

TCS Ti/TiAl-based Alloys Database (TCTI6)

Technical Information

Available Starting with Thermo-Calc Version 2024b



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

TCS Ti/TiAl-based Alloys Database (TCTI) is a thermodynamic and properties database developed for conventional Ti-based and newly emerging γ -TiAl based alloys. All necessary volume data (including molar volume and thermal expansion) for various solution and intermetallic phases is available.

This database 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

The database can be used with our entire suite of products: Thermo-Calc, the Add-on Modules, and all available SDKs.

In addition to thermodynamic data, it has thermophysical and elastic 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
- Elastic moduli and elastic constants



[TCTI: TCS Ti/TiAl-based Alloys Database Revision History](#). The current version of the database is TCTI6. See the link for any subversion release details.



The database is compatible with the TCS Ti-alloys Mobility Database (MOBTI). The current version is MOBTI5.



The thermophysical 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 elastic properties data is available starting with TCTI6.

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.



For more learning resources about CALPHAD and our databases, visit the video tutorials on our [website](#) or our [YouTube playlist](#).



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 TCTI6 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 thermophysical properties data (e.g. viscosity, surface tension, etc.), the elastic properties (elastic moduli and constants), a list of the included elements, and summaries of the database revision history by version.
- The *TCS Ti/TiAl-based Alloys Database (TCTI) Validation and Calculation 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 a Validation and Calculation 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.

TCTI6 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
- 423 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.

Thermophysical Properties Data

A variety of thermophysical 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, thermomechanical, and properties 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 thermophysical 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.
- Electrical resistivity and thermal conductivity are critically assessed with available data for liquid, BCC, HCP, FCC, and 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 THERMOPHYSICAL 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 an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property (and Graphical Mode Variable Name)	Model Parameters	Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)***
Molar volume	VO, VA	VM for a system $VM(PHI)$ for phase PHI
Electrical conductivity	ELQ**	ELCD for a system $ELCD(PHI)$ for phase PHI
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
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)**

* 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. As of 2024a, TCMG7, TCAL9, and TCHEA7. As of 2024b, TCSLD5.

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

*** The examples listed for the SDKs are using Console Mode syntax. The quantities can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. See the various model descriptions or the SDK help for details.

Elastic Properties Data

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

Starting with TCTI6, the elastic properties (elastic moduli and elastic constants) are added to the database.

GRAPHICAL MODE

In the **Plot Renderer** in Graphical Mode, elastic constants and moduli can be selected from the drop-down list of axis variables.

The independent elastic constants are selected on the **Plot Renderer** as an axis variable **Elastic constant** and then choose an option (**C11**, **C12**, **C13**, **C33**, or **C44**) from the drop-down list.

The elastic moduli, **Bulk modulus**, **Shear modulus**, and **Young's modulus**, are directly available from the **Axis variable** list.

All can be tabulated and plotted using the quantity names, with options for a specific phase or all phases.

CONSOLE MODE

The quantities corresponding to the individual elastic constants and elastic moduli (derived from the elastic constants) can be calculated in Console Mode for individual phases or all phases. The results can be shown in the POLY module with the command `SHOW_VALUE` or shown as a plot in the POST module with the command `PLOT_DIAGRAM` using:

- `Cij(<phase name>)` **OR** `Cij(*)`
- **Bulk modulus:** `BULKMOD(<phase name>)` **OR** `BULKMOD(*)`
- **Shear modulus:** `SHEARMOD(<phase name>)` **OR** `SHEARMOD(*)`
- **Young's modulus:** `YOUNGMOD(<phase name>)` **OR** `YOUNGMOD(*)`

TC-PYTHON AND TC-TOOLBOX FOR MATLAB®

For the Software Development Kits (SDKs), i.e. TC-Python and TC-Toolbox, the quantities of elastic constants, bulk modulus, shear modulus, and Young's modulus can be retrieved for individual phases or all phases via `get_value_of()` or `get_values_of()` from any equilibrium calculation types using:

- `Cij(<phase name>)` **OR** `Cij(ALL_PHASES/*)`
- `ThermodynamicQuantity.bulk_modulus(<phase name>)` **OR** `ThermodynamicQuantity.bulk_modulus(ALL_PHASES/*)`
- `ThermodynamicQuantity.shear_modulus (<phase name>)` **OR** `ThermodynamicQuantity.shear_modulus(ALL_PHASES/*)`
- `ThermodynamicQuantity.youngs_modulus(<phase name>)` **OR** `ThermodynamicQuantity.youngs_modulus(ALL_PHASES/*)`



See the relevant SDK documentation for details.

TCTI6 Systems

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TCTI6 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			

TCTI6 Phases

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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 (*).



TCTI6 Models for the Included Phases

<i>Name in the Database</i>	<i>Common Name and Description</i>
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.
B19_ORTHO*	This is the orthorhombic martensite in Ti-Ni-based alloys.
B19_PRIME*	This is the monoclinic martensite in Ti-Ni-based alloys.
B82_omega	This is the ω_0 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.

Name in the Database	Common Name and Description
M5Si3_D88	Ti ₅ Si ₃ is modeled as this phase.
O_PHASE	This is the orthorhombic phase stable in Ti-Al-Nb, Ti-Al-Ta and possibly in multicomponent TiAl alloys.
OMEGA*	The omega phase is a metastable phase which forms in titanium and its alloys with transition elements (like V, Mo, Nb, Fe, etc).
R_MARTE*	This is an intermediate martensite, R-phase, in Ti-Ni-based alloys.
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 ₂ N is modeled as this phase.
Ti2Ni3*	This is a tetragonal metastable precipitate in Ti-Ni alloys.
Ti3Ni4*	This is a metastable precipitate in Ti-Ni alloys.
Ti3B4	Ti ₃ B ₄ is modeled as this phase.
Ti3N2	η-Ti ₃ N _{2-x} phase in Ti-N binary.
Ti4N3	ζ-Ti ₄ N _{3-x} phase in Ti-N binary.
TiSi2_C54	TiSi ₂ is modeled as this phase.
Zr5Si4	Ti ₅ Si ₄ is modeled as this phase.

* Electrical resistivity and thermal conductivity are not assessed for this phase.

TCTI6 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	Info	Sublattices	Formula Unit
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6 ₃ /mmc)	Ti3Al	3	(AL, CO, CR, CU, MN, MO, NB, NI, TA, Ti, V, W, ZR)3.0(AL, C, CR, MO, NB, SI, SN, TA, Ti, V, W)1.0(H, O, VA)2.0
ALTI_L10	CuAu (L10)	L10	tP2	(123, P4/mmm)	TiAl	3	(AL, CO, CR, CU, MN, MO, NB, NI, PD, SN, TA, Ti, V, W, ZR)1.0(AL, CO, CR, CU, MN, MO, NB, NI, PD, SN, TA, Ti, V, W, ZR)1.0(C, H, O, Si, VA)2.0
B82_OMEGA	Ni2In (B82)	B82	hP6	(194, P6 ₃ /mmc)		3	(AL, SN, Ti)1.0(CO, CR, MO, NB, TA, Ti, ZR)1.0(AL, Ti)1.0
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	Metallic BCC_A2 solution. If BCC_B2 is defined, this phase will be combined to it.	2	(, AG, AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, PD, PT, RE, RU, SI, SN, TA, Ti, V, VA, W, Y, ZR)1.0(B, C, H, N, O, VA)3.0
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	Solution of ordered BCC_B2, having Gibbs energy contribution from BCC_A2	3	(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)3.0
FCC_B1	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	TiC, TiN, TiO	2	(AL, CR, HF, MO, NB, TA, Ti, V, VA, W, ZR)1.0(C, N, O, VA)1.0
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6 ₃ /mmc)	Metallic HCP_A3 solution, alpha_Ti	2	(AG, AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, PD, PT, RE, RU, SI, SN, TA, Ti, V, W, Y, ZR)1.0(B, C, H, N, O, VA)0.5
LIQUID	Liquid				Metallic LIQUID:L solution phase	1	(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, SNO, SNO2, TA, TA2/5O1, Ti, TiO3/2, V, V1O1, VO2, VO3/2, VO5/2, W, Y, Y2/3O1, ZR, ZR1/2O1)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
OMEGA	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	s metastable structure of Ti	1	(, AL, B, C, CO, CR, FE, HF, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W, Y, ZR)1.0
O_PHASE	NaHg		oS16	(63, Cmcm)	The O phase	3	(NB, TA, TI)0.5(AL, NB, TA, TI)0.25(NB, TA, TI)0.25
TI2X_OMEGA	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	Ordered Omega phase, B82 or C32 type	2	(TI)2.0(AL, B, C, CO, CR, FE, HF, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W, Y, ZR)1.0
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_3/mmc)		2	(AL, CO, CR, FE, HF, MN, MO, NB, NI, PD, RE, RU, TA, TI, V, W, Y, ZR)2.0(AL, CO, CR, FE, HF, MN, MO, NB, NI, PD, RE, RU, TA, TI, V, W, Y, ZR)1.0
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)		2	(AL, CO, CR, FE, HF, MN, MO, NB, SI, TA, TI, V, W, Y, ZR)2.0(AL, CO, CR, FE, HF, MO, NB, SI, TA, TI, V, W, Y, ZR)1.0
C16_THETA	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Hf2Al, Hf2Si, Zr2Si Zr2Co, Ta2Co, Hf2Ni, Ta2Ni, Zr2Ni	2	(AL, HF, TA, TI, ZR)2.0(AL, CO, FE, NI, SI)1.0
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_3/mmc)		2	(AL, CO, CR, FE, HF, MO, NB, TA, TI, ZR)2.0(AL, CO, CR, FE, HF, MO, NB, TA, TI, ZR)1.0
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(AL, CO, CR, FE, MN, MO, NB, NI, RE, RU, SI, SN, TA, TI, V, W, Y, ZR)1.0(B, C, H, VA)1.0
DIS_MU	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	Part of the description of MU_PHASE	1	(CO, FE, MN, MO, NB, NI, TA)1.0
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	DIS_MU contribution is introduced in the description of this phase	4	(CO, FE, MN, MO, NB, NI, TA)1.0(CO, FE, MN, MO, NB, NI, TA)2.0(CO, FE, MN, MO, NB, NI, TA)6.0(CO, FE, MN, MO, NB, NI, TA)4.0
DIS_SIG	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)		1	(CO, CR, FE, MN, MO, NB, NI, RE, RU, TA, V, W)1.0
ORD_SIG	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)		3	(CO, CR, FE, MN, MO, NB, NI, RE, RU, TA, V, W)10.0(CO, CR, FE, MN, MO, NB, NI, RE, RU, TA, V, W)4.0(CO, CR, FE, MN, MO, NB, NI, RE, RU, TA, V, W)16.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4 ₂ /mmm)		3	(AL, CO, CR, FE, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W)10.0(CO, CR, FE, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W)4.0(AL, CO, CR, FE, MN, MO, NB, NI, RE, RU, SI, TA, TI, V, W)16.0
GPHASE	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		4	(AL, CO)1.0(AL, TI)16.0(CO)7.0(TI)6.0
G_PHASE	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		3	(AL, CO, CU, FE, MN, NI, PD, TI)16.0(HF, TI, Y, ZR)6.0(CO, CU, FE, MN, NI, PD)7.0
H_L21	Heusler (L21)	L21	cF16	(225, Fm-3m)		3	(AL, NI, SN, TI)0.5(AL, NI, TI)0.5(CO, CU, NI, VA)1.0
L10_FCC	CuAu (L10)	L10	tP2	(123, P4/mmm)		2	(MN, NI)0.5(MN, NI)0.5
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(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
AF	FeGaO3		oP40	(33, Pna2 ₁)	Al2O3.Fe2O3	2	(AL2O3)1.0(Fe2O3)1.0
AG1TI2	CuZr2		tI6	(139, I4/mmm)		2	(AG)1.0(TI)2.0
AGTI	CdTi		tP4	(129, P4/nmm)		2	(AG, TI)1.0(AG, TI)1.0
AL11CR2	Al5Cr		mS732	(15, C2/c)		2	(AL)10.0(AL, CR, TI)2.0
AL11CR4	Al11Mn4		aP15	(2, P-1)		2	(AL)11.0(AL, CR, TI)4.0
AL11MN4_HT	Mn6(Mn0.5Al0.5)8Al25		oP156	(62, Pnma)		2	(AL, MN)29.0(MN)10.0
AL11MN4_LT	Al11Mn4		aP15	(2, P-1)		2	(AL)11.0(MN)4.0
AL11RE4	Al11Mn4		aP15	(2, P-1)		2	(AL)11.0(RE)4.0
AL12MN	Al12W		cl26	(204, Im-3)		2	(AL)12.0(MN)1.0
AL12W	Al12W		cl26	(204, Im-3)	also AL12RE and AL12MO	2	(AL)12.0(MO, RE, W)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL13CO4	Orthorhombic Co4Al13		oP102	(31, Pmn2_1)		2	(AL)13.0(CO)4.0
AL13FE4	Al13Fe4		mS102	(12, C2/m)	also Al13Ru4	3	(AL)0.6275(Fe, Ru)0.235(AL, VA)0.1375
AL17MO4	Al17Mo4		mS84	(5, C2)		2	(AL)17.0(MO)4.0
AL1RE2	CuZr2		tI6	(139, I4/mmm)	C11_b	2	(AL)1.0(RE)2.0
AL1ZR2	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)	also AlY2	2	(AL)1.0(Ti, Y, Zr)2.0
AL21PT8	Al21Pt8		tI116	(88, I4_1/a)	also Al21Pd8	2	(AL)21.0(PD, PT)8.0
AL21V2	Al10V		cF176	(227, Fd-3m)		2	(AL)21.0(V)2.0
AL22MO5	Al22Mo5		oF216	(43, Fdd2)		2	(AL)22.0(MO)5.0
AL23V4	Al23V4		hP54	(194, P6_3/mmc)		2	(AL)23.0(V)4.0
AL2CU_C16	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(AL)2.0(AL, CU)1.0
AL2FE	Al2Fe		aP18	(1, P1)		2	(AL)2.0(Fe)1.0
AL2N2TI3	(Al2Ti3N2)		hP22	(186, P6_3mc)		3	(AL)2.0(N)2.0(TI)3.0
AL2PD5	Unknown Structure					2	(AL)2.0(AL, PD)5.0
AL2TI	Ga2Hf		tI24	(141, I4_1/amd)		2	(AL, NB, TA, TI)2.0(AL, CO, CR, NB, TA, TI, V, ZR)1.0
AL2W	CrSi2 (C40)	C40	hP9	(180, P6_222)		2	(AL)2.0(W)1.0
AL2ZR3	Zr3Al2		tP20	(136, P4_2/mnm)	also Al2Hf3, Al2Y3	2	(AL)2.0(HF, TI, Y, ZR)3.0
AL3CO	Os4Al13		mS34	(12, C2/m)		2	(AL)3.0(CO)1.0

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AL3MO	MoAl3		mS32	(12, C2/m)		2	(AL)3.0(MO)1.0
AL3NI1	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(AL)0.75(NI)0.25
AL3NI2	Al3Ni2 (D513)	D513	hP5	(164, P-3m1)		3	(AL, PD)3.0(AL, NI, PD, RU)2.0(NI, RU, VA)1.0
AL3NI5	Ga3Pt5		oS16	(65, Cmmm)		2	(AL)0.375(NI)0.625
AL3PD1	(Al3Pd)		oP*	(33, Pna2_1)		2	(AL)3.0(PD)1.0
AL3PD5	Rh5Ge3		oP16	(55, Pbam)	also Al3Pt5	2	(AL)3.0(PD, PT)5.0
AL3TI_D022	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	also Al3V	2	(AL, MN, MO, NB, PD, SI, TI, V)3.0(AL, CO, CR, MN, MO, NB, NI, PD, SI, TA, TI, V, ZR)1.0
AL3TI_LT	Al3Ti-LT		tI32	(139, I4/mmm)		2	(AL, CR, NB, TI)3.0(AL, CR, NB, TI, V, ZR)1.0
AL3Y_HT	BaPb3		hR12	(166, R-3m)		2	(AL)0.75(Y)0.25
AL3Y_LT	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)		2	(AL)0.75(Y)0.25
AL3ZR2	Zr2Al3		oF40	(43, Fdd2)	also Al3Hf2	2	(AL)3.0(HF, ZR)2.0
AL3ZR4	Al3Zr4		hP7	(191, P6/mmm)	also Al3Hf4	2	(AL)3.0(HF, TI, ZR)4.0
AL3ZR5	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)		2	(AL)3.0(TI, ZR)5.0
AL3ZR_D023	Al3Zr (D023)	D023	tI16	(139, I4/mmm)	also Al3Hf	2	(AL)3.0(HF, TI, ZR)1.0
AL4V7	Al4V7		mS104	(12, C2/m)		2	(AL)45.0(V)7.0
AL4C3	Al4C3 (D71)	D71	hR7	(166, R-3m)		2	(AL)4.0(C)3.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL4CR	mu-Al4Mn		hP574	(194, P6 ₃ /mmc)		2	(AL)4.0(AL, CR, TI)1.0
AL4FE	AlmFe		tI110	(121, I-42m)		2	(AL)4.2(FE)1.0
AL4MN_R	lambda-Al4Mn		hP586	(194, P6 ₃ /mmc)		2	(AL)461.0(MN)107.0
AL4MN_U	mu-Al4Mn		hP574	(194, P6 ₃ /mmc)		2	(AL)4.0(MN)1.0
AL4PD	(Al4Pd)		hP*	(182, P6 ₃ 22)		2	(AL)4.0(PD)1.0
AL4RE	Unknown Structure					2	(AL)4.0(RE)1.0
AL4W	Al4W		mS30	(8, Cm)	also Al4Mo	2	(AL)4.0(MO, W)1.0
AL4ZR5	Ti5Ga4		hP18	(193, P6 ₃ /mcm)		2	(AL)4.0(ZR)5.0
AL5CO2_D811	Co2Al5 (D811)	D811	hP28	(194, P6 ₃ /mmc)		2	(AL)5.0(CO)2.0
AL5FE2	Al2.8Fe		oS24	(63, Cmc)		2	(AL)5.0(FE)2.0
AL5FE4	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		1	(AL, FE)1.0
AL5TI2	Al5Ti2		tP28	(123, P4/mmm)		2	(AL, CR, NB, TA, TI)5.0(AL, CR, NB, TA, TI, V, ZR)2.0
AL5TI3	Al5Ti3		tP32	(127, P4/mbm)		2	(AL)5.0(CR, NB, TA, TI)3.0
AL5W	Al5W		hP12	(182, P6 ₃ 22)	also Al5MO	2	(AL)5.0(MO, W)1.0
AL63MO37	Unknown Structure					2	(AL)63.0(MO)37.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL6MN	MnAl6 (D2h)	D2h	oS28	(63, Cmcm)		2	(AL)6.0(MN, RE, RU)1.0
AL77W23	Unknown Structure					2	(AL)77.0(W)23.0
AL7CR	Al45V7		mS104	(12, C2/m)		2	(AL)13.0(AL, CR, TI)2.0
AL7W3	Unknown Structure					2	(AL)7.0(W)3.0
AL8CR5_HT	gamma-brass (Cu5Zn8, D82)	D82	cl52	(217, I-43m)		4	(AL, CR)2.0(AL, CR, TI)3.0(CR)2.0(AL)6.0
AL8CR5_LT	Cr5Al8 (D810)	D810	hR26	(160, R3m)		3	(AL)12.0(CR)5.0(AL, CR, TI)9.0
AL8CR5_MT	Unknown Structure					4	(AL, CR, TI)2.0(AL, CR, TI)3.0(CR)2.0(AL)6.0
AL8MO3	Al8Mo3		mS22	(12, C2/m)		2	(AL)8.0(MO)3.0
AL8V5	gamma-brass (Cu5Zn8, D82)	D82	cl52	(217, I-43m)		2	(AL, MN, V)8.0(AL, MN, TI, V)5.0
AL9CO2	Co2Al9 (D8d)	D8d	mP22	(14, P2_1/c)		2	(AL)9.0(CO)2.0
ALB12	alpha-AlB12		tP216	(92, P4_12_12)		2	(AL, TI)1.0(B)12.0
ALCR2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(AL, CR, NI, PD)1.0(AL, CR, TI)2.0
ALCR3	Unknown Structure				AlCr3 super lattice	2	(AL, CR, TI)1.0(CR)3.0
ALCU_DEL	Al5Cu8		hR52	(160, R3m)		2	(AL)2.0(CU)3.0
ALCU_EPS	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(AL, CU)1.0(CU)1.0
ALCU_ETA	AlCu(r)		mS20	(12, C2/m)		2	(AL, CU)1.0(CU)1.0
ALCU_ZETA	Al9Cu11(h)		oF88	(42, Fmm2)		2	(AL)9.0(CU)11.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALH3	AlH3		oP24	(58, Pnm)		2	(Al)1.0(H)3.0
ALNTI2	AlCCr2		hP8	(194, P6 ₃ /mmc)		3	(Al)1.0(N)1.0(Ti)2.0
ALNTI3	Cubic Perovskite (CaTiO ₃ , E21)	E21	cP5	(221, Pm-3m)		3	(Al)1.0(N)1.0(Ti)3.0
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6 ₃ mc)		2	(Al)1.0(N)1.0
ALPHA_B19	beta'-AuCd (B19)	B19	oP4	(51, Pmma)		2	(PT, Ti)1.0(PT, Ti)1.0
ALPHA_SPINEL	Hausmannite (Mn ₃ O ₄)		tl28	(141, I4 ₁ /amd)		4	(CO+2, MN+2, MN+3, NI+2)1.0(AL+3, CR+3, FE+3, MN+2, MN+3, VA)2.0 (MN+2, VA)2.0(O-2)4.0
ALRE	gamma-CuTi (B11)	B11	tp4	(129, P4/nmm)		2	(Al)1.0(RE)1.0
ALS13TI2	Zr ₃ Al ₄ Si ₅		tl24	(141, I4 ₁ /amd)		3	(Al)0.166667(Si)0.5(Ti)0.333333
ALZR	CrB (B33)	B33	oS8	(63, Cmc)	also AlHf, AlY	2	(Al)1.0(HF, Y, Zr)1.0
ANDALUSITE	Andalusite (Al ₂ SiO ₅ , S02)	S02	oP32	(58, Pnm)	A high-pressure phase (Al ₂ O ₃ .SiO ₂)	4	(Al+3)1.0(AL+3)1.0(Si+4)1.0(O-2)5.0
B12ZR	UB12 (D2f)	D2f	cF52	(225, Fm-3m)	YB12, ZrB12	2	(B)12.0(Y, Zr)1.0
B19_ORTHO	beta'-AuCd (B19)	B19	oP4	(51, Pmma)	orthorhombic martensite in Ti-Ni-based alloys	2	(Cu, Ni, Ti)0.5(Cu, Ni, VA)0.5
B19_PRIME	NiTi		mP4	(11, P2 ₁ /m)	monoclinic martensite in Ti-Ni-based alloys	2	(Cu, Ni, Ti)0.5(Cu, Ni, VA)0.5
B2O3	B2O3		hP15	(152, P3 ₁ 21)		1	(B2O3)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
B3SI	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		3	(B)6.0(SI)2.0(B, SI)6.0
B4C	B13C2 B4C (D1g)	D1g	hR15	(166, R-3m)		2	(B11C, B12)1.0(B2, C2B, CB2, SI2)1.0
B5W2_X	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)		2	(B, C, VA)5.0(W)2.0
B6SI	SiB6		oP280	(58, Pnm)		3	(B)210.0(SI)23.0(B, SI)48.0
B9W2	W2B9		hP22	(147, P-3)		2	(B)9.0(W)2.0
BCT_A5	beta-Sn (A5)	A5	tI4	(141, I4_1/amd)		1	(AL, CU, SN, TI)1.0
BETAR_BORON	beta-B (R-105)		hR105	(166, R-3m)		2	(B)93.0(B, C, NB, SI, TI)12.0
DIS_BETA	V2H1.1		tI56	(141, I4_1/amd)	V-H binary	2	(H, VA)0.5(V)0.5
BETA_PHASE	V2H		mS6	(12, C2/m)	V-H binary	3	(H, VA)0.25(H, VA)0.25(V)0.5
BETA_V3O	CoO		tI4	(139, I4/mmm)		2	(V)1.0(O, VA)1.0
BNSI	alpha-B (hR12)		hR12	(166, R-3m)		3	(B)61.0(SI)1.0(B, SI)8.0
BN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)		2	(B)1.0(N)1.0
BW_ALPHA	MoB (Bg)	Bg	tI16	(141, I4_1/amd)		2	(B, C, VA)1.0(W)1.0
BW_BETA	CrB (B33)	B33	oS8	(63, Cmcm)		2	(B, C, VA)1.0(W)1.0
CEMENTITE	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)	D011	2	(FE, MN)3.0(C, N)1.0
CHI_A12	alpha-Mn (A12)	A12	cl58	(217, I-43m)		3	(RE)24.0(HF, MO, NB, TA, TI, W, ZR)10.0(MO, NB, RE, TA, W)24.0
CO11ZR2	(Co11Hf2)		oP*	(50, Pban)		2	(CO)11.0(ZR)2.0

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CO17Y2	Ni17Th2		hP38	(194, P6_3/mmc)		3	(CO ₂ , Y)1.0(CO ₂ , Y)2.0(CO)15.0
CO1SN1TI1	Unknown Structure					3	(CO, NI)1.0(SN)1.0(TI)1.0
CO1SN2	Khatyrkite (Al ₂ Cu, C16)	C16	tI12	(140, I4/mcm)		2	(CO)0.333(SN)0.667
CO1SN3	Au ₃ Zn		oS32	(64, Cmce)		2	(CO)0.25(SN)0.75
CO2SI_C23	Cotunnite (PbCl ₂ , C23)	C23	oP12	(62, Pnma)	also Ni ₂ Si(delta)	2	(AL, CO, NI, PD)2.0(AL, PD, SI)1.0
CO3SI	Ni ₃ Sn (D019)	D019	hP8	(194, P6_3/mmc)		2	(CO)3.0(SI)1.0
CO3SN2	Ni ₂ In (B82)	B82	hP6	(194, P6_3/mmc)		4	(CO)1.0(SN)1.0(CO, VA)0.5(CO, VA)0.5
CO3VV	Al ₃ Pu		hP24	(194, P6_3/mmc)		2	(CO, V)3.0(CO, V)1.0
CO3Y1	Ni ₃ Pu		hR12	(166, R-3m)		2	(CO)3.0(Y)1.0
CO3Y2	Unknown Structure		cP*			2	(CO)3.0(Y)2.0
CO3Y4	Co ₃ Ho ₄		hP22	(176, P6_3/m)		2	(CO)3.0(Y)4.0
CO5Y8	Co ₅ Y ₈		mP52	(14, P2_1/c)		2	(CO)5.0(Y)8.0
CO5Y_D2D	CaCu ₅ (D2d)	D2d	hP6	(191, P6/mmm)		3	(CO ₂ , Y)1.0(CO)4.0(CO, VA)1.0
CO7HF	(Co ₁₁ Hf ₂)		oP*	(50, Pban)		2	(CO)7.0(HF)1.0
CO7M2	(Co ₇ Nb ₂)		mS18	(12, C2/m)		2	(CO)7.0(NB, TA, TI)2.0
CO7MO6	Fe ₇ W ₆ (D85) mu-phase	D85	hR13	(166, R-3m)	mu phase	2	(CO, MO)7.0(CO, MO, TI)6.0
CO7W6	Fe ₇ W ₆ (D85) mu-phase	D85	hR13	(166, R-3m)	mu phase	4	(CO, W)4.0(CO, W)2.0(CO, W)1.0(CO, W)6.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CO7Y6	Unknown Structure					2	(CO)7.0(Y)6.0
COB	FeB (B27)	B27	oP8	(62, Pnma)		2	(CO)1.0(B)1.0
CORUNDUM	Corundum (Al ₂ O ₃ , D51)	D51	hR10	(167, R-3c)	corundum [Al ₂ O ₃], eskolaite [Cr ₂ O ₃], hematite [Fe ₂ O ₃], Ti ₂ O ₃ , V ₂ O ₃	3	(AL+3, CR+2, CR+3, FE+2, FE+3, MN+3, TI+3, V+3, V+4, VA)2.0(CR+3, FE+3, NI+2, VA)1.0(O-2)3.0
COSN	CoSn (B35)	B35	hP6	(191, P6/mmm)		2	(CO)0.5(SN)0.5
COY_BF	CrB (B33)	B33	oS8	(63, Cmcm)		2	(CO)1.0(Y)1.0
CR2B_ORTH	Mg ₂ Cu (Cb)	Cb	oF48	(70, Fddd)		2	(CR)2.0(B)1.0
CR2PD3_L12	Bogdanovite (Cu ₃ Au, L12)	L12	cP4	(221, Pm-3m)		2	(CR)0.4(PD)0.6
CR3MN5	alpha-Mn (A12)	A12	cl58	(217, I-43m)		2	(CR)3.0(MN)5.0
CR3SI_A15	Cr ₃ Si (A15)	A15	cP8	(223, Pm-3n)	Cr ₃ Ru, Mo ₃ Si, V ₃ Si, Mo ₃ Al, Nb ₃ Al, V ₃ Co, V ₃ Ni, V ₃ Sn, Nb ₃ Sn	3	(AL, CR, MO, NB, NI, PD, PT, RE, SI, SN, TI, V, ZR)3.0(AL, CO, CR, MO, NB, NI, PD, PT, RU, SI, SN, TI, V, ZR)1.0(VA)3.0
CR5B3	Cr ₅ B ₃ (D8I)	D8I	tl32	(140, I4/mcm)		2	(CR)0.625(B)0.375
CR8FE16TI5	alpha-Mn (A12)	A12	cl58	(217, I-43m)		2	(CR, FE)24.0(TI)5.0
CRB4	CrB ₄		ol10	(71, Immm)		2	(CR)0.2(B)0.8
CRISTOBALITE	Ideal beta-Cristobalite (SiO ₂ , C9)	C9	cF24	(227, Fd-3m)		1	(SiO ₂)1.0
CRNI2_OP6	MoPt ₂		ol6	(71, Immm)		2	(CR)1.0(NI)2.0
CRPD_L10	AuCu		tP4	(123,		2	(CR)0.5(PD)0.5

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				P4/mmm)			
CRS12_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)	also NbSi2, TaSi2, VSi2	2	(CR, MO, NB, SI, TA, TI, V, W)1.0(AL, CR, SI)2.0
CU10SN3	Cu10Sn3		hP26	(173, P6_3)		1	(CU, SN)1.0
CU15SI4_EPSILON	Cu15Si4 (D86)	D86	cl76	(220, I-43d)		2	(CU)0.789474(SI)0.210526
CU2TI	Au2V		oS12	(63, Cmc)		2	(CU, NI)2.0(TI)1.0
CU33SI7_DELTA	Unknown Structure					2	(CU)0.825(SI)0.175
CU3SN	Cu3Sn		oS80	(63, Cmc)		2	(CU, SN)3.0(CU, SN)1.0
CU3TI2	Cu3Ti2		tP10	(129, P4/nmm)		2	(CU, FE, NI)3.0(TI)2.0
CU41SN11	Cu41Sn11		cF416	(216, F-43m)		2	(CU, SN)41.0(CU, SN)11.0
CU4TI1	Au4Zr		oP20	(62, Pnma)		2	(CU, NI, TI)4.0(CU, NI, TI)1.0
CU4TI3	Cu4Ti3		tl14	(139, I4/mmm)		2	(CU, NI)4.0(TI)3.0
CU56SI11_GAMMA	Mg3Ru2		cP20	(213, P4_132)		2	(CU)0.835821(SI)0.164179
CU6SN5_HT	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		3	(CU)1.0(CU, SN)1.0(SN)1.0
CU6SN5_LT	Cu6Sn5		mS44	(15, C2/c)		3	(CU)1.0(CU, SN)1.0(SN)1.0
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		2	(AG, AL, CO, CR, FE, HF, MN, MO, NB, NI, RE, RU, SI, SN, TA, TI, V, W, Y, ZR)1.0 (B, C, H, VA)1.0
CUO	Tenorite (CuO, B26)	B26	mS8	(15, C2/c)		2	(CU+2)1.0(O-2)1.0
CUPRITE_C3	Cuprite (Cu2O, C3)	C3	cP6	(224, Pn-3m)		2	(CU+1)2.0(O-2)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CUSI_ETA	Cu3Si-h2		hR*	(162, P-31m)	Structure uncertain	2	(CU)0.76(SI)0.24
CUSN_GAMMA	BIF3 (D03)	D03	cF16	(225, Fm-3m)		1	(CU, SN)1.0
CUTI3	CuTi3 (L60)	L60	tP4	(123, P4/mmm)		2	(CU, TI)1.0(TI)3.0
CUTI_B11	gamma-CuTi (B11)	B11	tP4	(129, P4/nmm)		2	(CU, NI, TI)1.0(CU, NI, TI)1.0
CUZR2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	CuTi2	3	(CU, FE, NI, SI)1.0(NB, TI)2.0(O, VA)0.5
D0I_MO2B5	Mo2B5 (D8i)	D8i	hR7	(166, R-3m)		2	(MO, TI)0.32(B)0.68
D5A_M3B2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	TA3B2, NB3B2, V3B2	2	(FE, HF, MO, NB, TA, TI, V)3.0(B)2.0
DELTA_TIH2	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	delta dihydrides	2	(HF, NB, TI, V, Y, ZR)1.0(H, VA)2.0
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)		1	(AL, B, C, H, O, SI, SN)1.0
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	Metallic FCC_A1 solution, e.g. (Al), (Cu)	2	(AG, AL, CO, CR, CU, FE, HF, MN, MO, NB, NI, PD, PT, RE, RU, SI, SN, TA, TI, V, W, Y, ZR)1.0(B, C, H, N, O, VA)1.0
FE1SN2	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(FE)1.0(SN)2.0
FE2SI	AlNi2		hP6	(164, P-3m1)		2	(FE)0.666667(SI)0.333333
FE3SN2	Fe3Sn2		hR10	(166, R-3m)		2	(FE)3.0(SN)2.0
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	(221, Pm-3m)		2	(CO, CR, FE, MN, NI)4.0(N)1.0
FE5SN3	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(FE)5.0(SN)3.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FE7MO6	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	mu phase	3	(FE)7.0(MO, TI)2.0(FE, MO, TI)4.0
FE7W6	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		4	(FE, W)1.0(W)4.0(FE, W)2.0(FE, W)6.0
FECN_CHI	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(FE)2.2(C, N)1.0
FESI2_H	FeSi2-h		tP3	(123, P4/mmm)		2	(FE)0.3(SI)0.7
FESI2_L	FeSi2-l		oS48	(64, Cmce)		2	(FE)0.333333(SI)0.666667
FESI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	also CoSi, CrSi, ReSi	2	(CO, CR, FE, MN, NI, RE)1.0(AL, SI)1.0
FESN	CoSn (B35)	B35	hP6	(191, P6/mmm)		2	(FE)1.0(SN)1.0
FLUORITE_C1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(AL+3, CR+3, FE+2, HF+4, MN+2, MN+3, NI+2, SI+4, TI+4, Y+3, ZR, ZR+4)2.0(O-2, VA)4.0
GAMMA_D83	gamma-brass (Cu9Al4, D83)	D83	cP52	(215, P-43m)		3	(AL)4.0(AL, CU)1.0(CU)8.0
GAMMA_H	gamma-brass (Cu5Zn8, D82)	D82	cl52	(217, I-43m)		3	(AL)4.0(AL, CU)1.0(CU)8.0
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_3/mmc)		1	(B, C)1.0
HALITE	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)	Wustite [FeO], Bunsenite [NiO], MnO, CoO, high temperature TiO, VO	2	(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)1.0(O-2, VA)1.0
HF3NI7	Hf3Ni7		aP20	(2, P-1)		2	(HF)0.3(NI)0.7
HF8NI21	Hf8Ni21		aP29	(2, P-1)	also ZR8NI21	2	(HF, ZR)8.0(NI)21.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
HFMN	NiTi2		cF96	(227, Fd-3m)		2	(HF)0.5(MN)0.5
HFNI3_ALPHA	PdRh2Ta		hP40	(194, P6_3/mmc)		2	(HF)0.25(NI)0.75
HFNI3_BETA	BaPb3		hR12	(166, R-3m)		2	(HF)0.25(NI)0.75
HFNI_ALPHA	CrB (B33)	B33	oS8	(63, Cmcm)		2	(HF)0.5(NI)0.5
HFRE	Zr21Re25		hR92	(167, R-3c)		2	(HF)1.0(RE)1.0
HIGH_SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)		3	(MN)8.0(CR)4.0(CR, MN)18.0
KYANITE	Kyanite (Al2SiO5, S01)	S01	aP32	(2, P-1)		4	(AL+3)1.0(AL+3)1.0(SI+4)1.0(O-2)5.0
M23C6	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)		3	(CR, MN)20.0(CR, MN)3.0(C)6.0
M2B_TETR	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Co2B, Fe2B, Mn2B, Mo2B, Ni2B	2	(CO, FE, MN, MO, NI, RE, TA, TI, W)2.0(B)1.0
M2O3C	Bixbyite (Mn2O3, D53)	D53	cl80	(206, Ia-3)		3	(AL+3, CR+3, FE+3, MN+3, NI+2, Y, Y+3, ZR+4)2.0(O-2, VA)3.0(O-2, VA)1.0
M2O3H	La2O3 (D52)	D52	hP5	(164, P-3m1)	hexagonal Y2O3	3	(MN+3, Y, Y+3, ZR+4)2.0(O-2, VA)3.0(O-2, VA)1.0
M2P_C22	Revised Fe2P (C22)	C22(II)	hP9	(189, P-62m)		2	(TI, ZR)2.0(SI)1.0
M3C2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(CR)3.0(C)2.0
M3Si1	Ti3P		tP32	(86, P4_2/n)	Ti3Si, Ta3Si, Zr3Si	2	(NB, TA, TI, ZR)3.0(SI)1.0
M3Si2_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	Hf3Si2, Zr3Si2	2	(HF, ZR)3.0(SI)2.0
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(MN)5.0(C)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
M5Si3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_3/mcm)	Ti5Si3, Fe5Si3, Zr5Si3, Y5Si3, Hf5Si3, Mn5Si3, Zr5Sn3, Zr5Sn4	4	(CR, FE, HF, MN, MO, NB, SI, TI, W, Y, ZR)2.0(AL, SI, SN)3.0(CR, FE, HF, MN, MO, NB, TI, Y, ZR)3.0(C, CO, SN, VA)1.0
M7C3	C3Cr7 (D101)	D101	oP40	(62, Pnma)		2	(CR, MN)7.0(C)3.0
MB_B33	CrB (B33)	B33	oS8	(63, Cmcm)	CrB, NbB, NiB, TaB, VB	2	(CR, MO, NB, NI, TA, TI, V, W)1.0(B)1.0
MC_ETA	CMo		hP12	(194, P6_3/mmc)		2	(MO)1.0(C, VA)1.0
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	(187, P-6m2)		2	(MO, W)1.0(C, N)1.0
MN11Si19	Mn11Si19		tP120	(118, P-4n2)		2	(MN)11.0(SI)19.0
MN12Y	Mn12Th (D2b)	D2b	tI26	(139, I4/mmm)		2	(MN)12.0(Y)1.0
MN1O2	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mnm)		2	(MN)1.0(O)2.0
MN2B_D1F	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(MN)0.6707(B)0.3293
MN2SN	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		2	(MN)0.643(SN)0.357
MN3SI	BiF3 (D03)	D03	cF16	(225, Fm-3m)		2	(MN)3.0(SI)1.0
MN3SN2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(MN)3.0(SN)2.0
MN3TI	Unknown Structure					2	(MN)3.0(TI)1.0
MN4TI	R-(Co,Cr,Mo)		hR53	(148, R-3)		2	(MN)0.815(TI)0.185
MN6N4	Mn3N2		tI10	(139, I4/mmm)		2	(MN)6.0(N)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MN6N5	CoO		tI4	(139, I4/mmm)		2	(MN)6.0(N)5.0
MN6SI	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)		2	(MN)17.0(SI)3.0
MN9SI2	Mn9Si2		oI186	(71, Immm)		2	(MN)33.0(SI)7.0
MNB4	MnB4		mS10	(12, C2/m)		2	(MN)0.2(B)0.8
MNNI2	Unknown Structure					2	(MN, NI)1.0(NI)2.0
MNSN2	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(SN)2.0(MN)1.0
MNTA	Unknown Structure					2	(MN)1.0(TA)1.0
MNTI_HT	Unknown Structure		t**			2	(MN)0.515(TI)0.485
MNTI_LT	Zr21Re25		hR92	(167, R-3c)		2	(MN)1.0(TI)1.0
MO4O11	Mo4O11		oP60	(33, Pna2_1)		2	(MO)4.0(O)11.0
MO8O23	High-Temperature Mo8O23		mP62	(13, P2/c)		2	(MO)8.0(O)23.0
MO9O26	Mo9O26		mP70	(13, P2/c)		2	(MO)1.0(O)2.889
MOB4	MoB4		hP16	(194, P6_3/mmc)		2	(MO, TI)0.2(B)0.8
MONI4_BETA	Ni4Mo (D1a)	D1a	tI10	(87, I4/m)		2	(MO, W)1.0(NI)4.0
MONI_DELTA	MoNi		oP56	(19, P2_12_12_1)		3	(NI)24.0(MO, NI)20.0(MO)12.0
MOO2	VO2		mP12	(14, P2_1/c)		2	(MO)1.0(O)2.0
MOO3	gamma-WO3		mP32	(14, P2_1/c)		2	(MO)1.0(O)3.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(MO, W)1.0(SI)2.0
MSI2_C1	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)		2	(CO, NI)1.0(SI)2.0
MSI_B27	FeB (B27)	B27	oP8	(62, Pnma)	TiSi, HfSi, YSi, ZrSi (alpha), SiZr	2	(HF, TI, Y, ZR)1.0(AL, SI)1.0
MULLITE	Al(Al0.7Si0.3)2O4.8		oP24	(55, Pbam)		4	(AL+3)1.0(AL+3)1.0(AL+3, SI+4)1.0(O-2, VA)5.0
MZR3_E1A	MgCuAl2 (E1a)		oS16	(63, Cmcm)		2	(CO, FE, NI)1.0(Y, ZR)3.0
NB1O2	alpha-NbO2		tI96	(88, I4_1/a)		2	(NB)1.0(O)2.0
NB2B3	V2B3		oS20	(63, Cmcm)		2	(NB)2.0(B)3.0
NB2O5	Nb2O5		mP99	(10, P2/m)		2	(NB)2.0(O)5.0
NB3RU5	Rh5Ge3		oP16	(55, Pbam)		2	(NB, RU)0.375(RU)0.625
NBH_BETA	Ta2H		oS8	(21, C222)		2	(NB)1.0(H, VA)1.1
NBO	NbO		cP6	(221, Pm-3m)		2	(NB)1.0(O)1.0
NBSN2	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)		2	(NB, SN, V)1.0(NB, SN)2.0
NI10ZR7	Ni10Zr7		oS68	(64, Cmce)		2	(NI)23.0(HF, ZR)17.0
NI11ZR9	Pt11Zr9		tI40	(87, I4/m)		2	(NI, PD)11.0(HF, ZR)9.0
NI17Y2	Fe17Lu2		hP80	(194, P6_3/mmc)	also Fe17Y2	2	(FE, NI)1.0(Y)0.1176
NI2SI_TETA	AlNi2		hP6	(164, P-3m1)		3	(NI)1.0(NI, VA)1.0(SI)1.0
NI2TA	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(CO, NI)2.0(TA)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI2V	MoPt2		oI6	(71, Immm)		2	(NI, PD)2.0(V)1.0
NI2Y1	Ni2Tm		cF192	(216, F-43m)		2	(NI)2.0(Y)1.0
NI2Y3	Ni2Y3		tP80	(92, P4_12_12)		2	(NI)2.0(Y)3.0
NI31SI12	Ni31SI12		hP42	(150, P321)		2	(NI)5.0(SI)2.0
NI3B_D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(CO, NI)3.0(B)1.0
NI3SI2	Ni3Si2		oP80	(36, Cmc2_1)		2	(NI)3.0(SI)2.0
NI3SI_MONOCL	Ge9Pd25		hP34	(147, P-3)		2	(NI)3.0(SI)1.0
NI3SI_ORTHO	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(NI)3.0(SI)1.0
NI3SN2_HT	Ni2In (B82)	B82	hP6	(194, P6_3/mmc)		3	(NI)0.33333(NI, SN)0.33334(SN)0.33333
NI3SN2_LT	Ni3Sn2		oP20	(62, Pnma)		3	(SN)0.2(NI, SN)0.4(NI)0.4
NI3SN4	delta-Ni3Sn4 (D7a)	D7a	mS14	(12, C2/m)		3	(NI)0.25(NI, SN)0.25(SN)0.5
NI3SN_D019	Ni3Sn (D019)	D019	hP8	(194, P6_3/mmc)		2	(SN)1.0(MN, NI)3.0
NI3SN_HT	BIF3 (D03)	D03	cF16	(225, Fm-3m)		3	(NI, SN)0.25(NI, SN)0.25(NI)0.5
NI3TA_D0A	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)	also Ni3Mo, Ni3Nb	2	(AL, CO, NB, NI)3.0(AL, MO, NB, NI, TA, V)1.0
NI3TI_D024	Ni3Ti (D024)	D024	hP16	(194, P6_3/mmc)		2	(AL, CU, NI, PD, TI, ZR)0.75(AL, CU, NI, PD, TI, ZR)0.25
NI3Y	Ni3Pu		hR12	(166, R-3m)		2	(FE, NI)3.0(Y)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
NI4B3	m-Ni4B3		mS28	(15, C2/c)		2	(NI)0.57142857(B)0.42857143
NI4Y	Unknown Structure		hR*			2	(NI)4.0(Y)1.0
NI5ZR	AuBe5 (C15b)	C15b	cF24	(216, F-43m)	also Ni5Y, Ni5Hf	2	(NI)5.0(HF, Y, ZR)1.0
NI7ZR2	Ni7Zr2		mS36	(12, C2/m)		2	(CO, NI)7.0(HF, Y, ZR)2.0
NI8TA	Pt8Ti		tI18	(139, I4/mmm)		2	(NI)8.0(TA)1.0
NISI_B31	MnP (B31)	B31	oP8	(62, Pnma)		2	(NI)1.0(SI)1.0
NITi2	NiT _i 2		cF96	(227, Fd-3m)		2	(CO, CU, FE, MO, NI, PD, TI)1.0(AL, HF, NI, TA, TI)2.0
NIZR	CrB (B33)	B33	oS8	(63, Cmcm)		2	(NI)1.0(Y, ZR)1.0
PD2TI	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(PD)2.0(TI)1.0
PD3TI2	Pd3Ti2		oS20	(63, Cmcm)		2	(PD)3.0(TI)2.0
PD4ZR3	Pd4Pu3		hR14	(148, R-3)		2	(PD)4.0(ZR)3.0
PD5TI3	Pd5Ti3		tP8	(123, P4/mmm)		2	(PD)5.0(TI)3.0
PDZRM	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		3	(PD)1.0(ZR)1.0(PD, ZR)1.0
PDZR_ALPHA	(PdZr-alpha)		mS*	(8, Cm)		2	(PD)1.0(ZR)1.0
PDZR_BETA	CrB (B33)	B33	oS8	(63, Cmcm)		2	(PD)1.0(ZR)1.0
PSEUDO_BROOKITE	Pseudobrookite (Fe ₂ TiO ₅ , E41)	E41	oS32	(63, Cmcm)		3	(AL+3, TI+3, TI+4)1.0(AL+3, TI+3, TI+4)2.0(O-2)5.0
PT3TI4	Unknown Structure					2	(PT)3.0(TI)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
PT8TI	Pt8Ti		tI18	(139, I4/mmm)		2	(PT)8.0(TI)1.0
QUARTZ	alpha-Quartz (low Quartz)		hP9	(152, P3_121)		1	(SiO2)1.0
RE2O7	Re2O7		oP72	(19, P2_12_12_1)		1	(O7RE2)1.0
RE2Si	Re2Si		mP24	(14, P2_1/c)		2	(RE)2.0(SI)1.0
RE3B	Re3B		oS16	(63, Cmcm)		2	(RE)3.0(B)1.0
RE7B3	Fe3Th7 (D102)	D102	hP20	(186, P6_3mc)		3	(RE, RU)7.0(B)3.0(B, VA)3.0
REB2	ReB2		hP6	(194, P6_3/mmc)		3	(RE)1.0(B)2.0(B, VA)2.0
REO2	ReO2		mP14	(14, P2_1/c)		1	(O2RE1)1.0
REO3	alpha-ReO3 (D09)	D09	cP4	(221, Pm-3m)		1	(O3RE1)1.0
RESI2_C11B	Re4Si7		mS44	(8, Cm)		2	(RE)0.357(SI)0.643
REZR2	Zr21Re25		hR92	(167, R-3c)		2	(RE)1.0(ZR)2.0
RU1B2	RuB2		oP6	(59, Pmmn)		2	(RU)1.0(B)2.0
RU25Y44	Ru25Y44		oP276	(52, Pnna)		2	(RU)0.362(Y)0.638
RU2B3	Ru2B3		hP10	(194, P6_3/mmc)		2	(RU)2.0(B)3.0
RU2Si3	Ge3Ru2		oP40	(60, Pbcn)		2	(RU)2.0(SI)3.0
RU2Si_C37	Co2Si (C37)	C37	oP12	(62, Pnma)		2	(RU)2.0(SI)1.0
RU2SN3	Ru2Sn3		tP20	(116, P-4c2)		2	(RU)0.4(SN)0.6

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
RU2Y3	Er3Ru2		hP10	(176, P6_3/m)		2	(RU)0.4(Y)0.6
RU2Y5	Mn5C2 (Fe5C2 Hagg carbide)		mS28	(15, C2/c)		2	(RU)0.286(Y)0.714
RU3SN7	Ir3Ge7 (D8f)	D8f	cl40	(229, Im-3m)		2	(RU)0.3(SN)0.7
RU4Si3	Ru4Si3		oP28	(62, Pnma)		2	(RU)4.0(SI)3.0
RUB	Unknown Structure					2	(RU)1.0(B)1.0
RUSi	FeSi (B20)	B20	cP8	(198, P2_13)		2	(RU)1.0(SI)1.0
RUTILE_TIO2	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mnm)	TiO2, also the high-temperature VO2, RUO2	2	(AL+3, RU+4, SN+4, TI+4, V+4, ZR+4)1.0(O-2, VA-2)2.0
RUY3	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(RU)0.25(Y)0.75
R_MARTE	R_martensite		hP18	(157, P31m)	intermediate martensite in Ti-Ni-based alloys	2	(NI, TI)0.5(NI, VA)0.5
R_PHASE	R-(Co,Cr,Mo)		hR53	(148, R-3)		3	(FE)27.0(MO)14.0(FE, MO)12.0
SI3N4	Nierite (alpha-Si3N4)		hP28	(159, P31c)		2	(SI)3.0(N)4.0
SI5V6	Si5V6		ol44	(72, Ibam)		2	(SI)5.0(V)6.0
SIC	Zinblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(SI)1.0(B, C)1.0
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)		4	(AL+3, CO+2, CO+3, CR+2, CR+3, FE+2, FE+3, MN+2, NI+2)1.0(AL+3, CO+2, CO+3, CR+3, FE+2, FE+3, MN+2, MN+3, MN+4, NI+2, VA)2.0(CR+2, FE+2, MN+2, VA)2.0(O-2)4.0
T1CUNITI	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)		2	(CU, NI)2.0(TI)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
T2CUNITI	Cu3Ti2		tP10	(129, P4/nmm)		3	(CU)0.175(NI)2.825(TI)2.0
T4CUFETI	Unknown Structure				the Cu-Fe-Ti ternary phase, Tau4	2	(CU, FE)0.63(TI)0.37
T4CUNITI	BaPb3		hR12	(166, R-3m)		3	(CU, TI)0.075(CU, NI)0.675(TI)0.25
T5CUFETI	Unknown Structure				the Cu-Fe-Ti ternary phase, Tau5	2	(CU, FE)0.55(TI)0.45
T6CUNITI	Unknown Structure					3	(CU, TI)0.25(CU, NI)0.5(TI)0.25
TA1AL2	Al69Ta39		cF444	(216, F-43m)		2	(AL, TA, TI)0.6389(AL, TA, TI)0.3611
TA2H_EPSLON	Unknown Structure					2	(TA)2.0(H, VA)1.0
TA2O5_HT	Ta2O5-ht		tI44	(141, I4_1/amd)		2	(TA)2.0(O)5.0
TA2O5_LT	beta-Ta2O5		oP14	(49, Pccm)		2	(TA)2.0(O)5.0
TA5SI3_D8L	Cr5B3 (D8I)	D8I	tI32	(140, I4/mcm)		2	(HF, NB, TA, TI)5.0(AL, SI)3.0
TAAL	Al38Ta48		mP86	(14, P2_1/c)		2	(AL, TA, TI)0.8837(AL, TA, TI)1.1163
TAN_EPS	TaN-eps		hP6	(189, P-62m)		2	(TA)1.0(N)1.0
TAU	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)		4	(CO, HF, NI)20.0(B)6.0(B, VA)6.0(HF, TI)3.0
TI10O19	Unknown Structure					2	(TI)10.0(O)19.0
TI20O39	Ti20O39		aP118	(2, P-1)		2	(TI)20.0(O)39.0
TI2ALC	AlCCr2		hP8	(194, P6_3/mmc)	H, Ti2AlC1-x	3	(TI)2.0(AL)1.0(C, VA)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
TI2NIH	Ti2NiH		cF128	(227, Fd-3m)		3	(Ti)2.0(Ni)1.0(H)1.0
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	(136, P4_2/mmm)		2	(Ti)2.0(N)1.0
TI2NI3	Ti2Ni3		tI10	(139, I4/mmm)		2	(Ni)3.0(Ti)2.0
TI2SN3	Ti2Sn3		oS40	(64, Cmce)		2	(CR, Ti)2.0(SN)3.0
TI3AL1C2	CMo		hP12	(194, P6_3/mmc)	N, Ti3AlC2-x	3	(Ti)3.0(AL, Si)1.0(C, VA)2.0
TI3ALC	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	P, Ti3AlC1-x	3	(Ti)3.0(AL)1.0(C, VA)1.0
TI3B4	Ta3B4 (D7b)	D7b	oI14	(71, Immm)	Cr3B4, Mn3B4, Nb3B4, Ti3B4, V3B4	2	(B)4.0(AL, CR, HF, MN, NB, TA, TI, V)3.0
TI3NI4	Ti3Ni4		hR42	(148, R-3)		2	(Ni)4.0(Ti)3.0
TI3CO5B2	Ti3Co5B2		tP20	(127, P4/mbm)		3	(Ti)3.0(CO)5.0(B)2.0
TI3CU3O	Fe3W3C (E93)	E93	cF112	(227, Fd-3m)		3	(Ti)3.0(CU)3.0(O)1.0
TI3N2	TiS-9R		hR6	(166, R-3m)		2	(Ti)0.71(N)0.29
TI3O2	(Ti3O2)		hP5	(191, P6/mmm)		2	(Ti)3.0(O)2.0
TI3O5	V3O5-ht		mS32	(15, C2/c)		2	(Ti, V)3.0(O)5.0
TI4CU2O	W4Co2C		cF112	(227, Fd-3m)		3	(Ti)4.0(CU)2.0(O)1.0
TI4N3	Sc2Te3		hR8	(166, R-3m)		2	(Ti)0.685(N)0.315

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

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
V3H2	Unknown Structure					2	(V)0.6(H)0.4
V3O5_LT	V3O5-lt		mP32	(13, P2/c)		3	(V+3)2.0(V+4)1.0(O-2)5.0
V3O7	V3O7		mS120	(15, C2/c)		3	(V+5)2.0(V+4)1.0(O-2)7.0
V52O64	V13O16		tl116	(141, I4_1/amd)	delta-prime V-oxide	2	(V)52.0(O)64.0
V5B6	V5B6		oS22	(65, Cmmm)		2	(NB, TI, V)5.0(B)6.0
V6O13	V6O13		mS38	(12, C2/m)		3	(V+5)2.0(V+4)4.0(O-2)13.0
VO2_LT	VO2		mP12	(14, P2_1/c)		2	(V+4)1.0(O-2)2.0
W1O2	VO2		mP12	(14, P2_1/c)		1	(O2W1)1.0
W5Si3_D8M	W5Si3 (D8m)	D8m	tl32	(140, I4/mcm)		3	(CR, MO, NB, TI, V, W)4.0(CR, MO, NB, SI, TI, V, W)1.0(AL, SI, SN)3.0
WO2_72	Unknown Structure					1	(O2_72W1)1.0
WO2_90	Unknown Structure					1	(O2_90W1)1.0
WO2_96	Unknown Structure					1	(O2_96W1)1.0
WO3_HT	WO2.95		tP16	(113, P-42_1m)		1	(O3W1)1.0
WO3_LT	WO3		oP32	(60, Pbcn)		1	(O3W1)1.0
Y15C19_H	Unknown Structure					2	(C)19.0(Y)15.0
Y15C19_R	alpha-Y15C19		oP18	(55, Pbam)		2	(C)19.0(Y)15.0
Y1B6	CaB6 (D21)	D21	cP7	(221, Pm-3m)		2	(Y)1.0(B)6.0
Y2C3_H	Unknown Structure					3	(Y)2.0(C)2.0(C, VA)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
Y2C3_R	Sc3C4		tP70	(128, P4/mnc)		3	(Y)2.0(C)2.0(C, VA)1.0
Y3Si5_HT	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)		2	(Y)3.0(Si)5.0
Y3Si5_LT	Unknown Structure					2	(Y)3.0(Si)5.0
YB4	ThB4 (D1e)	D1e	tP20	(127, P4/mbm)		2	(Y)1.0(B)4.0
YB66	YB66		cF1936	(226, Fm-3c)		2	(Y)1.0(B)66.0
YC2_C11A	CaC2-I (C11a)	C11a	tI6	(139, I4/mmm)		1	(C2Y1)1.0
YC_GAMMA	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		2	(Y)1.0(C, C2, VA)1.0
YH3_EPSILON	H3Ho		hP24	(165, P-3c1)		2	(Y)1.0(H, VA)3.0
YSi2_HT	Unknown Structure					2	(Y)1.0(Si)2.0
ZR5Si4	Si4Zr5		tP36	(92, P4_12_12)	Ti5Si4, Hf5Si4, Y5Si4, Zr5Si4 (alpha)	2	(HF, MO, NB, Ti, Y, ZR)5.0(AL, Si)4.0
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	(14, P2_1/c)		2	(AL+3, CR+3, HF+4, TI+4, Y+3, ZR+4)2.0(O-2, VA)4.0
ZRO2_TETR	HgI2 (C13)	C13	tP6	(137, P4_2/nmc)		2	(AL+3, CR+3, FE+2, HF+4, MN+2, MN+3, NI+2, TI+4, Y+3, ZR+4)2.0(O-2, VA)4.0
ZRSi2_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)		2	(HF, NB, Y, ZR)1.0(Si)2.0
ZRSiO4	Zircon (ZrSiO4, S11)	S11	tI24	(141, I4_1/amd)		3	(Si+4)1.0(Y+3, ZR+4)1.0(O-2, VA)4.0
ZRTi2O6	Columbite (FeNb2O6, E51)	E51	oP36	(60, Pbcn)		3	(ZR+4)1.0(TI+4)2.0(O-2)6.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZRTIO4_ALPHA	Unknown Structure					3	(ZR+4)1.0(TI+4)1.0(O-2)4.0
ZRTIO4_BETA	zeta-Fe2N		oP12	(60, Pbcn)		2	(TI+4, ZR+4)2.0(O-2)4.0
GAS	Gas				Gas mixture	1	(AG, AG1AL1, AG1CU1, AG1H1, AG1O1, AG2, AL, AL1B1O2, AL1B3H12, AL1C1, AL1C2, AL1CU1, AL1H1, AL1H1O1_ALOH, AL1H1O1_HALO, AL1H1O2, AL1H2, AL1H2O2, AL1H3, AL1H3O3, AL1N1, AL1O1, AL1O2, AL2, AL2C2, AL2C6H18, AL2O1, AL2O2, AL2O3, B, B10H14, B1C1, B1C1H3O1, B1C2, B1C2H7O2, B1C3H9, B1C3H9O3, B1C6H15, B1H1, B1H1O1_BOH, B1H1O1_HBO, B1H1O2, B1H2, B1H2O1, B1H2O2, B1H3, B1H3O1, B1H3O2, B1H3O3, B1H6N1, B1N1, B1O1, B1O2, B2, B2C1, B2H4O4, B2H6, B2O1, B2O2, B2O3, B3H3O3, B3H3O6, B3H6N3, B5H9, C, C1H1, C1H1N1_HCN, C1H1N1_HNC, C1H1N1O1, C1H1O1, C1H1O2, C1H1SI1_1, C1H1SI1_2, C1H2, C1H2N4, C1H2O1, C1H2O2_CIS, C1H2O2_DIOXIRANE, C1H2O2_TRANS, C1H2SI1_1, C1H2SI1_2, C1H3, C1H3O1_CH2OH, C1H3O1_CH3O, C1H3SI1_1, C1H3SI1_2, C1H3SI1_3, C1H3SI1_4, C1H4, C1H4N2O1, C1H4O1, C1H4SI1_1, C1H4SI1_2, C1H4SI1_3, C1H5N1, C1H5SI1_1, C1H5SI1_2, C1H6SI1, C1N1, C1N1O1, C1N1O1_NCO, C1N2_CNN, C1N2_NCN, C1O1, C1O2, C1PT1, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2H1, C2H1OSI2, C2H1N1, C2H1SI1, C2H2, C2H2O1, C2H2SI1, C2H3, C2H3SI1_1, C2H3SI1_2, C2H4, C2H4O1_ACETALDEHYDE, C2H4O1_OXIRANE, C2H4O2_ACETICACID, C2H4O2_DIOXETANE, C2H4O3_123TRIOXOLANE, C2H4O3_124TRIOXOLANE, C2H4SI1_1, C2H4SI1_2, C2H5, C2H5SI1, C2H6, C2H6O1_1, C2H6O1_2, C2H6O1SI1, C2H6O2, C2H6SI1_1, C2H6SI1_2, C2H6SI1_3, C2H7SI1_1, C2H7SI1_2, C2H8SI1, C2H8SI1_2, C2N1_CCN, C2N1_CNC, C2N2, C2O1, C2SI1, C2SI2, C2SI3, C3, C3H1, C3H1O1SI1, C3H1N1, C3H4_1, C3H4_2, C3H6_1, C3H6_2, C3H6O1_1, C3H6O1_2, C3H8, C3H8SI1, C3H9SI1_1, C3H9SI1_2, C3N1, C3O2, C4, C4H1, C4H10_1, C4H10_2, C4H11SI1, C4H12SI1_1, C4H12SI1_2, C4H2_1, C4H2_2, C4H4_1, C4H4_2, C4H6_1, C4H6_2, C4H6_3, C4H6_4, C4H6_5, C4H8_1, C4H8_2, C4H8_3, C4H8_4, C4H8_5, C4H8_6, C4N1, C4N2, C4N1O4, C5, C5FE1O5, C5H1N1, C5N1, C6, C6H6, C6H6O1, C6MO1O6, C6N1, C6N2, C9N1, CO, CO1H1, CO1H1O1, CO1H2O2, CO1O1, CO2, CR, CR1H1, CR1H1O1, CR1H1O2, CR1H1O3, CR1H2O2, CR1H2O3, CR1H2O4, CR1H3O3, CR1H3O4, CR1H4O4, CR1H4O5, CR1N1, CR1O1, CR1O2, CR1O3, CR2, CR2O1, CR2O2, CR2O3, CU, CU1H1, CU1H1O1, CU1O1, CU2, FE, FE1H1, FE1H1O1, FE1H1O2, FE1H2O2, FE1O1, FE1O2, FE2, H, H1MN1, H1MN1O1, H1MO1O1, H1MO1O2, H1MO3, H1N1, H1N1O1, H1N1O2_CIS, H1N1O2_TRANS, H1N1O3, H1N3, H1N1I, H1N1I1O1, H1O1, H1O1W1, H1O2, H1O2W1, H1PT1, H1SI1, H1ZR1, H2, H2MO1O2, H2MO1O3, H2MO1O4, H2N1, H2N2_1_1N2H2, H2N2_CIS, H2N2_TRANS, H2N2O2, H2N1O2, H2O1, H2O2, H2O2W1, H2O3SI1, H2O3W1, H2O4W1, H2SI1, H3N1, H3N1O1, H3SI1, H4N2, H4O4SI1, H4SI1, H4SN1, H6SI2, 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, O1PD1, O1PT1, O1RE1, O1RU1, O1SI1, O1SN1, O1TA1, O1TI1, O1V1, O1W1, O1Y1, O1Y2, O1ZR1, O2, O2PT1, O2RE1, O2RU1,

<i>Name</i>	<i>Prototype</i>	<i>Strukturbericht</i>	<i>Pearson Symbol</i>	<i>Space Group</i>	<i>Info</i>	<i>Sublattices</i>	<i>Formula Unit</i>
							O2SI1, O2SI2, O2SN1, O2TA1, O2TI1, O2V1, O2W1, O2Y1, O2Y2, O2ZR1, O3, O3RE1, O3RU1, O3W1, O4RU1, O6RE2, O6W2, O7RE2, O8W3, O9W3, PD, PT, RE, RU, SI, SI2, SI3, SN, SN2, TA, TI, TI2, V, W, Y, ZR, ZR2)1.0

TCTI6 Properties Data

Model Descriptions

For more information about the various thermophysical, thermomechanical, and properties 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 a Validation and Calculation 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:	6.1
First release:	TCTI1 was released in 2017

Changes in the Most Recent Database Release

TCTI6.0 to TCTI6.1

Software release version 2025a (January 2025)

UNARY SYSTEMS

- Reassessed elastic constant model parameters to ensure that the calculated results at high temperatures align more closely with physically expected behavior.
 - FCC_A1: Ni
 - BCC_A2: Fe, Mo, Nb, Ta, Ti, V, W, Zr
 - HCP_A3: Co, Ti, Zr
- Reassessed elastic constant model parameters for metastable systems that enhance model consistency and improve composition profiles for both titanium-containing and non-titanium binary systems.
 - FCC_A1: Co, Cr
 - BCC_A2: Al
 - HCP_A3: Cr, Mo, Nb, V
- Fixed rounding error that affected the calculated accuracy of a few systems.

BINARY SYSTEMS

Reassessed binary interaction parameters affected by the adjustments made to unary elastic constant model parameters.

- BCC_A2:
 - Ti-X (X = Al, Cr, Mo, Nb, Sn, Ta, V, W, Zr)
 - Mo-X (X = Nb, Sn, Ta, W, Zr)
 - Nb-X (X = Al, Sn, Ta, V, W, Zr)
 - Sn-X (X = Ta, Zr)
 - W-X (X = Cr, Ta, V, Zr)
 - Zr-X (X = Ta, V)
- HCP_A3: Ti-X (X = Al, Cr, Mo, Nb, Sn, V, Zr)

Previous Releases

TCTI5.1 to TCTI6.0

Software release version: 2024b (June 2024)

NEW ELASTIC PROPERTIES

- New elastic moduli (bulk modulus, shear modulus, and Young's modulus) available.
- New elastic constants (C11, C12, C13, C33, and C44) available for the metallic elements for BCC, HCP, and FCC phases.

THERMODYNAMIC ASSESSMENTS

- The description of Ti-Ni system is updated for shape memory alloys. The B19_PRIME, B19_ORTHO, and R_MARTE martensite phases are included in addition to the metastable Ti_2Ni_3 , and Ti_3Ni_4 intermetallic phases which play an important role as precipitates in shape memory alloys.
- Related Ti-Ni-X systems are also updated: Ti-Al-Ni, Ti-B-Ni, Ti-Cu-Ni, Ti-H-Ni, Ti-Ni-Pd, and Ti-Ni-Sn.
- Ti-Al-Ta, Ti-Cr-Fe, Mn-W, and O-Sn are improved with more accurate prediction of phase stabilities.
- Full gas descriptions are updated.

OTHER IMPROVEMENTS

- Improved surface tension of Fe-Ni.
- Molar volumes of BCC_A2 phase are revised for the systems Al-V, Nb-Ti, Ta-Ti, Al-Ti-V, and Ti-V-Zr.

TCTI5.0 to TCTI5.1

Software release version: 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 version: 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 version: 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 α_2 and γ phases.
- Updated description of BCC_A2 in Mo-V and Mo-Ti-V.

TCTI2.2 to TCTI3.0

Software release version: 2021a (December 2020/January 2021)

- Added Copper (Cu), which is a minor-alloying element in titanium alloys.
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- 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 version: 2020b (June 2020)

- Improved description of liquid phase for calculations with yttrium.

TCTI2.0 to TCTI2.1

Software release version: 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 version: 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.