

# **TCS Ultra-high Temperature Materials Database (TCUHTM)**

## **Examples Collection**



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## About the Database Examples

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There are examples available to demonstrate both the *validity* of the database itself as well as to demonstrate some of its *calculation* capabilities when combined with Thermo-Calc software and its Add-on Modules and features.



For each database, the type and number of available examples varies. In some cases an example can belong to both a validation and calculation type.

- *Validation* examples generally include experimental data in the plot or diagram to show how close to the predicted data sets the Thermo-Calc calculations are. It uses the most recent version of the software and relevant database(s) unless otherwise specified.
- *Calculation* examples are intended to demonstrate a use case of the database. This might be showing a binary or ternary system calculated in a phase diagram, or demonstrate how the database and relevant software features would be applied to a heat treatment application, process metallurgy, soldering process, and so forth. In the case of heat treatment, it might include the result of calculating solidification segregation, determining homogenization temperature and then predicting the time needed to homogenize. There are many other examples specifically related to each database.



Where relevant, most references related to each example set are included at the end of the individual section. You can also find additional references specific to the database itself when using the database within Thermo-Calc. You can also contact us directly should you have any questions.



If you are interested in sharing your own examples using Thermo-Calc products in unique or surprising ways, or if you want to share your results from a peer reviewed paper, send an email to [info@thermocalc.com](mailto:info@thermocalc.com).

## TCS Ultra-high Temperature Materials Database (TCUHTM) Resources

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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.

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## TCUHTM Validation Examples

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Some diagrams are calculated with earlier versions of the database. Negligible differences might be observed if these are recalculated with the most recent version. The diagrams are updated when there are considerable or significant improvements.

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## Phase Stability Predictions

The TCS Ultra-high Temperature Materials Database (TCUHTM) can be used to calculate phase equilibria, including phase fractions and compositions, to reliably account for phase transformations. All the stable solution phases and intermetallic compounds that exist in the assessed and their extrapolated systems are included in the current database. TCUHTM1 is able to predict the stable phases for a given composition and condition within the recommended composition range of the database.

The table shows the calculated phases compared with experimental determined ones. TCS Ultra-high Temperature Materials Database (TCUHTM) is able to predict the phase types at each given composition correctly.

Reference	Composition	Temperature	Measured Phases	Calculated Phases
[2014Bai]	HfB <sub>2</sub> -ZrN	1600 °C	(Zr, Hf)N (Zr,Hf)B <sub>2</sub>	FCC_B1 which is (Zr,Hf)N MB2_C32, which is (Zr, Hf)B <sub>2</sub> And trace of BN
[2015Bas]	2ZrSi <sub>2</sub> -B <sub>4</sub> C-3C	1600 °C	ZrB <sub>2</sub> SiC	MB2_C32, which is ZrB <sub>2</sub> SiC
[2021Dod]	ZrB <sub>2</sub> /30SiC+8HfB <sub>2</sub>	1725 °C	(Zr,Hf)B <sub>2</sub> SiC	MB2_C32, which is (Zr,Hf)B <sub>2</sub> SiC

## References

- [2014Bai] M. C. Baier, M. A. Zuideveld, S. Mecking, Post-Metallocenes in the Industrial Production of Polyolefins. *Angew. Chemie Int. Ed.* 53, 9722–9744 (2014).
- [2015Bas] B. Basu, V. Parameswaran, H. Wang, S.-H. Lee, Dynamic compression behavior of reactive spark plasma sintered ultrafine grained (Hf, Zr)B<sub>2</sub>-SiC composites. *Ceram. Int.* 41, 8468–8474 (2015).
- [2021Dod] E. Dodi, Z. Balak, H. Kafashan, HfB<sub>2</sub> 2 -doped ZrB<sub>2</sub>-30 vol.% SiC composites: oxidation resistance behavior. *Mater. Res. Express.* 8, 045605 (2021).

## Melting Temperature Predictions

Melting temperature is one of the important properties for ultra-high temperature materials. The TCS Ultra-high Temperature Materials Database (TCUHTM) can be used to predict the phase transformation temperatures as a function of the chemical composition of typical industrial materials, including solidus and liquidus temperatures. This example shows the comparison of calculated and measured incipient melting temperatures and liquidus temperatures. The melting temperatures significantly decrease when silicates form. In most cases, the differences between measurements and the calculation are less than 5%.

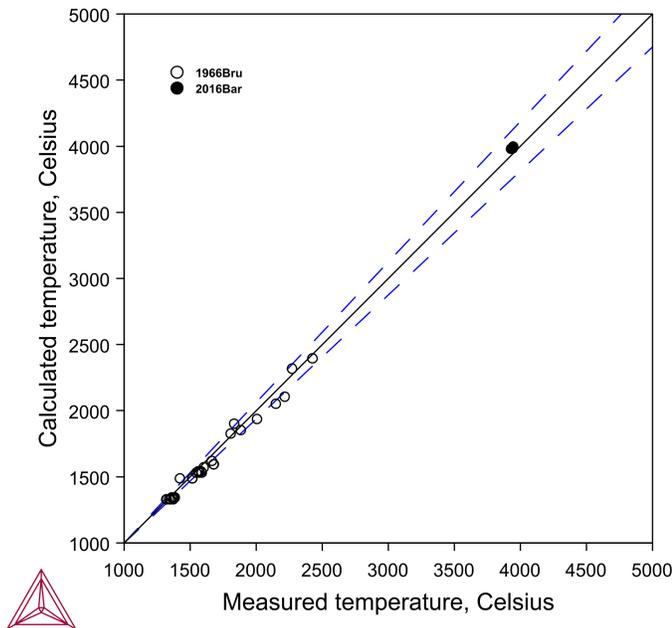


Figure 1: Comparison of calculated vs experimental melting temperatures [1966Bru; 2016Bar].

## References

- [1966Bru] C.E. Brukl and D.P. Harmon: "Ternary Phase Equilibria in Transition Metal-Boron-Carbon-Silicon Systems; Part II. Ternary Systems. Vol. 4. The Ti-Zr-C, Ti-Hf-C and Zr-Hf-C Systems," Tech. Rep. AFML-TR-65-2, Part II. Vol X, Air Force Materials Laboratory, Wright Patterson Air Force Base, OH, 1966.
- [2016Bar] O. Cedillos-Barraza, D. Manara, K. Boboridis, T. Watkins, S. Grasso, D. D. Jayaseelan, R. J. M. Konings, M. J. Reece, W. E. Lee, Investigating the highest melting temperature materials: A laser melting study of the TaC-HfC system. Sci. Rep. 6, 37962 (2016).

## Heat Capacity of HfN

TCS Ultra-high Temperature Materials Database (TCUHTM) can be used to calculate variety of thermodynamic properties. This example compares the calculated heat capacity of HfN (FCC\_B1) with the experimental data. The calculated heat capacity is consistent with the experimental data.

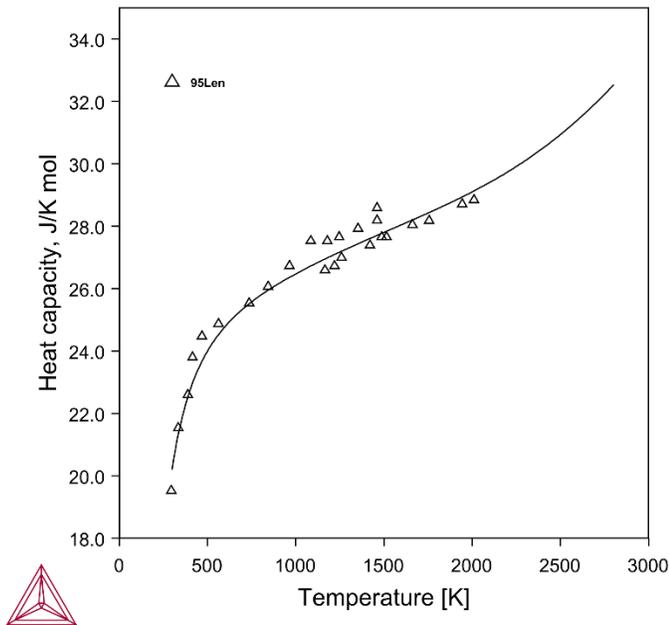


Figure 2: Calculated heat capacity of HfN with experimental data [1995Len].

### Reference

[1995Len] W. Lengauer, S. Binder, K. Aigner, P. Ettmayer, A. Guillou, J. Debuigne, G. Groboth, Solid state properties of group IVb carbonitrides. *J. Alloys Compd.* 217, 137–147 (1995).

## Pseudo Binary Phase Diagram of Oxides

The equilibria of the  $\text{HfO}_2\text{-Ta}_2\text{O}_5$  system is of interest for applications in high temperature material systems. Compositions within this system are currently used as thermal barrier coatings, and high temperature dielectrics. Understanding of the  $\text{HfO}_2\text{-Ta}_2\text{O}_5$  system is also of interest for the oxidation of other ultra-high temperature materials such as  $\text{HfC-TaC}$  and  $\text{HfN-TaN}$ , etc, and where you can use the TCS Ultra-high Temperature Materials Database (TCUHTM) for analysis.

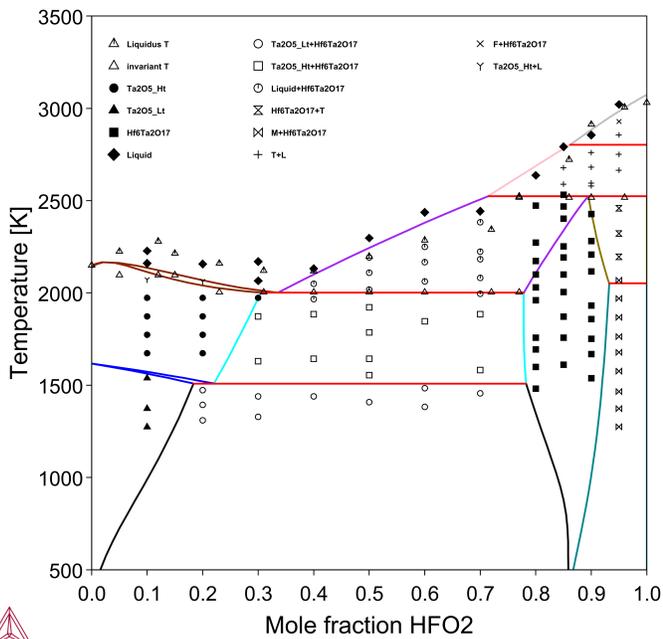


Figure 3: Calculated phase diagram for  $\text{Ta}_2\text{O}_5\text{-HfO}_2$  with experimental data from [2019McC].

### Reference

[2019McC] S. J. McCormack, K. Tseng, R. J. K. Weber, D. Kapush, S. V. Ushakov, A. Navrotsky, W. M. Kriven, In-situ determination of the  $\text{HfO}_2\text{-Ta}_2\text{O}_5$ -temperature phase diagram up to 3000°C. *J. Am. Ceram. Soc.* 102, 4848–4861 (2019).

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## TCUHTM Calculation Examples

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Some diagrams are calculated with earlier versions of the database. Negligible differences might be observed if these are recalculated with the most recent version. The diagrams are updated when there are considerable or significant improvements.

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## Binary Phase Diagrams

You can use the TCS Ultra-high Temperature Materials Database (TCUHTM) to plot binary phase diagrams in Thermo-Calc. Each assessed binary system is modeled to accurately describe experimental phase diagram data available in the literature. These examples show a selection of the important assessed systems that are the building blocks of the database itself when applying the CALPHAD method.



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

### Hf-B

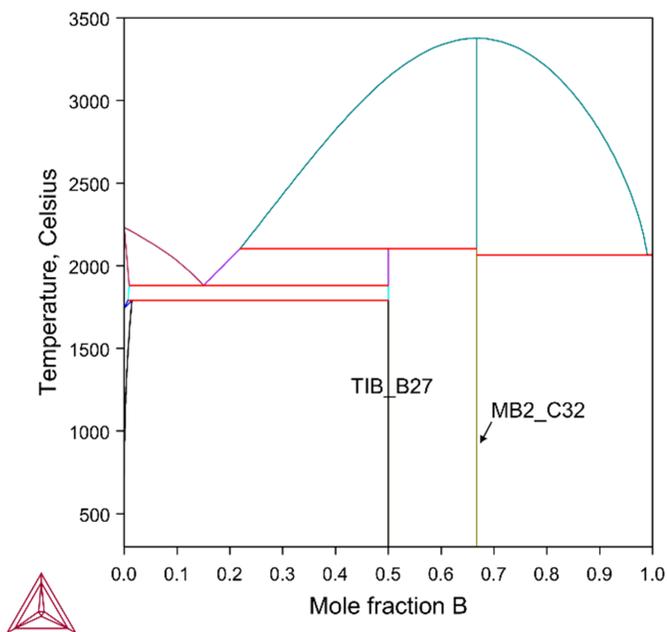


Figure 4: Calculated Hf-B phase diagram.

### Zr-B

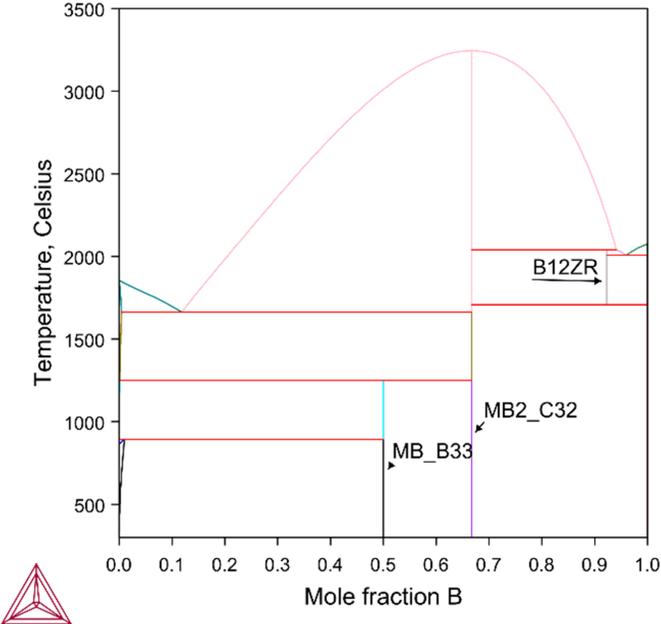


Figure 5: Calculated Zr-B phase diagram.

### Ta-C

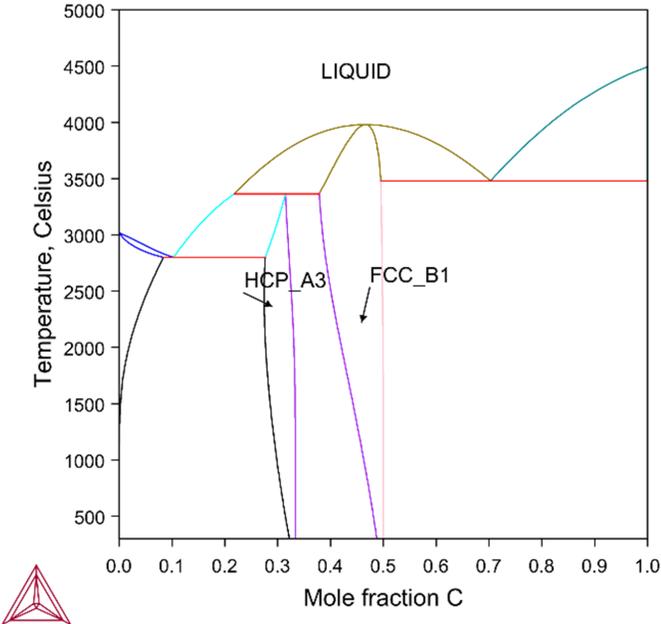


Figure 6: Calculated Ta-C phase diagram.

## Ta-Si

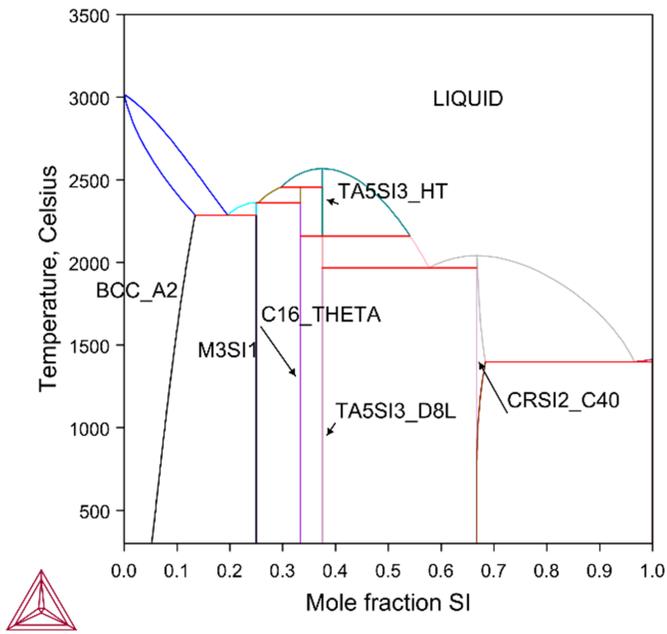


Figure 7: Calculated Ta-Si phase diagram.

## Zr-O

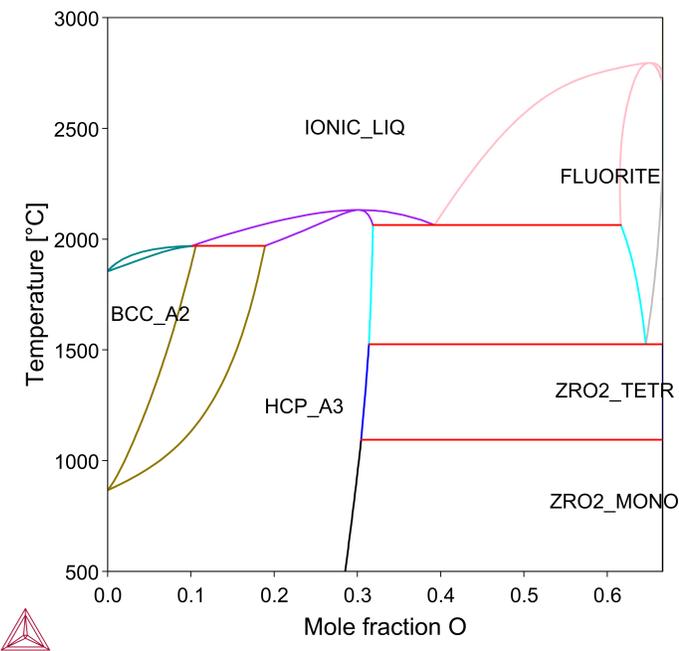


Figure 8: Calculated Zr-O phase diagram.

## Ternary Phase Diagrams

You can use the TCS Ultra-high Temperature Materials Database (TCUHTM) to plot ternary phase diagrams in Thermo-Calc. Each assessed ternary system is modeled to accurately describe experimental phase diagram data available in the literature. These examples show a selection of the important assessed systems that are the building blocks of the database itself when applying the CALPHAD method.



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



When working in Thermo-Calc with ternary diagrams you use either the Ternary Calculator (in Graphical Mode) or the Ternary module (in Console Mode). The fundamental calculation engine is the same but you access the settings in different ways.

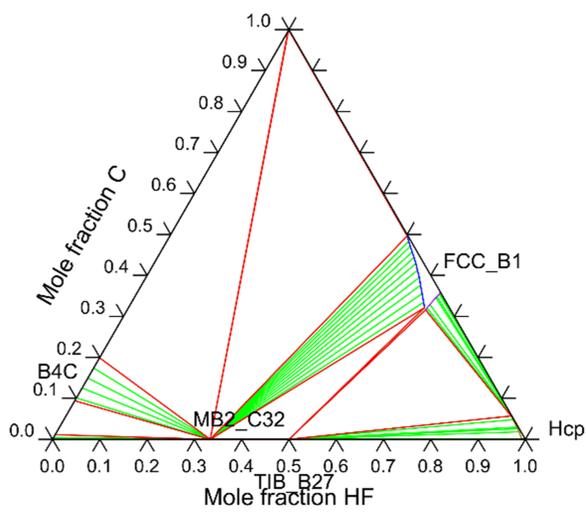


Figure 9: Calculated Hf-B-C isothermal section at 1773 K.

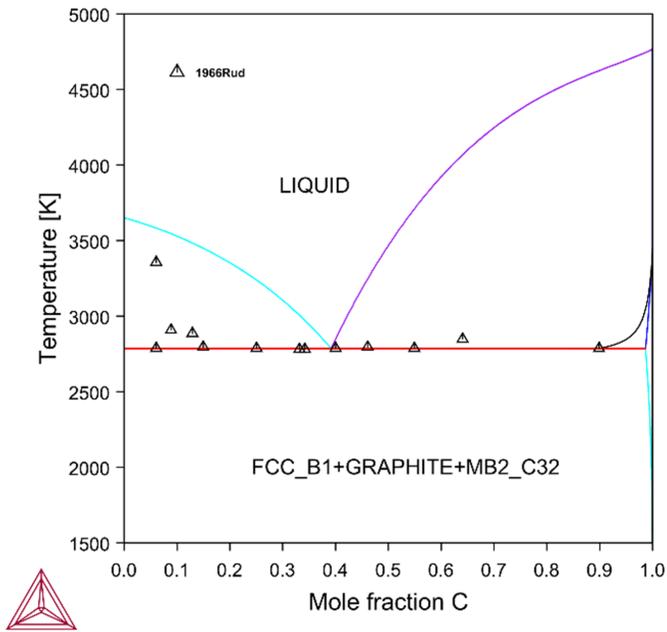


Figure 10: Calculated vertical section of at HfB<sub>2</sub>-C with experimental data from [1966Rud].

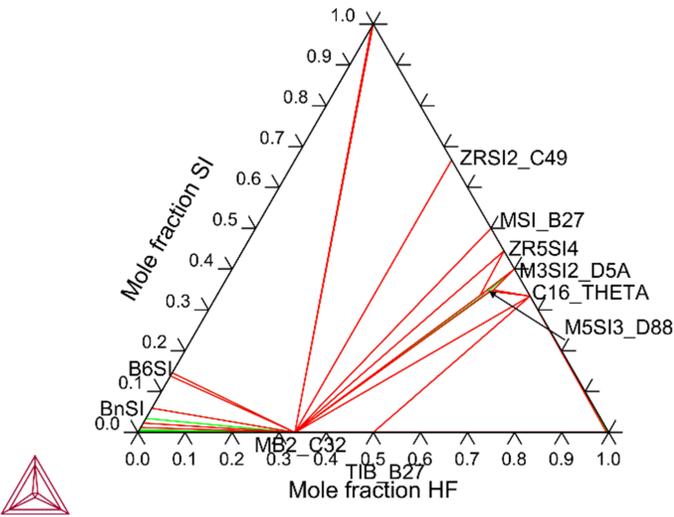


Figure 11: Calculated Hf-Si-B isothermal section at 1573 K.

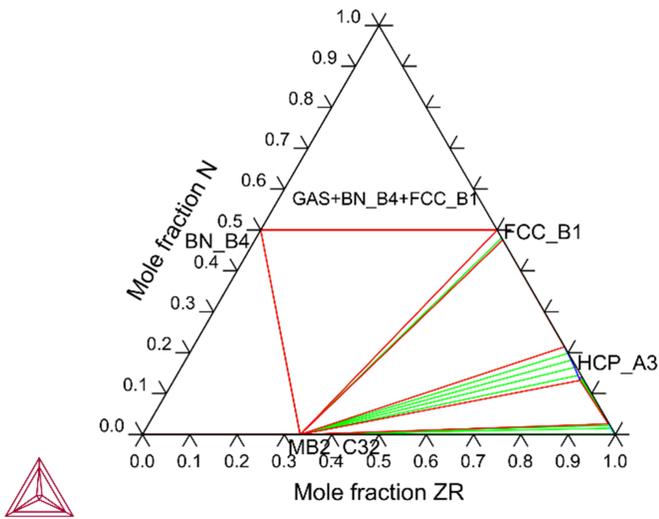


Figure 12: Calculated Zr-B-N isothermal section at 1773 K.

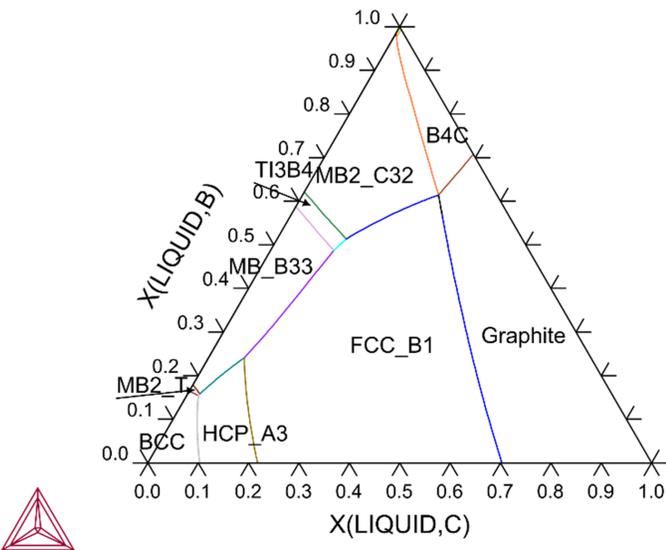


Figure 13: Calculated Ta-B-C liquidus projection.

## Reference

[1966Rud] E. Rudy and S. Windisch, & Ternary Phase Equilibria in Transition Metal-Boron-Carbon-Silicon Systems," Part II, Vol. XIII, Report AFML-TR-65-2, II, Vol XIII. Air Force Materials Laboratory, Wright Patterson Air Force Base, OH, 1966.