TCS Ti/TiAl-based Alloys Database (TCTI4)

Technical Information

Available Starting with Thermo-Calc Version 2022a

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Contents

About the TCS Ti/TiAl-based Alloys Database (TCTI)

TCS Ti/TiAl-based Alloys Database (TCTI) is a thermodynamic database developed for conventional Ti-based and newly emerging γ-TiAl based alloys. It can be used to calculate various phase diagrams and thermodynamic properties in assessed systems, but also to predict stable and metastable phase equilibria (β-transus temperature, evolution of phase fractions vs. temperature, martensitic temperature, and so on) for a wide range of multicomponent alloys of industrial relevance, with light impurities (O, N, H, etc.) taken into account. Ti- and γ-TiAl-based alloys of relevance that can be studied include, but are not limited to:

- Alpha and near-alpha alloys, such as Ti-6242Si
- Alpha-beta alloys, such as Ti64
- Beta or near-beta alloys, such as Ti 10-2-3
- γ-TiAl based alloys, such as TNM alloys

In addition to thermodynamic data, it has properties data available for:

- Molar volume with thermal expansion coefficients
- Viscosity of the metallic liquids
- Surface tension of liquid metallic alloys
- Electrical resistivity
- Thermal conductivity

TCTI: TCS Ti/TiAl-based Alloys Database Revision History. The current version of the database is TCTI4.

The properties data was gradually added to the database versions as follows. Molar volume with thermal expansion coefficients available starting with TCTI2, the viscosity of liquid and surface tension of liquid are available starting with TCTI3, and electrical resistivity and thermal conductivity starting with TCTI4.

The CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

Use Case Examples

There are examples available to both demonstrate the validation of the database and to showcase the types of calculations that can be used for different materials or application areas depending on the database.

Some use case examples of how the TCTI4 database can be used include:

- Calculate various phase diagrams and property diagrams in the assessed systems as well as extrapolated higher-order systems.
- Predict phase formation, phase fractions and phase compositions in multicomponent titanium alloys.
- Predict solidification behavior of Ti- and TiAl-based alloys with Scheil calculations in Thermo-Calc.
- Couple with a compatible atomic mobility database to study diffusion-controlled phase transformations with the add-on Diffusion Module (DICTRA) or multi-particle precipitation kinetics with the Precipitation Module (TC-PRISMA).

Calculations and simulations for higher-order systems might not be valid beyond the Ti-rich region and the Ti-Al vicinity.

Combining Databases

It is possible to combine several databases to make calculations using Thermo-Calc. For more information related to a specific type of problem, contact one of our support specialists at info@thermocalc.com. The experts are available to make recommendations on the most suitable database to use for your needs.

TCS Ti/TiAl-based Alloys Database (TCTI) Resources

Information about the database is available on our website and in the Thermo-Calc software online Help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online Help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCS Ti/TiAl-based Alloys Database (TCTI) Technical Information* PDF document contains version specific information such as the binary, ternary assessed systems, phases and models. It also includes details about the properties data (e.g. viscosity, surface tension, etc.), a list of the included elements, and summaries of the database revision history by version.
- The *TCS Ti/TiAl-based Alloys Database (TCTI) Examples Collection* PDF document contains a series of validation examples using experimental data, and a set of calculation examples showing some of the ways the database can be used.

Go to the Titanium and TiAl-based Alloys Databases page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to titanium and TiAl including links to resources such as examples, publications, and more.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

TCTI4 Elements, Systems, Phases, and Properties

Included Elements

There are 28 elements included in the most recent version of the database.

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

Assessed Systems and Phases

The most recent version of the database contains:

- 279 binary systems
- 110 ternary systems
- 435 solution and intermetallic phases. This includes nearly all stable phases in the assessed systems and most important metastable phases that may form in Ti- and TiAl-based alloys. The GAS phase is rejected by default when retrieving the data from the database; it needs to be manually restored when it is required for a calculation.

In Console Mode, you can list phases and constituents in the Database (TDB) module and the Gibbs (GES) module. For some phases, supplementary information is included in the definitions. To show the information, it is recommended in the Database (TDB) module to use the command LIST_SYSTEM with the option `Constituents`.

The ordered B2 phase with Bcc_A2 is modeled with the so-called partition model, which describes an ordered phase and its disordered counterpart using a single Gibbs energy function. This type of description is of importance to predict second order transformations between a disordered phase and its ordered structures.

Note About the Ternary Systems

Although the assessed ternary systems in TCTI are modeled by considering experimental data over quite wide (if not entire) compositions, this database prominently targets light elements, like O, C, N, and H, as impurities in alloys. Therefore, appending another appropriate database, for example the TCS Metal Oxide Solutions Database (TCOX) may be essential for calculations in pseudo-binary systems, as well as systems with a certain large amount of such elements.

Properties Data

A variety of properties data are included with the TCS Ti/TiAl-based Alloys Database (TCTI).

You can find information on our website about the thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

For more information about the various thermophysical models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

Notes About the Thermophysical Property Data in this Database

The properties data was gradually added to the database versions as follows. Molar volume with thermal expansion coefficients available starting with TCTI2, the viscosity of liquid and surface tension of liquid are available starting with TCTI3, and electrical resistivity and thermal conductivity starting with TCTI4.

- Molar volume data is critically assessed for most phases of importance to titanium alloys. All necessary volume data (including molar volume and thermal expansion) for various phases have been incorporated, which enables one to calculate volume fraction of phases, density and thermal expansivity, as well as lattice parameters for cubic structures using Thermo-Calc. However, note that the molar volume data only provides rough estimations and has no pressure dependence.
- Surface tension is modeled for the liquid phase in all pure elements and binary systems.
- The viscosity of the liquid is described for all pure elements and 141 binary systems.
- Electrical resistivity and thermal conductivity are critically assessed with available data in all binary systems for phases of importance to Ti/TiAl-based alloys. See Common Phases for Titanium Alloys for a list of these assessed phases and to review the phase descriptions for electrical resistivity and thermal conductivity.

Available Properties Data Parameters and Variables

Below is a summary of the available parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use the TC-Python SDK. More details are described in the online help.

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Electrical conductivity		ELCD for a system `ELCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI*	`SURF(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)` **
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)` **
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

* XI is not used in the TCS Metal Oxide Solutions Database (TCOX)
** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCTI4 Systems

In this section:

TCTI4 Assessed Binary Systems

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

Ti	Ag	Al	B	C	Co	Cr	Cu	Fe	H	Hf	Mn	Mo	N	Nb	Ni	O	Pd	Pt	Re	Ru	Si	Sn	Ta	V	W	Y	Zr
Ag	X																X										
Al		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
B			X	X	X	X		X	X	X	X	X	X	X	X	X			X	X	X	X	X	X	X	X	X
C				X	X	X		X	X	X	X	X		X	X				X	X	X		X	X	X	X	X
Co					X	X		X	X	X	X	X		X	X	X			X	X	X	X	X	X	X	X	X
Cr						X		X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X
Cu							X	X	X				X	X	X	X					X	X					
Fe								X	X	X	X	X	X	X	X	X			X	X	X	X	X	X	X	X	X
H									X	X	X	X	X	X	X	X			X	X	X	X	X	X	X	X	X
Hf										X	X	X		X	X	X			X	X	X		X	X	X	X	X
Mn											X	X	X	X	X	X			X	X	X	X	X	X	X	X	X
Mo												X	X	X	X	X	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	X
Ni															X	X	X		X	X	X	X	X	X	X	X	X
O																X			X	X	X	X	X	X		X	X
Pd																	X							X			X
Pt																		X									
Re																			X	X	X		X	X	X	X	X
Ru																				X	X	X	X	X	X	X	X
Si																					X	X	X	X	X	X	X
Sn																						X		X			X
Ta																							X	X	X	X	X
V																								X	X	X	X
W																									X	X	X
Y																										X	X
Zr																											X

TCTI4 Assessed Ternary Systems

Note About the Ternary Systems

Assessed Ternary Systems					
B-C-Si	Ti-Ag-Pd	Ti-Al-B	Ti-Al-C	Ti-Al-Co	Ti-Al-Cr
Ti-Al-Cu	Ti-Al-Fe	Ti-Al-H	Ti-Al-Mn	Ti-Al-Mo	Ti-Al-N
Ti-Al-Nb	Ti-Al-Ni	Ti-Al-O	Ti-Al-Pd	Ti-Al-Si	Ti-Al-Sn
Ti-Al-Ta	Ti-Al-V	Ti-Al-W	Ti-Al-Y	Ti-Al-Zr	Ti-B-Co
Ti-B-Cr	Ti-B-Hf	Ti-B-Mo	Ti-B-Nb	Ti-B-Ni	Ti-B-Si
Ti-B-Sn	Ti-B-Ta	Ti-B-V	Ti-B-W	Ti-B-Zr	Ti-C-Cr
Ti-C-Cu	Ti-C-Mo	Ti-C-Nb	Ti-C-Si	Ti-C-Ta	Ti-C-V
Ti-C-W	Ti-C-Zr	Ti-Co-Mo	Ti-Co-Sn	Ti-Co-Ta	Ti-Cr-Fe
Ti-Cr-H	Ti-Cr-Mn	Ti-Cr-Mo	Ti-Cr-N	Ti-Cr-Nb	Ti-Cr-O
Ti-Cr-Si	Ti-Cr-Sn	Ti-Cr-Ta	Ti-Cr-V	Ti-Cr-W	Ti-Cr-Zr
Ti-Cu-Fe	Ti-Cu-H	Ti-Cu-N	Ti-Cu-Nb	Ti-Cu-Ni	Ti-Cu-O
Ti-Cu-Si	Ti-Cu-Sn	Ti-Fe-Mo	Ti-Fe-V	Ti-H-Ni	Ti-H-O
Ti-H-Zr	Ti-Hf-Ta	Ti-Hf-Zr	Ti-Mo-N	Ti-Mo-Nb	Ti-Mo-O
Ti-Mo-Si	Ti-Mo-Sn	Ti-Mo-Ta	Ti-Mo-V	Ti-Mo-W	Ti-Mo-Zr
Ti-N-Nb	Ti-N-Ta	Ti-Nb-O	Ti-Nb-Si	Ti-Nb-Sn	Ti-Nb-Ta
Ti-Nb-V	Ti-Nb-W	Ti-Nb-Zr	Ti-Ni-Pd	Ti-Ni-Sn	Ti-O-Si
Ti-O-Ta	Ti-O-V	Ti-O-W	Ti-O-Zr	Ti-Pd-V	Ti-Si-W
Ti-Sn-V	Ti-Sn-Zr	Ti-Ta-V	Ti-Ta-W	Ti-Ta-Zr	Ti-V-W
Ti-V-Zr	Ti-W-Zr				

TCTI4 Phases

In this section:

Common Phases for Titanium Alloys

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key titanium alloys.

Electrical resistivity and thermal conductivity are only assessed for the phases listed here except those marked with an asterisk (*).

TCTI4 Models for the Included Phases

Name in the Database	*Common Name and Description*
ALTI_L10	This is the γ phase in TiAl-based alloys.
ALTI3_D019	This is the α_2 phase.
BCC_B2	This is the β phase. The ordered B2 phase with the disordered BCC_A2 has been modeled with the so-called partition model. It is always labeled as BCC_B2 in calculations with TCTI. It is necessary to check the constitution of the phase to find out whether it is ordered or not. Electrical resistivity and thermal conductivity are assessed for BCC_A2, BCC_B2 with available data.
B82_omega	This is the ω_o phase in TiAl-based alloys.
CUZR2_C11B	$CuTi_2$ is modeled as this phase.
CU4TI1	Cu_4Ti is modeled as this phase.
DELTA_TIH2	This is the delta dihydride (eg. TiH_2) with CaF_2 as prototype.
FCC_B1	Titanium carbide, nitride, oxide with NaCl as prototype
HCP_A3	This is the α phase. The descriptions of α' (Hcp martensite) and α" (orthorhombic martensite) are unified into HCP_A3 phase in the database by now.
Liquid	Metallic liquid solution
MSI_B27	TiSi is modeled as this phase.
M3SI1	Ti_3Si is modeled as this phase.
M5SI3_D88	Ti_5Si_3 is modeled as this phase.
O1_DIS	The disordered orthorhombic phase originating from the Ti- Al-Nb ternary system.

Name in the Database	*Common Name and Description*
O_PHASE	The ordered orthorhombic phase originating from the Ti-Al-Nb ternary system, which has different site occupancies compared with O1_DIS phase.
OMEGA*	The omega phase is a metastable phase which forms in titanium and its alloys with transition elements (like V, Mo, Nb, Fe, etc).
RUTILE_TIO2	TiO_2 is modeled as this phase.
TiB_B27	TiB is modeled as this phase.
TiB2_C32	TiB_2 is modeled as this phase.
Ti2N_C4	Ti_2N is modeled as this phase.
Ti3B4	Ti_3B_4 is modeled as this phase.
Ti3N2	η-Ti_3N_{2-x} phase in Ti-N binary
Ti4N3	ζ-Ti_4N_{3-x} phase in Ti-N binary
TiSi2_C54	$TiSi_2$ is modeled as this phase.
Zr5Si4	Ti_5Si_4 is modeled as this phase.
* Electrical resistivity and thermal conductivity are not assessed for this phase.	

TCTI4 Models for the Included Phases

For electrical resistivity and thermal conductivity thermophysical properties, see Common Phases for Titanium Alloys for a list of the assessed phases.

Name	*Prototype*	*Pearson*	*Spacegroup*	*Thermodynamic Model and phase Constitution*	*Notes*
AF	FeGaO3	oP40	Pna2_1	(Al2O3)1(Fe2O3)1	
AG1TI2	CuZr2	tI6	I4/mmm	(Ag)1(Ti)2	
AGTI	CdTi	tP4	P4/nmm	(Ag, Ti)1(Ag, Ti)1	
AL11CR2		oC584	Cmcm	(Al)10(Al, Cr, Ti)2	
AL11CR4	Al11Mn4	aP15	P-1	(Al)11(Al, Cr, Ti)4	
AL11MN4_HT	Al3Mn	oP156	Pnma	(Al, Mn)29(Mn)10	
AL11MN4_LT	Al11Mn4	aP15	P-1	(Al)11(Fe, Mn)4	
AL11RE4	Al11Mn4	aP15	P-1	(Al)11(Re)4	
AL12MN	Al12W	cI26	Im-3	(Al)12(Mn)1	
AL12W	Al12W	cI26	Im-3	(Al)12(Mo, Re, W)1	also AL12RE and AL12MO
AL13CO4	Al19Co6	mS100	C2/m	(Al)13(Co)4	
AL13FE4	Al13Fe4	mS102	C2/m	(Al)0.6275(Fe, Mn, Ru)0.235(Al, Si, Va)0.1375	also Al13Ru4
AL17MO4	Al17Mo4	mC84	C2	(Al)17(Mo)4	
AL1RE2	CuZr2	tI6	I4/mmm	(Al)1(Re)2	C11_b
AL1ZR2	Ni2In	hP6	P6_3/mmc	(Al)1(Ti, Y, Zr)2	also AlY2

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
AL21PT8	Al21Pt8	tI116	I4_1/a	(Al)21(Pd, Pt)8	also Al21Pd8
AL21V2	Al21V2	cF184	Fd-3m	(Al)21(V)2	
AL22MO5	Al22Mo5	oF216	Fdd2	(Al)22(Mo)5	
AL23V4	Al23V4	hP54	P6_3/mmc	(Al)23(V)4	
AL2CU_C16	Al2Cu	tI12	I4/mcm	(Al)2(Al, Cu)1	
AL2FE	Al2Fe	aP18	P1	(Al)2(Fe, Mn)1	
AL2N2TI3	Ti3Al2N2	hP22	P6_3mc	(Al)2(N)2(Ti)3	
AL2PD5	Ga2Pd5	oP28	Pnma	(Al)2(Al, Pd)5	
AL2TI	Ga2Hf	tI24	I4_1/amd	(Al, Nb, Ta, Ti)2(Al, Co, Cr, Nb, Ta, Ti, V, Zr)1	
AL2W	Cr2Si2	hP9	P6_222	(Al)2(W)1	
AL2ZR3	Al2Zr3	tP20	P4_2/mnm	(Al)2(Hf, Ti, Y, Zr)3	also Al2Hf3, Al2Y3
AL3CO	Al13Os4	mS34	C2/m	(Al)3(Co)1	
AL3MO	Al3MO	mC32	C2/m	(Al)3(Mo)1	
AL3NI1	Fe3C	oP16	Pnma	(Al)0.75(Ni)0.25	
AL3NI2	Al3Ni2	hP5	P-3m1	(Al, Pd, Si)3(Al, Ni, Pd, Ru)2(Ni, Ru, Va)1	
AL3NI5	Ga3Pt5	oS16	Cmmm	(Al)0.375(Ni)0.625	
AL3PD1	Al3Pd	oP*	Pna2_1	(Al)3(Pd)1	
AL3PD5	Ge3Rh5	oP16	Pbam	(Al)3(Pd, Pt)5	also Al3Pt5
AL3TI_D022	Al3Ti	tI8	I4/mmm	(Al, Mn, Mo, Nb, Pd, Si, Ti, V)3(Al, Co, Cr, Mn, Mo, Nb, Ni, Pd, Si, Ta, Ti, V, Zr)1	also Al3V

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
AL3TI_LT	Al3Ti	tI32	I4/mmm	(Al, Cr, Nb, Ti)3(Al, Cr, Nb, Ti, V, Zr)1	
AL3Y_HT	BaY3	hR36	R-3m	(Al)0.75(Y)0.25	
AL3Y_LT	Mg3Cd	hP8	P6_3/mmc	(Al)0.75(Y)0.25	
AL3ZR2	Al3Zr2	oF40	Fdd2	(Al)3(Hf, Zr)2	also Al3Hf2
AL3ZR4	Al3Zr4	hP7	P6/mmm	(Al)3(Hf, Ti, Zr)4	also Al3Hf4
AL3ZR5	Si3W5	tI32	I4/mcm	(Al)3(Ti, Zr)5	
AL3ZR_D023	Al3Zr	tI16	I4/mmm	(Al)3(Hf, Ti, Zr)1	also Al3Hf
AL45V7	Al45V7	mS104	C2/m	(Al)45(V)7	
AL4C3	Al4C3	hR21	R-3m	(Al, Si)4(C)3	
AL4CR	mu-Al4Mn	hP574	P6_3/mmc	(Al)4(Al, Cr, Ti)1	
AL4FE	AlmFe	tI110	I-42m	(Al)4.2(Fe)1	
AL4MN_R	lambda-Al4Mn	hP586	P6_3/mmc	(Al)461(Fe, Mn)107	
AL4MN_U	mu-Al4Mn	hP574	P6_3/mmc	(Al)4(Mn)1	
AL4PD	Al4Pd	hP*	P6_322	(Al)4(Pd)1	
AL4RE	Al4Re	aP71	P-1	(Al)4(Re)1	
AL4W	Al4W	mS30	Cm	(Al)4(Mo, W)1	also Al4Mo
AL4ZR5	Ga4Ti5	hP18	P6_3/mcm	(Al)4(Zr)5	
AL5CO2_D811	Al5Co2	hP28	P6_3/mmc	(Al)5(Co)2	
AL5FE2	Al2.8Fe	oS24	Cmcm	(Al)5(Fe, Mn)2	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
AL5FE4	Cu5Zn8	cI52	I-43m	(Al, Fe)1	
AL5TI2	Al5Ti2	tP28	P4/mmm	(Al, Cr, Nb, Ta, Ti)5(Al, Cr, Nb, Ta, Ti, V, Zr)2	
AL5TI3		tP*	P4/mbm	(Al)5(Cr, Nb, Ta, Ti)3	
AL5W	Al5W	hP12	P6_322	(Al)5(Mo, W)1	also AL5MO
AL63MO37	Unknown Structure			(Al)63(Mo)37	
AL6MN	MnAl6	oS28	Cmcm	(Al)6(Fe, Mn, Re, Ru)1	
AL77W23	Unknown Structure			(Al)77(W)23	
AL7CR	Al45V7	mC104	C2/m	(Al)13(Al, Cr, Ti)2	
AL7W3	Unknown Structure			(Al)7(W)3	
AL8CR5_HT	Cu5Zn8	cI52	I-43m	(Al, Cr)2(Al, Cr, Ti)3(Cr)2(Al)6	
AL8CR5_LT	Al8Cr5	hR26	R-3m	(Al)12(Cr)5(Al, Cr, Ti)9	
AL8CR5_MT	Unknown Structure			(Al, Cr, Ti)2(Al, Cr, Ti)3(Cr)2(Al)6	
AL8MO3	Al8Mo3	mS22	C2/m	(Al)8(Mo)3	
AL8V5	Cu5Zn8	cI52	I-43m	(Al, Mn, V)8(Al, Mn, Ti, V)5	
AL9CO2	Al9Co2	mP22	P2_1/c	(Al)9(Co)2	
ALB12		tP208	P4_12_12	(Al, Ti)1(B)12	
ALBMO	MoAlB	oS12	Cmcm	(Al)1(B)1(Mo)1	
ALCCR2	AlCCr2	hP8	P6_3/mmc	(Al)1(C)1(Cr)2	
ALCR2	MoSi2	tI6	I4/mmm	(Al, Cr, Ni, Pd)1(Al, Cr, Ti)2	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
ALCR3	Unknown Structure			(Al, Cr, Ti)1(Cr)3	AlCr3 super lattice
ALCU_DEL	Al5Cu8	hR52	R3m	(Al)2(Cu)3	
ALCU_EPS	Ni2In	hP6	P6_3/mmc	(Al, Cu)1(Cu)1	
ALCU_ETA	AlCu	mC20	C2/m	(Al, Cu)1(Cu)1	
ALCU_ZETA	Al9Cu11(r)	oI24	Imm2	(Al)9(Cu)11	
ALH3	FeF3	hR24	R-3c	(Al)1(H)3	
ALM3C_E21	CaTiO3	cP5	Pm-3m	(Al)1(Co, Fe)3(C)1	AlCo3C, AlFe3C, Perovskite
ALNTI2	AlCCr2	hP8	P6_3/mmc	(Al)1(N)1(Ti)2	
ALNTI3	CaTiO3	cP5	Pm-3m	(Al)1(N)1(Ti)3	
ALN_B4	Wurtzite (ZnS, B4)	hP4	P6_3mc	(Al)1(N)1	
ALPHA_B19	AuCd	oP4	Pmma	(Mo, Nb, Pt, Ti, V, Zr)1(Mo, Nb, Pt, Ti, V, Zr)1	
ALPHA_SPINEL	Mn3O4	tI28	I4_1/amd	(Co+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	
ALRE	gamma-CuTi	tP4	P4/nmm	(Al)1(Re)1	
ALSI3TI2	Zr3Al4Si5	tI24	I4_1/amd	(Al)0.166667(Si)0.5(Ti)0.333333	
ALTI3_D019	Ni3Sn	hP8	P6_3/mmc	(Al, Co, Cr, Cu, Mn, Mo, Nb, Ni, Ta, Ti, V, W, Zr)3(Al, C, Cr, Mo, Nb, Si, Sn, Ta, Ti, V, W)1(H, O, Va)2	Ti3Al
ALTI_L10	CuAu	tP2	P4/mmm	(Al, Co, Cr, Cu, Mn, Mo, Nb, Ni, Pd, Sn, Ta, Ti, V, W, Zr)1(Al, Co, Cr, Cu, Mn, Mo, Nb, Ni, Pd, Sn, Ta, Ti, V, W, Zr)1(C, H, O, Va)2	TiAl
ALZR	CrB	oS8	Cmcm	(Al)1(Hf, Y, Zr)1	also AlHf, AlY
ANDALUSITE	Al2(SiO4)O	oP32	Pnnm	(Al+3)1(Al+3)1(Si+4)1(O-2)5	A high-pressurephase (Al2O3.SiO2)

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
B12ZR	UB12	cF52	Fm-3m	(B)12(Y, Zr)1	YB12, ZrB12
B2O3	B2O3	hP15	P3_121	(B2O3)1	
B3SI	B4C	hR15	R-3m	(B)6(Si)2(B, Si)6	
B4C	B13C2	hR15	R-3m	(B11C, B12)1(B2, C2B, Cb2, Si2)1	
B5W2_X	Mo2B5	hR21	R-3m	(B, C, Va)5(W)2	
B6SI	B6Si	oP280	Pnnm	(B)210(Si)23(B, Si)48	
B82_OMEGA	Ni2In	hP6	P6_3/mmc	(Al, Sn)1(Co, Cr, Mo, Nb, Ta, Ti, Zr)1(Ti)1	
B9W2	BW4	hP20	P-3	(B)9(W)2	
BCC_A2	W	cI2	Im-3m	(Ag, Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Pd, Pt, Re, Ru, Si, Sn, Ta, Ti, V, Va, W, Y, Zr)1(B, C, H, N, O, Va)3	Metallic BCC_A2 solution. If BCC_B2 is defined, this phase will becombined to it.
BCC_B2	CsCl	cP2	Pm-3m	(Ag, Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Pd, Pt, Re, Ru, Si, Sn, Ta, Ti, V, Va, W, Y, Zr)0.5(Ag, Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Pd, Pt, Re, Ru, Si, Sn, Ta, Ti, V, Va, W, Y, Zr)0.5(B, C, H, N, O, Va)3	Solution of ordered BCC_B2, having Gibbs energy contribution from BCC_A2
BCT_A5	C	cF8	Fd-3m	(Al, Cu, Sn, Ti)1	
BETAR_BORON	B	hR423	R-3m	(B)93(B, C, Nb, Si, Ti)12	
BETA_PHASE		mC6	C21/m1	(H, Va)0.25(H, Va)0.25(V)0.5	V-H binary
BETA_V3O	CoO	tI4	I4/mmm	(V)1(O, Va)1	
BNSI	B	hR12	R-3m	(B)61(Si)1(B, Si)8	
BN_B4	Wurtzite (ZnS, B4)	hP4	P6_3mc	(B)1(N)1	
BW_ALPHA	MoB	tI16	I4_1/amd	(B, C, Va)1(W)1	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
BW_BETA	BCr	oS8	Cmcm	(B, C, Va)1(W)1	
C14_LAVES	MgZn2	hP12	P63/mmc	(Al, Co, Cr, Fe, Hf, Mn, Mo, Nb, Ni, Pd, Re, Ru, Si, Ta, Ti, V, W, Y, Zr)2(Al, Co, Cr, Fe, Hf, Mn, Mo, Nb, Ni, Pd, Re, Ru, Si, Ta, Ti, V, W, Y, Zr)1	
C15_LAVES	Cu2Mg	cF24	Fd-3m	(Al, Co, Cr, Fe, Hf, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zr)2(Al, Co, Cr, Fe, Hf, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zr)1	
C16_THETA	Al2Cu	tI12	I4/mcm	(Al, Hf, Mo, Nb, Ta, Ti, W, Zr)2(Al, Co, Cr, Fe, Ni, Si)1	Hf2Al, Hf2Si, Zr2Si Zr2Co,Ta2Co, Hf2Ni, Ta2Ni, Zr2Ni
C36_LAVES	MgNi2	hP246	P6_3/mmc	(Al, Co, Cr, Fe, Hf, Mo, Nb, Ni, Ta, Ti, V, W, Zr)2(Al, Co, Cr, Fe, Hf, Mo, Nb, Ni, Ta, Ti, V, W, Zr)1	
CBCC_A12	alpha-Mn	cI58	I-43m	(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zr)1(B, C, H, Va)1	
CEMENTITE	Fe3C	oP16	Pnma	(Co, Cr, Fe, Mn, Mo, Ni, V, W)3(C, N)1	D011
CFC2_FENBZR	MgCu2	cF24	Fd-3m	(Fe, Nb, Zr)2(Nb, Zr)1(Nb, Zr)3	
CHI_A12	alpha-Mn	cI58	I-43m	(Cr, Fe, Ni, Re)24(Al, Cr, Hf, Mo, Nb, Ta, Ti, W, Zr)10(Cr, Fe, Mo, Nb, Ni, Re, Ta, W)24	
CO11ZR2	Co11Hf2	oP*	Pban	(Co)11(Zr)2	
CO17Y2	Ni17Th2	hP38	P6_3/mmc	(Co2, Y)1(Co2, Y)2(Co)15	
CO1SN1TI1	Unknown Structure			(Co, Ni)1(Sn)1(Ti)1	
CO1SN2	Al2Cu	tI12	I4/mcm	(Co)0.333(Sn)0.667	
CO1SN3	PdSn3	oS32	Cmce	(Co)0.25(Sn)0.75	
CO2SI_C23	Co2Si	oP12	Pnma	(Al, Co, Cr, Fe, Ni, Pd, Ti)2(Al, Pd, Si)1	also Ni2Si(delta)
CO3SI	CdMg3	hP8	P6_3/mmc	(Co)3(Si)1	
CO3SN2	Co1.75Ge	hP6	P6_3/mmc	(Co)1(Sn)1(Co, Va)0.5(Co, Va)0.5	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
CO3VV	Al3Pu	hP24	P6_3/mmc	(Co, V)3(Co, V)1	
CO3Y1	Ni3Pu	hR12	R-3m	(Co)3(Y)1	
CO3Y2	Unknown Structure	cP*		(Co)3(Y)2	
CO3Y4	Co3Ho4	hP22	P6_3/m	(Co)3(Y)4	
CO5Y8	Co5Y8	mP52	P2_1/c	(Co)5(Y)8	
CO5Y_D2D	CaCu5	hP6	P6/mmm	(Co2, Y)1(Co)4(Co, Va)1	
CO7HF	(Co11Hf2)	oP*	Pban	(Co)7(Hf)1	
CO7M2	(Co7Nb2)	mS18	C2/m	(Co)7(Nb, Ta, Ti)2	
CO7MO6	W6Fe7	hR39	R-3m	(Co, Mo)7(Co, Mo, Ti)6	mu phase
CO7Y6	Unknown Structure			(Co)7(Y)6	
COB	FeB	oP8	Pnma	(Co, Re)1(B)1	
CORUNDUM	Al2O3	hR30	R-3c	(Al+3, Cr+2, Cr+3, Fe+2, Fe+3, Mn+3, Ti+3, V+3, V+4, Va)2(Cr+3, Fe+3, Ni+2, Va)1(O-2)3	corundum [Al2O3],eskolaite [Cr2O3], hematite [Fe2O3], Ti2O3, V2O3
COSN	CoSn	hP6	P6/mmm	(Co)0.5(Sn)0.5	
COY_BF	CrB	oC8	Cmcm	(Co)1(Y)1	
CR2B_ORTH	Mg2Cu	oF48	Fddd	(Cr, Fe, Mo, Re)2(B)1	
CR2PD3_L12	Cu3Au	cP4	Pm-3m	(Cr)0.4(Pd)0.6	
CR3MN5	alpha-Mn	cI58	I-43m	(Cr)3(Mn)5	
CR3NI5SI2	AlAu4	cP20	P2_13	(Cr)3(Ni)5(Si)2(C, Va)1	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
CR3SI_A15	Cr3Si	cP8	Pm-3n	(Al, Cr, Fe, Mo, Nb, Ni, Pd, Pt, Re, Si, Sn, Ta, Ti, V, Zr)3(Al, Co, Cr, Mo, Nb, Ni, Pd, Pt, Ru, Si, Sn, Ta, Ti, V, Zr)1(C, Va)3	Cr3Ru, Mo3Si, V3Si, Mo3Al,Nb3Al, V3Co, V3Ni, V3Sn, Nb3Sn
CR5B3	Cr5B3	tI32	I4/mcm	(Cr, Mo)0.625(B)0.375	
CR8FE16TI5	Ti5Re24	cI58	I-43m	(Cr, Fe)24(Ti)5	
CRB4	CrB4	oI10	Immm	(Cr)0.2(B)0.8	
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	cF24	Fd-3m	(Sio2)1	
CRNI2_OP6	MoPt2	oI6	Immm	(Cr, Mo, W)1(Mo, Ni, W)2	
CRPD_L10	In	tI2	I4/mmm	(Cr)0.5(Pd)0.5	
CRSI2_C40	CrSi2	hP9	P6_222	(Cr, Hf, Mo, Nb, Si, Ta, Ti, V, W)1(Al, Cr, Si)2	also NbSi2, TaSi2, VSi2
CU10SN3	Cu10Sn3	hP26	P6_3	(Cu, Sn)1	
CU15SI4_EPSILON	Cu15Si4 (D86)	cI76	I-43d	(Cu)0.789474(Si)0.210526	
CU2TI	Au2V	oS12	Cmcm	(Cu, Ni)2(Ti)1	
CU33SI7_DELTA	Unknown Structure	tP*		(Cu)0.825(Si)0.175	
CU3SN	Cu3Sn	oS80	Cmcm	(Cu, Sn)3(Cu, Sn)1	
CU3TI2	Cu3Ti2	tP10	P4/nmm	(Cu, Fe, Ni)3(Ti)2	
CU41SN11	Cu41Sn11	cF416	F-43m	(Cu, Sn)41(Cu, Sn)11	
CU4TI1	Au4Zr	oP20	Pnma	(Cu, Ni, Ti)4(Cu, Ni, Ti)1	
CU4TI3	Cu4Ti3	tI14	I4/mmm	(Cu, Ni)4(Ti)3	
CU56SI11_ GAMMA	Mg3Ru2	cP20	P4_132	(Cu)0.835821(Si)0.164179	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
CU6SN5_HT	Co1.75Ge	hP6	P6_3/mmc	(Cu)1(Cu, Sn)1(Sn)1	
CU6SN5_LT	Cu6Sn5	mS44	C2/c	(Cu)1(Cu, Sn)1(Sn)1	
CUB_A13	beta-Mn	cP20	P4_132	(Ag, Al, Co, Cr, Fe, Hf, Mn, Mo, Nb, Ni, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zr)1(B, C, H, Va)1	
CUO	CuO	mS8	C12/c1	(Cu+2)1(O-2)1	
CUPRITE_C3	Cu2O	cP6	Pn-3m	(Cu+1)2(O-2)1	
CUSI_ETA	Cu3Si-h2	hR*	P-31m	(Cu)0.76(Si)0.24	Structure uncertain
CUSN_GAMMA	BiF3	cF16	Fm-3m	(Cu, Sn)1	
CUTI3	CuTi3 (L60)	tP4	P4/mmm	(Cu, Ti)1(Ti)3	
CUTI_B11	CuTi	tP4	P4/nmm	(Cu, Ni, Ti)1(Cu, Ni, Ti)1	
CUZR2_C11B	CuZr2	tI6	I4/mmm	(Cu, Fe, Ni, Si)1(Nb, Ti)2(O, Va)0.5	CuTi2
D0I_MO2B5	Mo2B5	hR21	R-3m	(Mo, Ti)0.32(B)0.68	
D5A_M3B2	SI2U3	tP10	P4/mbm	(Fe, Hf, Mo, Nb, Ta, Ti, V)3(B)2	TA3B2, NB3B2, V3B2
DELTA_TIH2	CaF2	cF12	Fm-3m	(Hf, Nb, Ti, V, Y, Zr)1(H, Va)2	delta dihydrides
DIAMOND_A4	C	cF8	Fd-3m	(Al, B, C, H, O, Si, Sn)1	
DIS_BETA		tI56	I4_1/amd	(H, Va)0.5(V)0.5	V-H binary
DIS_MU	Fe7W6 (D85) mu-phase	hR13	R-3m	(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ta, W)1	Part of thedescription of MU_PHASE
DIS_SIG	sigma-CrFe	tP30	P4_2/mnm	(Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ru,Ta,V,W)1	
FCC_A1	Cu	cF4	Fm-3m	(Ag, Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Pd, Pt, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zr)1(B, C, H, N, O, Va)1	Metallic FCC_A1 solution,e.g. (Al), (Cu)

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
FCC_B1	NaCl	cF8	Fm-3m	(Al, Cr, Hf, Mo, Nb, Ta, Ti, V, Va, W, Zr)1(C, N, O, Va)1	TiC, TiN, TiO
FE1SN2	Al2Cu	tI12	I4/mcm	(Fe)1(Sn)2	
FE2SI	AlNi2	hP6	P-3m1	(Fe)0.666667(Si)0.333333	
FE3SN2	Fe3Sn2	hR30	R-3m	(Fe)3(Sn)2	
FE4N_LP1	Fe4N	cP5	Pm-3m	(Co, Cr, Fe, Mn, Ni)4(C, N)1	
FE5SN3	Co1.75Ge	hP6	P6_3/mmc	(Fe)5(Sn)3	
FE7MO6	W6Fe7	hR39	R-3m	(Fe)7(Mo, Ti)2(Fe, Mo, Ti)4	mu phase
FECN_CHI	Mn5C2	mS28	C2/c	(Fe)2.2(C, N)1	
FESI2_H	FeSi2-h	oC48	Cmca	(Fe)0.3(Si)0.7	
FESI2_L	FeSi2-l	tP3	P4/mmm	(Fe)0.333333(Si)0.666667	
FESI_B20	FeSi	cP8	P2_13	(Co, Cr, Fe, Mn, Ni, Re)1(Al, Si)1	also CoSi, CrSi, ReSi
FESN	CoSn	hP6	P6/mmm	(Fe)1(Sn)1	
FLUORITE_C1	CaF2	cF12	Fm-3m	(Al+3, Cr+3, Fe+2, Hf+4, Mn+2, Mn+3, Ni+2, Si+4, Ti+4, Y+3, Zr, Zr+4)2(O-2, Va)4	
GAMMA_D83	Al4Cu9	cP52	P-43m	(Al)4(Al, Cu)1(Cu)8	
GAMMA_H	Cu5Zn8	cI52	I-43m	(Al)4(Al, Cu)1(Cu)8	
GAS				(Al, Al1B1O2, Al1C1, Al1C2, Al1H1, Al1H2, Al1H3, Al1N1, Al1O1, Al1O2, Al2, Al2C2, Al2O1, Al2O2, Al2O3, B, B1C1, B1C2, B1N1, B1O1, B1O2, B2, B2C1, B2O1, B2O2, B2O3, C, C1N1, C1N1O1, C1N1O1_Nco, C1N2_Cnn, C1N2_Ncn, C1O1, C1O2, C1Si1, C1Si2, C1Si3, C1Si4, C2, C2N1_Ccn, C2N1_Cnc, C2N2, C2O1, C2Si1, C2Si2, C2Si3, C3, C3N1, C3O2, C4, C4N1, C4N2, C4Ni1O4, C5, C5Fe1O5, C5N1, C60, C6Mo1O6, C6N1, C6N2, C9N1, Co, Co1O1, Co2, Cr, Cr1N1, Cr1O1, Cr1O2, Cr1O3, Cr2, Cr2O1, Cr2O2, Cr2O3, Fe, Fe1O1, Fe1O2, Fe2, H, H2, H2O1, H2O2, Hf, Hf1O1, Hf1O2, Mn, Mn1O1, Mn1O2, Mo, Mo1N1, Mo1O1, Mo1O2, Mo1O3, 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, Ni, Ni1O1, Ni2, O, O10V4, O12W4, O15W5, O1Re1, O1Ru1, O1Si1, O1Sn1, O1Ta1, O1Ti1, O1V1, O1W1, O1Y1, O1Y2,	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
				O1Zr1, O2, O2Re1, O2Ru1, O2Si1, O2Si2, O2Sn1, O2Sn2, O2Ta1, O2Ti1, O2V1, O2W1, O2Y1, O2Y2, O2Zr1, O3, O3Re1, O3Ru1, O3W1, O4Ru1, O4Sn4, O6Re2, O6Sn6, O6W2, O7Re2, O8W3, O9W3, Re, Ru, Si, Si2, Si3, Sn, Ta, Ti, Ti2, V, W, Y, Zr, Zr2)1	
GPHASE	Mn23Th6	cF116	Fm-3m	(Al, Co)1(Al, Ti)16(Co)7(Ti)6	
GRAPHITE	C	hP4	P6_3/mmc	(B, C)1	
G_PHASE	Mn23Th6	cF116	Fm-3m	(Al, Co, Cu, Fe, Mn, Ni, Pd, Ti)16(Hf, Nb, Ti, Y, Zr)6(Co, Cu, Fe, Mn, Ni, Pd, Si)7	
HALITE	NaCl	cF8	Fm-3m	(Al+3, Co+2, Co+3, Cr+3, Fe+2, Fe+3, Mn+2, Mn+3, Ni+2, Ni+3, V, V+2, V+3, Va, Y+3, Zr+4)1(O-2, Va)1	Wustite [FeO], Bunsenite [NiO],MnO, CoO, high temperature TiO, VO
HCP_A3	Mg	hP2	P6_3/mmc	(Ag, Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Pd, Pt, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zr)1(B, C, H, N, O, Va)0.5	Metallic HCP_A3 solution,alpha_Ti
HF3NI7	Hf3Ni7	aP20	P-1	(Hf)0.3(Ni)0.7	
HF8NI21	Hf8Ni21	aP29	P-1	(Hf, Zr)8(Ni)21	also ZR8NI21
HFMN	NiTi2	cF96	Fd-3m	(Hf)0.5(Mn)0.5	
HFNI3_ALPHA	Ta(Rh0.33Pd0.67)3	hP40	P6_3/mmc	(Hf)0.25(Ni)0.75	
HFNI3_BETA	BaPb3	hR36	R-3m	(Hf)0.25(Ni)0.75	
HFNI_ALPHA	Til	oS8	Cmcm	(Hf)0.5(Ni)0.5	
HFRE	Zr21Re25	hR276	R-3c	(Hf)1(Re)1	
HIGH_SIGMA	CrFe	tP30	P4_2/mnm	(Mn)8(Cr)4(Cr, Mn)18	
H_L21	AlCu2Mn	cF16	Fm-3m	(Al, Ni, Sn, Ti)0.5(Al, Hf, Nb, Ni, Ta, Ti, Zr)0.5(Co, Cu, Ni, Ru, Va)1	
ION_LIQ	Liquid			(Al+3, Co+2, Cr+2, Fe+2, Hf+4, Mn+2, Mo+4, Nb+2, Ni+2, Re+4, Ru+4, Si+4, Ta+5, Ti+2, V+2, W+6, Y+3, Zr+4)64(Aln, Alo2-1, B, Bo3/2, C, Coo3/2, Cro3/2, Feo3/2, Mno3/2, Moo3, N, Nbo2, Nbo5/2, O-2, Reo7/2, Sio2, Sio4-4, Tio2, Va, Vo2, Vo5/2)57	IONIC_LIQ mixture, modeled by theionic two-sublattice model

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
KYANITE	Kyanite (Al2SiO5, S01)	aP32	P-1	(Al+3)1(Al+3)1(Si+4)1(O-2)5	
L10_FCC	In	tI2	I4/mmm	(Mn, Ni)0.5(Mn, Ni)0.5	
L12_FCC	Cu3Au	cP4	Pm-3m	(Ag, Al, Co, Cr, Cu, Fe, Mn, Ni, Pd, Pt, Ti, Zr)0.75(Ag, Al, Co, Cr, Cu, Fe, Mn, Ni, Pd, Pt, Si, Ta, Ti, Zr)0.25	
LIQUID				(Ag, Al, Al1N1, Al2/3O1, Al2O4Ti, Al4/3O2, B, Bo3/2, C, Co, Coo, Coo3/2, Cr, Cro, Cro3/2, Cu, Cu2O, Cuo, Fe, Feo, Feo3/2, H, H2O1, H2O2, Hf, Hf1/2O1, Mn, Mno, Mno3/2, Mo, Mo1/2O1, N, Nb, Nb1O1, Nbo2, Nbo5/2, Ni, Nio, O, O1Ti1, O2Ti1, Pd, Pt, Re, Re1/2O1, Reo7/2, Ru, Ru1/2O1, Si, Si1/2O1, Si2O4, Sio2, Sn, Sn1/2O1, Ta, Ta2/5O1, Ti, Tio3/2, V, V1O1, Vo2, Vo3/2, Vo5/2, W, Y, Y2/3O1, Zr, Zr1/2O1)1	
M12C	W6Fe6C	cF104	Fd-3m	(Co, Ni)6(Mo, W)6(C)1	
M23C6	Cr23C6	cF116	Fm-3m	(Co, Cr, Fe, Mn, Ni, Re, V)20(Co, Cr, Fe, Mn, Mo, Ni, Re, V, W)3(C)6	
M2B_TETR	Al2Cu	tI12	I4/mcm	(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ta, Ti, W)2(B)1	Co2B, Fe2B, Mn2B, Mo2B, Ni2B
M2O3C	(Mn0.5Fe0.5)2O3	cI80	Ia-3	(Al+3, Cr+3, Fe+3, Mn+3, Ni+2, Y, Y+3, Zr+4)2(O-2, Va)3(O-2, Va)1	
M2O3H	La2O3	hP5	P-3m1	(Mn+3, Y, Y+3, Zr+4)2(O-2, Va)3(O-2, Va)1	hexagonal Y2O3
M3B2	Mo2FeB2	tP10	P4/mbm	(Cr, Fe, Mo, Ni, W)0.4(Cr, Fe, Ni)0.2(B)0.4	
M3C2	Cr3C2-b	oP20	Pnma	(Cr, Mo, V, W)3(C)2	
M3SI1	Ti3P	tP32	P4_2/n	(Hf, Nb, Ta, Ti, Zr)3(Si)1	Ti3Si, Ta3Si, Zr3Si
M3SI2_D5A	Si2U3	tP10	P4/mbm	(Hf, Nb, Zr)3(Si)2	Hf3Si2, Zr3Si2
M5C2	Mn5C2	mC28	C2/c	(Fe, Mn)5(C)2	
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	hP16	P6_3/mcm	(Cr, Fe, Hf, Mn, Mo, Nb, Ni, Si, Ti, W, Y, Zr)2(Al, Si, Sn)3(Cr, Fe, Hf, Mn, Mo, Nb, Ni, Ti, Y, Zr)3(C, Co, Sn, Va)1	Ti5Si3, Fe5Si3, Zr5Si3, Y5Si3, Hf5Si3, Mn5Si3, Zr5Sn3, Zr5Sn4
M6C	W3Fe3C	cF112	Fd-3m	(Co, Fe, Ni)2(Mo, Nb, Ta, W)2(Co, Cr, Fe, Mo, Nb, Ni, Ta, V, W)2(C)1	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
M7C3	Cr7C3	oP40	Pnma	(Co, Cr, Fe, Mn, Mo, Ni, Re, V, W)7(C)3	
MB_B33	CrB	oC8	Cmcm	(Cr, Fe, Hf, Mo, Nb, Ni, Ta, Ti, V, W)1(B)1	CrB, NbB, NiB, TaB, VB
MC_ETA	MoC	hP12	P63/mmc	(Mo, V, W)1(C, Va)1	
MC_SHP	WC	hP2	P-6m2	(Mo, W)1(C, N)1	
MN11SI19	Mn11Si19	tP120	P-4n2	(Mn)11(Al, Si)19	
MN12Y	ThMn12	hI26	I4/mmm	(Mn)12(Y)1	
MN1O2	TiO2	tP6	P4_2/mnm	(Mn)1(O)2	
MN2B_D1F	Mg2Cu	oF48	Fddd	(Mn)0.6707(B)0.3293	
MN2SN	Co1.75Ge	hP6	P6_3/mmc	(Mn)0.643(Sn)0.357	
MN2YO5	DyMn2O5	oP32	Pbam	(Y+3)1(Mn+3)1(Mn+4)1(O-2)5	
MN3SI	BiF3	cF16	Fm-3m	(Fe, Mn)3(Al, Si)1	
MN3SN2	Ni3Sn	oP20	Pnma	(Mn)3(Sn)2	
MN3TI	Unknown Structure			(Mn)3(Ti)1	
MN4TI	Cr0.16Mo0.38Co0.46	hR159	R-3	(Mn)0.815(Ti)0.185	
MN6N4	Mn3N2	tI10	I4/mmm	(Mn)6(N)4	
MN6N5	CoO	tI4	I4/mmm	(Mn)6(N)5	
MN6SI	R-(Co,Cr,Mo)	hR53	R-3	(Al, Mn)17(Si)3	
MN9SI2	Mn9Si2	oI186	Immm	(Mn)33(Si)7	
MNB4	MnB4	mS10	C2/m	(Mn)0.2(B)0.8	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
MNNI2	Unknown Structure			(Mn, Ni)1(Ni)2	
MNSN2	Al2Cu	tI12	I4/mcm	(Sn)2(Mn)1	
MNTA	Unknown Structure			(Mn)1(Ta)1	
MNTI_HT	Unknown Structure	t**		(Mn)0.515(Ti)0.485	
MNTI_LT	Zr21Re25	hR276	R-3c	(Mn)1(Ti)1	
MNYO3_HEX	LuMnO3	hP30	P6_3cm	(Y+3)1(Mn+3)1(O-2)3	
MO4O11	Mo4O11	oP60	Pna2_1	(Mo)4(O)11	
MO8O23	Mo8O23	mP62	P2/c	(Mo)8(O)23	
MO9O26	Mo9O26	mP70	P2/c	(Mo)1(O)2.8890000000000002	
MOB4	MoB4	hP16	P6_3/mmc	(Mo, Ti)0.2(B)0.8	
MOCOB	TiNiSi	oP12	Pnma	(Mo, W)1(Co)1(B)1	
MONI4_BETA	MoNi4	tI10	I4/m	(Mo, W)1(Ni)4	
MONI_DELTA	MoNi	oP56	P2_12_12_1	(Co, Cr, Fe, Ni, Re)24(Co, Cr, Fe, Mo, Ni, Re, W)20(Mo, W)12	
MOO2	VO2	mP12	P2_1/c	(Mo)1(O)2	
MOO3	WO3	mP32	P2_1/c	(Mo)1(O)3	
MOSI2_C11B	MoSi2	tI6	I4/mmm	(Co, Fe, Mo, Ni, W)1(Al, Hf, Si, Ti, Zr)2	
MSI2_C1	CaF2	cF12	Fm-3m	(Co, Ni)1(Al, Si)2	
MSI_B27	FeB (B27)	oP8	Pnma	(Hf, Nb, Ti, Y, Zr)1(Al, Si)1	TiSi, HfSi, YSi,ZrSi (alpha), SiZr

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
MULLITE	Al3SiO6.5	oP24	Pbam	(Al+3)1(Al+3)1(Al+3, Si+4)1(O-2, Va)5	
MU_PHASE	Fe7W6 (D85) mu-phase	hR13	R-3m	(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ta, W)1(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ta, W)2(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ta, W)6(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ta, W)4	DIS_MUcontribution is introduced in the description of this phase
MZR3_E1A	Re3B	oS16	Cmcm	(Co, Fe, Ni)1(Y, Zr)3	
NB1O2	NbO2	tI96	I4_1/a	(Nb)1(O)2	
NB2B3	V2B3	oC20	Cmcm	(Nb)2(B)3	
NB2O5	Nb2O5	mP99	P2/m	(Nb)2(O)5	
NB3RU5	Rh5Ge3	oP16	Pbam	(Nb, Ru)0.375(Ru)0.625	
NBH_BETA	TaH0.5	oS8	C222	(Nb)1(H, Va)1.1	
NBO	NbO	cP6	Pm-3m	(Nb)1(O)1	
NBSN2	Mg2Cu	oF48	Fddd	(Nb, Sn, V)1(Nb, Sn)2	
NI10ZR7	Ni10Zr7	oS68	Cmce	(Ni)23(Hf, Zr)17	
NI11ZR9	Pt11Zr9	tI40	I4/m	(Ni, Pd)11(Hf, Zr)9	
NI17Y2	Fe17Lu2	hP80	P6_3/mmc	(Fe, Ni)1(Y)0.1176	also Fe17Y2
NI2SI_TETA	Ga3Ge6Ni13	hP66	P3_121	(Ni)1(Ni, Va)1(Al, Si)1	
NI2TA	MoSi2	tI6	I4/mmm	(Co, Ni)2(Ta)1	
NI2V	MoPt2	oI6	Immm	(Mo, Ni, Pd)2(Mo, Nb, Ta, V)1	
NI2Y1	Ni2Tm	cF192	F-43m	(Ni)2(Y)1	
NI2Y3	Ni2Y3	tP80	P4_12_12	(Ni)2(Y)3	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
NI31SI12	Ni31S12	hP42	P321	(Co, Cr, Fe, Ni)5(Si)2	
NI3B_D011	Fe3C	oP16	Pnma	(Co, Cr, Fe, Mo, Ni)3(B)1	
NI3SI2	Ni3Si2	hR15	R32	(Ni)3(Si)2	
NI3SI_MONOCL	Ge9Pt25	hP34	P-3	(Ni)3(Si)1	
NI3SI_ORTHO	Fe3C	oP16	Pnma	(Ni)3(Si)1	
NI3SN2_HT	Co1.75Ge	hP6	P6_3/mmc	(Ni)0.33333(Ni, Sn)0.33334(Sn)0.33333	
NI3SN2_LT	Ni3Sn2	oP20	Pnma	(Sn)0.2(Ni, Sn)0.4(Ni)0.4	
NI3SN4	Ni3Sn4	mS14	C2/m	(Ni)0.25(Ni, Sn)0.25(Sn)0.5	
NI3SN_D019	Ni3Sn	hP8	P6_3/mmc	(Sn)1(Mn, Ni)3	
NI3SN_HT	BiF3	cF16	Fm-3m	(Ni, Sn)0.25(Ni, Sn)0.25(Ni)0.5	
NI3TA_D0A	Ni3Ti	hP16	P6_3/mmc	(Al, Co, Cr, Fe, Nb, Ni)3(Al, Fe, Mo, Nb, Ni, Ta, Ti, V, W)1	also Ni3Mo, Ni3Nb
NI3TI_D024	Ni3Ti	hP16	P6_3/mmc	(Al, Co, Cr, Cu, Fe, Hf, Ni, Pd, Ta, Ti, W, Zr)0.75(Al, Cr, Cu, Hf, Mo, Nb, Ni, Pd, Si, Ta, Ti, W, Zr)0.25	
NI3Y	Ni3Pu	hR12	R-3m	(Fe, Ni)3(Y)1	
NI4B3	m-Ni4B3	mS28	C2/c	(Ni)0.57142857(B)0.42857143	
NI4Y	Unknown Structure	hR*		(Ni)4(Y)1	
NI5ZR	AuBe5	cF24	F-43m	(Ni)5(Hf, Y, Zr)1	also Ni5Y, Ni5Hf
NI7ZR2	Ni7Zr2	mS36	C2/m	(Al, Co, Cr, Ni)7(Hf, Y, Zr)2	
NI8TA	Pt8Ti	tI18	I4/mmm	(Ni)8(Nb, Ta)1	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
NISI_B31	MnP	oP8	Pnma	(Ni)1(Si)1	
NITI2	NiTi2	cF96	Fd-3m	(Co, Cr, Cu, Fe, Mo, Ni, Pd, Re, Ti)1(Al, Cr, Hf, Ni, Ta, Ti, Zr)2	
NIWO4	AgAuTe4	mP12	P2/c	(Co+2, Fe+2, Mn+2, Ni+2)1(W+6)1(O-2)4	
NIZR	CrB	oS8	Cmcm	(Ni)1(Ti, Y, Zr)1	
O1_DIS	NaHg	oC16	Cmcm	(Al, Nb, Ti)0.75(Al, Nb, Ti)0.25	The disordered O phase
OLIVINE	Mg2SiO4	oP28	Pnma	(Co+2, Fe+2, Mn+2, Ni+2)1(Co+2, Fe+2, Mn+2, Ni+2)1(Si+4)1(O-2)4	fayalite [Fe2SiO4],tephroite [Mn2SiO4], Ni2SiO4, Co2SiO4
OMEGA		hP3	P6/mmm	(Al, B, C, Co, Cr, Fe, Hf, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zr)1	s metastable structure of Ti
ORD_SIG	sigma-CrFe	tP30	P4_2/mnm	(Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ru, Ta, V, W)10(Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ru, Ta, V, W)4 (Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ru, Ta, V, W)16	
O_PHASE	NaHg	oC16	Cmcm	(Nb, Ta, Ti)0.5(Al, Nb, Ta, Ti)0.25(Nb, Ta, Ti)0.25	The O phase
PD2TI	MoSi2	tI6	I4/mmm	(Pd)2(Ti)1	
PD3TI2	Pd3Ti2	oS20	Cmcm	(Pd)3(Ti)2	
PD4ZR3	Pu3Pd4	hR42	R-3	(Pd)4(Zr)3	
PD5TI3	Pd5Ti3	tP8	P4/mmm	(Pd)5(Ti)3	
PDZRM	MoSi2	tI6	I4/mmm	(Pd)1(Zr)1(Pd, Zr)1	
PDZR_ALPHA	Tll	oS8	Cmcm	(Pd)1(Zr)1	
PDZR_BETA	Tll	oS8	Cmcm	(Pd)1(Zr)1	
PSEUDO_ BROOKITE	CaTi2O4	oS28	Cmcm	(Al+3, Ti+3, Ti+4)1(Al+3, Ti+3, Ti+4)2(O-2)5	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
PT3TI4	Unknown Structure			(Pt)3(Ti)4	
PT8TI	Pt8Ti	tI18	I4/mmm	(Pt)8(Ti)1	
P_PHASE	Cr9Mo21Ni20	oP56	Pnma	(Cr, Fe, Ni, Re)24(Cr, Fe, Mo, Ni, Re)20(Mo)12	
QUARTZ	alpha-Quartz	hP9	P3_121	(Sio2)1	
RE2O7	Re2O7	oP72	P2_12_12_1	(O7Re2)1	
RE2SI	Re2Si	mP24	P12_1/c1	(Re)2(Si)1	
RE3B	Re3B	oC16	Cmcm	(Cr, Mo, Re, Ta, W)3(B)1	
RE7B3	Th7Fe3	hP20	P6_3mc	(Co, Cr, Mo, Nb, Re, Ru, Ta, W)7(B)3(B, Va)3	
REB2	ReB2	hP6	P6_3/mmc	(Re)1(B)2(B, Va)2	
REO2	ReO2	mP14	P2_1/c	(O2Re1)1	
REO3	alpha-ReO3	cP4	Pm-3m	(O3Re1)1	
RESI2_C11B	Re4Si7	mS44	C1m1	(Re)0.357(Si)0.643	
REZR2	Re25Zr21	hR276	R-3c	(Ni, Re)1(Zr)2	
RHODONITE	MgSiO3	mP40	P2_1/c	(Mn+2)1(Si+4)1(O-2)3	This is MnO.SiO2
RU1B2	RuB2	oP6	Pmmm	(Ru)1(B)2	
RU25Y44	Ru25Y44	oP276	Pnna	(Ru)0.362(Y)0.638	
RU2B3	Ru2B3	hP10	P6_3/mmc	(Ru)2(B)3	
RU2SI3	Ge3Ru2	oP40	Pbcn	(Ru)2(Si)3	
RU2SI_C37	Co2Si	oP12	Pnma	(Ru)2(Si)1	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
RU2SN3	Ru2Sn3	tP20	P-4c2	(Ru)0.4(Sn)0.6	
RU2Y3	Ru2Er3	hP2	P6_3/m	(Ru)0.4(Y)0.6	
RU2Y5	C2Mn5	mS28	C2/c	(Ru)0.286(Y)0.714	
RU3SN7	Ru3Sn7	cI40	Im-3m	(Ru)0.3(Sn)0.7	
RU4SI3	Ru4Si3	oP28	Pnma	(Ru)4(Si)3	
RUB	Unknown Structure			(Ru)1(B)1	
RUSI	FeSi	cP8	P2_13	(Ru)1(Si)1	
RUTILE_TIO2	Rutile (TiO2, C4)	tP6	P4_2/mnm	(Al+3, Ru+4, Sn+4, Ti+4, V+4, Zr+4)1(O-2, Va-2)2	TiO2, alsothe high-temperature VO2, RUO2
RUY3	Fe3C	oP16	Pnma	(Ru)0.25(Y)0.75	
R_PHASE	Co5Cr2Mo3	hR53	R-3h	(Co, Cr, Fe, Ni, Re)27(Mo, W)14(Co, Cr, Fe, Mo, Ni, Re, W)12	
SI3N4	alpha-Si3N4	hP28	P31c	(Si)3(N)4	
SI5V6	Si5V6	oI44	Ibam	(Si)5(V)6	
SIC	ZnS	cF8	Fd-3m	(Si)1(B, C)1	
SIGMA	sigma-CrFe (D8b)	tP30	P4_2/mnm	(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W)10(Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W)4(Al, Co, Cr, Fe, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W)16	
SN3O4	Sn3O4	Unknown Structure		(Sn)3(O)4	
SNO	PbO	tP4	P4/nmm	(Sn)1(O)1	
SPINEL	Al2MgO4	cF56	Fd-3m	(Al+3, Co+2, Co+3, Cr+2, Cr+3, Fe+2, Fe+3, Mn+2, Ni+2)1(Al+3, Co+2, Co+3, Cr+3, Fe+2, Fe+3, Mn+2, Mn+3, Mn+4, Ni+2, Va)2(Cr+2, Fe+2, Mn+2, Va)2(O-2)4	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
T1CUNITI	MoSi2	tI6	I4/mmm	(Cu, Ni)2(Ti)1	
T2CUNITI	Cu3Ti2	tP10	P4/nmm	(Cu)0.175(Ni)2.825(Ti)2	
T4CUFETI	Unknown Structure			(Cu, Fe)0.63(Ti)0.37	the Cu-Fe-Ti ternaryphase, Tau4
T4CUNITI	BaPb3	hR12	R-3m	(Cu, Ti)0.075(Cu, Ni)0.675(Ti)0.25	
T5CUFETI	Unknown Structure			(Cu, Fe)0.55(Ti)0.45	the Cu-Fe-Ti ternaryphase, Tau5
T6CUNITI	Al3Ti (Ni3V)	tI8	I4/mmm	(Cu, Ti)0.25(Cu, Ni)0.5(Ti)0.25	
TA1AL2	Ta39Al69	cF444	F-43m	(Al, Ta, Ti)0.6389(Al, Ta, Ti)0.3611	
TA2H_EPSLON	Unknown Structure			(Ta)2(H, Va)1	
TA2O5_HT	Ta2O5	tI44	I4_1/amd	(Ta)2(O)5	
TA2O5_LT	Ta2O5	oP14	Pccm	(Ta)2(O)5	
TA5SI3_D8L	Cr5B3	tI32	I4/mcm	(Hf, Nb, Ta, Ti)5(Al, Si)3	
TAAL	Ta22Al21	mP86	P12_1/c1	(Al, Ta, Ti)0.8837(Al, Ta, Ti)1.1163	
TAN_EPS	TaN	hP6	P-62m	(Ta)1(N)1	
TAU	CR23C6	cF116	Fm-3m	(Co, Hf, Ni, Re)20(B)6(B, Va)6(Al, Cr, Hf, Mo, Re, Ta, Ti, V, W, Zr)3	
TI10O19	Unknown Structure			(Ti)10(O)19	
TI20O39		aP118	P-1	(Ti)20(O)39	
TI2ALC	Cr2AlC	hP8	P6_3/mmc	(Ti)2(Al)1(C, Va)1	H, Ti2AlC1-x
TI2NIH	Ti2NiH	cF128	Fd-3m	(Ti)2(Ni)1(H)1	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
TI2N_C4	Rutile (TiO2, C4)	tP6	P4_2/mnm	(Ti)2(N)1	
TI2SN3	Ti2Sn3	oS40	Cmca	(Cr, Ti)2(Sn)3	
TI2X_OMEGA	AlB2	hP3	P6/mmm	(Ti)2(Al, B, C, Co, Cr, Fe, Hf, Mn, Mo, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zr)1	Ordered Omega phase,B82 or C32 type
TI3AL1C2	MoC	hP12	P6_3/mmc	(Ti)3(Al, Si)1(C, Va)2	N, Ti3AlC2-x
TI3AL1O1	Unknown Structure			(Ti)3(Al)0.9(O)1.1	
TI3ALC	CaTiO3	cP5	Pm-3m	(Ti)3(Al)1(C, Va)1	P, Ti3AlC1-x
TI3B4	Ta3B4	oI14	Immm	(B)4(Al, Cr, Hf, Mn, Nb, Ta, Ti, V)3	Cr3B4, Mn3B4, Nb3B4,Ti3B4, V3B4
TI3CO5B2	Ti3Co5B2	tP20	P4/mbm	(Ti)3(Co)5(B)2	
TI3CU3O	W3Fe3C	cF112	Fd-3m	(Ti)3(Cu)3(O)1	
TI3N2	TiS	hR18	R-3m	(Ti)0.71(N)0.29	
TI3O2	Unknown Structure			(Ti)3(O)2	
TI3O5	Ti3O5-b	mS32	C12/m1	(Ti, V)3(O)5	
TI4CU2O	W4Co2C	cF112	Fd-3m	(Ti)4(Cu)2(O)1	
TI4N3	Sc0.67Te	hR24	R-3m	(Ti)0.685(N)0.315	
TI4O7	Ti4O7-a	aP22	P-1	(Ti, V)4(O)7	
TI5AL3O2			P4_232	(Ti)5(Al)3(O)2	Z- or X-phase
TI5O9	Ti5O9	aP28	P-1	(Ti, V)5(O)9	
TI6O11	Ti6O11	aP34	P-1	(Ti, V)6(O)11	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
TI6SI2B	K2UF6	hP9	P-62m	(Ti)6(Si)2(B)1	
TI6SN5	Ti6Sn5	oI44	Immm	(Cr, Mo, Nb, Ti, Zr)6(Al, Sn)5	
TI7O13	Ti7O13	aP40	P-1	(Ti, V)7(O)13	
TI8O15	Ti8O15	aP46	P-1	(Ti, V)8(O)15	
TI9O17	Ti9O17	aP52	P-1	(Ti)9(O)17	
TIB2_C32	AlB2	hP3	P6/mmm	(B)2(Al, Cr, Hf, Mn, Mo, Nb, Ta, Ti, V, Y, Zr)1	TiB2, ZrB2, etc
TIB_B27	FeB (B27)	oP8	Pnma	(B)1(Cr, Fe, Hf, Mn, Mo, Nb, Ta, Ti, V, W, Y, Zr)1	TiB, FeB, HfB, MnB etc
TIO_ALPHA	TiO	mS20	C12/m1	(Ti+2)1(O-2)1	
TISI2_C54	TiSi2 (C54)	oF24	Fddd	(Mo, Nb, Ru, Ti, Zr)1(Al, Si, Sn)2	
TRIDYMITE	SiO2	mS144	Cc	(Sio2)1	
V2B3	V2B3	oS20	Cmcm	(V)0.4(B)0.6	
V2O5	V2O5	oP14	Pmmm	(V+5)2(O-2)5	
V2O_SS	V7O3	mS20	C12/m1	(V)1(O, Va)0.5	Gamma (V)
V3C2	Sc2Te3	hR20	R-3m	(V)3(C)2	
V3H2	Unknown Structure			(V)0.6(H)0.4	
V3O5_LT	V3O5	mP32	P12/c1	(V+3)2(V+4)1(O-2)5	
V3O7	V3O7	mS120	C12/c1	(V+5)2(V+4)1(O-2)7	
V52O64	V13O16	tI116	I4_1/amd	(V)52(O)64	delta-prime V-oxide
V5B6	V5B6	oS22	Cmmm	(Nb, Ti, V)5(B)6	

Name	Prototype	Pearson	Spacegroup	Thermodynamic Model and phase Constitution	Notes
V6O13	V6O13	mS38	C12/m1	(V+5)2(V+4)4(O-2)13	
VO2_LT	VO2	mP12	P12_1/c1	(V+4)1(O-2)2	
W1O2	VO2	mP12	P12_1/c1	(O2W1)1	
W5SI3_D8M	W5Si3	tI32	I4/mcm	(Cr, Fe, Mo, Nb, Ti, V, W)4(Cr, Fe, Mo, Nb, Si, Ti, V, W)1(Al, Si, Sn)3	
WO2_72	Unknown Structure			(O2_72W1)1	
WO2_90	Unknown Structure			(O2_90W1)1	
WO2_96	Unknown Structure			(O2_96W1)1	
WO3_HT	WO3	tP16	P-42_1m	(O3W1)1	
WO3_LT	WO3	oP32	Pbcn	(O3W1)1	
Y15C19_H	Unknown Structure			(C)19(Y)15	
Y15C19_R	alpha-Y15C19	oP18	Pbam	(C)19(Y)15	
Y1B6	CaB6	cP7	Pm-3m	(Y)1(B)6	
Y2C3_H	Unknown Structure			(Y)2(C)2(C, Va)1	
Y2C3_R	Sc3C4	tP70	P4/mnc	(Y)2(C)2(C, Va)1	
Y3SI5_HT	GdSi1.4	oI12	Imma	(Y)3(Si)5	
Y3SI5_LT	AlB2	hP3	P6/mmm	(Y)3(Si)5	
YB4	UB4	tP20	P4/mbm	(Y)1(B)4	
YB66	YB66	cF1936	Fm-3c	(Y)1(B)66	
YC2_C11A	CaC2	tI6	I4/mmm	(C2Y1)1	

Name	*Prototype*	*Pearson*	*Spacegroup*	*Thermodynamic Model and phase Constitution*	*Notes*
YC_GAMMA	NaCl	cF8	Fm-3m	(Y)1(C, C2, Va)1	
YH3_EPSLON	H3Ho	hP24	P-3c1	(Y)1(H, Va)3	
YSI2_HT	AlB2	hP3	P6/mmm	(Y)1(Si)2	
ZR5SI4	Cr5B3 (D8l)	tI32	I4/mcm	(Hf, Mo, Nb, Ti, Y, Zr)5(Al, Si)4	Ti5Si4, Hf5Si4, Y5Si4,Zr5Si4(alpha)
ZRO2_MONO	ZrO2-m	mP12	P2_1/c	(Al+3, Cr+3, Hf+4, Ti+4, Y+3, Zr+4)2(O-2, Va)4	
ZRO2_TETR	HgI2	tP6	P4_2/nmc	(Al+3, Cr+3, Fe+2, Hf+4, Mn+2, Mn+3, Ni+2, Ti+4, Y+3, Zr+4)2(O-2, Va)4	
ZRSI2_C49	ZrSi2	oS12	Cmcm	(Hf, Nb, Y, Zr)1(Si)2	
ZRSIO4	Zr(SiO4)	tI24	I4_1/amd	(Si+4)1(Y+3, Zr+4)1(O-2, Va)4	
ZRTI2O6	Nb2FeO6	oP36	Pbcn	(Zr+4)1(Ti+4)2(O-2)6	
ZRTIO4_ALPHA	Unknown Structure			(Zr+4)1(Ti+4)1(O-2)4	
ZRTIO4_BETA	zeta-Fe2N	oP12	Pbcn	(Ti+4, Zr+4)2(O-2)4	

TCTI4 Properties Data

Model Descriptions

For more information about the various thermophysical models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

You can find information on our website about the thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

Examples

Go to the Titanium and TiAl-based Alloys Databases page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to titanium and TiAl including links to resources such as examples, publications, and more.

TCTI: TCS Ti/TiAl-based Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS Ti/TiAl-based Alloys Database (TCTI)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**4.0**
First release:	**TCTI1 was released in 2017**

Changes in the Most Recent Database Release

TCTI3 to TCTI4

Software release 2022a (December 2021/January 2022)

- Added thermophysical property data for electrical resistivity and thermal conductivity
- Two new assessed ternary systems: Ti-Al-Ni and Ti-Cu-Ni.
- Updated volume descriptions for α2 and γ phases.
- Updated description of BCC_A2 in Mo-V and Mo-Ti-V.

Previous Releases

TCTI2.2 to TCTI3.0

Software release 2021a (December 2020/January 2021)

- Added Copper (Cu), which is a minor-alloying element in titanium alloys.
- Ti-Cu, Cu-Fe, Cu-H, Cu-N, Cu-Nb, Cu-O, Cu-Si, Cu-Sn, Ti-Cu-C, Ti-Cu-Fe, Ti-Cu-H, Ti-Cu-N, Ti-Cu-Nb, Ti-Cu-O, Ti-Cu-Si, and Ti-Cu-Sn are modeled. Now it is possible to perform calculations for titanium alloys within the framework of Ti-Cu-Sn-Nb-Si. Moreover, the reliability can be enhanced by the availability of considering the effects from common impurities: C, Fe, H, N, and O.
- Al-Cu and Ti-Al-Cu are modeled, which is useful for both Ti- and TiAl-based alloys where alloying effects of Cu are of interest.
- Ti-Hf-Ta, Ti-B-Hf, Ti-Hf-Zr, and B-C-Si are modeled. These systems are of particular use for those involved in the development of biomedical materials because it combines cytocompatibility and improves mechanical properties.
- Viscosity and surface tension of liquid are included with the database as of this release.

TCTI2.1 to TCTI2.2

Software release 2020b (June 2020)

- Improved description of liquid phase for calculations with yttrium.

TCTI2.0 to TCTI2.1

Software release 2019b (June 2019)

- Improved description of liquidus temperature for Ti64 alloy.
- Adjusted phase stability of HCP_A3 and BCC_A2 in some systems.

TCTI1 to TCTI2

Software release 2019a (December 2018)

- Volume data for most of the phases assessed.
- 4 new elements: Ag, H, Pd, Pt
- 33 new binary systems are assessed: Ti-Ag, Ti-H, Ti-Pd, Ti-Pt, Ag-Pd, Al-Pd, Cr-Pd, Mo-Pd, Ni-Pd, Pd-V, Pd-Zr, Al-H, B-H, C-H, Co-H, Cr-H, Fe-H, Hf-H, Mn-H, Mo-H, N-H, Nb-H, Ni-H, O-H, Re-H, Ru-H, Si-H, Sn-H, Ta-H, V-H, W-H, Y-H, Zr-H. Most of these are H-containing.
- 24 new ternary systems are modeled: Ti-Ag-Pd, Ti-Al-Fe, Ti-Al-H, Ti-Al-Pd, Ti-Al-Y, Ti-B-Si, Ti-C-Si, Ti-Cr-H, Ti-Cr-O, Ti-Cr-Si, Ti-Fe-Mo, Ti-H-Ni, Ti-H-O, Ti-H-Zr, Ti-Mo-O, Ti-Nb-O, Ti-Nb-Si, Ti-Ni-Pd, Ti-O-Si, Ti-O-Ta, Ti-O-V, Ti-O-W, Ti-O-Zr, Ti-Pd-V.