TCS Ti/TiAl-based Alloys Database (TCTI5)

Technical Information

Available Starting with Thermo-Calc Version 2023a

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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 TCTI5. See the link for any subversion release details.

The database is compatible with the TCS Ti-alloys Mobility Database (MOBTI). The current version is MOBTI4.

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 TCTI5 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 and ternary assessed systems, plus 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.

TCTI5 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
- 111 ternary systems
- 433 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.

By default, the GAS phase is restored when retrieving the data from the database; it needs to be manually rejected when it is not 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 have been modeled by considering experimental data over quite wide (if not entire) compositions, this database most prominently targets light elements, like O, C, N,

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 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, it should be noted 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. Also see Common Phases for Titanium Alloys to review the phases with 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)` `SURF(ION)` **
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 TCOX database (all versions). As of 2023b it is also not used starting with the following versions of these databases: TCFE13, TCNI12.1, TCTI5.1, TCNOBL3, TCPMAG2, and TCCU6.

** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

TCTI5 Systems

In this section:

TCTI5 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

TCTI5 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-Si-Zr	Ti-Sn-V	Ti-Sn-Zr	Ti-Ta-V	Ti-Ta-W	Ti-Ta-Zr
Ti-V-W	Ti-V-Zr	Ti-W-Zr			

TCTI5 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 (*).

TCTI5 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.

Name in the Database	*Common Name and Description*
O_PHASE	The orthorhombic phase stable in Ti-Al-Nb ternary.
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.	

TCTI5 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*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
ALTI3_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194	Ti3Al	3	[3.0, 1.0, 2.0]	(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
ALTI_L10	CuAu (L10)	L10	tP2	P4/mmm	123	TiAl	3	[1.0, 1.0, 2.0]	(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, SI, VA)2
B82_OMEGA	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[1.0, 1.0, 1.0]	(AL, SN, TI)1(CO, CR, MO, NB, TA, TI, ZR)1(AL, TI)1
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229	Metallic BCC_A2 solution. If BCC_ B2 is defined, this phase will be combined to it.	2	[1.0, 3.0]	(, 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
BCC_B2	CsCl (B2)	B2	cP2	Pm-3m	221	Solution of ordered BCC_B2, having Gibbs energy contribution from BCC_A2	3	[0.5, 0.5, 3.0]	(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
FCC_B1	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225	TiC, TiN, TiO	2	[1.0, 1.0]	(AL, CR, HF, MO, NB, TA, TI, V, VA, W, ZR)1(C, N, O, VA)1
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194	Metallic HCP_A3 solution, alpha_Ti	2	[1.0, 0.5]	(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

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
LIQUID	Liquid					Metallic LIQUID:L solution phase	1	[1.0]	(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, MOO3, 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
OMEGA	Hexagonal omega (C32)	C32	hP3	P6/mmm	191	s metastable structure of Ti	1	[1.0]	(, AL, B, C, CO, CR, FE, HF, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W, Y, ZR)1
O_PHASE	NaHg		oS16	Cmcm	63	The O phase	3	[0.5, 0.25, 0.25]	(NB, TA, TI)0.5(AL, NB, TA, TI)0.25(NB, TA, TI)0.25
TI2X_OMEGA	Hexagonal omega (C32)	C32	hP3	P6/mmm	191	Ordered Omega phase, B82 or C32 type	2	[2.0, 1.0]	(TI)2(AL, B, C, CO, CR, FE, HF, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W, Y, ZR)1
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194		2	[2.0, 1.0]	(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 Cubic Laves (C15)	C15	cF24	Fd-3m	227		2	[2.0, 1.0]	(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	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140	Hf2Al, Hf2Si, Zr2Si Zr2Co, Ta2Co, Hf2Ni, Ta2Ni, Zr2Ni	2	[2.0, 1.0]	(AL, HF, MO, NB, TA, TI, W, ZR)2(AL, CO, CR, FE, NI, SI)1
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	P6_3/mmc	194		2	[2.0, 1.0]	(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 (A12)	A12	cI58	I-43m	217		2	[1.0, 1.0]	(AL, CO, CR, FE, MN, MO, NB, NI, RE, RU,

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
									SI, SN, TA, TI, V, W, Y, ZR)1(B, C, H, VA)1
DIS_MU	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	Part of the description of MU_PHASE	1	[1.0]	(AL, CO, CR, FE, MN, MO, NB, NI, RE, TA, W)1
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	DIS_MU contribution is introduced in the description of this phase	4	[1.0, 2.0, 6.0, 4.0]	(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_SIG	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		1	[1.0]	(CO, CR, FE, MN, MO, NB, NI, RE, RU, TA, V, W)1
ORD_SIG	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		3	[10.0, 4.0, 16.0]	(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
SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		3	[10.0, 4.0, 16.0]	(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
GPHASE	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		4	[1.0, 16.0, 7.0, 6.0]	(AL, CO)1(AL, TI)16(CO)7(TI)6
G_PHASE	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225		3	[16.0, 6.0, 7.0]	(AL, CO, CU, FE, MN, NI, PD, TI)16(HF, NB, TI, Y, ZR)6(CO, CU, FE, MN, NI, PD, SI)7
H_L21	Heusler (L21)	L21	cF16	Fm-3m	225		3	[0.5, 0.5, 1.0]	(AL, NI, SN, TI)0.5(AL, HF, NB, NI, TA, TI, ZR)0.5(CO, CU, NI, RU, VA)1
L10_FCC	CuAu (L10)	L10	tP2	P4/mmm	123		2	[0.5, 0.5]	(MN, NI)0.5(MN, NI)0.5
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.75, 0.25]	(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

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
AF	FeGaO3		oP40	Pna2_1	33	Al2O3.Fe2O3	2	[1.0, 1.0]	(AL2O3)1(FE2O3)1
AG1TI2	CuZr2		tI6	I4/mmm	139		2	[1.0, 2.0]	(AG)1(TI)2
AGTI	CdTi		tP4	P4/nmm	129		2	[1.0, 1.0]	(AG, TI)1(AG, TI)1
AL11CR2	Al5Cr		mS732	C2/c	15		2	[10.0, 2.0]	(AL)10(AL, CR, TI)2
AL11CR4	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(AL, CR, TI)4
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25		oP156	Pnma	62		2	[29.0, 10.0]	(AL, MN)29(MN)10
AL11MN4_LT	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(FE, MN)4
AL11RE4	Al11Mn4		aP15	P-1	2		2	[11.0, 4.0]	(AL)11(RE)4
AL12MN	Al12W		cI26	Im-3	204		2	[12.0, 1.0]	(AL)12(MN)1
AL12W	Al12W		cI26	Im-3	204	also AL12RE and AL12MO	2	[12.0, 1.0]	(AL)12(MO, RE, W)1
AL13CO4	Orthorhombic Co4Al13		oP102	Pmn2_1	31		2	[13.0, 4.0]	(AL)13(CO)4
AL13FE4	Al13Fe4		mS102	C2/m	12	also Al13Ru4	3	[0.6275, 0.235, 0.1375]	(AL)0.6275(FE, MN, RU)0.235(AL, SI, VA)0.1375
AL17MO4	Al17Mo4		mS84	C2	5		2	[17.0, 4.0]	(AL)17(MO)4
AL1RE2	CuZr2		tI6	I4/mmm	139	C11_b	2	[1.0, 2.0]	(AL)1(RE)2
AL1ZR2	Ni2In (B82)	B82	hP6	P6_3/mmc	194	also AlY2	2	[1.0, 2.0]	(AL)1(TI, Y, ZR)2
AL21PT8	Al21Pt8		tI116	I4_1/a	88	also Al21Pd8	2	[21.0, 8.0]	(AL)21(PD, PT)8
AL21V2	Al10V		cF176	Fd-3m	227		2	[21.0, 2.0]	(AL)21(V)2

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AL22MO5	Al22Mo5		oF216	Fdd2	43		2	[22.0, 5.0]	(AL)22(MO)5
AL23V4	Al23V4		hP54	P6_3/mmc	194		2	[23.0, 4.0]	(AL)23(V)4
AL2CU_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[2.0, 1.0]	(AL)2(AL, CU)1
AL2FE	Al2Fe		aP18	P1	1		2	[2.0, 1.0]	(AL)2(FE, MN)1
AL2N2TI3	(Al2Ti3N2)		hP22	P6_3mc	186		3	[2.0, 2.0, 3.0]	(AL)2(N)2(TI)3
AL2PD5	Unknown Structure						2	[2.0, 5.0]	(AL)2(AL, PD)5
AL2TI	Ga2Hf		tI24	I4_1/amd	141		2	[2.0, 1.0]	(AL, NB, TA, TI)2(AL, CO, CR, NB, TA, TI, V, ZR)1
AL2W	CrSi2 (C40)	C40	hP9	P6_222	180		2	[2.0, 1.0]	(AL)2(W)1
AL2ZR3	Zr3Al2		tP20	P4_2/mnm	136	also Al2Hf3, Al2Y3	2	[2.0, 3.0]	(AL)2(HF, TI, Y, ZR)3
AL3CO	Os4Al13		mS34	C2/m	12		2	[3.0, 1.0]	(AL)3(CO)1
AL3MO	MoAl3		mS32	C2/m	12		2	[3.0, 1.0]	(AL)3(MO)1
AL3NI1	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[0.75, 0.25]	(AL)0.75(NI)0.25
AL3NI2	Al3Ni2 (D513)	D513	hP5	P-3m1	164		3	[3.0, 2.0, 1.0]	(AL, PD, SI)3(AL, NI, PD, RU)2(NI, RU, VA)1
AL3NI5	Ga3Pt5		oS16	Cmmm	65		2	[0.375, 0.625]	(AL)0.375(NI)0.625
AL3PD1	(Al3Pd)		oP*	Pna2_1	33		2	[3.0, 1.0]	(AL)3(PD)1
AL3PD5	Rh5Ge3		oP16	Pbam	55	also Al3Pt5	2	[3.0, 5.0]	(AL)3(PD, PT)5
AL3TI_D022	Al3Ti (D022)	D022	tI8	I4/mmm	139	also Al3V	2	[3.0, 1.0]	(AL, MN, MO, NB, PD, SI, TI, V)3(AL, CO,

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									CR, MN, MO, NB, NI, PD, SI, TA, TI, V, ZR)1
AL3TI_LT	Al3Ti-LT		tI32	I4/mmm	139		2	[3.0, 1.0]	(AL, CR, NB, TI)3(AL, CR, NB, TI, V, ZR)1
AL3Y_HT	BaPb3		hR12	R-3m	166		2	[0.75, 0.25]	(AL)0.75(Y)0.25
AL3Y_LT	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[0.75, 0.25]	(AL)0.75(Y)0.25
AL3ZR2	Zr2Al3		oF40	Fdd2	43	also Al3Hf2	2	[3.0, 2.0]	(AL)3(HF, ZR)2
AL3ZR4	Al3Zr4		hP7	P6/mmm	191	also Al3Hf4	2	[3.0, 4.0]	(AL)3(HF, TI, ZR)4
AL3ZR5	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		2	[3.0, 5.0]	(AL)3(TI, ZR)5
AL3ZR_D023	Al3Zr (D023)	D023	tI16	I4/mmm	139	also Al3Hf	2	[3.0, 1.0]	(AL)3(HF, TI, ZR)1
AL45V7	Al45V7		mS104	C2/m	12		2	[45.0, 7.0]	(AL)45(V)7
AL4C3	Al4C3 (D71)	D71	hR7	R-3m	166		2	[4.0, 3.0]	(AL, SI)4(C)3
AL4CR	mu-Al4Mn		hP574	P6_3/mmc	194		2	[4.0, 1.0]	(AL)4(AL, CR, TI)1
AL4FE	AlmFe		tI110	I-42m	121		2	[4.2, 1.0]	(AL)4.2(FE)1
AL4MN_R	lambda-Al4Mn		hP586	P6_3/mmc	194		2	[461.0, 107.0]	(AL)461(FE, MN)107
AL4MN_U	mu-Al4Mn		hP574	P6_3/mmc	194		2	[4.0, 1.0]	(AL)4(MN)1
AL4PD	(Al4Pd)		hP*	P6_322	182		2	[4.0, 1.0]	(AL)4(PD)1
AL4RE	Unknown Structure						2	[4.0, 1.0]	(AL)4(RE)1
AL4W	Al4W		mS30	Cm	8	also Al4Mo	2	[4.0, 1.0]	(AL)4(MO, W)1
AL4ZR5	Ti5Ga4		hP18	P6_3/mcm	193		2	[4.0, 5.0]	(AL)4(ZR)5

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AL5CO2_D811	Co2Al5 (D811)	D811	hP28	P6_3/mmc	194		2	[5.0, 2.0]	(AL)5(CO)2
AL5FE2	Al2.8Fe		oS24	Cmcm	63		2	[5.0, 2.0]	(AL)5(FE, MN)2
AL5FE4	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		1	[1.0]	(AL, FE)1
AL5TI2	Al5Ti2		tP28	P4/mmm	123		2	[5.0, 2.0]	(AL, CR, NB, TA, TI)5(AL, CR, NB, TA, TI, V, ZR)2
AL5TI3	Al5Ti3		tP32	P4/mbm	127		2	[5.0, 3.0]	(AL)5(CR, NB, TA, TI)3
AL5W	Al5W		hP12	P6_322	182	also AL5MO	2	[5.0, 1.0]	(AL)5(MO, W)1
AL63MO37	Unknown Structure						2	[63.0, 37.0]	(AL)63(MO)37
AL6MN	MnAl6 (D2h)	D2h	oS28	Cmcm	63		2	[6.0, 1.0]	(AL)6(FE, MN, RE, RU)1
AL77W23	Unknown Structure						2	[77.0, 23.0]	(AL)77(W)23
AL7CR	Al45V7		mS104	C2/m	12		2	[13.0, 2.0]	(AL)13(AL, CR, TI)2
AL7W3	Unknown Structure						2	[7.0, 3.0]	(AL)7(W)3
AL8CR5_HT	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		4	[2.0, 3.0, 2.0, 6.0]	(AL, CR)2(AL, CR, TI)3(CR)2(AL)6
AL8CR5_LT	Cr5Al8 (D810)	D810	hR26	R3m	160		3	[12.0, 5.0, 9.0]	(AL)12(CR)5(AL, CR, TI)9
AL8CR5_MT	Unknown Structure						4	[2.0, 3.0, 2.0, 6.0]	(AL, CR, TI)2(AL, CR, TI)3(CR)2(AL)6
AL8MO3	Al8Mo3		mS22	C2/m	12		2	[8.0, 3.0]	(AL)8(MO)3
AL8V5	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		2	[8.0, 5.0]	(AL, MN, V)8(AL, MN, TI, V)5
AL9CO2	Co2Al9 (D8d)	D8d	mP22	P2_1/c	14		2	[9.0, 2.0]	(AL)9(CO)2

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ALB12	alpha-AlB12		tP216	P4_12_12	92		2	[1.0, 12.0]	(AL, TI)1(B)12
ALBMO	ZrSi2 (C49)	C49	oS12	Cmcm	63		3	[1.0, 1.0, 1.0]	(AL)1(B)1(MO)1
ALCCR2	AlCCr2		hP8	P6_3/mmc	194		3	[1.0, 1.0, 2.0]	(AL)1(C)1(CR)2
ALCR2	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[1.0, 2.0]	(AL, CR, NI, PD)1(AL, CR, TI)2
ALCR3	Unknown Structure					AlCr3 super lattice	2	[1.0, 3.0]	(AL, CR, TI)1(CR)3
ALCU_DEL	Al5Cu8		hR52	R3m	160		2	[2.0, 3.0]	(AL)2(CU)3
ALCU_EPS	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[1.0, 1.0]	(AL, CU)1(CU)1
ALCU_ETA	AlCu(r)		mS20	C2/m	12		2	[1.0, 1.0]	(AL, CU)1(CU)1
ALCU_ZETA	Al9Cu11(h)		oF88	Fmm2	42		2	[9.0, 11.0]	(AL)9(CU)11
ALH3	AlH3		oP24	Pnnm	58		2	[1.0, 3.0]	(AL)1(H)3
ALM3C_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221	AlCo3C, AlFe3C, Perovskite	3	[1.0, 3.0, 1.0]	(AL)1(CO, FE)3(C)1
ALNTI2	AlCCr2		hP8	P6_3/mmc	194		3	[1.0, 1.0, 2.0]	(AL)1(N)1(TI)2
ALNTI3	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221		3	[1.0, 1.0, 3.0]	(AL)1(N)1(TI)3
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186		2	[1.0, 1.0]	(AL)1(N)1
ALPHA_B19	beta'-AuCd (B19)	B19	oP4	Pmma	51		2	[1.0, 1.0]	(MO, NB, PT, TI, V, ZR)1(MO, NB, PT, TI, V, ZR)1
ALPHA_SPINEL	Hausmannite (Mn3O4)		tI28	I4_1/amd	141		4	[1.0, 2.0, 2.0, 4.0]	(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

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
ALRE	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[1.0, 1.0]	(AL)1(RE)1
ALSI3TI2	Zr3Al4Si5		tI24	I4_1/amd	141		3	[0.166667, 0.5, 0.333333]	(AL)0.166667(SI)0.5(TI)0.333333
ALZR	CrB (B33)	B33	oS8	Cmcm	63	also AlHf, AlY	2	[1.0, 1.0]	(AL)1(HF, Y, ZR)1
ANDALUSITE	Andalusite (Al2SiO5, S02)	S02	oP32	Pnnm	58	A high-pressure phase (Al2O3.SiO2)	4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(SI+4)1(O-2)5
B12ZR	UB12 (D2f)	D2f	cF52	Fm-3m	225	YB12, ZrB12	2	[12.0, 1.0]	(B)12(Y, ZR)1
B2O3	B2O3		hP15	P3_121	152		1	[1.0]	(B2O3)1
B3SI	B13C2 B4C (D1g)	D1g	hR15	R-3m	166		3	[6.0, 2.0, 6.0]	(B)6(SI)2(B, SI)6
B4C	B13C2 B4C (D1g)	D1g	hR15	R-3m	166		2	[1.0, 1.0]	(B11C, B12)1(B2, C2B, CB2, SI2)1
B5W2_X	Mo2B5 (D8i)	D8i	hR7	R-3m	166		2	[5.0, 2.0]	(B, C, VA)5(W)2
B6SI	SiB6		oP280	Pnnm	58		3	[210.0, 23.0, 48.0]	(B)210(SI)23(B, SI)48
B9W2	W2B9		hP22	P-3	147		2	[9.0, 2.0]	(B)9(W)2
BCT_A5	beta-Sn (A5)	A5	tI4	I4_1/amd	141		1	[1.0]	(AL, CU, SN, TI)1
BETAR_BORON	beta-B (R-105)		hR105	R-3m	166		2	[93.0, 12.0]	(B)93(B, C, NB, SI, TI)12
DIS_BETA	V2H1.1		tI56	I4_1/amd	141	V-H binary	2	[0.5, 0.5]	(H, VA)0.5(V)0.5
BETA_PHASE	V2H		mS6	C2/m	12	V-H binary	3	[0.25, 0.25, 0.5]	(H, VA)0.25(H, VA)0.25(V)0.5
BETA_V3O	CoO		tI4	I4/mmm	139		2	[1.0, 1.0]	(V)1(O, VA)1
BNSI	alpha-B (hR12)		hR12	R-3m	166		3	[61.0, 1.0, 8.0]	(B)61(SI)1(B, SI)8

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BN_B4	Wurtzite (ZnS, B4)	B4	hP4	P6_3mc	186		2	[1.0, 1.0]	(B)1(N)1
BW_ALPHA	MoB (Bg)	Bg	tI16	I4_1/amd	141		2	[1.0, 1.0]	(B, C, VA)1(W)1
BW_BETA	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(B, C, VA)1(W)1
CEMENTITE	Cementite (Fe3C, D011)	D011	oP16	Pnma	62	D011	2	[3.0, 1.0]	(CO, CR, FE, MN, MO, NI, V, W)3(C, N)1
CFC2_FENBZR	Cu2Mg Cubic Laves (C15)	C15	cF24	Fd-3m	227		3	[2.0, 1.0, 3.0]	(FE, NB, ZR)2(NB, ZR)1(NB, ZR)3
CHI_A12	alpha-Mn (A12)	A12	cI58	I-43m	217		3	[24.0, 10.0, 24.0]	(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	50		2	[11.0, 2.0]	(CO)11(ZR)2
CO17Y2	Ni17Th2		hP38	P6_3/mmc	194		3	[1.0, 2.0, 15.0]	(CO2, Y)1(CO2, Y)2(CO)15
CO1SN1TI1	Unknown Structure						3	[1.0, 1.0, 1.0]	(CO, NI)1(SN)1(TI)1
CO1SN2	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[0.333, 0.667]	(CO)0.333(SN)0.667
CO1SN3	Au3Zn		oS32	Cmce	64		2	[0.25, 0.75]	(CO)0.25(SN)0.75
CO2SI_C23	Cotunnite (PbCl2, C23)	C23	oP12	Pnma	62	also Ni2Si(delta)	2	[2.0, 1.0]	(AL, CO, CR, FE, NI, PD, TI)2(AL, PD, SI)1
CO3SI	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[3.0, 1.0]	(CO)3(SI)1
CO3SN2	Co1.75Ge		hP6	P6_3/mmc	194		4	[1.0, 1.0, 0.5, 0.5]	(CO)1(SN)1(CO, VA)0.5(CO, VA)0.5
CO3VV	Al3Pu		hP24	P6_3/mmc	194		2	[3.0, 1.0]	(CO, V)3(CO, V)1
CO3Y1	Ni3Pu		hR12	R-3m	166		2	[3.0, 1.0]	(CO)3(Y)1
CO3Y2	Unknown Structure		cP*				2	[3.0, 2.0]	(CO)3(Y)2

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CO3Y4	Co3Ho4		hP22	P6_3/m	176		2	[3.0, 4.0]	(CO)3(Y)4
CO5Y8	Co5Y8		mP52	P2_1/c	14		2	[5.0, 8.0]	(CO)5(Y)8
CO5Y_D2D	CaCu5 (D2d)	D2d	hP6	P6/mmm	191		3	[1.0, 4.0, 1.0]	(CO2, Y)1(CO)4(CO, VA)1
CO7HF	(Co11Hf2)		oP*	Pban	50		2	[7.0, 1.0]	(CO)7(HF)1
CO7M2	(Co7Nb2)		mS18	C2/m	12		2	[7.0, 2.0]	(CO)7(NB, TA, TI)2
CO7MO6	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	mu phase	2	[7.0, 6.0]	(CO, MO)7(CO, MO, TI)6
CO7Y6	Unknown Structure						2	[7.0, 6.0]	(CO)7(Y)6
COB	FeB (B27)	B27	oP8	Pnma	62		2	[1.0, 1.0]	(CO, RE)1(B)1
CORUNDUM	Corundum (Al2O3, D51)	D51	hR10	R-3c	167	corundum [Al2O3], eskolaite [Cr2O3], hematite [Fe2O3], Ti2O3, V2O3	3	[2.0, 1.0, 3.0]	(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
COSN	CoSn (B35)	B35	hP6	P6/mmm	191		2	[0.5, 0.5]	(CO)0.5(SN)0.5
COY_BF	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(CO)1(Y)1
CR2B_ORTH	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[2.0, 1.0]	(CR, FE, MO, RE)2(B)1
CR2PD3_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	Pm-3m	221		2	[0.4, 0.6]	(CR)0.4(PD)0.6
CR3MN5	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[3.0, 5.0]	(CR)3(MN)5
CR3NI5SI2	AlAu4		cP20	P2_13	198		4	[3.0, 5.0, 2.0, 1.0]	(CR)3(NI)5(SI)2(C, VA)1
CR3SI_A15	Cr3Si (A15)	A15	cP8	Pm-3n	223	Cr3Ru, Mo3Si, V3Si, Mo3Al, Nb3Al, V3Co,	3	[3.0, 1.0, 3.0]	(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,

Name	Prototype	Strukturbericht	Pearson_ Symbol	Space_ Group_ Symbol	SG#	Info	Sublattices	Sites	Formula_unit
						V3Ni, V3Sn, Nb3Sn			VA)3
CR5B3	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140		2	[0.625, 0.375]	(CR, MO)0.625(B)0.375
CR8FE16TI5	alpha-Mn (A12)	A12	cI58	I-43m	217		2	[24.0, 5.0]	(CR, FE)24(TI)5
CRB4	CrB4		oI10	Immm	71		2	[0.2, 0.8]	(CR)0.2(B)0.8
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	Fd-3m	227		1	[1.0]	(SIO2)1
CRNI2_OP6	MoPt2		oI6	Immm	71		2	[1.0, 2.0]	(CR, MO, W)1(MO, NI, W)2
CRPD_L10	AuCu		tP4	P4/mmm	123		2	[0.5, 0.5]	(CR)0.5(PD)0.5
CRSI2_C40	CrSi2 (C40)	C40	hP9	P6_222	180	also NbSi2, TaSi2, VSi2	2	[1.0, 2.0]	(CR, HF, MO, NB, SI, TA, TI, V, W)1(AL, CR, SI)2
CU10SN3	Cu10Sn3		hP26	P6_3	173		1	[1.0]	(CU, SN)1
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cI76	I-43d	220		2	[0.789474, 0.210526]	(CU)0.789474(SI)0.210526
CU2TI	Au2V		oS12	Cmcm	63		2	[2.0, 1.0]	(CU, NI)2(TI)1
CU33SI7_DELTA	Unknown Structure						2	[0.825, 0.175]	(CU)0.825(SI)0.175
CU3SN	Cu3Sn		oS80	Cmcm	63		2	[3.0, 1.0]	(CU, SN)3(CU, SN)1
CU3TI2	Cu3Ti2		tP10	P4/nmm	129		2	[3.0, 2.0]	(CU, FE, NI)3(TI)2
CU41SN11	Cu41Sn11		cF416	F-43m	216		2	[41.0, 11.0]	(CU, SN)41(CU, SN)11
CU4TI1	Au4Zr		oP20	Pnma	62		2	[4.0, 1.0]	(CU, NI, TI)4(CU, NI, TI)1
CU4TI3	Cu4Ti3		tI14	I4/mmm	139		2	[4.0, 3.0]	(CU, NI)4(TI)3

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
CU56SI11_ GAMMA	Mg3Ru2		cP20	P4_132	213		2	[0.835821, 0.164179]	(CU)0.835821(SI)0.164179
CU6SN5_HT	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[1.0, 1.0, 1.0]	(CU)1(CU, SN)1(SN)1
CU6SN5_LT	Cu6Sn5		mS44	C2/c	15		3	[1.0, 1.0, 1.0]	(CU)1(CU, SN)1(SN)1
CUB_A13	beta-Mn (A13)	A13	cP20	P4_132	213		2	[1.0, 1.0]	(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	Tenorite (CuO, B26)	B26	mS8	C2/c	15		2	[1.0, 1.0]	(CU+2)1(O-2)1
CUPRITE_C3	Cuprite (Cu2O, C3)	C3	cP6	Pn-3m	224		2	[2.0, 1.0]	(CU+1)2(O-2)1
CUSI_ETA	Cu3Si-h2		hR*	P-31m	162	Structure uncertain	2	[0.76, 0.24]	(CU)0.76(SI)0.24
CUSN_GAMMA	BiF3 (D03)	D03	cF16	Fm-3m	225		1	[1.0]	(CU, SN)1
CUTI3	CuTi3 (L60)	L60	tP4	P4/mmm	123		2	[1.0, 3.0]	(CU, TI)1(TI)3
CUTI_B11	gamma-CuTi (B11)	B11	tP4	P4/nmm	129		2	[1.0, 1.0]	(CU, NI, TI)1(CU, NI, TI)1
CUZR2_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139	CuTi2	3	[1.0, 2.0, 0.5]	(CU, FE, NI, SI)1(NB, TI)2(O, VA)0.5
D0I_MO2B5	Mo2B5 (D8i)	D8i	hR7	R-3m	166		2	[0.32, 0.68]	(MO, TI)0.32(B)0.68
D5A_M3B2	Si2U3 (D5a)	D5a	tP10	P4/mbm	127	TA3B2, NB3B2, V3B2	2	[3.0, 2.0]	(FE, HF, MO, NB, TA, TI, V)3(B)2
DELTA_TIH2	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225	delta dihydrides	2	[1.0, 2.0]	(HF, NB, TI, V, Y, ZR)1(H, VA)2
DIAMOND_A4	Diamond (A4)	A4	cF8	Fd-3m	227		1	[1.0]	(AL, B, C, H, O, SI, SN)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	Metallic FCC_A1 solution, e.g. (Al), (Cu)	2	[1.0, 1.0]	(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

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FE1SN2	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[1.0, 2.0]	(FE)1(SN)2
FE2SI	AlNi2		hP6	P-3m1	164		2	[0.666667, 0.333333]	(FE)0.666667(SI)0.333333
FE3SN2	Fe3Sn2		hR10	R-3m	166		2	[3.0, 2.0]	(FE)3(SN)2
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	Pm-3m	221		2	[4.0, 1.0]	(CO, CR, FE, MN, NI)4(C, N)1
FE5SN3	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[5.0, 3.0]	(FE)5(SN)3
FE7MO6	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	mu phase	3	[7.0, 2.0, 4.0]	(FE)7(MO, TI)2(FE, MO, TI)4
FECN_CHI	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[2.2, 1.0]	(FE)2.2(C, N)1
FESI2_H	FeSi2-h		tP3	P4/mmm	123		2	[0.3, 0.7]	(FE)0.3(SI)0.7
FESI2_L	FeSi2-l		oS48	Cmce	64		2	[0.333333, 0.666667]	(FE)0.333333(SI)0.666667
FESI_B20	FeSi (B20)	B20	cP8	P2_13	198	also CoSi, CrSi, ReSi	2	[1.0, 1.0]	(CO, CR, FE, MN, NI, RE)1(AL, SI)1
FESN	CoSn (B35)	B35	hP6	P6/mmm	191		2	[1.0, 1.0]	(FE)1(SN)1
FLUORITE_C1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		2	[2.0, 4.0]	(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	gamma-brass (Cu9Al4, D83)	D83	cP52	P-43m	215		3	[4.0, 1.0, 8.0]	(AL)4(AL, CU)1(CU)8
GAMMA_H	gamma-brass (Cu5Zn8, D82)	D82	cI52	I-43m	217		3	[4.0, 1.0, 8.0]	(AL)4(AL, CU)1(CU)8
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	P6_3/mmc	194		1	[1.0]	(B, C)1

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HALITE	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225	Wustite [FeO], Bunsenite [NiO], MnO, CoO, high temperature TiO, VO	2	[1.0, 1.0]	(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
HF3NI7	Hf3Ni7		aP20	P-1	2		2	[0.3, 0.7]	(HF)0.3(NI)0.7
HF8NI21	Hf8Ni21		aP29	P-1	2	also ZR8NI21	2	[8.0, 21.0]	(HF, ZR)8(NI)21
HFMN	NiTi2		cF96	Fd-3m	227		2	[0.5, 0.5]	(HF)0.5(MN)0.5
HFNI3_ALPHA	PdRh2Ta		hP40	P6_3/mmc	194		2	[0.25, 0.75]	(HF)0.25(NI)0.75
HFNI3_BETA	BaPb3		hR12	R-3m	166		2	[0.25, 0.75]	(HF)0.25(NI)0.75
HFNI_ALPHA	CrB (B33)	B33	oS8	Cmcm	63		2	[0.5, 0.5]	(HF)0.5(NI)0.5
HFRE	Zr21Re25		hR92	R-3c	167		2	[1.0, 1.0]	(HF)1(RE)1
HIGH_SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136		3	[8.0, 4.0, 18.0]	(MN)8(CR)4(CR, MN)18
ION_LIQ	Liquid					IONIC_LIQ mixture, modeled by the ionic two-sublattice model	2	[1.0, 1.0]	(, 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)1(, , 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)1
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	P-1	2		4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(SI+4)1(O-2)5
M12C	Fe6W6C		cF104	Fd-3m	227		3	[6.0, 6.0, 1.0]	(CO, NI)6(MO, W)6(C)1
M23C6	Cr23C6 (D84)	D84	cF116	Fm-3m	225		3	[20.0, 3.0, 6.0]	(CO, CR, FE, MN, NI, RE, V)20(CO, CR, FE, MN, MO, NI, RE, V, W)3(C)6
M2B_TETR	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140	Co2B, Fe2B, Mn2B, Mo2B,	2	[2.0, 1.0]	(AL, CO, CR, FE, MN, MO, NB, NI, RE, TA, TI, W)2(B)1

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						Ni2B			
M2O3C	Bixbyite (Mn2O3, D53)	D53	cI80	Ia-3	206		3	[2.0, 3.0, 1.0]	(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 (D52)	D52	hP5	P-3m1	164	hexagonal Y2O3	3	[2.0, 3.0, 1.0]	(MN+3, Y, Y+3, ZR+4)2(O-2, VA)3(O-2, VA)1
M2P_C22	Revised Fe2P (C22)		hP9	P-62m	189		2	[2.0, 1.0]	(TI, ZR)2(SI)1
M3B2	Si2U3 (D5a)	D5a	tP10	P4/mbm	127		3	[0.4, 0.2, 0.4]	(CR, FE, MO, NI, W)0.4(CR, FE, NI)0.2 (B)0.4
M3C2	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62		2	[3.0, 2.0]	(CR, MO, V, W)3(C)2
M3SI1	Ti3P		tP32	P4_2/n	86	Ti3Si, Ta3Si, Zr3Si	2	[3.0, 1.0]	(HF, NB, TA, TI, ZR)3(SI)1
M3SI2_D5A	Si2U3 (D5a)	D5a	tP10	P4/mbm	127	Hf3Si2, Zr3Si2	2	[3.0, 2.0]	(HF, NB, ZR)3(SI)2
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[5.0, 2.0]	(FE, MN)5(C)2
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	P6_3/mcm	193	Ti5Si3, Fe5Si3, Zr5Si3, Y5Si3, Hf5Si3, Mn5Si3, Zr5Sn3, Zr5Sn4	4	[2.0, 3.0, 3.0, 1.0]	(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
M6C	Fe3W3C (E93)	E93	cF112	Fd-3m	227		4	[2.0, 2.0, 2.0, 1.0]	(CO, FE, NI)2(MO, NB, TA, W)2(CO, CR, FE, MO, NB, NI, TA, V, W)2(C)1
M7C3	C3Cr7 (D101)	D101	oP40	Pnma	62		2	[7.0, 3.0]	(CO, CR, FE, MN, MO, NI, RE, V, W)7(C)3
MB_B33	CrB (B33)	B33	oS8	Cmcm	63	CrB, NbB, NiB, TaB, VB	2	[1.0, 1.0]	(CR, FE, HF, MO, NB, NI, TA, TI, V, W)1 (B)1
MC_ETA	CMo		hP12	P6_3/mmc	194		2	[1.0, 1.0]	(MO, V, W)1(C, VA)1

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MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	P-6m2	187		2	[1.0, 1.0]	(MO, W)1(C, N)1
MN11SI19	Mn11Si19		tP120	P-4n2	118		2	[11.0, 19.0]	(MN)11(AL, SI)19
MN12Y	Mn12Th (D2b)	D2b	tI26	I4/mmm	139		2	[12.0, 1.0]	(MN)12(Y)1
MN1O2	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136		2	[1.0, 2.0]	(MN)1(O)2
MN2B_D1F	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[0.6707, 0.3293]	(MN)0.6707(B)0.3293
MN2SN	Ni2In (B82)	B82	hP6	P6_3/mmc	194		2	[0.643, 0.357]	(MN)0.643(SN)0.357
MN2YO5	HoMn2O5		oP32	Pbam	55		4	[1.0, 1.0, 1.0, 5.0]	(Y+3)1(MN+3)1(MN+4)1(O-2)5
MN3SI	BiF3 (D03)	D03	cF16	Fm-3m	225		2	[3.0, 1.0]	(FE, MN)3(AL, SI)1
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62		2	[3.0, 2.0]	(MN)3(SN)2
MN3TI	Unknown Structure						2	[3.0, 1.0]	(MN)3(TI)1
MN4TI	R-(Co,Cr,Mo)		hR53	R-3	166		2	[0.815, 0.185]	(MN)0.815(TI)0.185
MN6N4	Mn3N2		tI10	I4/mmm	139		2	[6.0, 4.0]	(MN)6(N)4
MN6N5	CoO		tI4	I4/mmm	139		2	[6.0, 5.0]	(MN)6(N)5
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166		2	[17.0, 3.0]	(AL, MN)17(SI)3
MN9SI2	Mn9Si2		oI186	Immm	71		2	[33.0, 7.0]	(MN)33(SI)7
MNB4	MnB4		mS10	C2/m	12		2	[0.2, 0.8]	(MN)0.2(B)0.8
MNNI2	Unknown Structure						2	[1.0, 2.0]	(MN, NI)1(NI)2
MNSN2	Khatyrkite (Al2Cu, C16)	C16	tI12	I4/mcm	140		2	[2.0, 1.0]	(SN)2(MN)1

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MNTA	Unknown Structure						2	[1.0, 1.0]	(MN)1(TA)1
MNTI_HT	Unknown Structure		t**				2	[0.515, 0.485]	(MN)0.515(TI)0.485
MNTI_LT	Zr21Re25		hR92	R-3c	167		2	[1.0, 1.0]	(MN)1(TI)1
MNYO3_HEX	LuMnO3		hP30	P6_3cm	185		3	[1.0, 1.0, 3.0]	(Y+3)1(MN+3)1(O-2)3
MO4O11	Mo4O11		oP60	Pna2_1	33		2	[4.0, 11.0]	(MO)4(O)11
MO8O23	High-Temperature Mo8O23		mP62	P2/c	13		2	[8.0, 23.0]	(MO)8(O)23
MO9O26	Mo9O26		mP70	P2/c	13		2	[1.0, 2.889]	(MO)1(O)2.889
MOB4	MoB4		hP16	P6_3/mmc	194		2	[0.2, 0.8]	(MO, TI)0.2(B)0.8
MOCOB	MnCuP		oP12	Pnma	62		3	[1.0, 1.0, 1.0]	(MO, W)1(CO)1(B)1
MONI4_BETA	Ni4Mo (D1a)	D1a	tI10	I4/m	87		2	[1.0, 4.0]	(MO, W)1(NI)4
MONI_DELTA	MoNi		oP56	P2_12_12_1	19		3	[24.0, 20.0, 12.0]	(CO, CR, FE, NI, RE)24(CO, CR, FE, MO, NI, RE, W)20(MO, W)12
MOO2	VO2		mP12	P2_1/c	14		2	[1.0, 2.0]	(MO)1(O)2
MOO3	gamma-WO3		mP32	P2_1/c	14		2	[1.0, 3.0]	(MO)1(O)3
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[1.0, 2.0]	(CO, FE, MO, NI, W)1(AL, HF, SI, TI, ZR)2
MSI2_C1	Fluorite (CaF2, C1)	C1	cF12	Fm-3m	225		2	[1.0, 2.0]	(CO, NI)1(AL, SI)2
MSI_B27	FeB (B27)	B27	oP8	Pnma	62	TiSi, HfSi, YSi, ZrSi (alpha), SiZr	2	[1.0, 1.0]	(HF, NB, TI, Y, ZR)1(AL, SI)1
MULLITE	Al(Al0.7Si0.3)2O4.8		oP24	Pbam	55		4	[1.0, 1.0, 1.0, 5.0]	(AL+3)1(AL+3)1(AL+3, SI+4)1(O-2, VA)5

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MZR3_E1A	MgCuAl2 (E1a)		oS16	Cmcm	63		2	[1.0, 3.0]	(CO, FE, NI)1(Y, ZR)3
NB1O2	alpha-NbO2		tI96	I4_1/a	88		2	[1.0, 2.0]	(NB)1(O)2
NB2B3	V2B3		oS20	Cmcm	63		2	[2.0, 3.0]	(NB)2(B)3
NB2O5	Nb2O5		mP99	P2/m	10		2	[2.0, 5.0]	(NB)2(O)5
NB3RU5	Rh5Ge3		oP16	Pbam	55		2	[0.375, 0.625]	(NB, RU)0.375(RU)0.625
NBH_BETA	Ta2H		oS8	C222	21		2	[1.0, 1.1]	(NB)1(H, VA)1.1
NBO	NbO		cP6	Pm-3m	221		2	[1.0, 1.0]	(NB)1(O)1
NBSN2	Mg2Cu (Cb)	Cb	oF48	Fddd	70		2	[1.0, 2.0]	(NB, SN, V)1(NB, SN)2
NI10ZR7	Ni10Zr7		oS68	Cmce	64		2	[23.0, 17.0]	(NI)23(HF, ZR)17
NI11ZR9	Pt11Zr9		tI40	I4/m	87		2	[11.0, 9.0]	(NI, PD)11(HF, ZR)9
NI17Y2	Fe17Lu2		hP80	P6_3/mmc	194	also Fe17Y2	2	[1.0, 0.1176]	(FE, NI)1(Y)0.1176
NI2SI_TETA	AlNi2		hP6	P-3m1	164		3	[1.0, 1.0, 1.0]	(NI)1(NI, VA)1(AL, SI)1
NI2TA	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(CO, NI)2(TA)1
NI2V	MoPt2		oI6	Immm	71		2	[2.0, 1.0]	(MO, NI, PD)2(MO, NB, TA, V)1
NI2Y1	Ni2Tm		cF192	F-43m	216		2	[2.0, 1.0]	(NI)2(Y)1
NI2Y3	Ni2Y3		tP80	P4_12_12	92		2	[2.0, 3.0]	(NI)2(Y)3
NI31SI12	Ni31S12		hP42	P321	150		2	[5.0, 2.0]	(CO, CR, FE, NI)5(SI)2
NI3B_D011	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(CO, CR, FE, MO, NI)3(B)1

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NI3SI2	Ni3Si2		oP80	Cmc2_1	36		2	[3.0, 2.0]	(NI)3(SI)2
NI3SI_MONOCL	Ge9Pd25		hP34	P-3	147		2	[3.0, 1.0]	(NI)3(SI)1
NI3SI_ORTHO	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[3.0, 1.0]	(NI)3(SI)1
NI3SN2_HT	Ni2In (B82)	B82	hP6	P6_3/mmc	194		3	[0.33333, 0.33334, 0.33333]	(NI)0.33333(NI, SN)0.33334(SN)0.33333
NI3SN2_LT	Ni3Sn2		oP20	Pnma	62		3	[0.2, 0.4, 0.4]	(SN)0.2(NI, SN)0.4(NI)0.4
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	C2/m	12		3	[0.25, 0.25, 0.5]	(NI)0.25(NI, SN)0.25(SN)0.5
NI3SN_D019	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194		2	[1.0, 3.0]	(SN)1(MN, NI)3
NI3SN_HT	BiF3 (D03)	D03	cF16	Fm-3m	225		3	[0.25, 0.25, 0.5]	(NI, SN)0.25(NI, SN)0.25(NI)0.5
NI3TA_D0A	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59	also Ni3Mo, Ni3Nb	2	[3.0, 1.0]	(AL, CO, CR, FE, NB, NI)3(AL, FE, MO, NB, NI, TA, TI, V, W)1
NI3TI_D024	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194		2	[0.75, 0.25]	(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	166		2	[3.0, 1.0]	(FE, NI)3(Y)1
NI4B3	m-Ni4B3		mS28	C2/c	15		2	[0.57142857, 0.42857143]	(NI)0.571429(B)0.428571
NI4Y	Unknown Structure		hR*				2	[4.0, 1.0]	(NI)4(Y)1
NI5ZR	AuBe5 (C15b)	C15b	cF24	F-43m	216	also Ni5Y, Ni5Hf	2	[5.0, 1.0]	(NI)5(HF, Y, ZR)1
NI7ZR2	Ni7Zr2		mS36	C2/m	12		2	[7.0, 2.0]	(AL, CO, CR, NI)7(HF, Y, ZR)2

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
NI8TA	Pt8Ti		tI18	I4/mmm	139		2	[8.0, 1.0]	(NI)8(NB, TA)1
NISI_B31	MnP (B31)	B31	oP8	Pnma	62		2	[1.0, 1.0]	(NI)1(SI)1
NITI2	NiTi2		cF96	Fd-3m	227		2	[1.0, 2.0]	(CO, CR, CU, FE, MO, NI, PD, RE, TI)1(AL, CR, HF, NI, TA, TI, ZR)2
NIWO4	Sylvanite (AgAuTe4, E1b)	E1b	mP12	P2/c	13		3	[1.0, 1.0, 4.0]	(CO+2, FE+2, MN+2, NI+2)1(W+6)1(O-2)4
NIZR	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(NI)1(TI, Y, ZR)1
OLIVINE	Forsterite (Mg2SiO4, S12)	S12	oP28	Pnma	62	fayalite [Fe2SiO4], tephroite [Mn2SiO4], Ni2SiO4, Co2SiO4	4	[1.0, 1.0, 1.0, 4.0]	(CO+2, FE+2, MN+2, NI+2)1(CO+2, FE+2, MN+2, NI+2)1(SI+4)1(O-2)4
PD2TI	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(PD)2(TI)1
PD3TI2	Pd3Ti2		oS20	Cmcm	63		2	[3.0, 2.0]	(PD)3(TI)2
PD4ZR3	Pd4Pu3		hR14	R-3	148		2	[4.0, 3.0]	(PD)4(ZR)3
PD5TI3	Pd5Ti3		tP8	P4/mmm	123		2	[5.0, 3.0]	(PD)5(TI)3
PDZRM	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		3	[1.0, 1.0, 1.0]	(PD)1(ZR)1(PD, ZR)1
PDZR_ALPHA	(PdZr-alpha)		mS*	Cm	8		2	[1.0, 1.0]	(PD)1(ZR)1
PDZR_BETA	CrB (B33)	B33	oS8	Cmcm	63		2	[1.0, 1.0]	(PD)1(ZR)1
PSEUDO_ BROOKITE	Pseudobrookite (Fe2TiO5, E41)	E41	oS32	Cmcm	63		3	[1.0, 2.0, 5.0]	(AL+3, TI+3, TI+4)1(AL+3, TI+3, TI+4)2(O-2)5
PT3TI4	Unknown Structure						2	[3.0, 4.0]	(PT)3(TI)4

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PT8TI	Pt8Ti		tI18	I4/mmm	139		2	[8.0, 1.0]	(PT)8(TI)1
P_PHASE	Cr9Mo21Ni20		oP56	Pnma	62		3	[24.0, 20.0, 12.0]	(CR, FE, NI, RE)24(CR, FE, MO, NI, RE)20 (MO)12
QUARTZ	alpha-Quartz (low Quartz)		hP9	P3_121	152		1	[1.0]	(SIO2)1
RE2O7	Re2O7		oP72	P2_12_12_1	19		1	[1.0]	(O7RE2)1
RE2SI	Re2Si		mP24	P2_1/c	14		2	[2.0, 1.0]	(RE)2(SI)1
RE3B	Re3B		oS16	Cmcm	63		2	[3.0, 1.0]	(CR, MO, RE, TA, W)3(B)1
RE7B3	Fe3Th7 (D102)	D102	hP20	P6_3mc	186		3	[7.0, 3.0, 3.0]	(CO, CR, MO, NB, RE, RU, TA, W)7(B)3(B, VA)3
REB2	ReB2		hP6	P6_3/mmc	194		3	[1.0, 2.0, 2.0]	(RE)1(B)2(B, VA)2
REO2	ReO2		mP14	P2_1/c	14		1	[1.0]	(O2RE1)1
REO3	alpha-ReO3 (D09)	D09	cP4	Pm-3m	221		1	[1.0]	(O3RE1)1
RESI2_C11B	Re4Si7		mS44	Cm	8		2	[0.357, 0.643]	(RE)0.357(SI)0.643
REZR2	Zr21Re25		hR92	R-3c	167		2	[1.0, 2.0]	(NI, RE)1(ZR)2
RHODONITE	Rhodonite (MnSiO3-b)		aP50	P-1	2	This is MnO.SiO2	3	[1.0, 1.0, 3.0]	(MN+2)1(SI+4)1(O-2)3
RU1B2	RuB2		oP6	Pmmn	59		2	[1.0, 2.0]	(RU)1(B)2
RU25Y44	Ru25Y44		oP276	Pnna	52		2	[0.362, 0.638]	(RU)0.362(Y)0.638
RU2B3	Ru2B3		hP10	P6_3/mmc	194		2	[2.0, 3.0]	(RU)2(B)3
RU2SI3	Ge3Ru2		oP40	Pbcn	60		2	[2.0, 3.0]	(RU)2(SI)3

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RU2SI_C37	Co2Si (C37)	C37	oP12	Pnma	62		2	[2.0, 1.0]	(RU)2(SI)1
RU2SN3	Ru2Sn3		tP20	P-4c2	116		2	[0.4, 0.6]	(RU)0.4(SN)0.6
RU2Y3	Er3Ru2		hP10	P6_3/m	176		2	[0.4, 0.6]	(RU)0.4(Y)0.6
RU2Y5	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15		2	[0.286, 0.714]	(RU)0.286(Y)0.714
RU3SN7	Ir3Ge7 (D8f)	D8f	cI40	Im-3m	229		2	[0.3, 0.7]	(RU)0.3(SN)0.7
RU4SI3	Ru4Si3		oP28	Pnma	62		2	[4.0, 3.0]	(RU)4(SI)3
RUB	Unknown Structure						2	[1.0, 1.0]	(RU)1(B)1
RUSI	FeSi (B20)	B20	cP8	P2_13	198		2	[1.0, 1.0]	(RU)1(SI)1
RUTILE_TIO2	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136	TiO2, also the high-temperature VO2, RUO2	2	[1.0, 2.0]	(AL+3, RU+4, SN+4, TI+4, V+4, ZR+4)1(O-2, VA-2)2
RUY3	Cementite (Fe3C, D011)	D011	oP16	Pnma	62		2	[0.25, 0.75]	(RU)0.25(Y)0.75
R_PHASE	R-(Co,Cr,Mo)		hR53	R-3	166		3	[27.0, 14.0, 12.0]	(CO, CR, FE, NI, RE)27(MO, W)14(CO, CR, FE, MO, NI, RE, W)12
SI3N4	Nierite (alpha-Si3N4)		hP28	P31c	159		2	[3.0, 4.0]	(SI)3(N)4
SI5V6	Si5V6		oI44	Ibam	72		2	[5.0, 6.0]	(SI)5(V)6
SIC	Zincblende (ZnS, B3)	B3	cF8	F-43m	216		2	[1.0, 1.0]	(SI)1(B, C)1
SN3O4	Sn3O4		mP14	P2_1/c	14		2	[3.0, 4.0]	(SN)3(O)4
SNO	PbO		tP4	P4/nmm	129		2	[1.0, 1.0]	(SN)1(O)1

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SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	Fd-3m	227		4	[1.0, 2.0, 2.0, 4.0]	(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
T1CUNITI	MoSi2 (C11b)	C11b	tI6	I4/mmm	139		2	[2.0, 1.0]	(CU, NI)2(TI)1
T2CUNITI	Cu3Ti2		tP10	P4/nmm	129		3	[0.175, 2.825, 2.0]	(CU)0.175(NI)2.825(TI)2
T4CUFETI	Unknown Structure					the Cu-Fe-Ti ternary phase, Tau4	2	[0.63, 0.37]	(CU, FE)0.63(TI)0.37
T4CUNITI	BaPb3		hR12	R-3m	166		3	[0.075, 0.675, 0.25]	(CU, TI)0.075(CU, NI)0.675(TI)0.25
T5CUFETI	Unknown Structure					the Cu-Fe-Ti ternary phase, Tau5	2	[0.55, 0.45]	(CU, FE)0.55(TI)0.45
T6CUNITI	Unknown Structure						3	[0.25, 0.5, 0.25]	(CU, TI)0.25(CU, NI)0.5(TI)0.25
TA1AL2	Al69Ta39		cF444	F-43m	216		2	[0.6389, 0.3611]	(AL, TA, TI)0.6389(AL, TA, TI)0.3611
TA2H_EPSLON	Unknown Structure						2	[2.0, 1.0]	(TA)2(H, VA)1
TA2O5_HT	Ta2O5-ht		tI44	I4_1/amd	141		2	[2.0, 5.0]	(TA)2(O)5
TA2O5_LT	beta-Ta2O5		oP14	Pccm	49		2	[2.0, 5.0]	(TA)2(O)5
TA5SI3_D8L	Cr5B3 (D8l)	D8l	tI32	I4/mcm	140		2	[5.0, 3.0]	(HF, NB, TA, TI)5(AL, SI)3
TAAL	Al38Ta48		mP86	P2_1/c	14		2	[0.8837, 1.1163]	(AL, TA, TI)0.8837(AL, TA, TI)1.1163
TAN_EPS	TaN-eps		hP6	P-62m	189		2	[1.0, 1.0]	(TA)1(N)1
TAU	Cr23C6 (D84)	D84	cF116	Fm-3m	225		4	[20.0, 6.0, 6.0,	(CO, HF, NI, RE)20(B)6(B, VA)6(AL, CR,

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								3.0]	HF, MO, RE, TA, TI, V, W, ZR)3
TI10O19	Unknown Structure						2	[10.0, 19.0]	(TI)10(O)19
TI20O39	Ti20O39		aP118	P-1	2		2	[20.0, 39.0]	(TI)20(O)39
TI2ALC	AlCCr2		hP8	P6_3/mmc	194	H, Ti2AlC1-x	3	[2.0, 1.0, 1.0]	(TI)2(AL)1(C, VA)1
TI2NIH	Ti2NiH		cF128	Fd-3m	227		3	[2.0, 1.0, 1.0]	(TI)2(NI)1(H)1
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136		2	[2.0, 1.0]	(TI)2(N)1
TI2SN3	Ti2Sn3		oS40	Cmce	64		2	[2.0, 3.0]	(CR, TI)2(SN)3
TI3AL1C2	CMo		hP12	P6_3/mmc	194	N, Ti3AlC2-x	3	[3.0, 1.0, 2.0]	(TI)3(AL, SI)1(C, VA)2
TI3ALC	Cubic Perovskite (CaTiO3, E21)	E21	cP5	Pm-3m	221	P, Ti3AlC1-x	3	[3.0, 1.0, 1.0]	(TI)3(AL)1(C, VA)1
TI3B4	Ta3B4 (D7b)	D7b	oI14	Immm	71	Cr3B4, Mn3B4, Nb3B4, Ti3B4, V3B4	2	[4.0, 3.0]	(B)4(AL, CR, HF, MN, NB, TA, TI, V)3
TI3CO5B2	Ti3Co5B2		tP20	P4/mbm	127		3	[3.0, 5.0, 2.0]	(TI)3(CO)5(B)2
TI3CU3O	Fe3W3C (E93)	E93	cF112	Fd-3m	227		3	[3.0, 3.0, 1.0]	(TI)3(CU)3(O)1
TI3N2	TiS-9R		hR6	R-3m	166		2	[0.71, 0.29]	(TI)0.71(N)0.29
TI3O2	(Ti3O2)		hP5	P6/mmm	191		2	[3.0, 2.0]	(TI)3(O)2
TI3O5	V3O5-ht		mS32	C2/c	15		2	[3.0, 5.0]	(TI, V)3(O)5
TI4CU2O	W4Co2C		cF112	Fd-3m	227		3	[4.0, 2.0, 1.0]	(TI)4(CU)2(O)1
TI4N3	Sc2Te3		hR8	R-3m	166		2	[0.685, 0.315]	(TI)0.685(N)0.315

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TI4O7	Ti4O7-a		aP22	P-1	2		2	[4.0, 7.0]	(TI, V)4(O)7
TI5O9	Ti5O9		aP28	P-1	2		2	[5.0, 9.0]	(TI, V)5(O)9
TI6O11	Ti6O11		aP34	P-1	2		2	[6.0, 11.0]	(TI, V)6(O)11
TI6SI2B	K2UF6		hP9	P-62m	189		3	[6.0, 2.0, 1.0]	(TI)6(SI)2(B)1
TI6SN5	Sn5Ti6-beta		hP22	P6_3/mmc	194		2	[6.0, 5.0]	(CR, MO, NB, TI, ZR)6(AL, SN)5
TI7O13	Ti7O13		aP40	P-1	2		2	[7.0, 13.0]	(TI, V)7(O)13
TI8O15	Ti8O15		aP46	P-1	2		2	[8.0, 15.0]	(TI, V)8(O)15
TI9O17	Ti9O17		aP52	P-1	2		2	[9.0, 17.0]	(TI)9(O)17
TIB2_C32	Hexagonal omega (C32)	C32	hP3	P6/mmm	191	TiB2, ZrB2, etc	2	[2.0, 1.0]	(B)2(AL, CR, HF, MN, MO, NB, TA, TI, V, Y, ZR)1
TIB_B27	FeB (B27)	B27	oP8	Pnma	62	TiB, FeB, HfB, MnB etc	2	[1.0, 1.0]	(B)1(CR, FE, HF, MN, MO, NB, TA, TI, V, W, Y, ZR)1
TIO_ALPHA	alpha-TiO		mS20	C2/m	12		2	[1.0, 1.0]	(TI+2)1(O-2)1
TISI2_C54	TiSi2 (C54)	C54	oF24	Fddd	70		2	[1.0, 2.0]	(MO, NB, RU, TI, ZR)1(AL, SI, SN)2
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	Cc	9		1	[1.0]	(SIO2)1
V2B3	V2B3		oS20	Cmcm	63		2	[0.4, 0.6]	(V)0.4(B)0.6
V2O5	Shcherbinaite (V2O5) (Revised)		oP14	Pmmn	59		2	[2.0, 5.0]	(V+5)2(O-2)5
V2O_SS	V7O3		mS20	C2/m	12	Gamma (V)	2	[1.0, 0.5]	(V)1(O, VA)0.5
V3C2	Sc2Te3		hR8	R-3m	166		2	[3.0, 2.0]	(V)3(C)2

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V3H2	Unknown Structure						2	[0.6, 0.4]	(V)0.6(H)0.4
V3O5_LT	V3O5-lt		mP32	P2/c	13		3	[2.0, 1.0, 5.0]	(V+3)2(V+4)1(O-2)5
V3O7	V3O7		mS120	C2/c	15		3	[2.0, 1.0, 7.0]	(V+5)2(V+4)1(O-2)7
V52O64	V13O16		tI116	I4_1/amd	141	delta-prime V-oxide	2	[52.0, 64.0]	(V)52(O)64
V5B6	V5B6		oS22	Cmmm	65		2	[5.0, 6.0]	(NB, TI, V)5(B)6
V6O13	V6O13		mS38	C2/m	12		3	[2.0, 4.0, 13.0]	(V+5)2(V+4)4(O-2)13
VO2_LT	VO2		mP12	P2_1/c	14		2	[1.0, 2.0]	(V+4)1(O-2)2
W1O2	VO2		mP12	P2_1/c	14		1	[1.0]	(O2W1)1
W5SI3_D8M	W5Si3 (D8m)	D8m	tI32	I4/mcm	140		3	[4.0, 1.0, 3.0]	(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						1	[1.0]	(O2_72W1)1
WO2_90	Unknown Structure						1	[1.0]	(O2_90W1)1
WO2_96	Unknown Structure						1	[1.0]	(O2_96W1)1
WO3_HT	WO2.95		tP16	P-42_1m	113		1	[1.0]	(O3W1)1
WO3_LT	WO3		oP32	Pbcn	60		1	[1.0]	(O3W1)1
Y15C19_H	Unknown Structure						2	[19.0, 15.0]	(C)19(Y)15
Y15C19_R	alpha-Y15C19		oP18	Pbam	55		2	[19.0, 15.0]	(C)19(Y)15
Y1B6	CaB6 (D21)	D21	cP7	Pm-3m	221		2	[1.0, 6.0]	(Y)1(B)6

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
Y2C3_H	Unknown Structure						3	[2.0, 2.0, 1.0]	(Y)2(C)2(C, VA)1
Y2C3_R	Sc3C4		tP70	P4/mnc	128		3	[2.0, 2.0, 1.0]	(Y)2(C)2(C, VA)1
Y3SI5_HT	Hexagonal omega (C32)	C32	hP3	P6/mmm	191		2	[3.0, 5.0]	(Y)3(SI)5
Y3SI5_LT	Unknown Structure						2	[3.0, 5.0]	(Y)3(SI)5
YB4	ThB4 (D1e)	D1e	tP20	P4/mbm	127		2	[1.0, 4.0]	(Y)1(B)4
YB66	YB66		cF1936	Fm-3c	226		2	[1.0, 66.0]	(Y)1(B)66
YC2_C11A	CaC2-I (C11a)	C11a	tI6	I4/mmm	139		1	[1.0]	(C2Y1)1
YC_GAMMA	Rock Salt (NaCl, B1)	B1	cF8	Fm-3m	225		2	[1.0, 1.0]	(Y)1(C, C2, VA)1
YH3_EPSLON	H3Ho		hP24	P-3c1	165		2	[1.0, 3.0]	(Y)1(H, VA)3
YSI2_HT	Unknown Structure						2	[1.0, 2.0]	(Y)1(SI)2
ZR5SI4	Si4Zr5		tP36	P4_12_12	92	Ti5Si4, Hf5Si4, Y5Si4, Zr5Si4 (alpha)	2	[5.0, 4.0]	(HF, MO, NB, TI, Y, ZR)5(AL, SI)4
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	P2_1/c	14		2	[2.0, 4.0]	(AL+3, CR+3, HF+4, TI+4, Y+3, ZR+4)2(O-2, VA)4
ZRO2_TETR	HgI2 (C13)	C13	tP6	P4_2/nmc	137		2	[2.0, 4.0]	(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 (C49)	C49	oS12	Cmcm	63		2	[1.0, 2.0]	(HF, NB, Y, ZR)1(SI)2
ZRSIO4	Zircon (ZrSiO4, S11)	S11	tI24	I4_1/amd	141		3	[1.0, 1.0, 4.0]	(SI+4)1(Y+3, ZR+4)1(O-2, VA)4
ZRTI2O6	Columbite (FeNb2O6, E51)	E51	oP36	Pbcn	60		3	[1.0, 2.0, 6.0]	(ZR+4)1(TI+4)2(O-2)6

Name	*Prototype*	*Strukturbericht*	*Pearson_ Symbol*	*Space_ Group_ Symbol*	*SG#*	*Info*	*Sublattices*	*Sites*	*Formula_unit*
ZRTIO4_ALPHA	Unknown Structure						3	[1.0, 1.0, 4.0]	(ZR+4)1(TI+4)1(O-2)4
ZRTIO4_BETA	zeta-Fe2N		oP12	Pbcn	60		2	[2.0, 4.0]	(TI+4, ZR+4)2(O-2)4
GAS	Gas					Gas mixture	1	[1.0]	(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, 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

TCTI5 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 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:	**5.1**
First release:	**TCTI1 was released in 2017**

Changes in the Most Recent Database Release

TCTI5.0 to TCTI5.1

Software release 2023b (June 2023)

- The surface tension was re-assessed based on the Redlich-Kister-Muggianu (R-K-M) sub-regular solution model.

TCTI4 to TCTI5

Software release 2023a (December 2022/January 2023)

- Updates to Ti-Al-B, Ti-Al-C, Ti-Al-Cr, Ti-Al-Mo, Ti-Al-Nb, Ti-Al-O, Ti-Al-Si, Ti-Al-Sn, Ti-Al-W, and Ti-Al-Zr.
- Modeled the Ti-Si-Zr ternary system.
- Full gas descriptions are added.
- There is a change to default settings. From this release, the GAS phase is restored by default when retrieving the data from the database. In order to reject it when it is not required for a calculation, you have to now manually reject it.

The following volume parameters are updated for:

- Liquid in Ti-V and Ti-Al-V
- AlTi3_D019 in Ti-Al-O
- BCC_A2 in Ti-H
- HCP_A3 in Ti-O and Ti-N

Previous Releases

TCTI3 to TCTI4

Software release 2022a (December 2021/January 2022)

- Added 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.

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.
- Ti-Al-Cr is updated.
- 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.