

The Calfateria

Nathalie Dupin¹ Suzana G. Fries²

¹ Calcul Thermodynamique, 63670 Orcet, France

² Materials Research Department, Ruhr-Universität-Bochum, Universitätsstr. 150 44801 Bochum, Germany

nathdupin@cthermo.fr

Acknowledgements to Bengt Hallstedt, Christine Guéneau, Silvana Tuminello, Lina Kjellqvist, Ursula Kattner, Malin Selleby, Bo Sundman, Emily Corcoran, Nicholas Grundy, Karin Frisk, Klaus Richter



The Calphad Coffee Breaks on line



Selecting a system



The Calfateria - Open Binary Calphad Repository

Select system (e.g. Ag Al):

H																				He
Li	Be																			Ne
Na	Mg																			Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr			
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe			
Cs	Ba	Ln	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn			
Fr	Ra	An	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn									
		Ln	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
		An	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

● Show tiny phase diagrams when one element is selected

The Calfateria is a repository of binary Calphad descriptions, primarily based on [The SGTE collection of binary datasets published in 2025 by B. Hallstedt](#). A description can be accessed by selecting two elements. In some cases, additional descriptions for a given system are available and can be accessed by clicking the corresponding button. Connections between systems that share phases with identical crystallographic structures can be explored through the detailed information provided for each phase.

Furthermore, a range of figures calculated using Thermo-Calc [Thermo-Calc](#) (version 2026a) is provided. For each dataset, users can display calculated phase diagrams, enthalpy and Gibbs energy curves for each described phase, as well as the activities of the elements at equilibrium at a given temperature. The command files used to generate these figures are also available, allowing users to easily reproduce similar plots at different temperatures, adjust plotting scales, or limit the number of descriptions included for comparison.

For certain systems, comparison with experimental data are also provided.



Main contributors: N. Dupin: Hi, html, python, sh, javascript, TCM, exp files, S.G. Fries: the name and wanting always more

Acknowledgements for feedback and discussions : Bengt Hallstedt, Christine Guéneau, Silvana Tuminello, Lina Kjellvist, Ursula Kattner, Malin Selleby, Bo Sundman, Emily Corcoran, Nicho

Selecting a system

The CalFateria - Open Binary Calphad Repository

Select system (e.g. Ag-Al):

Show tiny phase diagrams when one element is selected

The CalFateria is a repository of binary Calphad descriptions, primarily based on [The ICSTI collection of binary datasets published in 2022 by B. Raftoyiannis](#). A description can be accessed by selecting two elements. In some cases, additional descriptions for a given system are available and can be accessed by clicking the corresponding button. Connections between systems that share phases with identical crystallographic structures can be explored through the detailed information provided for each phase.

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For certain systems, comparison with experimental data are also provided.

How to cite ?
To use figures from this site, cite <https://doi.org/10.21203/rs.3.rs-2120312/v1>. The bibliographic reference to the description and to the experimental or theoretical data shown here will be given.

How to contribute ?
You can send comments. You can send whatever files containing descriptions, macro commands to produce figures, experimental datasets, ...
Please put a date and the name of the contributor on the first line of every file, indicating the software (with version) able to handle the file would be nice.
Mail to Nathalie.Dupin.

The screenshot shows a periodic table where each element cell contains a small phase diagram. The 'Ag' element is selected in the search bar, and the 'Al' element is highlighted in the periodic table. A tooltip for the 'Ag-Al' system is visible over the intersection of Ag and Al.

As you feel

- ↪ Typing in the cell above the periodic table
 - Ag-Al
 - Al-Ag
 - ag al
 - ...
- ↪ Clicking on the two elements in the periodic table
- ↪ Clicking one element in the periodic table and one tiny phase diagram

Default description display

The CalFateria - Open Binary Calphad Repository

Select system (e.g. Ag-Al):

Ag	Al	Fe	Si	Co	Ni	Cr	Mn	Cu	Zn	Ga	Ge	As	Se	Te	Pb	Sb	Bi	Pt	Au	
Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Te	Pb	Sb	Bi	Pt	Au
Al	Si	P	S	Cl	Br	I	At													
Li	Na	K	Rb	Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Be	Mg	Ca	Str	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Ba	Hg
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Te	Pb	Sb	Bi	Pt	Au	Hg
Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Te	Pb	Sb	Bi	Pt	Au
Al	Si	P	S	Cl	Br	I	At													
Li	Na	K	Rb	Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Be	Mg	Ca	Str	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Ba	Hg
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Te	Pb	Sb	Bi	Pt	Au	Hg
Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Te	Pb	Sb	Bi	Pt	Au
Al	Si	P	S	Cl	Br	I	At													
Li	Na	K	Rb	Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Be	Mg	Ca	Str	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Ba	Hg
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Te	Pb	Sb	Bi	Pt	Au	Hg

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Furthermore, a range of figures calculated using Thermo-Calc [Thermo-Calc \(version 2024a\)](#) is provided. For each dataset, users can display calculated phase diagrams, enthalpy and Gibbs energy curves for each described phase, as well as the activities of the elements at equilibrium at a given temperature. The command files used to generate these figures are also available, allowing users to easily reproduce similar plots at different temperatures, adjust plotting scales, or limit the number of descriptions included for comparison. For certain systems, comparison with experimental data is also provided.

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System

Ag-Al

80Spe P.1. Spencer, O. Kubaschewski, unpublished, 1980. [Ag-Al_80Spe.TDB](#) [80Spe.TDB](#) [E7Spe.TDB](#) [V5Ag-48.TDB](#) [G6W9.TDB](#) [2016c.TDB](#) [Comparison](#)

Phase diagram

Thermo-Calc (2024.04.23.11.51) Ag-Al_80Spe.TDB

Files to download: [TCM](#) [exo](#) [exo](#)

Enthalpy of the phases

Thermo-Calc (2024.04.23.11.51) Ag-Al_80Spe.TDB 1000 K

Files to download: [TCM](#) [exo](#) [exo](#)

Activity of the elements

Thermo-Calc (2024.04.23.11.52) 1000 K Ag-Al_80Spe.TDB

Files to download: [TCM](#) [exo](#) [exo](#)

Comments in the TDB

Dataset created 2010.11.13 by Bengt Hallstedt, 2020.03.29: Modified for use with GESS.

This dataset does not work with the B7Spe lattice stabilities, but reasonably well with the SGTE lattice stabilities (except CUR_A13). The dataset has probably been modified since the original 80Spe dataset. Hcp is stable between fcc-ag and cur-a13 below 434 K.

Phases described in the database Ag-Al_80Spe.TDB

Name	Structure	Comment
LIQUID	[Ag, Al]	Liquid phase
FCC_A1	[Ag, Al](W)	Fcc (f4, fm-3m) and Max (cF8, fm-3m), magnetic model
BCC_A2	[Ag, Al](W)	Bcc (cI2, Im-3m), magnetic model
HCP_A3	[Ag, Al](W)	Hcp (hP2, P6_3/mmc) and Max2 (hR4s-type, hP4, P6_3/mmc, BB_1), magnetic model
CUR_A13	[Ag, Al](W)	Prototype beta-Mn (cP20, P4_132)

Click on the name of a phase to display more about this phase.

N. Dupin

The CalFateria

2026.06.08

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Default description display

The CalFateria - Open Binary Calphad Repository

Select system (e.g. Ag-Al):

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Please put a date and the name of the contributor on the first line of every file, indicating the software (with version) able to handle the file would be nice.
Mail to Nathalie.Duchin.

Link to the TDB file corresponding to this page

Source

Ag-Al

80Spe P.J. Spencer, O. Kubaschewski, unpublished, 1968 [Ag-Al_80Spe.TDB](#) [80Spe.TDB](#) [87Spe.TDB](#) [V5Am-UB.TDB](#) [G6W9.TDB](#) [2016c.TDB](#) Comparison

Phase diagram

Thermo-Calc (2026.04.23.11.51) Ag-Al_80Spe.TDB

Files to download: [TCM](#) [exo](#) [exo](#)

Enthalpy of the phases

Thermo-Calc (2026.04.23.11.51) Ag-Al_80Spe.TDB 1000 K

Files to download: [TCM](#) [exo](#) [exo](#)

Activity of the elements

Thermo-Calc (2026.04.23.11.52) 1000 K Ag-Al_80Spe.TDB

Files to download: [TCM](#) [exo](#) [exo](#)

Comments in the TDB

Dataset created 2010.11.13 by Bengt Hallstedt, 2020.03.29: Modified for use with GEM5.

This dataset does not work with the B75pe lattice stabilities, but reasonably well with the SGTE lattice stabilities (except CUB_A13). The dataset has probably been modified since the original 80Spe dataset. Hcp is stable between fcc-ag and cub-ai3 below 434 K.

Phases described in the database Ag-Al_80Spe.TDB

Name	Model	Comment
LIQUID	[Ag, Al]	Liquid phase
FCC_A1	[Ag, Al](W)	Fcc (fF4, Fm-3m) and Max (cF8, Fm-3m), magnetic model
BCC_A2	[Ag, Al](W)	Bcc (cI2, Im-3m), magnetic model
HCP_A3	[Ag, Al](W)	Hcp (hP2, P6_3/mmc) and Mg2X (hR4-type, hP4, P6_3/mmc, BB_1), magnetic model
CUB_A13	[Ag, Al](W)	Prototype beta-Mn (cP20, P4_132)

Click on the name of a phase to display more about this phase.

The default description is the first in chronological order.

Default description display

🔍 The CalFateria - Open Binary Calphad Repository

Select system (e.g. Ag-Al):

Ag	Al	As	Bi	Ca	Co	Cr	Cu	Fe	Ge	Ir	Li	Nb	Ni	Pb	Pt	Sb	Sn	Ta	Ti	V	Zn
Al	As	Bi	Ca	Co	Cr	Cu	Fe	Ge	Ir	Li	Nb	Ni	Pb	Pt	Sb	Sn	Ta	Ti	V	Zn	
Ag	Al	As	Bi	Ca	Co	Cr	Cu	Fe	Ge	Ir	Li	Nb	Ni	Pb	Pt	Sb	Sn	Ta	Ti	V	Zn
Al	As	Bi	Ca	Co	Cr	Cu	Fe	Ge	Ir	Li	Nb	Ni	Pb	Pt	Sb	Sn	Ta	Ti	V	Zn	
Ag	Al	As	Bi	Ca	Co	Cr	Cu	Fe	Ge	Ir	Li	Nb	Ni	Pb	Pt	Sb	Sn	Ta	Ti	V	Zn

Show tiny phase diagrams when one element is selected

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Furthermore, a range of figures calculated using Thermo-Calc [Thermo-Calc \(version 2024a\)](#) is provided. For each dataset, users can display calculated phase diagrams, enthalpy and Gibbs energy curves for each described phase, as well as the activities of the elements at equilibrium at a given temperature. The available, allow temperatures, are included for comparison. For certain systems.

How to cite ?
To use figures from this site, cite <https://calfateria.fr/TheCalFateria/>. The bibliographic reference to the description and to the experimental or theoretical data shown have also to be given.

How to contribute ?
You can send comments. You can send whatever files containing descriptions, macro commands to produce figures, experimental

Other descriptions and comparison

Ag-Al
80Spe P.J. Spencer, O. Kubaschewski, unpublished, 1980, [Ag-Al_80Spe.TDB](#)

[80Spe.TDB](#)
[87Spe.TDB](#)
[V5Am-UB.TDB](#)
[G6W9.TDB](#)
[2016c.TDB](#)
[Comparison](#)

Phase diagram

Files to download: [TCM](#) [exo](#) [exo](#)

Enthalpy of the phases

Files to download: [TCM](#) [exo](#) [exo](#)

Activity of the elements

Files to download: [TCM](#) [exo](#) [exo](#)

Comments in the TDB

Dataset created 2010.11.13 by Bengt Hallstedt, 2020.03.29: Modified for use with GESS.

This dataset does not work with the B7Spe lattice stabilities, but reasonably well with the SGT lattice stabilities (except CUR_A13). The dataset has probably been modified since the original 80Spe dataset. Hcp is stable between fcc-Ag and cur-A13 below 434 K.

Phases described in the database: Ag-Al_80Spe.TDB

Name	Model	Comment
LIQUID	[Ag, Al]	Liquid phase
FCC_A1	[Ag, Al](W)	Fcc (fF4, Fm-3m) and Max (cF8, Fm-3m), magnetic model
BCC_A2	[Ag, Al](W)	Bcc (cI2, Im-3m), magnetic model
HCP_A3	[Ag, Al](W) _{0.5}	Hcp (hP2, P6_3/mmc) and Max2X (hR4-type, hP4, P6_3/mmc, BB_1), magnetic model
CUR_A13	[Ag, Al](W)	Prototype beta-Mn (cP20, P4_132)

Click on the name of a phase to display more about this phase.

N. Dupin

The CalFateria

2026.06.08

5 / 10

Default description display

The CalFateria - Open Binary Calphad Repository

Select system (e.g. Ag-Al):

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Ag-Al

80Spa P.1. Spencer, O. Kubaschewski, unpublished, 1980. [Ag-Al_80Spa.TDB](#)

80Spa.TDB 87Spa.TDB V5Am-48.TDB G6W9.TDB 2016c.TDB

Phase diagram

Thermo-Calc (2026.04.23.11.51) Ag-Al_80Spa.TDB

Files to download: [TCM](#) [GIB](#) [GDS](#)

Enthalpy of the phases

Thermo-Calc (2026.04.23.11.51) Ag-Al_80Spa.TDB 1000 K

Files to download: [TCM](#) [GIB](#) [GDS](#)

Activity of the elements

Thermo-Calc (2026.04.23.11.52) 1000 K Ag-Al_80Spa.TDB

Files to download: [TCM](#) [GIB](#) [GDS](#)

Comments in the TDB

Dataset created 2010.11.13 by Bengt Hallstedt, 2020.03.29: Modified for use with GESS.

This dataset does not work with the B75pa lattice stabilisers, but reasonably well with the SGT lattice stabilisers (except CUR_A13). The dataset has probably been modified since the original 80Spa dataset. Hcp is stable between fcc-Ag and cub-A13 below 434 K.

Phases described in the database: [Ag-Al_80Spa.TDB](#)

Name	Material	Comment
LIQUID	[Ag, Al]	Liquid phase
FCC_A1	[Ag, Al](W)	Fcc (fF4, Fm-3m) and Max (cF8, Fm-3m), magnetic model
BCC_A2	[Ag, Al](W)	Bcc (cI2, Im-3m), magnetic model
HCP_A3	[Ag, Al](W) _{0.5}	Hcp (hP2, P6_3/mmc) and Mg2X (hR4-type, hP4, P6_3/mmc, BB_1), magnetic model
CUR_A13	[Ag, Al](W)	Prototype beta-Mn (cP20, P4_132)

Click on the name of a phase to display more about this phase.

Figures calculated with Thermo-Calc are shown.

Below each figure, there are links to download

- ↪ the TCM file used to make the figure,
- ↪ the exp file containing the coordinates of the curves,
- ↪ the graphical figure in png format.

Default description display

The CalFateria - Open Binary Calphad Repository

Full information on a range of figures calculated using Thermo-Calc 2026a (version 2026a) is provided. For each dataset, users can display calculated phase diagrams, enthalpy and Gibbs energy curves for each description phase, as well as the activities of the elements at equilibrium at a given temperature. The command files used to generate these figures are also available, allowing users to easily reproduce similar plots at different temperatures, adjust plotting scales or limit the number of descriptions included for comparison. For certain systems, comparison with experimental data is also provided.

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 Please put a date and the name of the contributor on the first line of every file. Indicating the software (with version) able to handle the file would be nice.
 Link to [Nathalie Dupin](#)

Ag-Al **805pe** P.J. Spencer, O. Kubaschewski, unpublished, 1980 Ag-Al_805pe.TDB 805pe.TDB 875pe.TDB HSLn-LB.TDB 04WLTDB 20TeTDB Comparison

Phase diagram

THERMO-CALC (2026.04.23:11:51) Ag-Al_805pe.TDB

Files to download: [TDB](#) [exo](#) [opt](#)

Enthalpy of the phases

THERMO-CALC (2026.04.23:11:51) Ag-Al_805pe.TDB 1000 K

Files to download: [TDB](#) [exo](#) [opt](#)

Activity of the elements

THERMO-CALC (2026.04.23:11:52) 1000 K Ag-Al_805pe.TDB

Files to download: [TDB](#) [exo](#) [opt](#)

Comments in the TDB

Dataset created 2010.11.13 by Bengt Hallstedt. 2020.03.29: Modified for use with GE56.
 This dataset does not work with the 875pe lattice stabilities, but reasonably well with the SGTE lattice stabilities (except CUB_A13). The dataset has probably been modified since the original 805pe dataset.
 Hcp is stable between fcc-Ag and cub-A13 below 434 K.

Phases described in the database: Ag-Al_805pe.TDB

Name	Model	Comment
LIQUID (Ag, Al)		Liquid phase
FCC_A1 (Ag, Al)(Va)		Fcc (cF4, Fm-3m) and MoX (cF8, Fm-3m), magnetic model
BCC_A2 (Ag, Al)(Va)3		Bcc (c12, Im-3m), magnetic model
HCP_A3 (Ag, Al)(Va)3.5		Hcp (hP2, P6_3/mmc) and Me2X (NiAs-type, hP4, hP6_3/mmc, BB_1), magnetic model
CUB_A13 (Ag, Al)(Va)		Prototype beta-Mn (#P20, P4_132)

Click on the name of a phase to display more about this phase.

```

$ Database for Ag-Al from P.J. Spencer and O. Kubaschewski 1980
$ P.J. Spencer, O. Kubaschewski, unpublished, 1980.
$ Dataset created 2010.11.13 by Bengt Hallstedt.
$ 2020.03.29: Modified for use with GE56.
$
$ This dataset does not work with the 875pe lattice stabilities, but
$ reasonably well with the SGTE lattice stabilities (except CUB_A13).
$ The dataset has probably been modified since the original 805pe dataset.
$
$ Hcp is stable between fcc-Ag and cub-A13 below 434 K.
$
$
$
$ TEMP-LIM 298.15 6000.00 !
$
$ SELEMENT NAME REF. STATE ATOMIC MASS H298-H0 S298 !
$
$ ELEMENT VA VACUUM 0.0 0.0 0.0 !
$ ELEMENT Ag FCC_A1 107.8682 5745. 42.55 !
$ ELEMENT Al FCC_A1 26.98154 4540. 28.30 !
$
$ Phase definitions
$
$ PHASE LIQUID:L % 1 1 !
$ CONST LIQUID:L : AG AL : !
$
$ Fcc (cF4, Fm-3m) and MoX (cF8, Fm-3m)
    
```

The source for the description and the comments in the TDB are taken from comment lines at the beginning of the file. This feature may be problematic if Bengt Hallstedt's usual layout is not followed.

Default description display

The CalFateria - Open Binary Calphad Repository

Full database: a range of figures calculated using Thermo-Calc 2022a (version 2026a) is provided. For each dataset, users can display calculated phase diagrams, enthalpy and Gibbs energy curves for each described phase, as well as the activities of the elements at equilibrium at a given temperature. The command files used to generate these figures are also available.

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Show tiny phase diagrams when one element is selected

Ag-Al

805pe P.J. Spencer

Phase diagram

THERMO-CALC (2026.04.23:11.51) Ag-Al_805pe.TDB

Files to download: [TCD](#) [exo](#) [opt](#)

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Phases described in the database: Ag-Al_805pe.TDB

Name	Model	Comment
LIQUID	(Ag, Al)	Liquid phase
FCC_A1	(Ag, Al)(Va)	Fcc (cF4, Fm-3m) and MoX (cF8, Fm-3m), magnetic model
BCC_A2	(Ag, Al)(Va) ₃	Bcc (cI2, Im-3m), magnetic model
HCP_A3	(Ag, Al)(Va) ₅	Hcp (hP2, P6_3/mmc) and Me2X (NiAs-type, hP4, P6_3/mmc, BB_1), magnetic model
CUB_A13	(Ag, Al)(Va)	Prototype beta-Mn (cP20, P4_132)

Click on the name of a phase to display more about this phase.

The comment for the phase is mainly taken from comment lines above the phase declaration. This feature is not very robust. Some comments like “magnetic model”, the fact that the phase is rejected by default or that there is a combination of several contributions are added from the analysis of the TYPE_DEFINITION commands.

```
$ Database for Ag-Al from P.J. Spencer and O. Kubaschewski 1980
$ P.J. Spencer, O. Kubaschewski, unpublished, 1980.
$ Dataset created 2010.11.13 by Bengt Hallstedt.
$ 2020.03.29: Modified for use with GE56.
$
$ This dataset does not work with the 875pe lattice stabilities, but
$ reasonably well with the SGTE lattice stabilities (except CUB_A13).
$ The dataset has probably been modified since the original 805pe dataset.
$
$ Hcp is stable between fcc-Ag and cub-A13 below 434 K.
$
$-----
$ TEMP-LIM 298.15 6000.00 !
$
$ELEMENT NAME REF. STATE ATOMIC MASS H298-H0 S298 !
$
$ ELEMENT VA VACUUM 0.0 0.0 0.0 !
$ ELEMENT AG FCC_A1 107.8682 5745. 42.55 !
$ ELEMENT AL FCC_A1 26.98154 4540. 28.30 !
$-----
$ Phase definitions
$
$ PHASE LIQUID:L % 1 1 !
$ CONST LIQUID:L : AG AL : !
$
$ Fcc (cF4, Fm-3m) and MoX (cF8, Fm-3m)
$
$ PHASE FCC_A1 %A 2 1 1 !
$ CONST FCC_A1 : AG% AL% : VA : !
$
$ Bcc (cI2, Im-3m)
$
$ PHASE BCC_A2 %B 2 1 3 !
$ CONST BCC_A2 : AG AL : VA : !
$
$ Hcp (hP2, P6_3/mmc) and Me2X (NiAs-type, hP4, P6_3/mmc, BB_1)
$
$ PHASE HCP_A3 %A 2 1 0.5 !
$ CONST HCP_A3 : AG AL : VA : !
$
$ Prototype beta-Mn (cP20, P4_132)
$
$ PHASE CUB_A13 % 2 1 1 !
$ CONST CUB_A13 : AG AL : VA : !
$-----
$ defaults
$
$ DEFINE-SYSTEM-DEFAULT ELEMENT 2 !
$ DEFAULT-COM DEFINE-SYSTEM-ELEMENT VA !
$ TYPE-DEF % SEQ %
$ TYPE-DEF A GE56-2020 PHASE-DESCRIPTION @ MAGNETIC -3 0.28 !
$ TYPE-DEF A GE56-2020 PHASE-DESCRIPTION @ MAGNETIC -1 0.4 !
$ FUNCTION ZERO 298.15 0; 6000 N !
$ FUNCTION UN_ASS 298.15 0; 6000 N !
$ FUNCTION R 298.15 +@J1451; 6000 N !
$-----
$ Element data
$
$ Ag
$
$ CUB_A13 added in unary 3.0
```

Default description display

The CalFateria - Open Binary Calphad Repository

Full database: a range of figures calculated using Thermo-Calc 2026.06.08 (version 2026a) is provided. For each dataset, users can display calculated phase diagrams, enthalpy and Gibbs energy curves for each described phase, as well as the activities of the elements at equilibrium at a given temperature. The command files used to generate these figures are also available, allowing users to easily reproduce similar plots at different temperatures, adjust plotting scales, or limit the number of descriptions included for comparison.

For certain systems, comparison with experimental data are also provided.

How to contribute ?

You can send comments. You can send whatever files containing descriptions, macro commands to produce figures, experimental datasets. ...

Please put a date and the name of the contributor on the first line of every file. Indicating the software (with version) able to handle the file would be nice.

Mail to [Nathalie Dupin](mailto:Nathalie.Dupin).

Database for Ag-Al from P.J. Spencer and O. Kubaschewski 1980

P.J. Spencer, O. Kubaschewski, unpublished, 1980.

Dataset created 2010.11.13 by Bengt Hallstedt.

2020.03.29: Modified for use with GE56.

This dataset does not work with the 875pe lattice stabilities, but reasonably well with the SGTE lattice stabilities (except CUB_A13).

The dataset has probably been modified since the original 805pe dataset.

Hcp is stable between fcc-Ag and cub-A13 below 434 K.

Ag-Al

805pe P.J. Spencer, O. Kubaschewski, unpublished, 1980. [Ag-Al_805pe.TDB](#) 805pe.TDB 875pe.TDB PSLm-LB.TDB G4WLTDB 20Te.TDB Comparison

Phase diagram

Thermo-Calc (2026.04.23:11.51) Ag-Al_805pe.TDB

Files to download: [TCD](#) [exo](#) [opt](#)

Enthalpy of the phases

Thermo-Calc (2026.04.23:11.51) Ag-Al_805pe.TDB 1000 K

Files to download: [TCD](#) [exo](#) [opt](#)

Activity of the elements

Thermo-Calc (2026.04.23:11.52) 1000 K Ag-Al_805pe.TDB

Files to download: [TCD](#) [exo](#) [opt](#)

Comments in the TDB

Dataset created 2010.11.13 by Bengt Hallstedt. 2020.03.29: Modified for use with GE56.

This dataset does not work with the 875pe lattice stabilities, but reasonably well with the SGTE lattice stabilities (except CUB_A13). The dataset has probably been modified since the original 805pe dataset.

Hcp is stable between fcc-Ag and cub-A13 below 434 K.

Phases described in the database: Ag-Al_805pe.TDB

Name	Model	Comment
LIQUID	(Ag, Al)	Liquid phase
FCC_A1	(Ag, Al)(Va)	Fcc (cF4, Fm-3m) and MeX (cF8, Fm-3m), magnetic model
BCC_A2	(Ag, Al)(Va) ₃	bcc (cI2, Im-3m), magnetic model
HCP_A3	(Ag, Al)(Va) ₆	Hcp (hP2, P6_3/mmc) and Me2X (NiAs-type, hP4, P6_3/mmc, BB_1), magnetic model
CUB_A13	(Ag, Al)(Va)	Prototype beta-Mn (cP20, P4_132)

Click on the name of a phase to display more about this phase.

```

$
$ Database for Ag-Al from P.J. Spencer and O. Kubaschewski 1980
$
$ P.J. Spencer, O. Kubaschewski, unpublished, 1980.
$
$ Dataset created 2010.11.13 by Bengt Hallstedt.
$ 2020.03.29: Modified for use with GE56.
$
$ This dataset does not work with the 875pe lattice stabilities, but
$ reasonably well with the SGTE lattice stabilities (except CUB_A13).
$ The dataset has probably been modified since the original 805pe dataset.
$
$ Hcp is stable between fcc-Ag and cub-A13 below 434 K.
$
$-----
$ TEMP-LIM 298.15 6000.00 !
$
$ ELEMENT NAME REF. STATE ATOMIC MASS H298-H0 S298 !
$
$ ELEMENT VA VACUUM 0.0 0.0 0.0 !
$ ELEMENT AG FCC_A1 107.8682 5745. 42.55 !
$ ELEMENT AL FCC_A1 26.98154 4540. 28.30 !
$
$ Phase definitions
$
$ PHASE LIQUID=L % 1 1 !
$ CONST LIQUID=L : AG AL : !
$
$ Fcc (cF4, Fm-3m) and MeX (cF8, Fm-3m)
$
$ PHASE FCC_A1 %A 2 1 1 !
$ CONST FCC_A1 : AG ALN : VA : !
$
$ Bcc (cI2, Im-3m)
$
$ PHASE BCC_A2 %B 2 1 3 !
$ CONST BCC_A2 : AG AL : VA : !
$
$ Hcp (hP2, P6_3/mmc) and Me2X (NiAs-type, hP4, P6_3/mmc, BB_1)
$
$ PHASE HCP_A3 %A 2 1 0.5 !
$ CONST HCP_A3 : AG AL : VA : !
$
$ Prototype beta-Mn (cP20, P4_132)
$
$ PHASE CUB_A13 %C 2 1 1 !
$ CONST CUB_A13 : AG AL : VA : !
$-----
$ Defaults
$
$ DEFINE-SYSTEM-DEFAULT ELEMENT 2 !
$ DEFAULT-COM DEFINE-SYSTEM-ELEMENT VA !
$ TYPE-DEF % 0 * !
$ TYPE-DEF GES AMEND PHASE-DESCRIPTION @ MAGNETIC -3 0.28 !
$ TYPE-DEF B GES AMEND PHASE-DESCRIPTION @ MAGNETIC -1 0.4 !
$ FUNCTION ZERO 298.15 0; 6000 N !
$ FUNCTION UN_ASS 298.15 0; 6000 N !
$ FUNCTION R 298.15 #+31451; 6000 N !
$-----
$ Element data
$-----
$ Ag
$
$ CUB_A13 added in unary 3.0
    
```

N. Dupin

The CalFateria

2026.06.08

5 / 10

More details on a phase

Ag-Al

80Spe P.J. Spencer, O. Kubaschewski, unpublished, 1980. [Ag-Al_80Spe.TDB](#)

[80Spe.TDB](#)

[87Spe.TDB](#)

[95Lim-LB.TDB](#)

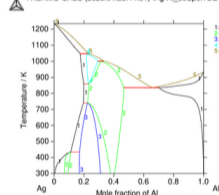
[04Wit.TDB](#)

[20Ter.TDB](#)

[Comparison](#)

Phase diagram

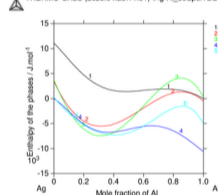
THERMO-CALC (2026.04.23:11.51) :Ag-Al_80Spe.TDB



Files to download: [TCM](#) [exp](#) [png](#)

Enthalpy of the phases

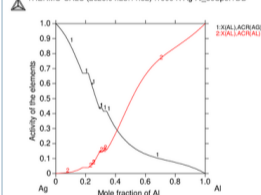
THERMO-CALC (2026.04.23:11.51) :Ag-Al_80Spe.TDB 1000 K



Files to download: [TCM](#) [exp](#) [png](#)

Activity of the elements

THERMO-CALC (2026.04.23:11.52) :1000 K Ag-Al_80Spe.TDB



Files to download: [TCM](#) [exp](#) [png](#)

Comments in the TDB

Dataset created 2010.11.13 by Bengt Hallstedt. 2020.03.29: Modified for use with GES6.

This dataset does not work with the 87Spe lattice stabilities, but reasonably well with the SGTE lattice stabilities (except CUB_A13). The dataset has probably been modified since the original 80Spe dataset. Hcp is stable between fcc-Ag and cub-A13 below 434 K.

Phases described in the database [Ag-Al_80Spe.TDB](#)

Name	Model	Comment
LIQUID	(Ag, Al)	Liquid phase
FCC_A1	(Ag, Al)(Va)	Fcc (cF4, Fm-3m) and MeX (cF8, Fm-3m), magnetic model
BCC_A2	(Ag, Al)(Va) ₃	Bcc (cI2, Im-3m), magnetic model
HCP_A3	(Ag, Al)(Va) _{0.5}	Hcp (hP2, P6_3/mmc) and Me2X (NiAs-type, hP4, P6_3/mmc, B8_1), magnetic model
CUB_A13	(Ag, Al)(Va)	Prototype beta-Mn (cP20, P4_132)

Click on the name of a phase to display more about this phase.

More details on a phase

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Ag-Al

[805pe.TDB](#) | [875pe.TDB](#) | [95Lm-LB.TDB](#) | [04WLi.TDB](#) | [207er.TDB](#) | [Comparison](#)

Phase diagram

THERMO-CALC (2006.04.23:11.51) ;Ag-Al_805pe.TDB

Files to download: [TCM exp one](#)

Enthalpy of the phases

THERMO-CALC (2006.04.23:11.51) ;Ag-Al_805pe.TDB 1000 K

Files to download: [TCM exp one](#)

Activity of the elements

THERMO-CALC (2006.04.23:11.52) ;1000 K;Ag-Al_805pe.TDB

Files to download: [TCM exp one](#)

Comments in the TDB

Dataset created 2010.11.13 by Bengt Hallstedt. 2020.03.29: Modified for use with GE56.
 This dataset does not work with the 875pe lattice stabilities, but reasonably well with the SGTE lattice stabilities (except CUB_A13). The dataset has probably been modified since the original 805pe dataset.
 Hcp is stable between fcc-Ag and cub-A13 below 434 K.

One phase described in the database: Ag-Al_805pe.TDB

Name	Descriptions with a phase having the same name
CUB_A13	Ag-Al_805pe Ag-Al_975pe Ag-Al_95Lm-LB Ag-Al_04WLi Ag-Al_207er Ag-Mn_906e
Model	Al-Mn_923m Al-Mn_983m Al-Mn_993a-LB Al-Mn_070a Al-Mn_1203a Al-Mn_1370a
(Ag, Al)(Va)	Al-Mn_107er-mod Al-Mn_107er Al-Mn_1994e B-Mn_105m B-Mn_1320a B-Mn_11Wm
Comment	C-Mn_893e C-Mn_904a-LB C-Mn_1023a C-Mn_107m C-Mn_1916e C-Mn_160e
Crystallographic structure	Cd-Mn_142m Ce-Mn_077m Ce-Mn_249e Ce-Mn_894a-LB Ce-Mn_933e-LB
Prototype beta-Mn (cP20, P4_132)	Ce-Mn_923e-mod Ce-Mn_923e-mod2 Cu-Mn_033Me-LB Cu-Mn_07Wm Cu-Mn_084e
Sublattice	Dy-Mn_09Wm Dy-Mn_19Wm Dy-Mn_249e Fe-Mn_0743a Fe-Mn_894a-LB
Fe-Mn	Fe-Mn_894e-mod9ed Fe-Mn_89Lee Fe-Mn_04WLi Fe-Mn_1993e-3e Fe-Mn_230ac
Fe-Mn	Fe-Mn_23Wb-3e Gd-Mn_01Gr-LB Gd-Mn_17Wm Ge-Mn_148e Ge-Mn_158e
H-Mn	H-Mn_110b H-Mn_10Li H-Mn_122h Hf-Mn_248r Ho-Mn_09Wm Ho-Mn_19Wm
In-Mn	In-Mn_15Wm La-Mn_12Wm La-Mn_162h Li-Mn_10Lm Lu-Mn_249e Mg-Mn_9ETb-LB
Mg-Mn	Mg-Mn_05Gr Mn-Mn_95Lee-mod Mn-Mn_95Lee-LB Mn-Ni_95Qb-LB Mn-Ni_95Qm-mod
Mn-Ni	Mn-Ni_12Li-alt Mn-Ni_12Li Mn-Ni_21Ym Mn-Ni_168m Mn-Ni_01D6e
Mn-Ni	Mn-Ni_07Fr-no-wilcards Mn-Ni_07Fr Mn-Ni_07Fr-2S Mn-Ni_08Li Mn-Ni_19Wb-4d
Mn-Ni	Mn-Ni_19Wb Mn-O_03Gr-LB Mn-O_10Kj Mn-P_01M6 Mn-P_073e Mn-P_14M6e

The items written in blue are links to the list of the descriptions with the same kind.

[Back to the table with all the phases in the database](#)

More details on a phase



The Calfateria - Open Binary Calphad Repository

[Mail to Nathalie Dupin](#)

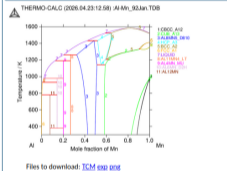
Al-Mn

92Jan A. Jansson, Metall. Trans. A, 23A, 2953-62(1992) [Al-Mn_92Jan.TDB](#)

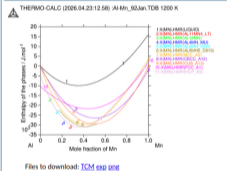
92Jan.TDB 98Jan.TDB 99Lu-LB.TDB 07Du.TDB 11Du.TDB 17Cu.TDB 18Zn-mod.TDB 18Zn.TDB 19Me.TDB

Comparison

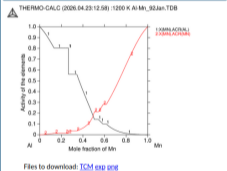
Phase diagram



Enthalpy of the phases



Activity of the elements



Comments in the TDB

Dataset created 2009.08.19 by Bengt Hallstedt. 2020.12.20: Modified for use with GE56.
There is an inverse miscibility gap with a minimum at 5202 K and x(Mn)=0.36.

One phase described in the database: [Al-Mn_92Jan.TDB](#)

Name	Descriptions with a phase having the same name
CUB_A13	Ag-Al_805pe Ag-Al_975pe Ag-Al_991m-LB Ag-Al_049te Ag-Al_207tr Ag-Mn_900e
Model	Al-Mn_92Jan Al-Mn_98Jan Al-Mn_99Lu-LB Al-Mn_07Du Al-Mn_11Du Al-Mn_17Cu
(Al, Mn)(Va)	Al-Mn_18Zn-mod Al-Mn_18Zn Al-Mn_19Me Bi-Mn_185m Bi-Mn_185m Bi-Mn_132a Bi-Mn_11Wm
Comment	C-Mn_87Kec C-Mn_90Kec-LB C-Mn_102a C-Mn_187m C-Mn_191Me Ca-Mn_160e
Crystallographic structure	Cd-Mn_142m Ce-Mn_07Jan Ce-Mn_249e Ce-Mn_89Kec-LB Cr-Mn_93Lee-LB
Prototype	Cr-Mn_92Lee-mod Cr-Mn_92Lee-mod2 Cu-Mn_03Mie-LB Cu-Mn_07Wm Cu-Mn_084e
Substructure	Dy-Mn_09Wm Dy-Mn_19Wm Er-Mn_249e Fe-Mn_074a Fe-Mn_89Kec-LB
Phase	Fe-Mn_89Kec-modRed Fe-Mn_89Lee Fe-Mn_049te Fe-Mn_198e-3e Fe-Mn_232ac
Group	Fe-Mn_23Wol-3e Gd-Mn_01Gro-LB Gd-Mn_17Wm Ge-Mn_148e Ge-Mn_158e
Phase	H-Mn_111ob H-Mn_18Lu H-Mn_122h Hf-Mn_248r Ho-Mn_09Wm Ho-Mn_19Wm
Phase	In-Mn_15Wm La-Mn_12Wm La-Mn_162h Li-Mn_181m Lu-Mn_249e Mg-Mn_9ETB-LB
Phase	Mg-Mn_05Gro Mn-Mn_95Lee-mod Mn-Mn_95Lee-LB Mn-Ni_93Qu-mod Mn-Ni_93Qu-mod
Phase	Mn-Ni_12Lu-alt Mn-Ni_12Lu Mn-Ni_21Van Mn-Ni_168m Mn-Ni_01Mie
Phase	Mn-Ni_07Tro-no-wildcards Mn-Ni_07Tro Mn-Ni_07Tro-2S Mn-Ni_08Lu Mn-Ni_19Wol-4e
Phase	Mn-Ni_19Wol Mn-O_03Gro-LB Mn-O_10Kie Mn-P_01Mie Mn-P_073e Mn-P_14Me

The items written in blue are links to the list of the descriptions with the same kind.

[Back to the table with all the phases in the database](#)

With experimental data



The Calfateria - Open Binary Calphad Repository

Cr-Ta

93Dup-LB N. Dupin, I. Ansara, J. Phase Equilib., 14, 451-56(1993), addendum, ibid, 15, 135(1994). [Cr-Ta_93Dup-LB.TDB](#)

93Dup-LB.TDB

012ha.TDB

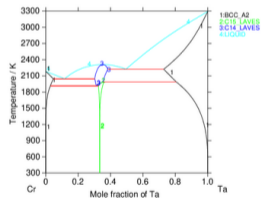
09Pav.TDB

Comparison

With experiments

Phase diagram

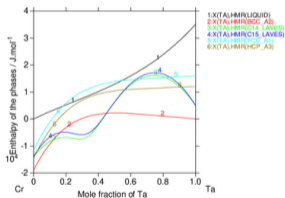
THERMO-CALC (2026.04.23:16:32) :Cr-Ta_93Dup-LB.TDB



Files to download: [TCM exp png](#)

Enthalpy of the phases

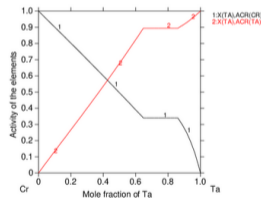
THERMO-CALC (2026.04.23:16:32) :Cr-Ta_93Dup-LB.TDB 2600 K



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Activity of the elements

THERMO-CALC (2026.04.23:16:32) :2600 K Cr-Ta_93Dup-LB.TDB



Files to download: [TCM exp png](#)

Comments in the TDB

Dataset created 2009.11.15 by Bengt Hallstedt. 2020.08.09: Modified for use with GES6.

Laves-C15 becomes more stable than Laves-C14 again at high temperature, as pointed out by F. Zhang et al. (Intermetallics, 9,

Phases described in the database Cr-Ta_93Dup-LB.TDB

Name	Model	Comment
LIQUID	(Cr, Ta)	Liquid phase
FCC_A1	(Cr, Ta)(Va)	Fcc (cF4, Fm-3m) and MeX (cF8, Fm-3m), magnetic model
BCC_A2	(Cr, Ta)(Va)	Bcc (cI2, Im-3m), magnetic model

With experimental data



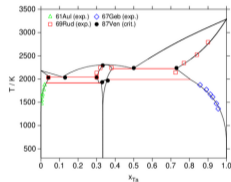
The CalFateria - Open Binary Calphad Repository

Cr-Ta

93Dup-LB N. Dupin, I. Ansara, J. Phase Equilib., 14, 451-56(1993), addendum, ibid, 15, 135(1994). Cr-Ta_93Dup-LB.TDB

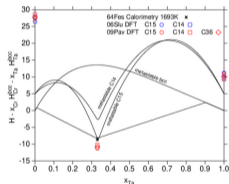
93Dup-LB.TDB 01Zha.TDB 09Pav.TDB Comparison With experiments

Calculated phase diagram



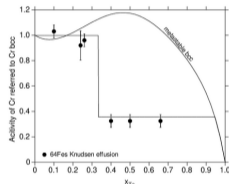
Files to download: [experimental data set](#) [TCM](#) [calculated exp](#) [png](#)

Enthalpy of formation at 1693K



Files to download: [experimental data set](#) [TCM](#) [calculated exp](#) [png](#)

Activity of Cr at 1472K



Files to download: [experimental data set](#) [TCM](#) [calculated exp](#) [png](#)

Divers files to download

Experimental or theoretical datasets

[Cr-Ta_dat.exp](#)

Command files

[Cr-Ta_93Dup-LB.TCM](#) [Cr-Ta_01Zha.TCM](#) [Cr-Ta_09Pav.TCM](#)

Descriptions

[Cr-Ta_93Dup-LB.TDB](#) [Cr-Ta_01Zha.TDB](#) [Cr-Ta_09Pav.TDB](#)

References

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With experimental data



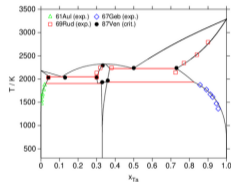
The CalFateria - Open Binary Calphad Repository

Cr-Ta

01Zha F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001)
1079-1083 Cr-Ta_01Zha.TDB

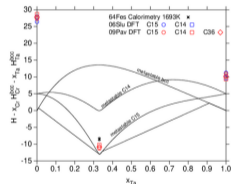
93Dup-LB.TDB 01Zha.TDB 09Pav.TDB Comparison With experiments

Calculated phase diagram



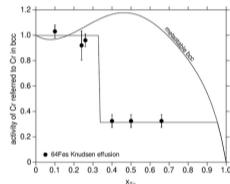
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Enthalpy of formation at 1693K



Files to download: [experimental data set](#) [TCM](#) [calculated exp](#) [png](#)

Activity of Cr at 1472K



Files to download: [experimental data set](#) [TCM](#) [calculated exp](#) [png](#)

Divers files to download

Experimental or theoretical datasets

[Cr-Ta_dat.exp](#)

Command files

[Cr-Ta_93Dup-LB.TCM](#) [Cr-Ta_01Zha.TCM](#) [Cr-Ta_09Pav.TCM](#)

Descriptions

[Cr-Ta_93Dup-LB.TDB](#) [Cr-Ta_01Zha.TDB](#) [Cr-Ta_09Pav.TDB](#)

References

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- 64Fes: P. Feschotte, O. Kubaschewski, Thermochemical Properties of the Laves Phase, Cr₂Ta, *Trans. Faraday Soc.*, 60, 1941-1946 (1964).
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- 67Mau: M. Muehleisen and J.B. Morrison, The Cr-Ta System, *Bull. Alloy Phase Diagrams*, 9(3), 113-114 (1989)

With experimental data



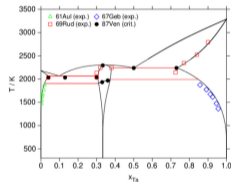
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Cr-Ta

09Pav J. Pavlu, J. Vrestal, M. Sob, Calphad, 33, 179-86(2009). Cr-Ta_09Pav.TDB

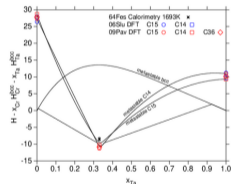
93Dup-LB.TDB 01Zha.TDB 09Pav.TDB Comparison With experiments

Calculated phase diagram



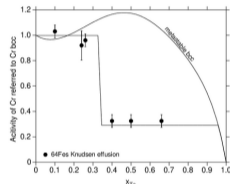
Files to download: [experimental data set](#) [TCM](#) [calculated exp](#) [png](#)

Enthalpy of formation at 1693K



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Activity of Cr at 1472K



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Experimental or theoretical datasets

[Cr-Ta_dat.exp](#)

Command files

[Cr-Ta_93Dup-LB.TCM](#) [Cr-Ta_01Zha.TCM](#) [Cr-Ta_09Pav.TCM](#)

Descriptions

[Cr-Ta_93Dup-LB.TDB](#) [Cr-Ta_01Zha.TDB](#) [Cr-Ta_09Pav.TDB](#)

References

- 48Kub: O. Kubaschewski and A. Speidel, Oxidation-Resistance and Some Phase Relationships in the System Cr-Ta-Ni, *J. Inst. Met.*, 75, 417-430 (1948-1949).
- 52Duv: P. Duwez and H. Martens, Crystal Structure of TaCr₂ and CbCr₂, *Trans. AIME*, 194, 72-74 (1952)
- 59Gr: A.T. Grigoriev, V.V. Kupfina, and N.A. Nedumov, Phase Diagram of the Cr-Ta System, *Russ. J. Inorganic Chem.*, 3(4), 296-297 (1959)
- 60Pi: G.O. Piloyan, A.M. Evseev, and Y.I. Gerasimov, Thermodynamic Properties of Alloys of the System Chromium-Tantalum, *Russ. J. Phys. Chem.*, 34, 1768-1772 (1960).
- 61Aul: J.H. Auld and N.E. Ryan, The Solid Solubility of Tantalum in Chromium, *J. Less-Common Met.*, 3, 221-225 (1961).
- 64Fes: P. Feschotte, O. Kubaschewski, Thermochemical Properties of the Laves Phase, Cr₂Ta, *Trans. Faraday Soc.*, 60, 1941-1946 (1964).
- 65Gus: L.N. Guseva, Phase Transformations in Chromium-Tantalum and Chromium-Niobium Alloys, *Inorganic Mater.*, 1(10), 1581-1583(1965).
- 67Geb: E. Gebhardt and J. Rexer, Precipitation Phenomena in Ta-Cr Solid Solutions, *Z. Metallkd.*, 58, 611-616 (1967).
- 69Rud: E. Rudy, Ternary Phase Equilibria in Transition Metal-Boron-Carbon-Silicon Systems, Part V: Compendium of Phase Diagram Data, *Tech. Rep. AFML-TR-65-2*, 23,137-141 (1969).
- 87Ven: M. Venzlshagen and J.B. Neumann, The Cr-Ta System, *Bull. Alloy Phase Diagrams*, 9(3), 113-114(1989)

With experimental data



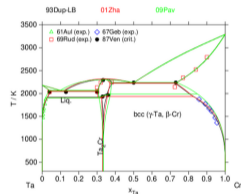
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Cr-Ta

93Dup-LB: N. Dupin, I. Ansara, J. Phase Equilib., 14, 451-56(1993),
addendum, Ibid, 15, 135(1994).
01Zha: F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001)
1070, 1082

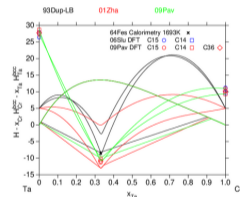
93Dup-LB.TDB 01Zha.TDB 09Pav.TDB Comparison With experiments

Calculated phase diagram



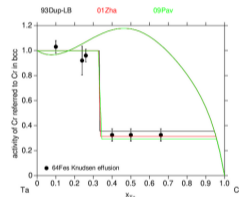
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Enthalpy of formation at 1693K



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Activity of Cr at 1472K



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Experimental or theoretical datasets

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Command files

[Cr-Ta_93Dup-LB.TCM](#) [Cr-Ta_01Zha.TCM](#) [Cr-Ta_09Pav.TCM](#)

Descriptions

[Cr-Ta_93Dup-LB.TDB](#) [Cr-Ta_01Zha.TDB](#) [Cr-Ta_09Pav.TDB](#)

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48Kub: O. Kubaschewski and A. Speidel, Oxidation-Resistance and Some Phase Relationships in the System Cr-Ta-Ni, J. Inst. Met., 75, 417-430 (1948-1949).

52Duw: P. Duwez and H. Martens, Crystal Structure of TaCr₂ and CbCr₂, Trans. AIME, 194, 72-74 (1952)

59Gr: A.T. Grigoriev, V.V. Kupfina, and N.A. Nedumov, Phase Diagram of the Cr-Ta System, Russ. J. Inorganic Chem., 3(4), 296-297 (1959)

60Pi: G.O. Piloyan, A.M. Evseev, and YI. Gerasimov, Thermodynamic Properties of Alloys of the System Chromium-Tantalum, Russ. J. Phys. Chem., 34, 1768-1772 (1960).

61Aul: J.H. Auld and N.E. Ryan, The Solid Solubility of Tantalum in Chromium, J. Less-Common Met., 3, 221-225 (1961).

64Fes: P. Feschotte, O. Kubaschewski, Thermochemical Properties of the Laves Phase, Cr₂Ta, Trans. Faraday Soc., 60, 1941-1946 (1964).

65Gus: L.N. Guseva, Phase Transformations in Chromium-Tantalum and Chromium-Niobium Alloys, Inorganic Mater., 1(10), 1581-1583(1965).

67Geb: E. Gebhardt and J. Rexer, Precipitation Phenomena in Ta-Cr Solid Solutions, Z. Metallkd., 58, 611-616 (1967).

69Rud: E. Rudy, Ternary Phase Equilibria in Transition Metal-Boron-Carbon-Silicon Systems, Part V: Compendium of Phase Diagram Data, Tech. Rep. AFML-TR-65-2, 23,137-141 (1969).

After CALPHAD2026

↪ The current status of The Calfateria will stay available online.



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CALPHAD2026

Mot de passe

Pwd4Calfat

Annuler Connexion

Ask for a personal login

- ↪ to secure your access
- ↪ to be informed of new release.

After CALPHAD2026

↪ The current status of The Calfateria will stay available online.

↪ The next releases will be open to people, institutes or companies forming a consortium

- contributing with data
 - . new descriptions
 - . new formats: dat, XTDB, py, ...
 - . experimental data
- supporting financially the work

↪ The evolution of The Calfateria will be defined by the members of the consortium according to the available data and funding.

↪ Let's talk during this week if you want to take part.



Thank you for your attention



Evolution of TDB format

The Calfrateria - Open Binary Calphad Repository

Cr-Ta

01Zha F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001) 1079-1083 Cr-Ta_01Zha.TDB

930up-48.TDB 01Zha.TDB 099hu.TDB Comparison With experiments

Phase diagram

Files to download: [TCM esp eng](#)

Enthalpy of the phases

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Activity of the elements

Files to download: [TCM esp eng](#)

When the **DATABASE_INFO** command is present in the TDB, it is used to define the comments in the TDB of the page.

Comments in the TDB

Edited by ND. Checked 2026/04/20

Cr-Ta: F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001)

Phases described in the database Cr-Ta_01Zha.TDB

Name	Model	Comment
LIQUID	{Cr, Ta}	LIQUID Liquid phase
FCC_A1	{Cr, Ta}(Va)	FCC_A1 fcc (cF4, Fm-3m), magnetic model
BCC_A2	{Cr, Ta}(Va) ₃	BCC_A2 bcc (cI2, Im-3m), magnetic model
HCP_A3	{Cr, Ta}(Va) _{0.5}	HCP_A3 hcp (hP2, P6_3/mmc), magnetic model
DIS_C14	{Cr, Ta}	DIS_C14 contribution to C14_LAVES
C14_LAVES	{Cr, Ta} _{0.67} {Cr, Ta} ₃₃	C14_LAVES Prototype MgZn2 (hP12, P6_3/mmc), disordered contribution from DIS_C14
DIS_C15	{Cr, Ta}	DIS_C15 contribution to C15_LAVES

DATABASE_INFO

Edited by ND. Checked 2026/04/20

Cr-Ta: F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001) 1079-1083

```

SNF DATABASE_REFERENCE 'F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001) 1079-1083' !
SNF
ELEMENT VA VACUUM 0.0 0.0 0.0 !
ELEMENT CR BCC A2 51.996 4658.8 23.5429 !
ELEMENT TA BCC A2 188.3479 5681.872 41.4718 !

DEFINE-SYSTEM-DEFAULT ELEMENT 2 !
DEFAULT.COM DEFINE-SYSTEM-ELEMENT VA !
TYPE-DEF % SEQ = 1 !
TYPE-DEF A GES AMEND PHASE-DESCRIPTION @ MAGNETIC -3 0.28 !
TYPE-DEF B GES AMEND PHASE-DESCRIPTION @ MAGNETIC -1 0.4 !
FUNCTION ZERO 298.15 0; 6000 N !
FUNCTION UN ASS 298.15 0; 6000 N !
FUNCTION R 298.15 +8.31451; 6000 N !

Phase definitions
...
SNF CRYSTALLO FCC A1 PROTOTYPE 'Cu' STRUKTUR_BERICHT 'A1' PEARSON 'cF4'
SNF SPACE_GROUP 'Fm-3m' !

PHASE BCC_A2 hP 2 1 3 1 !
CONST BCC_A2 : CRV TA% : VA : !

SNF COMMENT BCC_A2 'bcc (cI2, Im-3m) !
SNF CRYSTALLO BCC A2 PROTOTYPE 'W' STRUKTUR_BERICHT 'A2' PEARSON 'cI2'
SNF SPACE_GROUP 'Im-3m' !

PHASE HCP_A3 hA 2 1 0 5 1 !
CONST HCP_A3 : CR TA : VA : !

SNF COMMENT HCP_A3 'hcp (hP2, P6_3/mmc) !
SNF CRYSTALLO HCP A3 PROTOTYPE 'Mg' STRUKTUR_BERICHT 'A3' PEARSON 'hP4'
SNF SPACE_GROUP 'P6_3/mmc' !

PHASE DIS_C14 h 1 1 1 !
CONST DIS_C14 : CR TA : !

SNF COMMENT DIS_C14 'contribution to C14_LAVES' !
    
```

Evolution of TDB format

Cr-Ta
930up-48.TDB | 01Zha.TDB | 099hu.TDB | Comparison | With experiments

01Zha F. Zhang, S.-L. Chen, YA. Chang, W.A. Oates, Intermetallics 9 (2001) 1079-1083 [Cr-Ta_01Zha.TDB](#)

DATABASE_INFO ''''
 Edited by ND, Checked 2026/04/20''
 Cr-Ta: F. Zhang, S.-L. Chen, YA. Chang, W.A. Oates, 'Intermetallics 9 (2001) 1079-1083'
 !
 \$NF DATABASE_REFERENC 'F. Zhang, S.-L. Chen, YA. Chang, W.A. Oates, Intermetallics 9 (2001) 1079-1083' !
 \$NF
 ELEMENT VA VACUUM 0.0 0.0 0.0
 ELEMENT CR BCC A2 51.996 4050.0 23.5429 !
 ELEMENT TA BCC A2 180.9479 5681.072 41.4718 !
 DEFINE-SYSTEM-DEFAULT ELEMENT 2 !
 DEFAULT-COM DEFINE-SYSTEM ELEMENT VA !
 TYPE-DEF % SEQ = 1'
 TYPE-DEF A GES AMEND PHASE DESCRIPTION @ MAGNETIC -3 0.28 !
 TYPE-DEF B GES AMEND PHASE DESCRIPTION @ MAGNETIC -1 0.4 !
 FUNCTION ZERO 298.15 0; 6000 N !
 FUNCTION LN ASS 298.15 0; 6800 N !
 FUNCTION R 298.15 +8.31451; 6800 N !
 \$-----
 \$ Phase definitions
 \$-----
 PHASE LIQUID:L % 1 1 !
 CONST LIQUID:L : CR TA : !
 \$NF COMMENT LIQUID 'Liquid phase' !
 PHASE FCC A1 %A 2 1 1 !
 CONST FCC_A1 : CR TA : VA : !
 \$NF COMMENT FCC A1 'fcc (cF4, Fm-3m)' !
 \$NF CRYSTALLO FCC A1 PROTOTYPE 'Cu' STRUKTUR_BERICHT 'A1' PEARSON 'cF4'
 \$NF SPACE_GROUP 'Fm-3m' !
 PHASE BCC A2 %B 2 1 3 !
 CONST BCC_A2 : CRV TAV : VA : !
 \$NF COMMENT BCC A2 'bcc (cI2, Im-3m)' !
 \$NF CRYSTALLO BCC A2 PROTOTYPE 'W' STRUKTUR_BERICHT 'A2' PEARSON 'cI2'
 \$NF SPACE_GROUP 'Im-3m' !
 PHASE HCP A3 %A 2 1 0 5 !
 CONST HCP_A3 : CR TA : VA : !
 \$NF COMMENT HCP A3 'hcp (hP2, P6_3/mmc)' !
 \$NF CRYSTALLO HCP A3 PROTOTYPE 'Mg' STRUKTUR_BERICHT 'A3' PEARSON 'hP4'
 \$NF SPACE_GROUP 'P6_3/mmc' !
 PHASE DIS C14 % 1 1 !
 CONST DIS_C14 : CR TA : !
 \$NF COMMENT DIS_C14 'contribution to C14_LAVES' !

Phase diagram

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Enthalpy of the phases

Files to download: [TCM esp eng](#)

Activity of the elements

Files to download: [TCM esp eng](#)

Comments in the TDB

Edited by ND, Checked 2026/04/20

Cr-Ta: F. Zhang, S.-L. Chen, YA. Chang, W.A. Oates, Intermetallics 9 (2001)

Phases defined in the TDB

Name	Members	Comments
LIQUID	(Cr, Ta)	LIQUID Liquid phase
FCC_A1	(Cr, Ta)(Va)	FCC_A1 fcc (cF4, Fm-3m), magnetic model
BCC_A2	(Cr, Ta)(Va) ₃	BCC_A2 bcc (cI2, Im-3m), magnetic model
HCP_A3	(Cr, Ta)(Va) _{0.5}	HCP_A3 hcp (hP2, P6_3/mmc), magnetic model
DIS_C14	(Cr, Ta)	DIS_C14 contribution to C14_LAVES
C14_LAVES	(Cr, Ta) _{0.67} (Cr, Ta) ₃₃	C14_LAVES Prototype MgZn2 (hP12, P6_3/mmc), disordered contribution from DIS_C14
DIS_C15	(Cr, Ta)	DIS_C15 contribution to C15_LAVES

Lines beginning by **\$NF** correspond to comments more precise than those introduced by B. Hallstedt. They allow to define

- ↪ a reference for the database
- ↪ a comment for a phase
- ↪ the crystallography of a phase.

Evolution of TDB format

The Calfrateria - Open Binary Calphad Repository

Cr-Ta

01Zha F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001) 1079-1083 Cr-Ta_01Zha.TDB

930up-48.TDB 01Zha.TDB 099hu.TDB Comparison With experiments

Phase diagram

THERMO-CALC (2026.04.23.16.32) Cr-Ta_01Zha.TDB

Enthalpy of the phases

THERMO

Activity of the elements

It is suggested that in the future, removing the \$NF, these comments could become commands understood by the software and stored in the working space so that their content could be available interactively for the users.

Lines beginning by **\$NF** correspond to comments more precise than those introduced by B. Hallstedt. They allow to define

- ↪ a reference for the database
- ↪ a comment for a phase
- ↪ the crystallography of a phase.

Edited by ND. Checked 2026/04/20

Cr-Ta: F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001)

LIQUID (Cr, Ta)	LIQUID Liquid phase
FCC_A1 (Cr, Ta)(Va)	FCC_A1 fcc (cF4, Fm-3m), magnetic model
BCC_A2 (Cr, Ta)(Va) ₃	BCC_A2 bcc (cI2, Im-3m), magnetic model
HCP_A3 (Cr, Ta)(Va) _{0.5}	HCP_A3 hcp (hP2, P6_3/mmc), magnetic model
DIS_C14 (Cr, Ta)	DIS_C14 contribution to C14_LAVES
C14_LAVES (Cr, Ta) _{0.67} (Cr, Ta) ₃₃	C14_LAVES Prototype MgZn2 (hP12, P6_3/mmc), disordered contribution from DIS_C14
DIS_C15 (Cr, Ta)	DIS_C15 contribution to C15_LAVES

DATABASE_INFO '''

Edited by ND. Checked 2026/04/20'

Cr-Ta: F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001) 1079-1083'

\$NF DATABASE_REFERENC 'F. Zhang, S.-L. Chen, Y.A. Chang, W.A. Oates, Intermetallics 9 (2001) 1079-1083' !

```
ELEMENT VA VACUUM 0.0 0.0 0.0
ELEMENT CR BCC A2 51.996 4050.0 23.5429 !
ELEMENT TA BCC A2 180.9479 5681.072 41.4718 !
```

```
DEFINE-SYSTEM-DEFAULT ELEMENT 2 !
DEFAULT.COM DEFINE_SYSTEM_ELEMENT VA !
TYPE-DEF % SEQ = 1'
TYPE-DEF A GES AMEND PHASE DESCRIPTION @ MAGNETIC -3 0.28 !
TYPE-DEF B GES AMEND PHASE DESCRIPTION @ MAGNETIC -1 0.4 !
FUNCTION ZERO 298.15 0; 6000 N !
FUNCTION LN ASS 298.15 0; 6800 N !
FUNCTION R 298.15 +8.31451; 6800 N !
```

----- Phase definitions

```
PHASE LIQUID:L % 1 1 !
CONST LIQUID:L : CR TA : !
$NF COMMENT LIQUID 'Liquid phase' !
```

```
PHASE FCC_A1 %A 2 1 1 !
CONST FCC_A1 : CR TA : VA : !
$NF COMMENT FCC_A1 'fcc (cF4, Fm-3m)' !
$NF CRYSTALLO FCC_A1 PROTOTYPE 'Cu' STRUKTUR_BERICHT 'A1' PEARSON 'cF4'
$NF SPACE_GROUP 'Fm-3m' !
```

```
PHASE BCC_A2 %B 2 1 3 !
CONST BCC_A2 : CRV TAV : VA : !
$NF COMMENT BCC_A2 'bcc (cI2, Im-3m)' !
$NF CRYSTALLO BCC_A2 PROTOTYPE 'W' STRUKTUR_BERICHT 'A2' PEARSON 'cI2'
$NF SPACE_GROUP 'Im-3m' !
```

```
PHASE HCP_A3 %A 2 1 0.5 !
CONST HCP_A3 : CR TA : VA : !
$NF COMMENT HCP_A3 'hcp (hP2, P6_3/mmc)' !
$NF CRYSTALLO HCP_A3 PROTOTYPE 'Mg' STRUKTUR_BERICHT 'A3' PEARSON 'hP4'
$NF SPACE_GROUP 'P6_3/mmc' !
```

```
PHASE DIS_C14 % 1 1 !
CONST DIS_C14 : CR TA : !
```

\$NF COMMENT DIS_C14 'contribution to C14_LAVES' !