# TCS Mo-based Alloys Mobility Database (MOBMO1)

## Technical Information

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# Contents

# MOBMO1: TCS Mo-based Alloys Mobility Database

Molybdenum-based alloys are used in various applications due to their excellent mechanical, thermal, and corrosion-resistant properties. They are commonly used in aerospace components, electrical contacts, industrial machinery, and high-temperature furnace parts. Additionally, they are used in the production of high-strength steel alloys, which are crucial in construction and automotive industries for their durability and resistance to corrosion and heat.

The TCS Mo-based Alloys Mobility Database (MOBMO) is a kinetic database containing atomic mobility data for Mo-based refractory alloys. The database is compatible and primarily recommended for use with the most recent version of the TCS Mo-based Alloys Database (TCMO) (i.e. TCMO1).

The Mo-based alloys thermodynamic and kinetic databases (i.e. TCMO1 and MOBMO1) are available for refractory (e.g. Mo-base) superalloys that function at higher temperatures than the Ni-base superalloys. The Mo databases include the silicide and borosilicide phases to form $SiO_2$-based scales, which is to overcome the challenge of poor oxidation resistance that happens with these alloys that contain $MoO_3$.

The MOBMO1 database provides kinetic data for those working with the Add-on Modules—the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA). It can also be used together with the Thermo-Calc Software Development Kits (SDKs).

When the kinetic database is used with the Diffusion Module (DICTRA), and a thermodynamic database for Mo-based alloys (e.g. TCMO1) you can study diffusion-controlled phenomena in Mo/substrate systems, such as solidification, growth of interfacial compounds, dissolution of substrates, interdiffusion, and much more. Similarly, when used with the Precipitation Module (TC-PRISMA), it is suitable to simulate concurrent nucleation, growth, and coarsening of precipitates in Mo alloys.

## 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.

## Additional Resources

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

# MOBMO1 Elements and Phases

## Included Elements

There are 12 elements included in the most recent version of the database.

| | | | | | |
|---|---|---|---|---|---|
| Al | B | C | Cr | Fe | Hf |
| Mn | Mo | Re | Si | Ti | Zr |

## Included Phases

### Solution Phases

| *Solution Phases* | | | | |
|---|---|---|---|---|
| FCC_A1 | BCC_A2 | BCC_B2 | HCP_A3 | LIQUID |

### Compound Phases

| *Compound Phases* | | | | |
|---|---|---|---|---|
| MO5SI3_D8M | C15_LAVES | M6C | MOSI3_A15 | MOSI2_C11B |

The phases have diffusion data included in the database. You can include other phases in a diffusion simulation. However, these other phases are treated as so-called diffusion NONE, i.e. there is no diffusion considered in these other phases. Any phase not listed above is automatically entered as diffusion NONE (in Console Mode in the DICTRA module or in Graphical Mode with the Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA)), as long as a thermodynamic description for the phases is retrieved prior to reading data from the mobility database.

## Limits

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

# MOBMO1 Assessed Systems

The following systems have been either critically or tentatively assessed in this version of the database.

- 27 binary systems
- 8 ternary systems for solid phases
- 3 compounds

Parameters for self- and impurity- diffusivity of all the elements in the liquid phase are estimated using the Modified Sutherland equation. Mobility data for MO3SI_A15 are MOSI2_C11B are estimated.

## Binary Systems

### BCC_A2

| *Binary Systems (BCC_A2)* | | | | |
|---|---|---|---|---|
| Al-Fe | Al-Ti | Cr-Fe | Cr-Mo | Cr-Ti |
| Fe-Mn | Fe-Mo | Fe-Si | Fe-Ti | Hf-Mo |
| Hf-Ti | Hf-Zr | Mn-Ti | Mn-Zr | Mo-Ti |
| Mo-Zr | Zr-Ti | | | |

### FCC_A1

| *Binary Systems (FCC_A1)* | | | | | | |
|---|---|---|---|---|---|---|
| Al-Cr | Al-Fe | Al-Si | Al-Ti | Cr-Fe | Fe-Mn | Fe-Si |

### HCP_A3

| *Binary Systems (HCC_A3)* | | |
|---|---|---|
| C-Mo | Cr-Fe | Fe-Zr |

# Ternary Systems

## BCC_A2

| *Ternary Systems (BCC_A2)* | | | | | |
|---|---|---|---|---|---|
| Fe-Cr-Mo | Fe-Mn-Si | Ti-Al-Cr | Ti-Al-Fe | Ti-Al-Mo | Ti-Al-Zr |

## FCC_A1

| *Ternary Systems (FCC_A1)* | |
|---|---|
| Fe-Mn-Si | Fe-Cr-C |

# Compounds

| *Compounds* | | |
|---|---|---|
| MO5SI3_D8M: $Mo_5Si_3$ | C15_LAVES: $ZrMo_2$ | M6C: $Fe_3Mo_2C$ |