TCS Ultra-high Temperature Materials Database (TCUHTM2)

Technical Information

Available Starting with Thermo-Calc Version 2024b

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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.

TCS Ultra-high Temperature Materials Database (TCUHTM) is developed to be used with nearly our entire suite of products: Thermo-Calc, the Add-on Modules, except for the Additive Manufacturing Module, and all available SDKs.

The database does not currently have a corresponding mobility database.

TCUHTM: TCS Ultra-high Temperature Materials Database Revision History. The current version of the database is TCUHTM2. See the link for any subversion release details.

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 area.

The TCUHTM2 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.

TCS Ultra-high Temperature Materials Database (TCUHTM) 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 Ultra-high Temperature Materials Database (TCUHTM) 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 molar volume properties data, and a list of the included elements, and summaries of the database revision history by version.
- The *TCS Ultra-high Temperature Materials Database (TCUHTM) 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 Ultra-high Temperature Materials page on our website where you can access an 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 on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

TCUHTM2 Elements, Systems, Phases and Properties

Included Elements

There are 8 elements included in the database.

B	C	Hf	N	O	Si	Ta	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:

- 28 assessed binary systems
- 41 assessed ternary systems (31 critically assessed and 10 tentatively assessed)
- 47 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

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

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

TCUHTM2 Systems

In this section:

TCUHTM2 Assessed Binary Systems

Twenty-eight (28) binary systems are assessed.

	B	C	Hf	N	O	Si	Ta
C	x						
Hf	x	x					
N	x	x	x				
O	x	x	x	x			
Si	x	x	x	x	x		
Ta	x	x	x	x	x	x	
Zr	x	x	x	x	x	x	x

TCUHTM2 Assessed Ternary Systems

Fourty-one (41) ternary systems total are assessed.

Assessed Ternary Systems				
B-C-Hf	B-C-Si	B-C-Ta	B-C-Zr	B-Hf-N
B-Hf-Si	B-Hf-Zr	B-N-Zr	B-O-Si	B-O-Zr
B-Si-Zr	C-Hf-Si	C-Hf-Ta	C-Hf-Zr	C-N-Si
C-N-Zr	C-O-Zr	C-Si-Ta	C-Si-Zr	C-Ta-Zr
Hf-N-O	Hf-O-Si	Hf-O-Ta	Hf-O-Zr	N-O-Si
N-O-Zr	N-Si-Ta	N-Si-Zr	O-Si-Ta	O-Si-Zr
O-Ta-Zr				

Tentatively Assessed Ternary Systems				
B-Hf-O	B-Hf-Ta	B-N-O	B-N-Ta	B-Ta-Zr
C-Hf-N	C-Hf-O	C-N-Ta	Hf-N-Si	Nf-N-Ta

TCUHTM2 Phases

In this section:

Common Phases for Ultra-high Temperature Materials

TCUHTM2 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*
IONIC_LIQUID	Liquid phase, which covers the melt of ultra-high temperature materials
FCC_B1	Carbide and nitride-based phase, which covers HfC, HfN, TaC, TaN, ZrC, ZrN solution phase compositions.
HCP_A3	Hf, Zr, Ta2C, Ta2N solution phase
BCC_A2	Hf, Ta, Zr solution phase
MB2_C32	It covers HfB2, TaB2, ZrB2
M5Si3_D88	It covers Hf5Si3, Zr5Si3, Hf5Si3B, Hf5Si3C, Zr5Si3C, Zr5Si3N

TCUHTM2 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.

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
GAS	Gas					1	(B, B1C1, B1C2, B1N1, B1O1, B1O2, B2, B2C1, B2O1, B2O2, B2O3, C, C1N1, 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, HF, HF1O1, HF1O2, N, N1O1, N1O2, N1O3, N1SI1, N1SI2, N1ZR1, N2, N2O1, N2O2, N2O3, N2O4, N2O5, N3, O, O1SI1, O1TA1, O1ZR1, O2, O2SI1, O2SI2, O2TA1, O2ZR1, O3, SI, SI2, SI3, TA, ZR, ZR2)1.0
B12ZR	UB12 (D2f)	D2f	cF52	(225, Fm-3m)		2	(B)12.0(ZR)1.0
B2O3	B2O3		hP15	(152, P3_121)		2	(B+3)2.0(O-2)3.0
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
B6SI	SiB6		oP280	(58, Pnnm)		3	(B)210.0(SI)23.0(B, SI)48.0
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	Hf, Ta, Zr BodyCentered Cubic	2	(HF, SI, TA, VA, ZR)1.0(B, C, N, O, VA)3.0
BETAR_BORON	beta-B (R-105)		hR105	(166, R-3m)		2	(B)93.0(B, C, SI)12.0
BNSI	alpha-B (hR12)		hR12	(166, R-3m)	BnSi	3	(B)61.0(SI)1.0(B, SI)8.0
BN_B4	Wurtzite (ZnS, B4)	B4	hP4	(186, P6_3mc)	Wurtzite	2	(B)1.0(N)1.0
C16_THETA	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Hf2Si, Zr2Si	2	(HF, TA, ZR)2.0(SI)1.0
CRISTOBALITE	Ideal beta-	C9	cF24	(227, Fd-3m)	SiO2 with AlPO4	2	(SI+4)1.0(SIO4-4)1.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
	Cristobalite (SiO2, C9)				solubility.		
CRSI2_C40	CrSi2 (C40)	C40	hP9	(180, P6_222)	TaSi2, ZrSi2	2	(HF, SI, TA)1.0(SI)2.0
D5A_M3B2	Si2U3 (D5a)	D5a	tP10	(127, P4/mbm)	Ta3B2	2	(HF, TA)3.0(B)2.0
DIAMOND_A4	Diamond (A4)	A4	cF8	(227, Fd-3m)	Si	2	(B, C, SI)1.0(O, VA)1.0
FCC_B1	Rock Salt (NaCl, B1)	B1	cF8	(225, Fm-3m)		2	(HF, TA, VA, ZR)1.0(B, C, N, O, VA)1.0
FLUORITE	Fluorite (CaF2, C1)	C1	cF12	(225, Fm-3m)	This is cubic high temp HfO2 and ZrO2	2	(HF+4, SI+4, TA+5, VA, ZR, ZR+4)2.0(O-2, VA)4.0
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	(194, P6_ 3/mmc)	HfC, HfN, TaC, TaN, ZrC, ZrN solution phase	1	(B, C)1.0
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	(194, P6_ 3/mmc)	Hf, Zr, Ta2C, Ta2N solution phase	2	(HF, SI, TA, ZR)1.0(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
HF6TA2O17	Nb2Zr6O17		oI100	(46, Ima2)	Hf6Ta2O17 Zr6Ta2O17	2	(HF+4, TA+5, VA, ZR+4)8.0(O-2, VA)17.0
IONIC_LIQ	Liquid				Liquid metal and slag mixture.	2	(HF+4, SI+4, TA+5, ZR+4)1.0(B, BO3-3, BO3/2, C, N, O-2, SIN4/3, SIO2, SIO4-4, VA)1.0
M2B_TETR	Khatyrkite (Al2Cu, C16)	C16	tI12	(140, I4/mcm)	Ta2B	2	(TA)2.0(B)1.0
M3SI1	Ti3P		tP32	(86, P4_2/n)	Ta3Si, Zr3Si	2	(HF, TA, ZR)3.0(SI)1.0
M3SI2_D5A	Si2U3 (D5a)	D5a	tP10	(127,	Hf3Si2, Zr3Si2	2	(HF, ZR)3.0(SI)2.0

Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
				P4/mbm)			
M5SI3_D88	Mavlyanovite (Mn5Si3, D88)	D88	hP16	(193, P6_ 3/mcm)	Hf5Si3, Zr5Si3, Hf5Si3B, Hf5Si3C, Zr5Si3C, Zr5Si3N	3	(HF, ZR)5.0(SI)3.0(B, C, N, VA)1.0
MB2_C32	Hexagonal omega (C32)	C32	hP3	(191, P6/mmm)	HfB2, TaB2, ZrB2	2	(B)2.0(B, HF, TA, ZR)1.0
MB_B33	CrB (B33)	B33	oS8	(63, Cmcm)	TaB, ZrB	2	(HF, TA, ZR)1.0(B)1.0
MSI_B27	FeB (B27)	B27	oP8	(62, Pnma)	HfSi, ZrSi	2	(HF, ZR)1.0(SI)1.0
QUARTZ	alpha-Quartz (low Quartz)		hP9	(152, P3_121)	SiO2 with AlPO4 solubility.	2	(SI+4)1.0(SIO4-4)1.0
SI2N2O	Si2N2O		oS20	(36, Cmc2_1)		3	(SI)2.0(N)2.0(O)1.0
SI3N4	Nierite (alpha-Si3N4)		hP28	(159, P31c)		2	(SI)3.0(N)4.0
SIC	Zincblende (ZnS, B3)	B3	cF8	(216, F-43m)		2	(SI)1.0(B, C)1.0
TA2O5_HT	Ta2O5-ht		tI44	(141, I4_ 1/amd)		2	(HF+4, TA+5, ZR+4)2.0(O-2, VA)5.0
TA2O5_LT	beta-Ta2O5		oP14	(49, Pccm)		2	(HF+4, TA+5, ZR+4)2.0(O-2, VA)5.0
TA5SI3C	Unknown Structure				Ta5Si3C, Ta5Si3N	3	(TA)5.0(SI)3.0(C, N, VA)1.0
TA5SI3_D8L	Cr5B3 (D8l)	D8l	tI32	(140, I4/mcm)	Low temperature Ta5Si3	2	(HF, TA)5.0(SI)3.0
TA5SI3_HT	W5Si3 (D8m)	D8m	tI32	(140, I4/mcm)	Hightemperature Ta5Si3	2	(TA)5.0(SI)3.0
TI3B4	Ta3B4 (D7b)	D7b	oI14	(71, Immm)	Ta3B4	2	(B)4.0(HF, TA)3.0

Name	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group*	*Info*	*Sublattices*	*Formula Unit*
TIB_B27	FeB (B27)	B27	oP8	(62, Pnma)	HfB	2	(B)1.0(HF, TA, ZR)1.0
TRIDYMITE	Monoclinic (Cc) Low Tridymite (SiO2)		mS144	(9, Cc)	SiO2 with AlPO4 solubility.	2	(SI+4)1.0(SIO4-4)1.0
ZIRCON	Zircon (ZrSiO4, S11)	S11	tI24	(141, I4_ 1/amd)	This is HfSiO4, ZrSiO4, GdPO4, LaPO4 and YPO4.	3	(SI+4)1.0(HF+4, ZR+4)1.0(O-2)4.0
ZR5SI4	Si4Zr5		tP36	(92, P4_12_ 12)	Zr5Si4, Hf5Si4	2	(HF, ZR)5.0(SI)4.0
ZRO2_MONO	Baddeleyite (ZrO2, C43)	C43	mP12	(14, P2_1/c)	This is Monoclinic HfO2 and ZrO2	2	(HF+4, ZR+4)2.0(O-2)4.0
ZRO2_TETR	HgI2 (C13)	C13	tP6	(137, P4_ 2/nmc)	This is Tetragonal HfO2 and ZrO2	2	(HF+4, TA+5, VA, ZR+4)2.0(O-2, VA)4.0
ZRSI2_C49	ZrSi2 (C49)	C49	oS12	(63, Cmcm)	ZrSi2, HfSi2	2	(HF, ZR)1.0(SI)2.0

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:	**2.0**
First release:	**TCUHTM1 was released with 2022b**

Changes in the Most Recent Database Release

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.