TCNI9: TCS Ni-based Superalloys Database

Database name:	TCS Ni-based Superalloys Database	*Database acronym:*	TCNI
Database owner:	Thermo-Calc Software AB	*Database version:*	9.1

TCNI9 is a thermodynamic database for different kinds of Ni-based superalloys for use with Thermo-Calc and the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA). TCNI9 contains all the important Ni-based superalloy phases within a 28-element framework + Ar and H for the gas phase only.

Included Elements (30)

Al	Ar	B	C	Ca	Co	Cr	Cu	Fe	H
Hf	Mg	Mn	Mo	N	Nb	Ni	O	Pd	Pt
Re	Ru	S	Si	Ta	Ti	V	W	Y	Zr

Developed using the CALPHAD approach with industry input and support, TCNI9 is based on the critical evaluation of binary, ternary and, in some cases, higher order systems that enable predictions to be made for multicomponent systems and alloys of industrial importance. The database is validated where possible against higher order systems [2012, Bratberg].

All the necessary volume data (including molar volume and thermal expansion) for various alloy phases is 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 only provides rough estimations and has no pressure dependence.

The TCNI9 database also contains an extensive GAS mixture phase for the main purpose of considering oxygen/nitrogen-gas controls in alloy making processes, and different gas atmospheres under, for example, heat treatments. Note that argon (Ar) and hydrogen (H) are included in the gas phase only, and there is no solid solubility or condensed phase compounds with these elements included in the TCNI9 database.

All possible binary systems and most Ni-containing ternary systems have been assessed to the full range of composition.

- TCNI9 Assessed Binary Systems
- TCNI9 Assessed Ternary Systems

TCNI9 includes critically assessed thermodynamic descriptions for 30 elements and 680 phases. Most of the binary systems in this database have been assessed and can be calculated with the BINARY module in Thermo-Calc. TCNI9 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.

TCNI9 Calculation Examples

Ordered and disordered BCC (A2 and B2/β) 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 [2001b, Dupin].

TCP phases are modeled using more complex and physically correct models, which gives the ability to correctly predict site-fractions etc [2007, Hallstedt].

Oxygen has been implemented in an ambitious way using the Compound Energy Formalism (CEF) [2001, Hillert] for the solution phases, e.g. spinel, halite, corundum etc., and the ionic two-sublattice model [1985, Hillert; 1991, Sundman] for the metallic and ionized liquid.

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 in Thermo-Calc. 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 (β)).

Phases defined by default in TCNI9 lists of all the phases defined by default.

Models for the Included Phases in TCNI9 includes detailed description of all phases, e.g. number of sub lattices and elements on each sub lattice and if available also structure, Pearson symbol and Structur Bericht.

ACKNOWLEDGEMENT

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

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.

TCNI9 Assessed Binary Systems

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

	AL	B	C	Ca	Co	Cr	Cu	Fe	Hf	Mg	Mn	Mo	N	Nb	Ni	O	Pd	Pt	Re	Ru	S	Si	Ta	Ti	V	W	Y	Zr
AL																												
B	x																											
C	x	x																										
Ca	x	x	x																									
Co	x	x	x	x																								
Cr	x	x	x	x	x																							
Cu	x	x	x	x	x	x																						
Fe	x	x	x	x	x	x	x																					
Hf	x	x	x		x	x	x	x																				
Mg	x	x	x	x	x	x	x	x	x																			
Mn	x	x	x	x	x	x	x	x	x	x																		
Mo	x	x	x	x	x	x	x	x	x	x	x																	
N	x	x			x	x	x	x		x	x	x																
Nb	x	x	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	x														
O	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x													
Pd	x	x	x		x	x	x	x	x		x	x		x	x	x												
Pt	x	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	x	x										
Ru	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x									
S	x		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	x	x	x	x	x	x							
Ta	x	x	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	x	x					
V	x	x	x		x	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	x	x	x			
Y	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	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	x	x	

TCNI9 Assessed Ternary Systems

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

Al-B-Co	Al-Co-Mo	Al-Fe-Mn	Al-Mo-Re	Al-O-S	B-Cr-Fe
Al-B-Cr	Al-Co-Nb	Al-Fe-Mo	Al-Mo-Ru	Al-O-Si	B-Cr-Hf
Al-B-Fe	Al-Co-Ni	Al-Fe-N	Al-Mo-Si	Al-O-Ti	B-Cr-Mo
Al-B-Hf	Al-Co-O	Al-Fe-Nb	Al-Mo-Ta	Al-O-Y	B-Cr-Ni
Al-B-Mo	Al-Co-Si	Al-Fe-Ni	Al-Mo-Ti	Al-O-Zr	B-Cr-Re
Al-B-Ni	Al-Co-Ta	Al-Fe-O	Al-Mo-W	Al-Re-Ta	B-Fe-Mo
Al-B-Re	Al-Co-Ti	Al-Fe-Re	Al-Mo-Zr	Al-Re-W	B-Fe-Nb
Al-B-Ta	Al-Co-W	Al-Fe-Ru	Al-N-Ti	Al-Ru-Ta	B-Fe-Ni
Al-B-Ti	Al-Co-Zr	Al-Fe-S	Al-Nb-Ni	Al-Ru-Ti	B-Fe-W
Al-B-Zr	Al-Cr-Fe	Al-Fe-Ta	Al-Nb-Ru	Al-Ru-W	B-Hf-Nb
Al-C-Co	Al-Cr-Hf	Al-Fe-Ti	Al-Nb-Si	Al-Ta-Ti	B-Hf-Ni
Al-C-Cr	Al-Cr-Mo	Al-Fe-W	Al-Nb-Ta	Al-Ta-W	B-Hf-Re
Al-C-Fe	Al-Cr-Nb	Al-Hf-Mo	Al-Nb-W	Al-Ti-W	B-Hf-Ta
Al-C-Hf	Al-Cr-Ni	Al-Hf-Ni	Al-Ni-O	B-C-Hf	B-Hf-Ti
Al-C-Mo	Al-Cr-O	Al-Hf-Re	Al-Ni-Pd	B-C-Ti	B-Mo-Nb
Al-C-Ni	Al-Cr-Pt	Al-Hf-Ru	Al-Ni-Pt	B-C-W	B-Mo-Ni
Al-C-Si	Al-Cr-Ru	Al-Hf-Ta	Al-Ni-Re	B-C-Zr	B-Mo-Re
Al-C-Ta	Al-Cr-Ta	Al-Hf-Ti	Al-Ni-Ru	B-Co-Cr	B-Mo-Ti
Al-C-Ti	Al-Cr-Ti	Al-Hf-W	Al-Ni-S	B-Co-Hf	B-Nb-Re
Al-C-W	Al-Cr-W	Al-Hf-Zr	Al-Ni-Si	B-Co-Mo	B-Ni-Re
Al-C-Zr	Al-Cr-Zr	Al-Mn-Ni	Al-Ni-Ta	B-Co-Ni	B-Ni-Si
Al-Ca-O	Al-Cu-Fe	Al-Mn-O	Al-Ni-Ti	B-Co-Re	B-Ni-Ta
Al-Ca-Si	Al-Cu-Mn	Al-Mn-Si	Al-Ni-V	B-Co-Ta	B-Ni-Ti
Al-Co-Cr	Al-Cu-Ni	Al-Mn-Ti	Al-Ni-W	B-Co-Ti	B-Re-Ta
Al-Co-Fe	Al-Cu-S	Al-Mo-Nb	Al-Ni-Y	B-Co-W	B-Re-Ti
Al-Co-Hf	Al-Cu-Si	Al-Mo-Ni	Al-Ni-Zr	B-Co-Zr	B-Re-W

B-Re-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-Co-Zr
C-Cr-Fe
C-Cr-Hf
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C-Cr-Ni
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C-Cr-Ta
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C-Cr-V
C-Cr-W
C-Cr-Zr
C-Cu-Fe
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Co-Cr-Cu
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Ti-W-Zr

TCNI9 Calculation Examples

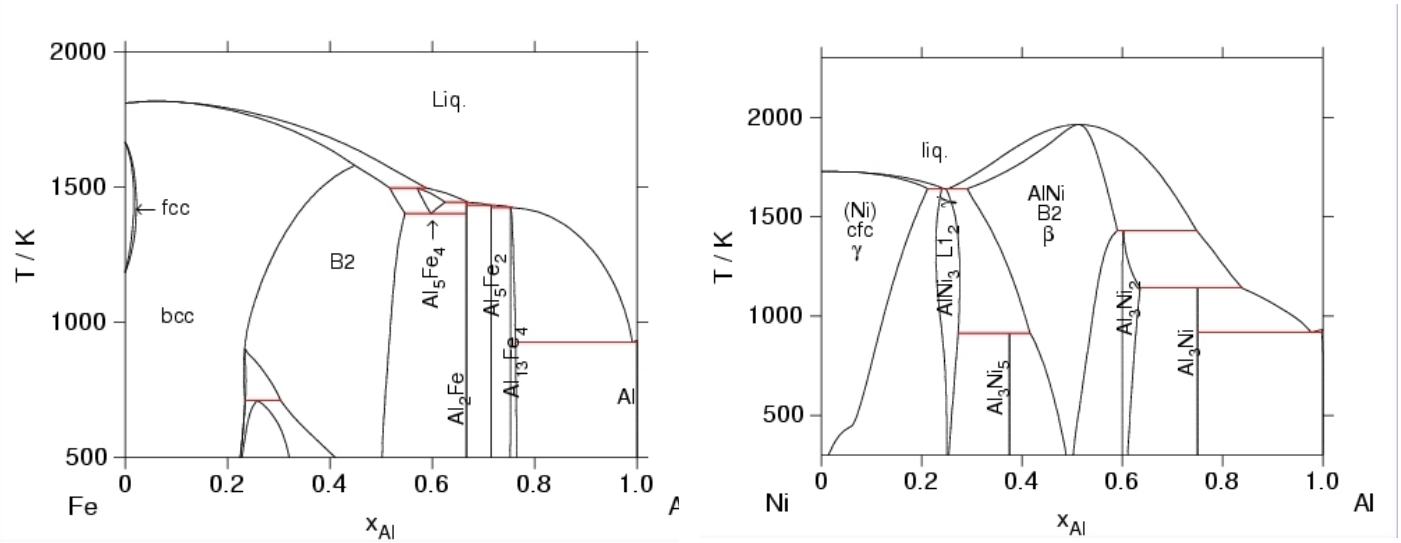

Figure 1: Phase diagrams calculated for Al-Fe [1993, Seiersten] and Al-Ni [1997, Ansara].

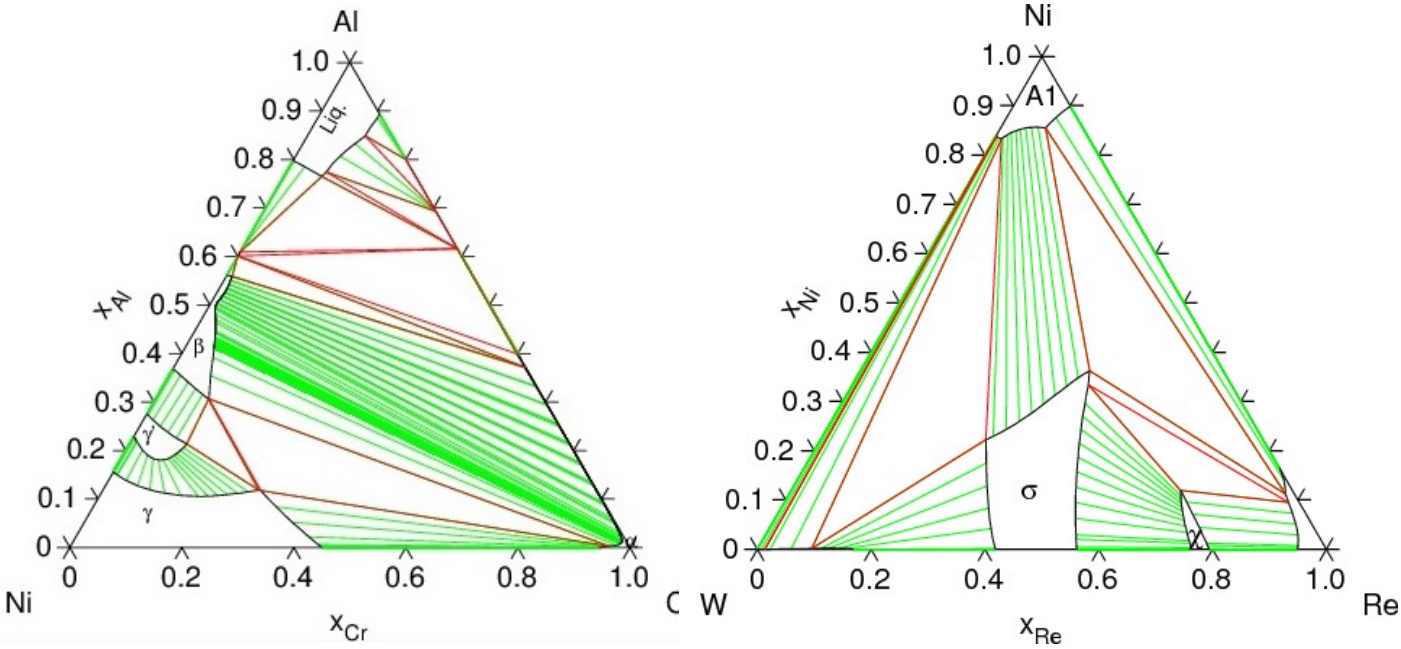

Figure 2: Isothermal sections of Al-Cr-Ni [2001a, Dupin] and Ni-Re-W [2000, Dupin] calculated at 1273 K.

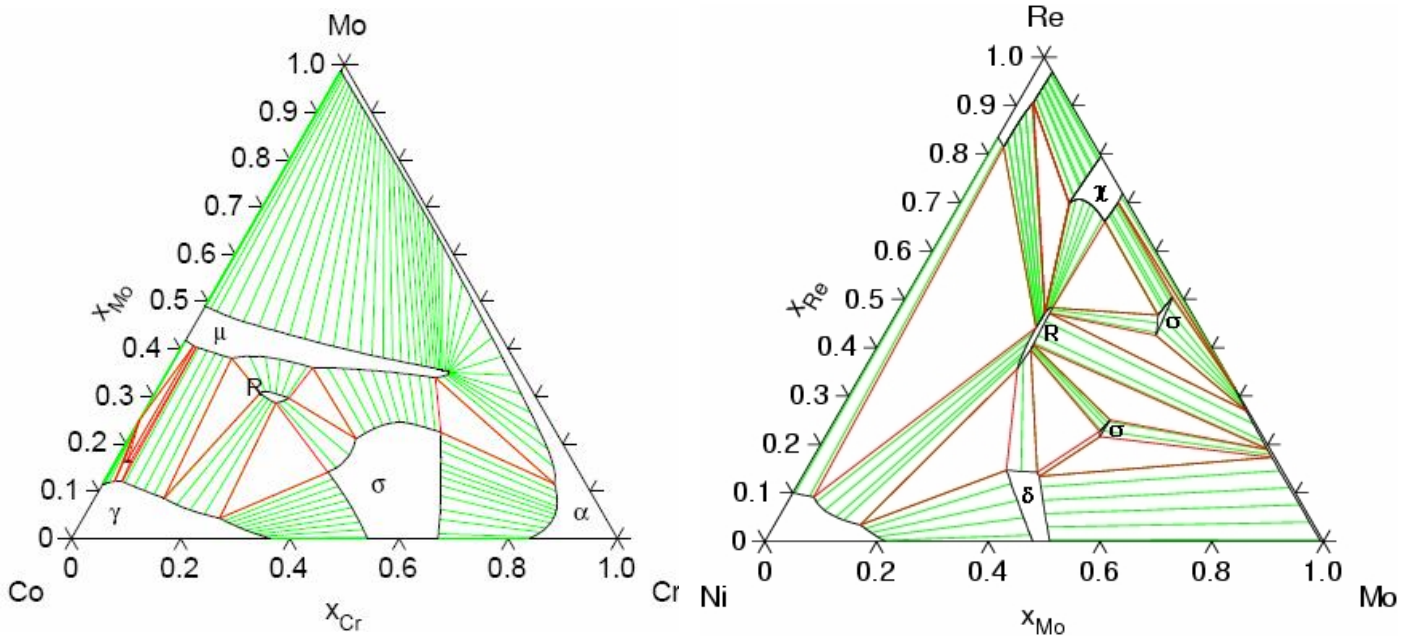

Figure 3: Isothermal sections of Co-Cr-Mo and Mo-Ni-Re [2000, Dupin] calculated at 1273 K.

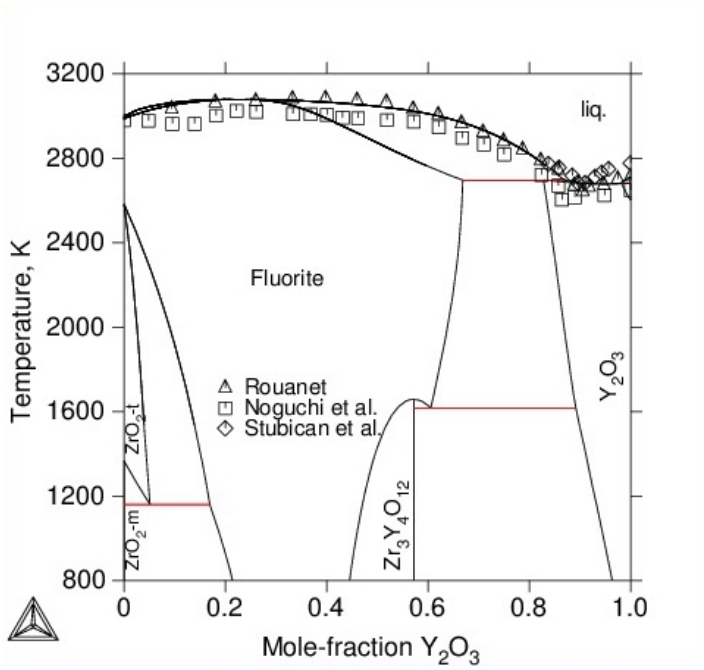

Figure 4: Section ZrO_2-Y_2O_3 compared with experimental information [1970, Noguchi; 1978, Stubican; 1968, Rouanet].

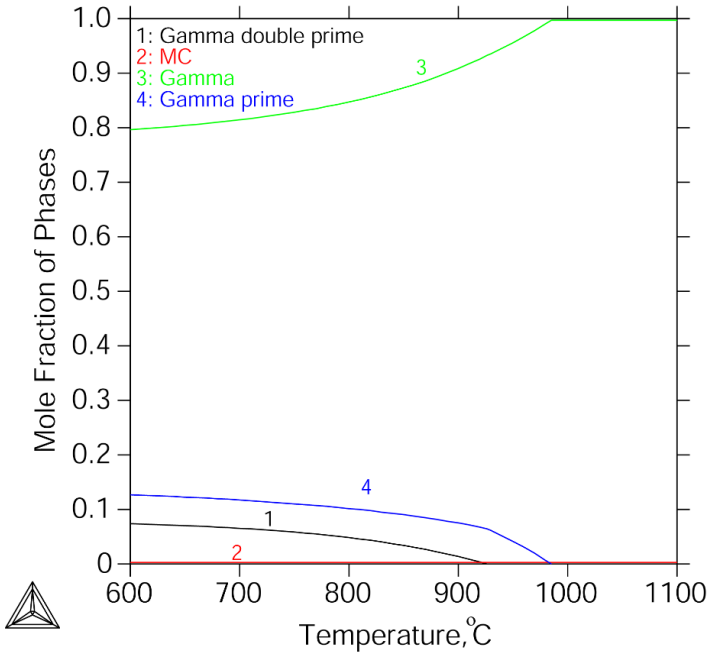

Figure 5: Predicted amount of phases (metastable calculation) at varying temperatures for a Ni-18Cr-18Fe-3Mo-0.5Al-1Ti-5.3Nb-0.02C (wt. %) alloy. Experimental γ'' (BCT_D022) solvus temperature [with experimental data from various sources] is close to 900 ºC and the γ'+γ'' fraction is between 15-20 %.

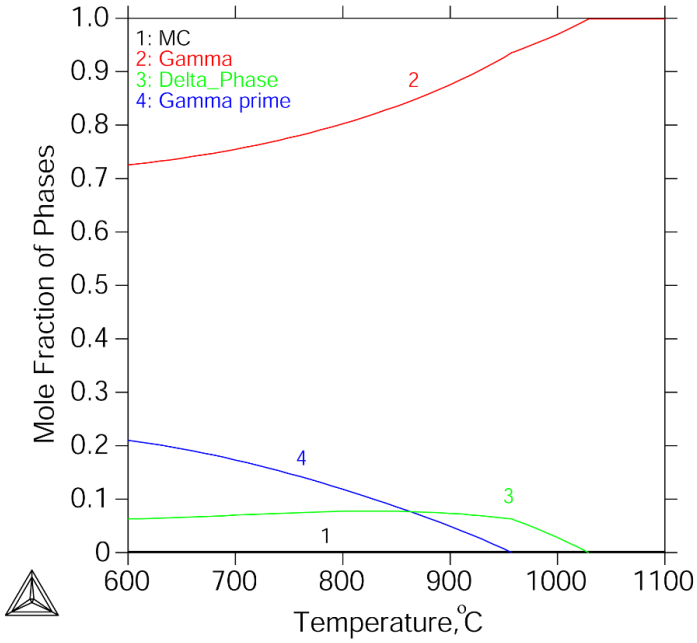

Figure 6: Predicted phase amounts at varying temperatures for a Ni-18Cr-10Fe-9Co-2.8Mo-1.5Al-0.7Ti-5.3Nb-0.02C (wt. %) alloy. Experimental γ′ solvus temperature [2007, Superalloys] is close to 950 ºC and delta (NI3TA_D0A) solvus close to 1010 ºC. The delta phase fraction measured around 8% and γ′ fraction around 20% at 760 ºC after 500 hour heat treatment.

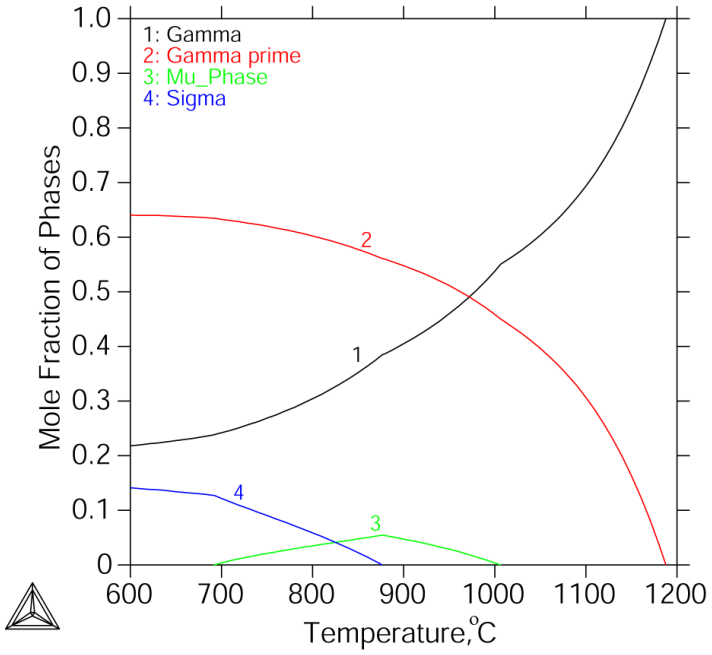

Figure 7: Predicted amount of phases at varying temperatures for a Ni-11.5Cr-15.5Co-6.5Mo-4.3Al-4.3Ti-0.5Hf (wt. %) alloy. Experimental γ′ solvus temperature[2009, Cui] is close to 1150 ºC and both σ and μ phases were observed at 760 ºC after 1000 hr heat treatment.

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 [2008].

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

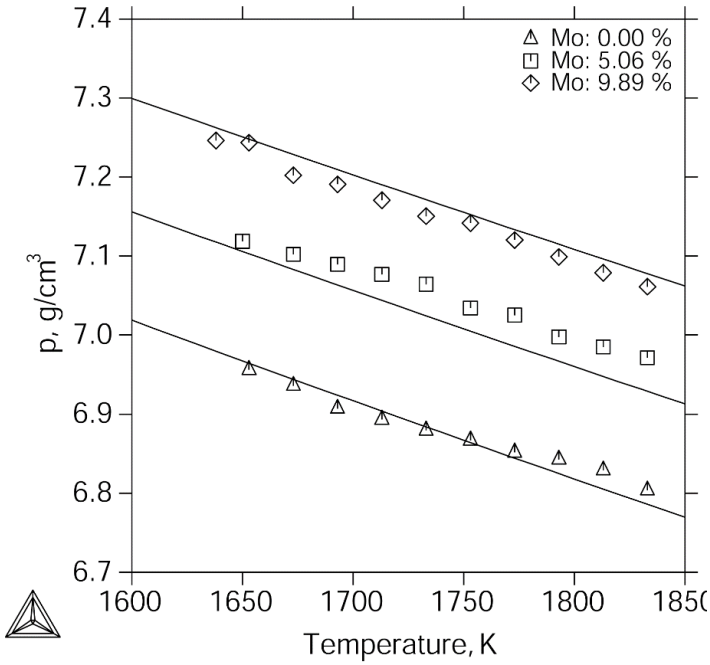

Figure 8: Predicted densities of liquid Ni-Cr-Al-Mo alloys where the molar ratio of Ni:Cr:Al is close to the average value for commercial superalloys INCO713, CM247LC and CMSX-4. Symbols are the experimental values from Fang [2006].

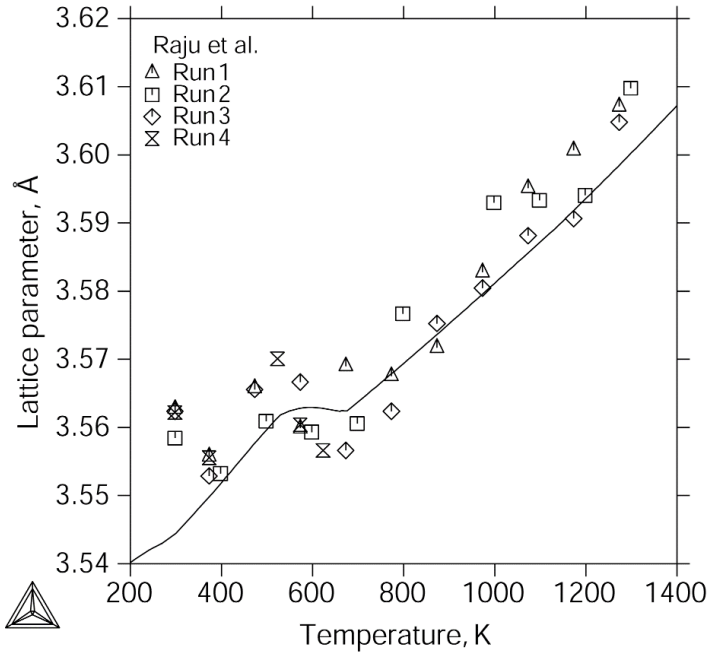

Figure 9: Predicted lattice parameters of disordered FCC of Inconel 600 at varying temperatures compared to X-ray diffraction values by Raju et.al [2004]. At low temperature the calculation gives, besides the disordered FCC, also an ordered L12 phase, which causes the kink in the curve.

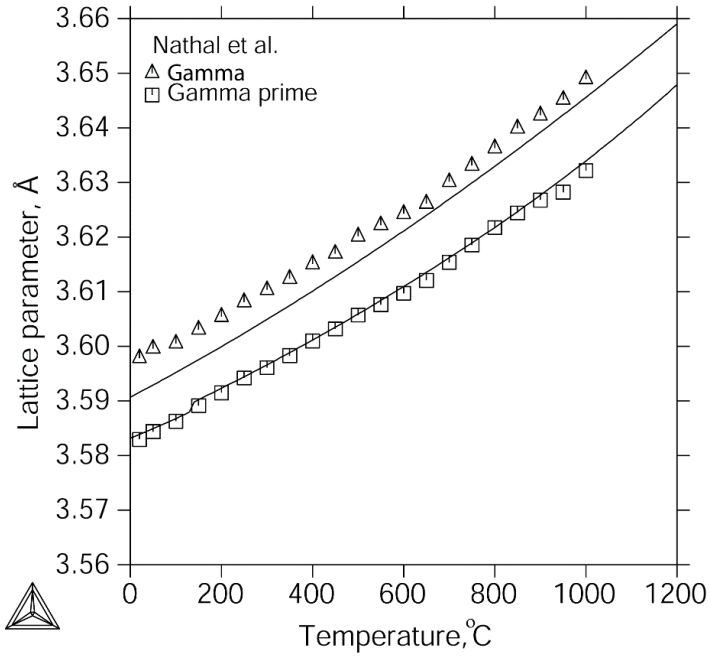

Figure 10: Predicted γ/γ′ lattice mismatch of a Ni-0.6Mo-0.92Ta-12.5Al-1.83Ti-10.5Cr-3.3W (at. %) compared to an experimental determination by Nathal [1985].

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Scientific Bibliography

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

Phases defined by default in TCNI9

AL2S3
ALABANDITE
ANHYDRITE
ANILITE
ANORTHITE:I
APATITE:I
BCC_A2
BCC_B2
BCT_D022
BETA_RHOMBO_B
C12A7:I
C13A6Z2:I
C14_LAVES
C1A1:I
C1A1F2:I
C1A2:I
C1A6:I
C2F:I
C3A1:I
C4WF4:I
C4WF8:I
CA15CU18O35:I
CA2ALNBO6
CA2CUO3:I
CA2NB2O7
CA2SIO4_ALPHA:I
CA2SIO4_ALPHA_PRIME:I

CA2ZRSI4O12
CA3CO2O6
CA3CO4O9
CA3COAL4O10:I
CA3NB2O8
CA3S3FE4OX
CA3Y2SI3O12:I
CA3Y2SI6O18:I
CA3ZRSI2O9
CA4NB2O9_HT11
CA4NB2O9_LT21
CA6ZR19O44:I
CACR2O4_A
CACRSI4O10:I
CACU2O3:I
CAMN2O4:I
CAMO3:I
CASFEO
CASO4_HT
CAV2O4:I
CAY4O7:I
CAYAL3O7:I
CAYALO4:I
CAZR4O9:I
CAZRO3_C:I
CBCC_A12
CEMENTITE

CF2:I
CHALCOCITE_ALPHA
CHALCOCITE_BETA
CHALCOPYRITE
CHI_A12
CLINO_PYROXENE:I
CO9S8
CORUNDUM:I
COVELLITE
CR1S1
CR2S3
CR3S4
CR5S6
CR7S8
CU2SO4
CU2SO5
CU2TI
CU3TI2
CU4TI1
CU4TI3
CUB_A13
CUCRS2
CUFES2_LT
CUMG2
CUTI3
CW3F:I
CWF:I

D5A_M3B2
DIAMOND_A4
DIGENITE
DIS_MU
DIS_SIG
DJURLEITE
FCC_A1
FCC_L12
FE2O12S3:I
FEAL2S4
G_PHASE
GARNET:I
GAS:G
GRAPHITE
H_L21
HALITE:I
HATRURITE:I
HCP_A3
HEAZLEWOODITE
HEAZLEWOODITE_B2
LAAP:I
LARNITE:I
LIQUID:L
M12C
M23C6
M2B_TETR
M2O3A:I
M2O3B:I
M2O3X:I
M3B2

M3C2
M6C
M7C3
MB_B33
MB2_C32
MC_ETA
MC_SHP
MELILITE:I
MG24Y5_A12
MG2NI
MG2SI
MG3N2_D53
MG6MN3NI
MN15NI45SI40
MN15NI50SI35
MN1NI1SI1
MN2NISI
MN3NI2SI
MN52NI29SI19
MN66NI4SI30
MN6NI16SI7
MN6NISI3
MN9SI3O14S1
MNNISI_T5
MNNISI_T6
MO1S2
MO2S3
MONOCLINIC_S
MU_PHASE
NI17Y2

NI3B_D011
NI3S2_LT
NI3TA_D0A
NI3TI_D024
NI5ZR
NI7S6
NI8ALY3
NI9S8
NIOCALITE_C10NS6
NIS_LT
ORTHO_PYROXENE:I
ORTHORHOMBIC_S
P_PHASE
PD16S7
PD3S
PD4S
PDS
PENTLANDITE
PROTO_PYROXENE:I
PSEUDO_WOLLASTONITE:I
PTS
PTS2
PYRITE
PYRRHOTITE
R_PHASE
RANKINITE:I
RE1S2
RE1S3
RE2S7
RU1S2

SIGMA
SIS2
SPINEL:I
TAU
THIOSPINEL
W1S2
WOLLASTONITE:I
Z_PHASE
ZRO8S2:I
ZRS2

Models for the Included Phases in TCNI9

The table lists all phases in TCNI9 and the thermodynamic model used to describe the phase.

Phase Name	Formula	Comments
AF	(AL2O3)1(FE2O3)1	This is Al2O3.Fe2O3. Prototype FeGaO3 (oP40 Pna21)
AL10CU10FE	(FE)1(AL,CU)10(AL)10	
AL10FEMN2	(FE,MN)3(AL)10	
AL10V	(AL)10(V)1	
AL11CR2	(AL)10(AL)1(CR)2	
AL11CU5MN3	(AL)11(MN)3(CU)5	
AL11MN4_HT	(AL,MN)29(MN)10	
AL11MN4_LT	(AL)11(MN,FE)4	
AL11RE4	(AL)11(RE)4	
AL11TI5	(AL)17(TI)8	
AL12MG17_A12	(MG)10(AL,MG)24(AL,MG)24	
AL12MN	(AL)12(MN)1	
AL12W	(AL)12(MO,RE,W)1	Also AL12RE and AL12MO
AL13CO4	(AL)13(CO)4	
AL13CR2	(AL)13(CR)2	
AL13FE2MN2	(FE,MN)4(AL)13	
AL13FE4	(AL,CU)0.63(FE,MN,RU)0.23(AL,SI,VA)0.14	
AL15SI2M4	(AL)14(FE,MN)4(AL,SI)5	Solution of Al-Mn-Si ternary phase tao 9 Al15(Mn Fe)3Si2
AL16FEMN3	(AL)4(FE,MN)1	
AL1MN1SI1	(AL)1(MN)1(SI)1	The Al-Mn-Si ternary phase tao3
AL21PD8	(AL)21(PD)8	
AL21PT5	(AL)0.81(PT)0.19	

Phase Name	Formula	Comments
AL21PT8	(AL)0.72(PT)0.28	
AL23CUFE4	(AL)23(CU)1(FE)4	
AL23V4	(AL)23(V)4	
AL28CU4MN7	(AL)28(MN)7(CU)4	
AL2CA_C15	(AL)2(CA)1	
AL2FE	(AL,CU)2(FE,MN)1	
AL2MN2SI3	(AL)2(MN)2(SI)3	The Al-Mn-Si ternary phase tao1
AL2MNSI3	(AL)2(MN)1(SI)3	The Al-Mn-Si ternary phase tao10
AL2N2TI3	(AL)2(N)2(TI)3	
AL2PD5	(AL)2(AL,PD)5	
AL2PT_C1	(AL)2(NI,PT)1(NI,VA)1	
AL2S3	(AL)2(S)3	
AL2TI	(AL)2(TI)1	
AL2W	(AL)2(W)1	
AL2ZR3	(AL)2(HF,Y,ZR)3	also Al2Hf3 Al2Y3
AL31MN6NI2	(AL)31(MN)6(NI)2	Orthorhombic ternary Al-Mn-Ni phase
AL3CO	(AL)3(CO)1	
AL3MN4SI2	(AL)3(MN)4(SI)2	the Al-Mn-Si ternary phase tao5
AL3MNSI2	(AL)3(MN)1(SI)2	the Al-Mn-Si ternary phase tao4
AL3NI1	(AL)0.75(NI)0.25	
AL3M2_D519	(AL,SI)3(AL,CU,NI,PT,RU)2(RU,NI,VA)1	
AL3NI5	(AL)0.38(NI)0.62	
AL3PD	(AL)3(PD)1	
AL3PD2	(AL,PD)3(AL,PD)2	
AL3PD5	(AL)3(PD)5	
AL3PT5	(AL)0.38(PT)0.62	

Phase Name	Formula	Comments
AL3Y_HT	(AL)0.75(Y)0.25	
AL3Y_LT	(AL)0.75(Y)0.25	
AL3ZR	(AL)3(HF,ZR)1	also Al3Hf
AL3ZR2	(AL)3(HF,ZR)2	also Al3Hf2
AL3ZR4	(AL)3(HF,ZR)4	also Al3Hf4
AL3ZR5	(AL)3(ZR)5	
AL4C3	(AL,SI)4(C)3	
AL4CA_D13	(AL)4(CA)1	
AL4CR	(AL)4(CR)1	
AL4MN_R	(AL)461(MN,FE)107	
AL4MN_U	(AL)4(MN)1	
AL4PD	(AL)4(PD)1	
AL4RE	(AL)4(RE)1	
AL4SIC4	(AL)4(SI)1(C)4	
AL4W	(AL)4(MO,W)1	also Al4Mo
AL4ZR5	(AL)4(ZR)5	
AL5CO2_D811	(AL)5(CO)2	D811
AL5FE2	(AL,CU)5(FE,MN)2	
AL5FE4	(AL,CU,FE)	
AL5MN6SI7	(AL)5(MN)6(SI)7	the Al-Mn-Si ternary phase tao2
AL5W	(AL)5(MO,W)1	also AL5MO
AL62CU25FE13	(FE)0.12(AL,CU)0.26(AL)0.62	
AL63MO37	(AL)63(MO)37	
AL6MN	(AL)6(FE,MN,RE,RU)1	
AL77W23	(AL)77(W)23	
AL7CU2FE	(FE,NI)1(CU)2(AL)7	Solution phase of the ternary compound Al7Cu2Fe
AL7CU4NI	(AL)1(FE,CU,NI,VA)1	

Phase Name	Formula	Comments
AL7V	(AL)7(V)1	
AL7W3	(AL)7(W)3	
AL8CR5_H	(AL)8(CR)5	
AL8CR5_L	(AL)8(CR)5	
AL8MN5	(AL,TI)12(MN)5(AL,CU,MN,SI,TI)9	
AL8MO3	(AL)8(MO)3	
AL8SIC7	(AL)8(SI)1(C)7	
AL8V5	(AL)8(V)5	
AL9CO2	(AL)9(CO)2	
AL9CR4_H	(AL)9(CR)4	
AL9CR4_L	(AL)9(CR)4	
ALABANDITE	(CA,CO,CR,CU,FE,MG,MN,Y,ZR)1(S)1	This is CaS (oldhamite) MnS (alabandite) (Mg Gd La Zr)S. Prototype NaCl.
ALB12_ALPHA	(AL)1(B)12	
ALBMO	(AL)1(B)1(MO)1	
ALCCR2	(AL)1(C)1(CR)2	
ALCR2	(AL)1(CR)2	
ALCR2B2	(AL)1(CR)2(B)2	
ALCR3B4	(AL)1(CR)3(B)4	
ALCU_DEL	(AL)2(CU,FE)3	
ALCU_EPS	(AL,CU,NI)1(CU,FE)1	
ALCU_ETA	(AL,CU)1(CU,FE,NI)1	
ALCU_PRIME	(AL)2(CU)1	
ALCU_ZETA	(AL)9(CU,FE)11	
ALCU3MN2	(AL)1(MN)2(CU)3	
ALFESI_ALPHA	(AL)0.66(FE)0.19(SI)0.05(AL,SI)0.1	
ALFESI_BETA	(AL)14(FE)3(SI)3	
ALFESI_DELTA	(AL)0.55(FE)0.15(SI)0.3	

Phase Name	Formula	Comments
ALFESI_GAMMA	(AL)3(FE)1(SI)1	
ALFESI_TAU1	(AL)2(FE)2(SI)1	
ALFESI_TAU3	(AL)2(FE)1(SI)1	
ALM3C_E21	(AL)1(CO,FE)3(C)1	AlCo3C AlFe3C Perovskite
ALMG_BETA	(AL)89(MG)	
ALMG_EPSILON	(AL)30(MG)23	
ALMNSI_T6	(AL,MN)4(SI)1	the Al-Mn-Si ternary phase tao6
ALMNSI_T8	(MN,VA)6(MN,VA)2(AL)12(AL,SI)6(AL,SI)2	
ALMO	(AL,MO)1(AL,MO)1	A2 badly described
ALN_B4	(AL)1(N)1	
ALNTI2	(AL)1(N)1(TI)2	
ALNTI3	(AL)1(N)1(TI)3	
ALPD2	(AL,NI,PD)1(AL,NI,PD)2	
ALPHA_B19	(MO,NB,PD,PT,TI,V,ZR)1(MO,NB,PD,PT,TI,V,ZR)1	
ALPHA_PD2SI	(PD,SI)2(SI)1	
ALPHA_PT17SI8	(PT)17(SI)8	
ALPHA_PT2SI	(PT)2(SI)1	
ALPHA_PT3SI	(PT)3(SI)1	
ALPHA_SPINEL	(CO+2,MG+2,MN+2,MN+3,NI+2)1(AL+3,CR+3,FE+3,MN+2,MN+3,VA)2 (MN+2,VA)2(O-2)4	Hausmannite [Mn3O4]
ALPT_B20	(AL)0.5(NI,PT)0.5	
ALPT2	(AL)0.33(PT)0.67	
ALRE	(AL)1(RE)1	
ALRE2	(AL)1(RE)2	
ALTI3_DO19	(AL,CO,CR,MN,MO,NI,PT,TA,TI,W)3(AL,CR,MO,NB,NI,PT,TA,TI,W)1	
ALZR	(AL)1(HF,Y,ZR)1	also AlHf AlY
ALZR2	(AL)1(Y,ZR)2	also AlY2
ANDALUSITE	(AL+3)1(AL+3)1(SI+4)1(O-2)5	A high-pressure phase (Al2O3.SiO2)

Phase Name	Formula	Comments
ANHYDRITE	(CA+2,CO+2,CU+2,FE+2,MN+2,NI+2)1(SO4-2)1	This is (Ca Cu Fe Mg Mn Ni)(SO4).
ANILITE	(CU)1.75(S)1	This is Cu7S4 orthorhombic structure.
ANORTHITE	(CA+2)1(AL+3)2(SI+4)2(O-2)8	This is CaO.Al2O3.2SiO2
APATITE	(CA+2,Y+3,ZR+4,VA)4(Y+3)6(SIO4-4)6(O-2,VA)2	This is Ca2(Gd Y)8 (SiO4)6O2 and Mg2 (Gd Y)8(SiO4)6O2
B11	(CO,CU,NI,PD,TI)1(CU,NI,TA,TI)1	
B12ZR	(B)12(Y,ZR)1	YB12 ZrB12
B2O3	(B2O3)1	
B2PD5	(B)2(PD)5	
B2PT3	(B)2(PT)3	
B3SI	(B)6(SI)2(B,SI)6	
B4C	(B11C,B12)1(B2,C2B,CB2)1	
B4TA3_D7B	(B)4(CR,HF,MN,NB,TA,TI,V)3	Prototype Ta3B4 also Cr3B4 Mn3B4 Nb3B4 Ti3B4 V3B4
B5W2_X	(B,C,VA)5(W)2	
B6SI	(B)23(SI)48(B,SI)	
B9W2	(B)9(W)2	
BCC_A2	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI,V,W,Y,ZR,VA)1 (B,C,N,O,VA)3	If BCC_B2 is defined this phase will be combined to it.
BCC_B2	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI,V,W,Y,ZR,VA)0.5 (AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI,V,W,Y,ZR,VA)0.5(B,C,N,O,VA)3	This phase has some contribution from BCC_A2.
BCT_D022	(AL,CR,FE,MO,NB,NI,PD,PT,TI,V)3(AL,CR,MO,NB,NI,PD,PT,TA,TI,V,SI)1	gamma double prime
BETA_PD2SI	(PD,SI)2(SI)1	
BETA_PT17SI8	(PT)17(SI)8	
BETA_PT2SI	(PT)2(SI)1	

Phase Name	Formula	Comments
BETA_PT3SI	(PT)3(SI)1	
BETA_RHOMBO_B	(B)93(B,C,CU,SI)12	
BM	(B,PT)1(CR,FE,HF,MN,MO,TI,Y)1	FeB MnB TiB HfB etc. and YPt StrukturBericht B27
BN_B4	(B)1(N)1	
BNSI	(B)61(SI)1(B,SI)8	
BPD3	(B)1(PD)3	
BPD5	(B)1(PD)5	
BPD6	(B)1(PD)6	
BPT2	(B)1(PT)2	
BPT3	(B)1(PT)3	
BW_ALPHA	(B,C,VA)1(W)1	
BW_BETA	(B,C,VA)1(W)1	prototype BCr
C12A7	(CA+2)6(AL+3)6(AL+3,FE+3)1(O-2)16.5	This is 12CaO.7Al2O3 (oS100 Cmc21) not stable under anhydrous conditions
C13A6Z2	(CA+2)13(AL+3)12(ZR+4)2(O-2)35	This is 13CaO.3Al2O3.2ZrO2.
C14_LAVES	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,SI,RE,RU,TA,TI,V,W,Y,ZR)2 (AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,SI,RE,RU,TA,TI,V,W,Y,ZR)1	prototype CuZn2
C15_LAVES	(AL,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,SI,RE,RU,TA,TI,V,W,Y,ZR)2 (AL,CO,CR,CU,FE,HF, MG,MO,NB,NI,SI,RE,RU,TA,TI,V,W,Y,ZR)1	
C16_THETA	(AL,HF,MO,NB,TA,TI,W,ZR)2(AL,CO,CR,CU,FE,NI,SI)1	Al2Cu Hf2Al Hf2Si Zr2Si Zr2Co Ta2Co Hf2Ni Ta2Ni Zr2Ni
C1A1	(CA+2)3(AL+3)5(AL+3,FE+3)1(O-2)12	This is CaO.Al2O3 (mP84 P121/c1) with solubility of Fe
C1A1F2	(CA+2)1(AL+3)1(FE+3)2(AL+3,FE+3)3(O-2)10	

Phase Name	Formula	Comments
C1A2	(CA+2)1(AL+3)3(AL+3,FE+3)1(O-2)7	This is CaO.2Al2O3 (mS48 C12/c1) with solubility of Fe
C1A6	(CA+2)1(AL+3,FE+3)12(O-2)19	This is CaO.6Al2O3 Prototype BaFe12O19 (hP66 P63/mmc) with solub of Fe
C2CA1_S	(C2CA1)1	
C2CA1_S2	(C2CA1)1	
C2F	(CA+2)2(AL+3,FE+3)2(O-2)5	This is 2CaO.Fe2O3 Prototype Sr2Fe2O5 (oI44 Imma) with solubility of Al.
C36_LAVES	(AL,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,TA,TI,W,ZR)2 (AL,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,TA,TI,W,ZR)1	
C3A1	(CA+2)3(AL+3,FE+3)2(O-2)6	This is 3CaO.Al2O3 (cP264 Pa-3) with some solubility of Fe
C4WF4	(CA+2)4(FE+2)1(FE+3)8(O-2)17	This is 4CaO.FeO.4Fe2O3 (mS60 C121)
C4WF8	(CA+2)4(FE+2)1(FE+3)16(O-2)29	This is 4CaO.FeO.8Fe2O3
CA15CU18O35	(CA+2)15(CU+2)14(CU+3)4(O-2)35	
CA2ALNBO6	(CA+2)2(AL+3)1(NB+5)1(O-2)6	
CA2CU	(CA)2(CU)1	
CA2CUO3	(CA+2)2(CU+2)1(O-2)3	
CA2NB2O7	(CA+2)2(NB+5)2(O-2)7	
CA2NI7	(CA)2(NI)7	
CA2SI_C37	(CA)2(SI)1	
CA2SIO4_ALPHA	(CA+2,MN+2,Y+3)3(CA+2,VA)1(SIO4-4)2	This is 2CaO.SiO2 and 3CaO.P2O5. Prototype Ca2[SiO4] (hP24 P63/mmc)
CA2SIO4_ ALPHA_PRIME	(CA+2,FE+2,MN+2,Y+3)3(CA+2,VA)1(SIO4-4)2	This is 2CaO.SiO2. Prototype Sr2[SiO4]

Phase Name	Formula	Comments
		(oP52 Pnma)
CA2ZRSI4O12	(CA2ZRSI4O12)1	This is 2CaO.ZrO2.4SiO2
CA3CO2O6	(CA+2)3(CO+3,CU+2)2(O-2,VA)6	
CA3CO4O9	(CA+2)3(CO+3,CU+2)4(O-2,VA)9	
CA3COAL4O10	(CA+2)3(CO+2)1(AL+3)4(O-2)10	
CA3NB2O8	(CA+2)3(NB+5)2(O-2)8	
CA3S3FE4OX	(CA+2)3(S-2)3(FE+2,FE+3)4(O-2,VA)6	This is 3CaS.4FeO and 3CaS.4Fe2O3.
CA3Y2SI3O12	(CA+2)3(Y+3)2(SI+4)3(O-2)12	This is 3CaO.(Gd Y)2O3.3SiO2.
CA3Y2SI6O18	(CA+2)3(Y+3)2(SI+4)6(O-2)18	This is 3CaO.(Gd Y)2O3.6SiO2.
CA3ZRSI2O9	(CA3ZRSI2O9)1	This is 3CaO.ZrO2.2SiO2
CA4NB2O9_HT11	(CA+2)6(CA+2,NB+5)3(NB+5)3(O-2,VA)3(O-2)15	
CA4NB2O9_LT21	(CA+2)6(CA+2,NB+5)4(CA+2)2(O-2,VA)3(O-2)15	
CA6ZR19O44	(CA+2)6(ZR+4)19(O-2)44	Space group hR*
CAB6	(CA)1(B)6	
CACR2O4_A	(CA+2)1(AL+3,CR+3,FE+3)2(O-2)4	With solubility of Al Fe. Prototype SrCr2O4 (oP28 Pmmn)
CACRSI4O10	(CA+2)1(CR+2)1(SI+4)4(O-2)10	This is CaO.CrO.4SiO2 Gillespite
CACU	(CA)1(CU)1	
CACU2O3	(CA+2)1(CU+2)2(O-2)3	
CACU5_D2D	(CA)1(CU)5	
CAMN2O4	(CA+2)1(MN+3)2(O-2)4	Prototype CaMn2O4 (Pbcm)
CAMO3	(CA+2,Y+3)1(MN+4,Y+3,ZR+4)1(O-2)3	This is CaMnO3 and low temp CaZrO3. Prototype GdFeO3 (oP20 Pnma)

Phase Name	Formula	Comments
CANI2	(NI)2(CA)1	
CANI3	(CA)0.25(NI)0.75	
CANI5	(CA)1(NI)5	
CASFEO	(CA+2)2(S-2)2(FE+2,FE+3)2(O-2,VA)3	This is CaS.FeO and CaS.Fe2O3.
CASI_B33	(CA)1(SI)1	
CASI2_C12	(CA)1(SI)2	
CASO4_HT	(CA+2,CO+2)1(SO4-2)1	This is high-temperature (Ca Co Mg)SO4.
CAV2O4	(CA+2)1(AL+3,CR+3,FE+3,Y+3)2(O-2)4	This is CaO.Fe2O3 b-CaCr2O4 CaY2O4. Prototype CaV2O4 (oP28 Pnma)
CAY4O7	(CA+2)1(Y+3)4(O-2)7	This is CaY4O7 and CaGd4O7.
CAYAL3O7	(CA+2)1(Y+3)1(AL+3)3(O-2)7	This is CaYAl3O7 and CaGdAl3O7
CAYALO4	(CA+2)1(Y+3)1(AL+3)1(O-2)4	This is CaYAlO4 and CaGdAlO4
CAZR4O9	(CA+2)1(ZR+4)4(O-2)9	Prototype CaZr4O9 (mS224 C12/c1)
CAZRO3_C	(CA+2,Y+3)1(Y+3,ZR+4)1(O-2)3	Prototype CaTiO3. This is the high-temperature phase (cP5 Pm-3m)
CBCC_A12	(AL,CO,CR,CU,FE,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W,Y,ZR)1(B,C,VA)1	
CEMENTITE	(CO,CR,FE,MN,MO,NI,V,W)3(C,N)1	D011
CF2	(CA+2)1(FE+3)4(O-2)7	This is CaO.2Fe2O3
CFC2_FENBZR	(FE,NB,ZR)2(NB,ZR)1(NB,ZR)3	s
CHALCOCITE_ ALPHA	(CU)2(S)1	This is Cu2S.
CHALCOCITE_ BETA	(CU)2(S)1	This is Cu2S.
CHALCOPYRITE	(CU,FE,VA)1(CU,VA)1(S)1	This is high-temperature

Phase Name	Formula	Comments
		nonstoichiometric CuFeS2.
CHI_A12	(CR,FE,NI,RE)24(AL,CR,HF,MO,NB,TA,TI,W,ZR)10(CR,FE,MO,NB,NI,RE,TA,W)24	
CLINO_ PYROXENE	(CA+2,FE+2,NI+2)1(CO+2,FE+2,NI+2)1(SI+4)2(O-2)6	clinoenstatite diopside niopside pigeonite hedenbergite & clinoferrosi
CO10CU57TI33	(CO)0.1(CU)0.57(TI)0.33	
CO11ZR2	(CO)11(ZR)2	
CO17Y2	(CO2,Y)1(CO2,Y)2(CO)15	
CO2SI_C23	(CO,CR,CU,FE,NI,TI)2(SI)1	Co2Si Ni2Si(delta) Prototype Co2Si
CO3AL2B5	(CO)3(AL)2(B)5	
CO3SI	(CO)3(SI)1	
CO3V	(CO,V)3(CO,V)1	
CO3Y	(CO)3(Y)1	
CO3Y2	(CO)3(Y)2	
CO3Y4	(CO)3(Y)4	
CO5Y_D2D	(CO2,Y)1(CO)4(CO,VA)1	
CO5Y8	(CO)5(Y)8	
CO7HF	(CO)7(HF)1	
CO7M2	(CO)7(NB,TA)2	
CO7Y6	(CO)7(Y)6	
CO9S8	(CO,FE,NI)9(S)8	
COB	(CO,RE)1(B)1	
CORUNDUM	(AL+3,CR+2,CR+3,FE+2,FE+3,MN+3,TI+3,V+3)2(CR+3,FE+3,NI+2,VA)1(O-2)3	corundum [Al2O3] eskolaite [Cr2O3] hematite [Fe2O3] Ti2O3 V2O3 prototype
COVELLITE	(CU)1(S)1	This is CuS.
COY_BF	(CO)1(Y)1	

Phase Name	Formula	Comments
CR1S1	(CR)1.03(S)1	This is low-temp CrS.
CR2B_ORTH	(CR,FE,MO,RE)0.67(B)0.33	Cr2B
CR2NI2SI	(CR)5(NI)5(SI)3	
CR2S3	(CR,FE)2(S)3	
CR3MN5	(CR)3(MN)5	
CR3NI5SI2	(CR)3(NI)5(SI)2(C,VA)1	
CR3S4	(CR,FE,MN,NI)3(S)4	
CR3SI_A15	(CR,FE,MO,NB,NI,PD,PT,RE,SI,TA,TI,V)3(AL,CO,CR,MO,NB,NI,PD,PT,RU,SI,TA,TI,V)1 (C,VA)3	Cr3Ru Cr3Si Mo3Si V3Si Mo3Al Nb3Al V3Co V3Ni Mo3Pt
CR5B3	(CR,MO)0.62(B)0.38	
CR5S6	(CR)5(S)6	
CR7S8	(CR)7(S)8	
CRB4	(CR)0.2(B)0.8	
CRISTOBALITE	(SIO2)1	
CRNBSI	(CR)1(NB)1(SI)1	hP9 Fe2P
CRNI2_OP6	(CR,MO,W)1(MO,NI,W)2	
CRSI2_C40	(CR,CU,HF,MO,NB,SI,TA,V)1(AL,CR,CU,SI)2	CrSi2 NbSi2 TaSi2 VSi2 Prototype CrSi2
CU10HF7	(CU)10(HF)7	
CU10ZR7	(CU)10(ZR)7	
CU15SI4_ EPSILON	(CU,MN)0.79(AL,SI)0.21	
CU2SO4	(CU+1)2(SO4-2)1	
CU2SO5	(CU2O5S1)1	
CU2TI	(CO,CU,NI)2(TI)1	
CU2TIZR	(CU)0.5(TI)0.25(ZR)0.25	
CU2Y_H	(CU)2(Y)1	
CU2Y_L	(CU)2(Y)1	
CU33SI7_DELTA	(CU)0.82(SI)0.17	

Phase Name	Formula	Comments
CU3TI2	(CU,NI,FE)3(CO,TI)2	
CU46NI25SI29	(CU)0.46(NI)0.25(SI)0.29	
CU4TI1	(CU,TI)4(CU,TI)1	
CU4TI3	(CO,CU,NI)4(TI)3	
CU4Y	(CU)4(Y)1	
CU51HF14	(CU)51(HF)14	
CU51ZR14	(CU)51(ZR)14	
CU56SI11_ GAMMA	(CU,MN,NI,SI)0.84(SI)0.16	
CU5MN4SI	(CU)0.5(MN)0.37(SI)0.13	
CU6NISI3	(CU,NI)0.73(SI)0.27	
CU7Y1	(CU2,Y)1(CU)5	
CU7Y2	(CU)7(Y)2	
CU8HF3	(CU)8(HF)3	
CU8ZR3	(CU)8(ZR)3	
CUB_A13	(AL,CO,CR,CU,FE,HF,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W,Y,ZR)1(B,C,VA)1	
CUCRS2	(CU)1(CR)1(S)2	
CUFES2_LT	(CU)1(FE)1(S)2	This is stoichiometric low-temperature CuFeS2.
CUMG2	(CU,NI)1(MG)2	
CUO	(CU+2)1(O-2)1	
CUPRITE_C3	(CU+1)2(O-2)1	
CUPT_L11	(CU,PT)0.5(CU,PT)0.5(VA)1	
CUSI_ETA	(CU,MN,NI)0.76(SI)0.24	
CUTI3	(CU,TI)1(TI)3	
CW3F	(CA+2)1(FE+2)3(FE+3)2(O-2)7	This is CaO.3FeO.Fe2O3 (oS52 Cmcm)
CWF	(CA+2)1(FE+2)1(FE+3)2(O-2)5	This is CaO.FeO.Fe2O3 (oS36 Cmcm)

Phase Name	Formula	Comments
D0I_MO2B5	(MO)0.32(B)0.68	
D5A_M3B2	(FE,HF,MO,NB,TA,V)3(B)2	TA3B2 NB3B2 V3B2 prototype U3SI2
DIAMOND_A4	(AL,B,C,O,SI)1	
DIGENITE	(CU,FE,MG,MN,VA)2(CU,VA)1(S)1	This is Cu2S with solubility of Fe Mg and Mn.
DIS_FCC_A1	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI,V,W,Y,ZR)1 (B,C,N,O,VA)1	
DIS_MU	(AL,CO,CR,CU,FE,MN,MO,NB,NI,RE,TA,TI,W)1	Part of the description of MU_ PHASE.
DIS_SIG	(AL,CO,CR,FE,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W)1	Part of the description of SIGMA phase.
DJURLEITE	(CU)1.93(S)1	This is Cu31S16.
FCC_A1	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI,V,W,Y,ZR)1 (B,C,N,O,VA)1	If FCC_L12 is defined this phase will be combined to it.
FCC_L10	(AL,CR,CU,MN,MO,NI,PD,PT,TA,TI,W)0.5(AL,CR,CU,MN,MO,NI,PD,PT,TA,TI,W)0.5	
FCC_L12	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI,V,W,Y,ZR)0.75 (AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,S,SI,TA,TI,V,W,Y,ZR)0.25 (B,C,N,O,VA)1	This phase has some contribution from FCC_A1.
FE2O12S3	(AL+3,CR+3,FE+3)2(SO4-2)3	This is (Al Cr Fe)2 (SO4)3
FE2SI	(FE)0.67(SI)0.33	
FE4N_LP1	(CO,CR,FE,MN,NI)4(C,N)1	
FE8SI2C	(FE)8(SI)2(C)1	
FEAL2S4	(FE)1(AL)2(S)4	
FECN_CHI	(FE)2.2(C,N)1	
FESI_B20	(CO,CR,FE,MN,NI,RE)1(AL,SI)1	CoSi CrSi ReSi Prototype FeSi
FESI2_H	(FE)0.3(SI)0.7	
FESI2_L	(FE)0.33(SI)0.67	

Phase Name	Formula	Comments
FEWB	(FE)1(W)1(B)1	prototype NiTiSi
FLUORITE_C1	(AL+3,CA+2,CR+3,FE+2,HF+4,MN+2,MN+3,NI+2,TI+4,Y+3,ZR,ZR+4)2(O-2,VA)4	
G_PHASE	(AL,CO,FE,MN,NI,TI)16(HF,NB,TI,Y,ZR)6(CO,FE,MN,NI,SI)7	Th6Mn23 prototype
GAMMA_D83	(AL,NI,SI)4(AL,CU,NI,SI)1(CU,FE,MN,NI)8	Al5Cu8 (rt)
GAMMA_H	(AL)4(AL,CU)1(CU,FE,MN,NI)8	Cu5Zn8-type Al8Cu5 (ht) phase
GARNET	(CA+2,MN+2)3(AL+3,CR+3)2(SI+4)3(O-2)12	This is Grossular Uvarovite and Spessartine.
GAS	(AL,AL1B1O2,AL1C1,AL1C2,AL1CU1,AL1CU1S1,AL1CU1S2, AL1H1, AL1H1O1_ ALOH,AL1H1O1_HALO,AL1H1O2,AL1H2,AL1H2O2,AL1H3, AL1H3O3,AL1N1,AL1O1,AL1O2,AL1S1,AL1S2,AL2,AL2C2,AL2O1,AL2O2, AL2O3,AL2S1,AL2S2,AR,B,B10H14,B1C1,B1C2,B1H1,B1H1O1_BOH, B1H1O1_ HBO,B1H1O2,B1H2,B1H2O1,B1H2O2,B1H3,B1H3O1,B1H3O2, B1H3O3,B1H6N1,B1N1,B1O1,B1O2,B2,B2C1,B2H4O4,B2H6,B2O1,B2O2, B2O3,B3H3O3,B3H3O6,B3H6N3,B5H9,C,C1H1,C1H1N1O1,C1H1N1_HCN, C1H1N1_HNC,C1H1O1,C1H1O2,C1H2,C1H2N4,C1H2O1,C1H2O2_CIS, C1H2O2_ DIOXIRANE,C1H2O2_TRANS,C1H3,C1H3O1_CH2OH,C1H3O1_CH3O, C1H4,C1H4N2O1,C1H4O1,C1H5N1,C1N1,C1N1O1,C1N1O1_NCO, C1N2_ CNN,C1N2_NCN,C1O1,C1O1S1,C1O2,C1PT1,C1S1,C1S2,C1SI1, C1SI2,C1SI3,C1SI4,C2,C2H1,C2H1N1,C2H2,C2H2O1,C2H3,C2H4, C2H4O1_ ACETALDEHYDE,C2H4O1_OXIRANE,C2H4O2_ACETICACID, C2H4O2_ DIOXETANE,C2H4O3_123TRIOXOLANE,C2H4O3_124TRIOXOLANE, C2H5,C2H6,C2H6O1,C2H6O1SI1,C2H6O2,C2H8SI1,C2N1_CCN,C2N1_CNC, C2N2,C2O1,C2SI1,C2SI2,C2SI3,C3,C3H1,C3H1N1,C3H4_1,C3H4_2,C3H6O1, C3H6_1,C3H6_2,C3H8,C3N1,C3O2,C4,C4H1,C4H10_1,C4H10_2,C4H12SI1, C4H2_1,C4H2_2,C4H4_1,C4H4_2,C4H6_1,C4H6_2,C4H6_3,C4H6_4,C4H6_5, C4H8_1,C4H8_2,C4H8_3,C4H8_4,C4H8_5,C4H8_6,C4N1,C4N2,C4NI1O4,C5, C5FE1O5,C5H1N1,C5N1,C60,C6H6,C6H6O1,C6MO1O6,C6N1,C6N2, C9N1,CA,CA1O1,CA1S1,CA2,CO,CO1H1,CO1H1O1,CO1H2O2,CO1O1, CO1S1,CO2,CR,CR1H1,CR1H1O1,CR1H1O2,CR1H1O3,CR1H2O2,CR1H2O3, CR1H2O4,CR1H3O3,CR1H3O4,CR1H4O4,CR1H4O5,CR1N1,CR1O1,CR1S1, CR1S2,CR1O2,CR1O3,CR2,CR2O1,CR2O2,CR2O3,CU,CU1H1,CU1H1O1, CU1O1,CU1S1,CU2,CU2S1,FE,FE1H1,FE1H1O1,FE1H1O2,FE1H2O2,FE1O1, FE1S1,FE1O2,FE2,H,H1MN1,H1MN1O1,H1MO1O1,H1MO1O2,H1MO3, H1N1,H1N1O1,H1N1O2_CIS,H1N1O2_TRANS,H1N1O3,H1N3,H1NI1, H1NI1O1,H1O1,H1O1W1,H1O2,H1O2W1,H1PT1,H1SI1,H1ZR1,H2, H2MO1O2,H2MO1O3,H2MO1O4,H2N1,H2N2O2,H2N2_1_1N2H2, H2N2_ CIS,H2N2_TRANS, H2NI1O2,H2O1,H2O2,H2O2W1,H2O3W1,H2O4W1,H2SI1, H3N1,H3N1O1,H3SI1,H4N2,H4SI1,H6SI2,HF,HF1O1,HF1O2,MN,MN1O1, MN1S1, MN1O2,MO,MO1N1,MO1O1,MO1O2,MO1O3,MO1S1,MO1S2, MO2,MO2O6,MO3O9,MO4O12,MO5O15,N,N1NB1,N1O1,N1O2,N1O3, N1SI1,N1SI2,N1TI1,N1V1,N1ZR1,N2,N2O1,N2O2,N2O3,N2O4,N2O5,N3 NB,NB1O1,NB1O2,NB1S1,NI,NI1O1,NI1S1,NI2,O10V4,O12W4,O15W5,	

Phase Name	Formula	Comments
	O1PD1,O1PT1,O1RE1,O1RU1,O1S1,O1S2,O1SI1,O1TA1,O1TI1,O1V1, O1W1,O1Y1,O1Y2,O1ZR1,O2,O2PT1,O2RE1,O2RU1,O2S1,O2SI1,O2SI2, O2TA1,O2TI1,O2V1,O2W1,O2Y1,O2Y2,O2ZR1,O3,O3RE1,O3RU1,O3W1, O4RU1,O6RE2,O3S1,O6W2,O7RE2,O8W3,O9W3,PD,PT,RE,RU,S,S1SI1, S1Y1,S1ZR1,S2,S2SI1,S2ZR1,S3,S4,S5,S6,S7,S8,SI,SI2,SI3,TA,TI,TI2,V,W,Y,ZR,ZR2)	
GRAPHITE	(B,C)1	
H_L21	(AL,CR,NI,TI)0.5(AL,HF,NB,NI,TA,TI,ZR)0.5(CO,NI,RU,VA)1	
HALITE	(AL+3,CA+2,CO+2,CO+3,CR+3,CU+2,FE+2,FE+3,MG+2,MN+2, MN+3,NI+2,NI+3,TI,TI+2,TI+3,V,V+2,V+3,VA,ZR+4,Y+3)1(O-2,VA)1	Wustite [FeO] Bunsenite [NiO] MnO CoO high temperature TiO VO prototy
HATRURITE	(CA+2,Y+3,VA)3(SIO4-4)1(O-2)1	This is 3CaO.SiO2 (hR81 R3m)
HCP_A3	(AL,CA,CO,CR,CU,FE,HF,MG,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W,Y,ZR)1 (B,C,N,O,VA)0.5	
HEAZLEWOODITE	(CO,FE,NI,VA)2(S)1	This is non-stoichiometric high temperature Ni3S2.
HEAZLEWOODITE_B2	(FE,NI,VA)2(S)1	This is non-stoichiometric high temperature Ni4S3.
HF2PD	(HF)2(PD)1	
HF3NI7	(HF)0.3(NI)0.7	
HF3PD4	(HF)3(PD)4	
HF8NI21	(HF,ZR)8(NI)21	also ZR8NI21
HFMN	(HF)0.5(MN)0.5	
HFNI_ALPHA	(HF)0.5(NI)0.5	
HFNI3_ALPHA	(HF)0.25(NI)0.75	
HFNI3_BETA	(HF)0.25(NI)0.75	
HFPD2	(HF)1(PD)2	
HFRE	(HF)1(RE)1	
HFSIO4	(HF+4)1(SI+4)1(O-2)4	
HIGH_SIGMA	(MN)8(CR)4(CR,MN)18	
IONIC_LIQ	(AL+3,CA+2,CO+2,CR+2,CU+1,FE+2,HF+4,MG+2,MN+2,MO+4,NB+2,NI+2,	IONIC_LIQ mixture

Phase Name	Formula	Comments
	PD+2,PT+2,RE+4,RU+4,SI+4,TA+5,TI+2,V+2,W+6,Y+3,ZR+4)1(ALO2-1,O-2,S-2,SO4-2,SIO4-4,VA,ALN,B,BO3/2,C,N,COO3/2,CRO3/2,CUO,FEO3/2,MNO3/2,MOO3,NBO2,NBO5/2,REO7/2,S,SIO2,TIO2,VO2,VO5/2)1	modeled by the ionic two-sublattice model.
KYANITE	(AL+3)1(AL+3)1(SI+4)1(O-2)5(,Al2O3.SiO2)	
LAAP	(CA+2,Y+3)1(AL+3,CO+3,CU+2,FE+3,NI+2)1(O-2,VA)3	This is Rhombohedral Perovskite)(LaAlO3 and LaCoO3 with sol. Ca Cu Ni Y
LARNITE	(CA+2)2(SI+4)1(O-2)4	This is 2CaO.SiO2 (metastable at 1 atm)
LIQUID	(AL,AL1N1,B,C,CA,CO,CR,CU,FE,HF,MG,MN,MO,N, NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W,Y,ZR)1	
M11SI8	(CR,NB)11(SI)8	oP76 Cr11Ge8
M12C	(CO,NI)6(MO,W)6(C)1	Prototype Mo6Ni6C
M23C6	(CO,CR,FE,MN,NI,RE,V)20(CO,CR,FE,MN,MO,NI,RE,V,W)3(C)6	Cr23C6
M2B_TETR	(AL,CO,CR,FE,MN,MO,NB,NI,RE,TA,W)2(B)1	Co2B Fe2B Mn2B Mo2B Ni2B
M2O3A	(CA+2,MG+2,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1	Prototype A-LA2O3? (P-3m1). AL2S3o hexagonal A-type structure of Gd2O3
M2O3B	(AL+3,CA+2,CO+3,MG+2,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1	Prototype B-GD2O3? (C2/m). This is monoclinic B-type structure of R2O3
M2O3C	(AL+3,CA+2,CR+3,FE+3,MG+2,MN+3,NI+2,Y,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1	Mn2O3 and cubic Y2O3
M2O3H	(CA+2,MG+2,MN+3,Y,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1	hexagonal Y2O3
M2O3X	(CA+2,MG+2,Y+3,ZR+4)2(O-2,VA)3(O-2,VA)1	Prototype X-LA2O3 (Ia3). This is AL2S3o HT cubic X-type structure of Gd2O3
M3B2	(CR,FE,MO,NI,W)0.4(CR,FE,NI)0.2(B)0.4	Mo2FeB2 Mo2CrB2
M3C2	(CO,CR,MO,V,W)3(C)2	Cr3C2

Phase Name	Formula	Comments
M3SI1	(HF,NB,TA,TI,ZR)3(SI)1	Ti3Si Ta3Si Zr3Si
M3SI2_D5A	(HF,NB,ZR)3(SI)2	Hf3Si2 Zr3Si2
M4SI3	(CR,NI)4(SI)3	
M5C2	(FE,MN)5(C)2	Mn5C2
M5SI3_D88	(CR,CU,FE,HF,MN,MO,NI,NB,SI,TI,Y,ZR)2(AL,CR,SI,TI)3 (CR,CU,FE,HF,MN,MO,NI,NB,TI,Y,ZR)3(C,VA)1	Fe5Si3 Ti5Si3 Zr5Si3 Y5Si3 Hf5Si3 Mo5Si3C Cr5Si3C prototype Mn5Si3
M6C	(CO,FE,NI)2(MO,NB,TA,W)2(CO,CR,FE,MO,NB,NI,TA,V,W)2(C)1	Prototype W3Fe3C
M6SI5	(CR,NB)6(SI)5	oI44 V6Si5
M7C3	(CO,CR,FE,MN,MO,NI,RE,V,W)7(C)3	Cr7C3
MB_B33	(CR,FE,HF,MO,NB,NI,TA,TI,V)1(B)1	CrB NbB NiB TaB VB
MB2_C32	(B)2(AL,CR,HF,MG,MN,MO,NB,TA,TI,V,Y,ZR)1	AlB2 CrB2 MnB2 MoB2 NbB2 TaB2 TiB2 VB2 YB2 ZrB2
MC_ETA	(MO,V,W)1(C,VA)1	MoC prototype TiAs
MC_SHP	(MO,W)1(C,N)1	Prototype WC also MoC low temperature
MELILITE	(CA+2)2(AL+3,CO+2,FE+2,FE+3)1(AL+3,SI+4)1(SI+4)1(O-2)7	
MG24Y5_A12	(MG)24(MG,Y)4(Y)1	
MG2C3	(MG)2(C)3	
MG2NI	(MG)2(CU,NI)1	
MG2SI	(MG)2(SI)1	
MG3N2_D53	(MG)3(N)2	
MG6MN3NI	(MG)3(MN)1(NI)2	
MGB4	(MG)1(B)4	
MGB7	(MG)1(B)7	
MGC2	(MG)1(C)2	
MN11SI19	(MN)11(AL,SI)19	
MN12Y	(MN)12(Y)1	
MN15NI45SI40	(MN)0.15(NI)0.45(SI)0.4	Mn-Ni-Si ternary

Phase Name	Formula	Comments
		phase T1 or N
MN15NI50SI35	(MN)0.15(NI)0.5(SI)0.35	Mn-Ni-Si ternary phase T2 or PHI
MN1NI1SI1	(MN)1(NI)1(SI)1	Mn-Ni-Si ternary phase T4 or E
MN2B_D1F	(MN)0.67(B)0.33	
MN2NISI	(MN,NI)3(SI)1	Mn-Ni-Si ternary phase T8 or S
MN2YO5	(Y+3)1(MN+3)1(MN+4)1(O-2)5	
MN3NI2SI	(MN)3(NI)2(SI)1	Mn-Ni-Si ternary phase T7 or Omega
MN3PD5	(MN)3(PD)5	
MN3SI	(MN,FE)3(AL,SI)1	
MN3TI	(MN)3(TI)1	
MN4TI	(MN)0.81(TI)0.18	
MN52NI29SI19	(MN)0.52(NI)0.29(SI)0.19	Mn-Ni-Si ternary phase T11 or W
MN66NI4SI30	(MN)0.66(NI)0.04(SI)0.3	Mn-Ni-Si ternary phase T10 or U
MN6N4	(MN)6(N)4	
MN6N5	(MN)6(N)5	
MN6NI16SI7	(MN)0.21(NI)0.55(SI)0.24	Mn-Ni-Si ternary phase T3 or G
MN6NISI3	(MN)0.61(NI)0.12(SI)0.27	Mn-Ni-Si ternary phase T9 or R
MN6SI	(AL,MN)17(SI)3	
MN9SI2	(MN)33(SI)7	
MN9SI3O14S1	(MN+2)9(SI+4)3(O-2)14(S-2)1	This is 8MnO.3SiO2.MnS
MNB4	(MN)0.2(B)0.8	
MNNI2	(MN,NI)1(NI)2	
MNNISI_T5	(MN)1(NI,SI)2	Mn-Ni-Si ternary phase T5 or "tao 1"
MNNISI_T6	(MN)1(NI,SI)2	Mn-Ni-Si ternary

Phase Name	Formula	Comments
		phase T6 or "tao 2"
MNPD2	(MN)1(PD)2	
MNPT7	(PT)6(PT)1(MN)1	
MNTA	(MN)1(TA)1	
MNTI_HT	(MN)0.52(TI)0.48	
MNTI_LT	(MN)1(TI)1	
MNYO3_HEX	(Y+3)1(MN+3)1(O-2)3	
MO1S2	(MO)1(S)2	
MO2S3	(MO)2(S)3	
MO3NI10B11	(MO)3(NI)10(B)11	
MO4O11	(MO)4(O)11	
MO8O23	(MO)8(O)23	
MO9O26	(MO)1(O)2.89	
MOB	(CR,FE,MO)1(B)1	MOB
MOB4	(MO)0.2(B)0.8	
MOCOB	(MO,W)1(CO)1(B)1	also WCoB
MONI_DELTA	(CO,CR,FE,NI,RE)24(CO,CR,FE,MO,NI,RE,W)20(CU,MO,W)12	
MONI4_BETA	(MO,W)1(NI)4	also WNi4
MONOCLINIC_S	(S)1	
MOO2	(MO)1(O)2	
MOO3	(MO)1(O)3	
MOSI2_C11B	(CO,CU,FE,MO,NI,PD,W)1(AL,HF,SI,TI,ZR)2	also WSi2 CuHf2 CuTi2 CuZr2 Prototype MoSi2
MSI_B27	(HF,NB,TI,Y,ZR)1(SI)1	TiSi HfSi YSi ZrSi (alpha) Prototype FeB
MSI2_C1	(CO,CU,MN,NI)1(AL,CU,SI)2	CoSi2 Prototype CaF2
MU_PHASE	(AL,CO,CR,CU,FE,MN,MO,NB,NI,RE,TA,TI,W)1 (AL,CO,CR,CU,FE,MN,MO,NB,NI,RE,TA,TI,W)2 (AL,CO,CR,CU,FE,MN,MO,NB,NI,RE,TI,TA,W)6 (AL,CO,CR,CU,FE,MN,MO,NB,NI,RE,TA,TI,W)4	DIS_MU contribution is introduced in the description of this

Phase Name	Formula	Comments
		phase
MULLITE	(AL+3)1(AL+3)1(AL+3,SI+4)1(O-2,VA)5	
MZR3_E1A	(CO,FE,NI)1(Y,ZR)3	COZR3 FEZR3 NiY3 COY3
NB13NI75TI12	(NB)0.13(NI)0.75(TI)0.12	
NB15NI56TI29	(NB)0.15(NI)0.56(TI)0.29	
NB15NI80TI5	(NB)0.15(NI)0.8(TI)0.05	
NB2O5	(NB)2(O)5	
NB3RU5	(NB,RU)0.38(RU)0.62	
NB5NI75TI20	(NB)0.05(NI)0.75(TI)0.2	
NB8NI9TI3	(NB)0.4(NI)0.45(TI)0.15	
NBO	(NB)1(O)1	
NBO2	(NB)1(O)2	
NI10ZR7	(NI)23(HF,ZR)17	
NI11ZR9	(NI)11(HF,ZR)9	
NI17Y2	(AL,FE,NI)1(Y)0.12	also Fe17Y2
NI2ALY2	(NI)2(AL)1(Y)2	
NI2SI_TETA	(CU,NI)1(NI,VA)1(AL,SI)1	
NI2TA	(CO,NI)2(TA,TI)1	
NI2V	(MO,NI,PD,PT)2(MO,NB,PT,TA,V)1	Ni2V Pd2Nb Pt2Nb Pt2V MoPt2
NI2Y	(NI)2(Y)1	
NI2Y3	(NI)2(Y)3	
NI31SI12	(CO,CR,CU,FE,NI)5(SI)2	
NI3ALY2	(NI)3(AL)1(Y)2	
NI3B_D011	(CO,CR,FE,MO,NI)3(B)1	Ni3B Co3B
NI3CR2B6	(NI)3(CR)2(B)6	
NI3S2_LT	(NI)3(S)2	
NI3SI_MONOCL	(NI)3(SI)1	
NI3SI_ORTHO	(NI)3(SI)1	
NI3SI2	(NI)3(SI)2	

Phase Name	Formula	Comments
NI3TA_D0A	(AL,CO,CR,FE,NI,NB,PT)3(AL,FE,MO,NB,NI,PT,TA,TI,V,W)1	also Ni3Mo Ni3Nb
NI3TI_D024	(AL,CO,CR,CU,FE,HF,NI,PD,PT,TA,TI,W,ZR)0.75 (AL,CR,CU,HF,MO,NB,NI,PD,PT,SI,TA,TI,W,ZR)0.25	also AlNi6Ta
NI3Y	(FE,NI)3(Y)1	also Fe3Y
NI4B3	(NI)0.57(B)0.43	
NI4SI2B	(NI)4.29(SI)2(B)1.43	
NI4Y	(NI)4(Y)1	
NI5ALB4	(NI)5(AL)1(B)4	
NI5ZR	(AL,CU,NI)5(HF,Y,ZR)1	also Ni5Y Ni5Hf Cu5Hf and Cu5Zr
NI6AL2Y3	(NI)6(AL)2(Y)3	
NI6MNO8	(NI+2)6(MN+4)1(O-2)8	
NI6SI2B	(NI)6(SI)2(B)1	
NI7S6	(FE,NI)7(S)6	
NI7ZR2	(AL,CO,CR,NI)7(HF,Y,ZR)2	also NI7HF2 NI7Y2 CO7Y2 and CO7HF2
NI8ALB11	(NI)8(AL)1(B)11	
NI8ALY3	(NI)8(AL)1(Y)3	
NI8TA	(NI)8(NB,TA)1	
NI9S8	(FE,NI)9(S)8	
NIAL2Y	(NI)1(AL)2(Y)1	
NIALY	(NI)1(AL)1(Y)1	
NICR3B6	(NI)0.1(CR)0.3(B)0.6	
NIMNO3	(MN+3,MN+4,NI+2)2(O-2)3	
NIMOO4	(NI+2)1(MO+6)1(O-2)4	
NIOCALITE_ C10NS6	(CA+2)10(NB+5)2(SI+4)6(O-2)27	This is 10CaO.Nb2O5.6SiO 2.
NIS_LT	(NI)1(S)1	This is low temperature NiS.
NISI_B31	(NI,PD)1(SI)1	
NITI2	(CO,CR,CU,FE,NI,RE,TI)1(AL,CR,CU,HF,NI,TA,TI,ZR)2	

Phase Name	Formula	Comments
NIWO4	(CO+2,FE+2,MN+2,NI+2)1(W+6)1(O-2)4	
NIZR	(NI)1(TI,Y,ZR)1	
OLIVINE	(CA+2,CO+2,CR+2,CU+2,FE+2,MN+2,NI+2)1 (CA+2,CO+2,CR+2,CU+2,FE+2,MN+2,NI+2)1(SI+4)1(O-2)4	This is 2CaO.SiO2 forsterite monticellite [CaO.MgO.SiO2] fayalite Ni2Si
ORTHO_ PYROXENE	(CA+2,FE+2)1(FE+2)1(SI+4)2(O-2)6	This is enstatite and orthodiopside
ORTHORHOMBIC_S	(S)1	
P_PHASE	(CR,FE,NI,RE)24(CR,FE,MO,NI,RE)20(MO)12	Prototype Cr9Mo21Ni20
PD11ZR9	(PD)11(ZR)9	
PD14SI3	(PD)14(SI)3	
PD15SI4	(PD)15(SI)4	
PD16S7	(PD)0.7(S)0.3	Prototype Pd16S7 (cI46 I-43m)
PD19SI10	(PD)19(SI)10	
PD21SI4	(PD,SI)21(SI)4	
PD2TA	(PD)2(TA)1	
PD2TI	(PD)2(TI)1	
PD2Y	(PD)2(Y)1	
PD2Y3	(PD)2(Y)3	
PD2Y5	(PD)2(Y)5	
PD39SI20	(PD)39(SI)20	
PD3S	(PD)0.75(S)0.25	Prototype Pd3S (oC16 Ama2)
PD3SI	(PD)3(SI)1	
PD3TI2	(PD)3(TI)2	
PD3Y2_HT	(PD)3(Y)2	
PD3Y2_LT	(PD)3(Y)2	
PD4S	(PD)0.8(S)0.2	Prototype Pd4Se (tP10 P-421C)

Phase Name	Formula	Comments
PD4Y3	(PD)4(Y)3	
PD4ZR3	(PD)4(ZR)3	
PD5SI	(PD)5(SI)1	
PD5TI3	(PD)5(TI)3	
PD7Y	(PD)7(Y)1	
PD9SI2	(PD)9(SI)2	
PDO	(PD)1(O)1	
PDS	(PD)0.5(S)0.5	Prototype PdS (tP16 P42/m)
PDY_HT	(PD,Y)1(Y)1	
PDY_LT	(PD,Y)1(Y)1	
PDY3	(PD)1(Y)3	
PDZR_ALPHA	(PD)1(ZR)1	
PDZR_BETA	(PD)1(ZR)1	
PDZRM	(PD)1(ZR)1(PD,ZR)1	
PENTLANDITE	(FE,NI)8(FE,NI)1(S)8	
PI	(CR)12.8(FE,NI)7.2(N)4	
PROTO_ PYROXENE	(CA+2,CO+2,CR+2,FE+2,NI+2)1(SI+4)1(O-2)3	This is proto-enstatite and protodiopside with Co Cr and Fe solubility.
PSEUDO_ BROOKITE	(TI+4)1(AL+3)2(O-2)5	
PSEUDO_ WOLLASTONITE	(CA+2)1(SI+4)1(O-2)3	This is CaO.SiO2 (mS120 C12/c1)
PT10ZR7	(PT)10(ZR)7	
PT25SI7	(PT)25(SI)7	
PT2TA	(PT)2(TA)1	
PT2Y	(PT)2(Y)1	
PT3O4	(PT)3(O)4	
PT3TA	(PT)3(TA)1	

Phase Name	Formula	Comments
PT3TI4	(PT)3(TI)4	
PT3Y5	(PT)3(Y)5	
PT3Y7	(PT)3(Y)7	
PT3ZR5	(PT,ZR)3(PT,ZR)5	
PT4Y3	(PT)4(Y)3	
PT4Y5	(PT)4(Y)5	
PT4ZR	(PT,ZR)4(PT,ZR)1	
PT4ZR3	(PT,ZR)4(PT,ZR)3	
PT5SI2	(PT)5(SI)2	
PT5Y	(PT)5(Y)1	
PT6SI5	(PT)6(SI)5	
PT8TI	(PT)8(TI)1	
PTO2	(PT)1(O)2	
PTS	(PT)1(S)1	Prototype PtS (tP4 P42/mmc)
PTS2	(PT)1(S)2	Prototype CdI2 (hP3 P-3m1)
PTSI	(PT)1(SI)1	
PTY2	(PT)1(Y)2	
PTY3	(PT)1(Y)3	
PYRITE	(CO,FE,MN,NI)1(S)2	This is (Co Fe Mn Ni)S2. Prototype FeS2 (cP12 Pa-3)
PYRRHOTITE	(AL,CO,CR,CU,FE,MG,MN,NB,NI,TI,V,ZR,VA)1(S)1	This is (Co Cr Fe Ni)S. Prototype NiAs (hP4 P63/mmc).
QUARTZ	(SIO2)1	
R_PHASE	(CO,CR,FE,NI,RE)27(MO,W)14(CO,CR,FE,MO,NI,RE,W)12	Prototype Co5Cr2Mo3
RANKINITE	(CA+2)3(SI+4)2(O-2)7	This is 3CaO.2SiO2 (mP48 P121/c1)
RE1S2	(RE)1(S)2	

Phase Name	Formula	Comments
RE1S3	(RE)1(S)3	
RE2O7	(O7RE2)1	
RE2S7	(RE)2(S)7	
RE2SI	(RE)2(SI)1	
RE3B	(CR,MO,RE,TA,W)3(B)1	
RE3CO3B2	(RE)3(CO)3(B)2	
RE5CO2B4	(RE)4(CO,RE)2(CO)1(B)4	
RE7B3	(CO,CR,MO,NB,RE,RU,TA,W)7(B)3(B,VA)3	Th7Fe3
REB2	(RE)1(B)2(B,VA)2	
RECOB	(RE)1(CO)1(B)1	
REO2	(O2RE1)1	
REO3	(O3RE1)1	
RESI2_C11B	(RE)0.36(SI)0.64	
REZR2	(NI,RE)1(ZR)2	
RHODONITE	(CA+2,MN+2)1(SI+4)1(O-2)3	This is MnO.SiO2
RU1S2	(RU)1(S)2	
RU25Y44	(RU)0.36(Y)0.64	
RU2B3	(RU)2(B)3	
RU2SI_C37	(RU)2(SI)1	
RU2SI3	(RU)2(SI)3	
RU2Y3	(RU)0.4(Y)0.6	
RU2Y5	(RU)0.29(Y)0.71	
RU4SI3	(RU)4(SI)3	
RUB	(RU)1(B)1	
RUB2	(RU)1(B)2	
RUSI	(RU)1(SI)1	
RUTILE_MO2	(AL+3,MN+4,RU+4,V+4,TI+4,ZR+4)1(O-2,VA)2	TiO2 also the high-temperature VO2 RUO2
RUY3	(RU)0.25(Y)0.75	
SI3N4	(SI)3(N)4	

Phase Name	Formula	Comments
SI5V6	(SI)5(V)6	
SIC	(SI)1(C)1	
SIGMA	(AL,CO,CR,FE,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W)10 (AL,CO,CR,FE,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W)4 (AL,CO,CR,FE,MN,MO,NB,NI,PD,PT,RE,RU,SI,TA,TI,V,W)16	DIS_SIG contribution is introduced in the description of this phase
SILLIMANITE	(AL+3)1(AL+3)1(SI+4)1(O-2)5	A high-pressure phase (Al2O3.SiO2)
SIS2	(SI)1(S)2	
SPINEL	(AL+3,CO+2,CO+3,CR+2,CR+3,CU+2,FE+2,FE+3,MG+2,MN+2,NI+2)1 (AL+3,CA+2,CO+2,CO+3,CR+3,CU+2,FE+2,FE+3,MG+2,MN+2,MN+3,MN+4,NI+2 ,VA)2(CR+2,FE+2,MG+2,MN+2,VA)2(O-2)4	magnetite [Fe3O4] FeAl2O4 NiAl2O4 FeCr2O4 NiCr2O4 NiFe2O4 Mn3O4 Co3O
T1_CU2TI	(CU,FE)2(TI)1	the Cu-Fe-Ti ternary phase Tau1
T1CUNITI	(CU,NI)2(TI)1	the Cu-Ni-Ti ternary phase Tau1
T2_CU3TI2	(CU,FE)3(TI)2	the Cu-Fe-Ti ternary phase Tau2
T2CUNITI	(CU)0.17(NI)2.83(TI)2	the Cu-Ni-Ti ternary phase Tau2
T3_CU4TI3	(CU,FE)4(TI)3	the Cu-Fe-Ti ternary phase Tau3
T4CUFETI	(CU,FE)0.63(TI)0.37	the Cu-Fe-Ti ternary phase Tau4
T4CUNITI	(CU)0.05(NI)0.7(TI)0.25	the Cu-Ni-Ti ternary phase Tau4
T5CUFETI	(CU,FE)0.55(TI)0.45	the Cu-Fe-Ti ternary phase Tau5
T6CUNITI	(CU)0.25(NI)0.5(TI)0.25	the Cu-Ni-Ti ternary phase Tau6
TA2O5_HT	(TA)2(O)5	
TA2O5_LT	(TA)2(O)5	
TA5SI3_D8L	(HF,NB,TA)5(AL,SI)3	
TAAL	(TA)0.52(AL)0.48	

Phase Name	Formula	Comments
TAAL2	(TA)0.35(AL)0.65	
TAN_EPS	(TA)1(N)1	
TAU	(CO,HF,NI,RE)20(B)6(B,VA)6(AL,CR,HF,MO,RE,TA,TI,V,W,ZR)3	ternary borides Prototype CR23C6
THIOSPINEL	(CO,CU,FE,MN,NI)1(CO,CR,NI)2(S)4	This is a sulphur spinel)((Cu Fe Mn)Cr2S4 Co3S4 FeNi2S4 and Ni3S4.
TI25MN9AL66_L12	(AL,MN,TI)0.25(AL,MN)0.08(AL,MN,TI)0.67	
TI2N_C4	(TI)2(N)1	
TI3N2	(TI)0.71(N)0.29	
TI3O2	(TI+2)2(TI)1(O-2)2	
TI3O5	(TI+3)2(TI+4)1(O-2)5	
TI3SIC2	(TI)3(SI)1(C)2	
TI4N3	(TI)0.69(N)0.32	
TIO_ALPHA	(TI+2)1(O-2)1	
TISI2_C54	(MO,NB,RU,TI)1(AL,SI)2	
TRIDYMITE	(SIO2)1	
V2B3	(V)0.4(B)0.6	
V2O_SS	(V)1(O,VA)0.5	Gamma (V)
V2O5	(V+5)2(O-2)5	
V3C2	(V)3(C)2	
V52O64	(V)52(O)64	delta-prime V-oxide
V5B6	(NB,V)5(B)6	
VO2_LT	(V+4)1(O-2)2	
W1S2	(W)1(S)2	
W2COB2	(MO,W)2(CO,NI)1(B)2	also Mo2NiB2 and Mo2CoB2
W3COC	(W)3(CO,NI)1(C)1	also W3NiC
W5SI3_D8M	(CR,FE,MO,NB,V,W)4(CR,FE,MO,NB,V,W,SI)1(AL,SI)3	Cr5Si3 Mo5Si3 W5Si3 protoype W5Si3

Phase Name	Formula	Comments
WO2	(O2W1)1	
WO2_72	(O2_72W1)1	
WO2_90	(O2_90W1)1	
WO2_96	(O2_96W1)1	
WO3_HT	(O3W1)1	
WO3_LT	(O3W1)1	
WOLLASTONITE	(CA+2,FE+2,MN+2)1(SI+4)1(O-2)3	This is CaO.SiO2 (aP30 P-1)
Y15C19_H	(C)19(Y)15	
Y15C19_R	(C)19(Y)15	
Y2C3_H	(Y)2(C)2(C,VA)1	
Y2C3_R	(Y)2(C)2(C,VA)1	
Y2CU2O5	(Y+3)2(CU+2)2(O-2)5	
Y2S2A_Y2SI2O7	(Y+3)1(Y+3)1(SI2O7-6)1	
Y2S2B_Y2SI2O7	(Y+3)1(Y+3)1(SI2O7-6)1	
Y2S2D_Y2SI2O7	(Y+3)1(Y+3)1(SI2O7-6)1	
Y2S2G_Y2SI2O7	(Y+3)1(Y+3)1(SI2O7-6)1	
Y2SIO5	(Y+3)1(Y+3)1(SIO4-4)1(O-2)1	
Y3SI5_HT	(Y)3(SI)5	
Y3SI5_LT	(Y)3(SI)5	
YAG	(AL+3,CR+3,FE+3)5(Y+3)3(O-2)12	
YAM	(AL+3,SI+4)2(CA+2,Y+3)4(O-2,VA)1(O-2)9	
YAP	(AL+3,CO+3,CR+3,FE+3,MN+3)1(CA+2,Y+3)1(O-2,VA)3	
YB4	(Y)1(B)4	
YB6	(Y)1(B)6	
YB66	(Y)1(B)66	
YC_GAMMA	(Y)1(C,C2,VA)1	
YC2_C11A	(C2Y1)1	
YCUO2	(Y+3)1(CU+1)1(O-2)2	
YSI2_HT	(Y)1(SI)2	

Phase Name	Formula	Comments
Z_PHASE	(CR,FE)1(MO,NB,V)1(N,VA)1	
ZR3Y4O12	(ZR+4)3(Y+3)4(O-2)12	
ZR5SI4	(HF,NB,TI,Y,ZR)5(SI)4	Hf5Si4 Ti5Si4 Y5Si4 Zr5Si4(alpha) prototype ZR5SI4
ZRO2_MONO	(AL+3,CA+2,CR+3,HF+4,TI+4,Y+3,ZR+4)2(O-2,VA)4	
ZRO2_TETR	(AL+3,CA+2,CR+3,FE+2,HF+4,MG+2,MN+2,MN+3,NI+2,TI+4,Y+3,ZR+4)2(O-2,VA)4	
ZRO8S2	(ZR+4)1(SO4-2)2	This is Zr(SO4)2
ZRS2	(ZR)1(S)2	
ZRSI2_C49	(ZR,Y,HF,NB)1(SI)2	ZrSi2 YSi2 HfSi2 Prototype ZrSi2
ZRSIO4	(SI+4)1(ZR+4)1(O-2)4	
ZRTI2O6	(ZR+4)1(TI+4)2(O-2)6	
ZRTIO4_ALPHA	(ZR+4)1(TI+4)1(O-2)4	
ZRTIO4_BETA	(TI+4,ZR+4)2(O-2)4	