The Calfateria

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

CALPHAD2026

The Calphad Coffee Breaks on line

The SGTE collection of binary datasets

2025 - The SGTE collection of binary datasets, Bengt Hallstedt
https://doi.org/10.1016/j.calphad.2025.102833

datasets.zip

CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 89 (2025) 102833

Contents lists available at ScienceDirect

Calphad

journal homepage: www.elsevier.com/locate/calphad

The SGTE collection of binary datasets

Bengt Hallstedt

Institute for Materials Applications in Mechanical Engineering (IWM), RWTH Aachen University, Augustinerbach 4, 52062, Aachen, Germany

ARTICLE INFO

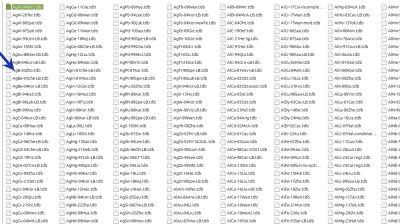
Handling Editor: Prof. Z.K. Liu

Keywords:
Calphad
Thermodynamic modelling
Binary systems

ABSTRACT

SGTE has collected (and also produced) binary assessments since the 1980's. This was documented with about 450 binary systems in five volumes of the Landolt-Börnstein series. These volumes were accompanied by a database with which the phase-diagrams could be calculated, but the database itself was encrypted. It is now time to make the SGTE collection of binary datasets publicly available. The collection now contains 2773 datasets from 1238 different binary systems. By providing this collection in open form it is hoped that Calphad modelling of, in particular, ternary and higher order systems can be further promoted.

2773 files



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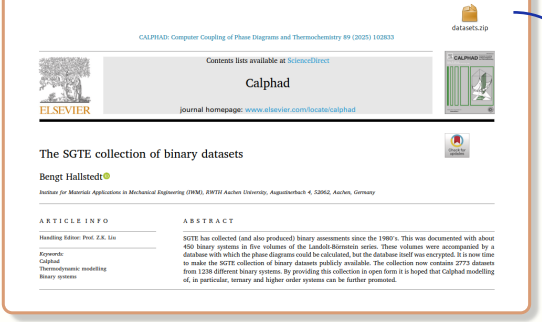
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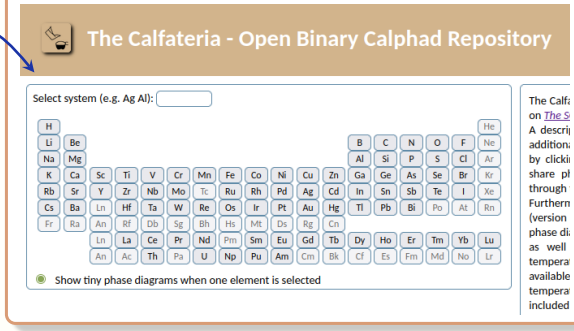
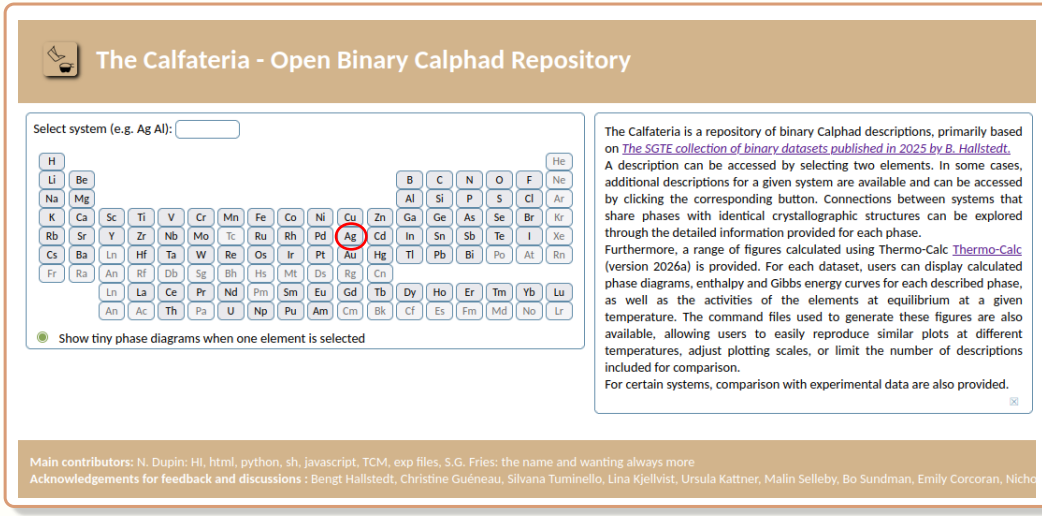

The Calfateria - Open Binary Calphad Repository

Select system (e.g. Ag Al):

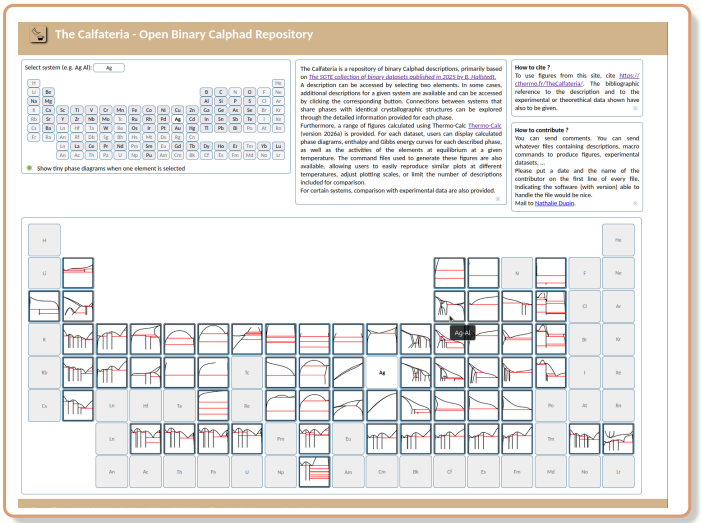
Show tiny phase diagrams when one element is selected

The Calfateria is a web page making easier many tasks needed before using one of these binary descriptions.

Selecting a system



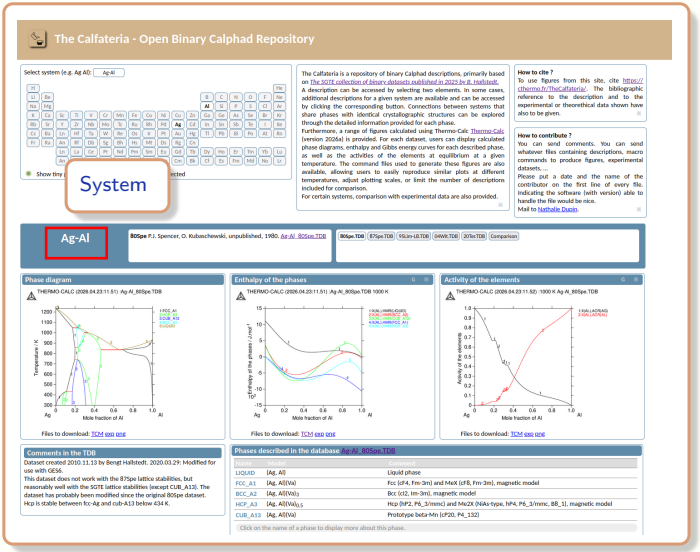
Selecting a system



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



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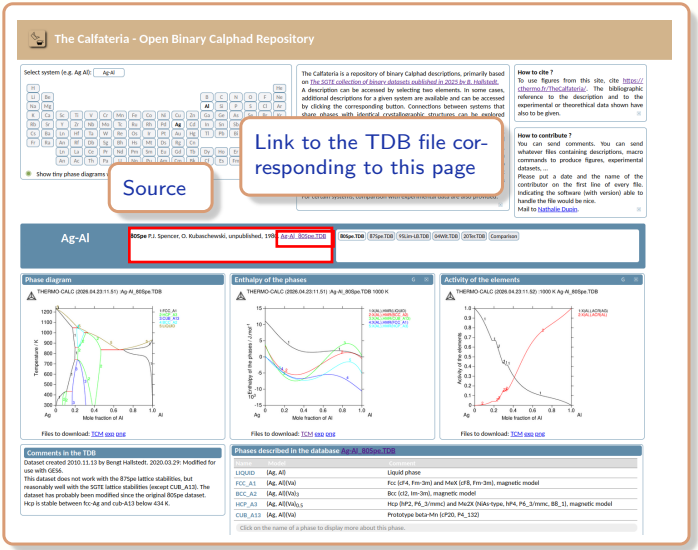
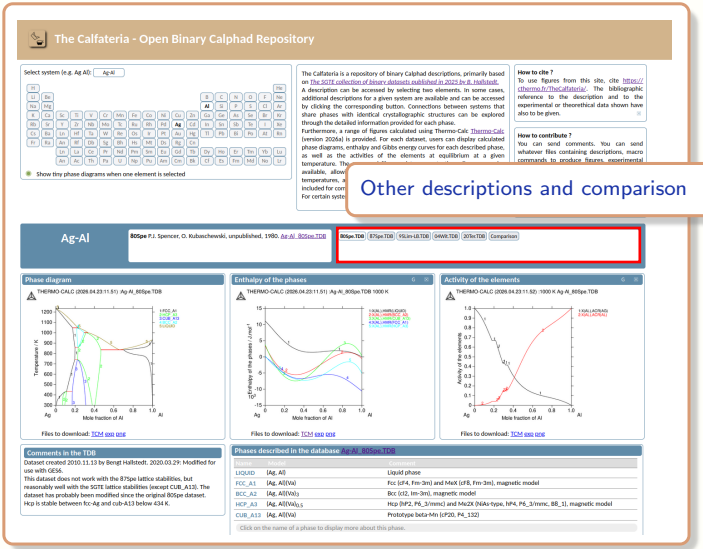
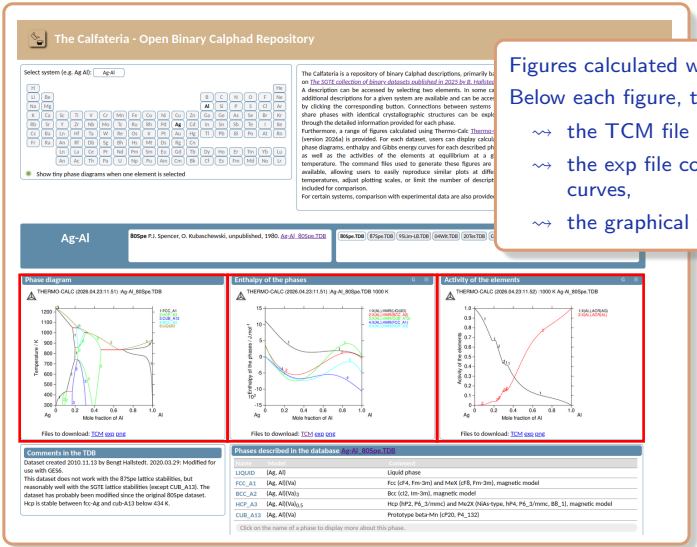


The default description is the first in chronological order.

Default description display



Default description display

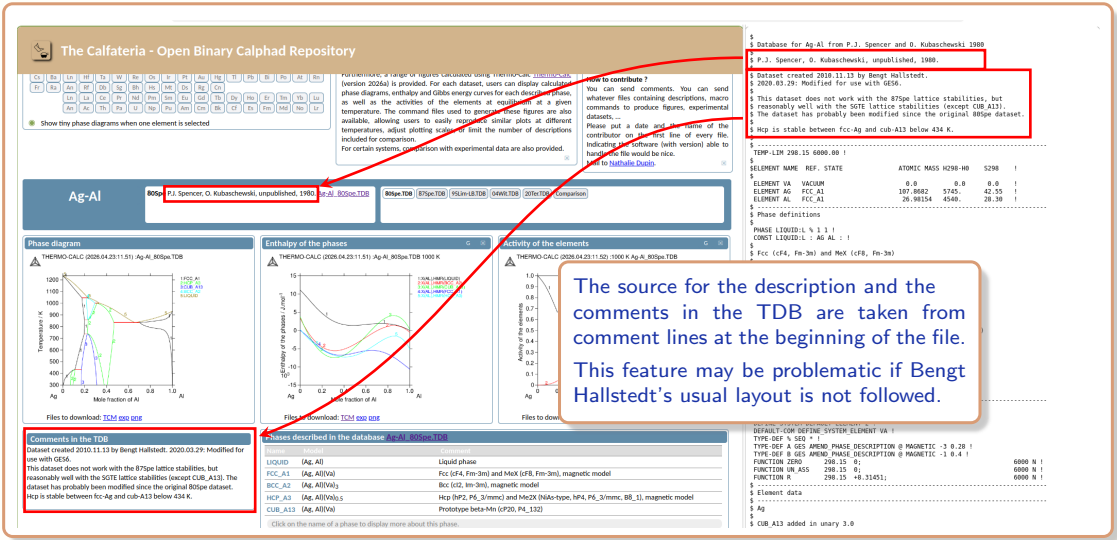


Figures calculated with Thermo-Calc are shown.

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.

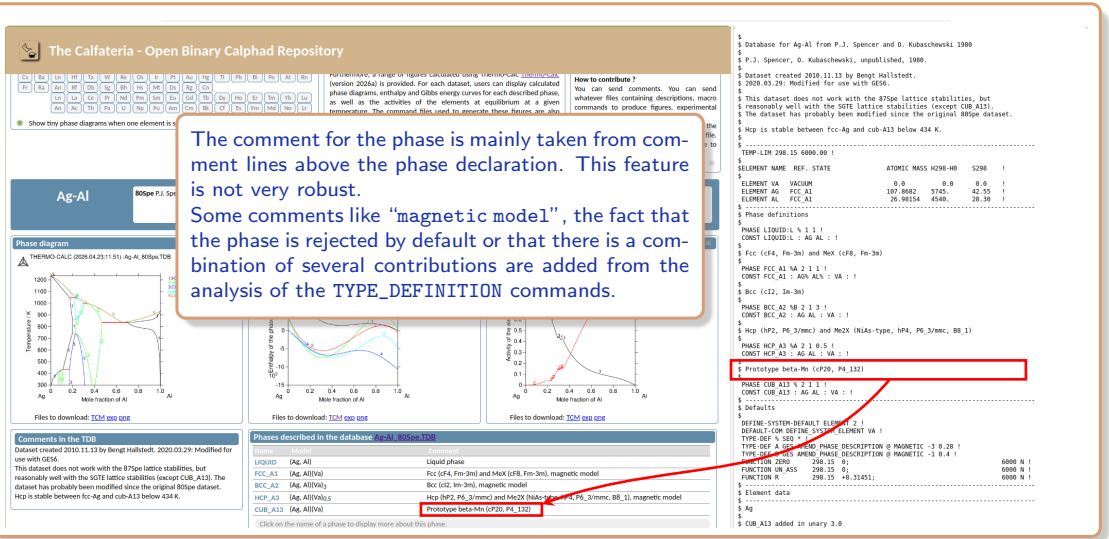
Default description display



The source for the description and the comments in the TDB are taken from comment lines at the beginning of the file.

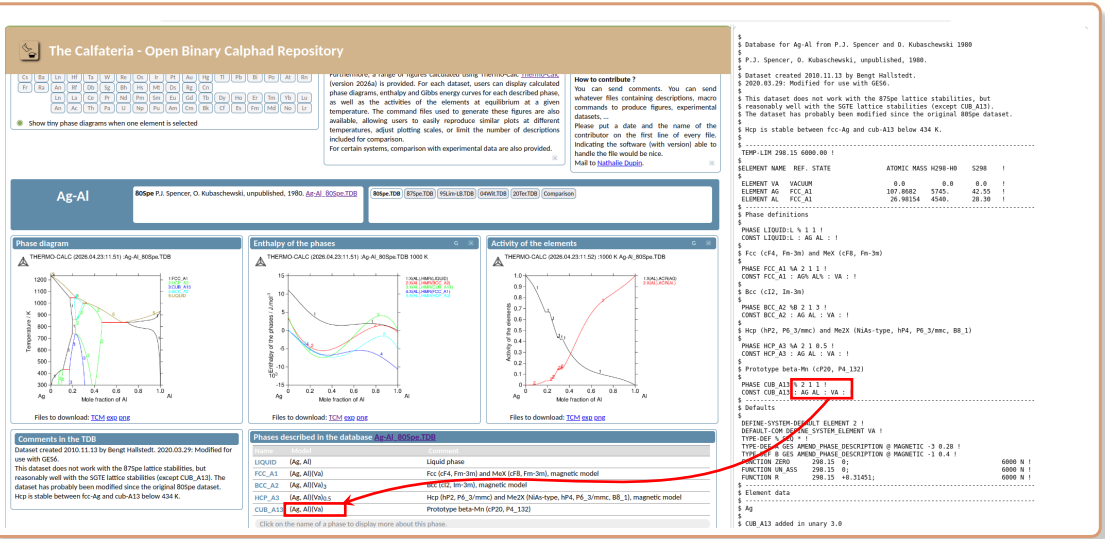
This feature may be problematic if Bengt Hallstedt's usual layout is not followed.

Default description display



The 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.

Default description display



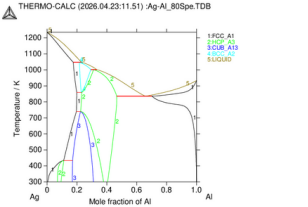
More details on a phase

Ag-Al

80Spe P.J. Spencer, O. Kubaschewski, unpublished, 1980. Ag-Al_80Spe.TDB

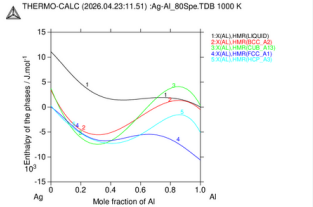
80Spe.TDB | 87Spe.TDB | 95Lim-LB.TDB | 04Wit.TDB | 20Ter.TDB | Comparison

Phase diagram



Files to download: TCM exp png

Enthalpy of the phases



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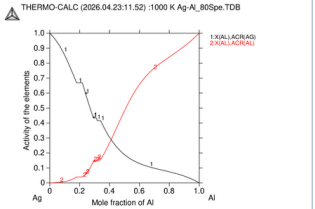
Activity of the elements



Files to download: TCM exp png

Comments in the TDB

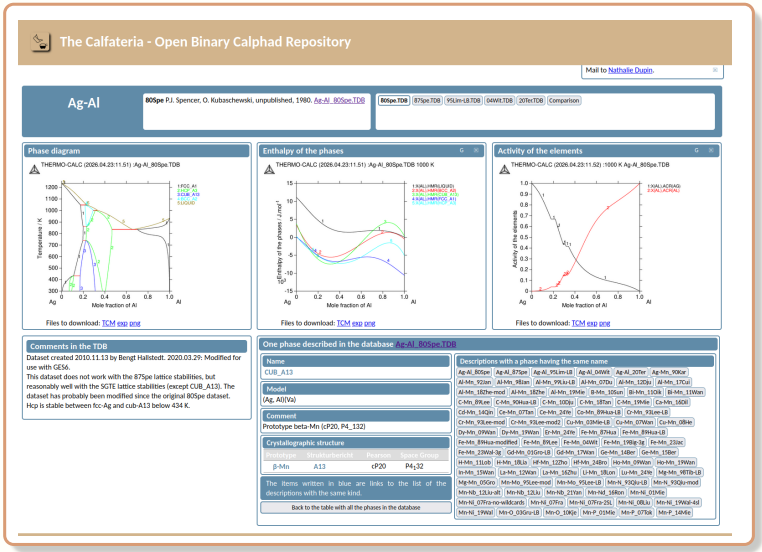
Dataset created 2010.11.13 by Bengt Hallstedt. 2020.03.29: Modified for use with GES6.
This dataset does not work with the 87Spe lattice stabilities, but reasonably well with the SGTE lattice stabilities (except CUB_A13). The dataset has probably been modified since the original 80Spe dataset.
Hcp is stable between fcc-Ag and cub-A13 below 434 K.

Phases described in the database Ag-Al_80Spe.TDB

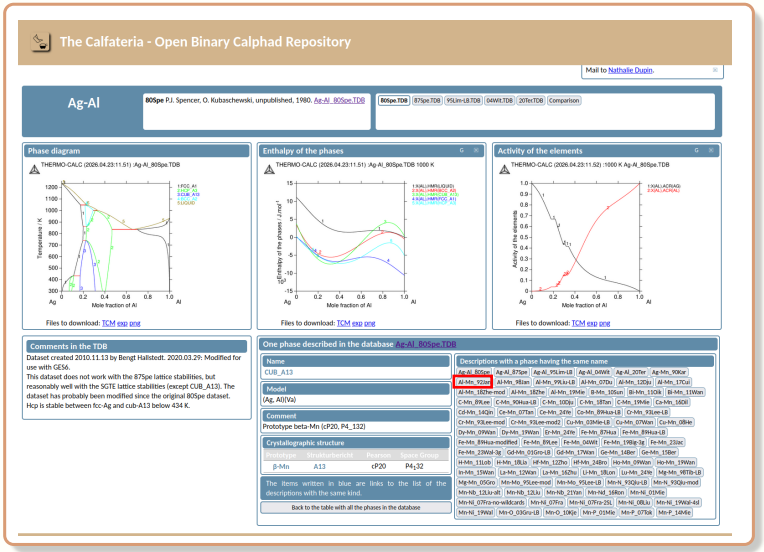
Name	Model	Comment
LIQUID	(Ag, Al)	Liquid phase
FCC_A1	(Ag, Al)(Va)	Fcc (cF4, Fm-3m) and MeX (cF8, Fm-3m), magnetic model
BCC_A2	(Ag, Al)(Va)$_3$	Bcc (cI2, Im-3m), magnetic model
HCP_A3	(Ag, Al)(Va)$_{0.5}$	Hcp (hP2, P6_3/mmc) and Me2X (NiAs-type, hP4, P6_3/mmc, B8_1), magnetic model
CUB_A13	(Ag, Al)(Va)	Prototype beta-Mn (cP20, P4_132)

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

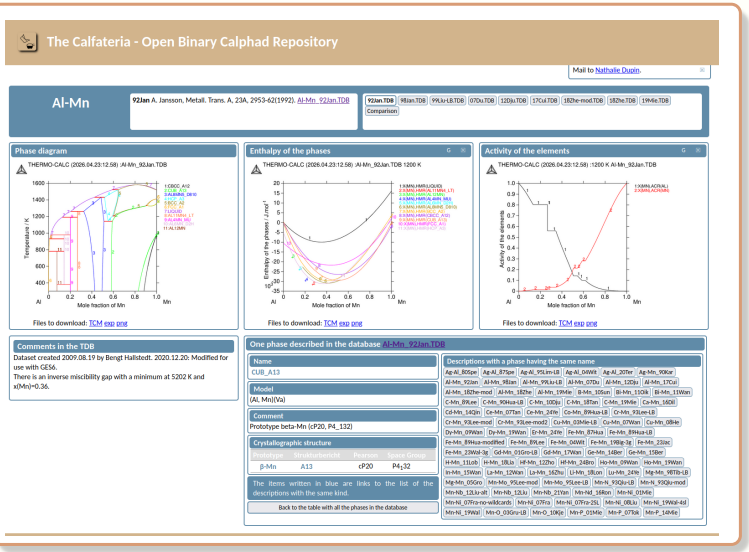
More details on a phase



More details on a phase



More details on a phase



With experimental data

The Calfateria - Open Binary Calphad Repository

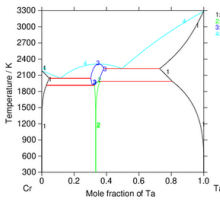
Cr-Ta

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

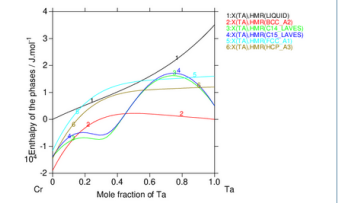
THERMO-CALC (2026.04.23:16.32) :Cr-Ta_93Dup-LB.TDB



Files to download: TCM exp png

Enthalpy of the phases

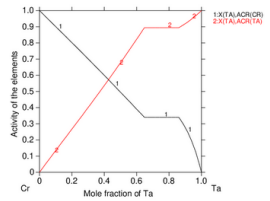
THERMO-CALC (2026.04.23:16.32) :Cr-Ta_93Dup-LB.TDB 2600 K



Files to download: TCM exp png

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

With experimental data

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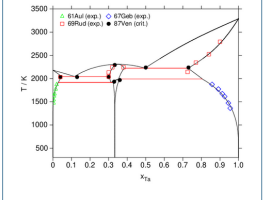
93Dup-LB N. Dupin, I. Ansara, J. Phase Equilib., 14, 451-56(1993), addendum, ibid, 15, 135(1994). Cr-Ta_93Dup-LB.TDB

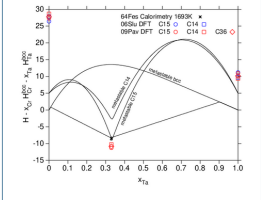
93Dup-LB.TDB | 01Zha.TDB | 09PavTDB | Comparison | With experiments

Calculated phase diagram



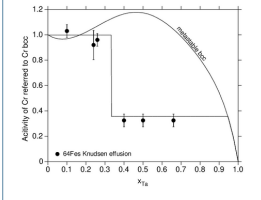
Files to download: experimental data set TCM calculated exp png

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

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)

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

60Pil: 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, ThermochemicalProperties 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. Venkatraman and J.P. Neumann, The Cr-Ta System, Bull Alloy Phase Diagrams, 8(2), 112-116(1987).

With experimental data

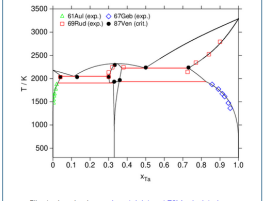
The Calfateria - Open Binary Calphad Repository

Cr-Ta

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

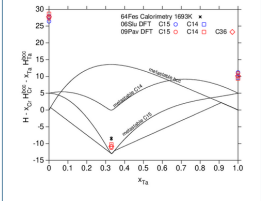
93Dup-LB.TDB | 01Zha.TDB | 09Pav.TDB | Comparison | With experiments

Calculated phase diagram



Files to download: experimental data set TCM calculated exp png

Enthalpy of formation at 1693K



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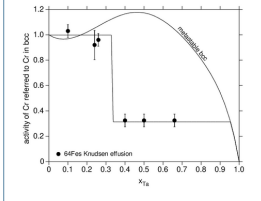
Activity of Cr at 1472K



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

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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).

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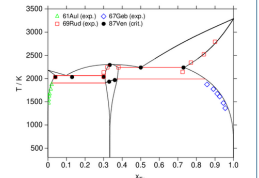
09Pav J. Pavlu, J. Vrestal, M. Sob, Calphad, 33, 179-86(2009). Cr-Ta_09Pav.TDB

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

Calculated phase diagram



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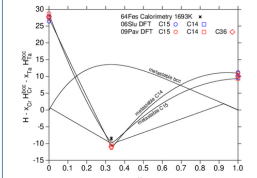
Enthalpy of formation at 1693K



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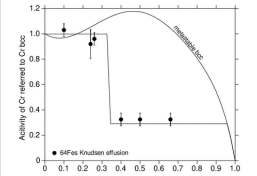
Activity of Cr at 1472K



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60Pil: 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, ThermochemicalProperties of the Laves Phase, Cr2Ta, Trans. Faraday Soc., 60, 1941-1946 (1964).

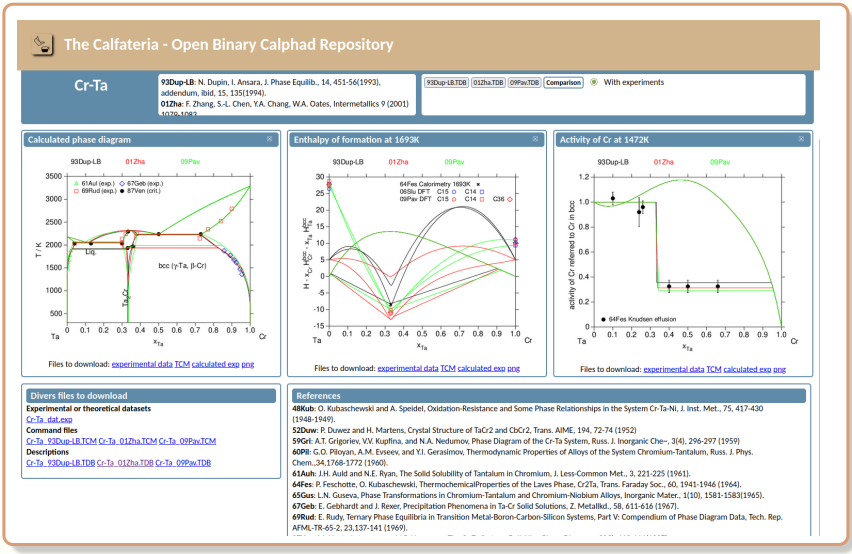
65Gus: L.N. Guseva, Phase Transformations in Chromium-Tantalum and Chromium-Niobium Alloys, Inorganic Mater., 1(10), 1581-1583(1965).

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).

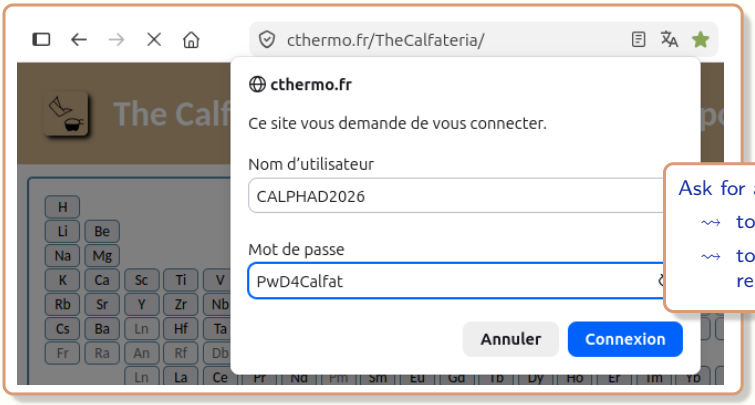
87Ven: M. Venkatraman and J.P. Neumann, The Cr-Ta System, Bull Alloy Phase Diagrams, 8(2), 112-116(1987)

With experimental data



After CALPHAD2026

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



Ask for a personnal 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

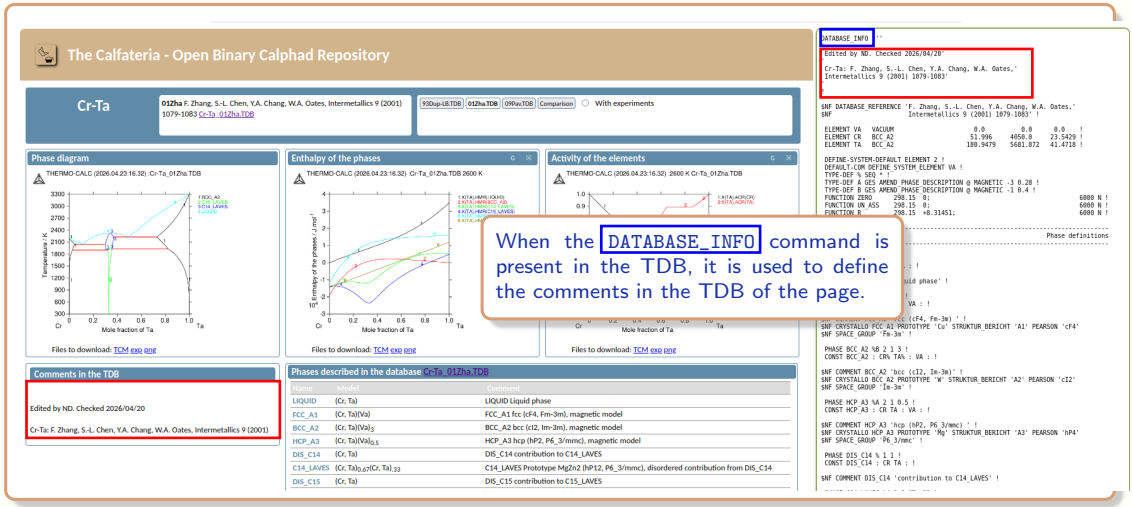
- contributing with data
  - new descriptions
  - new formats: dat, XTDB, py, ...
  - experimental data
- supporting financially the work

⇝ 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



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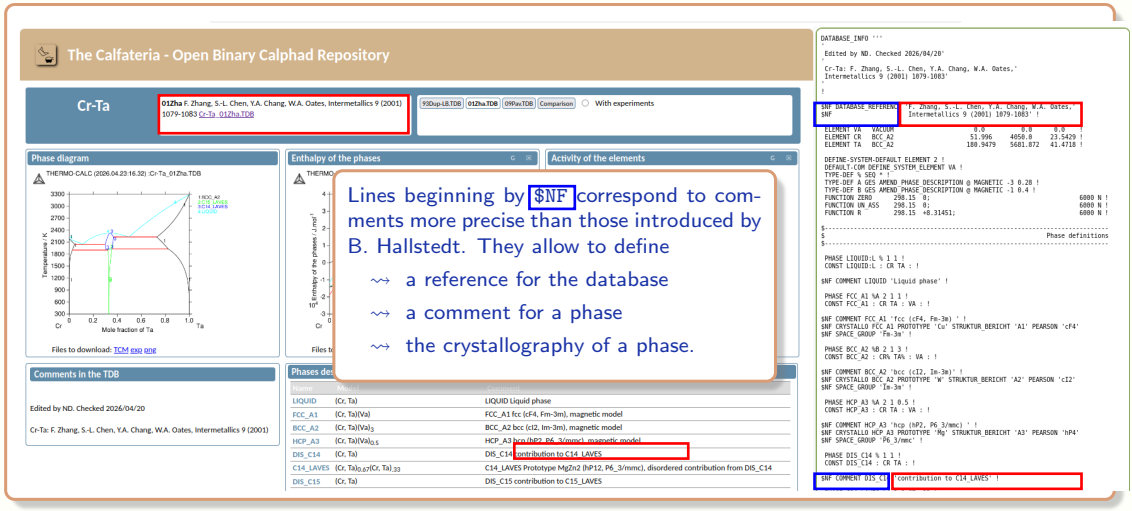
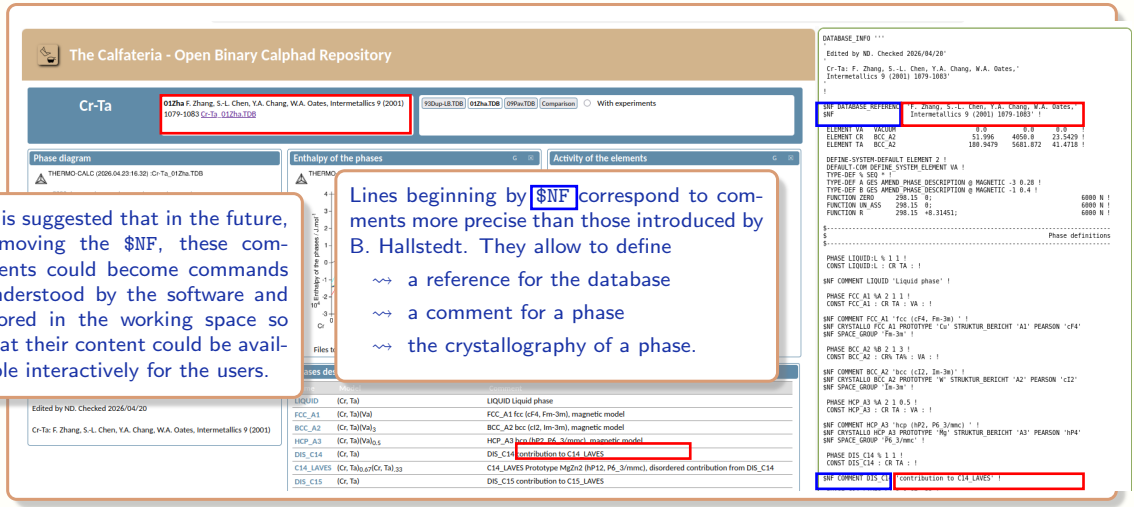


Evolution of TDB format



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.