Molten Salt Thermodynamic Database-Thermochemical 
(*MSTDB-TC*)

GitLab Documentation

Version 1.3

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Use the following references when citing *MSTDB-TC*


1. Introduction

The Molten Salt Thermal Properties Database-Thermochemical (MSTDB-TC) is a publicly available database of thermodynamic models and values for fluoride and chloride molten salt components and related systems of interest with respect to molten salt reactor technology. These include fuel or coolant salts, consequential fission product and transuranic elements, contaminants such as air and moisture, and likely corrosion product elements such as iron, nickel and chromium. Phases include gas/vapor, liquids (e.g., molten salts, noble metals), and solid compounds. Solutions include the fluoride-based and chloride-based liquid melts as well as several solid solutions. The database was developed in the ChemSage .dat format using the FactSage® commercial package and compatible with the open-source equilibrium code Thermochimica.

The models and values provided within MSTDB-TC are obtained through combinations of literature-reported information, first principles calculations, and experimental measurements. These have been used to a greater or lesser extent as needed in assessments for pseudo-binary, pseudo-ternary, and higher order systems. A system is said to be assessed when sufficient experimental and theoretical data are available to optimize adjustable thermochemical values and parameters for each model and species to represent each phase in that system. In essence, a system is assessed when models and values appropriately reproduce available phase equilibria (phase diagram) and attendant values such as heat capacity, enthalpy of mixing, and vapor pressures.

Maintaining consistency of pure compound thermodynamic values throughout the database is vital. Pure compound values provide the foundation from which solutions are modeled. As each compound in the solution can be a part of multiple different subsystems, the underlying pure compound values need to be the same across all solutions. In order to accomplish this, a single set of thermodynamic values need to be selected for each compound, which is used for all subsequent solutions. An effort has been made to select the best available thermodynamic values for pure compounds, as any need to change the values in the future may require a substantial re-assessment effort of all affected systems. Due to differences in pure compound values between different publications and those selected for the MSTDB-TC, it often became necessary to perform re-assessments of published solution models before being added to the database. If the pure compound values did not differ greatly, the re-assessment could be slight, or even unnecessary.

A note of caution: It is possible to perform thermodynamic equilibrium calculation with FactSage. Thermochimica, or other software using MSTDB-TC for salt melts that contain multiple cations. While the calculations may run smoothly, the results might not be accurate as the specific combination of the salt cations for the halide melt may not have been assessed and therefore known to reproduce observed behavior. The user is advised to check the listing of MSTDB-TC systems to be assured that their system of interest has been included.

2. Database Contents

The MSTDB-TC has been prepared for public release through the code.ornl GitLab repository hosted by Oak Ridge National Laboratory. The repository includes the following files for the latest version of the MSTDB-TC:

- The database .dat files in standard ChemSage ASCII format, which contain all compounds and solutions of the MSTDB-TC for the fluoride- and chloride-based systems, respectively (denoted by Fluorides or Chlorides in .dat file name). Separate sets of .dat files provided for compatibility with different software and versions:
  - FactSage 8.1 compatible .dat files end in *_8-1.dat
  - Generated in FactSage 8.1 with “include functions” selected.
**2.1 Pseudo-binary Systems**

**Fluorides**

- BeF$_2$-KF
- BeF$_2$-LiF
- BeF$_2$-NaF
- BeF$_2$-PuF$_3$
- BeF$_2$-ThF$_4$
- BeF$_2$-UF$_4$
- CaF$_2$-BeF$_2$
- CaF$_2$-KF
- CaF$_2$-LaF$_3$
- CaF$_2$-LiF
- CaF$_2$-NaF
- CaF$_2$-ThF$_4$

- CeF$_3$-LiF
- CeF$_3$-NaF
- CeF$_3$-ThF$_4$
- CsF-KF
- CsF-LiF
- CsF-NaF
- CsF-UF$_4$
- CsF-UF$_3$
- CsF-UF$_4$
- CsF-U$	ext{F}_3$
- KF-LiF
- KF-NaF
- KF-UF$_3$
- KF-UF$_4$
- LiF-NaF
- LiF-NdF$_3$
- LiF-NiF$_2$
- LiF-UF$_3$
- LiF-UF$_4$
- LiF-ThF$_4$
- LiF-ThF$_3$
- LiF-ThF$_4$
- LiF-ThF$_3$
- LiF-ThF$_4$

**Chlorides**

- AlCl$_3$-KCl
- AlCl$_3$-LiCl
- AlCl$_3$-MgCl$_2$
- AlCl$_3$-NaCl
- AlCl$_3$-NiCl$_2$
- AlCl$_3$-RbCl
- AlCl$_3$-NdCl$_3$
- AlCl$_3$-SrCl$_2$
- AlCl$_3$-ZrCl$_4$
- CaCl$_2$-KCl
- CaCl$_2$-LiCl
- CaCl$_2$-NaCl
- CaCl$_2$-RbCl
- CaCl$_2$-NdCl$_3$
- CaCl$_2$-SrCl$_2$
- CaCl$_2$-ZrCl$_4$
- CeCl$_3$-LiCl
- CeCl$_3$-MgCl$_2$
- CeCl$_3$-NaCl
- CeCl$_3$-KCl
- CeCl$_3$-LiCl
- CeCl$_3$-NaCl
- CeCl$_3$-KCl
- CsCl-KCl
- CsCl- LiCl
- CsCl- NaCl
- CsCl- PuCl$_3$
- CsCl-RbCl
- CsCl-NdCl$_3$
- CsCl-SrCl$_2$
- CsCl-ZrCl$_4$
- FeCl$_2$-FeCl$_3$
- FeCl$_2$-KCl
- FeCl$_2$-NaCl
- FeCl$_2$-MgCl$_2$
- FeCl$_2$-NdCl$_3$
- FeCl$_2$-SrCl$_2$
- FeCl$_2$-ZrCl$_4$
- LiCl-KCl
- LiCl-MgCl$_2$
- LiCl-NdCl$_3$
- LiCl-SrCl$_2$
- LiCl-ZrCl$_4$
- LiCl-Cl$_2$
- MgCl$_2$-KCl
- MgCl$_2$-NdCl$_3$
- MgCl$_2$-SrCl$_2$
- MgCl$_2$-ZrCl$_4$
- MgCl$_2$-RbCl
- MgCl$_2$-Cl$_2$
- MgCl$_2$-Cl$_2$
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- MgCl$_2$-Cl$_2$
2.2 Pseudo-ternary Systems

Fluorides

- BeF$_2$-LiF-PuF$_3$
- BeF$_2$-LiF-ThF$_4$
- BeF$_2$-LiF-UF$_4$
- BeF$_2$-NaF-PuF$_3$
- BeF$_2$-NaF-UF$_4$
- BeF$_2$-ThF$_4$-UF$_4$
- CaF$_2$-KF-LiF
- CaF$_2$-KF-NaF

- CaF$_2$-LaF$_3$-LiF
- CaF$_2$-LaF$_3$-NaF
- CaF$_2$-LiF-ThF$_4$
- CaF$_2$-LiF-NaF
- CeF$_3$-LiF-NaF
- CsF-KF-LiF
- KF-LiF-NaF
- KF-LiF-RbF
- LiF-LiF-NaF
- LiF-PuF$_3$-ThF$_4$
- LiF-PuF$_3$-UF$_4$
- LiF-ThF$_4$-UF$_4$
- LiF-ThF$_4$-BeF$_2$-LiBeThF$_7$
- LiF-NaF-PuF$_3$
- LiF-NaF-RbF
- LiF-NaF-ThF$_4$
- LiF-NaF-UF$_4$
- LiF-PuF$_3$-ThF$_4$
- LiF-PuF$_3$-UF$_4$
- LiF-ThF$_4$-UF$_4$
- NaF-ThF$_4$-UF$_4$
- NaF-UF$_4$-BeF$_2$-LiBeThF$_7$

- CaF$_2$-LaF$_3$-LiF
- CaF$_2$-LaF$_3$-NaF
- CaF$_2$-LiF-ThF$_4$
- CaF$_2$-LiF-NaF
- CeF$_3$-LiF-NaF
- CsF-KF-LiF
- KF-LiF-NaF
- KF-LiF-RbF
- LiF-LiF-NaF
- LiF-PuF$_3$-ThF$_4$
- LiF-PuF$_3$-UF$_4$
- LiF-ThF$_4$-UF$_4$
- LiF-ThF$_4$-BeF$_2$-LiBeThF$_7$
- LiF-NaF-PuF$_3$
- LiF-NaF-RbF
- LiF-NaF-ThF$_4$
- LiF-NaF-UF$_4$
- LiF-PuF$_3$-ThF$_4$
- LiF-PuF$_3$-UF$_4$
- LiF-ThF$_4$-UF$_4$
- NaF-ThF$_4$-UF$_4$
- NaF-UF$_4$-BeF$_2$-LiBeThF$_7$

Chlorides

- AlCl$_3$-KCl-LiCl
- AlCl$_3$-KCl-NaCl
- AlCl$_3$-LiCl-NaCl
- CaCl$_2$-CeCl$_3$-LiCl

- CaCl$_2$-CeCl$_3$-MgCl$_2$
- CaCl$_2$-CeCl$_3$-NaCl
- CeCl$_3$-KCl-LiCl
- CeCl$_3$-KCl-MgCl$_2$

- CeCl$_3$-KCl-NaCl
- CeCl$_3$-LiCl-MgCl$_2$
- LiCl-KCl-UCl$_3$

2.3 Solid Solutions

Fluorides

- SSaa = (Li, Na)$_7$Th$_6$F$_{31}$
- SSab = (Pu, Th)$_8$F$_{17}$
- SSac = Li$_7$(Th, U)$_4$F$_{31}$
- SSad = Li$_7$(Th, U)$_2$F$_9$
- SSae = Li$_7$(Th, U)$_6$F$_{31}$
- SSaf = Li$_7$(Th, U)$_6$F$_7$
- SSag = Na$_2$(Th, U)$_2$F$_9$
- SSah = Na$_7$(Th, U)$_3$F$_{31}$
- SSai = Na$_7$(Th, U)$_2$F$_9$
- SSam = (Li, Na, K, Rb, Cs)$_F$
- SSan = (Ce, Th)$_F$
- SSao = (Ca, Th)$_F$
- SSap = (Ca, La)$_F$LaF$_3$ destabilized
- SSaq = (Ca, La)$_F$(CaF$_2$ destabilized)
- SSar = (La, Pu)$_F$
- SSas = (Na, Th)$_F$
- SSat = (U, Pu)$_F$
- SSau = (U, Th)$_F$
- SSav = Li$_3$ThF$_7$-BeF$_2$-LiBeThF$_7$
- SSaw = (Li, Na)$_7$U$_5$F$_{31}$
- SSax = Na$_7$(Th, U)$_2$F$_{15}$
- SSay = Na$_3$Th$_2$F$_{11}$-Na$_8$U$_3$F$_{17}$
- SSaz = (Li,Ni)$_F$
- SSba = Na$_5$Nd$_5$F$_{32}$-NaF
- SSbb = (Na, Ce)$_F$
- UF$_{34}$ = UF$_{(3+x)}$

Chlorides

- SScb = (Li,K)Cl
- SScc = (Li,K)Cl
- SSce = (Li,Mg)Cl$_x$
- SScf = (Li,Mg)Cl$_x$
- SScg = (Na,K)$_2$CeCl$_5$
- SSch = (Na,K)$_3$CeCl$_6$
- SSci = (Na,K)$_3$Ce$_5$Cl$_{18}$
- SScj = (Fe,Mg)Cl$_2$
- SSck = (Mg,Ni)Cl$_2$
- SScl = (Mg,Ni)Cl$_2$
- SScm = (Fe,Ni)Cl$_2$
- SScn = (Fe,Ni)Cl$_2$
- SSco = (Li,Na)Cl
- SScq = (Na, Ca)Cl$_x$
- SScr = (Mg, Ca)Cl$_2$
- SScs = (Na, K, Rb, Cs)Cl
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<th>Authors</th>
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<th>Title</th>
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<td>Thermodynamic assessment of the LiF-NaF-BeF2-ThF4-UF4 system</td>
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<td>Thermodynamic evaluation and optimization of the LiF-NaF-KF-MgF2-CaF2 system using the modified quasi-chemical model</td>
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