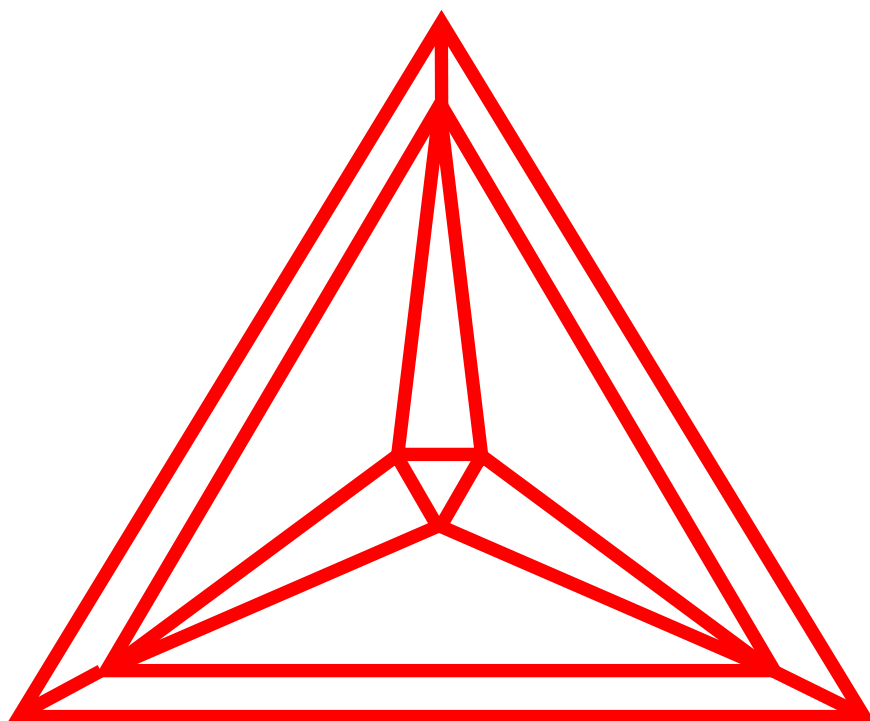


# **Thermo-Calc<sup>®</sup>**

## *Database Guide*

*(For Uses in TCC<sup>™</sup>/TCW<sup>™</sup>/DICTRA<sup>™</sup>)*



**Thermo-Calc Software AB  
Norra Stationsgatan 93 5 tr  
SE-113 64 Stockholm, Sweden**

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### **Availability of This Document:**

For the purpose of environment-friendliness, this *Thermo-Calc Database Guide* and all other operational manuals (User's Guides and Examples Books), as well as Reference Lists and other technical documentations, for the TCS-provided software, databases and programming interfaces are provided along the delivered TCS Standard Products CDs and installed on each of designated installation, which can be reviewed and accessed easily and conveniently. If desired and preferred, a user can locally print such a manual BUT it is only for the purpose of the user's internal use. For a hard copy of such a manual physically printed and delivered by TCS, a certain fee shall be applied.

To make manual updating more prompt and efficient, the later manual revisions or additions will be made available on the Internet. Our users may therefore download such revised documents from our company's web site [www.thermocalc.com](http://www.thermocalc.com).

### **Editors of This Document:**

Dr. Pingfang Shi  
Thermo-Calc Software AB (TCSAB)  
Norra Stationsgatan 93 Plan 5  
SE-113 64 Stockholm, SWEDEN  
E-Mail: [pingfang@thermocalc.se](mailto:pingfang@thermocalc.se)

Prof. Bo Sundman  
Dept. of Materials Science & Engineering  
Royal Institute of Technology (KTH)  
SE-100 44 Stockholm, SWEDEN  
E-Mail: [bosse@mse.kth.se](mailto:bosse@mse.kth.se)

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⇒ ***Revision History of the Thermo-Calc Database Guide:***  
Jun 2006 First (specialized) release (Edited by Pingfang Shi)  
Mar 2008 Second revised release (Edited by Pingfang Shi)

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## 1 Introduction

### 1.1 Thermo-Calc Software/Database/Interface Package

The Thermo-Calc software/database system covers more stoichiometric and non-ideal solution models and databases than any other available thermochemical software package. These models and databases can be used to describe steels, alloys, slags, salts, ceramics, solders, polymers, subcritical aqueous solutions, supercritical electrolyte solutions, non-ideal gases and hydrothermal fluids, organic substances, *etc.* over very wide ranges of temperature (up to 6000 K), pressure (up to 1 Mbar) and composition.

Good quality thermodynamic data for various materials is essential for obtaining reliable thermochemical calculations and simulations. As mentioned in *Part 3 (Section 3.3)* in the *Thermo-Calc Software System document*, such data must be established based on critical assessments. Great achievements have been made over the last two decades, and many internally-consistent databases or datasets have been built up, through varied international and national collaborations, such as CALPHAD community, SGTE society, Ringberg Forum, CAMPADA consortium, STT foundation, NIST institution, ThermoTech company, NPL laboratory, TGG program, UES/AEA corporation, *etc.*

#### 1.1.1 Thermo-Calc Software (TCC and TCW)

Thermo-Calc is a general and flexible software system (Sundman *et al.*, 1985; 1993; Jansson *et al.*, 1993; Sundman and Shi, 1997, Shi *et al.*, 2004), for all kinds of calculations of thermodynamic properties (as functions not only of temperature, pressure and composition, but also of magnetic contribution, chemical-/magnetic-ordering, crystallographic structures/defects, surface tension, amorphous glass-formation, mechanic-induced deformation, electro-static state, electronic potential, *etc.*), equilibrium and partial/local-equilibrium quantities, chemical driving forces (thermodynamic factors), and for various types of stable/meta-stable phase diagrams and property diagrams of multicomponent systems for many types of materials. It can efficiently handle a very complex multicomponent and heterogeneous interaction system defined with up to 40 elements, 1000 species and many different solution or stoichiometric phases. There are also powerful facilities to calculate many other types of diagrams, such as CVD/PVD depositions, CVM calculations of ordering/disordering phenomena, Scheil-Gulliver solidification simulations (with or without back-diffusions of fast-diffusing components), liquidus surface, Pourbaix diagrams, Ellingham diagrams, partition coefficients, partial pressures in gases, and so forth. It is the only software that can calculate arbitrary phase diagram sections with up to five independent variables in a defined system (which, is very useful, for instance, in finding the lowest melting temperature in a multicomponent alloy that has up to five independently-varying compositions), as well as the only software that can calculate chemical driving forces (thermodynamic factors, *i.e.*, the second derivatives of Gibbs free energy with respect to compositions) which are important fundamental information for kinetic simulations (such as in diffusion-controlled phase transformation, nucleation, particle growths/dissolutions, and so on).

Linked with various databases and interfaces, it stands for the **Thermo-Calc Software/Database/Interface Package**, or the *Thermo-Calc Databank*. The most important aim of the Thermo-Calc package is to make efficient and quick thermodynamic calculations available for applications in science and industry. The Thermo-Calc software system is based upon a powerful Gibbs Energy Minimizer, which has been further enhanced by the so-called Global Minimization Technique (that has been implemented in the current version). The Thermo-Calc software is especially designed for complex heterogeneous interaction systems with strongly non-ideal phases (which are specifically handled by a very wide range of sophisticated thermodynamic models), and can use many different thermodynamic databases, particularly those developed by the SGTE organization (*Scientific Group Thermodata Europe*, an international organization for collaborations on thermodynamic database developments) and CALPHAD community (*CALculations of PHase Diagrams*). Furthermore, there are several powerful application programming interfaces of the Thermo-Calc software engine, which can be utilized for user-written application programs or within third-party software packages for materials property calculations and materials process simulations.

There are two different user-interface types of the Thermo-Calc software, namely **TCC** (Thermo-Calc Classic) and **TCW** (Thermo-Calc Windows). The first version of TCC was released in 1981. Since 1999, TCW (as the second generation of the renowned Thermo-Calc software), with a completely GUI-driven (Graphic User Interface), has been made available to our users. There has been an update almost every year and the most recent ones, TCCS and TCW5, are released 2008.

Any modern PC (Microsoft Windows 7/VISTA/XP or Linux) can be used for running the Thermo-Calc and DICTRA software/database/interface packages.

The classical version TCC (and DICTRA) has an interactive user interface, extensive documentation, and on-line help facilities. The general GUI-driven (Graphic User Interface) version TCW has been made available for Windows environments, while such a general GUI version for Linux environments is still under development.

Thermo-Calc has gained a worldwide reputation as the best software for calculations of multicomponent phase diagrams. There are more than 1000 installations all over the world today, including academic institutions (universities and governmental institutes) and non-academic organizations (industrial companies and research companies), and is a reference in technical literature. It is the only software that can calculate chemical driving forces (thermodynamic factors, *i.e.*, the second derivatives of Gibbs free energy with respect to compositions) and arbitrary phase diagram sections with up to five independent variables in a very complex multicomponent and heterogeneous system (up to 40 elements in TCC and 20 elements in TCW, and up to 1000 species). There are also facilities to calculate many other types of diagrams, such as CVD depositions, Scheil-Gulliver solidification simulations, Pourbaix diagrams, partial pressures in gases, *etc.* Many application examples are given inside the **TCC Examples Book** and **TCW Examples Book**, and can also be found on our web site ([www.thermocalc.com](http://www.thermocalc.com)).

### 1.1.2 Thermo-Calc Databases

A thermodynamic software package is useless if without accurate and validated databases. Thermo-Calc allows you to utilize many critically-assessed and high-quality databases from various sources (such as SGTE, CAMPADA, CCT, ThermoTech, NPL, NIST, MIT, Theoretical Geochemistry Group, *etc.*). Such databases use different thermodynamic models for each phase in a certain heterogeneous interaction system. Currently-available Thermo-Calc databases cover a wide spectrum of materials, including steels, alloys, ceramics, melts, slag, slats, glasses, hard materials, semi-/super-conductors, solders, gas/fluids, aqueous solutions, organic substances, polymers, nuclear materials, earth materials, as well as geochemical and environmental systems, which can be applied to research and development in industrial engineering and natural systems: for instance, the SSUB/SSOL databases for substances and solutions in inorganic and metallurgic systems, TCFE for steels and Fe-alloys, TCNI/TTNi for Ni-based superalloys, TTAI/TTMg/TTTi for Al-/Mg-/Ti-based alloys, SLAG for slag, ION for carbides/nitrides/oxides/silicates/sulfides (solids/liquids/gases), TCMP for materials processing and applications to environmental problems associated with metallurgical, chemical and waste-treatment processes, particularly in recycling, remelting, sintering, incineration and combustion), SMEC for semi-conductors, NSLD/USLD for lead-free solders, SNOB for noble metals, NUMT/NUOX for nuclear substances and nuclear oxides, GCE for minerals, and TCAQ/AQS for aqueous solutions, *etc.* This **Thermo-Calc Database Guide** document gives all kinds of details about various available Thermo-Calc databases.

The Thermo-Calc and DICTRA groups at KTH-MSE have initiated and participated in many national and international projects in order to create general and validated databases. Thermo-Calc Software AB is now actively devoted to developments of more application-oriented databases of various industrial interests. There are also many users in various academic societies and industrial companies all over the world who have established their own databases or datasets under the assistance of the Thermo-Calc and DICTRA packages.

Both the TCC and DICTRA software also provide the users with a unique tool (the **PARROT** module) for critical assessment based upon varied experimental data such as PVT-EOS, thermochemical properties, phase equilibria, phase diagrams, diffusivity, and so on. By means of this module the user can efficiently expand some databases or reliably create various datasets or databases for some specific materials and applications. As a matter of fact, many of the existing databases and data-sets for various materials are really the products of R&D activities using the PARROT module.

### 1.1.3 Thermo-Calc Programming Interfaces

Any software has its limitations; this also applies to the Thermo-Calc and DICTRA software (and their associated databases). Many types of thermodynamic calculations and kinetic simulations can be efficiently and reliably performed with these two software; however, some of our users may wish to extend the Thermo-Calc and DICTRA capacities in order to additionally handle some other properties/systems/processes or in a different way to treat some problems. Application programming interfaces of the Thermo-Calc and DICTRA software with other user-written programs or third-party software packages for materials property calculations, materials structure simulations and materials process controls, have been rapidly developed. There are now different ways of conducting such application-oriented programming.

Two flexible programming interfaces (*i.e.*, **TQ** and **TCAPI**) allow the users to write their own application programs. TQ is available for all modern computer platforms (programming in FORTRAN), and TCAPI is currently for Windows and Linux based systems (programming in C/C++, VC, VB, JAVA or any other modern language). Powered by the Thermo-Calc software engine (plus some DICTRA extensions), such programming interfaces provide various kinds of calculations both for thermodynamic quantities and for local-/partial-equilibria and driving forces, which are needed by other user-written programs or third-party software packages in complex property modelling and process simulations. These facilities will greatly help you to reliably predict material compositions, structures and properties, and to efficiently optimise material processing and performance. The most successful examples are the comprehensive DICTRA<sup>®</sup> package, MICRESS<sup>™</sup> software (coupling via TQ) and PrecipiCalc<sup>™</sup> software (coupling via TCAPI).

Another powerful toolbox that is connected with specific third-party software (*i.e.*, **TC MATLAB Toolbox** in the MATLAB<sup>®</sup> software package) is also available. This unique toolbox has been developed, using the TCAPI programming interface. It allows an application (using this toolbox) to conduct all kinds of thermodynamic calculation precisely, which in return will enhance the performance of the MATLAB<sup>®</sup> applications in materials property calculations, materials process simulations and materials production controls. Recently, there have also been many other developments on coupling the Thermo-Calc/DICTRA engines through such programming interface with third-party software packages such as Fluent<sup>™</sup> and Phoenix<sup>™</sup>, as well as with FEM/PDE calculations and with Phase-Field simulations.

More sophisticated materials interface (using both Thermo-Calc and DICTRA as thermodynamic and kinetic engines) will be further developed.

### 1.1.4 Continuous Developments of the Thermo-Calc Package

Thermo-Calc and its sister software **DICTRA** (for Diffusion-Controlled phase TRAnsformation) have been developed originally at the *Department of Materials Science and Engineering of KTH (Royal Institute of Technology)*, Stockholm, Sweden, and further by our company **Thermo-Calc Software (TCS)** since 1997. They are the results of more than 35 years and 140 man-years R&D and many national/international collaborations through various R&D projects.

The copyrights for the Thermo-Calc and DICTRA software and several related databases belong to a non-profit organization, *Foundation of Computational Thermodynamics (STT)*, Stockholm. Since 1997, the further developments, marketing/sales, technical supports and all other activities concerning the Thermo-Calc and DICTRA packages are managed by our company TCS that is also owned by STT.

As mentioned above, there has been an update (normally as a major-version) almost every year. Such a great effort has efficiently been in place, not only for the Thermo-Calc (TCC/TCW) and DICTRA software, but also for the application programming interfaces (TQ, TCAPI and TC MATLAB Toolbox). Furthermore, some patches of various software and/or programming interfaces are released rather often, which our users can download from our web site ([www.thermocalc.com](http://www.thermocalc.com)) to replace some executable files in their existing installations, and can use such patches, if there is a relevant license (for the corresponding major-version) that is granted to the user, plus if there is a valid Software/Interface Maintenance & Support Subscription. This is why we encourage our users (who have valid licenses for the most-recent major-versions) to keep their eyes open on our web site for possibly available patches. We keep in mind that newly-implemented and improved

features/functionality, as well as necessary adjustments and corrections, made in an updated version (either a major-version or patch) of the TCC/TCW/DICTRA software, should usually be synchronized and transplanted into the new version of the programming interfaces, too. The most recent major-versions that are formally released in June 2008 are: TCCS, TCW5 and DICTRA26 (released in May 2010); TQ7, TCAPI5 and Toolbox5. For a rather complete list of the TCC software revision history (since TCCN), please refer to the [Section 1.4 of the TCCS User's Guide](#).

Some of the existing Thermo-Calc databases are also updated sometimes, but on a rather irregular basis due to the fact that a database update normally involves a tremendous amount of development work (assessments/evaluations and compilations) and validation tasks (testing, editing and applications), and often requires a long-enough period for many fruitful collaborations and discussions among our R&D partners and with some of our users. The major-version releases of such updated databases (such as TCFE6, SSOL4, TCMP2, SLAG2, ION3, TTNi7, TTTi3, TTAI7, TTMg4, TCAQ2, AQS2, GCE2, NOX2, NSLD2) are promptly announced on our web site ([www.thermocalc.com](http://www.thermocalc.com)) or in our company newsletters (which are also available at [www.thermocalc.com](http://www.thermocalc.com)) when they become available to our users (in cases of a public database, the updated major-version is freely and automatically included in a release/installation of the relevant major-version of the TCC/TCW/DICTRA software; whilst for a commercial database, a database version-upgrade can be applied to the existing users who have a valid license for an earlier version of a particular database). Sometimes, sub-versions of certain major-versions of particular databases may be made available: for instance, SLAG2.2 and TCMP2.2 are the second sub-versions of the second major-versions of the SLAG and TCMP databases, respectively. Such a database sub-version may cover some necessary improvements, adjustments, corrections, and occasionally additions (of parameters/functions, species, phases or even elements). A commercial database is always sold and licensed (via a new database license or a database version-upgrade) as of a major-version (e.g., SLAG2), while any database sub-version (e.g., SLAG2.2) is automatically distributed/installed together within a newly-purchased license for a corresponding database major-version, and/or is often freely (if not automatically then a special request can be placed to TCS or its agents by the users who have the corresponding database major-version) distributed/installed along with a renewed/enhanced license for a TCC/TCW/DICTRA software package (through a valid Software Maintenance & Support Subscription, a Software License-Upgrade, or a Software Version-Upgrade). For all kinds of details on updated databases (as of either major-versions or sub-versions) and for the possibility of getting a database version-upgrade (from an older major-version to the recent major-version) or obtaining a database version-enhancement (from an older sub-version to the recent sub-version, while remaining as of the same database major-version), please contact us at TCS and/or its agents.

At present and in future, TCS, STT and KTH-MSE are highly devoted to the further development on the Thermo-Calc and DICTRA software, as well on various databases and interfaced programs for different materials and processes. The continuous and close co-operations with many international R&D partners and Thermo-Calc and DICTRA users all over the world are very important for ensuring such developments.

*The mission of Thermo-Calc Software is to be extensively utilized as a powerful research and development tool for scientists and engineers in their daily work in laboratories or factories, and in teaching and training activities to bring new insight into realistic problems by linking fundamental models and critically assessed thermodynamic and kinetic data.*

*The ultimate purpose of Thermo-Calc Software is to assist you, to the highest degree, to save time and money in materials design, engineering and applications.*

*The development strategy of Thermo-Calc Software is to provide multiple applicability and increased efficiency to the materials industrials and R&D community.*

## 1.2 About This Document

This *Thermo-Calc Database Guide* document is a supplementary part of the following manual sets:

- *TCCS Manual Set* (*TCCS User's Guide* and *TCCS Examples Book*);
- *TCW5 Manual Set* (*TCW5 User's Guide* and *TCW5 Examples Book*); and
- *DICTRA26 Manual Set* (*DICTRA26 User's Guide* and *DICTRA26 Examples Book*).

This document comprise two major parts that used to be two chapters (i.e., *Chapter 4 - Thermo-Calc Database Descriptions* and *Chapter 6 - Database Manager Guide*) in the *TCC User's Guide*, but started from this version (TCCR), they have been extracted and separately prepared as an individual document.

The second part (*Thermo-Calc Database Descriptions*) of this document gives some brief descriptions on various available Thermo-Calc databases, which can be used within the Thermo-Calc software (TCC and TCW), DICTRA software, as well as various application programming interfaces. Such descriptions, however, will primarily include their elements and phases, specific applications, original producers and current contact persons; no detailed data will be given in this document.

The third part (*Database Manger Guide*) of this guide deals with all kinds of details regarding data structures and formats of the Thermo-Calc databases, as well as the DICTRA database-extensions. One should also refer to the relevant sections the document *Thermo-Calc Software System (Part 3 – Thermodynamic Data)* and of the *TCCS User's Guide (Chapter 5 – Database Module TDB)*.

Extensive descriptions and many application examples of the Thermo-Calc software/database/interface package are given inside the *TCCS Manual Set* and *TCW5 Manual Set*, which can be found within the TCCS/TCW5 installation and on our web site ([www.thermocalc.com](http://www.thermocalc.com)).

### *Editors of This Document:*

Dr. Pingfang Shi  
Thermo-Calc Software AB (TCSAB)  
Norra Stationsgatan 93 Plan 5  
SE-113 64 Stockholm, SWEDEN  
E-Mail: [pingfang@thermocalc.se](mailto:pingfang@thermocalc.se)

Prof. Bo Sundman  
Dept. of Materials Science & Engineering  
Royal Institute of Technology (KTH)  
SE-100 44 Stockholm, SWEDEN  
E-Mail: [bosse@mse.kth.se](mailto:bosse@mse.kth.se)

### 1.3 Availability of Thermo-Calc Databases

Within the SGTE community, enormous efforts have been put on establishing thermodynamic databases for various materials systems. Some unique databases have been made available on a wide range of elements, inorganic and metallurgical substances. Both KTH-MSE and TCS have been continuously devoted to the development of highly professional quality databases, under such collaborations.

Some other databases from independent sources (*e.g.*, ThermoTech Ltd., NIST, NPL, TGG) have been converted to the Thermo-Calc format, which are available from TCS and its agents.

*Table 1-1* outlines all the currently available Thermo-Calc databases from TCS or our collaborators. Each database will be described in the following pages.

**Please notice that some of the database names have been slightly modified, thanks to TCS's new strategy on systematical naming on software/database/interface products (valid from November 2002) for the purpose to avoid confusions regarding such products mentioned in various manuals, forms and informative documentations. For an abbreviated database name, there can be maximum 4 identical characters and optionally one digit for referring its version number if there are major updates (*e.g.*, PSUB1, PAQ2, PURE4, SSUB4, SSOL4, TCFE6, *etc.*). A full database name may refer to both the major update and minor sequential revision numbers, as well as to the release date(s), such as: PURE4 - SGTE Pure Elements Database (Version 4.6, 2002/2006/2008); SSOL4 - SGTE Alloy Solutions Database (Version 4.10, 2004//2005/2008). Those who may have any question about database names and database revision histories shall refer to the explanations in the specific Database Description Forms.**

Table 1-1. List of the Currently Available Thermo-Calc Databases

<i>Abbr. Name</i>	<i>Full Name (and version number &amp; release date)</i>	<i>Producers</i>	<i>Avail.</i>	<i>Updates</i>	<i>Page</i>
PURE4	SGTE Pure elements database (v4.6, 2002/2003/2006/2008)	SGTE	1	Y	2-2
PSUB	TC Public substances database (v1.1, 1998/2003)	TCS	1	N	2-3
PBIN	TC Public binary alloys database (v1.2, 1997/2003/2008)	SGTE, TCS	1	Y	2-3
PTER	TC Public ternary alloys database (v1.3, 1998/2003/2006/2008)	TCS	1	Y	2-3
PKP	Kaufman Binary alloys database (v1.1, 1990/2003)	LK	1	N	2-4
PCHAT	Chatenay-Malabry Post-transitional binary alloys database (v1.1, 1998/2003)	CM	1	N	2-5
COST2	COST507 Light alloys database (v2.1, 1998/2003)	COST507	5	N	2-6
SSUB4	SGTE Substances database (v4.0, 2006)	SGTE	2	Y	2-7
SSOL2	SGTE Solutions database (v2.1, 1999/2002/2003)	SGTE	2	Y	2-8
SSOL4	SGTE Solutions database (v4.10, 2003/2004/2006/2008)	SGTE	2	Y	2-9
TCBIN	TC Binary Solutions Database (v1.0, 2006)	TCS/SGTE	4	Y	2-10
TCFE1	TC Steels database (v1, 1992; TCFE_subset, TC-FE, TC-Alloy)	KTH-MSE	2	Y	2-12
TCFE2	TCS Steels/Fe-alloys database (v2.0, 1999)	TCS	2	Y	2-13
TCFE3	TCS Steels/Fe-alloys database (v3.0, 2002)	TCS	2	Y	2-14
TCFE4	TCS Steels/Fe-alloys database (v4.0, 2006)	TCS	2	Y	2-15
TCFE5	TCS Steels/Fe-alloys database (v5.0, 2007)	TCS	2	Y	2-16
TCFE6	TCS Steels/Fe-alloys database (v6.0, 2008)	TCS	2	Y	2-17
TCNI1	TCS Ni-based superalloys database (v1.2, 2000/2003/2008)	TCS, ND	2	Y	2-18
CCC1	CCT Cemented carbides database (v1.0, 2005)	CCT	2	Y	2-19
SLAG1	TC Fe-containing slag database (v1.2, 1992/1998/2006)	TCS	2	Y	2-20
SLAG2	TC Fe-containing slag database (v2.2, 2002/2003/2006)	TCS	2	Y	2-21
PION	TC Public ionic oxide solutions database (v1.1, 1998/2001)	TCS	1	N	2-22
ION1	TCS Ionic solutions database (v1.2, 1992/1994/2001)	TCS	2	Y	2-22
ION2	TCS Ionic solutions database (v2.3, 2002/2004/2005/2006)	TCS	2	Y	2-23
STBC1	SGTE Thermal Barrier Coating database (v1.0, 2005)	SGTE, MPIS	2	Y	2-24
SALT1	SGTE Molten salts database (v1.0, 1993)	SGTE	2	Y	2-25
TTNi7	TT Ni-based superalloys database (v7.0, 2006)	TT	3	Y	2-26
TTNF5	TT NiFe-based superalloys database (v5.0, 2002)	TT	3	Y	2-26
TTTi3	TT Ti-based alloys database (v3.0, 2006)	TT	3	Y	2-27
TTTA1	TT TiAl-based alloys database (v1.0, 1997)	TT	3	Y	2-27
TTAl6	TT Al-based alloys database (v6.1, 2007)	TT	3	Y	2-28
TTMg4	TT Mg-based alloys database (v4.1, 2007)	TT	3	Y	2-29
TTZr1	TT Zr-based alloys database (v1.0, 2006)	TT	3	Y	2-30
TCMP2	TCS Materials processing database (v2.5, 2002/2003/2004/2006/2008)	TCS, SG	2	Y	2-31
TCES1	TCS Sintering/Incineration/Combustion database (v1.1, 2000/2003)	TCS, SG	2	Y	2-32
PG35	ISC Group III-V Binary semiconductors database (v1.2, 1994/2003/2008)	ISC	1	N	2-33
SEMC2	TC Semiconductors database (v2.1, 2002/2003)	USTB-MSE	3	Y	2-34
PAQ2	TC Public aqueous database (SIT) for Pourbaix module (v2.4, 2002/03/06/08)	TCS	1	N	2-35
TCAQ2	TCS Aqueous solution database (SIT model; v2.5, 2002/2003/2004/2006/2008)	TCS	2	Y	2-36
PAQS2	TC Public aqueous database (HKF) for Pourbaix module (v2.4, 2002/03/06/08)	TCS	1	N	2-37
AQS2	TGG Aqueous solution database (HKF model; v2.5, 2000/02/03/04/06/08)	TGG	2	Y	2-38
PGE0	Saxena Minerals database (only substances) (v1.2, 1993/2003/2008)	TGG	1	N	2-39
GCE2	TGG Geochemical/Environmental database (v2.2, 2002/2003/2004)	TGG	2	Y	2-40
NUMT2	TCS/AEAT Pure radionuclides database (v2.0, 1999)	TCS	2	Y	2-41
NUOX4	TCS/AEAT Nuclear oxide solutions database (v4.0, 1999)	TCS	2	Y	2-42
SNUX6	SGTE In-vessel nuclear oxides database (v6.2, 2006)	SGTE/TCS	2	Y	2-43
NUTA	TCS/AEAT Ag-Cd-In ternary alloy solutions database (v1.0, 1991)	TCS	2	Y	2-44
NUTO	TCS/AEAT Si-U-Zr-O metal-metaloxide solutions database (v1.0, 1996)	TCS	2	Y	2-45
NOX2	NPL Oxide solutions database (v2.0, 2002)	NPL	3	Y	2-46
NSLD2	NPL Solder solutions database (v2.1, 2002)	NPL	3	Y	2-47
USLD1	NIST Solder solutions database (v1.0, 1999)	NIST	5	Y	2-48
SNOB1	SGTE Nobel metal alloys database (v1.2, 2003/2004/2008)	SGTE, SG	3	Y	2-49
<i>more *</i>					

**Producers:** CCT – Center of Computational Thermodynamics, Sweden; CM -- Chatenay-Malabry University, France; **COST507** -- European Cooperation in the field of Scientific and Technical research, Project 507; **FCT** -- Foundation of Computational Thermodynamics, Stockholm, Sweden; **ISC** -- an informal scientific collaboration (Ansara *et al.*, 1994); **KTH-MSE** -- Dept. of Materials Science and Engineering, KTH, Stockholm, Sweden; **LK** -- Larry Kaufman, MIT, USA; **MPIS** -- Max-plack Institute Stuttgart; **ND** -- Nathalie Dupin, France; **NIST** -- National Institute of Standards and Technology, USA; **NPL** -- National Physical Laboratory, UK; **SGTE** -- Scientific Group Thermodata Europe; **SG** -- Spencer Group, NY, USA; **TCS** -- Thermo-Calc Software AB, Stockholm, Sweden; **TGG** -- Theoretical Geochemistry Group, Florida International University, USA and Uppsala University, Sweden; **TT** -- ThermoTech Ltd., UK; **USTB-MSE** -- Dept. of Materials Science and Engineering, Univ. of Science and Technology, Beijing, China.

**Availability:** 1 -- Freely distributed with TCC and TCW, as well as with TCC-demo (TC4A) and TCW-demo (TC4W); 2 -- Commercially available from TCS and its agents; 3 -- Commercially available from TCS or the producers; 4 -- Freely distributed in encrypted form and can only be used in BIN module of the TCCR software and Binary Phase Diagram module of the TCW4 software; 5 -- Specially-distributed with TCC and TCW only under special requests.

**Updates:** Y -- Updates or expansions come irregularly; N -- No normal updates exist.

*more \** As new databases become available or any database is updated, the whole document *Thermo-Calc Database Description* will be promptly revised and published on our web site ([www.thermocalc.com](http://www.thermocalc.com)).

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## 2 Thermo-Calc Database Description Forms

This part gives some brief descriptions on various available Thermo-Calc databases, which can be used within the Thermo-Calc software (TCC and TCW), DICTRA software, as well as various application programming interfaces. Such descriptions, however, will primarily include their elements and phases, specific applications, original producers and current contact persons; no detailed data will be given in this document.

Please go to the individual *Thermo-Calc Database Description Form* page(s) for the specific database you are interested in and/or working with.

For more information on various new and updated Thermo-Calc databases, please regularly visit our web site [www.thermocalc.com](http://www.thermocalc.com).

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# PURE4

## SGTE Pure Elements Database (Version 4.6, 2002/2003/2006/2008)

**Producer:** SGTE, Scientific Group Thermodata Europe

**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The PURE4 Pure Elements Database contains critically assessed unary thermochemical data for the concerned elements in all stable and many metastable modifications from 298.15 K up to their liquid and gaseous states. All data are in SI units. The original unary database PURE1 was published by Dinsdale (1991).

This database can only be used to extract thermodynamic data of pure elements in performing assessment work for multicomponent systems, or in tabulating or plotting thermodynamic properties of the pure elements.

The same descriptions of all pure chemical elements have been utilized in the SGTE Substances Database SSUB and SGTE Solutions Database SSOL (SGTE, 1996, 2001, 2002, 2004, 2006, 2008), as well as in many specialized solution databases for alloys (*e.g.*, TCFE, TCNI, COST2, SEMC, TTAI/Mg/Ni/Ti/Zr, NSLD, etc.) and for other types of materials (*e.g.*, TCMP, TCES, ION, SLAG, SALT, TCAQ, AQS, GCE, NUMT, NUOX, etc.).

Status of the SGTE Pure Elements Database: The current version PURE4 (version 4.6) is based on the PURE4.5 sub-version of 2006 and PURE4.4 of 2003, which was updated by SGTE in 2001, and converted and edited into the TC database format by Bo Sundman and Pingfang Shi in Dec. 2002 and Jul. 2003). From PURE3 (available since 1998) to PURE4, the chemical framework has been extended from 83 elements to contain 16 additional elements (Ac-Ar-At-Cf-Cm-Es-Fm-Fr-He-Kr-Ne-Pm-Po-Ra-Rn-Xe) and 2 hydrogen isotopes (D-T). From PURE4.3 to PURE4.4, mainly includes improvements on functions for various elements in different structures; from PURE4.4 to PURE4.5 and (recently) to PURE4.6, minor corrections, modifications and improvements were made.

**Systems:** PURE4 now covers the totally 99 elements and 2 isotopes, as listed below:

Ac	Ag	Al	Am	Ar	As	At	Au	B	Ba
Be	Bi	Br	C	Ca	Cd	Ce	Cf	Cl	Cm
Co	Cr	Cs	Cu	Dy	Er	Es	Eu	F	Fe
Fm	Fr	Ga	Gd	Ge	H	He	Hf	Hg	Ho
I	In	Ir	K	Kr	La	Li	Lu	Mg	Mn
Mo	N	Na	Nb	Nd	Ne	Ni	Np	O	Os
P	Pa	Pb	Pd	Pm	Po	Pr	Pt	Pu	Ra
Rb	Re	Rh	Rn	Ru	S	Sb	Sc	Se	Si
Sm	Sn	Sr	Ta	Tb	Tc	Te	Th	Ti	Tl
Tm	U	V	W	Xe	Y	Yb	Zn	Zr	
D	T								

**Applications:** All kinds of applications.

**Availability:** Freely distributed with TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U.

**References:** Dinsdale A. (1991) SGTE data for pure elements, *Calphad*, **15**, 317-425.  
SGTE (1996) *The SGTE Casebook: Thermodynamics at Work* (Ed. Hack K.). The Institute of Materials, London, 227 p.  
SGTE (1993, 2000) The SGTE Solutions Database (SSOL version 1.2).  
SGTE (2001, 2002, 2004) The SGTE Substances Database (SSUB version 3.2).  
SGTE (1999, 2002, 2003) The SGTE Solutions Database (SSOL version 2.1).  
SGTE (2004, 2006) The SGTE Substances Database (SSUB version 4.0).  
SGTE (2004, 2006, 2008) The SGTE Solutions Database (SSOL version 4.0).

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## PSUB, PBIN and PTER

### TC Public Substances, Binary and Ternary Alloys Databases

(Version 1, 1997/1998/2003/2006/2008)

*Producer:* Thermo-Calc Software AB, Stockholm, Sweden

*Contact person:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* These three public databases were specially designed to demonstrate the uses of some particular databases or advanced modules: *i.e.*,

- PSUB for the POTENTIAL module, as well as for the SSUB and TCMP databases;
- PBIN for the BININAY module, as well as for the TCBIN and SSOL databases;
- PTER for the TERNARY module, as well as for the SSOL and other alloy databases.

Other public databases for the similar purposes also exist, *e.g.*,

- PION (for the ION Ionic Solution Database for oxides/sulfides/nitrides);
- PG35 (for the SEMC Semiconductors Database);
- PGEO (for the GCE Geochemical/Environmental Database);
- PAQ or PAQS (for the TCAQ or AQS Aqueous Solution Databases, as well as for the Pourbaix diagram calculations through either the POURBAIX module or TDBGES-POLY-POST routine).

Please note that all such public databases are designed only for demonstration and teaching purposes, and should not be used for any R&D activities whatsoever, due to their limitations of included elements, phases and data.

Such public databases contain only published data on some small-scaled systems. Some of them may be designed as subsets of commercially available databases, in order to show simple applications.

Status of the PSUB, PBIN and PTER Public Databases: These are the first versions of the PSUB, PBIN and PTER databases which were formally released as public Thermo-Calc databases in 1997 (PSUB, BIN97 and TERN98). Since April 2003, all such public databases are further revised and improved. Their most current sub-versions are PSUB1.1, PBIN1.2, PTERN1.3, respectively.

*Systems:* All such public databases are designed as limited systems:

#### TC Public Substance Database, **PSUB**

- ◆ covers the system **Cu-Fe-H-N-O-S**;
- ◆ contains a gas phase (with around 100 gas species) and about 50 condensed phases (solids or liquids, stoichiometric or solution phases).
- ◆ can be used in the POT module of the TCC software, *only for demonstration and teaching purposes.*

#### TC Public Binary Alloys Database, **PBIN** (Note it was previously called as **BIN97**)

- ◆ covers the 21-element system **Ag-Al-C-Co-Cr-Cu-Fe-Mn-Mo-N-Nb-Ni-O-Pb-S-Si-Sn-Ti-V-W-Zn**;
- ◆ contains about 40 binary solutions (liquids or solids), and many stoichiometric phases, as a subset of the SSOL database but containing only published data;
- ◆ is the appropriate database used in the BIN module of the TCC software, and in the “Binary Phase Diagram” module of the TCW software, *only for demonstration and teaching purposes.*

#### TC Public Ternary Alloys Database, **PTER** (Note it was previously called as **TER98**)

- ◆ covers the system **Al-C-Cr-Fe-Mg-Si-V**;
- ◆ contains two complete ternary subsystems (Al-Mg-Si and Fe-Cr-C) and a provisional ternary subsystem (Fe-V-C), as a subset of the TCFE and COST2 databases
- ◆ is the appropriate database used in the TERN module of the TCC software, *only for demonstration and teaching purposes.*

*Applications:* Alloy design and engineering.

## 2 Thermo-Calc Database Description Forms

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*Availability:* Freely distributed with TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U.



## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## PCHAT

### Chatenay-Malabry Post-Transitional Binary Alloys Database (Version 1.1, 1998/2003)

*Producer:* Laboratoire de Chimie Physique Minirale et Bioinorganique, Faculte de Pharmacie, Chatenay-Malabry, France.

*Contact person:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* This database consists of many post-transitional binary alloy solution systems. The systems have been optimized (without the gas phase) using the Lukas program, and the database file was converted to the Thermo-Calc format. A simple gaseous mixture phase was selectively appended from SSUB (the SGTE Substances Database), to complete this database for applications of heterogeneous interaction systems.

*Note the database was previously called as CHAT.*

*Status of the Chatenay-Malabry Post-Transitional Binary Alloys Database:* This is the first version of the PCHAT database which was formally released as a public Thermo-Calc database in Aug. 1998 (CHAT), with some minor modifications made in Apr. 2003 (PCHAT1.1).

*Systems:* This database includes the following 11 post-transitional elements:

**Au Bi Cd Ge Sb Se Si Sn Te Tl Zn**

Binary systems included in the database:

Au-Ge, Au-Si, Au-Te, Bi-Sb, Cd-Ge, Cd-Te, Cd-Zn, Ge-Sn, Se-Te, Si-Te, Zn-Te.

For the following binary systems, data were simply apoted from previous assessments:

Cd-Zn: L. Zabdyr and W. Zakulski (1993) *Archives of Metallurgy*, 38(1), 3-18.

Se-Te: G. Ghosh, H.L. Lukas, and L. Delaey (1988) *Calphad*, 12(3), 295-299.

Au-Ge: P.Y. Chevalier (1989) *Thermochimica Acta*, 141, 217-226.

However, the last one (Au-Ge) has been re-optimised to get a better temperature for the eutectic invariant.

Systems soon to be included are: Ge-Te, Sn-Se, Tl-Te.

Notes: Some problems occur with the gas phase in some binary systems:

1) For systems involving Se or Te, some values (-116522 and -42000 J/mol, respectively) were added to the Gibbs Energy functions of their gaseous species in order to get boiling points corresponding to the values given by ASM Handbook, V3, Alloy Phase Diagrams, Materials Park, Ohio, USA, 1992.

2) In the original version of CHAT, there was no Bi-bearing gaseous species, and the system Bi-Sb was presented without the gas phase.

In this revised version (Apr. 2003), PCHAT can also be directly used in the BIN module of the TCC software, and in the "Binary Phase Diagram" module of the TCW software. In addition, some Bi-bearing gaseous species have been added, and thus Bi-Sb binary is completed now.

*Applications:* Alloy design and engineering.

*Availability:* Freely distributed with TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U.

*References:* ASM (1992) *ASM Handbook, Volume 3, Alloy Phase Diagrams*, Materials Park, Ohio, USA.  
Chevalier P.Y. (1989) *Thermochimica Acta*, **141**, 217-226.  
Ghosh G., Lukas H.L., and Delaey L. (1988) *Calphad*, **12**(3), 295-299.  
Zabdyr L. and W. Zakulski W. (1993) *Archives of Metallurgy*, **38**(1), 3-18.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# COST2

## COST507 Light Alloys Database

*(Version 2.1, 1998/2003)*

*Producer:* COST507 Project: Round II, European Commission

*Contact person:* Pingfang Shi and Åke Jansson, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* This database is developed on the basis of the critical assessment work on light alloys established by the EU COST 507 Project, Round II (COST 1998). The project was devoted to the developments of new light alloys, with participants of 28 institutions from 14 EU countries (Austria, Belgium, Finland, France, Germany, Greece, Netherlands, Norway, Portugal, Spain, Sweden and UK) and Switzerland and Russia.

The database compiles the published assessment data, primarily on binary light alloys, resulted from the entire COST 507 Project. Some ternary systems are also included.

The quality of the assessed data may vary from one subsystem to another, and is therefore recommended that the use of this database should be always with care. Adjustment in some subsystems may be needed if the application is made for industrial alloys. This database presents a good resource for teaching and a fairly reasonable basis for academic research on light alloys.

*Status of the COST507 Light Alloys Database:* This is the second version of the COST2 database which was formally released as a free Thermo-Calc database in Jan. 1999 (COST2.0), with some minor modifications made in May 2003 (COST2.1).

*Systems:* This database includes the following 19 elements:

<b>Al</b>	<b>B</b>	<b>C</b>	<b>Ce</b>	<b>Cr</b>	<b>Cu</b>	<b>Fe</b>	<b>Li</b>	<b>Mg</b>	<b>Mn</b>
<b>N</b>	<b>Nd</b>	<b>Ni</b>	<b>Si</b>	<b>Sn</b>	<b>V</b>	<b>Y</b>	<b>Zn</b>	<b>Zr</b>	

192 possible phases have been considered in this database.

*Applications:* Light alloy design and engineering.

*Availability:* As a free database to be used together with TCC and TCW, **it is distributed only upon special requests to TCS (with a certain distribution fee).**

*References:* COST (1998) COST 507 -- Definition of Thermochemical and Thermophysical Properties to Provide a Database for the Development of New Light Alloys. European Cooperation in the Field of Scientific and Technical Research, European Commission.

*Vol 1.* Proceedings of the Final Workshop of COST 507, Vaals, the Netherlands, 1997

*Vol 2.* Thermochemical Database for Light Metal Alloys (Eds. Ansara I., Dinsdale A.T., and Rand M.H.)

*Vol 3.* Critical Evaluation of Ternary Systems (Ed. Effenberg G.)

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# SSUB4

## SGTE Substances Database

(Version 4.0, 2006)

**Producer:** SGTE, Scientific Group Thermodata Europe

**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The SSUB4 Pure Substances Database (version 4 within TCC/TCW software, while it was originally named by SGTE as *version 11*) was updated in 2005/2006, based upon its previous versions SSUB3 of 2001/2002/2004 and SSUB2 of 1998/1999. It now contains assessed thermochemical data for 5254 substances (2902 condensed compounds and 2356 gaseous species) within a chemical framework of 101 elements. The data has been generated by the SGTE organization or critically assessed from different sources, such as TCRAS, JANAF, Kubaschewski, Barin and Knacke, among others. For each compound or species, the literature reference is given. Data follow the new temperature scale ITPS 90. All thermodynamic data is for 1 bar. The reference state for all data are default set as the pure elements at 298.15 K and 1 bar.

The data for each compound or species consist of:

- The enthalpy of formation at 298.15 K (relative to pure elements),
- The entropy at 298.15 K (from 3rd law integrations or estimations),
- The temperature dependence of the heat capacity at constant pressure from 298.15 K up to the gaseous state.

This database is particularly useful for:

- Tabulation of thermochemical data,
- Computations and tabulations of reactions and equilibrium constants,
- Computation of complex gas equilibria for multicomponent systems with no solid solutions.

The descriptions of the elements are identical to those in PURE4, the SGTE Pure Elements Database (version 4), with explicit magnetic and pressure dependence functions.

The SSUB4 database can be appended to various multicomponent systems that have been primarily defined using certain solution databases (such as SSOL, TCFE/TCNI, TTNI/TTTi/TTAl/TTMg/TTZr, ION, NUOX, GCE, TCAQ, AQS, *etc.*), for a wide range of applications.

**Status of the SGTE Substances Database:** This database was completely revised by SGTE in 1994, 1998, 2001 and 2005, and has been updated irregularly and extended with some new compounds each time. The current version SSUB4 commercially distributed with Thermo-Calc is the updated version of 2005 (with some minor modifications made by Pingfang Shi in 2006 as SSUB4.0). From SSUB2 (available since 1998) to SSUB3 (with some minor modifications made by Bo Sundman and Pingfang Shi in 2002 as SSUB3.1 and further in 2004 as SSUB3.2), its chemical framework has been extended from 83 elements (as in SSOL2 and PURE3) to include 16 additional elements (Ac, Ar, At, Cf, Cm, Es, Fm, Fr, He, Kr, Ne, Pm, Po, Ra, Rn and Xe) and 2 hydrogen isotopes (D and T), and its content increased from about 4000 to about 5000 condensed compounds or gaseous species. From SSUB3 to SSUB4, its data has been further increased to 5254 substances (2902 condensed compounds and 2356 gaseous species), and some data have been corrected/modified/improved.

**Systems:** SSUB4 now covers the same chemical framework as in PURE4 (*i.e.*, 99 elements and 2 hydrogen isotopes; see *Thermo-Calc Database Description Form PURE4*), and contains about 5254 condensed compounds or gaseous species. The gaseous mixture phase is the only solution phase in the database, and it is treated as ideal (in both EOS and mixing) at all temperatures, pressures and compositions. For other solution phases, one can append data from separate databases for various specific alloy solutions, ionic oxide/sulfide/nitride/... solutions, slags, molten salts, solders, semi-conductors, minerals, nuclear materials, aqueous solutions, and organic substances/solutions, among others.

**Applications:** Alloy design and engineering; Inorganic materials.

**Availability:** Commercially available for uses with TCC and TCW; also together with its special subset SPOT4 for uses in the POTENTIAL module. *It is possible to upgrade from the older versions (SSUB1 of 1992, or SSUB2 of 1997, or SSUB3 of 2001/2002/2004) to SSUB4 upon a certain database upgrade fee.*

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

## SSOL2

### SGTE Solutions Database

(Version 2.1, 1999/2002/2003)

**Producer:** SGTE, Scientific Group Thermodata Europe

**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The SSOL2 Solutions Database is a sophisticated important thermochemical database for many non-ideal solution phases within a chemical framework of 83 elements. Combinations of several assessed systems can calculate and extrapolate higher order multicomponent systems. Such extrapolations require experience and understanding and the producer or vendor should be contacted if problems occur.

The descriptions of the elements are identical to the descriptions in PURE4, the SGTE Pure Elements Database (version 4). The SSOL2 database is compatible, among others, with PURE4, SSUB3 and TCAQ2 databases.

**Status of the SGTE Solutions Database:** This database was originally created by SGTE in 1992 and first released in TCC in November 1993. It was completely revised by SGTE in 1997, 1999 and later on. The actual systems included in a distribution may be different due to various updates and removal of inconsistencies. The particular version SSOL2.1 (which is commercially distributed with Thermo-Calc, and contains 222 complex alloy solution and intermetallic compound phases) is the updated version of 1999 (with some minor modifications made by Bo Sundman and Pingfang Shi in Nov. 2002 and Apr. 2003). In Sept. 2003, the SSOL database was updated to version 4.74B; for details see the *Thermo-Calc Database Description Form SSOLA*.

**Systems:** SSOL2 covers a chemical framework of 83 elements, as listed below:

Ag	Al	Am	As	Au	B	Ba	Be	Bi	Br
C	Ca	Cd	Ce	Cl	Co	Cr	Cs	Cu	Dy
Er	Eu	F	Fe	Ga	Gd	Ge	H	Hf	Hg
Ho	I	In	Ir	K	La	Li	Lu	Mg	Mn
Mo	N	Na	Nb	Nd	Ni	Np	O	Os	P
Pa	Pb	Pd	Pr	Pt	Pu	Rb	Re	Rh	Ru
S	Sb	Sc	Se	Si	Sm	Sn	Sr	Ta	Tb
Tc	Te	Th	Ti	Tl	Tm	U	V	W	Y
Yb	Zn	Zr							

Assessed data for condensed phases is in the following 106 binary systems:

Ag-Au, Ag-Cu, Ag-Ge, Ag-Pb, Ag-Si, Ag-Sn, Al-As, Al-Bi, Al-Ca, Al-Fe,  
Al-Ga, Al-Ge, Al-In, Al-Mg, Al-Mn, Al-Pb, Al-Si, Al-Sn, Al-Zn, As-Ga,  
As-Ge, As-In, Au-Bi, Au-Ge, Au-In, Au-Pb, Au-Sb, Au-Si, Au-Sn, Au-Tl,  
Bi-Cu, Bi-Ga, Bi-Ge, Bi-In, Bi-K, Bi-Sn, Bi-Tl, Bi-Zn, C-Co, C-Cr,  
C-Cu, C-Fe, C-Mn, C-Mo, C-Nb, C-Ni, C-Pb, C-Ti, C-V, C-W,  
Ca-Fe, Co-Cr, Co-Fe, Co-Mn, Co-Ni, Cr-Cu, Cr-Fe, Cr-Mo, Cr-N, Cr-Ni,  
Cr-V, Cr-W, Cs-K, Cs-Na, Cs-Rb, Cu-Fe, Cu-Mg, Cu-Ni, Cu-P, Cu-Pb,  
Cu-Si, Cu-Tl, Cu-Zn, Fe-Mn, Fe-Mo, Fe-N, Fe-Nb, Fe-Ni, Fe-Pb, Fe-S,  
Fe-Si, Fe-Ti, Fe-V, Fe-W, Ga-Ge, Ga-In, Ga-Pb, Ga-Sn, Ga-Zn, Ge-In,  
Ge-Pb, Ge-Sb, Ge-Sn, Ge-Tl, Ge-Zn, K-Rb, (Mg-Sb), Mg-Si, (Mg-Sn), Mo-N,  
Mo-Nb, Mo-Ni, Mo-W, N-Ni, N-Ti, Na-Rb, Ni-W, Pb-Si, Pb-Sn, Sb-Sn,  
Si-Mo, Si-Sn, Si-Ta, Si-Ti, Si-W, Si-Zn

Assessed data for the condensed phases is in the following ternary and higher order systems:

Ag-Au-Ge, Ag-Au-Si, Ag-Cu-Pb, Al-As-Ga-Ge, Al-Ga-Ge, Al-Ga-In, Al-Ge-Sn,  
Al-Mg-Si, Al-Si-Zn, Au-In-Pb, Bi-Ga-Zn, C-Co-Cr, C-Co-Cr-W, C-Co-Fe, C-Co-Fe-Ni,  
C-Co-Fe-Ni-W, C-Co-Fe-W, C-Co-Ni, C-Co-Ni-W, C-Co-W, C-Cr-Fe, C-Cr-Fe-Mo,  
C-Cr-Fe-Mo-W, C-Cr-Fe-W, C-Cr-Ni, C-Cr-W, C-Fe-Mn, C-Fe-Mn-V, C-Fe-Mo,  
C-Fe-Mo-W, C-Fe-N, C-Fe-Nb, C-Fe-Ni, C-Fe-Ni-W, C-Fe-Si, C-Fe-W, C-Mo-W,  
C-Ni-W, Co-Cr-W, Co-Fe-Mn, Co-Fe-Ni, Co-Fe-W, Co-Ni-W, Cr-Fe-Mo,  
Cr-Fe-Mo-W, Cr-Fe-N, Cr-Fe-N-Ni, Cr-Fe-Ni, Cr-Fe-Ni-Co, Cr-Fe-W, Cr-Mo-W,  
Cr-Ni-W, Cu-Fe-Ni, Cu-Fe-P, Fe-Mo-W, Fe-Ni-W, Ga-Ge-Sn, Mg-Sb-Sn, Sn-Pb-Te

**Applications:** Alloy design and engineering; Inorganic materials.

**Availability:** Commercially available for uses with TCC and TCW; also together with its special subset SBIN2 for uses in the BINARY module. *It is recommend to upgrade from this version or its older version (SSOL1 of 1992) to the latest version of the SSOL database (i.e., SSOLA) upon a database upgrade fee.*

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# SSOL4

## SGTE Solutions Database

(Version 4.10, 2004/2005/2008)

**Producer:** SGTE, Scientific Group Thermodata Europe

**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The SSOL4 Solutions Database is a sophisticated important thermochemical database for many non-ideal multicomponent solution phases within a chemical framework of 78 elements (compared with the SSOL2 solutions database, F-Cl-Br-I-H are excluded). The contents of this database (sub-version of SSOL4.10) have been greatly expanded from that of its previous version SSOL2, and extensively improved from its earlier sub-versions SSOL4.7 (of 2003), SSOL4.8 (of 2004) and SSOL4.9 (2005).

Combinations of several critically-assessed systems can calculate and extrapolate higher-order multicomponent systems. Such extrapolations require experience and understanding and the producer or vendor should be contacted if problems occur.

The descriptions of the elements are identical to the descriptions in PURE4, the SGTE Pure Elements Database (version 4). The SSOL4 database is compatible, among others, with PURE4 and SSUB4 databases.

Status of the SGTE Solutions Database: This database was originally created by SGTE in 1992 and first released in TCC in November 1993. It was completely revised by SGTE in 1997, 1999 and later on. The actual systems included in a distribution may be different due to various updates and removal of inconsistencies. The previous version SSOL2 commercially distributed with Thermo-Calc is the updated version of 1999 (with some minor modifications made by Bo Sundman and Pingfang Shi in April 2002).

This current version SSOL4 has been further developed on the basis of SSOL2, but mainly focused on alloy solution phases and important intermetallic compound phases. It was released as version 4.74B by SGTE in Sept. 2003, but converted into the Thermo-Calc database format and further modified by TCS during Nov. 2003 – Feb. 2004 (and formally released as to SSOL4.8 in Feb. 2004, and SSOL4.9 in Apr. 2005). **In the fall of 2008, a further sub-version SSOL4.10 will be released, which includes the unique on-line reference lists and many greatly-improved/modified descriptions.** Continuous developments of this database have been planned within the SGTE community.

**Systems:** SSOL4 covers the following 78 elements:

Ag	Al	Am	As	Au	B	Ba	Be	Bi	C
Ca	Cd	Ce	Co	Cr	Cs	Cu	Dy	Er	Eu
Fe	Ga	Gd	Ge	Hf	Hg	Ho	In	Ir	K
La	Li	Lu	Mg	Mn	Mo	N	Na	Nb	Nd
Ni	Np	O	Os	P	Pa	Pb	Pd	Pr	Pt
Pu	Rb	Re	Rh	Ru	S	Sb	Sc	Se	Si
Sm	Sn	Sr	Ta	Tb	Tc	Te	Th	Ti	Tl
Tm	U	V	W	Y	Yb	Zn	Zr		

Included thermodynamic data that have been critically assessed are available for many binary, ternary and higher-order subsystems in various multicomponent solution phases, as well as for many important intermetallic compound phases. **The total number of solution phases and intermetallic compound phases has been greatly increased from 222 (in SSOL2) to more than 600 (in SSOL4.10).**

**Applications:** Alloy design and engineering; Inorganic materials.

**Availability:** Commercially available for uses with TCC and TCW. *It can also be upgraded from its older versions (SSOL1 of 1992/1998 or SSOL2 of 1999/2002) to SSOL4, at a certain database upgrade fee. It is freely upgradeable from sub-versions SSOL4.7, 4.8 and 4.9 to SSOL4.10, when there is a valid TCC/TCW Software M&SS Subscription.*

## 2 Thermo-Calc Database Description Forms

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## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# TCBIN

## TC Binary Solutions Database

(Version 1.1, 2008)

*Producer:* Thermo-Calc Software AB, Stockholm, Sweden  
SGTE, Scientific Group Thermodata Europe

*Contact persons:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* TCBIN (TC Binary Solutions Database, Version 1.0) has been developed in 2005-2006, based on some previous assessment work within the SGTE community (during 2002-2005), as well as additional work made in TCS. It contains many critically-assessed thermochemical data for binary systems (mainly alloys), including contributions from magnetic and chemical ordering.

For each phase or species, the literature reference is given. Data follow the new temperature scale ITPS 90. All thermodynamic data is for 1 bar. The reference state for all data are default set as the pure elements at 298.15 K and 1 bar. The descriptions of the elements are identical to those in PURE3 (the SGTE Pure Elements Database, version 3), with explicit magnetic and pressure dependence functions. But the TCBIN database is not compatible with SSUB (SGTE Substances Database) and SSOL (SGTE Alloy Solutions Database), simply due to that TCBIN has a rather different strategy in naming and describing various binary intermediate solution/compound phases.

The database is particularly useful for:

- ☞ Calculation of binary alloy phase diagrams,
- ☞ Tabulation of thermochemical data of binary alloy joins.

*Systems:* TCBIN covers the following 67 elements:

Ag	Al	As	Au	B	Ba	Bi	C	Ca	Cd
Ce	Co	Cr	Cs	Cu	Dy	Er	Eu	Fe	Ga
Ge	H	Hf	Hg	Ho	In	Ir	K	La	Li
Mg	Mn	Mo	N	Na	Nb	Nd	Ni	O	Os
P	Pb	Pd	Pr	Pt	Rb	Re	Rh	Ru	S
Sb	Sc	Se	Si	Sn	Sr	Ta	Tb	Te	Ti
Tl	U	V	W	Y	Zn	Zr			

and contains totally 621 condensed phases (non-ideal alloy solutions that are handled by varied types of sophisticated thermodynamic models, and stoichiometric compounds) and one gaseous mixture phase. The gas phase is treated as ideal (in both EOS and mixing behaviors) under all temperatures, pressures and compositions.

TCBIN has 360 critically-assessed binary systems as listed below:

Ag-Al	Ag-Au	Ag-Bi	Ag-Cu	Ag-Ge	Ag-In	Ag-Ir	Ag-Mg	Ag-Os	Ag-Pb
Ag-Pd	Ag-Pt	Ag-Rh	Ag-Ru	Ag-Sb	Ag-Si	Ag-Sn	Ag-Ti	Ag-Tl	Ag-Zn
Ag-Zr	Al-As	Al-Au	Al-B	Al-Bi	Al-C	Al-Ca	Al-Ce	Al-Co	Al-Cr
Al-Cu	Al-Fe	Al-Ga	Al-Ge	Al-In	Al-Li	Al-Mg	Al-Mn	Al-Mo	Al-N
Al-Nb	Al-Nd	Al-Ni	Al-O	Al-P	Al-Pb	Al-Sb	Al-Si	Al-Sn	Al-Ta
Al-Ti	Al-V	Al-W	Al-Y	Al-Zn	Al-Zr	As-Au	As-Cu	As-Fe	As-Ga
As-Ge	As-In	As-P	As-Sb	Au-Bi	Au-C	Au-Cr	Au-Cu	Au-Ge	Au-In
Au-Pb	Au-Pd	Au-Rh	Au-Ru	Au-Sb	Au-Si	Au-Te	Au-Tl	B-C	B-Co
B-Cr	B-Fe	B-Hf	B-Mg	B-Mo	B-N	B-Nd	B-Ni	B-SC	B-Si
B-Ti	B-V	B-W	Ba-Cu	Ba-Eu	Ba-Sr	Ba-Y	Bi-Cu	Bi-Ga	Bi-Ge
Bi-In	Bi-K	Bi-Mg	Bi-O	Bi-Pb	Bi-Sb	Bi-Si	Bi-Sn	Bi-Tl	Bi-Zn
C-Co	C-Cr	C-Cu	C-Fe	C-Hf	C-Mn	C-Mo	C-Nb	C-Ni	C-Pb
C-Si	C-Ta	C-Ti	C-V	C-W	C-Y	C-Zr	Ca-Cu	Ca-Mg	Ca-Pb
Ca-Si	Ca-Zn	Cd-Ga	Cd-Ge	Cd-Hg	Cd-In	Cd-Pb	Cd-Sb	Cd-Sn	Cd-Te
Cd-Zn	Ce-Mg	Co-Cr	Co-Cu	Co-Dy	Co-Fe	Co-In	Co-Mn	Co-Mo	Co-N

## 2 Thermo-Calc Database Description Forms

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Co-Nb	Co-Ni	Co-Pd	Co-Pt	Co-Si	Co-Ta	Co-Ti	Co-V	Co-W	Cr-Cu
Cr-Mg	Cr-Mn	Cr-Mo	Cr-N	Cr-Nb	Cr-Ni	Cr-P	Cr-Pd	Cr-Pt	Cr-Si
Cr-Sn	Cr-Ta	Cr-Ti	Cr-V	Cr-W	Cr-Zn	Cr-Zr	Cs-K	Cs-Na	Cs-Rb
Cu-Fe	Cu-Ge	Cu-In	Cu-Li	Cu-Mg	Cu-Mn	Cu-N	Cu-Nb	Cu-Ni	Cu-O
Cu-P	Cu-Pb	Cu-S	Cu-Sb	Cu-Si	Cu-Sn	Cu-Sr	Cu-Ti	Cu-Tl	Cu-V
Cu-Y	Cu-Zn	Cu-Zr	Dy-Er	Dy-Ho	Er-Ho	Er-Tb	Fe-Mg	Fe-Mn	Fe-Mo
Fe-N	Fe-Nb	Fe-Nd	Fe-Ni	Fe-O	Fe-P	Fe-Pb	Fe-Pd	Fe-Pr	Fe-Pt
Fe-S	Fe-Si	Fe-Sn	Fe-Ti	Fe-V	Fe-W	Fe-Zn	Fe-Zr	Ga-Ge	Ga-Hg
Ga-In	Ga-P	Ga-Pb	Ga-Sb	Ga-Sn	Ga-Te	Ga-Zn	Ge-In	Ge-Pb	Ge-Sb
Ge-Si	Ge-Sn	Ge-Te	Ge-Tl	Ge-Zn	H-Nb	H-Zr	Hf-Ta	Hf-Si	Hf-Ti
Ho-Tb	In-P	In-Pb	In-Sb	In-Si	In-Sn	In-Zn	Ir-Pd	K-Rb	La-Ni
Li-Mg	Li-Zr	Mg-Mn	Mg-Ni	Mg-O	Mg-SC	Mg-Si	Mg-Y	Mg-Zn	Mg-Zr
Mn-Mo	Mn-N	Mn-O	Mn-Pb	Mn-Si	Mn-Ti	Mn-V	Mn-Y	Mn-Zr	Mo-N
Mo-Nb	Mo-Ni	Mo-Si	Mo-Ta	Mo-Ti	Mo-W	N-Nb	N-Ni	N-Ta	N-Ti
N-V	N-W	Na-Rb	Nb-Ni	Nb-O	Nb-Ti	Nb-V	Nb-W	Nb-Zr	Nd-Pr
Nd-Sb	Ni-P	Ni-Pd	Ni-Si	Ni-Ta	Ni-Ti	Ni-V	Ni-W	Ni-Y	Ni-Zr
O-Pb	O-Sn	O-Sr	O-Ti	O-Y	O-Zr	P-Sb	P-Si	Pb-Pd	Pb-Sb
Pb-Si	Pb-Sn	Pb-Tl	Pb-Zn	Pd-Ru	Pd-Sn	Pr-Sb	Pt-Rh	Pt-Ru	Re-Ta
Re-W	Sb-Si	Sb-Sn	Sb-Zn	Se-Sn	Se-Te	Se-Tl	Si-Sn	Si-Ta	Si-Te
Si-Ti	Si-U	Si-V	Si-W	Si-Y	Si-Zn	Si-Zr	Sn-Ti	Sn-Zn	Sn-Zr
Ta-Ti	Ta-V	Ta-W	Ta-Zr	Te-Zn	Ti-V	Ti-W	Ti-Zr	V-Zr	Y-Zr

**IMPORTANT NOTES:** The TCBIN database is free-of-charge included along with the TCC/TCW software (since TCCR/TCW4). However, unlike other databases, it will always be distributed in the encrypted database form, and can only be used inside the BIN module (of TCC) or Binary Phase Diagram module (of TCW).

*Other Limitations:* The ultimate and sole purpose of the TCBIN database is to demonstrate the BIN Module of the TCC software (and Binary Phase Diagram Module of the TCW software) in precisely calculating binary phase diagrams, property diagrams and various thermodynamic functions, based on critically-assess binary data; and the POLY3 files generated by the BIN Module may also be used in the POLY Module for some further calculations/simulations for the already-defined binary join and in the POST Module for other diagram plotting. However, the database can not be assessed directly from the TDB Module. Furthermore, it can not be used for calculations/simulations of multicomponent systems, since it only contains unary and binary data for each of individual binary systems.

*Applications:* Calculations of phase diagrams and property diagrams for binary systems (most alloys).

*Availability:* Freely distributed in encrypted form and can only be used within the BIN Module of TCC software and the Binary Phase Diagram Module of TCW software (since TCCR/TCW4).

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# TCFE1

## TC Steels/Fe-Alloys Database

(Version 1.1, Aug. 1992)

**Producer:** Division of Computational Thermodynamics, KTH-MSE, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCFE1 (TCFE\_subset) Steels/Fe-Alloys Database (previously named as TC-FE92 or TC-Alloy) consists of assessments of data for steels made by the division since 1978. It describes systems of interest for solidification and heat treatment of steels. This database supersedes an older database, called Fe-base, which was accumulated before 1978. In 1978, the description of pure Fe was changed to include an explicit magnetic description, which required a complete revision of all assessments. The TCFE1 database is a slightly modified subset of the SGTE solution database.

The last version of TCFE1 was released in 1992, while a revised sub-version named as FEDAT was released in 1996. During 1998-1999, the TCFE database was updated as TCFE2 to include seven more elements (Al, B, Cu, Mg, O, P and S), and to contain more experimental data in the systematical assessment (in which the models for some phases have been improved). The most updated database is the TCFE6 that was released in 2008 (for details see the *Thermo-Calc Database Description Form TCFE6*).

**Systems:** TCFE1 covers complete and critical assessments of binary and some ternary systems, as well as the iron rich corner of some higher order systems, within the 13-element framework:

**C Co Cr Fe Mn Mo N Nb Ni Si**  
**Ti V W**

The recommended limits for the alloying elements are (in weight percent):

Element	max	Element	max	Element	max	Element	max
C	5.0	Mn	15.0	Nb	5.0	Ti	1.0
Co	15.0	Mo	15.0	Ni	20.0	V	2.0
Cr	30.0	N	1.0	Si	1.0	W	20.0

The recommended temperature range is from 700 to 2000°C. Calculations slightly outside the recommended limits may give reasonable results but it requires experience and skill to correctly extrapolate data and interpret the calculation results. Comparisons with a known alloy should always be made to test the validity of the calculations before applying it to a new material. The data for liquid, austenite, ferrite, cementite, and the  $M_{23}$ ,  $M_7$  and  $M_6$  carbides are good. The data for nitrogen are mainly assessed for stainless steel *i.e.* austenite, ferrite, the epsilon phases and the MN nitride. Data for the intermetallics like  $\sigma$ ,  $\mu$ , Laves, are less reliable.

Note the use of the following phase names in the database

Phase	Database	Phase	Database	Phase	Database
Austenite	FCC#1	Ferrite	BCC	$\alpha$ -Mn	CBCC-A12
$M(C,N)_x$	FCC#2	$M_2(C,N)$	HCP#2	$\beta$ -Mn	CUB-A13

The number symbol, #, is used to denote different composition sets of the same phase.

This database is not updated regularly, but is compatible with the SGTE solution database.

**Applications:** Steel design and engineering.

**Availability:** Commercially available for uses with TCC and TCW. *It can be upgraded to the latest version of the TCFE database (i.e., TCFE6) upon a certain database upgrade fee.*

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# TCFE2

## TCS Steels/Fe-Alloys Database

(Version 2.0, Oct. 1999)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCFE2 Steels/Fe-Alloys Database was released by TCS in 1999, and was previously called TC-FE2000 or TCFE2K. In collaboration with the CAMPADA project at the Department of Materials Science and Engineering, KTH, TCS had developed a new steels/Fe-alloys database during 1998-1999. It was based on the TCFE1 steels database and includes all new assessments made up to 1998 for systems of interests for steels and Fe-alloys. The updating had been supervised by Dr. Byeong-Joo Lee and Prof. Bo Sundman.

**Systems:** TCFE2 covers complete and critical assessments of binary and some ternary systems, as well as the iron rich corner of some higher order systems, within the 20-element framework:

**Al B C Co Cr Cu Fe Mg Mn Mo**  
**N Nb Ni O P S Si Ti V W**

The database is applicable for steels with a Fe-minimum of 50wt% with the following alloying elements (with the recommended limits in weight percent):

Element	max	Element	max	Element	max	Element	max
Al	5.0	Cu	1.0	Nb	5.0	Si	5.0
B	<i>trace</i>	Mg	<i>trace</i>	Ni	20.0	Ti	2.0
C	5.0	Mn	20.0	O	<i>trace</i>	V	5.0
Co	15.0	Mo	10.0	P	<i>trace</i>	W	15.0
Cr	30.0	N	1.0	S	<i>trace</i>	Fe	<i>min 50</i>

The update was based on complete reassessments of binary and many ternary systems, mostly from published sources. Many of the intermediate compounds that do not occur in steels have been deleted from the database. Therefore, it is not suitable to calculate complete systems, but rather only in the iron rich corner. Each parameter in the database has a reference to its origin.

Sensible calculations cannot be expected if all alloying elements are at their highest limits. Some combinations of elements at high values will not give reasonable results; but, some alloying elements can exceed their limits considerably and the calculations will still give good results. Critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but TCS is interested to know about any significant deviations in order to improve any future release.

Compared to the previous TCFE1 database, the elements Al, B, Cu, Mg, O, P and S have been added. No elements have been added compared to SSOL but the alloying range has been extended considerably.

No ternary borides have been considered, but small amounts of B are possible to use. The elements O, P and S are included in the database to simplify calculations when the steel has traces of these elements, mainly in form of stable oxides, phosphides or sulphides. A careful matching of information on forming carbonitrides based on V, Nb and Ti has been made and the database should thus be applicable to HSLA steels

The description of highly alloyed steels has been improved by extending the alloying range (particularly for Mn) and including new classes of steels (particularly corrosion resistant high strength steels).

**Applications:** Steel design and engineering.

**Availability:** Commercially available for uses with TCC and TCW. *It can be upgraded to the latest version of the TCFE database (i.e., TCFE6) upon a certain database upgrade fee.*

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# TCFE3

## TCS Steels/Fe-Alloys Database

(Version 3.0, Dec. 2002)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCFE3 Steels/Fe-Alloys Database was released by TCS in 2002. It was based on the TCFE2 Steels/Fe-Alloys Database and includes all new assessments made up to 2002 for systems of interests for steels and Fe-alloys. The updating had been made by Prof. Bo Sundman.

**Systems:** TCFE3 covers complete and critical assessments of binary and some ternary systems, as well as the iron rich corner of some higher order systems, within the 20-element framework:

Al B C Co Cr Cu Fe Mg Mn Mo  
N Nb Ni O P S Si Ti V W

The database is applicable for steels with a Fe-minimum of 50wt%, and for alloying elements the recommended composition limits (in weight percent) are as follows:

Element	max	Element	max	Element	max	Element	max
Al	5.0	Cu	1.0	Nb	5.0	Si	5.0
B	trace	Mg	trace	Ni	20.0	Ti	2.0
C	5.0	Mn	20.0	O	trace	V	5.0
Co	15.0	Mo	10.0	P	trace	W	15.0
Cr	30.0	N	1.0	S	trace	Fe	min 50

The update was based on complete reassessments of binary and many ternary systems, mostly from published sources. Many intermediate compounds that do not occur in steels have been deleted from the database. Therefore, it is not suitable to calculate complete systems, but rather only in the iron rich corner. Each parameter in the database has a reference to its origin.

Sensible calculations cannot be expected if all alloying elements are at their highest limits. Some combinations of elements at high values will not give reasonable results; but, some alloying elements can exceed their limits considerably and the calculations will still give good results. Critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but TCS is interested to know about any significant deviations in order to improve any future release.

Compared with the TCFE2 database, a number of improvements have been made in order to increase the predictive capability of the TCFE3 database. Some of the major improvements are:

- Improved data for the important sigma phase in stainless steels.
- Addition of data for the binary Nb-Ni system.
- Improved data for the ternary Fe-Cr-Mo system.
- Improved data for the ternary Cr-Mo-Ni system.

Additionally some minor improvements on data for other systems have been made.

No ternary borides have been considered, but small amounts of B are possible to use. The elements O, P and S are included in the database to simplify calculations when the steel has traces of these elements, mainly in form of stable oxides, phosphides or sulphides. A careful matching of information on forming carbonitrides based on V, Nb and Ti has been made and the database should thus be applicable to HSLA steels.

The description of highly alloyed steels has been improved by extending the alloying range (particularly for Mn) and including new classes of steels (particularly corrosion resistant high strength steels).

**Applications:** Steel design and engineering.

**Availability:** Commercially available for uses with TCC and TCW. It can be upgraded to the latest version of the TCFE database (i.e., TCFE6) upon a certain database upgrade fee.

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# TCFE4

## TCS Steels/Fe-Alloys Database

(Version 4.0, May 2006)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCFE4 Steels/Fe-Alloys Database was released by TCS in 2006. It was based on the TCFE3 (that in turn is based on TCFE2 Steels/Fe-Alloys Database and includes all new assessments, made by Prof. Bo Sundman, up to 2002 for systems of interests for steels and Fe-alloys). **From TCFE3 to TCFE4, the main improvements are the additions of critically-assessed volume data (molar volume and thermal expansivity) for alloys and compounds as functions of temperature and compositions, that are recently made available by Thermo-Calc Software.**

**Systems:** TCFE4/TCFE3 covers complete and critical assessments of binary and some ternary systems, as well as the iron-rich corner of some higher order systems, within the 20-element framework:

Al B C Co Cr Cu Fe Mg Mn Mo  
N Nb Ni O P S Si Ti V W

The database is applicable for various types of steels/Fe-alloys with a Fe-minimum of 50wt%, and for alloying elements the recommended composition limits (in weight percent) are as follows:

Element	max	Element	max	Element	max	Element	max
Al	5.0	Cu	1.0	Nb	5.0	Si	5.0
B	trace	Mg	trace	Ni	20.0	Ti	2.0
C	5.0	Mn	20.0	O	trace	V	5.0
Co	15.0	Mo	10.0	P	trace	W	15.0
Cr	30.0	N	1.0	S	trace	Fe	min 50

The update was based on complete reassessments of binary and many ternary systems. Many intermediate compounds that do not occur in steels have been deleted from the database. Therefore, it is not suitable to calculate complete systems, but rather only in the iron rich corner. Each parameter in the database has a reference to its origin.

Sensible calculations cannot be expected if all alloying elements are at their highest limits. Some combinations of elements at high values will not give reasonable results; but, some alloying elements can exceed their limits considerably and the calculations will still give good results. Critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but TCS is interested to know about any significant deviations in order to improve any future release.

Compared with the TCFE3 database, all necessary volume data (including molar volume and thermal expansivity) for various alloy phases have been incorporated, in addition to the changes made in TCFE3, where a number of improvements (in comparison with the TCFE2 database) had been made in order to increase the predictive capability of the database. Some of the major improvements in the TCFE4 version are: improved data for the important sigma phase in stainless steels; addition of data for the binary Nb-Ni system; improved data for the ternary Fe-Cr-Mo system; improved data for the ternary Cr-Mo-Ni system; plus some minor improvements on data for other systems.

No ternary borides have been considered, but small amounts of B are possible to use. The elements O, P and S are included in the database to simplify calculations when the steel has traces of these elements, mainly in form of stable oxides, phosphides or sulphides. A careful matching of information on forming carbonitrides based on V, Nb and Ti has been made and the database should thus be applicable to HSLA steels.

The description of highly alloyed steels has been improved by extending the alloying range (particularly for Mn) and including new classes of steels (particularly corrosion resistant high strength steels).

**Applications:** Steel /Fe-alloys design and engineering.

**Availability:** Commercially available for uses with TCC and TCW. *It can be upgraded to the latest version of the TCFE database (i.e., TCFE6) upon a certain database upgrade fee.*

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# TCFE5

## TCS Steels/Fe-Alloys Database

(Version 5.0, Feb. 2007)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCFE5 Steels/Fe-Alloys Database was released by TCS in Feb. 2007. Its development was based on TCFE4 (2006) & TCFE3 (2002), and it includes many new critical assessments on thermodynamic data for multi-component systems of interests for various steels/Fe-alloys.

**Systems:** TCFE5 covers complete and critical assessments of binary and some ternary systems, as well as the iron-rich corner of some higher order systems, within the 20-element framework:

Al B C Co Cr Cu Fe Mg Mn Mo  
N Nb Ni O P S Si Ti V W

The database is applicable for various types of steels/Fe-alloys with a Fe-minimum of 50wt%, and for alloying elements the recommended composition limits (in weight percent) are as follows:

Element	max	Element	max	Element	max	Element	max
Al	5.0	Cu	2.0	Nb	5.0	Si	5.0
B	trace	Mg	trace	Ni	20.0	Ti	2.0
C	5.0	Mn	20.0	O	trace	V	5.0
Co	15.0	Mo	10.0	P	trace	W	15.0
Cr	30.0	N	1.0	S	trace	Fe	min 50

The update was based on complete reassessments of binary and many ternary systems. However, many intermediate compounds that do not occur in steels have been deleted from the database. Therefore, it is not suitable to calculate complete systems, but rather only in the iron rich corner. Each parameter in the database has a reference to its origin.

Sensible calculations cannot be expected if all alloying elements are at their highest limits. Some combinations of elements at high values will not give reasonable results; but, some alloying elements can exceed their limits considerably and the calculations will still give good results. Critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but TCS is interested to know about any significant deviations in order to improve any future release.

In its previous version TCFE4, all necessary volume data (including molar volume and thermal expansivity) for various alloy phases were incorporated; such volume data remain the same in TCFE5.

In order to further increase the predictive capability of the database, results from the CCT-Applied Stainless Steel project has been added in the TCFE5 version. The CCT (Centre of Computational Thermodynamics) is a collaboration among Thermo-Calc Software, KTH (Royal Institute of Technology), Kimab and Swedish industries. For details of all the major improvements, refer to the document "*TCFE5 Database Description Form*".

No ternary borides have been considered, but small amounts of B are possible to use. The elements O, P and S are included in the database to simplify calculations when the steel has traces of these elements, mainly in form of stable oxides, phosphides or sulphides. A careful matching of information (updated in TCFE5) on forming carbonitrides based on V, Nb and Ti has been made and the database should thus be applicable to HSLA steels. The description of highly alloyed steels has been improved by extending the alloying ranges (particularly for Mn and Cu) and by including new classes of steels (particularly for corrosion-resistant high strength steels and stainless steels).

**Applications:** Steel /Fe-alloys design and engineering.

**Availability:** Commercially available for uses with TCC and TCW. *It can be upgraded to the latest version of the TCFE database (i.e., TCFE6) upon a certain database upgrade fee.*

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# TCFE6

## TCS Steels/Fe-Alloys Database

(Version 6.0, Apr. 2008)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCFE6 Steels/Fe-Alloys Database was released by TCS in March 2008. Its development was based on TCFE5 (2007) & TCFE4 (2006), and it includes many new critical assessments on thermodynamic data for multi-component systems of interests for various steels/Fe-alloys.

**Systems:** TCFE6 covers complete and critical assessments of binary and some ternary systems, as well as the iron-rich corner of some higher order systems, within the 21-element framework:

Al B C Ca Co Cr Cu Fe Mg Mn  
Mo N Nb Ni O P S Si Ti V W

The database is applicable for various types of steels/Fe-alloys with a Fe-minimum of 50wt%, and for alloying elements the recommended composition limits (in weight percent) are as follows:

Element	max	Element	max	Element	max	Element	max
Al	5.0	Cr	30.0	N	5.0	S	trace
B	trace	Cu	5.0	Nb	5.0	Si	5.0
C	7.0	Mg	trace	Ni	20.0	Ti	3.0
Ca	trace	Mn	20.0	O	trace	V	15.0
Co	20.0	Mo	10.0	P	trace	W	15.0
Fe	min 50						

The update was based on complete reassessments of binary and many ternary systems. Many intermediate compounds that do not occur in steels have been deleted from the database. Therefore, it is not suitable to calculate complete systems, but rather only in the iron rich corner. Each parameter in the database has a reference to its origin.

Sensible calculations cannot be expected if all alloying elements are at their highest limits. Some combinations of elements at high values will not give reasonable results; but, some alloying elements can exceed their limits considerably and the calculations will still give good results. Critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but TCS is interested to know about any significant deviations in order to improve any future release.

In version TCFE4, all necessary volume data (including molar volume and thermal expansivity) for various alloy phases were incorporated; such volume data has been updated in TCFE6.

Results from the CCT-Applied Stainless Steel Project were incorporated into the TCFE5 version. The CCT (Centre of Computational Thermodynamics) is a collaboration among Thermo-Calc Software, KTH (Royal Institute of Technology), Swerea KIMAB and Swedish industries. In order to further increase the predictive capability of the database, many significant assessments and modifications have been performed by TCS and are introduced in TCFE6. The element Ca has been added and the alloying ranges for the elements C, Co, Cu, N, Ti and V have been extended. For details of all the major improvements, refer to the document "**TCFE6 Database Description Form**".

All the major improvements that have been implemented in TCFE6 make this database suitable to predict different thermodynamic properties with accurate results. It can be used with satisfying results for several types of alloys e.g. stainless steels, high-speed steels, tool steels, HSLA steels, cast iron and corrosion-resistant high strength steels and more.

The TCFE6 database contains a simple GAS mixture phase (Ar, O<sub>2</sub>, N<sub>2</sub> and S<sub>2</sub>) only for the main purpose of considering oxygen/nitrogen-gas controls in steel-making processes; however, it can be replaced by a large GAS phase appended from a compatible database (e.g. SSUB4, SLAG2 or TCMP2).

**Applications:** Steel /Fe-alloys design and engineering.

**Availability:** Commercially available for uses with TCC and TCW.

*It is highly recommended to upgrade from the older versions (TCFE1 of 1992, FEDAT of 1996, TCFE2 of 1999, TCFE3 of 2002, TCFE4 (of 2006) or TCFE5 (of 2007) to TCFE6 (upon a certain database upgrade fee).*

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# TCNI1

## TCS Ni-based Superalloys Database

(Version 1.2, 2000/2003/2008)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden  
Nathalie Dupin, France

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCNI database is developed for Ni-based superalloys. The thermodynamics of the  $\gamma$  and  $\gamma'$  phases are modeled with a single Gibbs energy function taking into account the crystallographic relations between these two phases after Ansara *et al.* (1997).

A brief presentation of the models used and the content of the database can be found in Dupin and Sundman (2000). The assessed agreement of the calculated equilibria with experimental data on the relevant ternary systems will be published in scientific journals.

Calculations with the current database in multicomponent systems validate its ability of extrapolation in a wide range of composition for Ni-based superalloys, for equilibria in the solid state as well as for solidification behavior (liquidus temperature and partition ratios).

Status of the TCS Ni-based Superalloys Database: This is the first version of the TCNI database which was formally released in Mar. 2000 (TCNI1.0), with some minor modifications made in Apr. 2003 (TCNI1.1) and in Jun. 2008 (TCNI1.2).

**Systems:** The database contains 7 elements:  
**Al Co Cr Ni Ti W Re**

All assessed binary systems constituting this database can be calculated with the BINARY Module in the Thermo-Calc software. The assessed ternary systems included in the database are the following:

Al-Co-Ni, Al-Cr-Ni, Al-Ni-Ti, Al-Ni-W, Co-Ni-W, Cr-Ni-Re, Cr-Ni-Ti, Cr-Ni-W,  
Ni-Re-Ti, Ni-Re-W, Ni-Ti-W, Al-Cr-Ti, Al-Ti-W

The extension of the present database to include Mo, Ta, Nb, Fe, Zr, Hf, C, B, *etc.* is ongoing.

**Applications:** Ni-based superalloy design and engineering.

**Availability:** Commercially available for uses with TCC and TCW.

**References:** Ansara I., Dupin N., Lukas H.L., and Sundman B (1997) *Journal of Alloys and Compounds*, **247**, 20-30.  
Dupin N. and Sundman B. (2000) *Proceedings of the Discussion Meeting on Thermodynamics of Alloys* (TOFA2000, Stockholm), *Scandinavian Journal of Metallurgy*.

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# CCC1

## CCT Cemented Carbides Database

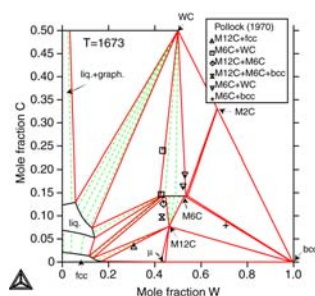
(Version 1.0, 2005)

**Producer:** CCT (Centre for Computational Thermodynamics) at KIMAB (Corrosion and Metals Research Institute), Stockholm, Sweden.

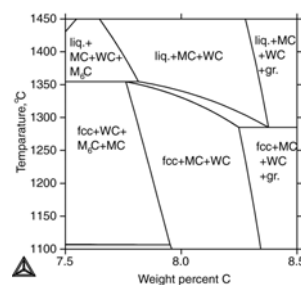
**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden.

**Description:** This database offers a high-accuracy thermodynamic description of systems relevant to production of cemented carbides. It has been developed within CCT (Centre for Computational Thermodynamics), involving a university (KTH - Royal Institute of Technology, Stockholm), a research institute (KIMAB - Corrosion and Metals Research Institute, Stockholm), and several Swedish industrial partners.

Descriptions are based on a recent evaluation of the C-Co-W based system [1]. All possible binary and ternary systems with a 6-element framework have been evaluated, and information from higher order systems has been taken into account. The solubility of Nb, Ta, Ti in the  $M_6C$  carbide and in the liquid phase, as well as the melting temperatures of the Co-binder phase, have also been adjusted to describe new experimental information [2]. For all phases a description of the molar volumes and thermal expansion is included [3], and thus the volume fractions of phases, densities, *etc.* for complex alloys can be calculated. The variation of the volumes with composition is described, too. Accurate calculations of the composition of the  $MC_x$  carbide in multi-component alloys can be made [4].



The Co-W-C diagram at 1673 K.  
From: Markström et al., *J. Phase Equilibria*, Vol. 26 No. 2 2005.



Calculated section through the C-Co-Nb-Ta-Ti-W system at 53%W, 8.3%Co, 1.5%Nb, 12.5%Ta, 16%Ti. From Frisk et al., *Proc. 16th Int. Plansee Seminar* (edited by G. Kneringer et al., Reutte, 2005).

**Status of the CCT Cemented Carbides Database:** The current version, CCC1, is the first version commercially released as a standard Thermo-Calc database. Work is currently in progress to include more elements and phases for a future update.

**Systems:** CCC1 covers the following 6 elements:

**C Co Nb Ta Ti W**

Equilibrium involving the following phases can be calculated with high accuracy:

Liquid, FCC, HCP,  $MC_x$ ,  $M_6C$ , WC, Graphite.

**Applications:** Cemented carbides (hard materials).

**Availability:** Commercially available for uses with TCC and TCW.

- References:**
- 1) Andreas Markström, Bo Sundman, and Karin Frisk (2005), "A revised thermodynamic description of the Co-W-C system", Research report IM-2003-143; Also accepted for publication in *Journal of Phase Equilibria and Diffusion*, 2005.
  - 2) Karin Frisk, Susanne Norgren, Jenni Zackrisson, Andreas Markström and Bo Jansson, (2005), "Phase equilibria in cemented carbides based on C-Co-W with Nb, Ta, Ti and V additions using thermodynamic calculations", to be published in: *Proc. 16th Int. Plansee Seminar* (edited by G. Kneringer et al., Reutte, 2005).
  - 3) Andreas Markström (2003), "Evaluation of molar volumes in cemented carbide systems", Internal report IM-2003-122, May 2003, Swedish Institute for Metals Research, Drottning Kristinas väg 48, 114 28 Stockholm, SWEDEN.

## 2 Thermo-Calc Database Description Forms

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- 4) Karin Frisk, Lucia Dumitrescu, Malin Ekroth, Bo Jansson, Olof Kruse, and Bo Sundman, (2001), "Development of a database for cemented carbides: Thermodynamic modelling and experiments", *Journal of Phase Equilibria*, 22(6), 645-655.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# SLAG1

## TCS Fe-Containing Slag Database (Version 1.2, 1992/1998/2006)

**Producers:** Thermo-Calc Software AB, Stockholm, Sweden  
IRSID (Institut de Recherches de la Siderurgie Francaise), France

**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** This database consists of data for the liquid slag and condensed oxides for the  $\text{Al}_2\text{O}_3$ -CaO-FeO- $\text{Fe}_2\text{O}_3$ -MgO-SiO<sub>2</sub> system. Data for Na, Cr, Ni, P and S were added, and it thus allows calculations of sulfide capacities of slags. The liquid slag is described with the cell model proposed by Kapoor-Frohberg and modified by Gaye. Composition variations in the solid oxides have not been considered.

The database also contains dilute solution parameters for about twenty elements in liquid iron compiled by Sigworth and Elliot and converted to regular solution parameters according to Hillert's suggestion.

Status of the TC Fe-containing Slag Database: The first release was in 1992 (SLAG1.0), and some modification was made in 1998 (SLAG1.1) and in 2006 (SLAG1.2). During 2002, the SLAG database was updated as SLAG2.0 (of Sept. 2002) to include four more elements (Ar, F, Mg and Na). In its latest updated version (SLAG2.2 of Jun. 2006), many thermodynamic parameters for the slag phase, Fe-rich liquid phase, and various solid phases have been improved and implemented, and a greatly enlarged phase description and thermodynamic properties for the gaseous mixture phase (within the framework of all covered 30 elements) has been included. For details see the *Thermo-Calc Database Description Form SLAG2*.

**Systems:** SLAG1.1 covers the following 26 elements (for Fe-containing slag systems):

<b>Ag</b>	<b>Al</b>	<b>B</b>	<b>C</b>	<b>Ca</b>	<b>Co</b>	<b>Cr</b>	<b>Cu</b>	<b>Fe</b>	<b>H</b>
<b>Mn</b>	<b>Mo</b>	<b>N</b>	<b>Nb</b>	<b>Ni</b>	<b>O</b>	<b>P</b>	<b>Pb</b>	<b>S</b>	<b>Si</b>
<b>Sn</b>	<b>Ti</b>	<b>U</b>	<b>V</b>	<b>W</b>	<b>Zr</b>				

Data are evaluated for diluted Fe-containing slag and the recommended limit of any minority component is only 0.1wt% but the user should carefully check each case. The database is suitable for activity and phase equilibrium calculations in metallurgical slag systems containing iron.

**Applications:** Alloy design and engineering; Metallurgy.

**Availability:** Commercially available for uses with TCC and TCW. *It can be upgraded to the latest version of the SLAG database (i.e., SLAG2) upon a certain database upgrade fee.*

**References:** IRSID (1984 & 1997) Thermodynamic data for slag in the Al-Ca-Cr-Fe-Mg-Mn-Na-Si-O-S-P-F system.  
Hillert M. (1986) *Met. Trans. A*, **17A**, 1878-1879.  
Gaye H., and J Welfringer J. (1984) *In: Fine H.A., and Gaskell D.R. (Eds) 2nd International Symposium on Metallurgical Slags and Fluxes*, Warrendale, PA, *Met Soc. of AIME*, 357.  
Sigworth G.K., and Elliot J.F. (1974) *Metal Science*, **8**, 298.

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# SLAG2

## TCS Fe-Containing Slag Database

(Version 2.2, 2002/2003/2006)

**Producers:** Thermo-Calc Software AB, Stockholm, Sweden  
IRSID (Institut de Recherches de la Siderurgie Francaise), France

**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** This updated SLAG2 Slag Database contains a liquid slag phase, as well as an Fe-rich liquid phase (dilute solution), a pure FeO liquid phase, a large gaseous mixture phase, and many stoichiometric solids and solid solution phases (*e.g.*, oxides, silicates, sulfides, phosphates, halites, *etc.*).

Thermodynamic data for the liquid slag phase and oxide/silicate solid phases within the  $\text{Al}_2\text{O}_3\text{-CaO-CrO-Cr}_2\text{O}_3\text{-FeO-Fe}_2\text{O}_3\text{-MgO-MnO-Na}_2\text{O-SiO}_2$  system were critically assessed by IRSID (1984), using the Kapoor-Frohberg-Gaye Quasichemical Cell Model, *i.e.*, the Kapoor-Frohberg Slag Model with the extensions introduced by Gaye and Welfringer (1984) for complex multicomponent slag solution systems.

Data for the additional components S, P and F (as sulfide, phosphate and fluoride species in the Al-Ca-Cr-Fe-Mg-Mn-Na-Si-O-S-P-F system) in the slag phase and solid phases, which were critically assessed by IRSID (1997), have been added to the database, and it thus allows calculations of sulfide capacities of slag. Composition-dependent parameters in the solid solution phases have not been considered in this particular database.

Data for a dilute solution of many elements in the Fe-rich liquid phase are critically assessed and converted to regular/subregular solution parameters according to Hillert (1986), with modified dilute solution parameters (plus a quadratic term) in liquid iron from Sigworth and Elliot (1974), so that it becomes a consistent thermodynamic model and also generally improves the agreements of calculated results with available experimental data.

**Status of the TC Fe-containing Slag Database:** The first release was in 1992 (SLAG1.0), and some modification was made in 1998 (SLAG1.1). During 2002, the SLAG database was updated as SLAG2.0 (of Sept. 2002) to include four more elements (Ar, F, Mg and Na). In its latest updated versions (SLAG2.1 of Aug. 2003, and SLAG2.2 of May 2006), many thermodynamic parameters for the slag phase, Fe-rich liquid phase, and various solid phases have been improved and implemented, and a greatly enlarged phase description and thermodynamic properties for the gaseous mixture phase (within the framework of all the covered 30 elements) has been included.

**Systems:** SLAG2.1 totally covers the following 30 elements:

<b>Ag</b>	<b>Al</b>	<b>Ar</b>	<b>B</b>	<b>C</b>	<b>Ca</b>	<b>Co</b>	<b>Cr</b>	<b>Cu</b>	<b>F</b>
<b>Fe</b>	<b>H</b>	<b>Mg</b>	<b>Mn</b>	<b>Mo</b>	<b>N</b>	<b>Na</b>	<b>Nb</b>	<b>Ni</b>	<b>O</b>
<b>P</b>	<b>Pb</b>	<b>S</b>	<b>Si</b>	<b>Sn</b>	<b>Ti</b>	<b>U</b>	<b>V</b>	<b>W</b>	<b>Zr</b>

The slag phase (containing oxide/silicate/sulfide/phosphate/fluoride species), as well as various oxide, silicate, sulfide, phosphate and fluoride solids phases, cover 12 elements (Al-Ca-Cr-Fe-Mg-Mn-Na-Si-O-S-P-F).

The Fe-Liquid solution phase includes 26 dilute components (Ag-Al-B-C-Ca-Co-Cr-Cu-H-Mg-Mn-Mo-N-Nb-Ni-O-P-Pb-S-Si-Sn-Ti-U-V-W-Zr). The recommended composition limit of any minority component, in the 27-component diluted Fe-rich liquid, is only 0.1wt%. In some cases, data could be used at much higher concentrations in the Fe-rich liquid phase, but the user must carefully check each of such cases. The database is suitable for activity and phase equilibrium calculations in metallurgical slag systems containing iron.

The gaseous mixture phase and many solid phases (stoichiometric or solution), as in the entire 30-element framework, are included.

For steels and various alloys, as well as other substance or solution phases, which are in interactions with the Fe-rich liquid phase or the liquid slag phase, thermodynamic data can be appended from other available databases, such as TCFE, TCNI, SSUB, SSOL, TCMP, TCES, TTAI/Mg/Ni/Ti, SALT, TCAQ, AQS, GCE, NUMT, NUOX, *etc.*

**Applications:** Alloy design and engineering; Metallurgy.

**Availability:** Commercially available for uses with TCC and TCW.

**References:** IRSID (1984 & 1997) Thermodynamic data for slag in the Al-Ca-Cr-Fe-Mg-Mn-Na-Si-O-S-P-F system.

Hillert M. (1986) *Met. Trans. A*, **17A**, 1878-1879.

Gaye H., and J Welfringer J. (1984) *In: Fine H.A., and Gaskell D.R. (Eds) 2nd International Symposium on Metallurgical Slags and Fluxes*, Warrendale, PA, *Met Soc. of AIME*, 357.

Sigworth G.K., and Elliot J.F. (1974) *Metal Science*, **8**, 298.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# ION1 and PION

## TCS Ionic Solutions Databases

(Version 1.5, 1992/1994/2001/2002/2004/2006)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The ION1 Ionic Solutions Database contains critically-assessed data for many oxides and silicates, as well as some carbides, nitrides, sulfides and arsenides in the 14-element system **Al-Bi-Ca-Cr-Cu-Fe-Mg-Ni-Si-O-C-N-S-As**, for various applications in R&D of ceramics, superconductors, metal/alloy processing, hard materials, materials corrosion, fusion processes, *etc.*

The primary thermodynamic models applied for various solution phases are: Ionic Two-Sublattice Model (Hillert *et al.*, 1985) for the ionic liquid solution phase; Compound-Energy Model with several sublattices and neutral or ionic constituents (*i.e.*, the general Sublattice Model; Hillert *et al.*, 1988) for metallic liquid mixture and solid solution phases; the Ideal Gas Model (for PVT EOS and mixing behavior) for the large gaseous mixture phase.

The data for specific subsystems are systematically assessed by including all possible elements in various ionic and neutral forms in their respective ionic liquid, metallic liquid, alloy solutions, or solid phases (metal/oxide/silicate/carbide/nitride/sulfide/arsenide/...). The Ionic Two-Sublattice Model is utilized for the ionic liquid phase over the whole composition range. Data for solubility in the metallic liquid mixture and various solid phases have also been taken into account.

Status of the TCS Ionic Solutions Database: The first release was in 1992 (ION1.0), and some modifications were made in 1994 (ION1.1), in 2001 (ION1.2), in 2002 (ION1.3), in 2004 (ION1.4) and further in 2006 (ION1.5). During 2002, the ION database was updated as ION2.0 (of Nov. 2002) to include three more elements (Ag-La-Sr). In its latest updated version (ION2.0 of 2002, ION2.1 of 2004, ION2.2 of 2005, ION2.3 of 2006), many thermodynamic parameters for ionic liquid, metallic liquid, alloy solutions, and various oxide/silicate/carbide/nitride/sulfide/arsenide phases (stoichiometric solids & solid solutions) have been improved and implemented, and a greatly enlarged gaseous mixture phase (within the framework of all the covered 17 elements) has been included. Dr. Bengt Hallstedt at Functional Ceramic Group of ETH, Switzerland, has contributed to the inclusions of critically-assessed data for the Ag-Bi-Sr-Ca-Cu-O and La-Sr-O subsystems. For details see the *Thermo-Calc Database Description Form ION2*.

**Systems:** The ION1.2 database currently contains:

- ◆ Binary Me-O systems: Al-O, Bi-O, Ca-O, Cr-O, Cu-O, Fe-O, Mg-O, Ni-O, Si-O
- ◆ Higher-order oxide containing systems (where all the lower-order subsystems have been evaluated): Al<sub>2</sub>O<sub>3</sub>-CaO-MgO, Al<sub>2</sub>O<sub>3</sub>-CaO-SiO<sub>2</sub>, CaO-MgO-SiO<sub>2</sub>, Al-Ca-Mg-Si-O, CaO-Fe-O-SiO<sub>2</sub>, Bi-Cu-O, Ca-Cu-O, Cr-Ni-O (provisional), Si-Al-O-N
- ◆ Binary Me-S systems: Fe-S, Cu-S
- ◆ Binary Me-As systems: Cu-As, Fe-As
- ◆ C/N-bearing systems: Al-Fe-N, Si-Al-O-N, Fe-Si-C-N (provisional)

For the ionic liquid phase (IONIC-LIQ), the edge metal systems have been included.

For the metallic liquid mixture and solid phases, the ION1 database is compatible with the SSOL, SSUB, TCFE and TCNI database. More solid phases can be obtained by appending the SSOL, SSUB, TCFE, TCNI and/or other appropriate databases.

The TC Public Ionic Oxide Solutions Database, PION (version 1.0, 1998), is a subset of the ION database but only with published data on the Ca-Si-O system. This small database is specially designed to demonstrate the use of ION database.

**Applications:** Ceramics, superconductors, metal/alloy processing, hard materials, materials corrosion, fusion processes

**Availability:** ION1 -- Commercially available for uses with TCC and TCW. *It can be upgraded to the latest version of the ION database (i.e., ION2) upon a certain database upgrade fee.*  
PION -- Freely distributed with TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U.

**References:** Hillert M., Jansson B., and Sundman B. (1988) *Z. Metallkde*, **79**, 81-87.  
Hillert M., Jansson B., Sundman B., and Ågren J. (1985) *Metall. Trans. A*, **16A**, 261-266.

### Thermo-Calc Database Description Form

# ION2 and PION

## TCS Ionic Solutions Databases

(Version 2.3, 2002/2004/2005/2006)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The ION2 Ionic Solutions Database contains critically-assessed data for many oxides and silicates, as well as some carbides, nitrides, sulfides and arsenides in the 17-element system **Al-Ag-Bi-Ca-Cr-Cu-Fe-La-Mg-Ni-Si-Sr-O-C-N-S-As**, for various applications in R&D of ceramics, superconductors, metal/alloy processing, hard materials, materials corrosion, fusion processes, *etc.*

The primary thermodynamic models applied for various solution phases are: Ionic Two-Sublattice Model (Hillert *et al.*, 1985) for the ionic liquid solution phase; Compound-Energy Model with several sublattices and neutral or ionic constituents (*i.e.*, the general Sublattice Model; Hillert *et al.*, 1988) for metallic liquid mixture and solid solution phases; the Ideal Gas Model (for PVT EOS and mixing behavior) for the large gaseous mixture phase.

The data for specific subsystems are systematically assessed by including all possible elements in various ionic and neutral forms in their respective ionic liquid, metallic liquid, alloy solutions, or solid phases (metal/oxide/silicate/carbide/nitride/sulfide/arsenide/...). The Ionic Two-Sublattice Model is utilized for the ionic liquid phase over the whole composition range. Data for solubility in the metallic liquid mixture and various solid phases have also been taken into account.

**Status of the TCS Ionic Solutions Database:** The first release was in 1992 (ION1.0), and some modifications were made in November, 1994 (ION1.1) and further in November, 2001 (ION1.2). During 2002, the ION database was updated as ION2.0 (of Nov. 2002) to include three more elements (Ag-La-Sr). In its latest updated version (ION2.0 of 2002, ION2.1 of 2004, ION2.2 of 2005, ION2.3 of 2006), many thermodynamic parameters for ionic liquid, metallic liquid, alloy solutions, and various oxide/silicate/carbide/nitride/sulfide/arsenide phases (stoichiometric solids & solid solutions) have been improved and implemented, and a greatly enlarged gaseous mixture phase (within the framework of all the covered 17 elements) has been included. Dr. Bengt Hallstedt at Functional Ceramic Group of ETH, Switzerland, has contributed to the inclusions of critically-assessed data for the Ag-Bi-Sr-Ca-Cu-O and La-Sr-O subsystems.

**Systems:** The ION2.0 database currently contains:

- ◆ Pure metallic systems:  
All possibly assessed binary, ternary and higher-order subsystems in the Al-Ag-Bi-Ca-Cr-Cu-Fe-La-Mg-Ni-Si-Sr system are included in the metallic liquid and alloy solution phases.
- ◆ Binary Me-O/C/N systems:  
Ag-O, Al-O, Bi-O, Ca-O, Cr-O, Cu-O, Fe-O, La-O, Mg-O, Ni-O, Si-O, Sr-O,  
Fe-C, Si-C, Al-N, Fe-N, Si-N
- ◆ Higher-order O/C/N-bearing systems (where all lower-order subsystems have been evaluated):  
Al<sub>2</sub>O<sub>3</sub>-CaO-MgO, Al<sub>2</sub>O<sub>3</sub>-CaO-SiO<sub>2</sub>, CaO-MgO-SiO<sub>2</sub>, Al-Ca-Mg-Si-O, CaO-Fe-O-SiO<sub>2</sub>,  
Si-Al-O-N, Al-Fe-N, Fe-Si-C-N (provisional), Cr-Ni-O (provisional),  
Ag-Bi-O, Ag-Cu-O, Bi-Ca-O, Bi-Cu-O, Bi-Sr-O, Ca-Cu-O, Ca-Sr-O, Cu-Sr-O,  
Ag-Ca-Cu-O, Ag-Cu-Sr-O, Bi-Ca-Cu-O, Bi-Ca-Sr-O, Bi-Cu-Sr-O, Ca-Cu-Sr-O,  
Bi-Ca-Cu-Sr-O, Ag-Bi-Ca-Cu-Sr-O
- ◆ Binary Me-S systems: Fe-S, Cu-S
- ◆ Binary Me-As systems: Cu-As, Fe-As

For the ionic liquid phase (IONIC-LIQ), the edge metal systems have been included.

For the metallic liquid mixture and solid phases, the ION2 database is compatible with the SSOL, SSUB, TCFE and TCNI database. More solid phases can be obtained by appending the SSOL, SSUB, TCFE, TCNI and/or other appropriate databases.

The TC Public Ionic Oxide Solutions Database, PION (version 1.0, 1998), is a subset of the ION database but only with published data on the Ca-Si-O system. This small database is specially designed to demonstrate the use of ION database.

**Applications:** Ceramics, superconductors, metal/alloy processing, hard materials, materials corrosion, fusion processes

**Availability:** ION2 -- Commercially available for uses with TCC and TCW.

PION -- Freely distributed with TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U.

**References:** Hillert M., Jansson B., and Sundman B. (1988) *Z. Metallkde*, **79**, 81-87.

Hillert M., Jansson B., Sundman B., and Ågren J. (1985) *Metall. Trans. A*, **16A**, 261-266.

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# STBC1

## SGTE Thermal Barrier Coating Database

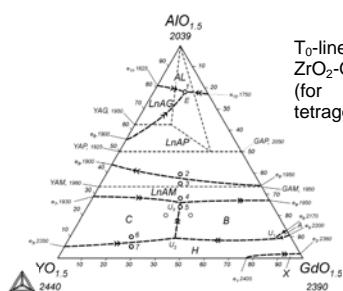
(Version 1.0, 2005)

**Producer:** MPI-MF, PML Stuttgart, Germany

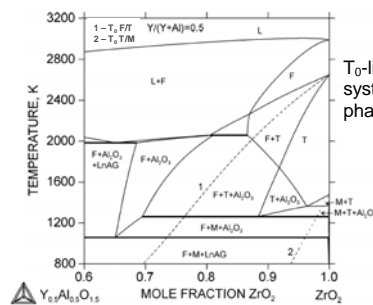
**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden.

**Description:** This database has been developed by MPI-MF, PML Stuttgart, Germany and been recently approved/released by SGTE as a so-called "SGTE application database". It contains critically-assessed thermodynamic data for the  $\text{Al}_2\text{O}_3$ - $\text{Gd}_2\text{O}_3$ - $\text{Y}_2\text{O}_3$ - $\text{ZrO}_2$  system, based on various experimental information such as phase equilibria (available from 1100 to 1300°C), as well as calorimetric measurements and vapour pressure determinations (over a wider temperature-composition range). It can be applied in many different fields of technology [for instance, yttria-stabilised-zirconia (YSZ), solid electrolyte (fluorite), thermal barrier coating (TBC using tetragonal oxides), and so forth], and most importantly the use of this database can further enhance such technologies.

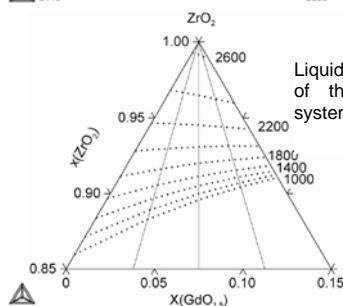
Beside phase equilibrium and phase diagram calculations, the Thermo-Calc (TCC/TCW) software also enables some specific calculations using this database, such as  $T_0$ -lines for diffusionless transformations (*e.g.*, fluorite  $\leftrightarrow$  tetragonal  $\text{M}_2\text{O}_3\text{A}$ , tetragonal  $\text{M}_2\text{O}_3\text{A} \leftrightarrow$  monoclinic  $\text{M}_2\text{O}_3\text{B}$ ), driving forces for partitioning of non-equilibrium phase to equilibrium assemblage, and so on.



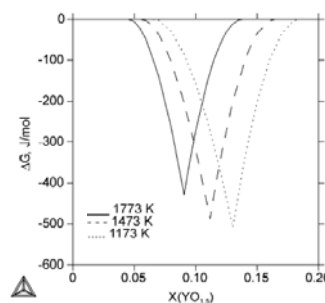
$T_0$ -lines projection of the  $\text{ZrO}_2$ - $\text{GdO}_{1.5}$ - $\text{YO}_{1.5}$  system  $\leftrightarrow$  (for fluorite tetragonal  $\text{M}_2\text{O}_3\text{A}$ ).



$T_0$ -lines in the  $\text{ZrO}_2$ - $\text{YO}_{1.5}$ - $\text{AlO}_{1.5}$  system, imposed on calculated phase diagram.



Liquidus surface projection of the  $\text{GdO}_{1.5}$ - $\text{YO}_{1.5}$ - $\text{AlO}_{1.5}$  system.



Driving forces for partitioning of F and T metastable phase to the F+T equilibrium assemblage in the  $\text{ZrO}_2$ - $\text{YO}_{1.5}$  system. F stands for fluorite, and T for tetragonal  $\text{M}_2\text{O}_3\text{A}$ .

Note that it is not appropriate to use this database to calculate phase equilibria in metallic or metal-oxygen system and in those involving a gas phase.

**Status of the SGTE Thermal Barrier Coating Database:** The current version, STBC1, is the first version commercially released as a standard Thermo-Calc database. Work is currently in progress to include more elements and phases for a future update.

**Systems:** STBC1 covers the following 5 elements:

**Al Gd Y Zr O**

The current version STBC1 covers many complex solution phases, *e.g.*, fluorite  $\text{ZrO}_2$ , tetragonal  $\text{ZrO}_2$ , monoclinic  $\text{ZrO}_2$ , cubic  $\text{M}_2\text{O}_3\text{C}$ , cubic  $\text{M}_2\text{O}_3\text{X}$ , monoclinic  $\text{M}_2\text{O}_3\text{B}$ , hexagonal  $\text{M}_2\text{O}_3\text{A}$ , hexagonal  $\text{M}_2\text{O}_3\text{H}$ ,  $\delta$ - $\text{Zr}_3\text{Y}_4\text{O}_{12}$ , pyrochlore  $\text{Gd}_2\text{Zr}_2\text{O}_7$ , monoclinic LnAM, perovskite LnAP, garnet LnAG, corundum, and liquid. It utilizes the Two-Sublattice Ionic Liquid Model for the liquid mixture phase, and the Compound-Energy Formalism (CEF) with ionic constrains for various solid solution phases.

**Applications:** Cemented carbides (hard materials).

**Availability:** Commercially available for uses with TCC and TCW.

**References:**

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# SALT1

## SGTE Molten Salts Database

(Version 1.2, 1993/2004/2005)

*Producer:* SGTE, Scientific Group Thermodata Europe

*Contact persons:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* The SALT Molten Salts Database originates from FACT, Montreal Canada, and has been modified by Alan Dinsdale at NPL, and adopted by SGTE in May 1993 (SGTE, 1996). The molten salt phase is described using the Two-Sublattice Ionic Model (Hillert *et al.*, 1985).

*Status of the SGTE Molten Salts Database:* This is the first version of the SALT database which was formally released in Jul. 1993 (SALT1.0), with minor modifications made in 2004 (SALT1.1) and 2005 (SALT1.2).

*Systems:* It contains data for many binary and some ternary molten salts within the **Cs-Li-K-Na-Rb-F-Cl-Br-I-SO<sub>4</sub>-CO<sub>3</sub>-CrO<sub>4</sub>-OH** system.

The database contains the following assessed systems:

KBr-KCl, KBr-KF, KBr-KI, KCl-KF, KCl-KI, KF-KI, CsBr-CsCl, CsBr-CsF, CsBr-CsI, CsCl-CsF, CsCl-CsI, CsF-CsI, LiBr-LiCl, LiBr-LiF, LiBr-LiI, LiCl-LiF, LiCl-LiI, LiF-LiI, NaBr-NaCl, NaBr-NaF, NaBr-NaI, NaCl-NaF, NaCl-NaI, NaF-NaI, RbBr-RbCl, RbBr-RbF, RbBr-RbI, RbCl-RbF, RbCl-RbI, RbF-RbI, CsBr-KBr, CsBr-LiBr, CsBr-NaBr, CsBr-RbBr, KBr-LiBr, KBr-NaBr, KBr-RbBr, LiBr-NaBr, LiBr-RbBr, NaBr-RbBr, CsCl-KCl, CsCl-LiCl, CsCl-NaCl, CsCl-RbCl, KCl-LiCl, KCl-NaCl, KCl-RbCl, LiCl-NaCl, LiCl-RbCl, NaCl-RbCl, CsF-KF, CsF-LiF, CsF-NaF, CsF-RbF, KF-LiF, KF-NaF, KF-RbF, LiF-NaF, LiF-RbF, NaF-RbF, CsI-KI, CsI-LiI, CsI-NaI, CsI-RbI, KI-LiI, KI-NaI, KI-RbI, LiI-NaI, LiI-RbI, NaI-RbI, K<sub>2</sub>CO<sub>3</sub>-LiCO<sub>3</sub>, K<sub>2</sub>CO<sub>3</sub>-Na<sub>2</sub>CO<sub>3</sub>, Li<sub>2</sub>CO<sub>3</sub>-Na<sub>2</sub>CO<sub>3</sub>, NaCl-Na<sub>2</sub>SO<sub>4</sub>, KCl-K<sub>2</sub>SO<sub>4</sub>, CaCl<sub>2</sub>-KCl, KCl-ZnCl<sub>2</sub>, CaCl<sub>2</sub>-ZnCl<sub>2</sub>, Na<sub>2</sub>CrO<sub>4</sub>-NaOH, NaCl-NaOH, NaCl-Na<sub>2</sub>CrO<sub>4</sub>, Na<sub>2</sub>CrO<sub>4</sub>-Na<sub>2</sub>SO<sub>4</sub>, NaOH-Na<sub>2</sub>SO<sub>4</sub>

*Applications:* High energy lamp design; Hot salt corrosion of alloys.

*Availability:* Commercially available for uses with TCC and TCW.

*References:* Hillert M., Jansson B., Sundman B., and Ågren J. (1985) *Metall. Trans. A*, **16A**, 261-266.

# 2 Thermo-Calc Database Description Forms

## Thermo-Calc Database Description Form

### TTNi7

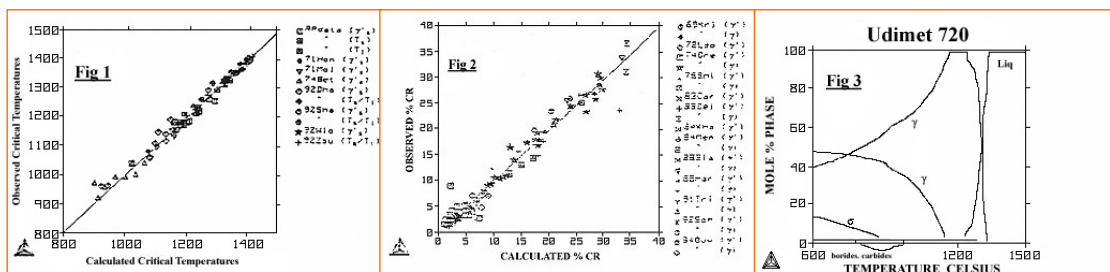
### TT Ni-based Superalloys Database (Version 7.0, Jan. 2006)

**Producer:** ThermoTech Ltd., Surrey Technology Center, Guildford, UK

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

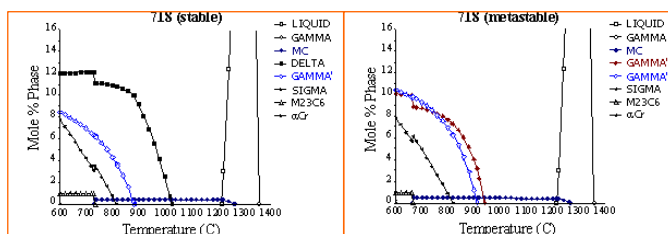
**Description:** This database has been developed by ThermoTech for commercial Ni-based superalloys, high Fe-containing Ni-based superalloys, single crystal Ni-based superalloys, and so on. Using the SCHEIL module in the TCC and TCW software, it is also possible to make solidification simulations that provide predictions for non-equilibrium micro-segregation, like  $f_s$  vs T plots and heat evolution. For more complex modeling, the calculations provide critical information that can otherwise only be found by expensive experimental techniques.

During validation process of the TTNi database, extensive comparison has been made between the simulated results and available experimental data for superalloys (Figures 1 and 2). The database performs at an accuracy close to the level expected of the experiments themselves. The database can be used for predictions of all types of equilibria, such as  $\gamma/\gamma'$ ,  $\gamma'$  solvus, solidus/liquidus relations (Figure 3 for U720 alloy as an example).



The TTNi database is specially created to meet the requirements of dealing with high Fe-containing Ni-based superalloys such as 706 and 718. NiFe-based superalloys can behave in a more complex fashion than predominantly Ni-based alloys. For example, the hardening mechanism often involves  $\gamma''$ , the metastable form of Ni<sub>3</sub>Nb. The TTNiFe database has proved capable of handling these very complex alloys providing excellent answers for both stable and metastable equilibrium. Furthermore, it has been used with excellent success in solidification modelling of such alloys. It also provides an accelerated route by which certain elements that are important to such alloys can be pursued. Further additions such as Si, P and S will be added. The figures on the right side show a phase% plot for a 718 alloy showing the stable behaviour where Ni<sub>3</sub>Nb is formed and its behaviour under more usual hardening conditions where sluggish kinetics cause  $\gamma''$  to form in preference to Ni<sub>3</sub>Nb. In these circumstances the alloy is hardened by a duplex precipitation of  $\gamma'$  and  $\gamma''$ .

From TTNi6 to TTNi7, extensive new work done on Si containing alloys to improve modelling of higher Si containing alloys. Also new modelling work undertaken for the Pt<sub>2</sub>Mo type ordered phase in NiCrMo based superalloys, which forms at low temperatures. Extensive new work on oxides based around the Ni-Al-Cr-Fe-Si-Ti-O system. Gamma' solvus temperatures improved for recently developed High Refractory Element Ni-based superalloys.



**Systems:** The database (Version 7.0) contains the following 22 elements (from TTNi6 to TTNi7, Ca-V-O are added):

Ni Al Co Cr Cu Fe Hf Mn Mo Nb  
Re Ru Si Ta Ti V W Zr B C N O

The TTNi database is currently designed as the following two individual database versions:

Name	Description	Elements
TTNi7	V7, complete, 22 elements	Ni-Al-Co-Cr-Cu-Fe-Hf-Mn-Mo-Nb-Re-Ru-Si-Ta-Ti-V-W-Zr-B-C-N-O
TTNF5	V5, NiFe-based, 14 elements	Ni-Fe-Al-Co-Cr-Mn-Mo-Nb-Si-Ti-Zr-B-C-N

Note that they are originally called as Ni-DATA and NiFe-Super, respectively.

The phases covered by the TTNi6 version are: Liquid,  $\gamma$ ,  $\gamma'$ ,  $\gamma''$ ,  $\eta$ ,  $\sigma$ ,  $\mu$ ,  $\alpha$ -(Cr,Mo,W), NiAl, Ni<sub>3</sub>Nb, Ni<sub>3</sub>Mo,  $\delta$ -NiMo, Laves\_C14, Laves\_C15, P\_phase, R\_phase, M(C,N), M<sub>23</sub>(B,C)<sub>6</sub>, M<sub>6</sub>C, M<sub>7</sub>(B,C)<sub>3</sub>, M<sub>2</sub>N, M<sub>3</sub>B, M<sub>3</sub>B<sub>2</sub>\_tetragonal, MB<sub>2</sub>\_tetragonal, MB<sub>2</sub>\_orthorhombic, MB\_orthorhombic, Cr<sub>2</sub>B<sub>3</sub>, TiB<sub>2</sub>, Ni<sub>3</sub>Si(h), Ni<sub>3</sub>Si<sub>2</sub>, Cr<sub>3</sub>Ni<sub>2</sub>Si<sub>3</sub>, B2\_BCC, A4B\_D1, Cub\_A15. From TTNi6 to TTNi7, added new phases are: Silicon rich G\_phase, Z and Pi nitrides, SiO<sub>2</sub>, MO\_B2, M3O4, M2O3, M2SiO4, Mullite, Spinel.

The phases covered by the TTNF5 version are: Liquid,  $\gamma$ ,  $\gamma'$ ,  $\gamma''$ ,  $\eta$ ,  $\sigma$ ,  $\mu$ ,  $\alpha$ -(Cr,Mo,W), NiAl, Ni<sub>3</sub>Nb, Ni<sub>3</sub>Mo,  $\delta$ -NiMo, Laves, P\_phase, M(C,N), M<sub>23</sub>(B,C)<sub>6</sub>, M<sub>6</sub>C, M<sub>7</sub>(B,C)<sub>3</sub>, M<sub>2</sub>N, M<sub>3</sub>B<sub>2</sub>\_tetragonal, TiB<sub>2</sub>, Ni<sub>3</sub>Si(h), Ni<sub>3</sub>Si<sub>2</sub>, Cub\_A15

**Applications:** Ni-based superalloy design and engineering.

**Availability:** Commercially available for uses with TCC and TCW.

**References:** Saunders N. and Miodownik A.P. (1998) CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide. Cambridge.



## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

## TTA16

### TT Al-based Alloys Database (Version 6.1, Jun. 2007)

**Producer:** ThermoTech Ltd., Surrey Technology Center, Guildford, UK

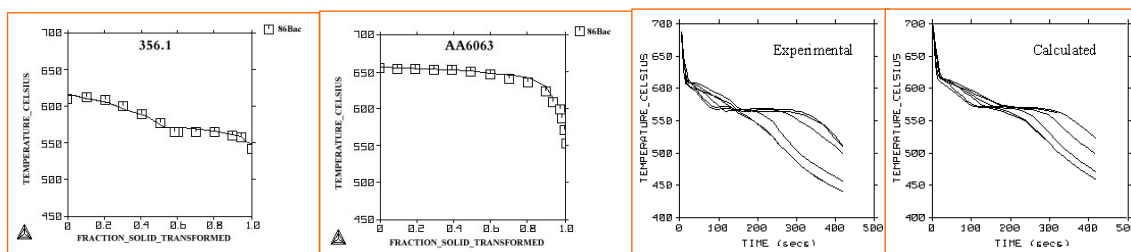
**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** This database has been developed by ThermoTech, and presents a comprehensive database for Al-alloys with a proven track record. It can be used for all major types of commercial Al-alloys ranging from commercial pure Al to complex alloys such as AA339.1, AA7075. *Note that it is originally called as Al-DATA.*

The database successfully predicts precipitation hardening reactions and provides excellent results for solution phase treatment temperatures and the formation of the “insoluble” compounds formed as part of the solidification process.

One of the striking successes of the database concerns prediction of the non-equilibrium solidification behavior of Al-alloys. Excellent agreements between the calculated results ( $f_s$  vs T) and experimental data from for instance Backerud *et al.* (1986) can be obtained using the SCHEIL module in the TCC and TCW software. The simulation also allows properties like heat evolution and the segregation patterns to be successfully predicted.

The phases predicted to form during the solidification process are well matched (as illustrated below). It is clear that the database provides very accurate predictions for the solidification behavior of Al-alloys in conditions that are well away from those associated with equilibrium. This provides a stringent test of the capabilities of the TTA1 database that it passes remarkably well.



From TTA13/TTA14 to TTA15, work has been done to take into model the various structural forms of Al<sub>3</sub>M compounds, DO22, DO23 and L12 that form with combinations Sc, Ti, V and Zr. From TTA15 to TTA16, three more elements (Co-Pb-Sn) have been added.

**Systems:** The database (Version 6.0) contains the following 22 elements:

Al B C Ca Co Cr Cu Fe H La  
Mg Mn Ni Pb Sc Si Sn Sr Ti V Zn Zr

The phases that are included in the database are list below:

Liquid, Al(fcc), Si, Graphite, SiC, (Al,Ti)B<sub>2</sub>, Al<sub>4</sub>C<sub>3</sub>, Al<sub>7</sub>Cr, Al<sub>2</sub>Cu, Al<sub>2</sub>CuMg, Al<sub>3</sub>(Fe,Mn,Ni,...), Al<sub>3</sub>Mg<sub>2</sub>, Al<sub>6</sub>(Mn,Fe,Cu,...), Al<sub>3</sub>Ni, Al<sub>3</sub>(Ni,Cu)<sub>2</sub>, Al<sub>4</sub>Sr, Al<sub>2</sub>Si<sub>2</sub>Sr, Al<sub>3</sub>(Ti,V,Zr,...), Mg<sub>2</sub>Si, Mg<sub>2</sub>Zn, MC\_carbide, Al<sub>18</sub>(Cr,Mn)<sub>2</sub>Mg<sub>3</sub>, Al<sub>13</sub>Cr<sub>4</sub>Si<sub>4</sub>, Al<sub>7</sub>Cu<sub>2</sub>Fe, Al<sub>20</sub>Cu<sub>2</sub>Mn<sub>3</sub>, Al<sub>7</sub>Cu<sub>4</sub>Ni, Al<sub>9</sub>(Fe,Ni)<sub>2</sub>,  $\alpha$ -AlFeSi,  $\beta$ -AlFeSi,  $\alpha$ -Al(Fe,Mn,Cu,Cr,...)<sub>2</sub>Si, Al<sub>2</sub>Mg<sub>3</sub>Zn<sub>3</sub>, Al<sub>4</sub>SiC<sub>4</sub>, Al<sub>8</sub>SiC<sub>7</sub>, Al<sub>5</sub>Cu<sub>2</sub>Mg<sub>8</sub>Si<sub>6</sub>, Al<sub>8</sub>FeMg<sub>3</sub>Si<sub>6</sub>, Laves, Al<sub>2</sub>CuMg, Al<sub>5</sub>(Fe,Mn,...), Mg(AlCuZn)<sub>2</sub>, E\_AlCrMgMn, T\_AlCuMgZn, TiC. From TTA14 to TTA15, added new REE phases are: Al<sub>11</sub>RE<sub>3</sub>, Al<sub>3</sub>RE\_DO19.

The Al-Cu-Mg-Zn quaternary has been reassessed based on its early version, so that it is fully compatible with the TTMg database.

**Applications:** Al-based alloy design and engineering.

**Availability:** Commercially available for uses with TCC and TCW.

**References:** Backerud L., Krol E., and Tamminen J. (1986) Solidification Characteristics of Aluminium Alloys, Vols 1 and 2. Tangen Trykk A/S, Oslo.  
Saunders N. and Miodownik A.P. (1998) CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide. Cambridge.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# TTMg4

## TT Mg-based Alloys Database

(Version 4.0, Jun. 2007)

**Producer:** ThermoTech Ltd., Surrey Technology Center, Guildford ,UK

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** This database has been developed by ThermoTech for uses with commercial Mg-based alloys. It is a sister database to TTAl and helps provides new insight into phase equilibria behaviour in complex Mg-alloys. Like TTAl it is well suited for use in the modelling of non-equilibrium solidification processes. *Note that it is originally called as Mg-DATA.*

As part of a validation process of the database, extensive comparison has been made between the simulated results and available experimental data for Mg-alloys. The database performs at accuracy close to the level expected of the experiments.

The Liquid and HCP-A3 phases are modeled as substitutional mixing phases, with the HCP-A3 phase corresponding to the Mg-rich solid solution. The other phases are often stoichiometric with respect to at least one element, although a number of other elements may mix in the phase. The nomenclature surrounding the various intermetallic phases can differ depending on which reference text is used as a basis.

The database can be used for predictions of all types of equilibria,  $\gamma/\gamma'$ ,  $\gamma'$  solvus, solidus/liquidus relations *etc.* Using the SCHEIL module in the TCC and TCW software, it is also possible to make solidification simulations which provide predictions for non-equilibrium micro-segregation,  $f_s$  vs T plots, heat evolution *etc.* For more complex modeling, the calculations provide critical information which can otherwise only be found by the use of expensive experimental techniques.

**Systems:** The database (Version 3.0) contains the following 16 elements (from TTMg2 to TTMg3, Ca-Sr-Nd-Y are added):

<b>Mg</b>	<b>Al</b>	<b>Ca</b>	<b>Ce</b>	<b>Cu</b>	<b>Ce</b>	<b>Fe</b>	<b>La</b>	<b>Mn</b>	<b>Nd</b>
<b>Si</b>	<b>Sn</b>	<b>Sr</b>	<b>Zn</b>	<b>Zr</b>	<b>Y</b>				

The important phases that are included in the database are list below:

**Liquid, Mg, Mg<sub>17</sub>Al<sub>12</sub>, Mg<sub>2</sub>Cu, MgCu<sub>2</sub>, MgZn<sub>2</sub>, Mg<sub>12</sub>RE, Mg<sub>2</sub>Si, MgZn, Mg<sub>2</sub>Zn<sub>3</sub>, Al<sub>4</sub>Mn, Al<sub>11</sub>Mn<sub>4</sub>, Al<sub>8</sub>Mn<sub>5</sub>, Al<sub>11</sub>RE<sub>3</sub>, Al<sub>3</sub>RE, Al<sub>2</sub>RE, Al<sub>2</sub>Zr,  $\Phi$ -AlMgZn, Q-Al<sub>7</sub>Cu<sub>3</sub>Mg<sub>6</sub>, T-AlCuMgZn,  $\alpha$ -Mn,  $\beta$ -Mn,  $\alpha$ -Zr**

**Applications:** Mg-based alloy design and engineering.

**Availability:** Commercially available for uses with TCC and TCW.

**References:** Saunders N. and Miodownik A.P. (1998) *CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide*. Cambridge.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# TTZr1

## TT Zr-based Alloys Database

(Version 1.0, Jan. 2006)

*Producer:* ThermoTech Ltd., Surrey Technology Center, Guildford ,UK

*Contact person:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* This database has been developed by ThermoTech for uses with commercial Zr-based alloys. Like other TT databases, it is well suited for use in the modelling of non-equilibrium solidification processes.

*Systems:* The database (Version 1.0) contains the following 12 elements:

**Zr Cr Fe Hf Nb Ni Si Sn C O**  
**N H**

*Applications:* Zr-based alloy design and engineering.

*Availability:* Commercially available for uses with TCC and TCW.

*References:* Saunders N. and Miodownik A.P. (1998) *CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide*. Cambridge.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## TCMP2

### TCS Materials Processing Database

(Version 2.5, 2002/2003/2004/2005/2008)

**Producers:** Thermo-Calc Software AB, Stockholm, Sweden  
Philip Spencer, The Spencer Group, Trumansburg, NY, USA.

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCMP2 database (its previous version was TCER) was developed for applications to materials processing, to process metallurgy, and to chemical and waste-treatment processes (particularly materials recycling and remelting, as well as sintering, incineration and combustion). For instance, in scrap remelting operations in an electric arc furnace, the resulting gradual concentration increases of minority elements in the metal that is of particular importance. Apart from a knowledge of the possible losses of these elements to the gas phase, and/or their transfer to the slag phase, information on the solubilities of minority elements in liquid and solid Fe-rich alloys is needed. This is because their presence can have deleterious effects on the properties of the produced steels/alloys.

The database allows calculations of, for example,

- ◆ composition of the gas phase, including concentrations of toxic species, resulting from the arc remelting process. Examples of potentially hazardous species are Cd, Zn, Pb, S, P, *etc.*, as well as CO, nitrogen oxides and Cl- and F-containing species.
- ◆ distribution of minority elements between the iron melt and an SiO<sub>2</sub>-CaO-Al<sub>2</sub>O<sub>3</sub>-FeO-MgO-based slag of variable composition.
- ◆ concentrations of undesirable solute elements in liquid and solid Fe-rich alloys as a function of alloy composition and temperature.

The calculations take into account all phases simultaneously, so that the distribution of a particular element between gas, slag and metal under defined process conditions is obtained in a single calculation. The optimum conditions for avoiding transformation of hazardous species to the environment can be quickly investigated.

Status of the TCS Materials Processing Database: The first version (called TCER, with 30 elements) was released in May 2000. In this gradually-updated version (TCMP2.0 of Aug. 2002, TCMP2.1 of Aug. 2003, TCMP2.2 of Apr. 2004, TCMP2.3 of Aug. 2004, TCMP2.4 of Aug. 2005 and TCMP2.5 of Mar. 2008), 5 more elements (Ag-Nb-U-V-W) are covered, many thermodynamic parameters for the liquid slag phase, metallic liquid phase, and various pure solid and solid solution phases have been improved and implemented, and a greatly enlarged phase description and thermodynamic properties for the gaseous mixture phase (within the framework of all the covered 35 elements) has been included.

**Systems:** This database currently contains the following 35 elements:

<b>Ag</b>	<b>Al</b>	<b>Ar</b>	<b>B</b>	<b>Bi</b>	<b>C</b>	<b>Ca</b>	<b>Cd</b>	<b>Cl</b>	<b>Co</b>
<b>Cr</b>	<b>Cu</b>	<b>F</b>	<b>Fe</b>	<b>H</b>	<b>K</b>	<b>Mg</b>	<b>Mn</b>	<b>Mo</b>	<b>N</b>
<b>Na</b>	<b>Nb</b>	<b>Ni</b>	<b>O</b>	<b>P</b>	<b>Pb</b>	<b>S</b>	<b>Sb</b>	<b>Si</b>	<b>Sn</b>
<b>Ti</b>	<b>U</b>	<b>V</b>	<b>W</b>	<b>Zn</b>					

Many types of multicomponent stoichiometric and non-ideal solution phases are available in the database, such as: melt (metallic/non-metallic liquid mixture); slag (oxide/silicate/sulfide/phosphate/fluoride... liquid mixture); gas (gaseous mixture); metallic/non-metallic solid solutions (*e.g.*, FCC, BCC, HCP, DIAMOND, BCT, TETRAGONAL, RHOMBOHEDRAL, CHI, CEMENTITE, M23C6, M3C2, M6C, M7C3, KSI\_CARBIDE, MONI\_DELTA, TI3M, M3SI, M5SI, LAVES, MU and SIGMA, and other carbides, nitrides, silicides, phosphides and borides); and many stoichiometric solids and solid solutions (*e.g.*, metals, oxides, hydroxides, silicates, sulfides, sulfates, nitrates, nitrites, phosphates, phosphites, carbonates, borates, halides, and other inter-metallic/non-metallic compounds).

Such phases are default treated by some appropriate thermodynamic models (*e.g.*, the Sublattice Model for solid solutions and liquid mixture phases, the Kapoor-Frohberg-Gaye Cell Model for slag phase, the Ideal Gas Model for gas mixture phase, the Inden Model for magnetic contributions, *etc.*), which are applicable over a wide temperature-pressure-composition range.

**Applications:** Materials processing and environmental controls in steel/alloy production and metallurgical engineering, Environment-friendly recycling/remelting/reprocessing treatments of industrial, chemical and nuclear wastes, as well as sintering, incineration and combustion processes.

**Availability:** Commercially available for uses with TCC and TCW.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# TCES1

## TCS Sintering/Incineration/Combustion Database

(Version 1.1, 2000/2003)

**Producers:** Thermo-Calc Software AB, Stockholm, Sweden  
Philip Spencer, The Spencer Group, Trumansburg, NY, USA.

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCES database was developed for simulations of environmental problems associated with metallurgical, chemical and waste-treatment processes (especially sintering, incineration and combustion processes). For instance, iron ore sintering is carried out prior to reduction processes and results in considerable, including toxic, emissions, which require comprehensive filtering operations to avoid transfer of hazardous species to the environment. In the sintering process, the ore is mixed with coke and sintered at temperatures up to 1200°C.

The present database allows calculations of, for example,

- ◆ the effect of variation of ore compositions, sintering temperature, water cooling of the sinter strand at different location, etc., on the concentrations of gaseous species produced along the strand.
- ◆ the condensed species formed from the gas phase on cooling and their formation temperatures.

The information provided by the calculations allows process parameters to be adjusted to minimize or eliminate emission of hazardous species and to select suitable filtering operations to maximize removal of both desirable and undesirable species condensing from the gas phase formed during the sintering process.

The database also allows calculations that regard the composition of gas phase forming during incineration and combustion processes, and their respective amounts and temperatures of condensation of species formed on cooling the gas.

Status of the TCS Sintering/Incineration/Combustion Database: The first version was released in May 2000, with some minor modifications made in Sept. 2003 (as to TCES1.1).

**Systems:** This database currently contains the following 30 elements:

<b>Al</b>	<b>As</b>	<b>Br</b>	<b>C</b>	<b>Ca</b>	<b>Cd</b>	<b>Cl</b>	<b>Cr</b>	<b>Cu</b>	<b>F</b>
<b>Fe</b>	<b>H</b>	<b>Hg</b>	<b>I</b>	<b>K</b>	<b>Mg</b>	<b>Mn</b>	<b>N</b>	<b>Na</b>	<b>Ni</b>
<b>O</b>	<b>P</b>	<b>Pb</b>	<b>S</b>	<b>Sb</b>	<b>Si</b>	<b>Sn</b>	<b>Te</b>	<b>Ti</b>	<b>Zn</b>

Many types of multicomponent stoichiometric and a solution phases are available in the database, such as: gas (gaseous mixture) and many stoichiometric solids (*e.g.*, metals; carbides, nitrides, silicides, phosphides, borides and other inter-metallic/non-metallic compounds; oxides, hydroxides, silicates, sulfides, sulfates, nitrates, nitrites, phosphates, phosphites, carbonates, borates, halides, *etc.*).

The gaseous mixture phases is default treated by the Ideal Gas Model.

Note that for multicomponent systems involving non-ideal solid solution phases, the TCER database (primarily for recycling and remelting processes, but also for sintering, incineration and combustion processes) should be used instead.

**Applications:** Environmental controls in steel and alloy production and metallurgical engineering, Environment-friendly treatments of industrial waste and nuclear waste.

**Availability:** Commercially available for uses with TCC and TCW.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## PG35

### ISC Group III-V Binary Semiconductors Database (Version 1.2, 1994/2003/2008)

*Producer:* An Informal Scientific Collaboration

*Contact person:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* The PG35 database contains all the 15 possible binary subsystems among the group III elements Al, Ga and In and the group V elements P, As and Sb. The database is a subset of the SEMC Semiconductors Database, and is compatible with PURE (the SGTE Pure Elements Database), SSUB (the SGTE Substances Database) and SSOL (the SGTE Solutions Database).

A liquid mixture phase containing all six elements and with possible binary interactions (in the liquid phase) is assessed. A gas phase with 40 gaseous species in the group III-V element system is included. Many stoichiometric solid and solid solution phases are also available.

*It was previously called as G35*, and it is a subset of the SEMC Semiconductors Database (for details see the *Thermo-Calc Database Description Form SEMC2*).

Please note that as a public database PG35 is designed only for demonstration and teaching purposes, and should not be used for any R&D activities whatsoever, due to its limitations of included elements, phases and data.

*Status of the ISC Public G35 Binary Semiconductors Database:* This is the first version of the PG35 database which was formally released in Nov. 1994 (G35), with some minor modifications made in May 2003 (PG35\_1.1), and in June 2008 (PG35\_1.2).

*Systems:* 15 binary alloys within the following system (6 elements):  
**Al-As-Ga-In-P-Sb.**

*Applications:* Semi-conductor design.

*Availability:* Freely distributed with all versions of Thermo-Calc (TCC, TCW, TC4A and TC4U).

*References:* Ansara I., Chatillon C., Lukas H.L., Nishizawa T., Ohtani H., Ishida K., Hillert M., Sundman B., Argent B.B., Watson A., Chart T. G., and Anderson T. (1994) A Binary Database for III-V Compound Semiconductor Systems, *Calphad*, **18**, 177-222.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## SEMC2

### TC Semiconductors Database

(Version 2.1, 2002/2003)

**Producer:** Department of Materials Science and Engineering, China University of Science and Technology, Beijing, China

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** This database contains all 15 possible binary subsystems, and 18 ternary subsystems, among the group III elements Al, Ga and In and the group V elements P, As and Sb. The binary subsystems are identical to the G35 database (Ansara *et al.*, 1994). The 18 ternary subsystems in the Al-As-Ga-In-P-Sb system were assessed by Li *et al.* (1999) and Ishida *et al.* (1998).

The gas phase has been extended on the basis of the G35 database, to include more species containing Al-As-Ga-In-P-Sb-(Pb-Sn-C-H) which were assessed by Tirtowidijoyo (1986), Jordan (1993), and SGTE (1992).

A liquid mixture phase, containing all six G35 elements (Al-As-Ga-In-P-Sb) and possible binary interactions, are assessed. Many stoichiometric solid and solid solution phases are also available.

It is compatible with PURE4 (the SGTE Pure Elements Database), SSUB3 (the SGTE Substances Database) and SSOL2 (the SGTE Solutions Database).

Status of the TC Semiconductors Database: The first version of the SMEC database was compiled in Dec. 2000 (SMEC1.0). During 2002-2003, the SMEC database was updated as to SMEC2.0 (of Nov. 2002) and SMEC2.1 (of Jun. 2003).

**Systems:** The whole database includes 10 elements as given below:

**Al-As-Ga-In-P-Sb-(Pb-Sn-C-H).**

#### Data Sources:

All 15 binary subsystems in Al-As-Ga-In-P-Sb: Ansara *et al.*, (1994)

18 ternary subsystems in Al-As-Ga-In-P-Sb:

5 from Ishida (1998):	Al-Ga-P	Al-In-P	Al-P-As	Al-P-Sb	Al-As-Sb
13 from Li <i>et al.</i> (1999):	Al-Ga-As	Al-Ga-Sb	Al-In-As	Al-In-Sb	Ga-In-P
	Ga-In-As	Ga-In-Sb	Ga-As-Sb	In-As-Sb	Ga-As-P
	In-As-P	Ga-Sb-P	In-Sb-P		

135 gas species in Al-As-Ga-In-P-Pb-Sb-Sn-C-H:

40 from Ansara <i>et al.</i> (1994):	in Al-As-Ga-In-P-Sb
59 from Tirtowidijoyo (1986) & Jordan (1993):	in Al-As-Ga-In-P-Sb-(Pb-Sn-C-H)
36 from the SGTE SSUB database:	in C-H-B-P-Al-As

**Applications:** Semi-conductors design and engineering,  
Electronic components processing and utility.

**Availability:** Commercially available for uses with TCC and TCW.

**References:** Ansara I., Chatillon C., Lukas H.L., Nishizawa T., Ohtani H., Ishida K., Hillert M., Sundman B., Argent B.B., Watson A., Chart T. G., and Anderson T. (1994) A Binary Database for III-V Compound Semiconductor Systems, *Calphad*, **18**, 177-222.  
Ishida K. (1998) *unpublished results*.  
Jordan A.S. (1993) *J. Crystal Growth*, **128**, 488-493.  
Li Jingbo, Li Chongrong, and Zhang Weijing (1999) *unpublished results*.  
Tirtowidijoyo M. (1986) *J. Crystal Growth*, **77**, 200-209.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## PAQ2

### TC Public Aqueous Database (SIT Model) for POUBAIX Module

(Version 2.4, 2002/2003/2006/2008)

**Producer:** Thermo-Calc Software, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The PAQ2 database is specifically designed for demonstrating the calculations of so-called Pourbaix diagrams through either the POURBAIX module or TDB-GES-POLY-POST routine in the TCC software, which calculate the pH-Eh relations and many properties for a heterogeneous interaction system with a certain bulk composition under a given temperature and pressure. Within such a specially designed database, there is an AQUEOUS solution phase, a GAS mixture phase (normally treated as an ideal phase, extracted from the SSUB Substances Database), and some stoichiometric solids and solid solution phases. The database is compatible with PURE, SSUB, SSOL, TCFE, SLAG, ION, TCNI, TCMP, TCES, TTNi/Ti/Al/Mg, and GCE databases.

The AQUEOUS solution part in the database is a very-much simplified subset adopted from the TCAQ2 Aqueous Solution Database, which has been extended and modified, based on evaluations available in literature, and at present contains about 350 aqueous solution species. The AQUEOUS solution phase in the TCAQ2/PAQ2 databases is described using the Extended SIT Model (Specific Interaction Theory). *Please note that as a public database PAQ2 is designed only for demonstration and teaching purposes, and should not be used for any R&D activities whatsoever, due to its limitations of included elements, phases and data.*

The POURBAIX module in TCC software can be used for heterogeneous interaction systems involving aqueous solution phase that is modelled by either the Extended SIT Model (Specific Interaction Theory; Ciavatta, 1990), the Complete Revised HKF Model (Helgeson *et al.*, 1981; Shi *et al.*, 1992), or the Generalized Pitzer Formalism (Pitzer, 1991). A user can choose any of the three available models (together with associated aqueous solution databases) for the Pourbaix-diagram calculations.

*Status of the TC Public Aqueous Solution Database (SIT Model) for POURBAIX Module:* The first version (called AQ) was released in 1997 and distributed with TCC and TCW, as well as with TC4A and TC4U for some time. This updated version PAQ2 (PAQ2.1 of 2002, PAQ2.1 of 2003, PAQ2.2 of 2006, and PAQ2.4 of 2008) has some modifications, and as a freely distributed database, is replacing both of those previous versions (AQ and PAQ) in the TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U installations, for testing and demonstration of easy calculations of so-called Pourbaix diagrams in heterogeneous interaction systems involving aqueous solution phase (modelled by the Extended SIT Model).

**Systems:** These databases includes the following 11 elements:

**H O C N S Cl Na Fe Co Ni Cr**

**Applications:** Materials corrosion processes; Hydro-metallurgy; Aqueous chemistry; Geochemistry; Environmental chemistry.

**Availability:** Freely distributed with TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U.

**References:** Ciavatta L. (1990) The specific interaction theory in equilibrium analysis. Some empirical rules for estimating interaction coefficients of metal ion complexes. *Ann Chim. (Rome)*, **80**, 255-263.  
Helgeson H.C., Kirkham D.H., and Flowers G.C. (1981) Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures. IV. Calculation of activity coefficients, osmotic coefficients, and apparent molal and standard and relative partial molal properties to 600°C and 5 kb. *American Sciences*, **281**, 1249-1516.  
Pitzer K.S. (1991) Ion interaction approach: theory and data correlation. In: Pitzer K.S. (Ed.) *Activity Coefficients in Electrolyte Solutions*. 2nd Edition, CRC Press, pp. 75-153.  
Shi Pingfang, Saxena S.K., and Eriksson G. (1992) Thermodynamic models, methods and databases used in studying geochemical processes of hydrothermal systems. Uppsala University.

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Shi Pingfang and Saxena S.K. (1995) The TGG aqueous solution database (AQS) and its applications.  
Uppsala University.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## TCAQ2

### TCS Aqueous Solution Database (Version 2.5, 2002/2003/2004/2006/2008)

**Producer:** Thermo-Calc Software AB, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The TCAQ2 database was developed for calculating thermodynamic properties of aqueous solutions. It can be applied to conditions of temperatures up to 350°C, room pressure, and aqueous concentrations up to 3 molality. The database contains an AQUEOUS solution phase which consists of various free cations and anions, inorganic and organic complexes. The hypothetical phase, REFERENCE\_ELECTRODE, is introduced to calculate the electric potential (based on the standard hydrogen electrode) and other properties of the electron in the interaction system. Connected with this database, the non-ideality of the EOS and thermodynamic properties of H<sub>2</sub>O is calculated, using an empirical expression of the simplified HGK model (Haar, Gallagher and Kell, 1984). The non-ideality of the AQUEOUS solution phase in this database is described using the Extended SIT Model (Specific Interaction Theory; Ciavatta, 1990), *i.e.*, taking into account of the Debye-Hückel Limiting Law term, as well the binary, ternary and higher-order interaction terms.

This database is compatible with PURE, SSUB, SSOL, TCFE, SLAG, ION, TCNI, TCMP, TCES, TTNi/Ti/Al/Mg, and GCE databases. Some phases from other appropriate databases, such as gaseous mixtures and stoichiometric solids from SSUB, and solid solutions from SSOL or TCFE, should be appended to make heterogeneous equilibrium calculations in complex systems involving aqueous solutions.

The TCAQ2 database can be used in the POURBAIX module in the TCC software, if the multiple database option is chosen with appended gas and solid phases from other available databases (*e.g.*, SSUB and SSOL). Another aqueous solution database, AQS2 (developed by TGG Group; Shi and Saxena, 1995), is recommended for calculations of complex heterogeneous interactions under high temperature, pressure and concentration conditions. The AQS2 database is connected with the complete Revised HKF model implemented in the TCC and TCW software.

Status of the TCS Aqueous Solution Database: The TCAQ database was originally developed by the Thermo-Calc Group in 1996 (Shi and Sundman, 1996), and the first version was formally released in Feb. 1999. Since then it has been extended and modified by Thermo-Calc Software, based on evaluations available in literature. In Apr. 1999, more aqueous species of Cu-Co-Ni-Zn-W, obtained through the CAMPADA Project and other assessment work, were added. Further modifications were made during 2002 (TCAQ2.0), 2003 (TCAQ2.1), 2004 (TCAQ2.2) and 2006 (TCAQ2.3). At present it contains about 350 aqueous solution species. More aqueous species (mainly complex species) will be gradually added into the database in future.

**Systems:** This complete aqueous database covers all elements in always the same framework as in SSUB and SSOL. Below is a list of all 76 elements available in the TCAQ2 aqueous solution database:

Ag Al Ar As Au B Ba Be Br C Ca Cd Ce Cl Co Cr Cs Cu Dy Er  
Eu F Fe Ga Gd H He Hg Ho I In K Kr La Li Lu Mg Mn Mo N  
Na Nd Ne Ni O Os P Pb Pd Pr Pt Ra Rb Re Ru S Sb Sc Se Si  
Sm Sn Sr Tb Te Th Tl Tm U V W Xe Y Yb Zn Zr

The PAQ2 databases (which covers C-Cl-Co-Cr-Fe-H-N-Na-Ni-O-S and contains some related pure solid, solid solution and gas species), freely distributed together with TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U, is adopted from TCAQ2 and specifically designed for uses with the POURBAIX module in the TCC software.

**Applications:** Materials corrosion processes; Hydro-metallurgy; Aqueous chemistry; Geochemistry; Environmental chemistry.

**Availability:** Commercially available for uses with TCC and TCW.

**References:** Ciavatta L. (1990) The specific interaction theory in equilibrium analysis. Some empirical rules for estimating interaction coefficients of metal ion complexes. *Ann Chim. (Rome)*, **80**, 255-263.  
Haar L., Gallagher J.S., and Kell G.S. (1984) *NBS/NRC Steam Tables. Thermodynamic and Transport Properties and Computer Programs for Vapor and Liquid States of Water in SI Units*. Hemisphere Publishing Corp., McGraw-Hill, New York, 318 p.

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### Thermo-Calc Database Description Form

## PAQS2

### TC Public Aqueous Database (HKF Model) for POUBAIX Module (Version 2.4, 2002/2005/2007/2008)

**Producer:** Thermo-Calc Software, Stockholm, Sweden

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The PAQS2 database is specifically designed for demonstrating the calculations of so-called Pourbaix diagrams through either the POURBAIX module or TDB-GES-POLY-POST routine in the TCC software, which calculate the pH-Eh relations and many properties for a heterogeneous interaction system with a certain bulk composition under a given temperature and pressure. Within such a specially designed database, there is an AQUEOUS solution phase, a GAS mixture phase (normally treated as an ideal phase, extracted from the SSUB Substances Database), and some stoichiometric solids and solid solution phases. The database is compatible with PURE, SSUB, SSOL, TCFE, SLAG, ION, TCNI, TCMP, TCES, TTNi/Ti/Al/Mg, and GCE databases.

The AQUEOUS solution part in the database is a very-much simplified subset adopted from the AQS2 Aqueous Solution Database, which has been extended and modified, based on evaluations available in literature, and at present contains about 1600 aqueous solution species. The AQUEOUS solution phase in the AQS2/PAQS2 database is described using the Complete Revised HKF Model (Helgeon-Kirkham-Flowers). *Please note that as a public database PAQS2 is designed only for demonstration and teaching purposes, and should not be used for any R&D activities whatsoever, due to its limitations of included elements, phases and data.*

The POURBAIX Module in TCC software can be used for heterogeneous interaction systems involving aqueous solution phase that is modelled by either the Extended SIT Model (Specific Interaction Theory; Ciavatta, 1990), the Complete Revised HKF Model (Helgeson *et al.*, 1981; Shi *et al.*, 1992), or the Generalized Pitzer Formalism (Pitzer, 1991). A user can choose any of the three available models (together with associated aqueous solution databases) for the Pourbaix-diagram calculations.

Status of the TC Public Aqueous Solution Database (HKF Model) for POURBAIX Module:  
This version (PAQS2) was released in 2008 and distributed with TCCS and TCW5, for testing and demonstration of easy calculations of so-called Pourbaix diagrams in heterogeneous interaction systems involving aqueous solution phase (modelled by the Complete Revised HKF Model).

**Systems:** These databases includes the following 11 elements:

**H O C N S Cl Na Fe Co Ni Cr**

**Applications:** Materials corrosion processes; Hydro-metallurgy; Aqueous chemistry; Geochemistry; Environmental chemistry.

**Availability:** Freely distributed with TCC, TCW, TCC-Demo/TC4A and TCW-Demo/TC4U.

**References:** Ciavatta L. (1990) The specific interaction theory in equilibrium analysis. Some empirical rules for estimating interaction coefficients of metal ion complexes. *Ann Chim. (Rome)*, **80**, 255-263.  
Helgeson H.C., Kirkham D.H., and Flowers G.C. (1981) Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures. IV. Calculation of activity coefficients, osmotic coefficients, and apparent molal and standard and relative partial molal properties to 600°C and 5 kb. *American Sciences*, **281**, 1249-1516.  
Pitzer K.S. (1991) Ion interaction approach: theory and data correlation. In: Pitzer K.S. (Ed.) *Activity Coefficients in Electrolyte Solutions*. 2nd Edition, CRC Press, pp. 75-153.  
Shi Pingfang, Saxena S.K., and Eriksson G. (1992) Thermodynamic models, methods and databases used in studying geochemical processes of hydrothermal systems. Uppsala University.  
Shi Pingfang and Saxena S.K. (1995) The TGG aqueous solution database (AQS) and its applications. Uppsala University.

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

## AQS2

### TGG Aqueous Solution Database (Version 2.5, 2000/2002/2003/2004/2006/2008)

- Producer:** TGG (Theoretical Geochemistry Group), Uppsala, Sweden and Florida, USA
- Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden
- Description:** This database is developed for calculating thermodynamic properties of aqueous solutions at conditions of temperatures up to 1000°C, pressures up to 5 kbar, and aqueous concentrations up to 6 molality (at room temperature and pressure) or higher (at high temperature and pressure). The database contains an AQUEOUS solution phase which consists of various free cations and anions, inorganic and organic complexes. The hypothetical phase, REFERENCE\_ELECTRODE, is introduced to calculate the electric potential (based on the standard hydrogen electrode) and other properties of the electron in the interaction system. Connected with this database, the non-ideality of the EOS, thermodynamic, electrostatic and transport properties of H<sub>2</sub>O is calculated using the comprehensive Johnson-Norton model (Johnson and Norton, 1991) that is implemented in the Thermo-Calc software. The non-ideality of the AQUEOUS solution phase in this database is described using the Complete Revised HKF (Helgeon-Kirkham-Flowers) Model (Helgeson *et al.*, 1981; Shock *et al.*, 1992; Shi *et al.*, 1992), *i.e.*, taking into account of the Debye-Hückel Limiting Law term, ionic solvation, ionic association, as well the binary, ternary and higher-order interaction terms.
- This database is compatible with PURE, SSUB, SSOL, TCFE, SLAG, ION, TCNI, TCMP, TCES, TTNi/Ti/Al/Mg, and GCE databases. Some phases from other appropriate databases, such as gaseous mixtures from the SSUB database (*i.e.*, ideal gaseous species and mixtures) or the SUPERFLUID model (*i.e.*, non-ideal EOS and mixing for the C-H-O-S-N-Ar fluids; Shi and Saxena, 1992), stoichiometric solids from the SSUB database, and solid solutions from the SSOL or TCFE database(s), should be appended to make heterogeneous equilibrium calculations in complex systems involving aqueous solutions.
- Status of the TGG Aqueous Solution Database:** The AQS database was originally developed by the Theoretical Geochemistry Group in 1995 (Shi and Saxena, 1995), and was converted and modified by Thermo-Calc Software in 1999. The current version AQS2 (AQS2.0 of 2000, AQS2.1 of 2002, AQS2.2 of 2003, AQS2.3 of 2004, AQS2.4 of 2006 and AQS2.5 of 2008) contains about 1600 aqueous solution species. More aqueous species (mainly complex species) will be gradually added into the database in future.
- Systems:** This complete aqueous database covers the following 83 elements:  
Ag Al Ar As Au B Ba Be Bi Br C Ca Cd Ce Cl Co Cr Cs Cu Dy  
Er Eu F Fe Fr Ga Gd H He Hf Hg Ho I In K Kr La Li Lu Mg  
Mn Mo N Na Nb Nd Ne Ni O P Pb Pd Pm Pr Pt Ra Rb Re Rh Rn  
Ru S Sb Sc Se Si Sm Sn Sr Tb Tc Th Ti Tl Tm U V W Xe Y  
Yb Zn Zr
- The AQS2 database can be used in the POURBAIX module in the TCC software, if the multiple database option is chosen with appended gas and solid phases from other available databases (*e.g.*, SSUB, SSOL, TCFE, TCNI, TCMP, TCES, TTNi/Ti/Al/Mg, and GCE).
- Applications:** Materials corrosion processes; Hydro-metallurgy; Aqueous chemistry; Geochemistry; Environmental chemistry.
- Availability:** Commercially available for uses with TCC and TCW.
- References:** Helgeson H.C., Kirkham D.H., and Flowers G.C. (1981) Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures. IV. Calculation of activity coefficients, osmotic coefficients, and apparent molal and standard and relative partial molal properties to 600°C and 5 kb. *American Sciences*, **281**, 1249- 1516.  
Shi Pingfang and Saxena S.K. (1992) Thermodynamic modeling of the C-H-O-S fluid system. *American Mineralogist*, **77**, 1038-1049.  
Shi Pingfang and Saxena S.K. (1995) The AQS Aqueous Solution Database and Its Applications. Uppsala University.  
Shi Pingfang, Saxena S.K., and Eriksson G. (1992) Thermodynamic models, methods and databases used in studying geochemical processes of hydrothermal systems. Uppsala University.  
Shock E.L., Oelkers E.H., Johnson J.W., Sverjensky D.A., and Helgeson H.C. (1992) Calculation of the thermodynamic properties of aqueous species at high pressures and temperatures. Effective electrostatic radii, dissociation constants and standard partial molal properties to 1000°C and 5 kbar. *J. Chem. Soc. Faraday Trans.*, **88**(6), 803-826.

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### Thermo-Calc Database Description Form

## PGEO

### Saxena Minerals Database (Version 1.2, 1993/2003/2007)

**Producer:** TGG (Theoretical Geochemistry Group), Uppsala, Sweden and Florida, USA

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** This The PGEO database contains assessed temperature and pressure dependent data for minerals (Saxena *et al.*, 1993), that covers 15 elements that are important for geochemical, geophysical and environmental systems. The Murnaghan model for pressure dependence is used. The applicable temperature range is from 298.15 K to about 6000 K and the pressure range from 1 bar to 200 kbar (20 GPa). The compounds are treated as stoichiometric (pure phases) and there are no data for liquids. Solid solution phases are not included in this particular database, but are available in GCE2 database. It is also compatible with the PURE, SSUB, ION, TCAQ/PAQ and AQS/PAQS databases, to some extends.

*Note the database was previously called as GEO, and it is a subset of the GCE2 TGG Geochemical/Environmental Database (for details see the Thermo-Calc Database Description Form GCE2), while the latter one is substantially extended to include 46 elements, to cover stoichiometric and solid solution phases, sub-/super-critical fluid mixture, and to imply the Birch-Murnaghan model (that can also be applied at pressures above 20 GPa).*

Please also note that as a public database PG35 is designed only for demonstration and teaching purposes, and should not be not for any R&D activities whatsoever, due to its limitations of included elements, phases and data.

Status of the Saxena Minerals Database: This is the first version of the PGEO database which was formally released in Oct. 1993 (GEO), with some minor modifications made in May 2003 (PGEO1.1) and in Oct 2007 (PGEO1.2).

**Systems:** 150 silicates and oxides, mainly rock-forming minerals within the following 15-element framework:

<b>Al</b>	<b>C</b>	<b>Ca</b>	<b>H</b>	<b>K</b>	<b>Fe</b>	<b>Mg</b>	<b>Mn</b>	<b>N</b>	<b>Na</b>
<b>Ni</b>	<b>S</b>	<b>Si</b>	<b>Ti</b>	<b>O</b>					

**Applications:** This database is useful for geochemical applications and for teaching thermodynamics.

**Availability:** Freely distributed with all versions of Thermo-Calc (TCC, TCW, TC4A and TC4U).

**References:** Saxena S.K., Chatterjee N., Fei Y.W., and Shen G.Y. (1993) *An Assessment of Thermodynamics of Oxides and Silicates*. Springer-Verlag, New York.  
Murnaghan F. D. (1944) *Proc. Natl. Acad. Sci.*, Vol 30, 244-247.

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

## GCE2

### TGG Geochemical/Environmental Database

(Version 2.3, 2002/2003/2004/2008)

**Producer:** TGG (Theoretical Geochemistry Group), Uppsala, Sweden and Florida, USA

**Contact person:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** This database contains critically-assessed temperature-, pressure- and composition-dependent data for minerals. The Birch-Murnaghan model for the pressure dependence is used. The applicable temperatures range from 298.15 K to about 6000 K and pressures range from 1 bar to 1000 kbar (100 GPa). The compounds are treated as either stoichiometric or solution phases, but there are no data for liquid phases.

Compared with its subset, the PGEO database (Saxena Minerals Database), extensions have been made in various directions:

<i>Extended Respect</i>	<i>PGEO Database</i>	<i>GCE2 Database</i>
Element number	15	46
Model for P-dependence	Murnaghan model	Birch-Murnaghan model, so that it can be applied to ultra-high pressure systems.
Phases	stoichiometric	stoichiometric and solution phases.
Minerals	silicates, oxides	silicates, oxides, hydroxides, halides, carbonates, sulfides, sulfates, nitrates, phosphates, <i>etc.</i> , so that it can also be applied to low temperature and pressure processes.
Interactions with gases/fluids	ideal gas	C-H-O-S-N-Ar sub-/super-critical fluid mixture (code in the SUPERFLUID program).
Interactions with aqueous solutions	simple aqueous	complex aqueous solutions, using the SIT, HKF or PITZ models, over a wide TPX ranges.
Interactions with melts	(no plan)	<i>It is planned to add a MELT phase to include various types of melt mixtures.</i>

This database is compatible with PURE, SSUB, SSOL, TCFE, SLAG, ION, TCNI, TCMP, TCES and AQS databases. For simulations of complex heterogeneous interactions among minerals, aqueous solutions and sub-/super-critical fluids over a wide temperature-pressure-composition range, the AQS database and the SUPERFLUID model (which is implemented into the Thermo-Calc GES system) can be appended.

The GCE database (previously called as GEOCHEM) was originally developed by the Theoretical Geochemistry Group in 1995 (Shi and Saxena, 1995), and was converted and further modified by Thermo-Calc Software in 2002 (as GCE2.0), 2003 (GCE2.1), 2004 (GCE2.2) and 2008 (GCE2.3). The current version GCE2.3 contains about 600 minerals which are stable at either low or high temperatures and pressures. More minerals are expected to add into the database.

**Systems:** The following 46 elements are the building blocks to silicates, oxides, hydroxides, halides, carbonates, sulfides, sulfates, nitrates, phosphates, and other rock-forming and environmentally-important minerals:

Ag Al Ar As Au B Ba Be Br C Ca Cd Cl Co Cr Cs Cu F Fe Ga  
Gd H Hg I K Li Mg Mn Mo N Na Ni O P Pb Rb S Se Si Sn  
Sr Ti U V W Zn

**Applications:** Geochemistry; Geophysics; Hydro-metallurgy; Aqueous chemistry; Environmental chemistry

**Availability:** Commercially available for uses with TCC and TCW.

**References:** Saxena S.K., Chatterjee N., Fei Y.W., and Shen G.Y. (1993) *An Assessment of Thermodynamics of Oxides and Silicates*. Springer-Verlag, New York.  
Murnaghan F. D. (1944) *Proc. Natl. Acad. Sci.*, Vol 30, 244-247.  
Shi Pingfang and Saxena S.K. (1995) *The GEOCHEM Geochemical/Environmental Database and Its Applications*. Uppsala University.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## NUMT2

### TCS/AEAT Pure Radionuclides Database

(Version 2.0, 1999)

- Producer:** AEA Technology plc., UK
- Owner:** Thermo-Calc Software, Stockholm, Sweden (Intellectual property was completely brought from previous owners AEAT-UES-ESI in May 2004).
- Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden  
Paul Mason, Thermo-Calc Software Inc., Pittsburgh, PA, USA
- Description:** The NUMT Pure Radionuclides Database was originally developed by UES Software (AEA Technology) as a supplement to be used in conjunction with the SSUB Substances Database. Version 1.0 of the database contained data for 546 substances, which were of relevance to calculations for nuclear applications. The current version (2.0, released September 1999) of the database has been both updated and expanded to now contain 596 condensed and gas phase substances. On the basis of the Version 1.0, data for 76 of the substances were amended, and data for 50 new substances were added.
- It includes a gas mixture phase. Hence, for vaporization calculations, the database can also be used in conjunction with any other database (such as NUOX) which requires the gas phase species. It is compatible with PURE (the SGTE Pure Elements Database), SSUB (the SGTE Substances Database), SSOL (the SGTE Solutions Database), and NUOX (the UES Nuclear Oxides Database).
- It should be stressed that this current database is still only intended as a supplement to other pure substance databases (such as SSUB) for applications in nuclear materials related systems. The reference state of the Gibbs Energy function is the enthalpy of the elements in their standard states at 298.15 K [*i.e.*, G-H(SER)].
- Systems:** The current version of the database contains pure radionuclides within the following 15-element framework:
- |           |           |           |          |           |           |           |           |           |           |
|-----------|-----------|-----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|
| <b>Ba</b> | <b>Ce</b> | <b>Cs</b> | <b>I</b> | <b>La</b> | <b>Mo</b> | <b>Pd</b> | <b>Pr</b> | <b>Pu</b> | <b>Rh</b> |
| <b>Ru</b> | <b>Sr</b> | <b>Te</b> | <b>U</b> | <b>Zr</b> |           |           |           |           |           |
- However, for other related pure substances (and gas mixture species), the following 44 elements are covered by the database:
- |           |           |           |           |           |           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| <b>Ag</b> | <b>Al</b> | <b>Am</b> | <b>B</b>  | <b>Ba</b> | <b>Bi</b> | <b>C</b>  | <b>Ca</b> | <b>Cd</b> | <b>Ce</b> |
| <b>Cl</b> | <b>Co</b> | <b>Cr</b> | <b>Cs</b> | <b>Eu</b> | <b>F</b>  | <b>Fe</b> | <b>H</b>  | <b>I</b>  | <b>In</b> |
| <b>Kr</b> | <b>La</b> | <b>Mg</b> | <b>Mn</b> | <b>Mo</b> | <b>Na</b> | <b>Nb</b> | <b>Nd</b> | <b>Ni</b> | <b>O</b>  |
| <b>Pd</b> | <b>Pr</b> | <b>Pu</b> | <b>Rh</b> | <b>Ru</b> | <b>Sb</b> | <b>Si</b> | <b>Sn</b> | <b>Sr</b> | <b>Tc</b> |
| <b>Te</b> | <b>U</b>  | <b>Xe</b> | <b>Zr</b> |           |           |           |           |           |           |
- It is planned to develop the NUMT database to a stand-alone compilation of critically-assessed data relevant to nuclear applications. This final version will be significantly larger since many other elements and substances will be considered. The future substances included in the database will be based on extensive analyses of thermodynamic calculations at typical nuclear related conditions.
- Applications:** This database can be applied to a wide range of nuclear related applications, which can be modeled adequately, or to a first approximation, using pure substances. However, It can also be coupled with other pure substance databases (*e.g.*, SSUB) or solution databases (*e.g.*, NUOX, SSOL, TCFE) to increase the range of applications which can be studied.
- Availability:** Commercially available for uses with TCC and TCW.
- References:** Ball R.G.J., Mason P.K., and Mignanelli, M.A. (1996) Application of phase equilibrium calculations to the analysis of severe accidents in nuclear reactors. In: SGTE (1996) *The SGTE Casebook: Thermodynamics at Work* (Ed. Hack K.). The Institute of Materials, London.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# NUOX4

## TCS/AEAT Nuclear Oxide Solutions Database

(Version 4.0, 1999)

- Producer:** AEA Technology plc., UK
- Owner:** Thermo-Calc Software, Stockholm, Sweden (Intellectual property was completely brought from previous owners AEAT-UES-ESI in May 2004).
- Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden  
Paul Mason, Thermo-Calc Software Inc., Pittsburgh, PA, USA
- Description:** This database was originally based on work performed by UES Software (AEA Technology), National Physical Laboratory (UK) and Thermodata (France) for the system  $\text{UO}_2\text{-ZrO}_2\text{-SiO}_2\text{-CaO-Al}_2\text{O}_3\text{-MgO-BaO-SrO-La}_2\text{O}_3$  (in versions 1&2). The database has been independently extended since then by AEA Technology to include  $\text{CeO}_2$  and  $\text{Ce}_2\text{O}_3$  (in versions 3&4).
- It contains data for a collection of assessed binary and ternary systems relevant to nuclear applications. The current version (version 4.0, released in September 1999), like the previous versions, does not include gas phase data. Hence, for vaporization calculations, the database must be used in conjunction with another database which includes the gas phase species such as NUMT or SSUB (the SGTE Substances Database). The next upgrade to NUOX will include appropriate, critically-assessed gas phase data enabling self-consistent calculations to be made from a single database.
- It is compatible with PURE (the SGTE Pure Elements Database), SSUB (the SGTE Substances Database), SSOL (the SGTE Solutions Database), and NUMT (the UES Pure Radionuclides Database).
- Systems:** The current database has a full description of the following system:  
 **$\text{UO}_{2+x}\text{-ZrO}_2\text{-SiO}_2\text{-CaO-Al}_2\text{O}_3\text{-MgO-BaO-SrO-La}_2\text{O}_3\text{-CeO}_2\text{-Ce}_2\text{O}_3$**   
where all the component binary interactions have been assessed. A description of the fuel hyperstoichiometry in the FCC\_FLUORITE phase ( $\text{UO}_{2+x}$ ) is included.  
A new major upgrade to the database, planned for release in 2001, will include the introduction of iron oxides.
- Applications:** The database has been developed primarily for studying molten core-concrete interactions. However, it can also be applied to any relevant system or application which comprises essentially the constituent oxides. It can also be coupled with pure substance databases (*e.g.*, NUMT, SSUB) or solution databases (*e.g.*, SSOL, TCFE) to increase the range of applications which can be studied.
- Availability:** Commercially available for uses with TCC and TCW.
- References:** Ball R.G.J., Mason P.K., and Mignanelli, M.A. (1996) Application of phase equilibrium calculations to the analysis of severe accidents in nuclear reactors. In: SGTE (1996) *The SGTE Casebook: Thermodynamics at Work* (Ed. Hack K.). The Institute of Materials, London.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

## SNUX6

### SGTE In-Vessel Nuclear Oxides Database

(Version 6.2, Apr. 2006)

- Producer:** ThermoData (INPG – CNRS), France & AEA-Technology plc., UK
- Owner:** SGTE (Scientific Group Thermodata Europe)
- Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden  
Paul Mason, Thermo-Calc Software Inc., Pittsburgh, PA, USA
- Description:** This database was originally based on work performed by UES Software (AEA Technology), National Physical Laboratory (UK) and Thermodata (France) for the system  $\text{UO}_2\text{-ZrO}_2\text{-SiO}_2\text{-CaO-Al}_2\text{O}_3\text{-MgO-BaO-SrO-La}_2\text{O}_3$  (in versions 1&2). The database has been independently extended since then by AEA Technology to include  $\text{CeO}_2$  and  $\text{Ce}_2\text{O}_3$  (in versions 3&4).
- It contains data for a collection of assessed binary and ternary systems relevant to nuclear applications. The current version (version 4.0, released in September 1999), like the previous versions, does not include gas phase data. Hence, for vaporization calculations, the database must be used in conjunction with another database which includes the gas phase species such as NUMT or SSUB (the SGTE Substances Database). The next upgrade to NUOX will include appropriate, critically-assessed gas phase data enabling self-consistent calculations to be made from a single database.
- It is compatible with PURE (the SGTE Pure Elements Database), SSUB (the SGTE Substances Database), SSOL (the SGTE Solutions Database), and NUMT (the UES Pure Radionuclides Database).
- Systems:** The current database has a full description of the following system:  
 **$\text{UO}_{2+x}\text{-ZrO}_2\text{-SiO}_2\text{-CaO-Al}_2\text{O}_3\text{-MgO-BaO-SrO-La}_2\text{O}_3\text{-CeO}_2\text{-Ce}_2\text{O}_3$**   
where all the component binary interactions have been assessed. A description of the fuel hyperstoichiometry in the FCC\_FLUORITE phase ( $\text{UO}_{2+x}$ ) is included.
- A new major upgrade to the database, planned for release in 2001, will include the introduction of iron oxides.
- Applications:** The database has been developed primarily for studying molten core-concrete interactions. However, it can also be applied to any relevant system or application which comprises essentially the constituent oxides. It can also be coupled with pure substance databases (*e.g.*, NUMT, SSUB) or solution databases (*e.g.*, SSOL, TCFE) to increase the range of applications which can be studied.
- Availability:** Commercially available for uses with TCC and TCW.
- References:** Ball R.G.J., Mason P.K., and Mignanelli, M.A. (1996) Application of phase equilibrium calculations to the analysis of severe accidents in nuclear reactors. In: SGTE (1996) *The SGTE Casebook: Thermodynamics at Work* (Ed. Hack K.). The Institute of Materials, London.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# NUTA

## TCS/AEAT Ag-Cd-In Ternary Alloy Solutions Database (Version 1.0, 1991)

- Producer:* AEA Technology plc., UK
- Owner:* Thermo-Calc Software, Stockholm, Sweden (Intellectual property was completely brought from previous owners AEAT-UES-ESI in May 2004).
- Contact persons:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden  
Paul Mason, Thermo-Calc Software Inc., Pittsburgh, PA, USA
- Description:* This database was originally developed by UES Software (AEA Technology) to model the Ag-Cd-In ternary alloy, which is an important control rod material in many nuclear reactors.
- Systems:* The current database (version 1.0) describes the **Ag-Cd-In** ternary system.
- Applications:* Calculations pertaining to control rods in nuclear reactors.
- Availability:* Commercially available for uses with TCC and TCW.
- References:* Horrocks P.J. (1991) *Phase Diagram and Thermodynamics of the Ag-Cd-In Ternary Alloy System*, PhD Thesis, University of Manchester.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# NUTO

## TCS/AEAT Si-U-Zr-O Metal-Metaloxide Solutions Database

(Version 1.0, 1996)

- Producer:* AEA Technology plc., UK
- Owner:* Thermo-Calc Software, Stockholm, Sweden (Intellectual property was completely brought from previous owners AEAT-UES-ESI in May 2004).
- Contact persons:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden  
Paul Mason, Thermo-Calc Software Inc., Pittsburgh, PA, USA
- Description:* This database was originally developed by UES Software (AEA Technology) to model the metal-metal/metal-oxide/oxide-oxide interactions for the U-Zr-Si-O system. The database is based on assessments for the binary constituent systems available in the open literature and also assessments made by UES Software (AEA Technology).
- Systems:* The current database (version 1.0) describes the **U-Zr-Si-O** system. Future work is planned to implement Fe into the database.
- Applications:* The database models the hyper- and hypo-stoichiometry of UO<sub>2</sub> in the presence of metallic zirconium and silicon. This database has applications for modeling in-vessel and ex-vessel fuel-clad interactions.
- Availability:* Commercially available for uses with TCC and TCW.
- References:* Ball R.G.J., Mason P.K., and Mignanelli, M.A. (1996) Application of phase equilibrium calculations to the analysis of severe accidents in nuclear reactors. *In: SGTE (1996) The SGTE Casebook: Thermodynamics at Work* (Ed. Hack K.). The Institute of Materials, London.

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# NOX2

## NPL Oxide Solutions Database (Version 2.0, 2002)

*Producer:* NPL (National Physical Laboratory), UK

*Contact persons:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* The NOX2 database contains critically-assessed and recently updated thermodynamic data for many multicomponent oxide/silicate solution phases in a wide range of temperature and composition. Thermodynamic data for the liquid oxide phase and oxide/silicate solid phases in the  $\text{Al}_2\text{O}_3$ -CaO-FeO- $\text{Fe}_2\text{O}_3$ -MgO-SiO<sub>2</sub> system were critically assessed by NPL, using the Associate Model for oxide liquid mixture phase, and the generalized CEF (Compound-Energy-Formulism) model that treats other phases (with both neutral and charged species). The database was converted to the Thermo-Calc database format in Dec. 2002, and was further modified in Apr. 2003. It can be used with the TCC and TCW software.

*Systems:* This database covers a chemical framework of 6 elements:

**Al Ca Fe Mg Si O**

The contained solution phases are of two types:

By CEF model with neutral species:

Liquid\_Oxide, Melilite, Cordierite,  
CaAF<sub>2</sub>O<sub>4</sub>\_CF, Ca<sub>2</sub>AF<sub>2</sub>O<sub>5</sub>\_C2F, Ca<sub>3</sub>AF<sub>2</sub>O<sub>6</sub>\_C3A, CaAF<sub>4</sub>O<sub>7</sub>\_CA2, Ca<sub>3</sub>AF<sub>6</sub>O<sub>12</sub>\_CA,  
CaAF<sub>6</sub>O<sub>10</sub>\_CAF2, CaAF<sub>12</sub>O<sub>19</sub>\_CA6, Ca<sub>12</sub>AF<sub>14</sub>O<sub>33</sub>\_C12A7 [where AF=(Al,Fe)]

By CEF model with charged (ionic) species:

Spinel, Olivine, Halite, Mullite, Corundum, Wollastonite, Plagioclase\_H,  
Clinopyroxene, Low-Clinopyroxene, Orthopyroxene, Protopyroxene,  
CM<sub>2</sub>SiO<sub>4</sub>\_C2S, CMF<sub>2</sub>SiO<sub>4</sub>\_C2S [where CM=(Ca,Mg) and CMF=(Ca,Mg,Fe)]

The contained stoichiometric phases are:

Fe\_Liquid, Fe\_FCC, Fe\_BCC, Fe\_HCP, Quartz, Cristobalite, Tridymite,  
Pseudo\_Wollastonite, Merwinite, Bredigite, Hatrurite, Rankinite,  
CaFe<sub>4</sub>O, CaFe<sub>3</sub>O<sub>5</sub>, CaFe<sub>2</sub>O<sub>7</sub>, Ca<sub>4</sub>Fe<sub>9</sub>O<sub>17</sub>, Ca<sub>4</sub>Fe<sub>17</sub>O<sub>29</sub>, Al<sub>2</sub>Fe<sub>2</sub>O<sub>6</sub>, Al<sub>4</sub>Ca<sub>3</sub>MgO<sub>10</sub>

For various applications in materials processing, the NOX2 database can be appended to multicomponent systems which are primarily defined using SSOL, SSUB, TCFE, TTAI, TTMg and/or other appropriate databases.

*Status of the NPL Oxide Solutions Database:* The first release was in 1999, and second in 2002, both in MTDATA. It was converted in the Thermo-Calc database format and slightly improved in 2002/2003, and was released as NOX2 in Apr. 2003.

*Applications:* Ceramics, metal/alloy processing, mineral processing, materials corrosion, etc.

*Availability:* Commercially available for uses with TCC and TCW.

*References:*

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

## NSLD2

### NPL Solder Solutions Database (Version 2.3, 2002/2004)

*Producer:* NPL (National Physical Laboratory), UK

*Contact persons:* Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

*Description:* This solder alloy solution database was developed for thermodynamic calculations of solder systems (Pb-containing/Pb-free), by NPL and SGTE. The database was converted to the Thermo-Calc database format in Dec. 2002, and was further modified in Apr. 2003. It can be used with the TCC and TCW software.

It is desirable, where practicable, to remove some lead-containing components from commercial products for critical environmental considerations. One area where lead is extensively used is in lead-based solders. New lead-free solders must have the appropriate melting temperatures and freezing ranges, in order to be compatible with the existing equipment and components. Ultimately, all the toxic elements (Pb,Cd,As,Sb,...) and environmentally problematic elements (Bi,...) should be eliminated from commercial solders.

This solder alloy solution database can be used to predict various thermodynamic properties, and to show the effects of non-equilibrium solidification. The results from these predictions can be used to eliminate candidate solder alloys for which the calculations reveal unsuitable freezing temperature and range from further testing.

*Status of the NPL Oxide Solutions Database:* The first major release was in 1999, and second in 2002, both in MTDATA. It was converted in the Thermo-Calc database format and further improved in 2002/2003/2004, and was released within the TCC/TCW software as NSLD2.1 in Apr. 2003 and NSLD2.3 in Jun. 2004. Further updated versions of this database are now under continuous developments at NPL and SGTE, for the inclusions of more alloying elements and more critically-assessed ternary and higher-order systems.

*Systems:* The current version of this database covers 12 elements:

**Ag Al Au Bi Cu Ge In Pb Sb Si Sn Zn**

Critically assessments and extrapolations have been conducted in the development of this database.

Available binary subsystems are:

	Ag	Al	Au	Bi	Cu	Ge	In	Pb	Sb	Si	Sn	Zn
Ag	-	x	x	x	x	x	x	x	x	x	x	x
Al		-	x	x	x	x	x	x	x	x	x	x
Au			-	x	x	x	x	x	x	x	x	x
Bi				-	x	x	x	x	x	x	x	x
Cu					-	x	x	x	x	x	x	x
Ge						-	x	x	x	x	x	x
In							-	x	x	x	x	x
Pb								-	x	x	x	x
Sb									-	x	x	x
Si										-	x	x
Sn											-	x
Zn												-

Available ternary subsystems are:

Ag-Au-Pb    Bi-In-Pb    Ag-Sb-Sn    Al-Cu-Zn    Al-In-Sb    Cu-Si-Zn

For many other ternary and higher-order subsystems, the analytical descriptions of lower-order constituent subsystems are combined and used to predict multicomponent systems, even for compositions and temperatures which have not been experimentally evaluated. Depending on the complexity of multicomponent systems, such an analytical prediction will be more or less accurate.

*Applications:* Thermodynamic calculations of solder systems (Pb-containing and Pb-free).

*Availability:* Commercially available for uses with TCC and TCW.

*References:*

## 2 Thermo-Calc Database Description Forms

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### Thermo-Calc Database Description Form

# USLD1

## NIST Solder Solutions Database

(Version 1.0, 1999)

- Producer:** NIST (National Institute of Standards and Technology), Gaithersburg, MD, USA
- Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden  
Ursula R. Kattner, NIST Materials Science and Engineering Laboratory, Gaithersburg, MD, USA
- Description:** This solder alloy solution database was developed for thermodynamic calculations of solder systems (Pb-containing/Pb-free), by NIST Materials Science and Engineering Laboratory.
- It is desirable, where practicable, to remove some lead-containing components from commercial products for critical environmental considerations. One area where lead is extensively used is in lead-based solders. New lead-free solders must have the appropriate melting temperatures and freezing ranges, in order to be compatible with the existing equipment and components. Ultimately, all the toxic elements (Pb, Cd, As, Sb, ...) and environmentally problematic elements (Bi, ...) should be eliminated from commercial solders.
- This solder alloy solution database can be used to predict various thermodynamic properties, and to show the effects of non-equilibrium solidification. The results from these predictions can be used to eliminate candidate solder alloys for which the calculations reveal unsuitable freezing temperature and range from further testing. Different types of calculated systems have been distinguished in the development of this solder alloy solution database:
- *Critically assessed systems:* A critical evaluation of available experimental data was used to derive a proper thermodynamic description of the multicomponent system. If such experimental data were only available or considered for part of the system, then a partial assessment is possible.
  - *Extrapolated systems:* The analytical descriptions of constituent subsystems are combined and used to predict the multicomponent system, even for compositions and temperatures which have not been experimentally evaluated. Depending on the complexity of the multicomponent system, such an analytical prediction will be more or less accurate.
- The database was originally compiled by Ursula R. Kattner at NIST, and its Thermo-Calc form was further edited and completed by Pingfang Shi at Thermo-Calc Software.
- Systems:** The current version of this solder solution database covers 6 elements: **Ag-Bi-Cu-Pb-Sb-Sn**.
- Critically assessed binary systems:
- |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|
| Ag-Bi | Ag-Cu | Ag-Pb | Ag-Sb | Ag-Sn | Bi-Cu | Bi-Pb | Bi-Sn |
| Cu-Pb | Cu-Sn | Pb-Sn | Sb-Sn |       |       |       |       |
- Critically assessed ternary systems:
- |          |          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|----------|
| Ag-Bi-Cu | Ag-Bi-Pb | Ag-Bi-Sn | Ag-Cu-Pb | Ag-Cu-Sn | Ag-Pb-Sn | Ag-Sb-Sn |
| Bi-Cu-Pb | Bi-Cu-Sn | Bi-Pb-Sn | Cu-Pb-Sn |          |          |          |
- Note that some Sb-bearing subsystems are not yet fully implemented or completely assessed. In the next release this will be improved.
- Further updated versions of this database are now under continuous developments at NIST, for the inclusions of more alloying elements (*e.g.*, Al-Au-In-Ga-Ge-Si-Zn).
- Applications:** Thermodynamic calculations of solder systems (Pb-containing and Pb-free).
- Availability:** As a free database to be used together with TCC and TCW, *it is distributed only upon special requests to TCS (with a certain distribution fee).*
- References:** Kattner U.R. (2002) Phase diagrams for lead-free solder alloys. *JOM*, **54**(12), 45-51.  
Kattner U.R. and Handwerker C.A. (2001) Calculation of phase equilibria in candidate solder alloys. *Zeitschrift für Metallkunde*, **92**, 740-746.  
Moon K.W., Boettinger W.J., Kattner U.R., Biancaniello F.S., and Handwerker C.A. (2000) Experimental and thermodynamic assessment of Sn-Ag-Cu solder alloys. *J. El. Mater.*, **29**, 1122-1136.  
Moon K.W., Boettinger W.J., Kattner U.R., Handwerker C.A., and Lee D.J. (2001) The Effect of Pb contamination on the solidification behavior of Sn-Bi solders. *J. El. Mater.*, **30**, 45-52.

## 2 Thermo-Calc Database Description Forms

### Thermo-Calc Database Description Form

# SNOB1

## SGTE Nobel Metal Alloys Database

(Version 1.2, 2003/2004/2007)

**Producer:** The Spencer Group Inc., Trumansburg, NY, USA;  
GTT-Technologies, Herzogenrath, Germany.

**Contact persons:** Pingfang Shi, Thermo-Calc Software AB, Stockholm, Sweden

**Description:** The database contains evaluated thermodynamic parameters for alloys of **Ag, Au, Ir, Os, Pd, Pt, Rh, Ru** which are alloyed amongst themselves and also in alloys with the following elements: **Al, As, Bi, C, Co, Cr, Cu, Fe, Ge, In, Mg, Ni, Pb, Sb, Si, Sn, Ta, Te, Ti, Tl, Zn, Zr.**

The evaluated parameters in this database are based on data collected from publications and internal project reports or have been assessed as part of the development of the database.

In only a few cases are the assessed parameters based on a large amount of experimental information. For many systems, very few, or even no thermodynamic measurements are available. This has necessitated use of published phase boundary information only, with a combination of estimated and optimized mixing parameters to provide a thermodynamic description of the systems concerned. For some inter-noble metal alloys, where complete ranges of solid and liquid solutions are observed, the descriptions should still be fairly reliable. For others, while a reasonable phase diagram description may have been obtained, the thermodynamic values for the different phases may have large errors associated with them.

The database provides a good starting basis for development of data for higher-order noble metal systems. At the same time, the assessed data it contains for the binary and ternary sub-systems of Au-Pd-Pt-Sn allow calculations relevant to dental alloy development.

Most of the binary alloy systems have been assessed over the entire composition range. Only a few ternary and higher-order parameters are available.

The database is generally valid for the temperature range 300°C to 2500°C. Phase boundaries and thermodynamic properties measured at lower temperatures may not correspond to the equilibrium state of the alloy, even after very long annealing times.

The database makes use of the SGTE Pure Element Data and, as such, is compatible with other SGTE Solution and Application Databases.

In the present assessments, some phases with narrow ranges of composition have been simplified to compounds with no compositional variation. Others have been modeled using the compound energy, sublattice formalism.

Specific information on each alloy system can be obtained from the list of references below.

Status of the SGTE Nobel Metal Alloys Database: The first version (v1.0) was released in Oct. 2003. The current subversion (v1.1) includes some further modifications, corrections and improvements implemented by Thermo-Calc Software.

**Systems:** This database currently contains the following 30 elements:

<b>Al</b>	<b>Ag</b>	<b>As</b>	<b>Au</b>	<b>Bi</b>	<b>C</b>	<b>Ca</b>	<b>Co</b>	<b>Cr</b>	<b>Cu</b>
<b>Fe</b>	<b>Ge</b>	<b>In</b>	<b>Ir</b>	<b>Mg</b>	<b>Ni</b>	<b>Os</b>	<b>Pb</b>	<b>Pd</b>	<b>Pt</b>
<b>Rh</b>	<b>Ru</b>	<b>Sb</b>	<b>Si</b>	<b>Ta</b>	<b>Te</b>	<b>Ti</b>	<b>Tl</b>	<b>Zn</b>	<b>Zr</b>

#### Systems assessed over complete range of composition:

Ag-Al	Ag-Au	Ag-Bi	Ag-Cu	Ag-Ge	Ag-In	Ag-Ir	Ag-Mg	Ag-Os	Ag-Pb
Ag-Pd	Ag-Pt	Ag-Rh	Ag-Ru	Ag-Sb	Ag-Si	Ag-Sn	Ag-Ti	Ag-Tl	Ag-Zn
Ag-Zr									
Au-Al	Au-As	Au-Bi	Au-C	Au-Cr	Au-Cu	Au-Ge	Au-In	Au-Pb	Au-Pd
Au-Pt	Au-Rh	Au-Ru	Au-Sb	Au-Si	Au-Sn	Au-Te*	Au-Ti	Au-Tl	
Pd-Co	Pd-Fe	Pd-Ir	Pd-Ni	Pd-Pb	Pd-Pt	Pd-Ru	Pd-Sn**	Pd-Ti	
Pt-Co	Pt-Cr	Pt-Rh	Pt-Ru	Pt-Sn	Pt-Ta	Pt-Ti			
Rh-Ru	Sn-In (crude description)			Sn-Zn	In-Zn				

#### Systems assessed over a partial range of composition:

Au-Zn:	to 50 at% Zn (crude description)
Pd-In:	to 35 at% In
Pd-Zn:	to 50 at% Zn (no reliable phase diagram information available)
Pt-In:	to 30 at% In

## 2 Thermo-Calc Database Description Forms

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Pt-Zn:	only estimated data for the compounds Pt <sub>3</sub> Zn and PtZn
Ag-Cu-Pb:	liquid
Au-In-Pb:	liquid
Au-Pd-Pt:	fcc
Pd-Pt-Sn:	liquid, (Pd,Pt) <sub>2</sub> Sn, (Pd,Pt) <sub>3</sub> Sn <sub>2</sub> , (PdPt) <sub>5</sub> Sn <sub>3</sub> ,
Pd-Pt-Ti:	(Pd,Pt)Ti, (Pd,Pt) <sub>3</sub> Ti
Au-Pd-Pt-Sn:	(Au,Pd,Pt)Sn, (Au,Pd,Pt) <sub>3</sub> Sn, (Au,Pd,Pt)Sn <sub>4</sub>

- \* Please note that the gas phase should be included in calculations involving the Au-Te system, otherwise an inverted miscibility gap is predicted in the liquid phase for Te-rich alloys.
  - \*\* Please note that 2 descriptions of the Pd-Sn system are provided. The first description uses a simplified, stoichiometric modeling of the compound phases, which is compatible with the assessed parameters for the Pd-Pt-Sn and Au-Pd-Pt-Sn systems. The compound phases denoted by `_ggt` should be used with the LIQ-gtt and FCC-gtt phases. The second description provides a more rigorous modeling of the binary Pd-Sn system. In this case the phases with no additional definition should be used with the LIQUID and FCC phases.
- N.B. Pure element Gibbs energy data have been included in the form of Me\_SGPS expressions for a number of elements. This is to facilitate calculations for systems where the primary solid solution range is negligible. However, to avoid incorrect phase boundary calculations, it is preferable to suppress these parameters in most cases.

The phase diagrams of all the binary systems listed above were checked on 10th June, 2003.

**Applications:** Noble metals and their alloys have a wide variety of applications, and calculations of relevant phase equilibria in particular cases are important *e.g.* for optimizing suitable alloy compositions or predicting reaction products in chemically aggressive environments.

Some examples of noble metal alloy uses are:

- Jewellery and decoration
- Electronic components; micro-electronic contact materials
- Solders and brazes
- Dental alloys
- Fission products
- Catalysts
- New minority alloy components, *e.g.* in turbine alloys
- Scientific equipment, *e.g.* thermocouples, crucibles, calorimeters

Because of their values, noble metal alloys undergo extensive recycling. For this reason, information on dilute ranges of impurity elements in precious metals is important with respect to different methods of refining. Among such methods are oxygen refining and some use of halogens. In such cases, the database should be used in conjunction with the SGTE Pure Substances Database to take into account relevant condensed and gaseous oxides and halides.

The database will often be used with one of the noble metals as major component, but in a number of applications, large concentrations of alloying elements are present. For this reason, and whenever possible, the assessed parameters in the noble metal alloys database cover the entire composition range of the alloys involved (see below for information on relevant ranges for specific alloys).

There are very few ternary interaction parameters available in the database and it must be realized that *calculation of phase boundaries in higher-order systems by combination of binary alloy data only may give very unreliable results.*

In its present development stage, the database can best be used for calculations relating to Ag-, Au-, Pd- and Pt-rich alloys containing small amounts (3-5%) of impurity or alloying elements.

The critically assessed values for the Au-Pd-Pt-Sn system allow theoretical investigation of phase equilibria in certain dental alloys.

**Availability:** Commercially available for uses with TCC and TCW.

**Disclaimer:** The Spencer Group Inc. and GTT-Technologies assumes no responsibility for the validity of results from a calculation using data from the noble metal alloy database and is not liable for any damage or loss, subsequential or otherwise, caused by the application of results.

**References:** A complete reference for the SNOB1 database can be obtained from Thermo-Calc Software on requests.

## 3 Database Manager's Guide

### 3.1 Introduction

Thermo-Calc is a sophisticated software for thermochemical calculations and automatic mapping of phase diagrams. It uses the method of minimizing the global Gibbs energy for a given set of conditions. The actual data that describe the thermochemical properties of a given phase is not included in the program. Instead, the thermodynamic quantities needed for the calculation were provided by a set of general subroutines called the **Gibbs Energy System (GES)**.

The subroutines and calculation program was refined several times before a thermochemical calculation interface was defined. Until then, the Gibbs energy parameters needed by GES for a given system had more or less been typed in by hand and stored on individual files. It was thus natural that, along with the calculation interface, there were additional developments of an interface to a databank and a data structure storing all available thermodynamic parameters.

However, when the work on the software for the present database began, it was thought that the interface and the data structure might be too limited to take full advantage of important facilities in GES. On the other hand, the suggested data structure was based on a linked list concept and efficient search algorithms could easily be written. The actual implementation had probably to be done using a "relational database" software making the databank extremely hardware dependent since each computer manufacturer has its own such software. Other drawbacks with the original data structure were connected with the updating and maintenance of it.

To gain further experience, it was decided to use a much simpler scheme, utilizing sequential files and data stored as character codes. The maintenance of data could then be performed with a standard text editor. This method allowed the software and data to be more portable to other computers and operating systems. The module developed was named as the **Thermodynamic DataBase module**, in the following text always referred to as **TDB**  $\Rightarrow$ .

As need arises for larger and larger databases, the original program has been slightly amended to incorporate different types of random access files for data storage.

In recent years, the software for simulation of Diffusion-Controlled phase TRANSformations (**DICTRA**) has been developed at the Department of Materials Science and Engineering of KTH (Royal Institute of Technology), Stockholm, Sweden. In addition to thermodynamic data, DICTRA needs kinetic data, *i.e.*, diffusion or mobility data. The basis of DICTRA is the accumulated package of thermodynamic calculation and data management routines mentioned above. Thus, the kinetic data was extended to the original set of keywords valid for the database definition file presented below. The extensions were made in such a way that the TDB module can now be easily adapted for any additional kinds of kinetic data used by calculation programs. The DICTRA extensions are given in a separate section (*Section 6.4*).

---

$\Rightarrow$  **Revision History of the Database Manager's Guide:**

Nov 1986	First release (Edited by Jan-Olof Andersson and Björn Jönsson)
Oct 1993	Second revised and extended release (Edited by Bo Sundman)
Jun 2000	Third revised and extended release (Edited by Pingfang Shi)
Nov 2002	Fourth revised release (Edited by Pingfang Shi)
Jun 2004	Fifth revised release (Edited by Pingfang Shi)
Jun 2006	Sixth revised release (Edited by Pingfang Shi)
Mar 2008	Seventh revised release (Edited by Pingfang Shi)

## 3.2 Initialization of the TDB Module

The following paragraphs will present how a *database initiation file* (or called *database directory file*) is constructed to work with the TDB module. Upon starting, TDB looks for this special file that has information on the available predefined databases (whether freely distributed with the TCC/TCW/DICTRA packages, purchased from TCS or its agents, or created by the users).

The database initiation file is currently called TC\_INITD (or TC\_INITD.TDB) on PC Windows, or `initd.tdb` on PC Linux. Each user could have his own TC\_INITD (or `initd.tdb`) file, but a better way is to define an environment variable with the name TC\_INITD (or `initd.tdb`) translating to an initiation file name that is common for all users at one installation. This common file is automatically copied by the TCC/TCW/DICTRA installation script to the `\DATA\` area that is under the directory defined by the `TCPATH` parameter (on Windows), or the `/data/` area that is under the directory defined by the `TC_DATA` parameter (on Linux). The database manager can find it on a local computer for an independent installation locates or a connected server for a server installation.

When editing or modifying the definitions of initiation parameter (including short-names, paths and subdirectories, database definition file names, and instructive database descriptions) for the available databases in the TC\_INITD or `initd.tdb` file, a specific format should be used, with the three sequent fields as explained below:

- ◆ The *first* field gives the abbreviated name for the database (currently restricted to maximum 5 characters)
- ◆ The *second* field specifies a path & filename (maximum 78 characters), containing the database path definition and the actual database definition (`setup`) file name. The `setup` file name must consist of a main part and an extension of maximum 3 characters under Windows (such as `SSOL4SETUP.TDB`) or various Linux platforms (such as `ssol4setup.tdb`). For the database path definition, the backslash “\” is used with Windows, and the forward-slash “/” is used with PC Linux. All databases should be normally located in subdirectories that are under the directory defined by the `TCPATH` parameter (under Windows) or by the `TC_DATA` parameter (under Linux), or under its subdirectory `\DATA\` or `/data/`.
- ◆ The *third* field (maximum 60 characters) details an optional full name for the database description.

Each entry record (*i.e.*, for one single database) must end with an exclamation mark “!”. There should be no spaces or commas within the first and second fields since such characters are taken as field separators, while spaces or commons can be used within the third field.

Although that it is always OK to write each database entry in one or two lines (till its ending mark,!), it is usually recommended that the third field may be added on the same line as the first and second fields for PC Windows environments, or on the following line for all kinds of Linux platforms. The following is an example of an initiation file defining three databases named PURE4, SSOL2 and TCFE2:

*Under PC Windows environment:*

```
SSOL2 TCPATH\DATA\SSOL2\SSOL2SETUP.TDB  SGTE Solutions Database version 2 !
PURE4 TCPATH\DATA\PURE4\PURE4SETUP.TDB  SGTE Pure Elements Database version 4 !
TCFE2 TCPATH\DATA\TCFE2\TCFE2SETUP.TDB  TCS Steels/Fe-Alloys Database version 2 !
```

*Under Linux platforms:*

```
ssol2 TC_DATA/data/ssol2/ssol2setup.tdb
      SGTE Solutions Database 1 version 2 !
pure4 TC_DATA/data/pure4/pure4setup.tdb
      SGTE Pure Elements Database version 4 !
tcfe2 TC_DATA/data/tcfe2/tcfe2setup.tdb
      TCS Steels/Fe-Alloys Database version 2 !
```

Under PC Windows environment, a TCW installation normally shares many directories with TCC, including the `\DATA\` area and the database initiation file TC\_INITD. A DICTRA installation (under PC Windows) does the same: the installation script automatically locates the DICTRA databases in the `\DATA\` area, and the database manager or user shall copy the database initiation lines for the DICTRA databases (normally saved in the

TC\_INITD.ADD file attached on the DICTRA distribution media) to the end of the database initiation file TC\_INITD.

For your convenience when switching/ appending your self-generated databases or lately purchase databases from TCS or its agents, you can simply add them to the predefined database list in the database initiation file TC\_INITD or `initd.tdb` of your installed TCC/TCW/DICTRA packages; please also refer to *Section 2.2.2.2*.

It is possible to write some comment lines, always starting with a “\$” sign, in the database initiation file; such lines are ignored by the TDB module. This is also applicable if the database manager or user wants to temporarily disable any database from the predefined database list for common uses.

If there are too many databases in the `\DATA\` area that the TDB module may not be able to properly handle, the \$ sign can also be used to temporarily comment out some of the uncommon databases.

Since TCCM, the `NEW_DICTORY_FILE` command (see *Section 5.4.16*) was implemented so that TCC can use several additional database initiation files that define accessing paths for various databases located in different subdirectories under the directory defined by the `TCPATH` or `TC_DATA` parameter. If TCC is used under a Windows environment, such additional database initiation files can be located at any directory of any driver, on either a local computer or connected server. The `NEW_DICTORY_FILE` command will pop up an *Open file* window to access a database initiation file if the file name or its path is not given on the same line of the `NEW_DICTORY_FILE` command, or if it is incomplete or incorrect, so that the path (in the **Look in** box) and database initiation file name (in the **File name** box) can be appropriately selected. However, if TCC is run on a Linux platform, these files must be located in the current working directory (where TCC is started).

In an additional database initiation file, the first database entry may need to have the same path definition structure as in the ordinary database initiation file `TC_INITD` or `initd.tdb`. So it is advisable to simply copy the entry line(s) for some common databases from the original `TC_INITD` or `initd.tdb` file to such a database initiation file. The entries of the additional databases follow. Similarly to the standard databases predefined in the `TC_INITD` or `initd.tdb` file, all databases should be normally located in subdirectories that are under the directory defined by the `TCPATH` parameter (on Windows) or by the `TC_DATA` parameter (on Linux), or under its subdirectory `\DATA\` or `/data/`.

Given below is an example of an additional database initiation file, named like `MYINITD1`, for uses under Windows:

```
$
$ DATABASES TCC (Additional TCC Databases)
PURE4 TCPATH\DATA\PURE4\PURE4SETU.TDB  SGTE Pure Elements Database version 4 !
AD1   TCPATH\DATA\ADD1\AD1SETUP.TDB    TCS ADD1 Solution Database !
AD2   TCPATH\ADDDATA\ADD2\AD2SETUP.TDB  TCS ADD2 Solution Database !
$AD2o TCPATH\ADDDATA\ADD2old\AD2SETUP.TDB TCS ADD2 Database (old) !
AD3   TCPATH\DATA\NEWDATA\ADD3\AD3SETUP.TDB TCS ADD3 Solution Database !
AD4   TCPATH\DATA\NEWDATA\MYPROJ1\ADD4\AD4SETUP.TDB
      MYPROJECT1 ADD4 Solution Database !
$
$ DATABASES DIC (Additional DICTRA Databases)
DCAD1 TCPATH\DICDATA\DCADD1\DCAD1SET.TDB
      TCS DCADD1 Mobility Database !
```

### 3.3 Database Definition File Syntax

The database definition file consists of a set of keyword codes each followed by one or several parameters (arguments). A complete keyword entry must end with an exclamation mark "!". It can be up to 2000 characters long, but the maximum length of a line in a TDB file is 78 characters, so it may be necessary to continue the keyword's parameters (arguments) in several lines, and the exclamation mark "!" must be written at the end of the last line. It is recommended to *always have at least one empty space at the beginning of each continuation line for keyword's parameters (arguments)*; otherwise, the TDB module may issue some error messages when reading the keyword entry. The keyword and its various parameters (arguments) are separated by a space or a comma. A dollar sign "\$" in the first position of the line indicates that the line is a comment line, which is ignored by the TDB module.

TDB completely reads the definition file only once, from beginning to end, when the database is selected. Much checking is done by TDB when reading the definition file. This implies that (nearly) everything must be declared or defined before it is used in any other way. For example, if the graphite phase is to be included in the database definition, the element carbon and the phase graphite must be defined before declaring that carbon dissolves in graphite. This definition order is necessary to build the internal data structure acceptable by the TDB module (during its consistency checking).

This section gives a description of the available keywords and their appropriate arguments. The reader is assumed to have basic knowledge of the Gibbs Energy System module.

The following syntax is used:

```
KEYWORD [arg.1]*# [arg.2]*## {optional arg.3}!
```

The keywords are in the text written in full length but can be abbreviated as long as the abbreviation is unique. A keyword may have syntax consisting of several arguments and optional arguments. The number, # or ##, in the notation, [...] \*# or [...] \*##, indicates an argument with a maximum length of ASCII characters. Arguments within square brackets [...] *must* always be given, while such in curly braces {...} are *optional*.

#### 3.3.1 ELEMENT

```
ELEMENT [element name]*2 [ref. state]*24 [mass] [H298] [S298] !
```

The **element name** (maximum 2 characters) is meant to be the one found in the periodic chart but there is no restriction on naming conventions. However, the GES module only recognizes UPPER-case element names (if the Upper Case Mode has been selected by the GES command REINITIATE), implying lower-cases (if defined in a database) is automatically converted to UPPER-cases by the TDB/GES module. The elements are automatically entered as species using the same names of the elements. If, for instance, the species corresponding to FE by some reasons needs to be named FE1, it is possible to define the species as FE1, resulting in an element named FE and a species named FE1. Vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or as ZE in an aqueous solution phase), if used, need to be also entered as special elements for correct handling by the TDB module.

The **reference state** (maximum 24 characters) is the stable phase (at 298.15 K and 1 bar) that should contain this element and should be used as the reference state for all thermodynamic data of this element. The **mass**, given in gram per mole, is used in various calculation programs and should always be given the correct value. **H298** and **S298** denote the enthalpy and entropy difference between 0 and 298.15 K for the element in SI units. If they are unknown, the values can be set to zero. All these information (**reference state**, **H298** and **S298**) precisely define the so-called **SER (Stable Element Reference State)**.

Examples:

```
ELEMENT /- ELECTRON_GAS      0.0  0.0  0.0  !
ELEMENT VA VACUUM            0.0  0.0  0.0  !
ELEMENT ZE UNIT_CHARGE       0.0000000001  0.0  0.0  !
ELEMENT AL FCC Al            26.98154  4577.296  28.3215  !
ELEMENT C GRAPHITE           12.011  1054.0  5.74  !
```

```

ELEMENT FE BCC_A2          55.847  4489    27.28 !
ELEMENT O  1/2_MOLE_O2(G) 15.9994 4341    102.5158 !
ELEMENT TI HCP_A3          47.88   4810    30.648 !
ELEMENT ZR HCP_A3          91.224  5566.27  39.181 !
ELEMENT ZY DUMMY           1         1         1 !

```

### 3.3.2SPECIES

**SPECIES** [*species name*]\*24 [*stoichiometric formula*] !

This keyword defines species in the data structure. Every **species name** (maximum 24 characters) must be unique. The species are built from the already defined set of elements in the stoichiometric formula. If a non-defined element is referred, TDB will issue an error message and the data structure is probably damaged. The species names do not necessarily have to be the same as the stoichiometry formula, but it is often recommended to do so for most cases. The elements are automatically entered as species using the same names of the elements. One can define a species name as a mixture of UPPER-case and lower-case in a database, but the TDB module will automatically convert all lower-cases to UPPER-cases, as the GES module only recognizes UPPER-case species names. If wished for some convenience in naming the species in a database, one can also use some special characters [such as +, -, \_, / and .] in species names, but one should avoid using other special characters [such as ( and )].

The **stoichiometric formula** is written with a simplified chemical notation, in which the chemical elements should always be given in UPPER-cases and in any preferred order, and their stoichiometric coefficients can be written in either real numerical factor or integer digits. It is important that the numerical factor of 1 cannot be left out. Subgroups are not allowed in a stoichiometry formula; however, if wished for some convenience in specifying the stoichiometry formula for a specific species in a database, one can specify it in a way that some elements (always together with their corresponding partial stoichiometric coefficients) can be repeated (as shown below in some examples).

*Examples:*

```

SPECIES AL2O3      AL2O3 !
SPECIES Silica    SI1O2 !
SPECIES NaSb_6OH  NA1SB1O6H6 !
SPECIES FE+2      FE/+2 !
SPECIES SB-3      SB/-3 !
SPECIES AlCl2/3   AL.33333CL.666667 !
SPECIES AL1CL1H2O2 AL1CL1H2O2 !
SPECIES AlCl3_3H2O AL1CL3H6O3 !
SPECIES AlO2H2Cl.H6O3 AL1O2H2CL1H6O3 !
SPECIES AlCl2-OH.3H2O AL1CL2O1H1H6O3 !
SPECIES AlCl2OH.3Water AL1O1H1CL2H6O3 !

```

### 3.3.3PHASE

**PHASE** [*phase name*]\*24 [*data-type code*]\*8 [*numb. subl.*] [*sites in subl. 1*] [*sites in subl. 2*] etc... {*auxiliary text string*} !

This keyword defines a phase and its properties (except for what species are allowed to enter it and for its thermodynamic parameters).

The **phase name** (maximum 24 characters) must be unique; otherwise the TDB module sees it as an attempt to redefine a previously defined phase. This mistake causes TDB to issue an error message and ignore the rest of the line. The phase name can also be attached with a colon sign : and a letter for a legal GES phase-type code (e.g., IONIC-LIQ:Y and GAS:G); see more examples below.

Legal GES phase-type codes are:

G ⇒ Bit set for a gaseous mixture phase.

A ⇒ Bit set for an aqueous solution phase.

Y ⇒ Bit set for an ionic liquid solution phase (that is specially treated by the Ionic Two-Sublattice Liquid Model).

L ⇒ Bit set for a liquid solution phase [but not A (aqueous) or Y (ionic liquid)].

I ⇒ Bit set for a phase with charged species [but not G (gaseous), A (aqueous) or Y (ionic liquid)].

F  $\Rightarrow$  Bit set for an ordered FCC or HCP solution phase with 4 substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).

B  $\Rightarrow$  Bit set for an ordered BCC solution phase with 4 substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).

Note that other invalid characters (*e.g.* M or P) will be eventually treated, together with the colon sign “:”, as a part of a phase name.

A G phase (gaseous mixture) or an A phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and that an L phase (ordinary liquid solution) is normally (but not always) modelled as a substitutional phase without sublattice, too.

Since TCCS/TCW5, the phase-type F has been extended, and the new phase-type B has been implemented. These two phase-types are useful for ordered FCC (or HCP) and BCC solution phases handled by the so-called *Four Substitutional-Sublattice Ordering Model*, which always require that the solution phase must have 4 sublattices for substitutional ordering and can additionally have an interstitial sublattice.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices all of which are the nearest neighbours. A *Normal 4-Sublattice Model* requires that all the G parameters for each of end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option F means that the G parameters need be given only once. The possible permutations are handled automatically. *To be more clarified:* An A–B binary solution phase (with the element A locates on one sublattice site and B on three sublattice sites) treated by the Normal 4-Sublattice Model has to have 4 G parameters for 4 end-members, *i.e.*,  $G(\text{phase}, A:B:B:B)$ ,  $G(\text{phase}, B:A:B:B)$ ,  $G(\text{phase}, B:B:A:B)$  and  $G(\text{phase}, B:B:B:A)$ , because of that in the general case these G parameters can be different from each other. But for the FCC and HCP orderings, they are identical and thus all G parameters of such end-members need be given only once, and the possible permutations are then automatically handled by the GES module. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

Previously (within versions prior to TCCS/TCW4), no excess interaction parameters were allowed with the phase-type option F, but this has been modified since TCCS/TCW5. However, there are restrictions on the excess parameters allowed with the phase-type option F. One can only have excess parameters of the following types:

L (phase, A, B : \* : \* : \* ; 0...9)

L (phase, A, B : C, D : \* : \* ; 0...9)

The asterisk “\*” means that the interaction parameter is independent of the constituents on its corresponding sublattice. No ternary interaction parameters (*i.e.*, with 3 elements on one sublattice site) are allowed. The reason for this restriction is that it would be too complicated to handle all possible permutations. In the current *Four Substitutional-Sublattice Ordering Model*, the binary interaction between A and B atoms is thus independent of the constituents on the other sublattices, where there are many other parameters to model the composition-dependence of the Gibbs energy (both in the ordered and disordered parts of the phase). The model for these ordered phases are always partitioned in a disordered part (with a single substitutional sublattice) and an ordered part (with 4 substitutional sublattices for ordering).

For ordered BCC phases, the phase-type option B means the same thing but the situation is a bit more complicated, as the 4-substitutional-sublattice ordering phase represents an irregular tetrahedron with 2 pairs of sites that are next nearest neighbours. Thus, for an A–B binary solution phase (with the element A locates on two sublattice site and B on two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the  $G(\text{phase}, A:A:B:B)$  term has 4 nearest neighbor bonds between A and B atoms, whereas the end-member described by the  $G(\text{phase}, A:B:A:B)$  term has 2 nearest neighbour bonds between A and B atoms and 2 next nearest neighbor bonds (for detailed reference one may visit the Crystal Lattice Structure web page <http://cst-www.nrl.navy.mil/lattice/index.html>).

The first end-member [described by the  $G(\text{phase}, A:A:B:B)$  term] represents B2-ordering and the second [described by the  $G(\text{phase}, A:B:A:B)$  term] stands for B32-ordering. There are 2 permutations of the  $G(\text{phase}, A:A:B:B)$  term and 4 permutations of the  $G(\text{phase}, A:B:A:B)$  term, automatically conducted in the *Four Substitutional-Sublattice Ordering Model*. And there are also two kinds of reciprocal interaction parameters, *i.e.*,



### 3.3.4 CONSTITUENT

**CONSTITUENT** [**phase name**]\*24 [**constituent description**]\*2000 !

This keyword (and the **ADD\_CONSTITUENT** keyword for large solution phase) defines the *phase-constitution* as a list of *constituents* (for a substitutional phase with no sublattice) or of *constituent arrays* (for a sublattice phase).

The **phase name** (maximum 24 characters) must be an already defined phase (*i.e.*, already through the **PHASE** keyword). Specifying the phase name always in UPPER-cases is recommended; however, if one would prefer to write it as a mixture of UPPER-case and lower-case in a database, the TDB module will then automatically convert all lower-cases to UPPER-cases, as the GES module only recognizes UPPER-case phase names. It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the **PHASE** keyword; such as **GAS:G**, **LIQUID:L**, **IONIC-LIQ:Y**, **SPINEL:I**, **FCC\_L12:F**, **HCP\_D021:F**, **BCC\_B2:B**, **AQUEOUS:A**), such a valid phase-type code must also always be attached to the phase name in the **CONSTITUENT** keyword (and the **ADD\_CONSTITUENT** keyword).

The **constituent description** (maximum 2000 characters) is a list of the species that enter a phase. The list starts with a colon “:”, indicating the start of the sub-list of species for the first sublattice, and different sublattices are separated by colons. The complete sequence ends with a final colon. Optionally, each sublattice may specify which species are considered to be so-called major constituents. This is done by adding a “%” (percent sign) directly on the species name. The start values on the site fractions of the major constituents should sum to 0.99 on a specific sublattice. Thus, the so-called minor constituents (*i.e.*, those without a “%”) adds up to 0.01. Maximum 2000 characters can be coded in the constituent description, continuing in sequent lines. If the phase has a constituent description longer than 2000 characters, the rest can be coded in one or several **ADD\_CONSTITUENT** keywords.

*Examples:*

```
CONSTITUENT BCC_A2 :FE
CONSTITUENT IONIC-LIQ:Y :FE+2 : SB-3: !
CONSTITUENT M23C6 :CR FE :FE CR W MO : C: !
CONSTITUENT AQUEOUS:A :H2O% AG+1 AGF AGCL AGCL2-1 AGI3-2 AGSO4-1 AGC2H4+1
  AGN2H6+1 AGC2N2-1 AGC2H4NO2 AL+3 ALF3 ALO2-1, ... : !
CONSTITUENT SPINEL:I : AL+3% CR+3 FE+2% FE+3 MG+2% NI+2
  : AL+3% CA+2 CR+3 FE+2 FE+3 MG+2% NI+2 VA
  : FE+2 MG+2 VA%
  : N-3 O-2% :!
```

### 3.3.5 ADD\_CONSTITUENT

**ADD\_CONSTITUENT** [**phase name**]\*24 [**constituent description**]\*2000 !

This keyword adds more constituents to a phase that has already some constituents. **Its syntax is the same as for the CONSTITUENT keyword.** This keyword can be used several times, if the phase is very large, *e.g.*, a gaseous mixture or a complex aqueous solution. This is useful when there are so many constituents in a phase that the 2000 characters available for the constituent description list are not enough.

Note that constituents are not necessary on all sublattices. In the second example below, no addition is made to the first sublattice.

*Examples:*

```
ADD_CONSTITUENT GAS :S1 S2 S3 ... : !
ADD_CONSTITUENT IM-PHASE : :CR:W ... : !
ADD_CONSTITUENT AQUEOUS:A :CUCL+1 CUCL2 CUCL3-2 CUOH+1 CUO2H2 CUO3H3-1
  CUO4H4-2 CU2OH+3 CU2O2H2+2 CU3O4H4+2 NIO2H2 NIO3H3-1 NIO4H4-2 NI2OH+3
  NI4O4H4+4 ZNOH+1 ZNO2H2 ZNO3H3-1 ZNO4H4-2 ... : !
```

### 3.3.6 COMPOUND\_PHASE

**COMPOUND\_PHASE** [phase name]\*24 [data-type code]\*8 [constituent] !

The keyword is a compact way to simultaneously define a species, a compound phase (maximum 24 characters) and its phase-constituent. It is useful for stoichiometric phases with constant compositions. The species name and stoichiometric formula must be identical, *i.e.*, being the given constituent. The phase will have this species as its only constituent. This keyword was implemented to make the database definition file for a large substance database more compact; it is just a combination of the SPECIES, PHASE and CONSTITUENT keywords.

*Examples:*

```
COMPOUND_PHASE AL2O3 % AL2O3 !
COMPOUND_PHASE MAGNETITE %MF FE3O4 !
COMPOUND_PHASE QUARTZ % SIO2 !
```

### 3.3.7 ALLOTROPIC\_PHASE

**ALLOTROPIC\_PHASE** [phase name]\*24 [data-type code]\*8 [constituent] !

This keyword does the same as the COMPOUND\_PHASE keyword for entering an allotropic phase (maximum 24 characters), but does not enter the constituent as a species to the data structure; it should therefore be used if the species is already defined.

*Examples:*

```
ALLOTROPIC_PHASE BETHA-AL2O3 % AL2O3 !
ALLOTROPIC_PHASE CRISTOBALITE % SIO2 !
ALLOTROPIC_PHASE TRIDYMITTE % SIO2 !
```

### 3.3.8 TEMPERATURE\_LIMITS

**TEMPERATURE\_LIMITS** [lower limit] [upper limit] !

This keyword sets the default upper and lower temperature limits used by the GES module for Gibbs energy parameters and functions. It can be used only once in one database definition file and all its sequential files.

*Example:*

```
TEMPERATURE_LIMITS 500.0 1800.0 !
```

### 3.3.9 DEFINE\_SYSTEM\_DEFAULT

**DEFINE\_SYSTEM\_DEFAULT** [keyword] {G-ref. type index} !

This keyword sets the default value to ELEMENT or SPECIES in the TDB command DEFINE\_SYSTEM (see Section 5.4.7). For a substance database, it might be appropriate to have ELEMENT as default value whereas a large solution database can benefit from having SPECIES as default value. A proper default value is beneficial for a beginner, but an advanced user will probably use the TDB commands DEFINE\_ELEMENT and DEFINE\_SPECIES to override the default value.

{G-ref. type index} is an integer indicating the reference state type for an element when entering and listing data in the GES module. The following lists legal numbers and their corresponding meaning (the reference state type for an element):

- 1 ⇒ symbol: G
- 2 ⇒ symbol: H298
- 3 ⇒ symbol: H0

*Example:*

```
DEFINE_SYSTEM_DEFAULT element 2 !
```

### 3.3.10 DEFAULT\_COMMAND

**DEFAULT\_COMMAND** [secondary keyword and parameters] !

The keyword specifies commands to be executed by the TDB module at database initialization. The syntax of the available commands is currently not the same as the user available TDB commands but the actions are similar. The available secondary keywords and parameters in syntax for **DEFAULT\_COMMAND** are,

```
DEFINE_SYSTEM_ELEMENT [element names]
DEFINE_SYSTEM_SPECIES [species names]
DEFINE_SYSTEM_CONSTITUENT [phase] [sublattice] [species]
REJECT_SYSTEM_ELEMENT [element names]
REJECT_SYSTEM_SPECIES [species names]
REJECT_SYSTEM_CONSTITUENT [phase] [sublattice] [species]
REJECT_PHASE [phase names]
RESTORE_PHASE [phase names]
```

*Examples:*

```
DEFAULT_COMMAND DEFINE_SYSTEM_ELEMENT FE VA !
DEFAULT_COMMAND REJECT_SYSTEM_CONSTITUENT LIQUID 2 C !
DEFAULT_COMMAND REJECT_PHASE LIQUID !
DEFAULT_COMMAND RESTOR_PHASE GAS !
```

### 3.3.11 DATABASE\_INFORMATION

**DATABASE\_INFORMATION** [text]\*8000 !

This keyword defines a text for the detailed description of the current database. The text can be listed with the TDB command **DATABASE\_INFORMATION**. An apostrophe, “'”, can be used in the text to indicate a new line; and two apostrophe, “''”, can be used in the text to indicate a new line plus an empty line. **Note that the continuous text length (each line with max 78 characters) has been extended from 2000 to 8000 characters since TCCP/TCW2.**

*Example:*

```
DATABASE INFORMATION This is the XXX-Alloy Solution Database '
    in the A-B-C-D-..... System. '
    Developed by TCS, released in May 2001. ''
... more ... !
```

### 3.3.12 TYPE\_DEFINITION

**TYPE\_DEFINITION** [data-type code]\*1 [secondary keyword with parameters] !

This keyword couples phases to an action performed by the TDB module when the TDB command **GET\_DATA** is executed. The available secondary keywords and associated parameters in syntax for **TYPE\_DEFINITION** are:

```
SEQ [filename]
RND# [filename]
GES [valid GES command with parameters]
POLY [valid POLY command with parameters]
TDB [valid TDB command with parameters]
IF [conditional statement] THEN [keyword with parameters]
AFTER [valid GES command with parameters]
```

The secondary keyword **SEQ** specifies a sequential file that stores parameters belonging to the phases using the associated data type code (which is defined by this **TYPE\_DEFINITION** keyword). A special case where the filename is given as an asterisk, \*, implies that the database definition file also acts as a sequential data storage file. This case makes it possible to have a single file for a small database, which is especially suited for personal databases.

The secondary keyword **RND** should be concatenated with a positive integer # to indicate the type of the *random file*. Currently, there are three types of random files. Type **RND0**, the default type, is used for complete Gibbs

energy expressions (G0 parameters), where the search field is the unabbreviated parameter name. Type RND1 is designated for functions, where the function name is used as the search field. Type RND2 is reserved for binary interaction parameters, where its search field is also the unabbreviated parameter name without any interaction order notation. Note that ternary and higher order interaction parameters must be specified on a sequential file. Moreover, the internal structures of these random files are subject to changes with different versions of TDB, and with implementations of TDB on various computer systems. For further information, one may consult the FORTRAN program **TDBSORT**, which is available from Thermo-Calc Software AB.

The secondary keyword **GES**, **POLY**, or **TDB** specifies a modification of, or addition to, phases having the associated data type code, such as magnetic contribution, another excess model, or any other valid GES/POLY/TDB command that applies to a certain phase. By implementing this as a call to the interactive GES/POLY/TDB module, much flexibility is achieved. If a new type of addition is implemented in GES/POLY/TDB module, it can immediately be used in the database definition file without reprogramming the TDB module. Note, in several examples given below, the use of an “@” (at) sign indicates any phase to which the relevant type definition (*e.g.*, A, B, 4, or E) applies.

The secondary keyword **IF/THEN** allows specification of a conditional statement structured with respect to the phase constitution that controls the execution of a following type-definition [keyword with parameters] string. See the last four examples below.

The secondary keyword **AFTER** is similar to the GES keyword except the defined GES command will be executed after all parameters have been entered. The reason for this is that the command has no effect unless there is a parameter. After “AFTER” keyword a GES command must be given and it is executed AFTER entering the parameters of the phase.

The **data-type** code (always as one string) can be any normal or special character, *e.g.*, 0, 5, A, F, M, %, &, (, *etc.*, and is referred in the definition keywords (PHASE, COMPOUND\_PHASE and ALLOTROPIC\_PHASE) for various phases.

Since TCCS/TCW5, a phase can have several so-called **ADDITIONAL** parts of different types (that are enforced by certain **TYPE\_DEFINITIONS** which call the GES command **AMEND\_PHASE\_DESCRIPTION** for describing various contributions to Gibbs energy); however, the TDB/GES modules will automatically delete any early-defined **ADDITIONAL** part(s) of the same type.

Since TCCS/TCW5, the TDB module can now selectively retrieve functions which are necessary for a defined system from a database that has functions stored in its **setup** file or **SEQ** sequential function file, while all other functions irrelevant for the defined system are simply ignored and will not be saved in associated **GES5** and **POLY3** workspaces. Previously, this can only done for large databases that have functions stored in **RND1** random or **FTP** function files.

#### Examples:

```

TYPE_DEF % SEQ TCPATH\DATA\[DATABASE]\PARAMETERS.TDB !
TYPE_DEF I SEQ TCPATH\DATA\[DATABASE]\INTERACTION-PARAMS.TDB !
TYPE_DEF G RND0 TCPATH\DATA\[DATABASE]\GZERO-PARAMS.TDB !
TYPE_DEF F RND1 TCPATH\DATA\[DATABASE]\FUNCTIONS.TDB !
TYPE_DEF & RND2 TCPATH\DATA\[DATABASE]\BINARY-INTERACTIONS.TDB !
TYPE_DEF A GES AM_PH_DES @ MAGNETIC -1 0.40 !
TYPE_DEF B GES AM_PH_DES @ MAGNETIC -3 0.28 !
TYPE_DEF 4 GES AM_PH_DES @ EXCESS_MODEL REDLICH-KISTER_KOHLER !
TYPE_DEF 5 GES AM_PH_DES AQUEOUS EXCESS_MODEL HKF !
TYPE_DEF 6 GES AM_PH_DES AQUEOUS HKF ELECTROSTATIC !
TYPE_DEF 7 GES AM_PH_DES AQUEOUS STATUS 02084000,,, !
TYPE_DEF 8 GES AM_PH_DES AQUEOUS MAJOR_CONST 1 H2O !
TYPE_DEF E AFTER AM_PH_DES LIQUID EXCESS MIXED-EXCESS
          A B LEGENDRE C A POLYNOM ,,,, !
TYPE_DEF T AFTER AM_PH_DES LIQUID TERN-EXT TOOP-KOHLER B A C ,,,, !
TYPE_DEF Q AFTER AM_PH_DES LIQUID TERN-EXT KOHLER FE CR NI !
TYPE_DEF C IF (PD AND PT AND SN) THEN TDB RESTORE_PHASE BCT_A5 !
TYPE_DEF D IF (PD AND (PT OR SN)) THEN TDB REJECT_PHASE BCC_A2 !
TYPE_DEF E IF ((NB OR TI OR V) AND (C OR N)) THEN
          GES AM_PH_DES @ COMP_SET ,, CR NB TI V: C N: !
TYPE_DEF F IF (ALO3/2 OR CRO3/2 OR FEO OR MNO OR SIO2) THEN
          GES AM_PH_DES LIQUID COMP_SET ,, ALN%,ALO3/2%,CRO3/2%,
          FEO%,FEO3/2%,MNO3/2%,MNS%,SIO2%,TIO2% : !

```

```

TYPE_DEF R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS Fe 0 0.6
      Ag 0 0.01 Al 0 0.05 Ca 0 0.05 Co 0 0.01 Cr 0 0.01
      Cu 0 0.02 Mg 0 0.05 Mn 0 0.05 Mo 0 0.05 Nb 0 0.05
      Ni 0 0.05 Pb 0 0.05 Si 0 0.10 Sn 0 0.02 Ti 0 0.05
      U 0 0.01 V 0 0.02 W 0 0.02 Zr 0 0.03
      B 0 0.01 C 0 0.01 H 0 0.01 N 0 0.01 O 0 0.01
      P 0 0.01 S 0 0.01 !

```

### 3.3.13 FTP\_FILE

**FTP\_FILE [filename] !**

The FTP file is a special function random file whose function names correspond to the record numbers where these record names and their functions are stored. The FTP file dramatically decreases search time for the associated database in the TDB module. The file is used for large substance databases along with a SEQ sequential or RND0 random file for storage of G0 parameters referring the functions named **FxxxxT** that are stored in the FTP file. The integer number **xxxx** is a search code used by TDB when such files are processed. No modification of this file type is allowed.

*Example:*

```
FTP_FILE TCPATH\DATA\[DATABASE]\FTP-FILE.TDB !
```

### 3.3.14 FUNCTION

```

FUNCTION [function name]*8 [lowest temp. limit]
      [expression 2]; [upper temp. limit 2] Y
      [expression 1]; [upper temp. limit 1] Y
      [expression 3]; [upper temp. limit 2] Y
      ..... ; ..... Y
      [expression n-1]; [upper temp. limit n-1] Y
      [expression n]; [upper temp. limit n] N {Ref. Index} !

```

GES has the capability to use predefined functions in the expression (TP-Function) of a Gibbs energy parameter or in other functions. This is often used when several parameters (or functions) have a common sub-expression, such as for metastable modifications of elements. The FUNCTION keyword can appear in both files for database definition and sequential storage, but not in FTP files. A valid function name can have up to 8 characters.

A function always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) that are coded as mathematical relations of constants, functions of stable variables (T and P) and other entered functions (normally with a # suffix, e.g. +3\*GHSERAL#). For further information, see *Section 11.2.5* (Functions of Temperature and Pressure). The expression is a FORTRAN-like expression and operators +, -, \*, = and \*\* can be used (\*\* only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. Each expression (TP-Function) should end with a semicolon “;”, and be followed by its upper applicable temperature limit and a continuation indicator (Y for continuing with the next expression, or N for ending the function's expression). If there is no continuation after a specific expression (TP-Function), the reference index can optionally be given after the N indicator.

A complete/valid function entry can be written in several continuation lines if the function's expression (TP-Function) is too long or if there are more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.

One should avoid entering functions like

```

FUNCTION GHSERXY 298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !

```

Such a function will be read by the TDB module as 1000+1058\*T-38.9\*T\*LOG(T)+GFUNXY#, rather than as -1000+1058\*T-38.9\*T\*LOG(T)+GFUNXY#.

The reason for this is that the TDB module will concatenate all lines and remove extra spaces before trying to enter the function in the GES5 workspace. Thus, the - sign will be taken as delimiter between 298.15 and 1000, and the function will wrongly become

```
FUNCTION GHSERXY 298.15 1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

This mistake can be avoided by giving at least one empty space as the first character of a new line, such as

```
FUNCTION GHSERXY 298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

which will be correctly read as

```
FUNCTION GHSERXY 298.15 -1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Therefore, it is recommended to *always have at least one empty space at the beginning of each continuation line*. Otherwise, the TDB module may issue some error messages when reading the function entry.

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a function is normally set by default as 298.15 K, in most cases; however, one may set another limit when it is applicable (according to experimental data and assessments). An upper-temperature limit (in Kelvin; followed by an Y or N sign) for the applicability of each TP-Function in a function must be given after the semicolon “;” sign immediately following the specific TP-Function; and the highest-temperature limit (in Kelvin) for the applicability of the current function is always followed by the N sign. If a negative number is given as the lowest-temperature limit, it will be assumed that there are breakpoints in pressure for this function; in such a case, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function will also be taken as pressure limit values (in Pascal).

The temperature/pressure limits for the functions are checked during calculations. An indicator will be set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation will be conducted using the TP-Function valid in the nearest temperature/pressure range.

Note that, in general, a function must be defined before it is referred. However, this rule may be neglected by suffixing a number sign “#” directly on the function name (such as +3\*GHSERAL#). However, this has been further simplified since TCCN/TCW1, where functions no longer need to be suffixed with #. A function that is used in a parameter (or other functions) but has never defined in the currently-used database will be listed at the end of the TDB command GET\_DATA. A user of an unsolicited database should beware when he gets such a list, and contact the database supplier.

The optional reference index {Ref. Index} is an integer number indicating where to find the particular function in a special reference file. The references are listed when doing the GET\_DATA command in the TDB module. They may also be listed in the GES module with the command LIST\_DATA with the option R. For accounting the reference indices, see also the keyword REFERENCE\_FILE.

The reference index field can also be an abbreviation (such as REF:250, REF\_002, or REF-SGTE) simply denoting the original reference; in this case, the reference may not be obtained when issuing the TDB command GET\_DATA or the GES command LIST\_DATA (with the option R).

However, since TCCN/TCW1, the references directly coded in the database definition file (\*\*\*)setup.TDB that starts with a letter can be shown when issuing the TDB command GET\_DATA or the GES command LIST\_DATA (with the option N or R). Normally, such references must be located after the LIST\_OF\_REFERENCE keyword. It is recommended to use reference code names such as REF001, REF018, etc. The reference list, which is generated by the GES command LIST\_DATA <file> with the N or R option, is thus also possible to be directly read by the TDB module.

Since TCCS/TCW5, the TDB module can now selectively retrieve functions which are necessary for a defined system from a database that has functions stored in its setup file or SEQ sequential function file, while all other functions irrelevant for the defined system are simply ignored and will not be saved in associated GES5 and POLY3 workspaces. Previously, this can only done for large databases that have functions stored in RND1 random or FTP function files.

*Examples:*

```
FUNCTION GFREE 298.15 1000+GFUNXY#; 6000 N !
FUNCTION GFUNXY 298.15 -1000+200*T+30*T*LOG(T); 6000 N 505 !
FUNCTION GO_CAO 298.15 -663538.11+352.67749*T-57.7533*T*LN(T)
```

```
+5.3895E-03*T**2-8.879385E-07*T**3+575530*T**(-1);  
1400.00 Y -625196.99+78.896993*T-20.40145*T*LN(T)  
-1.112923E-02*T**2+5.1896733E-07*T**3-6917350*T**(-1);  
2900.00 Y -499226.55-490.37695*T+51.95912*T*LN(T)  
-2.961051E-02*T**2+1.4033905E-06*T**3-48114685*T**(-1);  
3172.00 Y -587711.89+375.04117-62.76*T*LN(T);  
6000.00 N REF020 !
```

### 3.3.15 PARAMETER

```
PARAMETER [GES parameter name] [lowest temp. limit]
  [expression 1]; [upper temp. limit 1] Y
  [expression 2]; [upper temp. limit 2] Y
  [expression 3]; [upper temp. limit 2] Y
  ..... ; ..... Y
  [expression n-1]; [upper temp. limit n-1] Y
  [expression n]; [upper temp. limit n] N {Ref. Index} !
```

The PARAMETER keyword can appear in both files for database definition and sequential storage, but not in FTP files. After the keyword PARAMETER, a valid **GES parameter name** should be given.

It is used for defining standard Gibbs energies (*i.e.*, the G parameters for Gibbs energy of formations) of all valid end-members of various stoichiometric and solution phases, and excess Gibbs energies (*i.e.*, the L parameters for Gibbs energy of interactions) of all binary, ternary, quaternary or higher-order interactions in various solution phases; both standard Gibbs energies and excess energies can also have parameters for contributions from PT-depended volume variations (*i.e.*, the V0, VA, VB, VC and VK parameters for molar volume, thermal expansivity, bulk modulus, isothermal compressibility and high-pressure fitting parameter), magnetic ordering (*i.e.*, the TC and BM parameters for Curie temperature and Bohr magneton number) and hypothetical electrostatic interactions (*i.e.*, BM parameter for Born functions  $\omega_{Pr,Tr}$  of aqueous solute species).

As described in *Section 11.4 (Thermodynamic Parameters)* in the *Chapter 11 (GES – Gibbs Energy System)* of the **TCCS User's Guide**, the general form of a parameter is:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx> <expression> <yyy>
  <keyword Y or N> <zzz> !
```

where

identifier	is the parameter type;
phase	is the phase name (maximum 24 characters);
constituent array	is the specific constituent array in the phase;
digit	is the degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted;
expression	is the mathematical relation to describe the parameter;
xxx and yyy	are the low and high temperature limits respectively for the applicable temperature range of the parameter expression;
keyword Y or N	is the indicator on if there is continuation for the parameter expression or not;
zzz	is the reference index/number for the assessment of this parameter; and
sign “!”	is used to indicate that the current parameter definition is ended.

Also as described in *Section 11.10.5 (ENTER\_PARAMETER)* in the *Chapter 11 (GES – Gibbs Energy System)* of the **TCCS User's Guide**, The **GES parameter name** has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Examples of parameter names:

G (GAS, C1O2)	The Gibbs energy of formation of a CO2 molecule in gas.
G (FCC, Fe:VA)	The Gibbs energy of formation of fcc Fe with interstitials.
L (LIQ, Fe, Cr;0)	The regular solution parameter for Fe and Cr in liquid.
L (LIQ, Fe, Cr;1)	The sub-regular solution parameter.
TC (BCC, Fe:Va)	The Curie temperature of bcc Fe.
BMAGN (BCC, Fe:Va)	The Bohr magneton number parameter of bcc Fe.

The **GES parameter name** consists of several parts. The first is a *type-identifier*. The following *type-identifiers* are legal:

- ☞ G Standard energy parameter (Gibbs energy of formation);
- ☞ L Excess energy parameter (Gibbs energy of interaction);
- ☞ TC Curie temperature for magnetic ordering;
- ☞ BMAGN or BM Bohr magneton number for magnetic ordering  
(or Born function  $\omega_{Pr,Tr}$  for aqueous solute species).

One may also use G for interaction parameters; and on output list (performed by the GES command LIST\_PARAMETER or LIST\_PHASE\_DATA) the type-identifier L is always used for interaction parameters. Note that the type-identifier BM is also used for Born functions  $\omega_{Pr,Tr}$  of aqueous solute species since TCCP/TCW2.

The following new types of identifiers are available since TCCN/TCW1 and are further expanded since TCCR/TCW4:

- ☞ V0 Molar volume at 298.15 K and 1 bar (a numeric value only);
- ☞ VA Integrated thermal expansivity  $\int_{298.15}^T \alpha(T) dT$
- ☞ VB Bulk modulus at 1 bar;
- ☞ VC Isothermal compressibility;
- ☞ VK High-pressure fitting parameter.

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.

Specifying the phase name always in UPPER-cases is recommended; however, if one would prefer to write it as a mixture of UPPER-case and lower-case in a database, the TDB module will then automatically convert all lower-cases to UPPER-cases, as the GES module only recognizes UPPER-case phase names. It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, LIQUID:L, IONIC-LIQ:Y, SPINEL:I, FCC\_L12:F, HCP\_D021:F, BCC\_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name in the PARAMETER keyword.

The constituent array consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, *e.g.*, the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents. Note that solution phases with sublattices may have interacting constituents in each sublattice.

One may use an asterisk, “\*”, to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, L (FCC\_L12,AL,NI:\*) means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the FCC\_L12 solution phase, while it is independent of all constituents on the second sublattice. A interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk “\*” is calculated with the term of  $[1 - \sum Y(\text{specified constituents})]$ , which implies that in an A-B binary system the following three L parameters are identical (but in higher-order systems, they are different):

- L (phase,A,B) is multiplied with  $X(A) * X(B)$
- L (phase,A,\*) is multiplied with  $X(A) * (1 - X(A))$
- L (phase,B,\*) is multiplied with  $X(B) * (1 - X(B))$

A parameter always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) that are coded as mathematical relations of constants, functions of stable variables (T and P) and entered functions (normally with a # suffix, *e.g.* +3\*GSERAL#). However, this has

been further simplified since TCCN/TCW1, where functions no longer need to be suffixed with #. For further information, see *Section 11.2.5* (Functions of Temperature and Pressure). The expression is a FORTRAN-like expression and operators +, -, \*, = and \*\* can be used (\*\* only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. Each expression (TP-Function) should end with a semicolon “;”, and be followed by its upper applicable temperature limit and a continuation indicator (Y for continuing with the next expression, or N for ending the parameter's expression). If there is no continuation after a specific expression (TP-Function), the reference index can optionally be given after the N indicator.

A complete/valid parameter entry can be written in several continuation lines if the parameter's expression (TP-Function) is too long or if there are more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.

One should avoid entering parameters like

```
PARAMETR G(LIQUID,A,B) 298.15
-2000+4568*T+2*GFUNAB#; 6000 N !
```

Such a parameter will be read by the TDB module as 2000+4568\*T+2\*GFUNAB#, rather than as -2000+4568\*T+2\*GFUNAB#.

The reason for this is that the TDB module will concatenate all lines and remove extra spaces before trying to enter the parameter in the GES5 workspace. Thus, the - sign will be taken as delimiter between 298.15 and 2000, and the parameter will wrongly become

```
PARAMETR G(LIQUID,A,B) 298.15 2000+4568*T+2*GFUNAB#; 6000 N !
```

This mistake can be avoided by giving at least one empty space as the first character of a new line, such as

```
PARAMETR G(LIQUID,A,B) 298.15
 -2000+4568*T+2*GFUNAB#; 6000 N !
```

which will be correctly read as

```
PARAMETR G(LIQUID,A,B) 298.15 -2000+4568*T+2*GFUNAB#; 6000 N !
```

Therefore, it is recommended to ***always have at least one empty space at the beginning of each continuation line***. Otherwise, the TDB module may issue some error messages when reading the parameter entry.

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a parameter is normally set by default as 298.15 K, in most cases; however, one may set another limit when it is applicable (according to experimental data and assessments). An upper-temperature limit (in Kelvin; followed by an Y or N sign) for the applicability of each TP-Function in a parameter must be given after the semicolon “;” sign immediately following the specific TP-Function; and the highest-temperature limit (in Kelvin) for the applicability of the current parameter is always followed by the N sign. If a negative number is given as the lowest-temperature limit, it will be assumed that there are breakpoints in pressure for this parameter; in such a case, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current parameter will also be taken as pressure limit values (in Pascal).

The temperature/pressure limits for the parameters are checked during calculations. An indicator will be set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation will be conducted using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index {Ref. Index} is an integer number indicating where to find the particular parameter in a special reference file. The references are listed when doing the GET\_DATA command in the TDB module. They may also be listed in the GES module with the command LIST\_DATA with the option R or N. For accounting the reference indices, see also the keyword REFERENCE\_FILE.

The reference index field can also be an abbreviation (such as REF:250, REF\_002, or REF-SGTE) simply denoting the original reference; in this case, the reference may not be obtained when issuing the TDB command GET\_DATA or the GES command LIST\_DATA (with the option R or N).

However, since TCCN/TCW1, the references directly coded in the database definition file (\*\*setup.TDB) that starts with a letter can be shown when issuing the TDB command GET\_DATA or the GES command LIST\_DATA (with the option R or N). Normally, such references must be located after the

LIST\_OF\_REFERENCE keyword. It is recommended to use reference code names such as REF001, REF018, *etc.* The reference list, which is generated by the GES command LIST\_DATA <file> with the N option, is thus also possible to be directly read by the TDB module.

*Examples:*

```
PARAMETER G(BCC,FE:VA) 298.15 1000+200*T+...; 6000 N 91DIN !
PARAMETER TC(BCC,FE:VA) 298.15 +1043; 6000 N 91DIN !
PARAMETER BMAGN(BCC,FE:VA) 298.15 +2.22; 6000 N 91DIN !
PARAMETER G(SIGMA,FE:CR:CR;0) 298.15 1000+200*T+...; 6000 N 101 !
PARAMETER G(LIQUID,AL;0) 298.15 +11005.553-11.840873*T
+7.9401E-20*T**7+GHSERAL#;
933.60 Y +10481.974-11.252014*T+1.234264E+28*T**(-9)+GHSERAL#;
2900.00 N REF:283 !
PARAMETER G(BCC_A2,PB:C) 298.15 UN_ASS#; 300 N REF:0 !
PARAMETER G(BCC_A2,NI:C;0) 298.15 +GHSERNI#+3*GHSERCC#
+400000-100*T; 6000 N REF071 !
PARAMETER G(BCC_A2,MN:VA) 298.15 +GMNBCC#; 6000 N REF285 !
PARAMETER BM(AQUEOUS,OH-1) 298.15 +Z0002PW0#; 1600 N 155 !
PARAMETER L(BCC,FE,CO:VA;0) 298.15 1000+200*T+...; 6000 N !
PARAMETER L(BCC,FE,CO:VA;1) 298.15 1000+200*T+...; 6000 N !
PARAMETER L(BCC,FE,CO:VA;2) 298.15 1000+200*T+...; 6000 N !
PARAM TC(BCC_A2,CO,MO:VA;0) 298.15 -3700; 6000 N R454 !
PARAM TC(BCC_A2,CO,MO:VA;1) 298.15 +2300; 6000 N R454 !
PARAM BMAGN(BCC_A2,CO,MO:VA;0) 298.15 -3.445; 6000 N R454 !
PARAM V0(BCC_A2,CR,FE:VA;0) 298.15 +ZERO#; 6000 N REF06V !
PARAM V0(BCC_A2,CR,FE:VA;1) 298.15 -1.10524097E-7; 6000 N REF06V !
PARAM V0(BCC_A2,CR,FE:VA;2) 298.15 +1.40024130E-7; 6000 N REF06V !
PARAM VA(BCC_A2,CR,FE:VA;0) 298.15 -6.49444634E-6*DELTAT#; 6000 N REF06V !
PARAM VA(BCC_A2,CR,FE:VA;1) 298.15 +2.91269321E-5*DELTAT#; 6000 N REF06V !
```

### 3.3.16 OPTIONS

**OPTIONS** /[alloy name]([composition limitations for all alloying elements]) !

The OPTIONS keyword defines an “alloy” in a database. It has been available since TCCM. An alloy has a name, a major component and a number of alloying elements. The purpose for defining an alloy is to be able to inform the user about applicable composition limits of the current database in applications to that particular type of alloy. It is possible to have several alloys in the same database. The alloys are given after the OPTIONS keyword in the database.

The alloy name must be preceded by a slash “/” and terminated by the opening parenthesis, and no spaces are allowed in between. The alloy name is maximum 8 characters. After the parenthesis, follows the major element and a parenthesis with its minimum mass and minimum mole percent given inside. Then, follows the alloying element names, each with its maximum mass and mole percent given within parenthesis. There must a space between definitions for each alloying element. The alloy definition is terminated by a closing parenthesis, and the whole OPTIONS keyword by the exclamation mark “!”.

*Example:*

```
OPTIONS /SSteel(Fe(60,60) CR(30,30) NI(15,15) SI(1,1) N(.1,1)) !
```

### 3.3.17 TABLE

**TABLE** [name]\*8 [start temp] [end temp] [delta temp] [table values] !

The TABLE keyword can appear in both files for database definition and sequential storage, but not in FTP files. It makes a table of Gibbs energy as a function of temperature where the values are given from the start temperature to the end temperature, at a step of the delta temperature.

It is also recommended to *always have at least one empty space at the beginning of each continuation line.* Otherwise, the TDB module may issue some error messages when reading the table entry.

*Example:*

```
TABLE DEMENTAB 1000.0 1500.0 100.0 -2912.9008 -2834.2416 -2755.5824
-2677.7600 -2600.7744 -2524.2072 !
```



### 3.3.18 ASSESSED\_SYSTEMS

**ASSESSED\_SYSTEM** [descriptions on special treatments for specific assessed systems]\*8000 !

The keyword `ASSESSED_SYSTEMS` can be included in the database definition file (the `***setup.TDB` file). A maximum of 8000 characters after the keyword (to describe some special options when the TDB, GES and POLY models deal with the existing systems with assessed data) is allowed until the exclamation mark "!".

*Since TCCP/TCW2 and DICTRA22, several `ASSESSED_SYSTEMS` keywords can be used in the same TDB file in order to have more lists of assessed systems; in other word, the number of the `ASSESSED_SYSTEMS` keyword entries in the same TDB file is not limited.*

The assessed systems in the database, and their special treatment options, are typed after the keyword. The elements (should always be in UPPER CASE) in each assessed system must be in alphabetical order and be separated by a hyphen, like `C-FE` for the Fe-C system. A space must be between each assessed system. Information on assessed binary, ternary or higher-order systems may also be given in this way. Note that a ternary system like `C-CR-FE` does not imply that the binary `C-CR`, `C-FE` and `CR-FE` are assessed! There is no way to indicate partially assessed systems.

There is a field to give some descriptive information for a specific system, with various options on:

- ◆ How to reject or restore phase(s) from the current database in the TDB module;
- ◆ How to set major constituent(s) in the first composition set and to set a second composition set for a specific phase available in the current database in the GES module; *and*
- ◆ How to calculate this specific system in the POLY module.

This is the facility used by the BIN (binary phase diagrams) and TERN (ternary phase diagrams) modules in the Thermo-Calc software/database package.

The descriptive information must immediately follow the specific system name, and must be enclosed within parenthesis "(" and ")", and the left parenthesis must follow directly after the system, such as

```
AL-NI (TDB +L12 ;G5 C-S:L12/NI:AL:VA ;P3 STP:.8/1200/1 STP:.2/600/1)
```

The information is specific to Thermo-Calc, and intended to be cryptic. As in the above example,

- The syntax `TDB` means that the commands to the TDB module proceed, and `+L12` in the example means that the phase called `L12` should be restored (it has been rejected by default).
- The directive `;G5` means that the following are commands to the GES module. `C_S`: means creating a second composition set, after the colon follows the phase name and after the slash the major constituents.
- After the directive `;P3` follows commands to the POLY module. `STP:` means setting a start point with the value of the X-axis first (composition for the second element in a binary system), the slash separates the Y-axis value (temperature), and possibly one or more directions (-1, 1, -2 or 2).

A summary of the allowed syntax is:

- TDB accepts
  - `+phase` and `-phase` for restore/reject (the syntax `-*` to reject all phases should not be used).
- ;G5 accepts
  - `MAJ:phase/constituent-array` for major constituents of the first composition set.
  - `C_S:phase/constituent-array` for a second composition set.
- ;P3 accepts
  - `TMM:lt/ht` for the low-/high-temperature limits (`lt` and `ht`; for instance `TMM:500/4000`) suitable for calculating phase diagrams and property diagrams of a binary system.
  - \* for a default start point which is set as
    - for a binary system:* at the composition  $X(2^{\text{nd}} \text{ element}) = .1234$ , temperature  $T = 1100 \text{ K}$  and with the default directions; *or*
    - for a ternary system:* at the compositions  $X(2^{\text{nd}} \text{ element}) = .1234$  and  $X(3^{\text{rd}} \text{ element}) = .1234$  and with the default directions.

STP:x/t/d1/d2/d3 for a specific start point in a binary system which is set as at the composition  $X(2^{\text{nd}} \text{ element})=x$  and temperature  $T=t$  (in K), and with the directions d1, d2 and/or d3.

STP:x1/x2/d1/d2/d3 for a specific start point in a ternary system which is set as at the compositions  $X(2^{\text{nd}} \text{ element})=x1$  and  $X(3^{\text{rd}} \text{ element})=x2$  and with the directions d1, d2 and/or d3.

The direction(s) can be defined as -1, 1, -2 or 2. If no direction is specified, all default directions will be used (meaning no ADD command will be enforced in the POLY module).

If only one start point is specified, the direction(s) may be omitted; if more than one start point are specified, at least one direction for each start point must be given for all start points.

Each entry for a specific binary or ternary sub-system can be written in one or several lines (each line with 78 characters).

Some other examples given below may clarify:

```

ASSESSED_SYSTEMS
AL-NI(TDB +L12 +BCC_B2 ;G5 C_S:L12/NI:AL:VA
      ;P3 STP:.8/1000/1 STP:.45/700/1 STP:.7/700/1)
AL-PB(TDB -HCP -BCC
      ;G5 MAJ:LIQ/AL MAJ:FCC/AL:VA C-S:LIQ/PB C-S:FCC/PB:VA ;P3 *)
CR-FE(;G5 C-S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
AG-CU(;G5 MAJ:FCC/AG:VA C_S:FCC/CU:VA ;P3 STP:.3/1000)
C-NB(;P3 STP:.9/1100/1)
C-SI(;P3 *)
CO-CR(;G5 MAJ:FCC/CO:VA C_S:FCC/CR:VA ;P3 STP:.1/1100)
CR-FE(TDB -HCP ;G5 C_S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
CR-NI(;P3 *)
CR-W(;G5 MAJ:BCC/W:VA C_S:BCC/CR:VA
      ;P3 TMM:500/4000 STP:.3/700/1 STP:.3/1800/2 )
CU-FE(TDB -HCP ;G5 MAJ:LIQ/CU MAJ:FCC/FE:VA C_S:FCC/CU:VA
      ;P3 STP:.9/1400)
FE-N(TDB +FE4N ;P3 *)
FE-O(TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:O-2 MAJ:ION_LIQ/FE+2:VA
      ;P3 STP:.2/2000/1 )
FE-S(TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:S MAJ:ION_LIQ/FE+2:S-2 ;P3 *)
AL-MG-SI(;P3 *)
C-CR-FE ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA ;P3 *) !

```

Note that the semicolon “;” is a part of the ;G5 and ;P3 directives. A long descriptive information can be written in more than one line, such as for the AL-NI, AL-PB, CU-FE and FE-O systems shown above.

The directive “;P3 \*” is needed if the default start point should be used. If there is no ;P3 directive, the BIN or TERN module will generate some 20 different start points in order to cover all possible compositions and temperatures (for a binary system) or all possible compositions (for a ternary system under any specific temperature).

Since TCCS/TCW5, the GES-action parts (enforced by the syntaxes MAJ:phase/constituent-array for major constituents of the first composition set, and C\_S:phase/constituent-array for a second composition set) and POLY-action parts (enforced by the syntax STP:x/t/d1/d2/d3 for a specific start point in a binary system, or STP:x1/x2/d1/d2/d3 for a specific start point in a ternary system) becomes much less important (and usually unnecessary for some cases), thanks to that the implemented Global Minimization Technique and further improved stepping/mapping routines can automatically detect and create appropriate additional composition set(s) where it is necessary and can generally handle the starting point(s) in an automatic and comprehensive way. However, if the POLY-action syntaxes STP:x/t/d1/d2/d3 or STP:x1/x2/d1/d2/d3 are used in the database, the TCCS/TCW5 software-version will assume that the user (database-manager) knows exactly what he is doing (regarding enforced starting points), and thus no automatic starting points will be created/used during the BIN/TERN-module calculations.

### 3.3.19 REFERENCE\_FILE

**REFERENCE\_FILE** [file name] !

The keyword `REFERENCE_FILE` takes a reference file name as its argument. This reference file (*that must be edited in a very restrictive way and must also be saved as a blocked file with a fixed line-length for each line in the file, as described below*) contains a complete list of the references for the various parameters (and sometimes functions) in the database. The file must have a fixed record structure: each reference entry with one or several records, and each record with 78 characters written in one single line; and no empty space is allowed at the beginning of all lines in the file. If there are more than one record entered for a reference entry, all the continuation lines must start with a "&" sign. The line number of the first record for a specific reference entry is then accounted as the unique integer for that specific reference, which will be referred when a parameter or function calls this integer as the optional {Ref. Index}. See keyword `PARAMETER` or `FUNCTION` about specifying a reference index.

*Example:*

```

/-1<G>                T.C.R.A.S. Class 1
AG1.64TE1            THERMODATA 01/93
&28/01/93
&SILVER 1.64-TELLURIDE. Solid Standard State.
AG1                  HULTGREN SELECTED VAL.          SGTE **
&AT.WEIGHT 107.870,STANDARD STATE:CODATA KEY VALUE.MPT=1234.93K.
&--U.D. 30/10/85 .
AG1<G>                T.C.R.A.S Class: 1
AG1/+1<G>            T.C.R.A.S Class: 1
AG1BR1              N.P.L.                          SGTE **
&Tfusion uncertain and heat vaporization estimated.
AG1BR1<G>            THERMODATA 01/93
&28/01/93
&Gaseous Standard State.
AG1BR103            BARIN & KNACKE.SUPPL.REF:62,* SGTE **
&AGO3BR             SILVER OXYTRIBROMIDE

```

In the above example, the unique integers of related references (for assessed elements, species, phases, interactions, etc.) are:

```

1  /-1<G>
2  AG1.64TE1
5  AG1
8  AG1<G>
9  AG1/+1<G>
10 AG1BR1
12 AG1BR1<G>
15 AG1BR103

```

### 3.3.20 LIST\_OF\_REFERENCE

**LIST\_OF\_REFERENCE**

**NUMBER SOURCE**

[REFxxx] '[Detailed reference]'

.....  
 ..... !

The keyword `LIST_OF_REFERENCE` starts a reference list that is directly coded in the database definition file (`***setup.TDB`). This is a new feature since the TCC version N. Its argument begins on the following line, and normally has an explanation line (`NUMBER SOURCE`) that is followed by various reference codes. Each reference code may occupy one or more lines (each line with maximum 78 characters), but must have a reference code name (that starts with a letter) and the detailed reference information (that is written within two single-quotation marks, "' ..... '"). It is recommended to use reference code names such as `REF001`,

REF018, etc. A maximum of 40000 characters (in TCCP/TCW2, extended from 2000 in TCCN/TCW1) after the keyword is allowed until the exclamation mark “!”.

Such a reference list can be shown when issuing the TDB command `GET_DATA` or the GES command `LIST_DATA` (with the R option). The reference list, which is generated by the GES command `LIST_DATA <file>` with the N option, has this structure, and is thus possible to be directly read by the TDB module.

*Example:*

```
LIST_OF_REFERENCES
NUMBER SOURCE
REF283 'Alan Dinsdale, SGTE Data for Pure Elements,
      Calphad Vol 15(1991) p 317-425,
      also in NPL Report DMA(A)195 Rev. August 1990'
REF224 'P-Y Chevalier, Thermochimica Acta, 130 (1988) p 33-41; AG-SI'
!
```

### 3.3.21 ADD\_REFERENCE

```
ADD_REFERENCE
[REFxxx] '[Detailed reference]'
.....
..... !
```

With the directive `LIST_OF_REFERENCES`, it has been possible to include the references in the same file as that containing parameters for a long time. But for large databases the space for references has not been big enough. Now a new directive called `ADD_REFERENCES` makes it possible to have virtually unlimited number of references. The use of this directive is the same as that of `LIST_OF_REFERENCES`, and must be used after the `LIST_OF_REFERENCE` section. Several `ADD_REFERENCES` section can be used in a single database, if there are too many references.

However, it is recommended to always start with an empty one (such as the `DUMP0` reference in the following example) as the first entry to make sure that all references will be listed out appropriately as retrieving data by issuing the `GET_DATA` command.

*Example:*

```
ADD_REFERENCES
DUMP0 'Empty reference 1'
REF275 'A. Fernandez Guillermet, Z. Metallkde. Vol 79(1988) p.524-536,
      TRITA-MAC 362 (1988); C-CO-NI AND C-CO-FE-NI'
REF393 'K. Frisk, Metall. Trans. Vol 21A (1990) p 2477-2488,
      TRITA 0409 (1989); CR-FE-N'
REF1096 'P. Gustafson, Metall. Trans. 19A(1988) p 2547-2554,
      TRITA-MAC 348, (1987); C-CR-FE-W'
!
```

### 3.3.22 CASE and ENDCASE

```
CASE [ELEMENT/SPECIE/PHASE] !
  IF (boolean algebra on element, species or phase names) THEN
    [GES/POLY/TDB command] !
ENDCASE !
```

The keyword CASE takes, as its argument, a definition on which type of the following boolean algebra will operate. A simple boolean algebra using AND and OR with a maximum of 4 levels of parentheses will work. The CASE construction must end with the ENDCASE keyword. This makes it possible to have additional TDB, GES or POLY commands executed depending on the user selection of elements, species or phases.

*Example 1:*

```
CASE [ELEMENT] !
  IF ((CR OR TI OR V) AND N)
  THEN GES AM_PH_DES @ C_S ,, CR MO TI V:C N: !
ENDCASE !
```

*Example 2:*

```
CASE ELEMENT !
  IF (O) THEN TDB DEFINE_SYSTEM_ELEMENTS /- !
ENDCASE !
```

### 3.3.23 VERSION\_DATA

```
VERSION_DATE [string]*78 !
```

The string (denoted as the version date of the database) is shown when the TDB command DATABASE\_INFORMATION is performed.

### 3.4 DICTRA Extensions to the Database Definition File Syntax

Software packages for simulation of diffusional phase transformations, such as DICTRA, needs both thermodynamic data and kinetic data (*i.e.*, diffusivities or mobilities). Naturally, the handling and storage of kinetic data will also benefit from the use of some kind of database management. Thus, the TDB database definition file syntax has been extended to incorporate some new keywords needed for storing kinetic data.

#### 3.4.1 PARAMETER

```
PARAMETER [special GES parameter name] [low temp. limit]
          [expression 1]; [upper temp. limit 1] Y
          [expression 2]; [upper temp. limit 2] Y
          [expression 3]; [upper temp. limit 2] Y
          ..... ; ..... Y
          [expression n-1]; [upper temp. limit n-1] Y
          [expression n]; [upper temp. limit n] N {Ref. Index} !
```

The keyword `PARAMETER` allows to enter all types of normal GES parameters for thermodynamic data (as previously presented in *Section 6.3.15*), as well as five special extensions suitable for kinetic data used in the DICTRA software. Valid extensions to special GES parameter names are:

- MQ ⇒ Activation enthalpy for mobility equation.
- MF ⇒ Pre-exponential factor for mobility equation.
- DQ ⇒ Activation enthalpy for diffusivity equation.
- DF ⇒ Pre-exponential factor for diffusivity equation.
- VS ⇒ Volume counted per mole of volume carrying species.

*Examples:*

```
PARAMETER MQ(BCC,FE:VA) 298.15 1000+200*T+...; 6000 N !
PARAMETER MF(BCC,CO:VA) 298.15 1000+200*T+...; 6000 N !
PARAMETER DQ(FCC,FE:VA) 298.15 1043+...; 6000 N 10 !
PARAMETER DF(FCC:CR:C ) 298.15 1000+200*T+...; 6000 N 10 !
PARAMETER VS(FCC) 298.15 1000+200*T+...; 6000 N 11 !
```

#### 3.4.2 DIFFUSION

```
DIFFUSION [model keyword] [phase name] [additional parameter(s)] !
```

The keyword `DIFFUSION` specifies what type of diffusion model to use for a phase if the default model is not desired. The default model calculates the full diffusion matrix. A diffusivity is calculated from the different mobilities and the thermodynamic factors. The former ones are calculated as:

$$M = \exp(\sum MF/RT) \exp(\sum MQ/RT) / RT$$

where  $\sum$  stands for a weighted summation of the different MF's and MQ's plus possibly a Redlich-Kister term. Valid model keyword are:

- NONE  
no diffusion in this phase
- DILUTE  
constitution list of dependent species in each sublattice must be given as an additional parameter. Only the diagonal terms in the diffusion matrix are calculated.  $D = \exp(\sum DF/RT) \exp(\sum DQ/RT)$
- SIMPLE  
constitution list of dependent species in each sublattice must be given as additional parameter. Only the diagonal terms in the diffusion matrix are calculated.  $D = \sum DF + \sum DQ$
- MAGNETIC

the so-called ALPHA and ALPHA2 parameters must be given as additional parameters. ALPHA is for the substitutional magnetic model and ALPHA2 for the interstitial one. By appending an "&" (the and sign) and a species name after the alpha keyword one can supply individual values for the different species. The full diffusion matrix is calculated.

*Examples:*

```
DIFFUSION NONE SIGMA !
DIFFUSION DILUTE CEMENTITE : FE : C : !
DIFFUSION MAGNETIC BCC_A2 ALPHA=0.3 ALPHA2&C=1.8 ALPHA2&N=0.6 !
```

### 3.4.3 ZERO\_VOLUME\_SPECIES

**ZERO\_VOLUME\_SPECIES [list of species] !**

In the DICTRA software, the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes. The keyword ZERO\_VOLUME\_SPECIES uses a list of which species are to be considered as zero volume ones for an argument.

*Example:*

```
ZERO_VOLUME_SPECIES VA C N !
```

## 3.5 Examples of Database Definition Files

### 3.5.1 Example 1: A small steel database

```

TEMP-LIM 500.0 2000.0 !
$
$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !
ELEMENT VA VACUUM          0.0    0.0 0.0 !
ELEMENT C GRAPHITE         12.011 0.0 0.0 !
ELEMENT V BCC              50.9415 0.0 0.0 !
ELEMENT CR BCC-PARAMAGNETIC 51.996 0.0 0.0 !
ELEMENT FE FCC-PARAMAGNETIC 55.847  0.0 0.0 !
ELEMENT NI FCC-PARAMAGNETIC 58.69   0.0 0.0 !
ELEMENT MO BCC             95.94    0.0 0.0 !
ELEMENT W BCC              183.85  0.0 0.0 !
$
$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !
PHASE BCC      B1M  2 1.0 3.0 !
PHASE FCC      F2M  2 1.0 1.0 !
PHASE HCP      0    2 2.0 1.0 !
PHASE LIQUID   3    2 1.0 1.0 !
PHASE CEMENTITE 4    2 3.0 1.0 !
PHASE M23C6    4    2 23.0 6.0 !
PHASE M7C3     4    2 7.0 3.0 !
PHASE M6C      4    4 2.0 2.0 2.0 1.0 !
PHASE SIGMA    0    3 10.0 4.0 16.0 !
PHASE MU-PHASE 0    3 7.0 2.0 4.0 !
PHASE R-PHASE  0    3 27.0 14.0 12.0 !
PHASE GRAPHITE 4    1 1.0 !
$
$CONSTITUENT, PHASE-NAME : CONSTITUENTS !
CONSTITUENT BCC :V CR FE NI MO W:VA C: !
CONSTITUENT FCC :V CR FE NI MO W:VA C: !
CONSTITUENT HCP :CR FE NI:VA C N: !
CONSTITUENT LIQUID :C V CR FE NI MO W VA:VA C: !
CONSTITUENT CEMENTITE :CR FE:C: !
CONSTITUENT M23C6 :CR FE:C: !
CONSTITUENT M7C3 :CR FE:C: !
CONSTITUENT M6C :FE:W:FE W:C: !
CONSTITUENT SIGMA :FE:V CR MO:FE V CR MO: !
CONSTITUENT MU-PHASE :FE:MO W:FE MO W: !
CONSTITUENT R-PHASE :FE:MO :FE MO: !
CONSTITUENT GRAPHITE :C: !
$
$TYPE DEFINITIIONS:
TYPE-DEFINITION 0 SEQ TCPATH\DATA\METDATA\TC-THEREST.TDB !
TYPE-DEFINITION 1 SEQ TCPATH\DATA\METDATA\TC-BCC.TDB !
TYPE-DEFINITION 2 SEQ TCPATH\DATA\METDATA\TC-FCC.TDB !
TYPE-DEFINITION 3 SEQ TCPATH\DATA\METDATA\TC-LIQUID.TDB !
TYPE-DEFINITION 4 SEQ TCPATH\DATA\METDATA\TC-CARBIDES.TDB !
TYPE-DEFINITION M SEQ TCPATH\DATA\METDATA\TC-CURIE-BOHR.TDB !
TYPE-DEFINITION B GES AM-PH BCC MAGNETIC -1 .4 !
TYPE-DEFINITION F GES AM-PH FCC MAGNETIC -3 .28 !
$
$DEFAULT_COMMANDS:
DEFAULT-COMMAND DEF_ELEMENT VA !
DEFAULT-COMMAND REJ_SYS-CONST LIQUID 1 VA !
$
$DATABASE INFORMATION:
DATABASE-INFO The following binary and ternary systems are available: '
  FE-CR-NI by Hertzman'
  FE-MO      Fernandez'
  FE-CR-C    Andersson'
  FE-W-C     Gustafson'
  FE-W       Andersson & Gustafson' !

```

## 3.5.2 Example 2: A personal database for the Sb-Sn system

```

$
$
$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !
ELEM VA VACUUM          0.0  0.0 0.0 !
ELEM MG HCP (A3)        24.305 0.0 0.0 !
ELEM SB RHOMBOHEDRAL (A7) 121.75 0.0 0.0 !
ELEM SN BCT (A5)        118.69 0.0 0.0 !
ELEM /- ELECTRON-GAS    0      0  0 !
$
$SPECIES, NAME, STOICHIOMETRIC-FORMULA !
SPECIE MG1 MG1!
SPECIE MG2 MG2!
SPECIE MG2+ MG/+2!
SPECIE SB1 SB1!
SPECIE SB2 SB2!
SPECIE SB4 SB4!
SPECIE SB3- SB/-3!
SPECIE SB5- SB/-5!
SPECIE SN1 SN1!
SPECIE SN4- SN/-4!
$
$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !
PHASE BCT              Z 1 1.0!
PHASE HCP              Z 1 1.0!
PHASE RHOMBO          Z 1 1.0!
PHASE GAS:G           Z 1 1.0!
PHASE LIQUID:L        Z 1 1.0!
PHASE IONICLIQ:Y     Z 2 1 1!
PHASE SPLIQ:Y         Z 2 1 1!
PHASE BMG3SB2:I      Z 2 3 2!
PHASE AMG3SB2:I      Z 2 3 2!
PHASE MG2SN:I         Z 2 2 1!
PHASE SBSN            Z 2 1 1!
PHASE SB2SN3         Z 2 2 3!
$
$CONSTITUENT, PHASE-NAME : CONSTITUENTS !
CONSTITUENT RHOMBO :SB SN:!
CONSTITUENT HCP :MG SN:!
CONSTITUENT BCT :SB SN:!
CONSTITUENT GAS:G :MG1 MG2 SB1 SB2 SB4 SN1:
  > Gas phase, using the Ideal EOS and Mixing Model. !
CONSTITUENT LIQUID:L :SB SN:!
CONSTITUENT IONICLIQ:Y :MG2+:SB SB3- SN SN4- VA:
  > This is the Ionic Liquid Solution Phase. !
CONSTITUENT SPLIQ:Y :MG2+:SB SB3- SN SN4- VA:!
CONSTITUENT BMG3SB2:I :MG2+:SB3- SB5- VA SN4-:!
CONSTITUENT AMG3SB2:I :MG2+:SB3- VA SN4-:!
CONSTITUENT MG2SN:I :MG2+ VA:SB3- SN4-:!
CONSTITUENT SBSN :SB SN:SB SN:!
CONSTITUENT SB2SN3 :SB:SN:!
$
$DEFAULT_COMMANDS:
DEFAULT-COM DEF-ELEM VA /-!
DEFAULT-COM REJ-PHASE LIQUID!
DEFAULT-COM REJ-PHASE SPLIQ!
$
$TYPE_DEFINITIONS:
TYPE-DEFINITION Z SEQ * !
$
$DATABASE_INFORMATION:
DATABASE_INFO The Sb-Sn system with isentropic temperatures!
$
$VERSION_DATE:
VERSION_DATE Last update 1986-05-18 11:39:49 !
$
$
$
$ HERE COMES THE THERMODYNAMIC DATA (expressed in functions & parameters):
$
FUNCTION MGLIQUID 298.15 -4630.90976+192.994374*T-34.0888057*T*LOG(T)
  -36544605.6*T**(-2); 6000 N!

```

```

$
FUNCTION MGSOLID 298.15 -8367.34+143.677876*T-26.1849785*T*LOG(T)
+4.858E-4*T**2-1.393669E-6*T**3+78950*T**(-1);
923.00 Y -13804.4772 +202.909445*T-34.0888057*T*LOG(T)
-3.65446056E7*T**(-2) +1.06753982E28*T**(-9); 6000 N!
$
FUNCTION SBLIQUID 298.15 9071.98+146.800*T-31.38*T*LOG(T)
-2.441646E8*T**(-2); 6000 N!
$
.....
..... <more>
$
FUNCTION LFCT 298.15 -17325.6+5.03600*T; 6000 N!
FUNCTION GFCTSBSN 298.15 LFCT+SBSOLID+SNSOLID+2948.291+3721.286;
6000 N!
FUNCTION ISB 298.15 15000; 6000 N!
FUNCTION ISN 298.15 47199.9-95.6270*T; 6000 N!
$
.....
..... <more>
$
PARAMETER G(RHOMBO,SB;0) 298.15 SBSOLID; 6000 N!
PARAMETER G(RHOMBO,SN;0) 298.15 2035+SNSOLID; 6000 N!
$
PARAMETER G(HCP,MG;0) 298.15 MGSOLID; 6000 N!
PARAMETER G(HCP,SN;0) 298.15 32000+SNSOLID; 6000 N!
PARAMETER G(HCP,MG,SN;0) 298.15 -69566-9.23183*T; 6000 N!
$
PARAMETER G(BCT,SN;0) 298.15 SNSOLID; 6000 N!
PARAMETER G(BCT,SB;0) 298.15 1000+SBSOLID; 6000 N!
PARAMETER G(BCT,SB,SN;0) 298.15 0.5*ISB+0.5*ISN; 6000 N!
PARAMETER G(BCT,SB,SN;1) 298.15 0.5*ISB-0.5*ISN; 6000 N!
$
PARAMETER G(IONICLIQ,MG2+:SB3-;0) 298.15 -204389-4.98506*T
-2.75637E9*T**(-2)+3*MGLIQUID+2*SBLIQUID; 6000 N!
PARAMETER G(IONICLIQ,MG2+:SN4-;0) 298.15 -98639.5+881.073*T
-174.523*T*LOG(T)-1.79808E9*T**(-2); 6000 N!
PARAMETER G(IONICLIQ,MG2+:SB;0) 298.15 SBLIQUID; 6000 N!
$
.....
..... <more>
$

```

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