TCS Nb-based Alloys Database (TCNB1)

Technical Information

Available Starting with Thermo-Calc Version 2024b

Document created 5/29/2024

Contents

TCNB1: TCS Nb-based Alloys Database **3**

TCS Nb-based Alloys Database (TCNB) Resources **5**

TCNB1 Elements, Systems, Phases and Properties **6**

TCNB1 Systems **8**

TCNB1 Assessed Binary Systems 9

TCNB1 Assessed Ternary Systems 10

TCNB1 Phases **11**

Common Phases for Niobium Materials 12

TCNB1 Models for the Included Phases 13

TCNB1 Properties Data **20**

Examples 20

TCNB1: TCS Nb-based Alloys Database

Niobium-based alloys find applications in various industries due to their unique properties. They are commonly used in aerospace and aviation industries for manufacturing superalloys, which are heat-resistant and can withstand high-stress environments, such as jet engines and gas turbines. Niobium-based alloys are also used in medical implants due to their biocompatibility and corrosion resistance. Additionally, these are used in the production of superconductors for applications like MRI machines and particle accelerators. In the automotive sector, Nb-based alloys are used for lightweighting and improving the strength of structural components.

The thermodynamic TCS Nb-based Alloys Database (TCNB) is available for refractory alloys (Nb-based) that exhibit high melting temperature and low density compared to Ni-superalloys. The database can be used to study the influence of alloying by the addition of elements on various properties.

The database is compatible with the TCS Nb-based Alloys Mobility Database (MOBNB). The current version is MOBNB1.

In addition to thermodynamic data, TCNB1 has properties data available for:

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

When combined with the kinetic database you can also use the Add-on Modules — Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA). The thermodynamic database is also compatible with the Additive Manufacturing (AM) Module. Both the thermodynamic and kinetic databases can be used together with the Thermo-Calc Software Development Kits (SDKs).

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.

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 Nb-based Alloys Database (TCNB) 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 Nb-based Alloys Database (TCNB) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, and the phases and models. It also includes details about the properties data (e.g. viscosity, surface tension, etc.), and a list of the included elements.
- The *TCS Nb-based Alloys Database (TCNB) 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 Niobium-based Alloys page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database.

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

TCNB1 Elements, Systems, Phases and Properties

Included Elements

There are 12 elements included in the database.

Al	C	Cr	Hf	Mo	Nb
Si	Ta	Ti	V	W	Zr

Assessed Systems and Phases

A hybrid approach of experiments, first-principles calculations and CALPHAD modeling have been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges.

All the stable solution phases and intermetallic compounds that exist in each assessed system are included.

The database contains:

- 66 assessed binary systems
- 76 assessed ternary systems
- 101 phases

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`.

Properties Data

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.

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	V0, 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.

TCNB1 Systems

In this section:

TCNB1 Assessed Binary Systems 9
TCNB1 Assessed Ternary Systems 10

TCNB1 Assessed Binary Systems

66 binary systems are assessed.

	Al	C	Cr	Hf	Mo	Nb	Si	Ta	Ti	V	W	Zr
Al	Al											
C	x	C										
Cr	x	x	Cr									
Hf	x	x	x	Hf								
Mo	x	x	x	x	Mo							
Nb	x	x	x	x	x	Nb						
Si	x	x	x	x	x	x	Si					
Ta	x	x	x	x	x	x	x	Ta				
Ti	x	x	x	x	x	x	x	x	Ti			
V	x	x	x	x	x	x	x	x	x	V		
W	x	x	x	x	x	x	x	x	x	x	W	
Zr	x	x	x	x	x	x	x	x	x	x	x	Zr

TCNB1 Assessed Ternary Systems

76 ternary systems are assessed.

Assessed Ternary Systems				
Al-C-Ti	Al-Cr-Nb	Al-Cr-V	Al-Mo-Nb	Al-Nb-Si
Al-Nb-Ti	Al-Nb-V	Al-Nb-W	Al-Si-Ti	Al-Ti-Zr
C-Cr-Hf	C-Cr-Nb	C-Cr-Si	C-Cr-V	C-Cr-Zr
C-Hf-Mo	C-Hf-Nb	C-Hf-Si	C-Hf-Ta	C-Mo-Nb
C-Mo-Ti	C-Mo-V	C-Mo-W	C-Mo-Zr	C-Nb-Ta
C-Nb-Ti	C-Nb-V	C-Nb-W	C-Nb-Zr	C-Si-Ta
C-Ta-Ti	C-Ta-W	C-Ta-Zr	C-Ti-V	C-Ti-W
C-Ti-Zr	Cr-Hf-Nb	Cr-Mo-Nb	Cr-Mo-Ti	Cr-Nb-Si
Cr-Nb-Ta	Cr-Nb-Ti	Cr-Nb-V	Cr-Nb-W	Cr-Nb-Zr
Cr-Si-Ti	Cr-Ti-W	Hf-Nb-Si	Hf-Nb-Ti	Hf-Si-Ti
Hf-Ti-Zr	Mo-Nb-Si	Mo-Nb-Ta	Mo-Nb-V	Mo-Nb-Zr
Mo-Si-Ti	Mo-Ta-Ti	Mo-Ti-V	Mo-Ti-W	Mo-Ti-Zr
Nb-Si-Ta	Nb-Si-Ti	Nb-Si-V	Nb-Si-W	Nb-Si-Zr
Nb-Ta-Ti	Nb-Ti-V	Nb-V-Zr	Si-Ti-W	Ta-Ti-V
Ta-Ti-W	Ta-Ti-Zr	Ti-V-W	Ti-V-Zr	Ti-W-Zr
V-W-Zr				

TCNB1 Phases

In this section:

Common Phases for Niobium Materials 12
TCNB1 Models for the Included Phases 13

Common Phases for Niobium Materials

TCNB1 Models for the Included Phases

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

Name in the Database	*Common Name and Description*
LIQUID	Liquid phase, which covers the melt of Nb alloys.
BCC_B2	BCC type solid solution phase (β), which is the matrix phase for Nb alloys. 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 this database. It is necessary to check the constitution of the phase to find out whether it is ordered or not.
C14_Laves	Laves_C14 phase, which covers some Cr/Nb etc.-compounds.
C15_Laves	Laves_C15 phase, which covers compounds, Cr_2Nb, Cr_2Ta, Cr_2Ti etc.
FCC_A1	FCC type solid solution phase, as well as carbide, which covers HfC, NbC, TaC, ZrC etc. solution phase compositions
M5SI3_D88	Ti-rich M_5Si_3 phase, dissolving other elements. It also covers Hf_5Si_3, Zr_5Si_3, Hf_5Si_3C, and Zr_5Si_3C compounds.
M3SI1	It covers Nb_3Si, Ti_3Si, Ta_3Si and dissolving other elements.
NB5Si3_D8M	It covers αNb_5Si_3 and Ta_5Si and dissolving other elements
W5Si3_D8L	It covers Cr_5Si_3, Mo_5Si_3, βNb_5Si_3, V_5Si_3 and W_5Si_3 and solutions between them.

TCNB1 Models for the Included Phases

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

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
AL11CR2	Al5Cr		mS732	(15, C2/c)		3	(AL)10.0(AL)1.0(CR)2.0
AL12W	Al12W		cI26	(204, Im-3)	also Al12Mo, Al12Re.	2	(AL)12.0(MO, W)1.0
AL13CR2	Al45V7		mS104	(12, C2/m)		2	(AL)13.0(CR)2.0
AL17MO4	Al17Mo4		mS84	(5, C2)		2	(AL)17.0(MO)4.0
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
AL2TI_LT	Ga2Hf		tI24	(141, I4_ 1/amd)		2	(AL, NB, TI)2.0(AL, NB, TA, TI, V, ZR)1.0
AL2ZR3	Zr3Al2		tP20	(136, P4_ 2/mnm)	also Al2Hf3, Al2Y3.	2	(AL)2.0(HF, TI, ZR)3.0
AL3MO	MoAl3		mS32	(12, C2/m)		2	(AL)3.0(MO, NB)1.0
AL3TI_D022	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	gamma double prime, AL3TI_D022, Al3M, Ni3V.	2	(AL, CR, MO, NB, SI, TI, V, W)3.0(AL, CR, MO, NB, SI, TA, TI, V, W, ZR)1.0
AL3TI_LT	Al3Ti-LT		tI32	(139, I4/mmm)		2	(AL, TI)3.0(AL, TI, ZR)1.0
AL3ZR2	Zr2Al3		oF40	(43, Fdd2)	also Al3Hf2.	2	(AL)3.0(HF, ZR)2.0
AL3ZR4	Al3Zr4		hP7	(191,	also Al3Hf4.	2	(AL)3.0(HF, TI, ZR)4.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				P6/mmm)			
AL3ZR5_D8M	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, Zn3Zr.	2	(AL)3.0(HF, TI, ZR)1.0
AL45V7	Al45V7		mS104	(12, C2/m)	aka Al7V	2	(AL)45.0(V)7.0
AL4C3_D71	Al4C3 (D71)	D71	hR7	(166, R-3m)		2	(AL, SI)4.0(C)3.0
AL4CR	mu-Al4Mn		hP574	(194, P6_3/mmc)		2	(AL)4.0(CR)1.0
AL4SIC4_E94	Al5C3N (E94)	E94	hP18	(186, P6_3mc)		3	(AL)4.0(SI)1.0(C)4.0
AL4W	Al4W		mS30	(8, Cm)	also Al4Mo.	2	(AL)4.0(MO, NB, W)1.0
AL4ZR5	Ti5Ga4		hP18	(193, P6_3/mcm)		2	(AL)4.0(ZR)5.0
AL5TI2_HT	Al5Ti2		tP28	(123, P4/mmm)		2	(AL, TI)5.0(AL, NB, TA, TI, V, ZR)2.0
AL5TI3	Al5Ti3		tP32	(127, P4/mbm)		2	(AL)5.0(TA, TI)3.0
AL5W	Al5W		hP12	(182, P6_322)	also AL5MO.	2	(AL)5.0(MO, W)1.0
AL63MO37	Unknown Structure				Mo3Al5_HT	2	(AL)63.0(MO)37.0
AL8CR5_LT_D810	Cr5Al8 (D810)	D810	hR26	(160, R3m)		2	(AL)8.0(CR, V)5.0
AL8MO3	Al8Mo3		mS22	(12, C2/m)		2	(AL)8.0(MO, NB)3.0
AL8SIC7	Unknown Structure		hP16			3	(AL)8.0(SI)1.0(C)7.0
AL8V5_D82	gamma-brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)		2	(AL, V)8.0(AL, CR, V, ZR)5.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL9CR4_HT	Unknown Structure					2	(AL)9.0(CR)4.0
AL9CR4_LT	Unknown Structure					2	(AL)9.0(CR)4.0
ALCR2C	AlCCr2		hP8	(194, P6_ 3/mmc)	MAX_PHASE.	3	(AL)1.0(C)1.0(CR)2.0
ALPHA_B19	beta'-AuCd (B19)	B19	oP4	(51, Pmma)	an ordered HCP.	2	(MO, NB, TI, V, ZR)1.0(MO, NB, TI, V, ZR)1.0
ALSI3TI2	Zr3Al4Si5		tI24	(141, I4_ 1/amd)	aka Ti7Al5Si12, Tau1	3	(AL)0.166667(SI)0.5(TI)0.333333
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	also Ni3Sn_LT, Mn3Sn, Ti3Sn.	2	(AL, CR, MO, NB, TA, TI, V, W, ZR)3.0(AL, C, CR, MO, NB, SI, TA, TI, V, W)1.0
ALTI_L10	CuAu (L10)	L10	tP2	(123, P4/mmm)	Solid solution of ordered L10.	2	(AL, CR, MO, NB, TA, TI, V, W, ZR)1.0(AL, CR, MO, NB, TA, TI, V, W, ZR)1.0
ALZR2_B82	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		2	(AL)1.0(TI, ZR)2.0
ALZR_B33	CrB (B33)	B33	oS8	(63, Cmcm)	also AlHf, ALY_B33.	2	(AL)1.0(HF, ZR)1.0
Al2W_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)		2	(AL)2.0(W)1.0
B82_OMEGA	Ni2In (B82)	B82	hP6	(194, P6_ 3/mmc)		3	(AL)1.0(NB, TA, TI)1.0(TI)1.0
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	BCC_A2 will be combined to BCC_B2 if defined.	2	(AL, CR, HF, MO, NB, SI, TA, TI, V, VA, W, ZR)1.0(C, VA)3.0
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	This phase has some contribution from BCC_ A2.	3	(AL, CR, HF, MO, NB, SI, TA, TI, V, VA, W, ZR)0.5(AL, CR, HF, MO, NB, SI, TA, TI, V, VA, W, ZR)0.5(C, VA)3.0
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	also CuZn2.	2	(AL, CR, HF, MO, NB, SI, TA, TI, V, W, ZR)2.0(AL, CR, HF, MO, NB, SI, TA, TI, V, W, ZR)1.0
C15_LAVES	Cu2Mg Cubic Laves	C15	cF24	(227, Fd-3m)		2	(AL, CR, HF, MO, NB, SI, TA, TI, V, W, ZR)2.0(AL, CR, HF, MO, NB, SI, TA, TI,

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
	(C15)						V, W, ZR)1.0
C16_THETA	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)		2	(AL, HF, MO, NB, TA, TI, V, W, ZR)2.0(AL, CR, SI)1.0
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)		2	(AL, CR, HF, MO, NB, TA, TI, W, ZR)2.0(AL, CR, HF, MO, NB, TA, TI, W, ZR)1.0
CBCC_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)		2	(AL, CR, MO, NB, SI, TA, TI, V, W, ZR)1.0(C, VA)1.0
CEMENTITE_ D011	Cementite (Fe3C, D011)	D011	oP16	(62, Pnma)		2	(CR, MO, V, W)3.0(C)1.0
CHI_A12	alpha-Mn (A12)	A12	cI58	(217, I-43m)	also M5Re24, Mo2Re8, Ta3Re7, WRe3.	3	(CR)24.0(AL, CR, HF, MO, NB, TA, TI, W, ZR)10.0(CR, MO, NB, TA, W)24.0
CR3SI_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	also Cr3X, Nb3X, Ti3X, V3X.	3	(AL, CR, MO, NB, SI, TA, TI, V, W, ZR)3.0(AL, CR, MO, NB, SI, TA, TI, V, W, ZR)1.0(C, VA)3.0
CRNBSI	ZrNiAl		hP9	(189, P-62m)		3	(CR)1.0(NB)1.0(SI)1.0
CRNI2_OP6	MoPt2		oI6	(71, Immm)		2	(CR, MO, W)1.0(MO, W)2.0
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)	also NbSi2, TaSi2, VSi2.	2	(CR, HF, MO, NB, SI, TA, TI, V, W, ZR)1.0(AL, CR, SI)2.0
CUB_A13	beta-Mn (A13)	A13	cP20	(213, P4_132)		2	(AL, CR, HF, MO, NB, SI, TA, TI, V, W, ZR)1.0(C, VA)1.0
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	Pure C, Si or solid solution phases based on them.	1	(AL, C, SI)1.0
DIS_MU	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	Part of the description for the MU_PHASE	1	(AL, CR, MO, NB, TA, TI, W)1.0
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	FCC_A1 will be combined to FCC_L12 if defined.	2	(AL, CR, HF, MO, NB, SI, TA, TI, V, W, ZR)1.0(C, VA)1.0
GAS	Gas					1	(AL, AL1C1, AL1C2, AL2, AL2C2, C, C1SI1, C1SI2, C1SI3, C1SI4, C2, C2SI1, C2SI2, C2SI3, C3, C4, C5, C60, CR, CR2, HF, MO, MO2, NB, SI, SI2, SI3, TA, TI,

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
							TI2, V, W, ZR, ZR2)1.0
GRAPHITE_A9	Hexagonal Graphite (A9)	A9	hP4	(194, P6_ 3/mmc)		1	(C)1.0
G_PHASE_D8A	Th6Mn23 (D8a)	D8a	cF116	(225, Fm-3m)		3	(AL, TI)16.0(HF, NB, TI, ZR)6.0(SI)7.0
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	Disordered HCP_A3 solution phase.	2	(AL, CR, HF, MO, NB, SI, TA, TI, V, W, ZR)1.0(C, VA)0.5
HEUSLER_L21	Heusler (L21)	L21	cF16	(225, Fm-3m)	aka H_L21.	3	(AL, CR, TI)0.5(AL, HF, NB, TA, TI, ZR)0.5(VA)1.0
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)		2	(AL, CR, TI, ZR)0.75(AL, CR, SI, TA, TI, ZR)0.25
LIQUID	Liquid					1	(AL, C, CR, HF, MO, NB, SI, TA, TI, V, W, ZR)1.0
M11SI8	Cr11Ge8		oP76	(62, Pnma)	also Cr11Si8, Nb11Si8.	2	(CR, NB)11.0(SI)8.0
M23C6_D84	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)		3	(CR, V)20.0(CR, MO, V, W)3.0(C)6.0
M3C2_D510	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)		2	(CR, MO, V, W)3.0(C)2.0
M3SI1	Ti3P		tP32	(86, P4_2/n)	also Nb3Si, Ta3Si, Ti3Si, Zr3Si.	2	(HF, NB, TA, TI, ZR)3.0(SI)1.0
M3SI2_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	also Hf3Si2, Zr3Si2.	2	(HF, NB, ZR)3.0(SI)2.0
M4SI3	Ru4Si3		oP28	(62, Pnma)	also Cr4Si3, Nb4Si3.	2	(CR)4.0(SI)3.0
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)	also M5Sn3, M5Si3C.	4	(CR, HF, MO, NB, SI, TI, W, ZR)2.0(AL, CR, SI, TI)3.0(CR, HF, MO, NB, TI, ZR)3.0(C, VA)1.0
M6SI5	Si5V6		oI44	(72, Ibam)	also Cr6Si5, Nb6Si5.	2	(CR, NB, TI, V)6.0(SI)5.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
M7C3_D101	C3Cr7 (D101)	D101	oP40	(62, Pnma)		2	(CR, MO, V, W)7.0(C)3.0
MC_ETA	CMo		hP12	(194, P6_ 3/mmc)		2	(MO, V, W)1.0(C, VA)1.0
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	(187, P-6m2)	also MoC_LT, Strukturbericht Bh	2	(MO, W)1.0(C)1.0
MONI_DELTA	MoNi		oP56	(19, P2_12_ 12_1)		3	(CR)24.0(CR, MO, W)20.0(MO, W)12.0
MOSI2_C11B	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	also AlCr2, Ti2Zn, ZnZr2, CUZR2_C11B.	2	(AL, MO, W)1.0(AL, CR, HF, SI, TI, ZR)2.0
MSI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	also CoSi, CrSi, MnSi, ReSi.	2	(CR)1.0(AL, SI)1.0
MSI_B27	FeB (B27)	B27	oP8	(62, Pnma)	also TiSi, HfSi, YSi, ZrSi (alpha).	2	(HF, NB, TI, ZR)1.0(AL, SI)1.0
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	(166, R-3m)	DIS_MU contribution added onto it.	4	(AL, CR, MO, NB, TA, TI, W)1.0(AL, CR, MO, NB, TA, TI, W)2.0(AL, CR, MO, NB, TA, TI, W)6.0(AL, CR, MO, NB, TA, TI, W)4.0
NI3TA_D0A	beta-TiCu3 (D0a)	D0a	oP8	(59, Pmmn)	also delta, Ni3Mo, Ni3Nb.	2	(AL, CR, NB)3.0(AL, MO, NB, TA, TI, V, W)1.0
NI3TI_D024	Ni3Ti (D024)	D024	hP16	(194, P6_ 3/mmc)	also Eta, AlNi6Ta.	2	(AL, CR, HF, TA, TI, W, ZR)0.75(AL, CR, HF, MO, NB, SI, TA, TI, W, ZR)0.25
NITI2	NiTi2		cF96	(227, Fd-3m)		2	(CR, TI)1.0(AL, CR, HF, TA, TI, ZR)2.0
O_PHASE	NaHg		oS16	(63, Cmcm)	aka Ti2NbAl, the O phase.	3	(NB, TA, TI)0.5(AL, NB, TA, TI)0.25(NB, TA, TI)0.25
R_PHASE	R-(Co,Cr,Mo)		hR53	(148, R-3)		3	(CR)27.0(MO, W)14.0(CR, MO, W)12.0
SIC_B3	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(SI)1.0(C)1.0
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_ 2/mnm)	DIS_SIG contribution added onto it.	3	(AL, CR, MO, NB, TA, TI, V, W)10.0(CR, MO, NB, TA, TI, V, W)4.0(AL, CR, MO, NB, SI, TA, TI, V, W)16.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
TA1AL1	Al38Ta48		mP86	(14, P2_1/c)		2	(TA)0.51515(AL)0.48485
NB5SI3_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	also alpha-Nb5Si3 and Ta5Si3.	2	(CR, HF, MO, NB, TA, TI, V, W, ZR)5.0(AL, SI)3.0
TAAL2_HT	Al69Ta39		cF444	(216, F-43m)		2	(TA)0.35(AL)0.65
TA5SI3C	TA5SI3C	TA5SI3C	TA5SI3C	TA5SI3C	TA5SI3C	TA5SI3C	TA5SI3C
TI2ALC	AlCCr2		hP8	(194, P6_ 3/mmc)	i.e. Ti2AlC1-x.	3	(TI)2.0(AL)1.0(C, VA)1.0
TI3ALC2	Ti3SiC2		hP12	(194, P6_ 3/mmc)		3	(TI)3.0(AL, SI)1.0(C, VA)2.0
TI3ALC_E21	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	i.e. Ti3AlC1-x.	3	(TI)3.0(AL)1.0(C, VA)1.0
TI3SIC2	Ti3SiC2		hP12	(194, P6_ 3/mmc)		3	(TI)3.0(SI)1.0(C)2.0
TISI2_C54	TiSi2 (C54)	C54	oF24	(70, Fddd)	also MoSi2, RuAl2, ZrSn2.	2	(MO, NB, TI, ZR)1.0(AL, SI)2.0
W5SI3_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	also Cr5Si3, Mo5Si3, Nb5Si3, V5Si3.	3	(CR, MO, NB, TA, TI, V, W)4.0(CR, MO, NB, SI, TA, TI, V, W)1.0(AL, SI)3.0
ZR5SI4_TP36	Si4Zr5		tP36	(92, P4_12_ 12)	also Hf5Si4, Ti5Si4.	2	(HF, MO, NB, TI, ZR)5.0(AL, SI)4.0
ZRSI2_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	also HfSi2.	2	(HF, NB, ZR)1.0(SI)2.0
Z_PHASE	CrNbN		tP6	(129, P4/nmm)		3	(CR)1.0(MO, NB, V)1.0(VA)1.0

TCNB1 Properties Data

This section lists the assessed systems for each of the properties.

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 Niobium-based Alloys page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database.