

TCS Noble Metals Mobility Database (MOBNOBL2)

Technical Information

Available Starting with Thermo-Calc Version 2025b



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MOBNOBL2: TCS Noble Metal Alloys Mobility Database

TCS Noble Metal Alloys Mobility Database (MOBNOBL) is a kinetic database containing mobility data for noble metal alloys. It can be used for the atomic mobility descriptions of Ag-Au-Cu-Pd-Pt-based alloys for the fcc and liquid phases.

MOBNOBL2 is intended for use in combination with the TCNOBL4 TCS Noble Metal Alloys thermodynamic database.

Together with the Diffusion Module (DICTRA) and a thermodynamic database for noble metals, it can be used to study diffusion-controlled phenomena in noble metals e.g. microsegregation during solidification, homogenization kinetics, growth/dissolution kinetics of precipitates, interdiffusion, and so forth. You can also use it with the Precipitation Module (TC-PRISMA) to simulate concurrent nucleation, growth, and coarsening of precipitates in noble metal alloys.

MOBNOBL: TCS Noble Metals Mobility Database Revision History. The current version of the database is MOBNOBL2. See the link for any subversion release details.

The CALPHAD Method

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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 <u>CALPHAD Method</u> and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our <u>website</u> or our <u>YouTube playlist</u>.

Additional Resources

Go to the <u>Noble Metal Alloys Databases</u> page on our website where you can access this Technical Information plus learn more about the compatible thermodynamic database and its Validation and Calculation Examples Collection. Also explore further <u>applications of</u> <u>Thermo-Calc to Precious Metals</u> including links to other resources such as publications and examples.

MOBNOBL2 Assessed Systems

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

- 48 binary systems
- 3 ternary systems

Binary Systems

FCC_A1

Binary Systems (FCC_A1)					
Ag-Al	Ag-Au	Ag-Cu	Ag-Ge	Ag-Mn	Ag-Pd
Ag-Sn	Ag-Zn	Al-Cu	Al-Li	Al-Ni	Al-Pt
Al-Si	Al-Zn	Au-Cu	Au-Fe	Au-Ni	Au-Pt
Co-Cu	Co-Fe	Co-Ga	Co-Mn	Co-Ni	Co-Pd
Co-Pt	Co-Si	Co-Ti	Cu-Fe	Cu-Ge	Cu-Mn
Cu-Ni	Cu-Pt	Cu-Sn	Cu-Ti	Cu-Zn	Fe-Mn
Fe-Ni	Fe-Pd	Fe-Pt	Ni-Pt	Ni-Re	Ni-Rh
Ni-Ru	Pd-Pt				

Liquid

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

Binary Systems (Liquid)					
Ag-Cu	Ag-Sn	Al-Cu	Cu-Sn		

Ternary Systems

FCC_A1

Ternary Systems (FCC_A1)					
Ag-Al-Cu	Ag-Au-Cu	Cu-Ag-Sn			

MOBNOBL2 Elements and Phases

Included Elements

There are 26 elements included in the most recent version of the database.

Included Elements									
Ag	AI	Au	Са	Со	Cr	Cu	Fe	Ga	Ge
In	lr	Li	Mn	Ni	Pd	Pt	Re	Rh	Ru
Sb	Sc	Si	Sn	Ti	Zn				

Included Phases

FCC_A1 and LIQUID.

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

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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.

MOBNOBL: TCS Noble Metals Mobility Database Revision History

Current Database Version

Database name (acronym):	TCS Noble Metal Alloys Mobility Database (MOBNOBL)
Database owner:	Thermo-Calc Software AB
Database version:	2.0
First release:	MOBNOBL1 was released with 2022a

Changes in the Most Recent Database Release

MOBNOBL1 to MOBNOBL2

Software release version 2025b (June 2025)

New Elements

- Five (5) new elements added to the database to align with the thermodynamic database: Ca, Li, Sb, Sc, and Si. Now it is a 26 element framework.
- Parameters for the new elements Ca, Li, Sb, Sc, and Si in the liquid phase are estimated using the Modified Sutherland equation.

BINARY SYSTEMS

Nineteen (19) newly assessed binary systems for FCC_A1 phase (total 44): Ag-Ge, Al-Li, Al-Ni, Al-Si, Al-Zn, Co-Fe, Co-Ga, Co-Mn, Co-Ni, Co-Si, Co-Ti, Cu-Ge, Cu-Ti, Fe-Mn, Fe-Ni, Fe-Pt, Ni-Re, Ni-Rh, and Ni-Ru.

THERMOPHYSICAL PROPERTIES

• Added viscosity, surface tension and THCD/ELRS descriptions for the above newly added systems.