-Re B-Ni-Ta B-Re-Ta B-Re-Ti B-Re-W B-Re-Zr C-Co-Cr C-Co-Mo C-Co-Ti C-Co-W C-Co-Zr C-Cr-Hf C-Cr-Mo C-Cr-Ni C-Cr-Re C-Cr-Ta C-Cr-Ti C-Cr-W C-Cr-Zr C-Hf-Mo C-Hf-Ni C-Hf-Re C-Hf-Ta C-Hf-Ti C-Hf-W C-Hf-Zr C-Mo-Ni C-Mo-Ta C-Mo-Ti C-Mo-W C-Mo-Zr C-N-Ta C-Nb-Re C-Nb-W C-Ni-Ti C-Ni-W C-Ni-Zr C-Re-Ta C-Re-W C-Ta-Ti C-Ta-W C-Ta-Zr C-Ti-W C-Ti-Zr C-W-Zr Co-Cr-Mo Co-Cr-Nb Co-Cr-Ni Co-Cr-Re Co-Cr-Ti Co-Cr-W Co-Fe-Nb Co-Fe-Ti Co-Hf-W Co-Mo-Ta Co-Mo-W Co-Ni-Re Co-Ni-Ta Co-Ni-W Co-Re-W Co-Ta-W Co-Ti-W Co-Ti-Zr Co-W-Zr Cr-Fe-Mo Cr-Fe-N Cr-Fe-Ni Cr-Fe-Si Cr-Fe-W Cr-Hf-Nb Cr-Mo-Ni Cr-Nb-Ni Cr-Nb-Si Cr-Ni-Re Cr-Ni-Si Cr-Ni-Ta Cr-Ni-Ti Cr-Ni-W Cr-Ni-Zr Cr-W-Zr Fe-Mo-Ni Fe-Mo-W Fe-Nb-Ni Fe-Nb-Zr Fe-Ni-W Hf-Mo-Ni Hf-Nb-Si Hf-Ni-Ta Mo-Nb-Ni Mo-Ni-Re Mo-Ni-Ta Mo-Ni-Ti Mo-Ni-W Mo-Re-Ta Nb-Ni-Ti Nb-Ni-W Nb-Re-Ta Nb-Re-W Ni-Re-Ta Ni-Re-Ti Ni-Re-W Ni-Re-Zr Ni-Ta-W Ni-W-Zr Re-Ta-W Re-Ta-Zr Re-W-Zr Ta-W-Zr Ti-W-Zr

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Example Calculations using TCNI5

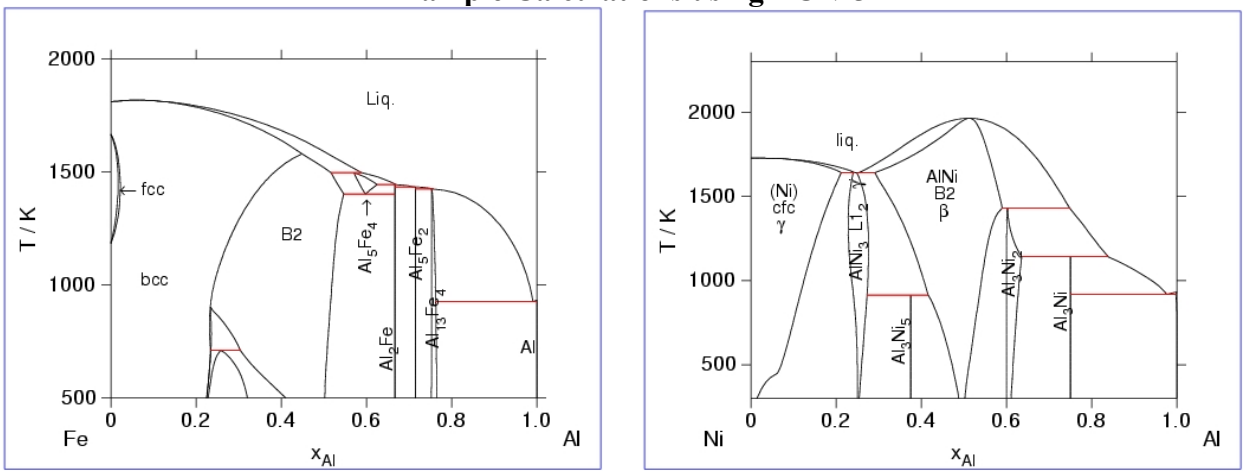

Figure 1. Phase diagrams calculated for Al-Fe[1] and Al-Ni[2].

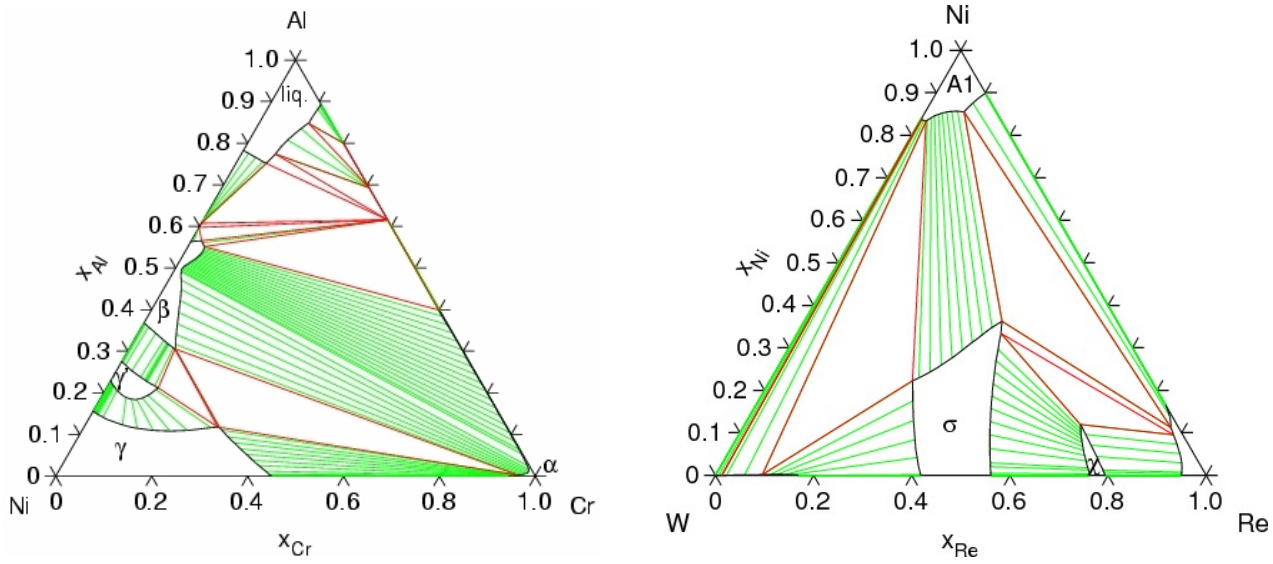

Figure 2. Isothermal sections of Al-Cr-Ni[3] and Ni-Re-W[4] calculated at 1273 K.

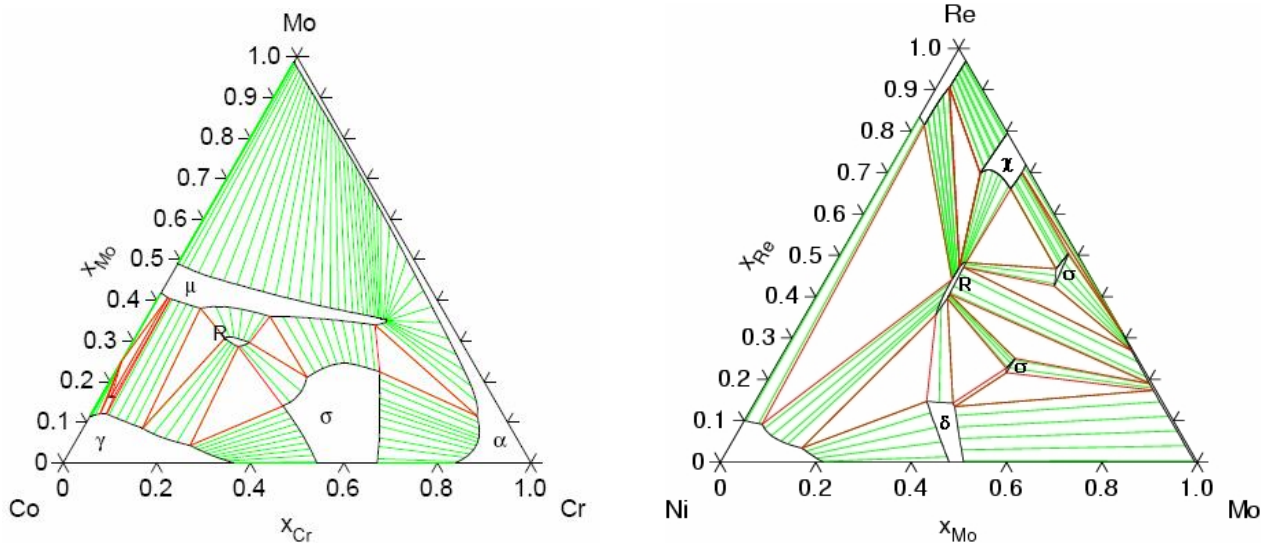

Figure 3. Isothermal sections of Co-Cr-Mo[5] and Mo-Ni-Re[6] calculated at 1273 K.

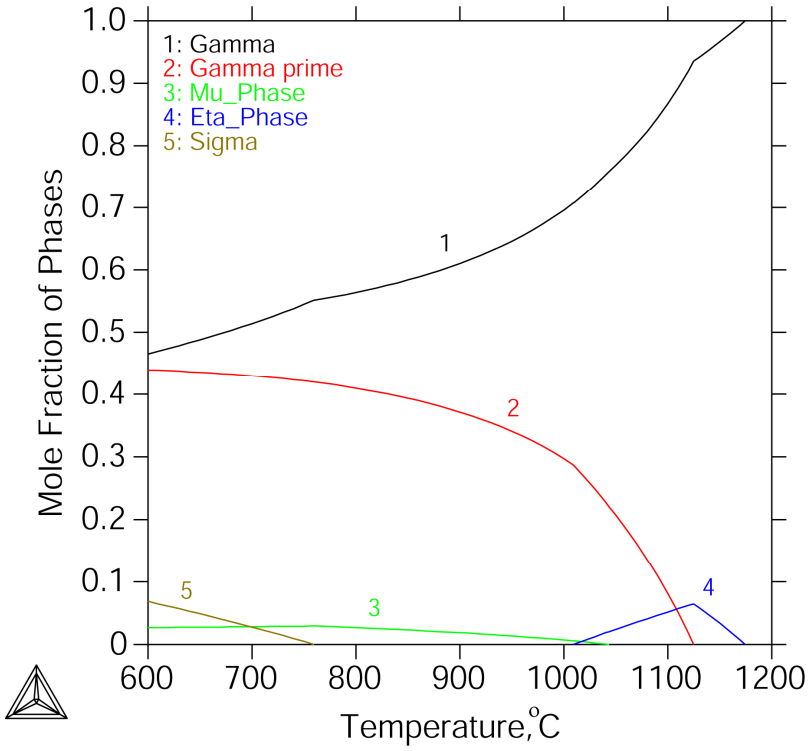

Figure 4. Predicted amount of phases (NI3TI_D024 is eta phase) at varying temperatures for a Ni-15Cr-26Co-2.8Mo-1.1W-1.9Al-6Ti (wt. %) alloy. The experimental determination[7] of the stable eta phase region is between 1030 ºC to 1170 ºC.

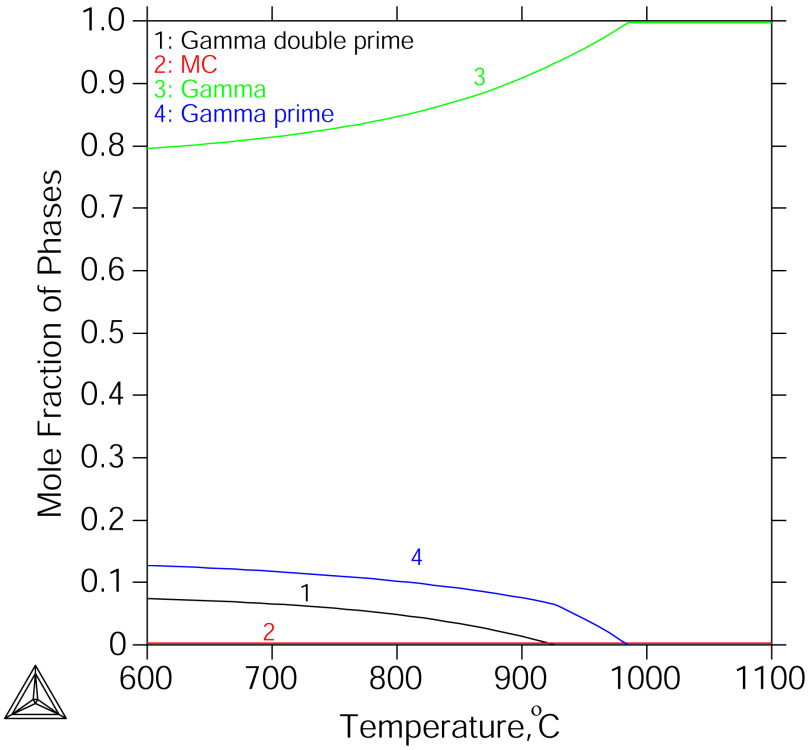

Figure 5. Predicted amount of phases (metastable calculation) at varying temperatures for a Ni-18Cr-18Fe-3Mo-0.5Al-1Ti-5.3Nb-0.02C (wt. %) alloy. Experimental γ'' (BCT_D022) solvus temperature[8] is close to 900 ºC and the γ'+γ'' fraction is between 15-20 %.

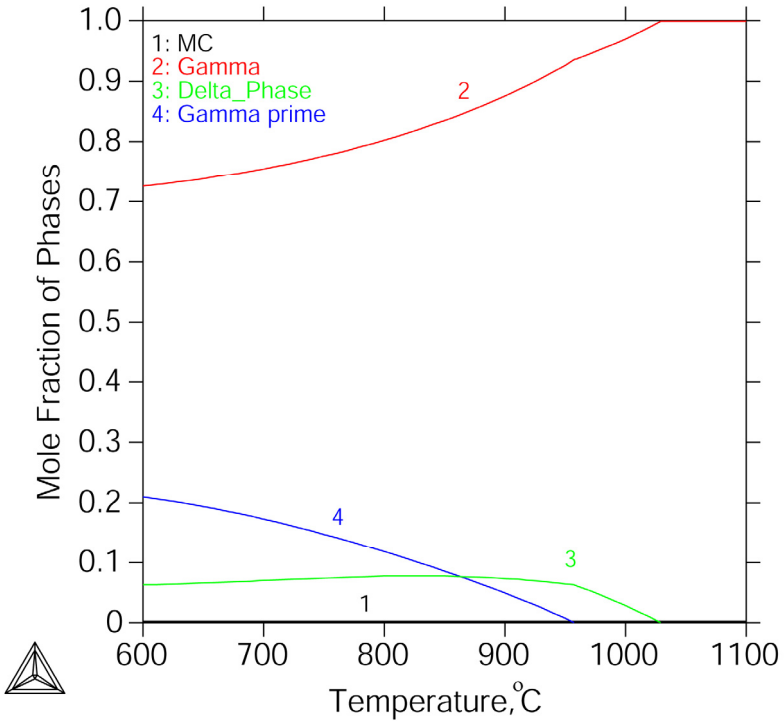

Figure 6. Predicted amount of phases at varying temperatures for a Ni-18Cr-10Fe-9Co-2.8Mo-1.5Al-0.7Ti-5.3Nb-0.02C (wt. %) alloy. Experimental γ' solvus temperature[9] is close to 950 ºC and delta (NI3TA_D0A) solvus close to 1010 ºC. The delta phase fraction was measured around 8 % and γ' fraction around 20% at 760 ºC after 500 hr heat treatment.

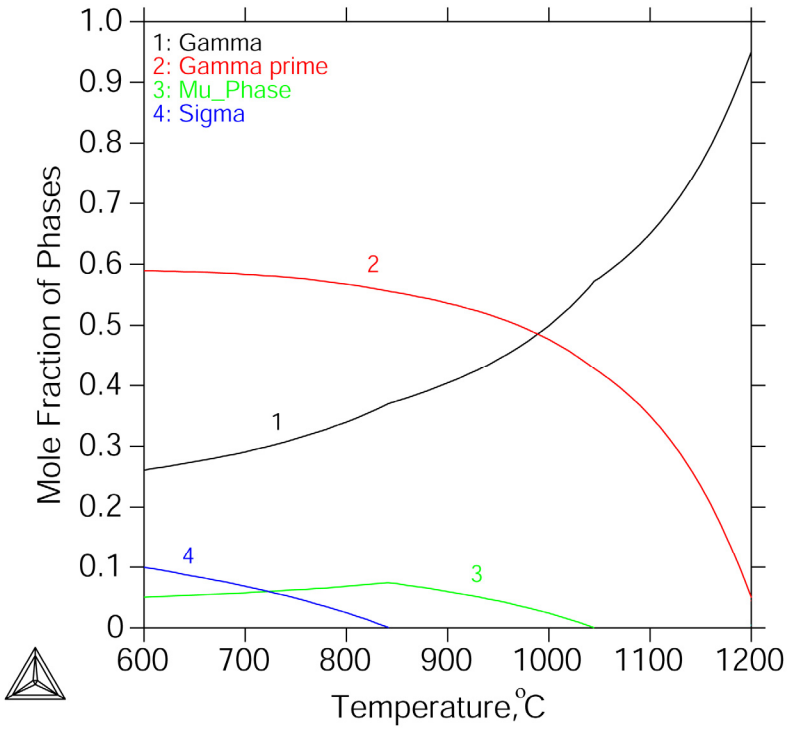

Figure 7. Predicted amount of phases at varying temperatures for a Ni-11.5Cr-15.5Co-6.5Mo-4.3Al-4.3Ti-0.5Hf (wt. %) alloy. Experimental γ' solvus temperature[10] is close to 1150 ºC and both σ and μ phases were observed at 760 ºC after 1000 hr heat treatment.

at.%	Ni	Al	Cr	W	Experimental γ' fraction	Predicted γ' fraction
Ni-9.8Al-8.3Cr γ	82.9 (82.7)	8.51 (8.43)	8.61 (8.86)	-		
Ni-9.8Al-8.3Cr γ'	76.7 (76.6)	16.7 (17.4)	6.63 (5.99)	-	18.9	15.8
Ni-9.7Al-8.5Cr-2W γ	81.4 (81.8)	6.75 (6.23)	9.51 (10.48)	2.35 (1.54)		
Ni-9.7Al-8.5Cr-2W γ'	76.2 (76.2)	16.4 (16.9)	6.19 (3.94)	1.21 (3.00)	30.8	30.5

Table 1. Predicted compositions of γ and γ' as well as the fraction in two Ni-base alloys compared with measurements (in brackets) from Sudbrack et al.[11]

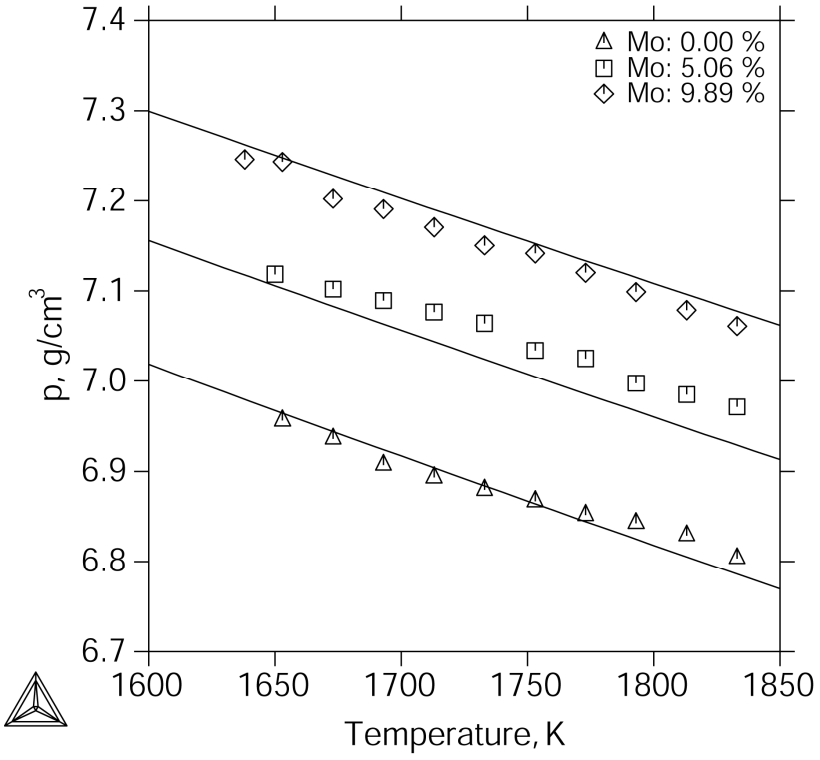

Figure 8. Predicted densities of liquid Ni-Cr-Al-Mo alloys where the molar ratio of Ni:Cr:Al is close to the average value for commercial superalloys INCO713, CM247LC and CMSX-4. Symbols are the experimental values from Fang et al.[12]

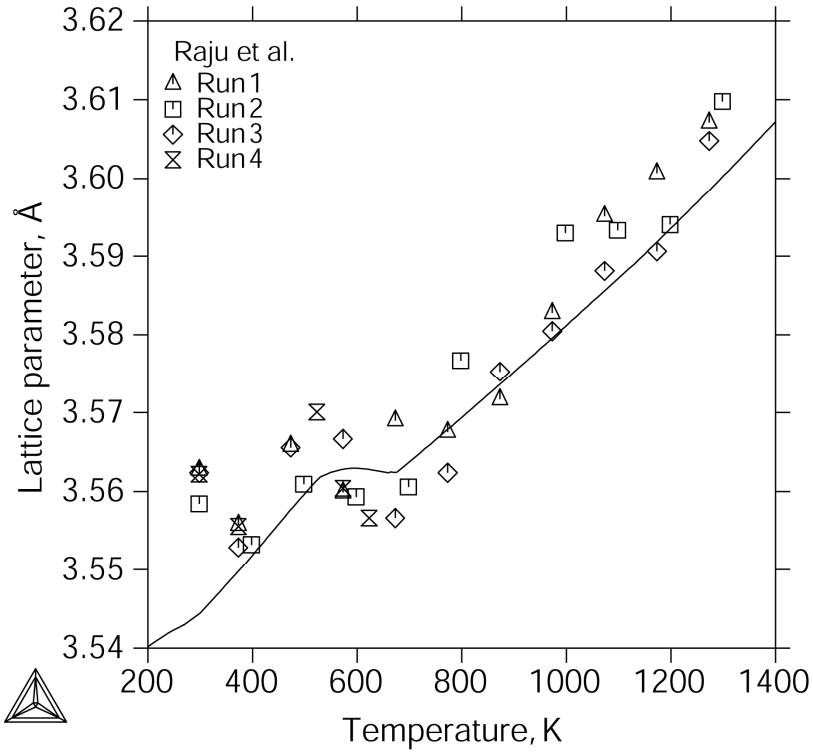

Figure 9. Predicted lattice parameters of disordered FCC of Inconel-600 at varying temperatures compared to X-ray diffraction values by Raju et al.[13] At low temperature the calculation gives, besides the disordered FCC, also an ordered L12 phase, which causes the kink in the curve.

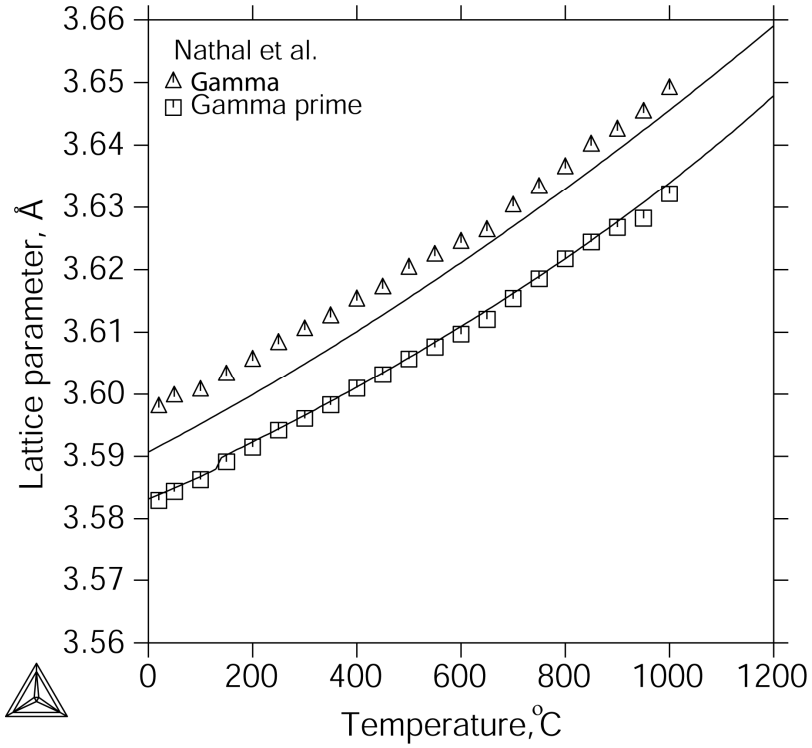

Figure 10. Predicted γ/γ' lattice mismatch of a Ni-0.6Mo-0.92Ta-12.5Al-1.83Ti-10.5Cr-3.3W (at. %) compared to an experimental determination by Nathal et al.[14]

Acknowledgement

Dr Nathalie Dupin and Prof Bo Sundman are acknowledged for many valuable discussions and important contributions.

References

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List of all phases included in TCNI5.

LIQUID
FCC_L12#1 (Austenite/γ)
FCC_L12#2 (γ')
FCC_L12#3 (carbonitride)
BCC_B2#1 (disordered BCC)
BCC_B2#2 (ordered BCC)
NI3TI_D024 (Eta)
NI3TA_D0A (Delta)
BCT_D022 (γ'')
HCP_A3
DIAMOND_A4
BETA_RHOMBO_B
GRAPHITE
D019_HCP
C14_LAVES
MU_PHASE
SIGMA
R_PHASE
P_PHASE
CHI_A12
MONI_DELTA
NISI_B31
MC_ETA
MC_SHP
M23C6
CEMENTITE
M12C
M3C2
M6C
M7C3
TAU
MB_B33
MB2_C32
M3B2
M2B_TETR
ALPT
ALTI_L10
NIZR
ALZR
ALPHA_B19
B11
AL2PT
C15_LAVES
C36_LAVES
NI2TA
NI2V
C16_THETA
NITI2
REZR2
CO3M
ALTI3_DO19
AL3ZR
MZR3_E1A
H_L21
G_PHASE
AL21PD8
AL2PD5
AL3PD
AL3PD2
AL3PD5
AL4PD
ALPD2
AL21PT5
AL21PT8
AL3PT2
AL3PT5
ALPT2
AL2ZR3
AL3ZR4
AL3ZR2
AL3NI2
AL12W
AL4W
HF2PD
HF3PD4
HFPD2
BPD3
BPD5
BPD6
B2PD5
BPT3
BPT2
B2PT3
MONI4_BETA
AL5W
NI7ZR2
NI11ZR9
NI10ZR7
NI5ZR
PD21SI4
PD5SI
PD14SI3
PD9SI2
PD15SI4
PD3SI
PD39SI20
PD19SI10
ALPHA_PD2SI
BETA_PD2SI
PD2TA
PD2TI
PD3TI2
PD5TI3
PD11ZR9
PD4ZR3
PDZRM
PDZR_ALPHA
PDZR_BETA
PTSI
PT6SI5
ALPHA_PT2SI
BETA_PT2SI
ALPHA_PT17SI8
BETA_PT17SI8
PT5SI2
BETA_PT3SI
ALPHA_PT3SI
PT25SI7
PT2TA
PT3TA
PT3TI4
PT8TI
PT4ZR3
PT4ZR
PT3ZR5
PT10ZR7
HF8NI21
AL13FE4
NI8TA
CO7M2
W3COC
ALM3C_E21
AL4C3
BM
COB
MOB
BW_ALPHA
BW_BETA
CR2B_ORTH
MOCOB
NI3B_D011
RE3B
B4TA3_D7B

B5W2_X
RE7B3
D5A_M3B2
W2COB2
CR5B3
V5B6
Z_PHASE
FE4N_LP1
FECN_CHI
PI
ALN_B4
SI3N4
BN_B4
TI2N_C4
TAN_EPS
TI3N2
TI4N3
ALNTI2
ALNTI3
AL2N2TI3
M5SI3_D88
W5SI3_D8M
TA5SI3_D8L
ZR5SI4
CR3SI_A15
M3SI1
CO2SI_C23
MSI_B27
FESI_B20
CRSI2_C40
MOSI2_C11B
ZRSI2_C49
TISI2_C54
MSI2_C1
M3SI2_D5A
NI31SI12
CR3NI5SI2
GAS
ALB12_ALPHA
AL13CO4
AL3CO
AL5CO2_D811
AL9CO2
AL11CR2
AL13CR2
AL4CR
AL8CR5_H
AL8CR5_L
AL9CR4_H
AL9CR4_L
ALCR2
AL2FE
AL5FE2
AL5FE4
AL63MO37
AL8MO3
ALMO
AL3NI1
AL3NI5
AL11RE4
AL4RE
AL6RE
ALRE2
ALRE
TAAL
TAAL2
AL11TI5
AL2TI
AL10V
AL7V
AL23V4
AL8V5
AL77W23
AL7W3
AL2W
ALZR2
AL3ZR5
AL4ZR5
B4C
CRB4
D0I_MO2B5
MOB4
NI4B3
REB2
B3SI
B6SI
BNSI
V2B3
B9W2
B12ZR
SIC
V3C2
CO7HF
CO3SI
CO3V
CO11ZR2
FE2SI
FESI2_H
FESI2_L
HFNI3_ALPHA
HFNI3_BETA
HF3NI7
HFNI_ALPHA
HFRE
NI3SI_MONOCL
NI3SI_ORTHO
NI3SI2
NI2SI_TETA
RE2SI
RESI2_C11B
SI5V6
CO3AL2B5
ALCR2B2
ALCR3B4
ALBMO
NI5ALB4
NI8ALB11
ALCCR2
AL4SIC4
AL8SIC7
ALFESI_ALPHA
ALFESI_BETA
ALFESI_GAMMA
ALFESI_DELTA
ALFESI_TAU1
ALFESI_TAU3
RECOB
RE5CO2B4
RE3CO3B2
NI3CR2B6
NICR3B6
FEWB
MO3NI10B11
NI6SI2B
NI4SI2B
FE8SI2C
TI3SIC2
CRNBSI
M11SI8
M6SI5
CR2NI2SI
M4SI3
CFC2_FENBZR
NB15NI56TI29
NB8NI9TI3
NB5NI75TI20
NB13NI75TI12
NB15NI80TI5

LIQUID
  CONSTITUENTS:
AL,AL1N1,B,C,CO,CR,FE,HF,MO,N,NB,NI,PD,PT,RE,SI,TA,TI,V,W,ZR

AL10V
 2 SUBLATTICES, SITES 10: 1
  CONSTITUENTS: AL : V

AL11CR2
 3 SUBLATTICES, SITES 10: 1: 2
  CONSTITUENTS: AL : AL : CR

AL11RE4
 2 SUBLATTICES, SITES 11: 4
  CONSTITUENTS: AL : RE

AL11TI5
 2 SUBLATTICES, SITES 17: 8
  CONSTITUENTS: AL : TI

AL12W
2 SUBLATTICES, SITES 12: 1
  CONSTITUENTS: AL : MO,RE,W

AL13CO4
 2 SUBLATTICES, SITES 13: 4
  CONSTITUENTS: AL : CO

AL13CR2
 2 SUBLATTICES, SITES 13: 2
  CONSTITUENTS: AL : CR

AL13FE4
3 SUBLATTICES, SITES .6275: .235: .1375
  CONSTITUENTS: AL : FE : AL,SI,VA

AL21PD8
 2 SUBLATTICES, SITES 21: 8
  CONSTITUENTS: AL : PD

AL21PT5
 2 SUBLATTICES, SITES .8077: .1923
  CONSTITUENTS: AL : PT

AL21PT8
 2 SUBLATTICES, SITES .7241: .2759
  CONSTITUENTS: AL : PT

AL23V4
2 SUBLATTICES, SITES 23: 4
CONSTITUENTS: AL : V

AL2FE
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: AL : FE

AL2N2TI3
3 SUBLATTICES, SITES 2: 2: 3
CONSTITUENTS: AL : N : TI

AL2PD5
2 SUBLATTICES, SITES 2: 5
CONSTITUENTS: AL : AL,PD

AL2PT
2 SUBLATTICES, SITES .66667: .33333
CONSTITUENTS: AL : PT

AL2TI
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: AL : TI

AL2W
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: AL : W

AL2ZR3
2 SUBLATTICES, SITES 2: 3
CONSTITUENTS: AL : HF,ZR

AL3CO
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: AL : CO

AL3NI1
2 SUBLATTICES, SITES .75: .25
CONSTITUENTS: AL : NI

AL3NI2
3 SUBLATTICES, SITES 3: 2: 1
CONSTITUENTS: AL,SI : AL,NI,PT : NI,VA

AL3NI5
2 SUBLATTICES, SITES .375: .625
CONSTITUENTS: AL : NI

AL3PD
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: AL : PD

AL3PD2
2 SUBLATTICES, SITES 3: 2
CONSTITUENTS: AL,PD : AL,PD

AL3PD5
2 SUBLATTICES, SITES 3: 5
CONSTITUENTS: AL : PD

AL3PT2
2 SUBLATTICES, SITES .6: .4
CONSTITUENTS: AL : PT

AL3PT5
2 SUBLATTICES, SITES .375: .625
CONSTITUENTS: AL : PT

AL3ZR
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: AL : HF,ZR

AL3ZR2
2 SUBLATTICES, SITES 3: 2
CONSTITUENTS: AL : HF,ZR

AL3ZR4
2 SUBLATTICES, SITES 3: 4
CONSTITUENTS: AL : HF,ZR

AL3ZR5
2 SUBLATTICES, SITES 3: 5
CONSTITUENTS: AL : ZR

AL4C3
2 SUBLATTICES, SITES 4: 3
CONSTITUENTS: AL,SI : C

AL4CR
2 SUBLATTICES, SITES 4: 1
CONSTITUENTS: AL : CR

AL4PD
2 SUBLATTICES, SITES 4: 1
CONSTITUENTS: AL : PD

AL4RE
2 SUBLATTICES, SITES 4: 1
CONSTITUENTS: AL : RE

AL4SIC4
3 SUBLATTICES, SITES 4: 1: 4
CONSTITUENTS: AL : SI : C

AL4W
2 SUBLATTICES, SITES 4: 1
CONSTITUENTS: AL : MO,W

AL4ZR5
2 SUBLATTICES, SITES 4: 5
CONSTITUENTS: AL : ZR

AL5CO2_D811
2 SUBLATTICES, SITES 5: 2
CONSTITUENTS: AL : CO

AL5FE2
2 SUBLATTICES, SITES 5: 2
CONSTITUENTS: AL : FE

AL5FE4
CONSTITUENTS: AL,FE

AL5W
2 SUBLATTICES, SITES 5: 1
CONSTITUENTS: AL : MO,W

AL63MO37
2 SUBLATTICES, SITES 63: 37
CONSTITUENTS: AL : MO

AL6RE
2 SUBLATTICES, SITES 6: 1
CONSTITUENTS: AL : RE

AL77W23
2 SUBLATTICES, SITES 77: 23
CONSTITUENTS: AL : W

AL7V
2 SUBLATTICES, SITES 7: 1
CONSTITUENTS: AL : V

AL7W3
2 SUBLATTICES, SITES 7: 3
CONSTITUENTS: AL : W

AL8CR5_H
2 SUBLATTICES, SITES 8: 5
CONSTITUENTS: AL : CR

AL8CR5_L
2 SUBLATTICES, SITES 8: 5
CONSTITUENTS: AL : CR

AL8MO3
2 SUBLATTICES, SITES 8: 3
CONSTITUENTS: AL : MO

AL8SIC7
3 SUBLATTICES, SITES 8: 1: 7
CONSTITUENTS: AL : SI : C

AL8V5
2 SUBLATTICES, SITES 8: 5
CONSTITUENTS: AL : V

AL9CO2
2 SUBLATTICES, SITES 9: 2
CONSTITUENTS: AL : CO

AL9CR4_H
2 SUBLATTICES, SITES 9: 4
CONSTITUENTS: AL : CR

AL9CR4_L
2 SUBLATTICES, SITES 9: 4
CONSTITUENTS: AL : CR

ALB12_ALPHA
2 SUBLATTICES, SITES 1: 12
CONSTITUENTS: AL : B

ALBMO
3 SUBLATTICES, SITES 1: 1: 1
CONSTITUENTS: AL : B : MO

ALCCR2
3 SUBLATTICES, SITES 1: 1: 2
CONSTITUENTS: AL : C : CR

ALCR2
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: AL : CR

ALCR2B2
3 SUBLATTICES, SITES 1: 2: 2
CONSTITUENTS: AL : CR : B

ALCR3B4
3 SUBLATTICES, SITES 1: 3: 4
CONSTITUENTS: AL : CR : B

ALFESI_ALPHA
4 SUBLATTICES, SITES .6612: .19: .0496: .0992
CONSTITUENTS: AL : FE : SI : AL,SI

ALFESI_BETA
3 SUBLATTICES, SITES 14: 3: 3
CONSTITUENTS: AL : FE : SI

ALFESI_DELTA
3 SUBLATTICES, SITES .55: .15: .3
CONSTITUENTS: AL : FE : SI

ALFESI_GAMMA
3 SUBLATTICES, SITES 3: 1: 1
CONSTITUENTS: AL : FE : SI

ALFESI_TAU1
3 SUBLATTICES, SITES 2: 2: 1
CONSTITUENTS: AL : FE : SI

ALFESI_TAU3
3 SUBLATTICES, SITES 2: 1: 1
CONSTITUENTS: AL : FE : SI

ALM3C_E21
3 SUBLATTICES, SITES 1: 3: 1
CONSTITUENTS: AL : CO,FE : C

ALMO
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: AL,MO : AL,MO

ALNTI2
3 SUBLATTICES, SITES 1: 1: 2
CONSTITUENTS: AL : N : TI

ALNTI3
3 SUBLATTICES, SITES 1: 1: 3
CONSTITUENTS: AL : N : TI

ALN_B4
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: AL : N

ALPD2
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: AL,NI,PD : AL,NI,PD

ALPHA_B19
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: NB,PD,PT,TI,V,ZR : NB,PD,PT,TI,V,ZR

ALPHA_PD2SI
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: PD,SI : SI

ALPHA_PT17SI8
2 SUBLATTICES, SITES 17: 8
CONSTITUENTS: PT : SI

ALPHA_PT2SI
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: PT : SI

ALPHA_PT3SI
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: PT : SI

ALPT
2 SUBLATTICES, SITES .5: .5
CONSTITUENTS: AL : PT

ALPT2
2 SUBLATTICES, SITES .33333: .66667
CONSTITUENTS: AL : PT

ALRE
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: AL : RE

ALRE2
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: AL : RE

ALTI3_DO19
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: AL,CR,MO,NI,TA,TI,W : AL,CR,MO,NI,TA,TI,W

ALTI_L10
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: AL,CR,MO,TA,TI,W : AL,CR,MO,TA,TI,W

ALZR
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: AL : HF,ZR

ALZR2
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: AL : ZR

B11
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: PD : TA

B12ZR
2 SUBLATTICES, SITES 12: 1
CONSTITUENTS: B : ZR

B2PD5
2 SUBLATTICES, SITES 2: 5
CONSTITUENTS: B : PD

B2PT3
2 SUBLATTICES, SITES 2: 3
CONSTITUENTS: B : PT

B3SI
3 SUBLATTICES, SITES 6: 2: 6
CONSTITUENTS: B : SI : B,SI

B4C
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: B11C,B12 : B2,C2B,CB2

B4TA3_D7B
2 SUBLATTICES, SITES 4: 3
CONSTITUENTS: B : CR,HF,NB,TA,TI,V

B5W2_X
2 SUBLATTICES, SITES 5: 2
CONSTITUENTS: B,C,VA : W

B6SI
3 SUBLATTICES, SITES 210: 23: 48
CONSTITUENTS: B : SI : B,SI

B9W2
2 SUBLATTICES, SITES 9: 2
CONSTITUENTS: B : W

BCC_A2
THIS PHASE IS THE DISORDERED PART OF BCC_B2
2 SUBLATTICES, SITES 1: 3
CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,VA,W,ZR : B,C,
N,VA

BCC_B2
THIS PHASE HAS A DISORDERED CONTRIBUTION FROM BCC_A2
3 SUBLATTICES, SITES .5: .5: 3
CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,VA,W,ZR : AL,
CO,CR,FE,HF,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,VA,W,ZR : B,C,N,VA

BCT_D022
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: AL,CR,FE,MO,NI,PD,PT,TI,V : AL,CR,MO,NB,NI,PD,PT,SI,TA,TI,V

BETA_PD2SI
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: PD,SI : SI

BETA_PT17SI8
2 SUBLATTICES, SITES 17: 8
CONSTITUENTS: PT : SI

BETA_PT2SI
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: PT : SI

BETA_PT3SI
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: PT : SI

BETA_RHOMBO_B
2 SUBLATTICES, SITES 93: 12
CONSTITUENTS: B : B,C,SI

BM
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: B : CR,FE,HF,MO,TI

BNSI
3 SUBLATTICES, SITES 61: 1: 8
CONSTITUENTS: B : SI : B,SI

BN_B4
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: B : N

BPD3
2 SUBLATTICES, SITES 1: 3
CONSTITUENTS: B : PD

BPD5
2 SUBLATTICES, SITES 1: 5
CONSTITUENTS: B : PD

BPD6
2 SUBLATTICES, SITES 1: 6
CONSTITUENTS: B : PD

BPT2
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: B : PT

BPT3
2 SUBLATTICES, SITES 1: 3
CONSTITUENTS: B : PT

BW_ALPHA
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: B,C,VA : W

BW_BETA
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: B,C,VA : W

C14_LAVES
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,RE,SI,TA,TI,W,ZR : AL,CO,CR,FE,HF,
MO,NB,NI,RE,SI,TA,TI,W,ZR

C15_LAVES
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,RE,SI,TA,TI,V,W,ZR : AL,CO,CR,FE,
HF,MO,NB,NI,RE,SI,TA,TI,V,W,ZR

C16_THETA
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: HF,MO,NB,TA,TI,W,ZR : AL,CO,CR,FE,NI,SI

C36_LAVES
 2 SUBLATTICES, SITES 2: 1
  CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,TA,TI,W,ZR : AL,CO,CR,FE,HF,MO,NB,
  NI,TA,TI,W,ZR

CEMENTITE
 2 SUBLATTICES, SITES 3: 1
  CONSTITUENTS: CO,CR,FE,MO,NI,V,W : C,N

CFC2_FENBZR
 3 SUBLATTICES, SITES 2: 1: 3
  CONSTITUENTS: FE,NB,ZR : NB,ZR : NB,ZR

CHI_A12
 3 SUBLATTICES, SITES 24: 10: 24
  CONSTITUENTS: CR,FE,NI,RE : AL,CR,HF,MO,NB,TA,TI,W,ZR : CR,FE,MO,NB,NI,
  RE,TA,W

CO11ZR2
 2 SUBLATTICES, SITES 11: 2
  CONSTITUENTS: CO : ZR

CO2SI_C23
 2 SUBLATTICES, SITES 2: 1
  CONSTITUENTS: CO,CR,FE,NI,TI : SI

CO3AL2B5
 3 SUBLATTICES, SITES 3: 2: 5
  CONSTITUENTS: CO : AL : B

CO3M
 2 SUBLATTICES, SITES 3: 1
  CONSTITUENTS: CO,NI : MO,NB,TA,TI,W

CO3SI
 2 SUBLATTICES, SITES 3: 1
  CONSTITUENTS: CO : SI

CO3V
 2 SUBLATTICES, SITES 3: 1
  CONSTITUENTS: CO,V : CO,V

CO7HF
 2 SUBLATTICES, SITES 7: 1
  CONSTITUENTS: CO : HF

CO7M2
 2 SUBLATTICES, SITES 7: 2
  CONSTITUENTS: CO : NB,TA

COB
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: CO,RE : B

CR2B_ORTH
2 SUBLATTICES, SITES .666667: .333333
CONSTITUENTS: CR,FE,MO,RE : B

CR2NI2SI
3 SUBLATTICES, SITES 5: 5: 3
CONSTITUENTS: CR : NI : SI

CR3NI5SI2
4 SUBLATTICES, SITES 3: 5: 2: 1
CONSTITUENTS: CR : NI : SI : C,VA

CR3SI_A15
3 SUBLATTICES, SITES 3: 1: 3
CONSTITUENTS: CR,FE,MO,NB,NI,PD,PT,RE,SI,TA,TI,V : AL,CO,CR,NB,NI,PD,PT,
SI,TA,TI,V : C,VA

CR5B3
2 SUBLATTICES, SITES .625: .375
CONSTITUENTS: CR,MO : B

CRB4
2 SUBLATTICES, SITES .2: .8
CONSTITUENTS: CR : B

CRNBSI
3 SUBLATTICES, SITES 1: 1: 1
CONSTITUENTS: CR : NB : SI

CRSI2_C40
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: CR,HF,MO,NB,SI,TA,V : AL,CR,SI

D019_HCP
3 SUBLATTICES, SITES .75: .25: 1
CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,RE,SI,TA,TI,W,ZR : AL,CO,CR,FE,HF,
MO,NB,NI,RE,SI,TA,TI,W,ZR : VA

D0I_MO2B5
2 SUBLATTICES, SITES .32: .68
CONSTITUENTS: MO : B

D5A_M3B2
2 SUBLATTICES, SITES 3: 2
CONSTITUENTS: FE,HF,MO,NB,TA,V : B

DIAMOND_A4
  CONSTITUENTS: B,C,SI

DIS_MU
 THIS PHASE IS THE DISORDERED PART OF MU_PHASE
  CONSTITUENTS: AL,CO,CR,FE,MO,NB,NI,RE,TA,W

DIS_SIG
 THIS PHASE IS THE DISORDERED PART OF SIGMA
  CONSTITUENTS: AL,CO,CR,FE,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,W

FCC_A1
 THIS PHASE IS THE DISORDERED PART OF FCC_L12
2 SUBLATTICES, SITES 1: 1
  CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,W,ZR : B,C,N,VA

FCC_L12
 THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
3 SUBLATTICES, SITES .75: .25: 1
  CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,W,ZR : AL,CO,
  CR,FE,HF,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,W,ZR : B,C,N,VA

FE2SI
 2 SUBLATTICES, SITES .666667: .333333
  CONSTITUENTS: FE : SI

FE4N_LP1
 2 SUBLATTICES, SITES 4: 1
  CONSTITUENTS: CO,FE,NI : N

FE8SI2C
 3 SUBLATTICES, SITES 8: 2: 1
  CONSTITUENTS: FE : SI : C

FECN_CHI
 2 SUBLATTICES, SITES 2.2: 1
  CONSTITUENTS: FE : N

FESI2_H
 2 SUBLATTICES, SITES .3: .7
  CONSTITUENTS: FE : SI

FESI2_L
 2 SUBLATTICES, SITES .333333: .666667
  CONSTITUENTS: FE : SI

FESI_B20
 2 SUBLATTICES, SITES 1: 1
  CONSTITUENTS: CO,CR,FE,NI,RE : AL,SI

FEWB
3 SUBLATTICES, SITES 1: 1: 1
CONSTITUENTS: FE : W : B

GRAPHITE
CONSTITUENTS: B,C

G_PHASE
3 SUBLATTICES, SITES 16: 6: 7
CONSTITUENTS: AL,CO,FE,NI,TI : HF,NB,TI,ZR : CO,FE,NI,SI

HCP_A3
2 SUBLATTICES, SITES 1: .5
CONSTITUENTS: AL,CO,CR,FE,HF,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,W,ZR : B,C,N,VA

HF2PD
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: HF : PD

HF3NI7
2 SUBLATTICES, SITES .3: .7
CONSTITUENTS: HF : NI

HF3PD4
2 SUBLATTICES, SITES 3: 4
CONSTITUENTS: HF : PD

HF8NI21
2 SUBLATTICES, SITES 8: 21
CONSTITUENTS: HF,ZR : NI

HFNI3_ALPHA
2 SUBLATTICES, SITES .25: .75
CONSTITUENTS: HF : NI

HFNI3_BETA
2 SUBLATTICES, SITES .25: .75
CONSTITUENTS: HF : NI

HFNI_ALPHA
2 SUBLATTICES, SITES .5: .5
CONSTITUENTS: HF : NI

HFPD2
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: HF : PD

HFRE
 2 SUBLATTICES, SITES 1: 1
  CONSTITUENTS: HF : RE

H_L21
 3 SUBLATTICES, SITES .5: .5: 1
  CONSTITUENTS: AL,NI,TI : AL,HF,NB,NI,TA,TI,ZR : CO,NI,VA
M11SI8
 2 SUBLATTICES, SITES 11: 8
  CONSTITUENTS: CR,NB : SI

M12C
 3 SUBLATTICES, SITES 6: 6: 1
  CONSTITUENTS: CO,NI : MO,W : C

M23C6
 3 SUBLATTICES, SITES 20: 3: 6
  CONSTITUENTS: CO,CR,FE,NI,RE,V : CO,CR,FE,MO,NI,RE,V,W : C

M2B_TETR
 2 SUBLATTICES, SITES 2: 1
  CONSTITUENTS: AL,CO,CR,FE,MO,NB,NI,RE,TA,W : B

M3B2
 3 SUBLATTICES, SITES .4: .2: .4
  CONSTITUENTS: CR,FE,MO,NI,W : CR,FE,NI : B

M3C2
 2 SUBLATTICES, SITES 3: 2
  CONSTITUENTS: CR,MO,V,W : C

M3SI1
 2 SUBLATTICES, SITES 3: 1
  CONSTITUENTS: HF,NB,TA,TI,ZR : SI

M3SI2_D5A
 2 SUBLATTICES, SITES 3: 2
  CONSTITUENTS: HF,NB,ZR : SI

M4SI3
 2 SUBLATTICES, SITES 4: 3
  CONSTITUENTS: CR,NI : SI

M5SI3_D88
 4 SUBLATTICES, SITES 2: 3: 3: 1
  CONSTITUENTS: CR,FE,HF,MO,NB,SI,TI,ZR : CR,SI,TI : CR,FE,HF,MO,NB,TI,ZR
  : C,VA

M6C
4 SUBLATTICES, SITES 2: 2: 2: 1
CONSTITUENTS: CO,FE,NI : MO,NB,TA,W : CO,CR,FE,MO,NB,NI,TA,V,W : C

M6SI5
2 SUBLATTICES, SITES 6: 5
CONSTITUENTS: CR,NB : SI

M7C3
2 SUBLATTICES, SITES 7: 3
CONSTITUENTS: CO,CR,FE,MO,NI,RE,V,W : C

MB2_C32
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: B : AL,CR,HF,MO,NB,TA,TI,V,ZR

MB_B33
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: CR,FE,HF,MO,NB,NI,TA,TI,V : B

MC_ETA
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: MO,V,W : C,VA

MC_SHP
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: MO,W : C,N

MO3NI10B11
3 SUBLATTICES, SITES 3: 10: 11
CONSTITUENTS: MO : NI : B

MOB
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: CR,FE,MO : B

MOB4
2 SUBLATTICES, SITES .2: .8
CONSTITUENTS: MO : B

MOCOB
3 SUBLATTICES, SITES 1: 1: 1
CONSTITUENTS: MO,W : CO : B

MONI4_BETA
2 SUBLATTICES, SITES 1: 4
CONSTITUENTS: MO,W : NI

MONI_DELTA
3 SUBLATTICES, SITES 24: 20: 12
CONSTITUENTS: CO,CR,FE,NI,RE : CO,CR,FE,MO,NI,RE,W : MO,W

MOSI2_C11B
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: MO,PD,W : AL,SI,TI

MSI2_C1
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: CO,NI : AL,SI

MSI_B27
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: HF,NB,TI,ZR : SI

MU_PHASE
THIS PHASE HAS A DISORDERED CONTRIBUTION FROM DIS_MU
4 SUBLATTICES, SITES 1: 2: 6: 4
CONSTITUENTS: AL,CO,CR,FE,MO,NB,NI,RE,TA,W : AL,CO,CR,FE,MO,NB,NI,RE,TA,
W : AL,CO,CR,FE,MO,NB,NI,RE,TA,W : AL,CO,CR,FE,MO,NB,NI,RE,TA,W

MZR3_E1A
2 SUBLATTICES, SITES 1: 3
CONSTITUENTS: CO,FE : ZR

NB13NI75TI12
3 SUBLATTICES, SITES .13: .75: .12
CONSTITUENTS: NB : NI : TI

NB15NI56TI29
3 SUBLATTICES, SITES .15: .56: .29
CONSTITUENTS: NB : NI : TI

NB15NI80TI5
3 SUBLATTICES, SITES .15: .8: .05
CONSTITUENTS: NB : NI : TI

NB5NI75TI20
3 SUBLATTICES, SITES .05: .75: .2
CONSTITUENTS: NB : NI : TI

NB8NI9TI3
3 SUBLATTICES, SITES .4: .45: .15
CONSTITUENTS: NB : NI : TI

NI10ZR7
2 SUBLATTICES, SITES 23: 17
CONSTITUENTS: NI : HF,ZR

NI11ZR9
2 SUBLATTICES, SITES 11: 9
CONSTITUENTS: NI : HF,ZR

NI2SI_TETA
3 SUBLATTICES, SITES 1: 1: 1
CONSTITUENTS: NI : NI,VA : AL,SI

NI2TA
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: CO,NI : TA

NI2V
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: NI,PD,PT : NB,TA,V

NI31SI12
2 SUBLATTICES, SITES 5: 2
CONSTITUENTS: CO,CR,FE,NI : SI

NI3B_D011
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: CO,CR,FE,MO,NI : B

NI3CR2B6
3 SUBLATTICES, SITES 3: 2: 6
CONSTITUENTS: NI : CR : B

NI3SI2
2 SUBLATTICES, SITES 3: 2
CONSTITUENTS: NI : SI

NI3SI_MONOCL
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: NI : SI

NI3SI_ORTHO
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: NI : SI

NI3TA_D0A
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: AL,CO,CR,FE,NB,NI,PT : AL,FE,MO,NB,NI,PT,TA,TI,V,W

NI3TI_D024
2 SUBLATTICES, SITES .75: .25
CONSTITUENTS: AL,CO,CR,FE,HF,NI,PD,PT,TA,TI,W,ZR : AL,CR,HF,MO,NB,NI,PD,
PT,SI,TA,TI,W,ZR

NI4B3
2 SUBLATTICES, SITES .571429: .428571
CONSTITUENTS: NI : B

NI4SI2B
3 SUBLATTICES, SITES 4.29: 2: 1.43
CONSTITUENTS: NI : SI : B

NI5ALB4
3 SUBLATTICES, SITES 5: 1: 4
CONSTITUENTS: NI : AL : B

NI5ZR
2 SUBLATTICES, SITES 5: 1
CONSTITUENTS: NI : HF,ZR

NI6SI2B
3 SUBLATTICES, SITES 6: 2: 1
CONSTITUENTS: NI : SI : B

NI7ZR2
2 SUBLATTICES, SITES 7: 2
CONSTITUENTS: AL,CO,CR,NI : HF,ZR

NI8ALB11
3 SUBLATTICES, SITES 8: 1: 11
CONSTITUENTS: NI : AL : B

NI8TA
2 SUBLATTICES, SITES 8: 1
CONSTITUENTS: NI : NB,TA

NICR3B6
3 SUBLATTICES, SITES .1: .3: .6
CONSTITUENTS: NI : CR : B

NISI_B31
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: NI,PD : SI

NITI2
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: CO,CR,FE,NI,RE,TI : AL,CR,HF,NI,TA,TI,ZR

NIZR
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: NI : TI,ZR

PD11ZR9
2 SUBLATTICES, SITES 11: 9
CONSTITUENTS: PD : ZR

PD14SI3
2 SUBLATTICES, SITES 14: 3
CONSTITUENTS: PD : SI

PD15SI4
2 SUBLATTICES, SITES 15: 4
CONSTITUENTS: PD : SI

PD19SI10
2 SUBLATTICES, SITES 19: 10
CONSTITUENTS: PD : SI

PD21SI4
2 SUBLATTICES, SITES 21: 4
CONSTITUENTS: PD,SI : SI

PD2TA
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: PD : TA

PD2TI
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: PD : TI

PD39SI20
2 SUBLATTICES, SITES 39: 20
CONSTITUENTS: PD : SI

PD3SI
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: PD : SI

PD3TI2
2 SUBLATTICES, SITES 3: 2
CONSTITUENTS: PD : TI

PD4ZR3
2 SUBLATTICES, SITES 4: 3
CONSTITUENTS: PD : ZR

PD5SI
2 SUBLATTICES, SITES 5: 1
CONSTITUENTS: PD : SI

PD5TI3
2 SUBLATTICES, SITES 5: 3
CONSTITUENTS: PD : TI

PD9SI2
2 SUBLATTICES, SITES 9: 2
CONSTITUENTS: PD : SI

PDZRM
3 SUBLATTICES, SITES 1: 1: 1
CONSTITUENTS: PD : ZR : PD,ZR

PDZR_ALPHA
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: PD : ZR

PDZR_BETA
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: PD : ZR

PI
3 SUBLATTICES, SITES 12.8: 7.2: 4
CONSTITUENTS: CR : FE,NI : N

PT10ZR7
2 SUBLATTICES, SITES 10: 7
CONSTITUENTS: PT : ZR

PT25SI7
2 SUBLATTICES, SITES 25: 7
CONSTITUENTS: PT : SI

PT2TA
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: PT : TA

PT3TA
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: PT : TA

PT3TI4
2 SUBLATTICES, SITES 3: 4
CONSTITUENTS: PT : TI

PT3ZR5
2 SUBLATTICES, SITES 3: 5
CONSTITUENTS: PT,ZR : PT,ZR

PT4ZR
2 SUBLATTICES, SITES 4: 1
CONSTITUENTS: PT,ZR : PT,ZR

PT4ZR3
2 SUBLATTICES, SITES 4: 3
CONSTITUENTS: PT,ZR : PT,ZR

PT5SI2
2 SUBLATTICES, SITES 5: 2
CONSTITUENTS: PT : SI

PT6SI5
2 SUBLATTICES, SITES 6: 5
CONSTITUENTS: PT : SI

PT8TI
2 SUBLATTICES, SITES 8: 1
CONSTITUENTS: PT : TI

PTSI
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: PT : SI

P_PHASE
3 SUBLATTICES, SITES 24: 20: 12
CONSTITUENTS: CR,FE,NI,RE : CR,FE,MO,NI,RE : MO

RE2SI
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: RE : SI

RE3B
2 SUBLATTICES, SITES 3: 1
CONSTITUENTS: CR,MO,RE,TA,W : B

RE3CO3B2
3 SUBLATTICES, SITES 3: 3: 2
CONSTITUENTS: RE : CO : B

RE5CO2B4
4 SUBLATTICES, SITES 4: 2: 1: 4
CONSTITUENTS: RE : CO,RE : CO : B

RE7B3
3 SUBLATTICES, SITES 7: 3: 3
CONSTITUENTS: CO,CR,MO,NB,RE,TA,W : B : B,VA

REB2
 3 SUBLATTICES, SITES 1: 2: 2
  CONSTITUENTS: RE : B : B,VA

RECOB
 3 SUBLATTICES, SITES 1: 1: 1
  CONSTITUENTS: RE : CO : B

RESI2_C11B
 2 SUBLATTICES, SITES .357: .643
  CONSTITUENTS: RE : SI

REZR2
 2 SUBLATTICES, SITES 1: 2
  CONSTITUENTS: NI,RE : ZR

R_PHASE
 3 SUBLATTICES, SITES 27: 14: 12
  CONSTITUENTS: CO,CR,FE,NI,RE : MO,W : CO,CR,FE,MO,NI,RE,W

SI3N4
 2 SUBLATTICES, SITES 3: 4
  CONSTITUENTS: SI : N

SI5V6
 2 SUBLATTICES, SITES 5: 6
  CONSTITUENTS: SI : V

SIC
 2 SUBLATTICES, SITES 1: 1
  CONSTITUENTS: SI : C

SIGMA
 THIS PHASE HAS A DISORDERED CONTRIBUTION FROM DIS_SIG
 3 SUBLATTICES, SITES 10: 4: 16
  CONSTITUENTS: AL,CO,CR,FE,MO,NB,NI,PD,PT,RE,SI,TA,TI,V,W : AL,CO,CR,FE,
  MO,NB,NI,PD,PT,RE,SI,TA,TI,V,W : AL,CO,CR,FE,MO,NB,NI,PD,PT,RE,SI,TA,TI,
  V,W

TA5SI3_D8L
 2 SUBLATTICES, SITES 5: 3
  CONSTITUENTS: HF,NB,TA : AL,SI

TAAL
 2 SUBLATTICES, SITES .51515: .48485
  CONSTITUENTS: TA : AL

TAAL2
2 SUBLATTICES, SITES .35: .65
CONSTITUENTS: TA : AL

TAN_EPS
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: TA : N

TAU
4 SUBLATTICES, SITES 20: 6: 6: 3
CONSTITUENTS: CO,HF,NI,RE : B : B,VA : AL,CR,HF,MO,RE,TA,TI,V,W,ZR
TI2N_C4
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: TI : N

TI3N2
2 SUBLATTICES, SITES .71: .29
CONSTITUENTS: TI : N

TI3SIC2
3 SUBLATTICES, SITES 3: 1: 2
CONSTITUENTS: TI : SI : C

TI4N3
2 SUBLATTICES, SITES .685: .315
CONSTITUENTS: TI : N

TISI2_C54
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: MO,NB,TI : AL,SI

V2B3
2 SUBLATTICES, SITES .4: .6
CONSTITUENTS: V : B

V3C2
2 SUBLATTICES, SITES 3: 2
CONSTITUENTS: V : C

V5B6
2 SUBLATTICES, SITES 5: 6
CONSTITUENTS: NB,V : B

W2COB2
3 SUBLATTICES, SITES 2: 1: 2
CONSTITUENTS: MO,W : CO,NI : B

W3COC
3 SUBLATTICES, SITES 3: 1: 1
CONSTITUENTS: W : CO,NI : C

W5SI3_D8M
3 SUBLATTICES, SITES 4: 1: 3
CONSTITUENTS: CR,FE,MO,NB,V,W : CR,FE,MO,NB,SI,V,W : AL,SI

ZR5SI4
2 SUBLATTICES, SITES 5: 4
CONSTITUENTS: HF,NB,TI,ZR : SI

ZRSI2_C49
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: HF,NB,ZR : SI

Z_PHASE
3 SUBLATTICES, SITES 1: 1: 1
CONSTITUENTS: CR,FE : MO,NB,V : N,VA

GAS
CONSTITUENTS:
AL,AL1C1,AL1C2,AL1H1,AL1H1O1_ALOH,AL1H1O1_HALO,AL1H1O2,AL1H2,AL1H2O2,AL1H3,AL1H3O3,AL1N1,AL1O1,AL1O2,AL2,AL2C2,AL2O1,AL2O2,AL2O3,AR,C,C1H1,C1H1N1O1,C1H1N1_HCN,C1H1N1_HNC,C1H1O1,C1H1O2,C1H2,C1H2O1,C1H2O2_CIS,C1H2O2_DIOXIRANE,C1H2O2_TRANS,C1H3,C1H3O1_CH2OH,C1H3O1_CH3O,C1H4,C1H4O1,C1N1,C1N1O1,C1N1O1_NCO,C1N2_CNN,C1N2_NCN,C1O1,C1O2,C2,C2H1,C2H1N1,C2H2,C2H2O1,C2H3,C2H4,C2H4O1_ACETALDEHYDE,C2H4O1_OXIRANE,C2H4O2_ACETICACID,C2H4O2_DIOXETANE,C2H4O3_123TRIOXOLANE,C2H4O3_124TRIOXOLANE,C2H5,C2H6,C2H6O1,C2H6O2,C2N1_CCN,C2N1_CNC,C2N2,C2O1,C3,C3H1,C3H1N1,C3H4_1,C3H4_2,C3H6,C3H6O1,C3H6_2,C3H8,C3N1,C3O2,C4,C4H1,C4H10_1,C4H10_2,C4H2,C4H4,C4H4_1_3,C4H6_1,C4H6_2,C4H6_3,C4H6_4,C4H6_5,C4H8,C4H8_1,C4H8_2,C4H8_3,C4H8_4,C4H8_5,C4N1,C4N2,C5,C5H1N1,C5N1,C60,C6H6,C6H6O1,C6N1,C6N2,C9N1,H,H1N1,H1N1O1,H1N1O2_CIS,H1N1O2_TRANS,H1N1O3,H1N3,H1O1,H1O2,H2,H2N1,H2N2O2,H2N2_1_1N2H2,H2N2_CIS,H2N2_TRANS,H2O1,H2O2,H3N1,H3N1O1,H4N2,N,N1O1,N1O2,N1O3,N2,N2O1,N2O3,N2O4,N2O5,N3,O,O2,O3