TCS Ultra-high Temperature Materials Database (TCUHTM3)

Technical Information

Available Starting with Thermo-Calc Version 2026b

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Contents

About the TCS Ultra-high Temperature Materials Database (TCUHTM)

The TCS Ultra-high Temperature Materials Database (TCUHTM) is a thermodynamic database for ultra-high temperature materials that can be used for applications including hypersonic aircraft and space vehicles. These materials are typically non-oxides with melting/decomposition temperatures in excess of 3000°C. Examples include borides, nitrides, and carbides of Group IV-V metals in the periodic table, such as ZrB_2, HfB_2, ZrC, HfC, TaC, and HfN. Si is also included as SiC can be used to improve oxidation resistance. The database can be used to calculate phase diagrams and thermodynamic properties of assessed systems, but also for predicting phase equilibria, melting temperatures, and simulating operation processes for a wide range of compositions.

In addition to thermodynamic data, it has properties data available for molar volume with thermal expansion coefficients.

TCUHTM3 enables predictions (such as multicomponent phase equilibria calculations, equilibrium solidification simulations, and Scheil solidification simulations) to be made for multicomponent systems and alloys of industrial importance. This means that the database can be used to extrapolate to higher-order systems by combining several critically assessed systems.

Interconnectivity to Other Products

TCS Ultra-high Temperature Materials Database (TCUHTM) can be used with Thermo-Calc and all available SDKs. The database does not currently have a corresponding mobility database. It also cannot be used with the Additive Manufacturing (AM) Module.

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 area.

The TCUHTM3 database enables predictions (such as multicomponent phase equilibria calculations, equilibrium solidification simulations, and Scheil solidification simulations) to be made for multicomponent systems and alloys of industrial importance. This means that the database can be used to extrapolate to higher-order systems by combining several critically assessed systems.enables predictions (such as multicomponent phase equilibria calculations, equilibrium solidification simulations, and Scheil solidification simulations) to be made for multicomponent systems and alloys of industrial importance. This means that the database can be used to extrapolate to higher-order systems by combining several critically assessed systems.

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.

Release History

TCUHTM: TCS Ultra-high Temperature Materials Database Revision History. The current version of the database is TCUHTM3. See the link for any subversion release details.

TCS Ultra-high Temperature Materials Database (TCUHTM) Resources

Database technical content and examples are available in different formats (html help files or PDFs).

Go to these locations to access the same content:

- **Locally Installed Help**: When in Thermo-Calc, press F1 to open the current version of the help in a local browser. You can also click **Online Help** from the **My Project** page to open the file. Then search or navigate to the **Databases** folder to browse the contents.
- **Web Help**: Go to the Documentation page to link to the most recent version of the web help. Then search or navigate to the **Databases** folder to browse the contents.
- **Website resources**: The individual database technical information and examples are also available in PDF format from the website. Download the *current version* of the PDFs for each database.

About 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. Also visit the video tutorials on our website or our YouTube playlist.

Learn More

Go to the Ultra-high Temperature Materials Database page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information*. Also explore further applications of Thermo-Calc including links to resources such as examples, publications, and more.

For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what properties can be calculated with Thermo-Calc and the Add-on Modules.

TCUHTM3 Elements, Systems, and Phases

This section summarizes the available elements, assessed systems, and total number of phases in the TCS Ultra-high Temperature Materials Database (TCUHTM).

Included Elements

There are 13 elements included in the database.

Included Elements									
Al	B	C	Cr	Hf	N	Nb	O	Si	Ta
Ti	V	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.

In most cases phases having the same crystal structure had been merged as the same phase.

The database contains:

- 78 assessed binary systems
- 100 assessed ternary systems (88 critically assessed and 12 tentatively assessed)
- 167 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`.

TCUHTM3 Thermophysical Properties

This section summarizes the available properties. In addition to thermodynamic data, the TCS Ultra-high Temperature Materials Database (TCUHTM) has properties data available for molar volume with thermal expansion coefficients.

Thermophysical Parameters and Variables

Below is a summary of the available thermophysical parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode (CM) versus Graphical Mode (GM) as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

Examples

In Thermo-Calc, press F1 and search or navigate to the relevant database to discover the Validation and Calculation Examples Collection, which is also available in PDF format on our website.

Go to the Ultra-high Temperature Materials Database page on our website where you can access a *Validation and Calculation Examples Collection* and the *Technical Information*. Also explore further applications of Thermo-Calc including links to resources such as examples, publications, and more.

Learn More

For more information about the various thermophysical, thermomechanical, elastic, and properties models, and when in Thermo-Calc, press F1 to search the online help. The details are found under the *General Reference* section. You can also see the brochure on our website that lists what properties can be calculated with Thermo-Calc and the Add-on Modules.

TCUHTM3 Systems

In this section:

TCUHTM3 Assessed Binary Systems

These are the assessed binary systems in the latest version of the database.

	Al	B	C	Cr	Hf	N	Nb	O	Si	Ta	Ti	V	Zr
Al	Al												
B	x	B											
C	x	x	C										
Cr	x	x	x	Cr									
Hf	x	x	x	x	Hf								
N	x	x	x	x	x	N							
Nb	x	x	x	x	x	x	Nb						
O	x	x	x	x	x	x	x	O					
Si	x	x	x	x	x	x	x	x	Si				
Ta	x	x	x	x	x	x	x	x	x	Ta			
Ti	x	x	x	x	x	x	x	x	x	x	Ti		
V	x	x	x	x	x	x	x	x	x	x	x	V	
Zr	x	x	x	x	x	x	x	x	x	x	x	x	Zr

TCUHTM3 Assessed Ternary Systems

These are the assessed ternary systems in the latest version of the database. Those with an asterisk (*) are tentatively assessed.

Assessed Ternary Systems							
Al-C-Cr	Al-C-Nb	Al-C-Si	Al-C-Ta	Al-C-Ti	Al-C-V	Al-C-Zr	Al-Cr-V
Al-Hf-O	Al-N-Nb	Al-N-Ti	Al-N-Zr*	Al-Nb-O	Al-Nb-Ti	Al-O-V	Al-O-Zr
Al-Ta-Ti	Al-Ti-Zr	Al-V-Zr	B-C-Hf	B-C-Si	B-C-Ta	B-C-Ti	B-C-Zr
B-Hf-N	B-Hf-O*	B-Hf-Si	B-Hf-Ta*	B-Hf-Ti	B-Hf-Zr	B-N-O*	B-N-Ta*
B-N-Zr	B-Nb-O	B-Nb-Ti	B-O-Si	B-O-Zr	B-Si-Zr	B-Ta-Zr*	B-Ti-V
B-Ti-Zr	C-Cr-Hf	C-Cr-Nb	C-Hf-N*	C-Hf-Nb	C-Hf-O*	C-Hf-Si	C-Hf-Ta
C-Hf-Ti	C-Hf-Zr	C-N-Si	C-N-Ta*	C-N-Ti	C-N-Zr	C-Nb-Ti	C-Nb-V
C-Nb-Zr	C-O-Zr	C-Si-Ta	C-Si-Ti	C-Si-Zr	C-Ta-Ti	C-Ta-V	C-Ta-Zr
C-Ti-V	C-Ti-Zr	C-V-Zr	Cr-Nb-O	Cr-Nb-Si	Cr-Nb-V	Cr-Nb-Zr	Cr-O-Ti
Cr-O-V	Cr-O-Zr	Hf-N-O	Hf-N-Si*	Hf-N-Ta*	Hf-Nb-Si	Hf-O-Si	Hf-O-Ta
Hf-O-Ti	Hf-O-Zr	Hf-Si-Ti	N-O-Si	N-O-Zr	N-Si-Ta	N-Si-Zr	N-Ta-Ti*
Nb-O-Ta	Nb-O-Ti	Nb-O-Zr	Nb-Si-Ta	Nb-Si-Ti	Nb-Si-V	Nb-Si-Zr	O-Si-Ta
O-Si-Zr	O-Ta-Zr	O-Ti-Zr	Ti-V-Zr				
* tentatively assessed systems							

TCUHTM3 Phases

In this section:

Common Phases for Ultra-high Temperature Materials

TCUHTM3 Models for the Included Phases

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

Name in the Database	*Common Name and Description*
AlCCr2	211 type MAX phase, Cr_2AlC, Nb_2AlC, Ta_2AlC, Ti_2AlC, Ti_2AlN, and V_2AlC
BCC_A2	Hf, Ta, Zr solution phase
FCC_A1	Fcc metal, carbide, and nitride-based phase, which covers Al, HfC, HfN, TaC, TaN, ZrC, ZrN solution phase compositions
HCP_A3	Hf, Zr, Ta_2C, Ta_2N solution phase
IONIC_LIQUID	Liquid phase, which covers the melt of ultra-high temperature materials
M4AlX3	413 type MAX phase, Nb_4AlC_3, Ti_4AlN_3, and V_4AlC_3
M5Si3_D88	It covers Hf_5Si_3, Zr_5Si_3, Hf_5Si_3B, Hf_5Si_3C, Zr_5Si_3C, Zr_5Si_3N
MB2_C32	It covers HfB_2, TaB_2, ZrB_2
Ti3Al1C2	312 type MAX phase, Ti_3AlC_2, and Ti_3SiC_2

TCUHTM3 Models for the Included Phases

The table lists all phases and the thermodynamic model used to describe the phase. Also see Common Phases for Ultra-high Temperature Materials.

Phase Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
GAS	Gas	-	-	-	-	1	(AL, AL1B1O2, AL1C1, AL1C2, AL1N1, AL1O1, AL1O2, AL2, AL2C2, AL2O1, AL2O2, AL2O3, B, B1C1, B1C2, B1N1, B1O1, B1O2, B2, B2C1, B2O1, B2O2, B2O3, C, C1N1, C1N1O1_NCO, C1N1O1, 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, C5, C5N1, C60, C6N1, C6N2, C9N1, CR, CR1N1, CR1O1, CR1O2, CR1O3, CR2, CR2O1, CR2O2, CR2O3, HF, HF1O1, HF1O2, N, N1NB1, N1O1, N1O2, N1O3, N1SI1, N1SI2, N1TI1, N1V1, N1ZR1, N2, N2O1, N2O2, N2O3, N2O4, N2O5, N3, NB, NB1O1, NB1O2, O, O10V4, O1SI1, O1TA1, O1TI1, O1V1, O1ZR1, O2, O2SI1, O2SI2, O2TA1, O2TI1, O2V1, O2ZR1, O3, SI, SI2, SI3, TA, TI, TI2, V, ZR, ZR2)1
AL11CR2	Al5Cr	-	mS732	(15, C2/c)	-	3	(AL)10(AL)1(CR)2
AL1ZR2	InNi2 (B82)	B82	hP6	(194, P6_3/mmc)	also AlY2	2	(AL)1(TI, ZR)2
AL21V2	Al10V	-	cF176	(227, Fd-3m)	-	2	(AL)21(V)2
AL23V4	Al23V4	-	hP54	(194, P6_3/mmc)	-	2	(AL)23(V)4
AL2TI	Ga2Hf	-	tI24	(141, I4_1/amd)	-	2	(AL, NB, TI)2(AL, CR, NB, TA, TI, V, ZR)1
AL2ZR3	Zr3Al2	-	tP20	(136, P4_2/mnm)	also Al2Hf3, Al2Y3	2	(AL)2(HF, TI, ZR)3
AL3TI_D022	Al3Ti (D022)	D022	tI8	(139, I4/mmm)	also Al3V	2	(AL, NB, TI, V)3(AL, CR, NB, TA, TI, V, ZR)1
AL3TI_LT	Al3Ti-LT	-	tI32	(139, I4/mmm)	-	2	(AL, TI)3(AL, CR, TI, ZR)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
AL3ZR2	Zr2Al3	-	oF40	(43, Fdd2)	also Al3Hf2	2	(AL)3(HF, ZR)2
AL3ZR4	Al3Zr4	-	hP7	(191, P6/mmm)	also Al3Hf4	2	(AL)3(HF, TI, ZR)4
AL3ZR_D023	Al3Zr (D023)	D023	tI16	(139, I4/mmm)	also Al3Hf	2	(AL)3(HF, TI, ZR)1
AL45V7	Al45V7	-	mS104	(12, C2/m)	-	2	(AL)45(V)7
AL4C3	Al4C3 (D71)	D71	hR7	(166, R-3m)	-	2	(AL)4(C)3
AL4CR	mu-Al4Mn	-	hP574	(194, P6_3/mmc)	-	2	(AL)4(AL, CR, TI)1
AL4SIC4_E94	Al5C3N (E94)	E94	hP18	(186, P6_3mc)	-	3	(AL)4(SI)1(C)4
AL4ZR5	Ti5Ga4	-	hP18	(193, P6_3/mcm)	-	2	(AL)4(ZR)5
AL5TI2	Al5Ti2	-	tP28	(123, P4/mmm)	-	2	(AL, TI)5(AL, CR, NB, TA, TI, V, ZR)2
AL5TI3	Al5Ti3	-	tP32	(127, P4/mbm)	-	2	(AL)5(TA, TI)3
AL13CR2	Al45V7	-	mS104	(12, C2/m)	-	2	(AL)13(CR)2
AL8CR5_HT	gamma-Brass (Cu5Zn8, D82)	D82	cI52	(217, I-43m)	-	2	(AL, V)8(AL, CR, TI, V, ZR)5
AL8CR5_LT	Cr5Al8 (D810)	D810	hR26	(160, R3m)	-	2	(AL)8(CR, V)5
AL8SIC7	Unknown Structure	-	hP16	-	-	3	(AL)8(SI)1(C)7
AL9CR4_HT	Unknown Structure	-	-	-	-	2	(AL)9(CR)4
AL9CR4_LT	Unknown Structure	-	-	-	-	2	(AL)9(CR)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALB12	alpha-AlB12	-	tP216	(92, P4_12_12)	-	2	(AL, TI)1(B)12
AL18B4O33	Al5BO9	-	oS60	(36, Cmc2_1)	-	3	(AL+3)18(B+3)4(O-2)33
AL4B2O9	Al4B1.5[BO3]0.5O7.5	-	mS124	(12, C2/m)	-	3	(AL+3)4(B+3)2(O-2)9
ALCR2	MoSi2 (C11b)	C11b	tI6	(139, I4/mmm)	-	2	(AL)1(CR, TI)2
ALCCR2	AlCCr2	-	hP8	(194, P6_3/mmc)	AlNTi2	3	(AL)1(C, N, VA)1(CR, NB, TA, TI, V, ZR)2
TI3AL1C2	CMo	-	hP12	(194, P6_3/mmc)	N, Ti3AlC2-x	3	(TI)3(AL, SI)1(C, VA)2
M4ALX3	AlN3Ti4	-	hP16	(194, P6_3/mmc)	-	4	(NB, TA, TI, V)4(AL)1(C, N)2(C, N, VA)1
AL2NNB3	beta-Mn (A13)	A13	cP20	(213, P4_132)	-	3	(AL)2(N)1(NB)3
TI3ALC	Cubic Perovskite (CaTiO3, E21)	E21	cP5	(221, Pm-3m)	P, Ti3AlC1-x	3	(TI)3(AL)1(C, N, VA)1
AL3CTA5	CuHf5Sn3	-	hP18	(193, P6_3/mcm)	Al3CTa5	3	(AL)3(C)1(TA, ZR)5
AL3C4ZR2	U2Al3C4	-	hP18	(186, P6_3mc)	AL3C4ZR2	3	(AL)3(C)5(ZR)2
AL3C5ZR3	Hf3Al3C5	-	hP22	(186, P6_3mc)	Al3C5-xZr3	3	(AL)3(C)5(ZR)3
AL3NZR5	CuHf5Sn3	-	hP18	(193, P6_3/mcm)	Al3NZR5	3	(AL)3(N, VA)1(ZR)5
ALNZR3	Cr3B0.5C0.5C	-	Os20	(63, Cmcm)	AlNZr3	3	(AL)1(N)1(ZR)3
ALSI3TI2	Zr3Al4Si5	-	tI24	(141, I4_1/amd)	-	3	(AL)0.166667(SI)0.5(TI)0.333333

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ALTI3_D019	Ni3Sn (D019)	D019	hP8	(194, P6_ 3/mmc)	Ti3Al	2	(AL, NB, TA, TI, V, ZR)3(AL, TI, C)1
ALTI_L10	CuAu(I) (L10)	L10	tP2	(123, P4/mmm)	TiAl	3	(AL, TI, ZR)1(AL, CR, NB, TA, TI, V, ZR)1(C, VA)2
ALZR	CrB (B33)	B33	oS8	(63, Cmcm)	also AlHf, AlY	2	(AL)1(HF, ZR)1
B82_OMEGA	InNi2 (B82)	B82	hP6	(194, P6_ 3/mmc)	-	3	(AL)1(NB, TA, TI)1(TI)1
BETA_V_O	CoO	-	tI4	(139, I4/mmm)	-	2	(V)1(O, VA)1
C14_LAVES	MgZn2 Hexagonal Laves (C14)	C14	hP12	(194, P6_ 3/mmc)	-	2	(AL, CR, HF, SI, TA, TI, V, ZR)2(AL, CR, HF, NB, TA, TI, V, ZR)1
C15_LAVES	Cu2Mg Cubic Laves (C15)	C15	cF24	(227, Fd-3m)	-	2	(AL, CR, HF, NB, SI, TA, TI, V, ZR)2(CR, HF, NB, TA, TI, V, ZR)1
C36_LAVES	MgNi2 Hexagonal Laves (C36)	C36	hP24	(194, P6_ 3/mmc)	-	2	(CR, TI, ZR)2(CR, TI, ZR)1
CORUNDUM	Corundum (alpha-alumina, Al2O3, D51)	D51	hR10	(167, R-3c)	This is Al2O3, Cr2O3, Fe2O3, Ti2O3, V2O3 + (Co, Fe, Mg, Mn, Ni, Zn)TiO3 Ilmenite.	2	(AL+3, CR+3, TI+3, TI+4, V+3, V+4, VA)2(O-2)3
CR2B_ORTH	Mg2Cu (Cb)	Cb	oF48	(70, Fddd)	-	2	(CR)2(B)1
CR3SI_A15	Cr3Si (A15)	A15	cP8	(223, Pm-3n)	Cr3Ru, Mo3Si, V3Si, Mo3Al, Nb3Al, V3Co, V3Ni, V3Sn, Nb3Sn	2	(AL, CR, NB, SI, TI, V, ZR)3(AL, CR, NB, SI, V)1
CR5B3	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	-	2	(CR)0.625(B)0.375
CRB4	CrB4	-	oI10	(71, Immm)	-	2	(CR)0.2(B)0.8
MSI_B20	FeSi (B20)	B20	cP8	(198, P2_13)	also CoSi, CrSi,	2	(CR)1(SI)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
					ReSi		
L12_FCC	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	2	(AL, ZR)0.75(AL, ZR)0.25
M23C6	Cr23C6 (D84)	D84	cF116	(225, Fm-3m)	-	3	(CR)20(CR)3(C)6
M3C2	Tongbaite (Cr3C2, D510)	D510	oP20	(62, Pnma)	-	2	(CR)3(C)2
M7C3	C3Cr7 (D101)	D101	oP40	(62, Pnma)	-	2	(CR)7(C)3
NB2O5	Nb2O5	-	mP99	(10, P2/m)	-	2	(NB+5, TA+5, V+5, ZR+4)2(O-2, VA)5
NBO1	NbO	-	cP6	(221, Pm-3m)	-	2	(NB+2)1(O-2)1
NBO2	alpha-NbO2	-	tI96	(88, I4_1/a)	This is NbO2	2	(NB+4)1(O-2)2
SPINEL	Spinel (Al2MgO4, H11)	H11	cF56	(227, Fd-3m)	This is MgAl2O4, Fe3O4, Mn3O4 (ht) and many more.	4	(CR+2, CR+3)1(CR+3, VA)2(CR+2, VA)2(O-2)4
V2B3	V2B3	-	oS20	(63, Cmcm)	-	2	(NB, V)2(B)3
V5B6	V5B6	-	oS22	(65, Cmmm)	-	2	(NB, V)5(B)6
SIGMA	sigma-CrFe (D8b)	D8b	tP30	(136, P4_2/mnm)	DIS_SIG contribution added onto it.	3	(AL, NB, TA, TI)10(NB, TA, TI)4(AL, NB, TA, TI)16
TA1AL2	Al69Ta39	-	cF444	(216, F-43m)	-	2	(AL, TA, TI)0.6389(AL, TA, TI)0.3611
TAAL	Al38Ta48	-	mP86	(14, P2_1/c)	-	2	(AL, TA, TI)0.8837(AL, TA, TI)1.1163
B12ZR	UB12 (D2f)	D2f	cF52	(225, Fm-3m)	-	2	(B)12(ZR)1
B2O3	B2O3	-	hP15	(152, P3_121)	-	2	(B+3)2(O-2)3
B3SI	B13C2 "B4C" (D1g)	D1g	hR15	(166, R-3m)	-	3	(B)6(SI)2(B, SI)6

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
B4C	B13C2 "B4C" (D1g)	D1g	hR15	(166, R-3m)	-	2	(B11C, B12)1(B2, C2B, CB2, SI2)1
B6SI	SiB6	-	oP280	(58, Pnnm)	-	3	(B)210(SI)23(B, SI)48
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	Hf, Ta, Zr BodyCentered Cubic	2	(AL, CR, HF, NB, SI, TA, TI, V, VA, ZR)1(B, C, N, O, VA)3
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	Solution of ordered BCC_B2, having Gibbs energy contribution from BCC_A2	3	(AL, CR, HF, NB, SI, TA, TI, VA, V, ZR)0.5(AL, CR, HF, NB, SI, TA, TI, VA, V, ZR)0.5(B, C, N, O, VA)3
BETAR_BORON	beta-B (R-105)	-	hR105	(166, R-3m)	-	2	(B)93(B, C, NB, SI)12
BNSI	alpha-B (R-12)	-	hR12	(166, R-3m)	BnSi	3	(B)61(SI)1(B, SI)8
ALN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	-	2	(AL)1(N)1
BN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	Wurtzite	2	(B)1(N)1
C16_THETA	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Hf2Al, Hf2Si, Zr2Si	2	(HF, NB, TA, TI, V, ZR)2(AL, SI)1
M2B_TETR	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Ta2B	2	(TA, TI)2(B)1
CRISTOBALITE	Ideal beta-Cristobalite (SiO2, C9)	C9	cF24	(227, Fd-3m)	SiO2 with AlPO4 solubility.	2	(SI+4)1(SIO4-4)1
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)	also NbSi2, TaSi2, VSi2	2	(CR, HF, NB, SI, TA, TI, V, ZR)1(CR, SI)2
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	Si	2	(AL, B, C, SI)1(VA, O)1
FCC_A1	Rock Salt/Halite (NaCl, B1)	B1	cF8	(225, Fm-3m)	Al solution, NbC, TaC etc.	2	(AL, CR, HF, NB, SI, TA, TI, V, VA, ZR)1(B, C, N, O, VA)1
FLUORITE	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is cubic high temp HfO2 and	2	(AL+3, CR+3, HF+4, NB+5, SI+4, TA+5, TI+4, ZR, ZR+4, VA)2(O-2, VA)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
					ZrO2		
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_ 3/mmc)	HfC, HfN, TaC, TaN, ZrC, ZrN solution phase	1	(B, C)1
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	Hf, Zr, Ta2C, Ta2N solution phase	2	(AL, CR, HF, NB, SI, TA, TI, V, ZR)1(B, C, N, O, VA)0.5
HF3N2	TiS-9R	-	hR6	(166, R-3m)	-	2	(HF)0.64(N)0.36
HF4N3	Sc2Te3	-	hR8	(166, R-3m)	-	2	(HF)0.61(N)0.39
TI4N3	Sc2Te3	-	hR8	(166, R-3m)	-	2	(TI)0.685(N)0.315
HF6TA2O17	Nb2Zr6O17	-	oI100	(46, Ima2)	Hf6Ta2O17 Zr6Ta2O17	2	(HF+4, NB+5, TA+5, ZR+4, VA)8(O-2, VA)17
IONIC_LIQ	Liquid	-	-	-	Liquid metal and slag mixture.	2	(AL+3, CR+2, HF+4, NB+2, SI+4, TA+5, TI+2, V+2, ZR+4)P(ALO2-1, BO3-3, O-2, SIO4-4, VA, ALN, B, BO3/2, C, CrO3/2, N, NBO5/2, SIN4/3, SIO2, TIO3/2, TIO2, VO2, VO3/2, VO5/2)Q
M3SI1	Ti3P	-	tP32	(86, P4_2/n)	Ta3Si, Zr3Si	2	(HF, NB, TA, TI, ZR)3(SI)1
D5A_M3B2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	Ta3B2	2	(HF, NB, TA, TI, V)3(B)2
M11SI8	Cr11Ge8	-	oP76	(62, Pnma)	also Cr11Si8, Nb11Si8.	2	(CR, NB)11(SI)8
M3SI2_D5A	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	Hf3Si2, Zr3Si2	2	(HF, NB, ZR)3(SI)2
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)	Hf5Si3, Zr5Si3, Hf5Si3B, Hf5Si3C, Zr5Si3C, Zr5Si3N	3	(CR, HF, NB, TI, ZR)5(SI)3(B, C, N, VA)1
M4O7	Ti4O7-a	-	aP22	(2, P-1)	This is Ti4O7 and V4O7 .	2	(AL, TI, V)4(O)7

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
M6O11	Ti6O11	-	aP34	(2, P-1)	This is Ti6O11 and V6O11.	2	(TI, V)6(O)11
M7O13	Ti7O13	-	aP40	(2, P-1)	This is Ti7O13 and V7O13.	2	(TI, V)7(O)13
M8O15	Ti8O15	-	aP46	(2, P-1)	This is Ti8O15 and V8O15.	2	(TI, V)8(O)15
MB2_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	HfB2, TaB2, ZrB2	2	(B)2(AL, CR, B, HF, NB, TA, TI, V, ZR)1
MB_B33	CrB (B33)	B33	oS8	(63, Cmcm)	CrB, NbB, TaB, VB	2	(CR, HF, NB, TA, TI, V, ZR)1(B)1
MSI_B27	FeB (B27)	B27	oP8	(62, Pnma)	HfSi, ZrSi	2	(HF, NB, TI, ZR)1(SI)1
MULLITE	Al(Al0.7Si0.3)2O4.8	-	oP24	(55, Pbam)	With solubility of B, Cr and Fe.	3	(AL+3)2(AL+3, SI+4)1(O-2, VA)5
O_PHASE	NaHg	-	oS16	(63, Cmcm)	The O phase	3	(NB, TI)0.5(AL)0.25(NB, TA, TI)0.25
PSEUDO_ BROOKITE	Pseudobrookite (Fe2TiO5, E41)	E41	oS32	(63, Cmcm)	This is Fe2TiO5, Ti3O5, Al2TiO5 and (Co, Fe, Mg, Mn)Ti2O5.	3	(AL+3, TI+3, TI+4)1(AL+3, TI+3, TI+4)2(O-2)5
QUARTZ	alpha-Quartz (low Quartz)	-	hP9	(152, P3_121)	SiO2 with AlPO4 solubility.	2	(SI+4)1(SIO4-4)1
RUTILE	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)	This is MnO2, PbO2, TiO2 and ht-VO2.	2	(AL+3, HF+4, TI+3, TI+4, V+4, ZR+4)1(O-2, VA)2
SI2N2O	Si2N2O	-	oS20	(36, Cmc2_1)	-	3	(SI)2(N)2(O)1
SI3N4	Nierite (alpha-Si3N4)	-	hP28	(159, P31c)	-	2	(SI)3(N)4
SI5V6	Si5V6	-	oI44	(72, Ibam)	-	2	(SI)5(CR, NB, TI, V)6

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
SIC	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)	-	2	(SI)1(B, C)1
TA2O5_HT	Ta2O5-ht	-	tI44	(141, I4_ 1/amd)	-	2	(HF+4, NB+5, TA+5, ZR+4)2(O-2, VA)5
TA2O5_LT	beta-Ta2O5	-	oP14	(49, Pccm)	-	2	(HF+4, NB+5, TA+5, ZR+4)2(O-2, VA)5
TA5SI3C	Unknown Structure	-	-	-	Ta5Si3C, Ta5Si3N	3	(TA)5(SI)3(C, N, VA)1
TA5SI3_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	Low temperature Ta5Si3	2	(CR, HF, NB, TA, TI, V, ZR)5(SI)3
W5SI3_D8M	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	also Cr5Si3, Nb5Si3, V5Si3.	3	(CR, NB, TA, TI, V)4(CR, NB, TA, TI, V, SI)1(SI)3
AL3ZR5	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	-	2	(AL)3(TI, ZR)5
TI2N_C4	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)	-	2	(TI)2(C, N)1
TI3B4	Ta3B4 (D7b)	D7b	oI14	(71, Immm)	Ta3B4	2	(B)4(AL, CR, HF, NB, TI, TA, V)3
TI3N2	TiS-9R	-	hR6	(166, R-3m)	-	2	(TI)0.71(N)0.29
TI10O19	Unknown Structure	-	-	-	-	2	(TI)10(O)19
TI20O39	Ti20O39	-	aP118	(2, P-1)	-	2	(TI)20(O)39
TI3O2	(Ti3O2)	-	hP5	(191, P6/mmm)	-	3	(TI+2)2(TI)1(O-2)2
TI5O9	Ti5O9	-	aP28	(2, P-1)	Ti5O9 with solubility of V.	2	(TI, V)5(O)9
V2O5	Shcherbinaite (V2O5) (Revised)	-	oP14	(59, Pmmn)	-	2	(V+5)2(O-2)5
V2O_SS	V7O3	-	mS20	(12, C2/m)	-	2	(V)1(O, VA)0.5

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
V3O5_HT	V3O5-ht	-	mS32	(15, C2/c)	This is ht-V3O5 with solubility of Al, Cr, Mg, Mn, Ti and Zn.	2	(AL, CR, TI, V)3(O)5
V3O5_LT	V3O5-lt	-	mP32	(13, P2/c)	-	2	(V)3(O)5
V3O7	V3O7	-	mS120	(15, C2/c)	-	2	(V)3(O)7
V52O64	V13O16	-	tI116	(141, I4_ 1/amd)	-	2	(V)52(O)64
V5O9	Ti5O9	-	aP28	(2, P-1)	V5O9 with solubility of Ti.	2	(TI, V)5(O)9
V6O13	V6O13	-	mS38	(12, C2/m)	-	2	(V)6(O)13
VO2_LT	VO2	-	mP12	(14, P2_1/c)	This is lt-VO2, MoO2 and WO2.	2	(V+4)1(O-2)2
TI9O17	Ti9O17	-	aP52	(2, P-1)	-	2	(TI)9(O)17
TIO_ALPHA	alpha-TiO	-	mS20	(12, C2/m)	-	2	(TI+2)1(O-2)1
TIB_B27	FeB (B27)	B27	oP8	(62, Pnma)	HfB TiB	2	(B)1(HF, NB, TA, TI, V, ZR)1
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)	-	mS144	(9, Cc)	SiO2 with AlPO4 solubility.	2	(SI+4)1(SIO4-4)1
V3C2	Sc2Te3	-	hR8	(166, R-3m)	-	2	(V)3(C)2
ZIRCON	Zircon (ZrSiO4, S11)	S11	tI24	(141, I4_ 1/amd)	This is HfSiO4, ZrSiO4, GdPO4, LaPO4 and YPO4.	3	(SI+4)1(HF+4, ZR+4)1(O-2)4
ZR5SI4	Si4Zr5	-	tP36	(92, P4_12_ 12)	Zr5Si4, Hf5Si4	2	(HF, NB, TI, ZR)5(SI)4
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	(14, P2_1/c)	This is Monoclinic HfO2 and ZrO2	2	(CR+3, HF+4, TI+4, ZR+4)2(O-2, VA)4

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
ZRO2_TETR	Coccinite (Red HgI2, C13)	C13	tP6	(137, P4_ 2/nmc)	This is Tetragonal HfO2 and ZrO2	2	(AL+3, CR+3, HF+4, NB+5, TA+5, TI+4, ZR+4, VA)2(O-2, VA)4
ZRSI2_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	ZrSi2, HfSi2	2	(HF, ZR)1(SI)2
ZRTIO4_BETA	zeta-Fe2N	-	oP12	(60, Pbcn)	This is (Hf, Zr)TiO4 solid solution with Al solubility.	3	(AL+3, HF+4, TI+4, ZR+4)2(AL+3, VA)1(O-2)4
TISI2_C54	TiSi2 (C54) Nowotony Chimney-Ladder	C54	oF24	(70, Fddd)	-	2	(TI)1(SI)2
ALNB11O29	(Ti0.17Nb0.83)12O29	-	mS82	(12, C2/m)	-	3	(AL+3)1(NB+5)11(O-2)29
ALNB49O124	Unknown Structure	-	-	-	-	3	(AL+3)1(NB+5)49(O-2)124
MGWO4_TYPE	Huanzalaite (MgWO4, H06)	H06	mP12	(13, P2/c)	This is (Al, Fe)NbO4 and (Co, Fe, Mg, Mn, Ni, Zn)WO4.	3	(AL+3, NB+5, VA)1(NB+5)1(O-2)4
FEVO4	Zn[MoO4]	-	aP36	(2, P-1)	This is FeVO4 and AlVO4.	3	(AL+3)1(V+5)1(O-2)4
NB3BO9	Unknown Structure	-	-	-	-	3	(NB+5)3(B+3)1(O-2)9
TI6SI2B	K2UF6	-	hP9	(189, P-62m)	-	3	(TI)6(SI)2(B)1
CRNB25O64	Unknown Structure	-	-	-	-	3	(CR+3)1(NB+5)25(O-2)64
CRNB49O124	Unknown Structure	-	-	-	-	3	(CR+3)1(NB+5)49(O-2)124
CRNB9O24	Unknown Structure	-	-	-	-	3	(CR+3)1(NB+5)9(O-2)24
CRNBO4	Rutile (TiO2, C4)	C4	tP6	(136, P4_ 2/mnm)	-	3	(CR+3, VA)1(CR+3, NB+5)1(O-2, VA)4
CRNBSI	ZrNiAl	-	hP9	(189, P-62m)	-	3	(CR)1(NB)1(SI)1

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
CR2TI2O7	Unknown Structure	-	-	-	with solubility of Al2O3 and Fe2O3.	3	(CR+3)2(TI+4)2(O-2)7
CR2V4O13	Cr2P4O13	-	mP76	(14, P2_1/c)	This is Cr2P4O13, Cr2V4O13 and Fe2V4O13.	3	(CR+3)2(V+5)4(O-2)13
CRVO4	MgSO4	-	oS24	(63, Cmcm)	-	3	(CR+3)1(V+5)1(O-2)4
TI2NB10O29	(Ti0.17Nb0.83)12O29	-	mS82	(12, C2/m)	-	3	(TI+4)2(NB+5)10(O-2)29
TINB24O62	(Ti0.04Nb0.96)25O62	-	mS174	(5, C2)	-	3	(TI+4)1(NB+5)24(O-2)62
TINB2O7	(Ti0.33Nb0.67)3O7	-	mS60	(12, C2/m)	-	3	(TI+4)1(NB+5)2(O-2)7
NB4TA2O15	Unknown Structure	-	-	-	-	3	(NB+5)4(TA+5)2(O-2)15
ZRTI2O6	Columbite (FeNb2O4, E51)	E51	oP36	(60, Pbcn)	-	3	(ZR+4)1(TI+4)2(O-2)6
ZRTIO4_ALPHA	Unknown Structure	-	-	-	-	3	(ZR+4)1(TI+4)1(O-2)4

TCUHTM: TCS Ultra-high Temperature Materials Database Revision History

Current Database Version	
Database name (acronym):	TCS Ultra-high Temperature Materials Database (TCUHTM)
Database owner:	Thermo-Calc Software AB
Database version:	3.0
First release:	TCUHTM1 was released with 2022b

TCUHTM2 to TCUHTM3

Software release version: 2026b (June 2026)

Elements and Phases

- Added Al, Cr, Nb, Ti and V, making it a 13-element framework.
- 120 new phases (167 phases in total).
- The FCC_A1 and FCC_B1 structures were combined into the FCC_A1 phase to have a better description of the solubilities.

Binary Systems

- Added 50 new binary systems, where all Al-, Cr-, Nb-, Ti-, and V- related binaries are assessed.
- Two (2) binary systems are reassessed: B-Zr and Hf-N.

Ternary Systems

- 59 newly assessed ternary systems, including:
- MAX phases related ternaries: Al-C-Cr, Al-C-Nb, Al-C-Ta, Al-C-Ti, Al-C-V, Al-C-Zr, Al-N-Nb, Al-N-Ti, Al-N-Zr, and C-Si-Ti.

- And other Al-, Cr-, Nb-, Ti-, V- related ternaries: Al-C-Si, Al-Cr-V, Al-Hf-O, Al-Nb-O, Al-Nb-Ti, Al-O-V, Al-O-Zr, Al-Ta-Ti, Al-Ti-Zr, Al-V-Zr, B-C-Ti, B-Hf-Ti, B-Nb-O, B-Nb-Ti, B-Ti-V, B-Ti-Zr, C-Cr-Hf, C-Cr-Nb, C-Hf-Nb, C-Hf-Ti, C-N-Ti, C-Nb-Ti, C-Nb-V, C-Nb-Zr, C-Ta-Ti, C-Ta-V, C-Ti-V, C-Ti-Zr, C-V-Zr, Cr-Nb-O, Cr-Nb-Si, Cr-Nb-V, Cr-Nb-Zr, Cr-O-Ti, Cr-O-V, Cr-O-Zr, Hf-Nb-Si, Hf-O-Ti, Hf-Si-Ti, N-Ta-Ti, Nb-O-Ta, Nb-O-Ti, Nb-O-Zr, Nb-Si-Ta, Nb-Si-Ti, Nb-Si-V, Nb-Si-Zr, O-Ti-Zr, and Ti-V-Zr.

Thermophysical Properties

- Molar volumes are included with the additions of new elements of Al, Cr, Nb, Ti and V.

TCUHTM1.0 to TCUHTM2.0

Software release version: 2024b (June 2024)

Oxygen is added to this version of the database because oxidation is a well-known bottleneck in the development of high-temperature materials. By well-describing the oxygen-related phase equilibria, we want to provide help to explore ultra-high temperature oxidation resistance materials.

New Element and Phases

- One new element oxygen (O) for an 8 element framework.
- 12 new oxide phases.
- The IONIC_LIQUID model is used for the liquid phase.

Binary Systems

- 28 assessed binary systems are now included.
- 7 new binary systems: B-O, C-O, Hf-O, N-O, O-Si, O-Ta, and O-Zr.

Ternary Systems

- 41 assessed ternary systems are now included.
- 15 new ternary systems: B-Hf-O (T), B-N-O (T), B-O-Si, B-O-Zr, C-Hf-O (T), C-O-Zr, Hf-N-O, Hf-O-Si, Hf-O-Ta, Hf-O-Zr, N-O-Si, N-O-Zr, O-Si-Ta, O-Si-Zr, and O-Ta-Zr. (T: tentatively assessed)

Other Updates

- Molar volume property data added.