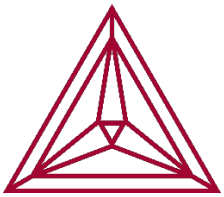
Database Manager User Guide

Version 2015b



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1. Contents

2. Thermodynamic and Kinetic/Mobility Databases

This document describes how to define and construct a thermodynamic or kinetic database. It includes details about the data structures and formats of the Thermo-Calc databases as well as the DICTRA database-extensions.

The Thermo-Calc databases are created and maintained in the Thermo-Calc Database Format (TDB) which is an international standard for the CALPHAD-type thermodynamic calculations and kinetic simulations. This document gives a full description of the TDB format (with the DICTRA database extension) and is a comprehensive guide about how to create and manage a Thermo-Calc (and DICTRA) database.

Usually, a Thermo-Calc or DICTRA database is constructed as a single text file with an extension of TDB, for example, `PAQS2setup.TDB`. For some databases (especially large databases used with older versions of Thermo-Calc or DICTRA) a database may consist of one primary-definition file (`***setup.TDB`) and several additional-definition TDB files (such as `***param.TDB`, `***funct.TDB`, `***refer.TDB`, etc. These are built for a variety of defined parameters, functions, references and so forth, and are linked to the `***setup.TDB` file through the correct use of the TYPE_DEFINITION and/or FTP_FILE commands inside the `***setup.TDB` file.

With a current version of Thermo-Calc, TC-PRISMA and Thermo-Calc Software Development Kits (SDKs), you can code everything into a single *****setup.TDB** file for a database at any scale.

In this section:

2.1 Typographical Conventions

Convention	*Definition*
Forward arrow →	The forward arrow symbol > instructs you to select a series of menu items in a specific order. For example, **Tools→Options** is equivalent to: From the **Tools** menu, select **Options**.
Boldface font	A **boldface** font indicates that the given word(s) are shown that way in on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as **Tools→Options**, or to click **Save**.
Italic font	An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
HELP	Text in blue and underline is a link to another section. In this document commands are also sections. Clicking this link will take you to more detail about a particular command.

Convention	*Definition*
`code`	A `code` font shows a programming code or code example.

A note. The information can be of use to you. It is recommended that you read the text

Important. Indicates that additional important information is located in the hyperlinked or named section.

2.2 Help Resources

Online Help

- To access online help, open Thermo-Calc and select **Help →Online Help**.
- To access some feature help in Graphical Mode, in the lower left corner of the Configuration window, click the help button for information about the active tab or node.

In Console Mode at the command line prompt, you can access help in these ways:

- For a list of all the available commands in the current module, at the prompt type a question mark (`?`) and press <Enter>.
- For a description of a specific command, type `Help` followed by the name of the command. You can only get online help about a command related to the current module you are in.
- For general system information type `Information`. Specify the subject or type `?` and the available subjects are listed. This subject list is specific to the current module.

PDFs

- On the Thermo-Calc Software website.
- Wherever the software is installed, folders containing the PDFs versions of the documentation are also downloaded. See the *Thermo-Calc Installation Guide* for details of where these are installed for your operating system.

2.3 The Database Checker Program

The Thermo-Calc software package includes a program to check that the syntax of unencrypted Thermo-Calc or DICTRA database files is correct. The program applies the syntax rules set out in this document and reports errors and issues warnings.

Thermo-Calc and DICTRA accept deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and DICTRA.

The executable **DatabaseChecker** file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→Database Checker** from the main menu.

3. Initialization of the DATA Module

The following explains how a database initiation file (or a database directory file) is constructed to work with the DATA module. When you start, DATA looks for this file that has information about the available predefined databases (whether freely distributed with the Thermo-Calc/DICTRA packages, purchased from Thermo-Calc Software or its agents, or created by a user).

The *database initiation file* is called:

- Windows: `TC_INITD.TDB` (or `TC_INITD`)
- Linux/UNIX: `initd.tdb`

You can have your own file, but it is more efficient to define an environment variable with the default name as above, and then during installation, translate it to a common initiation file name. The common file is automatically copied by the Thermo-Calc/DICTRA installation script to the following directories:

- Windows: `\DATA\` under the directory defined by the `TCPATH` parameter
- Linux/UNIX:`/data/` under the directory defined by the `TC_DATA` parameter.

The database manager can find the file on a local computer (independent installations) or a connected server (server installations).

When editing or modifying the definitions of initiation parameters (including short-names, paths and subdirectories, database definition file names, and instructive database descriptions) for the available databases in the database initiation file a specific format is used with the fields:

- The first field gives the abbreviated name for the database (to a maximum of five characters)
- The second field specifies a path and filename (maximum 78 characters) containing the database path definition and the actual database definition (*setup*) file name, where the extension is either `TDB` (which stands for original textual TDB file) or `TDC` (which is encrypted from the original TDB file). There are differences between platforms with respect to entering parameters as listed in Table 1.
- The third field (maximum 60 characters) details an optional full name (and version/subversion numbers) for the brief database description.

Table 1: Initiation parameter examples.

Parameter	Windows	Linux/Unix
The `setup` file name must consist of a main part and an extension of a maximum of three characters:	For example, `SSOL5SETUP.TDB`	For example, `ssol5setup.tdb`
Database path definition	Use a back-slash `\`	Use a forward-slash `/`
All databases should be normally located in subdirectories that are under the directory defined by the:	`TCPATH` parameter or under its subdirectory `\DATA\`	`TC_DATA` parameter or under its subdirectory `/data/`

Each entry record (i.e. for a single database) must finish with an exclamation mark !. There should be no spaces or commas within the first and second fields since these characters are taken as field separators, while spaces or commas can be used in the third field.

You can write each database entry on one or two lines (up to the!), it is recommended that the third field is added as follows:

- Windows: on the same line as the first and second fields.
- Linux/UNIX: on the following line.

The following is an example of an initiation file defining three databases named PURE5, SSOL5 and TCFE8:

Windows

```
SSOL5 TCPATH\DATA\SSOL5\SSOL5SETUP.TDC  SGTE Solutions Database
version 5.1 !

PURE5 TCPATH\DATA\PURE5\PURE5SETUP.TDB  SGTE Pure Elements
Database version 5.2 !

TCFE8 TCPATH\DATA\TCFE8\TCFE8SETUP.TDC  TCS Steels/Fe-Alloys
Database version 8.0 !
```

Linux/UNIX

```
ssol5 TC_DATA/data/ssol5/ssol5setup.tdc
     SGTE Solutions Database version 5.1  !
pure5 TC_DATA/data/pure5/pure4setup.tdb
     SGTE Pure Elements Database version 5.2 !
Tcfe8 TC_DATA/data/tcfe8/tcfe8setup.tdc
     TCS Steels/Fe-Alloys Database version 8.0 !
```

3.1 DICTRA and the Databases

A DICTRA installation shares directories with Thermo-Calc, including the `\DATA\` (or `/data/`) area and the database initiation file (`TC_INITD.TDB` or `initd.tdb`).

When you want to switch or add self-generated databases/data-sets or any new database, use the predefined database list in the database initiation file as part of the Thermo-Calc/DICTRA installation packages.

You can add comment lines in the database initiation file, which must start with a $ sign. These lines are ignored by the DATA module. This is also applicable if the database manager or user wants to temporarily disable a database in the predefined database list. If there are too many databases in the \DATA\ area that the DATA module cannot handle properly, the $ sign can be used to temporarily comment about the uncommon databases. However, this does not often happen.

If Thermo-Calc is used with a Windows platform, 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 displays an **Open** 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 Thermo-Calc is run on a Linux/UNIX platform, these files must be located in the current working directory (where Thermo-Calc 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. Copy the entry line(s) for common databases from the original file to a database initiation file. The entries of the additional databases follow. Similar to the standard databases predefined in the database initiation file, all databases should normally be located in subdirectories under the directory as defined by the `TCPATH` parameter (Windows) or the `TC_DATA` parameter (Linux/UNIX), or under its subdirectory `\DATA\` or `/data/`.

For a Windows platform, the following example is an additional database initiation file, called `MYINITD1.TDB`:

```
$
$ DATABASES TCC (Additional TCC Databases)
PURE5 TCPATH\DATA\PURE5\PURE5SETU.TDB   SGTE Pure Elements
Database, version 5 !
AD1   TCPATH\DATA\ADD1\AD1SETUP.TDB     TCS ADD1 Solution
Database, version 1 !
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 !
```

4. The Database Definition File and Keywords

4.1 Database Definition File Syntax

The database definition (*.TDB) file (normally named `***setup.TDB`) 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 (!).
- A single keyword entry can be up to 2000 characters long. However, the maximum length of a line in an *.TDB file is 78 characters--it may be necessary to continue the keyword parameter (arguments) on several lines. The ! must be 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 the keyword parameters (arguments); otherwise, the DATA module can misunderstand the parameters (or arguments), or issue an error message.
- 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 DATA module.

When the database is selected the DATA module only reads the database definition file (***setup.TDB) once, from beginning to end. The DATA module checks continuously 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 C (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 DATA module (during its consistency checking).

This section gives a description of the available keywords and the appropriate arguments. A basic knowledge of the Gibbs Energy System (GIBBS) module is assumed.

This syntax is used:

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

The keywords are 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, but are optional when enclosed in curly brackets {...}.

4.2 ELEMENT

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

The *element name* (maximum two characters) is the one found in the periodic chart but there are no naming restrictions. However, the GIBBS module only recognizes UPPER-case element names (if the `Upper Case Mode` is selected by the GIBBS command REINITIATE), which means that lower-case (if defined in a database) is automatically converted to UPPER-case by the DATA/GIBBS module.

The elements are automatically entered as species using the same names of the elements. If, for example, the species corresponding to FE needs to be named FE1, you can define the species as FE1, which results in an element named FE and a species named FE1. Vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase), need to be entered as special elements for correct handling by the DATA module.

The *reference (ref.) state* (maximum 24 characters) is the stable phase (at 298.15 K and 1 bar) that should contain this element and be used as the reference state for all element thermodynamic data. 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 these are unknown, the values can be set to zero. All this information (reference state, H298 and S298) define the 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_A1              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 !
```

4.3 SPECIES

```
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 predefined set of elements in the stoichiometric formula. If an undefined element is referenced, DATA displays an error message and the data structure is probably damaged.

The species names do not have to be the same as the stoichiometry formula, although in general this is recommended. The elements are automatically entered as species using the same names of the elements.

You can define a species name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case species names.

When naming the species in a database, use special characters (such as +, -, _, / and .) in species names. 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-case and in any preferred order, and the stoichiometric coefficients are written in either real numerical factors or integer digits.

It is important that the numerical factor of 1 is not left out. Subgroups are not allowed in a stoichiometry formula; however, while specifying the stoichiometry formula for a specific species in a database, you can specify it in a way that some elements (always together with the corresponding partial stoichiometric coefficients) are repeated (as in the examples below).

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 !
```

4.4 PHASE

```
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 parameters). The *phase name* (maximum 24 characters) must be unique; otherwise the DATA module sees it as an attempt to redefine a previously defined phase. This causes DATA to display an error message and ignore the rest of the line. A phase name can be suffixed by an underscore (`_`) and letters to identify the physical state(s) or structure type(s) of the phase. Examples of recommended suffixes are:

Suffix	*Definition*
`ABC_S`	The `ABC` phase in solid state.
`ABC_S2`	The `ABC` phase in solid state 2.
`ABC_S3`	The `ABC` phase in solid state 3.
`ABC_LT`	The `ABC` phase in solid state at low temperatures.
`ABC_HT`	The `ABC` phase in solid state at high temperatures.
`ABC_L`	The `ABC` phase in liquid state.
`ABC_LIQ`	The `ABC` phase in liquid state.
`FCC_A1`	The `FCC` phase in disordered structure type A1.
`FCC_L12`	The `FCC` phase in ordered structure type L12.

The *phase name* can also be attached with a colon sign (`:`) and a letter for a legal GIBBS phase-type code (e.g. `IONIC_LIQ:Y` and `GAS:G`).

Legal GIBBS phase-type codes are:

Code	*Definition*
`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 (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`	Bit set for an ordered FCC or HCP solution phase using the *Four Substitutional-Sublattice Ordering Model* (additionally, such a phase can also have interstitial sublattices).
`B`	Bit set for an ordered BCC solution phase using the *Four Substitutional-Sublattice Ordering Model* (additionally, such a phase can also have interstitial sublattices).

Other invalid characters (e.g. M or P) are eventually treated, together with the colon (:) 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 an `L` phase (ordinary liquid solution) is normally (but not always) modelled as a substitutional phase without sublattice, too.

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, as shown in Figure 1. A *Normal 4-Sublattice Model* requires that all the `G` parameters for each of the 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.

4.4.1 Additional Clarification

An `A-B` binary solution phase (with the element A located on one sublattice site and `B` on the other three sublattice sites) treated by the Normal 4-Sublattice Model has to have four `G` parameters for four end-members, i.e.

- `G(phase,A:B:B:B)`
- `G(phase,B:A:B:B)`
- `G(phase,B:B:A:B,` and
- `G(phase,B:B:B:A)`

This is because 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 to be given only once, and the possible permutations are then automatically handled by the GIBBS module. Also, only one of the identical permutations is listed; in this example, `G(phase,A:B:B:B)` where it is alphabetically the first in the list of permutations. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

For ordered BCC phases, the phase-type option `B` means the same thing but it is more complicated since the 4-substitutional-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours as shown in Figure 2. For an end member described by the parameter `G (phase,A:B:C:D)` A and B are next nearest neighbours, as are C and D. And the nearest neighbours of A (or B) are C and D. Thus, for an `A-B` binary solution phase (with the element A located on two sublattice sites and `B` on two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the `G(phase,A:A:B:B)` term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the `G(phase,A:B:A:B)` term has two nearest neighbour bonds between A and B atoms and three next nearest neighbour bonds.

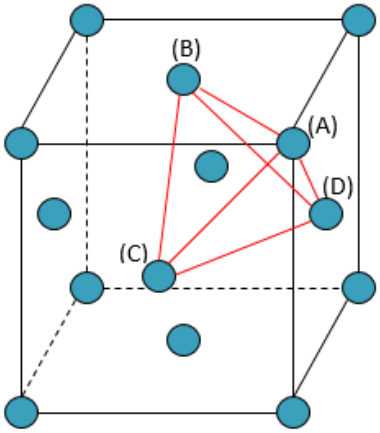

Figure 1: An FCC unit cell with the lattice positions indicated that correspond to the G (FCC,A:B:C:D) end member. All lattice positions are equivalent for a four substitutional-sublattice ordering model.

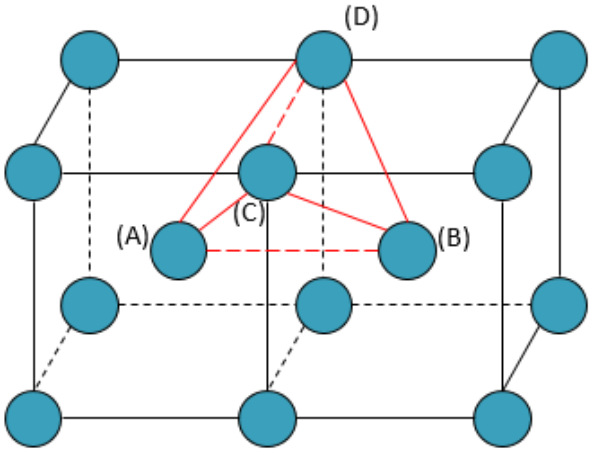

Figure 2: Two BCC unit cells with the lattice positions indicated that correspond to the G (BCC,A:B:C:D,0) end member. Lattice positions (A) and (B) are equivalent, as are lattice positions (C) and (B) for a four substitutional-sublattice ordering model.

The first end-member (described by the `G(phase,A:A:B:B)` term) represents B2-ordering and the second (described by the `G(phase,A:B:A:B)` term) stands for B32-ordering. There are two permutations of the `G(phase,A:A:B:B)` term and four permutations of the `G(phase,A:B:A:B)` term, automatically conducted in the *Four Substitutional-Sublattice Ordering Model*. If you enter the unary, binary, ternary and quaternary parameters you are dealing with 1, 6, 21, 55 parameters for BCC:B, 1, 5, 15, 35 parameters for FCC:F and 1, 16, 81, 256 parameters for phases without F/B.

An additional feature with the phase-type options `F` and `B` is that a composition set that represents the solution phase has a suffix (indicating what ordering the phase has) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams). Such suffix indications can be:

Solution Phase	*Suffix for Disordered Phase*	*Suffix for Ordered Phase*
FCC_PHASE	FCC_A1	FCC_L12
		FCC_L10
BCC_PHASE	BCC_A2	BCC_B2
		BCC_B32
		BCC_D03
		BCC_L21
HCP_PHASE	HCP_A3	HCP_D019
		HCP_B19

If you want to convert an existing database TDB-file to use the F/B feature, add the phase-type code to the corresponding phase name in the PHASE and CONSTITUENT commands in the TDB-file, then when running the LIST_DATA command in the GES module. The created database file is in this less verbose format.

The *data-type code* consists of 1 to 8 characters where each character must stand for an action, which is to be coupled to this phase. The keyword TYPE_DEFINITION, described below, must be used in the current database to specify what action should be taken by DATA for each character code.

The data entries `[numb. subl.] [sites in subl. 1] [sites in subl. 2]` etc., specify the total number of sublattices (always as an integer digit) and the sites (i.e. stoichiometric coefficients) of each of the sublattices (given in either integer digits or real numerical factors) for the phase.

Optionally, an *auxiliary text string* (maximum 78 characters) can be given after the last [sites in sublattice #] but before the exclamation mark `!`. This string displays in connection with the phase name in some listings within the DATA module.

Examples:

```
PHASE GAS:G  % 1 1.0 !
PHASE LIQUID:L %ZCDQ  2  1.0  1.0
> Metallic liquid solution, modelled by CEF Model. !
PHASE IONIC-LIQ:Y %ZCDQ  2  1.0  1.0
> Ionic liquid solution, modelled by Ionic Two-Sublattice Model. !
PHASE SPINEL:I    %ZA   4   1  2  2  4
> Complex Spinel Solution, by CEF model with ionic constraints. !
PHASE M23C6  % 3 20.0 3.0 6.0 !
PHASE FCC_A1    %&A  2  1 1
> Disordered FCC phase; also as MX carbides/nitrides. !
PHASE FCC_L10   %&AX  3  0.75 0.25 1
> Ordered FCC phase, modelled by 2-Sublattice Model for Ordering.
!
```

```
PHASE FCC_L12:F %&AX  5  0.25 0.25 0.25 0.25 1.0

> Ordered FCC phase, modelled by 4-Sublattice Model for Ordering.
!

PHASE AQUEOUS:A %HIJMR 1 1.0

> Aqueous Solution: using the Complete Revised HKF Model. !
```

4.5 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 a predefined phase (i.e. already through the PHASE keyword).

Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS 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, SLAG:L, 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 major constituents. This is done by adding a percent sign (%) directly to 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 minor constituents (i.e. those without a %) add up to 0.01. A maximum of 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% :!
```

4.6 ADD_CONSTITUENT

```
ADD_CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword adds more constituents to a phase that already has 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 is not enough.

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 CUCL2-1 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 ... : !
```

4.7 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 has this species as its only constituent. This keyword allows the database definition file for a large substance database to be more compact; it is a combination of the SPECIES, PHASE and CONSTITUENT keywords.

Examples

```
COMPOUND_PHASE AL2O3 % AL2O3 !
```

```
COMPOUND_PHASE MAGNETITE %MF FE3O4 !
```

```
COMPOUND_PHASE QUARTZ % SIO2 !
```

4.8 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. Use this if the species is already defined.

Examples:

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

4.9 TEMPERATURE_LIMITS

```
TEMPERATURE_LIMITS [lower limit] [upper limit] !
```

This keyword sets the default upper and lower temperature limits used by the GIBBS 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 !
```

4.10 DEFINE_SYSTEM_DEFAULT

```
DEFINE_SYSTEM_DEFAULT [keyword] {G-ref. type index} !
```

This keyword sets the default value to ELEMENT or SPECIES in the DATA command DEFINE_SYSTEM (see the *Thermo-Calc User Guide*). For a substance database, it can be appropriate to have ELEMENT as a default value whereas a large solution database can benefit from having SPECIES as a default value. A proper default value is useful for beginners. An advanced user is more likely to use the DATA 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 GIBBS module. The following lists legal numbers and the corresponding meaning (the reference state type for an element):

Number	*Definition*
1	symbol: G
2	symbol: H298
3	symbol: H0

Example

```
DEFINE_SYSTEM_DEFAULT element 2 !
```

4.11 DEFAULT_COMMAND

```
DEFAULT_COMMAND [secondary keyword and parameters] !
```

This keyword specifies commands to be executed by the DATA module at database initialization. The syntax of the available command is currently not the same as the user available DATA commands but the actions are similar. The available *secondary keyword and parameters* in syntax 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 !
```

4.12 DATABASE_INFORMATION

```
DATABASE_INFORMATION [text]*10000 !
```

This keyword defines a text for the detailed description of the current database. The text can be listed with the DATA command DATBASE_INFORMATION. An apostrophe (') can be used in the text to indicate a new line; and two apostrophes, ('') can be used in the text to indicate a new line plus an empty line.

 The continuous text length (each line with max 78 characters) is 10,000 characters.

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 ... !
```

4.13 TYPE_DEFINITION

```
TYPE_DEFINITION [data-type code]*1 [secondary keyword with
parameters] !
```

This keyword couples phases to an action performed by the DATA module when the DATA command GET_DATA is executed.

4.13.1 Secondary keywords

The secondary keywords and associated parameters in syntax are:

```
SEQ [filename]
RND# [filename]
GES [valid GIBBS command with parameters]
POLY3 [valid POLY command with parameters]
TDB [valid DATA command with parameters]
IF [conditional statement] THEN [keyword with parameters]
AFTER [valid GIBBS 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 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 these types of random files:

- `RND0`, the default, is used for complete Gibbs energy expressions (G0 parameters), where the search field is the unabbreviated parameter name.
- `RND1` is designated for functions, where the function name is used as the search field.
- `RND2` is reserved for binary interaction parameters, where its search field is also the unabbreviated parameter name without any interaction order notation.

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 DATA, and with implementations of DATA on various computer systems. For more information, see the FORTRAN program TDBSORT, which is available from Thermo-Calc Software AB.

The secondary keywords `GES`, `POLY3`, 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 GIBBS/POLY/DATA command that applies to a certain phase. By implementing this as a call to the interactive GIBBS/POLY/DATA module, flexibility is achieved. If a new type of addition is implemented in a GIBBS/POLY/DATA module, it can be immediately used in the database definition file without reprogramming the DATA module.

In several examples below, the use of the at (@) sign indicates any phase to which the relevant type definition (e.g. A, B, 4, or E) applies.

The secondary keywords IF and THEN allow 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.

The secondary keyword AFTER is similar to the GES keyword except the defined GIBBS command is executed after all parameters are entered. The reason for this is that the command has no effect unless there is a parameter. Following the AFTER keyword, a GIBBS 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, %, &, and so forth, and is referred in the definition keywords PHASE, COMPOUND_PHASE and ALLOTROPIC_PHASE for various phases.

A phase can have several ADDITIONAL parts of different types (that are enforced by certain TYPE_DEFINITIONS which call the GIBBS command AMEND_PHASE_DESCRIPTION for describing various contributions to Gibbs energy). However, the DATA/GIBBS module automatically deletes any early-defined ADDITIONAL part(s) of the same type.

The DATA module can selectively retrieve functions that 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 ignored and are not saved in associated GIBBS and POLY workspaces.

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  !
```

4.13.2 Ordered phase restores disorder contribution

When an ordered phase with disordered contribution is restored, the disordered contribution is automatically restored as well. You can also restore the disordered phase *without* restoring the ordered phase.

However the DIS_PART TYPE_DEFINITION must always be set on the ordered phase. It is important that the disordered phase is declared before the ordered phase. Otherwise it causes an error when DIS_PART TYPE_DEFINITION is executed and then either the ordered or disordered phase is rejected.

Example

```
TYPE_DEFINITION & GES A_P_D FCC_A1 MAGNETIC  -3.0    2.80000E-01 !
PHASE FCC_A1  %&  2 1   1 !
    CONSTITUENT FCC_A1  :CR,NI% : C%,VA :  !
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
TYPE_DEFINITION ' GES AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART
FCC_A1,,,!
TYPE_DEFINITION ( GES A_P_D FCC_L12 MAGNETIC  -3.0    2.80000E-01
!
PHASE FCC_L12  %'(  3 .75   .25   1 !
    CONSTITUENT FCC_L12  :CR,NI% : CR,NI% : C,VA% :  !
```

For example a GES command such as the following only affects phases defined above or at the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( GES A_P_D FCC_L12 DIS_PART FCC_A1,,, !
```

For example a TDB command such as the following only affects phases defined *below* the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( TDB RESTORE_PHASE FCC_A1 !
```

4.14 FTP_FILE

```
FTP_FILE [filename] !
```

FTP_FILE is a special function random file and the function names correspond to the record numbers where these record names and the functions are stored. The FTP_FILE decreases search time for the associated database in the DATA 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 DATA when such files are processed.

No modification of this file type is allowed.

Example

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

4.15 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} !
```

GIBBS can 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. This 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 more information, see the ENTER_PARAMETER command in the *Thermo-Calc Console Mode Command Reference*.

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` to continue with the next expression or `N` to end 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 is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.


It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may misunderstand the expression or issue some error messages when reading the function entry. Avoid entering functions like the one below.

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

Such a function is read by the DATA module as

```
1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

rather than

```
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

This is because the DATA module concatenates all lines and removes extra spaces before trying to enter the function in the GIBBS workspace. Thus, the - sign is taken as a delimiter between 298.15 and 1000, and the function incorrectly becomes:

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

Avoid this mistake 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 is read correctly as

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

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, you can set another limit when it is applicable (according to experimental data and assessments).

An upper-temperature limit (in Kelvin; followed by a `Y` or `N` sign) for the applicability of each TP-Function in a function must be given after the semicolon (`;`) immediately following the specific TP-Function. 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 assumes there are breakpoints in pressure for this function. In these cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function is also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done 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 function in a special reference file. The references are listed when doing the GET_DATA command in the DATA module. They can also be listed in the GIBBS module with the command LIST_DATA with the option R. For accounting for the reference indices, also see the keyword REFERENCE_FILE.

The reference index field can also be an abbreviation (such as REF:250, REF_002, or REF-SGTE) which denotes the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option R).

However, the references directly coded in the database definition file (***setup.TDB) starting with a letter can be shown when issuing the DATA command GET_DATA or the GIBBS 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 GIBBS command LIST_DATA <file> with the N or R option, is also possible to be directly read by the DATA module.

The DATA module can 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 ignored and are not saved in associated GIBBS and POLY workspaces. Previously, this can only be 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 G0_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 !
```

4.16 PARAMETER

```
PARAMETER [GIBBS 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} !
```

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

It is used to define 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).

The general form of a parameter is:

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

Where it is defined as below.

Name	*Description*
identifier	The parameter type.
phase	The phase name (maximum 24 characters).
constituent array	The specific constituent array in the phase.
digit	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	The mathematical relation to describe the parameter.
xxx and yyy	The low and high temperature limits respectively for the applicable temperature range of the parameter expression
keyword Y or N	The indicator on if there is continuation for the parameter expression or not
zzz	The reference index/number for the assessment of this parameter;
!	The exclamation mark is used to indicate that the current parameter definition is ended

GIBBS parameter name

The GIBBS parameter name has a general form of:

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

Examples of parameter names:

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

Type-Identifier	**Definition**
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).
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

You can also use `G` for interaction parameters; and on output list (performed by the GIBBS 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.

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 in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS 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, SLAG: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.

Be careful about the sign of odd terms, for example, `L(BCC, B, A:VA;1)` is treated as `L(BCC,A,B:VA;1)`, i.e. it is always put into alphabetical order.

Solution phases with sublattices may have interacting constituents in each sublattice.

You can 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-∑y(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) coded as mathematical relations of constants, functions of stable variables (`T` and `P`) and entered functions (normally with a `#` suffix, e.g. `+3*GSERAL#`).

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 ends with a semicolon (`;`) and be followed by its upper applicable temperature limit and a continuation indicator (`Y` to continue with the next expression, or `N` to end the parameter's expression). If there is no continuation after a specific expression (TP-Function), the reference index can be optionally 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 is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.


It is recommended to always have at least one empty space at the beginning of each continuation line. Avoid entering parameters such as:

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

Such a parameter is read by the DATA module as `2000+4568*T+2*GFUNAB#`, rather than as `-2000 +4568*T+2*GFUNAB#`.

Avoid this mistake 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 !
```

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, you can set another limit when it is applicable (according to experimental data and assessments). An upper-temperature limit (in Kelvin; followed by a `Y` or `N` sign) for the applicability of each TP-Function in a parameter must be given after the semicolon (`;`) 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 is assumed that there are breakpoints in pressure for this parameter. In such cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current parameter are also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the parameters are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done 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 DATA module. These can also be listed in the GIBBS module with the command LIST_DATA and the option `R` or `N`. For accounting the reference indices, also see the keyword REFERENCE_FILE.

The reference index field can also be an abbreviation (such as `REF:250`, `REF_002`, or `REF-SGTE`) denoting the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option `R` or `N`).

However, the references directly coded in the database definition file (`***setup.TDB`) that starts with a letter can be shown when issuing the DATA command `GET_DATA` or the GIBBS 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 GIBBS command LIST_DATA `<file>` with the `N` option, is thus also possible to be directly read by the DATA 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 !
```

4.17 OPTIONS

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

This keyword defines an alloy in a database. 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 tell you 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 keyword in the database.

The alloy name must be proceeded by a slash (`/`) and terminated by the opening parenthesis, with 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, the alloying element names, each with its maximum mass and mole percent are 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)) !
```

4.18 TABLE

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

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

Example

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

4.19 ASSESSED_SYSTEMS

```
ASSESSED_SYSTEM [descriptions on special treatments for specific
assessed systems]*8000 !
```

This keyword 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 DATA, GIBBS and POLY models deal with the existing systems with assessed data) is allowed until the exclamation mark (`!`).

Several ASSESSED_SYSTEMS keywords can be used in the same TDB file in order to have more lists of assessed systems. There is no limit to the number of the entries in the same TDB file.

The assessed systems in the database, and the special treatment options, are typed after the keyword. The elements (always in UPPER CASE) in each assessed system must be in alphabetical order and be separated by a hyphen, such as `C-FE` for the Fe-C binary system, and `C-CR-FE` for the Fe-Cr-C ternary 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.

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 about how to:
- Reject or restore phase(s) from the current database in the DATA module;
- 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 GIBBS module; *and*
- 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 syntax TDB means that the commands to the DATA 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 GIBBS 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.

- ;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(2nd element)=.1234, temperature T=1100 K and with the default directions; or
- for a ternary system: at the compositions X(2nd element)=.1234 and X(3rd 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(2nd 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(2nd element)=x1 and X(3rd 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 are used (meaning no ADD command is enforced in the POLY module).
- If only one start point is specified, the direction(s) may be omitted; if more than one start points 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).

Other examples:

```
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 *) !
```

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 generates 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).

4.20 REFERENCE_FILE

```
REFERENCE_FILE [file name] !
```

This keyword takes a reference file name as its argument. This reference file (that must be edited in a restrictive way and 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 exactly 78 characters written in one single blocked 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 an ampersand (`&`). The line number of the first record for a specific reference entry is then accounted as the unique integer for that specific reference, which is 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.
AG1BR1O3          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 AG1BR1O3
```

4.21 LIST_OF_REFERENCE

```
LIST_OF_REFERENCE
NUMBER SOURCE
  [REFxxx]  '[Detailed reference]'
.........
.......... !
```

This keyword starts a reference list that is directly coded in the database definition file (`***setup.TDB`). 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 400,000 characters after the keyword is allowed until the exclamation mark (`!`).

Such a reference list can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the R option). The reference list, which is generated by the GIBBS command LIST_DATA <file> with the N option, has this structure, and is thus possible to be directly read by the DATA 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'
 !
```

4.22 ADD_REFERENCE

```
ADD_REFERENCE
  [REFxxx]  '[Detailed reference]'
.........
......... !
```

Use this keyword to have an unlimited number of references. The use of this is the same as that of LIST_OF_REFERENCE, and is used after it. Several ADD_REFERENCES sections can be used in a single database if there are too many references.

It is recommended to always start with a so-called *empty reference* (such as the DUMP0 reference in the following example) as the first entry in each of the ADD_REFERENCE sections to make sure that all references are listed appropriately as retrieving data by issuing the GET_DATA command.

Example

```
ADD_REFERENCE
   DUMP0  'Empty reference 0'
   REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-
92
          TRITA 0270 (1986); CR-FE'
   REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
          TRITA 0207 (1986); C-CR-FE'
   REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys
Database,
          v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
          at high temperatures.'
```

```
   ... ...
 !
ADD_REFERENCE
   DUMP1  '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'
   ... ...
 !
```

4.23 CASE and ENDCASE

```
CASE [ELEMENT/SPECIE/PHASE] !
  IF (boolean algebra on element, species or phase names) THEN
       [GIBBS/POLY/DATA command] !
ENDCASE !
```

This keyword takes as its argument, a definition on which type of the following Boolean algebra operates. A simple Boolean algebra using `AND` and `OR` with a maximum of four levels of parentheses works. The `CASE` construction must end with the `ENDCASE` keyword. This makes it possible to have additional GIBBS or POLY commands executed depending on the user selection of elements, species or phases. The DATA commands that can be given as secondary keyword to DEFAULT_COMMAND can also be executed.

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_ELEMENT /- !
 ENDCASE !
```

Example 3:

```
CASE ELEMENT !
   IF(AL AND FE)
```

```
    THEN TDB_DEF_SYS_ELEMENT VA !
  ENDCASE !
```

4.24 VERSION_DATA

```
VERSION_DATE [string]*78 !
```

The string is denoted as the version/revision date and database manager of the database. Nowadays, this directive is used mainly for the purpose of keeping the development and revision history mostly updated.

Example

```
VERSION_DATE Last update and adjustment: Database Manager, 2015-
09-25 !
```

5. DICTRA Extensions to Database Definition File Syntax

Software packages for simulation of diffusional phase transformations, such as DICTRA, need both thermodynamic data and kinetic data (i.e. diffusivities or mobilities). Naturally, the handling and storage of kinetic data also benefits 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 - PARAMETER, DIFFUSION, and ZERO_VOLUME_SPECIES.

5.1 PARAMETER

```
PARAMETER [special GIBBS 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} !
```

This keyword allows you to enter all types of normal GIBBS parameters for thermodynamic data as well as five special extensions suitable for kinetic data used in the DICTRA software.

Valid extensions to special GIBBS 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 !
```

5.2 DIFFUSION

```
DIFFUSION [model keyword] [phase name] [additional parameter(s)] !
```

This keyword specifies the 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 (∑MF/RT) exp (∑MQ/RT) / RT
```

where ∑ stands for a weighted summation of the different MF's and MQ's plus possibly a Redlich-Kister term.

Valid model keywords are:

Keyword	Description
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 (∑ DF/RT) exp (∑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 = ∑ DF + ∑ 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 & 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 !
```

5.3 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. This keyword uses a list of which species are to be considered as zero volume ones for an argument.

Example

```
ZERO_VOLUME_SPECIES VA C N !
```

6. Database Definition File Examples

6.1 Example 1: A 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' !
```

6.2 Example 2: A Custom Database for the Sb-Sn Binary 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_DEFINITIIONS:
 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>
$
```

6.3 Example 3: A Public Database for the Fe-Cr-C Ternary System

[discussed with Qing, perhaps this example can be deleted as it is long and there are 2 other examples]

```
$
$   Revision history:
$       Created as PDEMO  by Pingfang Shi  on 2004-10-05
$       Renamed to DFeCrC by Pingfang Shi  on 2006-10-25
$
$ FURTHER MODIFICATIONS:
$ ======================
$ pfs: /20041005 (PDEMO)
$       * Retrieved all definitions from PTERN for the Fe-Cr-C ternary !
$
```

```
$ pfs: /20061025 (DFeCrC)
$       * Ignore ELEMENT /- definition.
$       * Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$         parameters, in order to avoid BCC-appearance (Fe-C)
$         at temperatures higher than 3900 K.
$           $L(BCC_A2,CR:C,VA;0) 298.15 -190*T;           6000 N REF1 !
$            L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REF1 !
$           $L(BCC_A2,FE:C,VA;0) 298.15 -190*T;           6000 N REF3 !
$            L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REF3 !
$       * Add Cr into HCP_A3 phase, and
$         add all necessary G0/L parameters (according to SSOL2/TCFE3):
$           G(HCP_A3,CR:VA;0)
$           TC(HCP_A3,CR:VA;0)
$           BMAGN(HCP_A3,CR:VA;0)
$           G(HCP_A3,FE:C;0)
$           G(HCP_A3,CR:C;0)
$           L(HCP_A3,CR:C,VA;0)
$           L(HCP_A3,CR,FE:VA;0)
$       * Add "TMM:300/3000" limits to all three binary joins in the
$           ASSESSED_SYSTEM section.
$       * Change the reference indices, e.g., 101 to REF1, in order to
$           always get the reference list correctly.
$       * Re-arrange database format slightly.
$       * Updated the DATABASE_INFO section.
$-----------------------------------------------------------------------
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ DATABASE INFORMATION:
$**********************************************************************
$
 DATABASE_INFO                                        DFeCrC '
                TCS Demo Fe-Cr-C Alloy Solutions Database'
          (only for demonstration purposes in TCC-Demo/TCW-Demo)'
       ********************************************************** '
                        (Version 1.2, Oct. 2006) ''
          Copyright @ 2004-2012: Thermo-Calc Software AB, Sweden ''
The DFeCrC database (previously called PDEMO) is the TCS Demo Fe-Cr-C '
Alloy Solutions Database, which is especially designed for primarily '
demonstrating the uses of: '
```

```
  * TCC-Demo software: BIN, TERN, SCHEIL and some other modules; '
  * TCW-Demo software: '
     "Binary" module calculations of phase diagrams and property
diagrams'
                  in available binary systems; '
     "Ternary" module calculations of phase diagrams (e.g., isothermal'
                  sections, monovariant lines involving liquid, liquidus'
                  surface projections) and property diagrams in available'
                  ternary systems; '
     "Scheil" module simulations of alloy solidifications; and/or '
     "Equilibrium" calculation routines for phase diagrams and property'
                  diagrams in available binary or ternary systems. '
It can also be used for other types of calculations/simulations in both'
TCC and TCW software, and in their application programming interfaces.''
It includes critically-assessed data for all possible three binary joins'
(i.e. Cr-C, Fe-Cr and Fe-Cr) and one complete ternary alloy solutions '
within the Fe-Cr-C system. However, due to the fact that experimental'
data for the Fe-C and Cr-C binary joins and Fe-Cr-C ternary system at '
extremely-high temperatures are not sufficient, the available assessed'
data can not be applied to temperature conditions higher than 4000 K.''
Included thermodynamic data are available for various stoichiometric '
and solution phases, e.g. liquid mixture, various alloy solutions and '
intermetallic phases. But the gaseous mixture phase is excluded in this'
DEMO version.''
The DFeCrC database can be used not only in calculating various types '
of phase diagrams (binary phase diagrams, ternary isothermal sections,'
ternary monovariant lines involving liquid, ternary liquidus surface '
projections, ternary isopleth sections, etc.) and property diagrams '
(the easiest ways are through the BIN and TERN modules), but also in '
simulating alloy solidification processes (with the SCHEIL module) of'
Fe-based or Cr-based alloys (but limited within the Fe-Cr-C ternary '
system in this DEMO version). Many unique features of the TCC/TCW '
software can be demonstrated using this and other specially-designed '
DEMO databases. ''
However, this DFeCrC database (similar to other DEMO and/or PUBLIC TC '
databases) is provided within the TCC-Demo/TCW-Demo software only for '
the purposes of demonstration, testing and evaluation. For R&D projects'
and teaching activities, you are highly encouraged to only use the FULL'
versions of the TCC and/or TCW software together with some commercial '
```

```
databases that are appropriate for your specific applications. Please '
contact us for all kinds of details. ''
Release History: Version 1.1 with minor improvements,  Oct. 2004 '
                 Version 1.2 with minor modifications, Oct. 2006 ''
Edited by: Dr. Pingfang Shi (Thermo-Calc Software, Oct. 2006). ''
 !

$ ----------------------------------------------------------------------
$VERSION_DATE Last update and adjustment: Pingfang Shi, 2004-10-05 !
 VERSION_DATE Last update and adjustment: Pingfang Shi, 2006-10-25 !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Definition of Elements in the Database System:
$----------------------------------------------------------------------
$ELEM NAME STABLE_ELEMENT_REF         ATOMIC MASS  H298-H0     S298 !
$----------------------------------------------------------------------
$ELEMENT /-   ELECTRON_GAS            0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT VA   VACUUM                  0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT C    GRAPHITE                1.2011E+01  1.0540E+03  5.7400E+00!
 ELEMENT CR   BCC_A2                  5.1996E+01  4.0500E+03  2.3560E+01!
 ELEMENT FE   BCC_A2                  5.5847E+01  4.4890E+03  2.7280E+01!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ TYPE_DEFINITIONS for data inclusions:
$----------------------------------------------------------------------
 TYPE_DEFINITION % SEQ *!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$  TYPE_DEFINITIONS for phase descriptions:
$----------------------------------------------------------------------
$... For magnetic contributions:
 TYPE_DEFINITION A GES AMEND_PHASE_DES @ MAGNETIC  -1.0  4.00000E-01 !
 TYPE_DEFINITION B GES AMEND_PHASE_DES @ MAGNETIC  -3.0  2.80000E-01 !

$... For Cr/Fe-C in FCC phase and Cr/Fe-C in HCP phase:
 TYPE_DEFINITION C IF(C) THEN GES AMEND_PHASE_DES @ C_S ,, :C: !
```

```
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Default Commands:
$-----------------------------------------------------------------------
$DEFINE_SYSTEM_DEFAULT SPECIES 2 !
 DEFINE_SYSTEM_DEFAULT ELEMENT 2 !

 DEFAULT_COMMAND DEF_SYS_ELEMENT VA !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ FUNCTIONS for various phases:
$-----------------------------------------------------------------------
$
 FUNCT GHSERCC  298.15 -17368.441+170.73*T-24.3*T*LN(T)
     -4.723E-04*T**2+2562600*T**(-1)-2.643E+08*T**(-2)
     +1.2E+10*T**(-3); 6000 N!
 FUNCT GHSERCR  298.15 -8856.94+157.48*T-26.908*T*LN(T)
     +.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);  2180 Y
      -34869.344+344.18*T-50*T*LN(T)-2.88526E+32*T**(-9); 6000 N!
 FUNCT GHSERFE  298.15 +1225.7+124.134*T-23.5143*T*LN(T)
     -.00439752*T**2-5.8927E-08*T**3+77359*T**(-1);  1811.00 Y
     -25383.581+299.31255*T-46*T*LN(T)+2.29603E+31*T**(-9); 6000 N!

 FUNCT GFELIQ   298.15 +GHSERFE#+12040.17-6.55843*T
     -3.6751551E-21*T**7;  1811 Y
      -10839.7+291.302*T-46*T*LN(T);  6000 N!
 FUNCT GFEFCC   298.15 +GHSERFE#-1462.4+8.282*T
     -1.15*T*LN(T)+6.4E-04*T**2;  1811 Y
      -27098.266+300.25256*T-46*T*LN(T)+2.78854E+31*T**(-9);  6000 N!
 FUNCT GFECEM   298.15 +GPCEM1#-10745+706.04*T-120.6*T*LN(T); 6000 N!
 FUNCT GFEM23C6  298.15 +7.666667*GFECEM#-1.666667*GHSERCC#
     +66920-40*T; 6000 N!

 FUNCT GCRFCC   298.15 +GHSERCR#+7284+.163*T;  6000 N!
 FUNCT GCRM23C6 298.15 -521983+3622.24*T-620.965*T*LN(T)
     -.126431*T**2;   6000 N!
 FUNCT GCRM3C2  298.15 -100823.8+530.66989*T-89.6694*T*LN(T)
```

```
    -.0301188*T**2;  6000 N!
FUNCT GCRM7C3  298.15 -201690+1103.128*T-190.177*T*LN(T)
    -.0578207*T**2;  6000 N!

FUNCT GPCLIQ   298.15 +YCLIQ#*EXP(ZCLIQ#);    6000 N!
FUNCT ACLIQ    298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!
FUNCT BCLIQ    298.15 +1+3.2E-10*P;               6000 N!
FUNCT CCLIQ    298.15 1.6E-10;                    6000 N!
FUNCT DCLIQ    298.15 +1*LN(BCLIQ#);              6000 N!
FUNCT ECLIQ    298.15 +1*LN(CCLIQ#);              6000 N!
FUNCT VCLIQ    298.15 +7.626E-06*EXP(ACLIQ#);     6000 N!
FUNCT XCLIQ    298.15 +1*EXP(.5*DCLIQ#)-1;        6000 N!
FUNCT YCLIQ    298.15 +VCLIQ#*EXP(-ECLIQ#);       6000 N!
FUNCT ZCLIQ    298.15 +1*LN(XCLIQ#);              6000 N!

FUNCT GPCGRA   298.15 +YCGRA#*EXP(ZCGRA#);    6000 N!
FUNCT ACGRA    298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!
FUNCT BCGRA    298.15 +1+3.6E-10*P;               6000 N!
FUNCT CCGRA    298.15 3.3E-10;                    6000 N!
FUNCT DCGRA    298.15 +1*LN(BCGRA#);              6000 N!
FUNCT ECGRA    298.15 +1*LN(CCGRA#);              6000 N!
FUNCT VCGRA    298.15 +5.259E-06*EXP(ACGRA#);     6000 N!
FUNCT XCGRA    298.15 +1*EXP(.9166667*DCGRA#)-1;  6000 N!
FUNCT YCGRA    298.15 +VCGRA#*EXP(-ECGRA#);       6000 N!
FUNCT ZCGRA    298.15 +1*LN(XCGRA#);              6000 N!

FUNCT GPCFCC   298.15 +YCFCC#*EXP(ZFEFCC#);   6000 N!
FUNCT ACFCC    298.15 +1.44E-04*T;              6000 N!
FUNCT VCFCC    298.15 +1.031E-05*EXP(ACFCC#);   6000 N!
FUNCT YCFCC    298.15 +VCFCC#*EXP(-EFEFCC#);    6000 N!

FUNCT GPCRLIQ  298.15 +YCRLIQ#*EXP(ZCRLIQ#);    6000 N!
FUNCT ACRLIQ   298.15 +1.7E-05*T+9.2E-09*T**2;  6000 N!
FUNCT BCRLIQ   298.15 +1+4.65E-11*P;            6000 N!
FUNCT CCRLIQ   298.15 3.72E-11;                 6000 N!
FUNCT DCRLIQ   298.15 +1*LN(BCRLIQ#);           6000 N!
FUNCT ECRLIQ   298.15 +1*LN(CCRLIQ#);           6000 N!
FUNCT VCRLIQ   298.15 +7.653E-06*EXP(ACRLIQ#);  6000 N!
FUNCT XCRLIQ   298.15 +1*EXP(.8*DCRLIQ#)-1;     6000 N!
```

```
FUNCT YCRLIQ   298.15 +VCRLIQ#*EXP(-ECRLIQ#);   6000 N!
FUNCT ZCRLIQ   298.15 +1*LN(XCRLIQ#);           6000 N!

FUNCT GPCRBCC  298.15 +YCRBCC#*EXP(ZCRBCC#);  6000 N!
FUNCT ACRBCC   298.15 +1.7E-05*T+9.2E-09*T**2;  6000 N!
FUNCT BCRBCC   298.15 +1+2.6E-11*P;             6000 N!
FUNCT CCRBCC   298.15 2.08E-11;                 6000 N!
FUNCT DCRBCC   298.15 +1*LN(BCRBCC#);           6000 N!
FUNCT ECRBCC   298.15 +1*LN(CCRBCC#);           6000 N!
FUNCT VCRBCC   298.15 +7.188E-06*EXP(ACRBCC#);  6000 N!
FUNCT XCRBCC   298.15 +1*EXP(.8*DCRBCC#)-1;     6000 N!
FUNCT YCRBCC   298.15 +VCRBCC#*EXP(-ECRBCC#);   6000 N!
FUNCT ZCRBCC   298.15 +1*LN(XCRBCC#);           6000 N!

FUNCT GPFELIQ  298.15 +YFELIQ#*EXP(ZFELIQ#);  6000 N!
FUNCT AFELIQ   298.15 +1.135E-04*T;                              6000 N!
FUNCT BFELIQ   298.15 +1+4.98009787E-12*P+3.20078924E-14*T*P;    6000 N!
FUNCT CFELIQ   298.15 +4.22534787E-12+2.71569924E-14*T;          6000 N!
FUNCT DFELIQ   298.15 +1*LN(BFELIQ#);                            6000 N!
FUNCT EFELIQ   298.15 +1*LN(CFELIQ#);                            6000 N!
FUNCT VFELIQ   298.15 +6.46677E-06*EXP(AFELIQ#);                 6000 N!
FUNCT XFELIQ   298.15 +1*EXP(.8484467*DFELIQ#)-1;                6000 N!
FUNCT YFELIQ   298.15 +VFELIQ#*EXP(-EFELIQ#);                    6000 N!
FUNCT ZFELIQ   298.15 +1*LN(XFELIQ#);                            6000 N!

FUNCT GPFEFCC  298.15 +YFEFCC#*EXP(ZFEFCC#);  6000 N!
FUNCT AFEFCC   298.15 +7.3097E-05*T;                             6000 N!
FUNCT BFEFCC   298.15 +1+3.25236341E-11*P+3.36607808E-16*T*P;    6000 N!
FUNCT CFEFCC   298.15 +2.62285341E-11+2.71455808E-16*T;          6000 N!
FUNCT DFEFCC   298.15 +1*LN(BFEFCC#);                            6000 N!
FUNCT EFEFCC   298.15 +1*LN(CFEFCC#);                            6000 N!
FUNCT VFEFCC   298.15 +6.688726E-06*EXP(AFEFCC#);                6000 N!
FUNCT XFEFCC   298.15 +1*EXP(.8064454*DFEFCC#)-1;                6000 N!
FUNCT YFEFCC   298.15 +VFEFCC#*EXP(-EFEFCC#);                    6000 N!
FUNCT ZFEFCC   298.15 +1*LN(XFEFCC#);                            6000 N!

FUNCT GPFEBCC  298.15 +YFEBCC#*EXP(ZFEBCC#);  6000 N!
FUNCT AFEBCC   298.15 +2.3987E-05*T+1.2845E-08*T**2;             6000 N!
FUNCT BFEBCC   298.15 +1+2.80599565E-11*P+3.06481523E-16*T*P;    6000 N!
```

```
 FUNCT CFEBCC   298.15 +2.20949565E-11+2.41329523E-16*T;       6000 N!
 FUNCT DFEBCC   298.15 +1*LN(BFEBCC#);                        6000 N!
 FUNCT EFEBCC   298.15 +1*LN(CFEBCC#);                        6000 N!
 FUNCT VFEBCC   298.15 +7.042095E-06*EXP(AFEBCC#);            6000 N!
 FUNCT XFEBCC   298.15 +1*EXP(.7874195*DFEBCC#)-1;            6000 N!
 FUNCT YFEBCC   298.15 +VFEBCC#*EXP(-EFEBCC#);                6000 N!
 FUNCT ZFEBCC   298.15 +1*LN(XFEBCC#);                        6000 N!

 FUNCT GPFEHCP  298.15 +YFEHCP#*EXP(ZFEHCP#);  6000 N!
 FUNCT AFEHCP 298.15 +7.3646E-5*T;                           6000 N!
 FUNCT BFEHCP 298.15 +1+32.5236341E-12*P+3.36607808E-16*P*T; 6000 N!
 FUNCT CFEHCP 298.15 +26.2285341E-12+2.71455808E-16*T;       6000 N!
 FUNCT DFEHCP 298.15 +LOG(BFEHCP#);                          6000 N!
 FUNCT EFEHCP 298.15 +LOG(CFEHCP#);                          6000 N!
 FUNCT VFEHCP 298.15 +6.59121E-6*EXP(AFEHCP#);               6000 N!
 FUNCT XFEHCP 298.15 +EXP(0.8064454*DFEHCP#)-1;              6000 N!
 FUNCT YFEHCP 298.15 +VFEHCP#*EXP(-1*EFEHCP#);               6000 N!
 FUNCT ZFEHCP 298.15 +LOG(XFEHCP#);                          6000 N!

 FUNCT GPCEM1   298.15 +VCEM1#*P;     6000 N!
 FUNCT ACEM1    298.15 -1.36E-05*T+4E-08*T**2;    6000 N!
 FUNCT VCEM1    298.15 +2.339E-05*EXP(ACEM1#);    6000 N!

 FUNCT GPSIG1   298.15 +1.09E-04*P;        6000 N!
 FUNCT GPSIG2   298.15 +1.117E-04*P;       6000 N!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Define the various Phase and their Constituents, and
$ Assign parameters to phases:
$---------------------------------------------------------------------------
$PHASE  NAME:TYPE  MARKCODE  #SUBL  SITES_IN_EACH_SUBL. !
$---------------------------------------------------------------------------

$***** LIQUID (Solution) ********************************************
 PHASE LIQUID:L %  1  1.0
  > This is metallic liquid solution phase, with C species !
 CONST LIQUID:L  : C,CR,FE :  !
```

```
 PARAM G(LIQUID,C;0)  298.15 +GHSERCC#+GPCLIQ#
                             +117369-24.63*T; 6000 N REF0 !
 PARAM G(LIQUID,CR;0)  298.15 +GHSERCR#+GPCRLIQ#
                +24339.955-11.420225*T+2.37615E-21*T**7;  2180 Y
                             +GHSERCR#+GPCRLIQ#
                +18409.36-8.563683*T+2.88526E+32*T**(-9); 6000 N REF0 !
 PARAM G(LIQUID,FE;0)  298.15 +GFELIQ#+GPFELIQ#;  6000 N REF0 !

 PARAM L(LIQUID,C,CR;0)  298.15 -90526-25.9116*T; 6000 N REF1 !
 PARAM L(LIQUID,C,CR;1)  298.15 +80000;           6000 N REF1 !
 PARAM L(LIQUID,C,CR;2)  298.15 +80000;           6000 N REF1 !
 PARAM L(LIQUID,C,FE;0)  298.15 -124320+28.5*T;  6000 N REF3 !
 PARAM L(LIQUID,C,FE;1)  298.15  +19300;         6000 N REF3 !
 PARAM L(LIQUID,C,FE;2)  298.15  +49260-19*T;    6000 N REF3 !
 PARAM L(LIQUID,CR,FE;0)  298.15 -14550+6.65*T;   6000 N REF4 !
 PARAM L(LIQUID,C,CR,FE;0)  298.15 -496063;  6000 N REF2 !
 PARAM L(LIQUID,C,CR,FE;1)  298.15  +57990;  6000 N REF2 !
 PARAM L(LIQUID,C,CR,FE;2)  298.15  +61404;  6000 N REF2 !

$***** FCC_A1 (Solution) ********************************************
$PHASE FCC_A1  %BC  2 1   1 !
$ Note the C TYPE_DEF for 2nd FCC composition-set (MC) is not necessary
$    for the (Fe,Cr)-C system.
 PHASE FCC_A1  %B   2 1   1 !
 CONST FCC_A1   : CR,FE%
                : C,VA% :  !

 PARAM G(FCC_A1,CR:VA;0)  298.15 +GCRFCC#+GPCRBCC#;  6000 N REF0 !
 PARAM TC(FCC_A1,CR:VA;0)     298.15 -1109;  6000 N REF0 !
 PARAM BMAGN(FCC_A1,CR:VA;0)  298.15 -2.46;  6000 N REF0 !
 PARAM G(FCC_A1,FE:VA;0)  298.15 +GFEFCC#+GPFEFCC#;  6000 N REF0 !
 PARAM TC(FCC_A1,FE:VA;0)     298.15 -201;  6000 N REF0 !
 PARAM BMAGN(FCC_A1,FE:VA;0)  298.15 -2.1;  6000 N REF0 !

 PARAM G(FCC_A1,CR:C;0)  298.15 +GHSERCR#+GHSERCC#
                                  +1200-1.94*T;     6000 N REF2 !
 PARAM G(FCC_A1,FE:C;0)  298.15 +GFEFCC#+GHSERCC#+GPCFCC#
                                  +77207-15.877*T;  6000 N REF3 !
 PARAM TC(FCC_A1,FE:C;0)     298.15 -201;  6000 N REF3 !
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 PARAM BMAGN(FCC_A1,FE:C;0)  298.15 -2.1;  6000 N REF3 !

 PARAM L(FCC_A1,CR:C,VA;0)  298.15 -11977+6.8194*T; 6000 N REF2 !
 PARAM L(FCC_A1,FE:C,VA;0)  298.15 -34671;          6000 N REF3 !
 PARAM L(FCC_A1,CR,FE:VA;0) 298.15 +10833-7.477*T;  6000 N REF4 !
 PARAM L(FCC_A1,CR,FE:VA;1) 298.15  +1410;          6000 N REF4 !
 PARAM L(FCC_A1,CR,FE:C;0)  298.15 -74319+3.2353*T; 6000 N REF2 !

$***** BCC_A2 (Solution) ********************************************
 PHASE BCC_A2  %A  2 1   3 !
 CONST BCC_A2  : CR%,FE%
               : C,VA% :  !

 PARAM G(BCC_A2,CR:VA;0)  298.15 +GHSERCR#+GPCRBCC#;  6000 N REF0 !
 PARAM TC(BCC_A2,CR:VA;0)     298.15 -311.5;  6000 N REF0 !
 PARAM BMAGN(BCC_A2,CR:VA;0)  298.15   -.01;  6000 N REF0 !
 PARAM G(BCC_A2,FE:VA;0)  298.15 +GHSERFE#+GPFEBCC#;  6000 N REF0 !
 PARAM TC(BCC_A2,FE:VA;0)     298.15 1043;  6000 N REF0 !
 PARAM BMAGN(BCC_A2,FE:VA;0)  298.15 2.22;  6000 N REF0 !

 PARAM G(BCC_A2,CR:C;0)  298.15 +GHSERCR#+3*GHSERCC#+GPCRBCC#+3*GPCGRA#
                                +416000;            6000 N REF1 !
 PARAM TC(BCC_A2,CR:C;0)     298.15 -311.5;  6000 N REF1 !
 PARAM BMAGN(BCC_A2,CR:C;0)  298.15  -.008;  6000 N REF1 !
 PARAM G(BCC_A2,FE:C;0)  298.15 +GHSERFE#+3*GHSERCC#+GPFEBCC#+3*GPCGRA#
                                +322050+75.667*T;   6000 N REF3 !
 PARAM TC(BCC_A2,FE:C;0)     298.15 1043;  6000 N REF3 !
 PARAM BMAGN(BCC_A2,FE:C;0)  298.15 2.22;  6000 N REF3 !

$ PF-20061025: Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$         parametera, in order to avoid BCC-appearance (Fe-C)
$         at temperatures higher than 3900 K.
$PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T;           6000 N REF1 !
 PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REFS !
$PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T;           6000 N REF3 !
 PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REFS !
$
 PARAM L(BCC_A2,CR,FE:VA;0) 298.15 +20500-9.68*T;   6000 N REF4 !
 PARAM TC(BCC_A2,CR,FE:VA;0)     298.15 1650;  6000 N REF4 !
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 PARAM TC(BCC_A2,CR,FE:VA;1)      298.15  550;  6000 N REF4 !
 PARAM BMAGN(BCC_A2,CR,FE:VA;0)   298.15 -.85;  6000 N REF4 !

 PARAM L(BCC_A2,CR,FE:C;0)  298.15 -1250000+667.7*T; 6000 N REF2 !
 PARAM TC(BCC_A2,CR,FE:C;0)    298.15 1650;  6000 N REF5 !
 PARAM TC(BCC_A2,CR,FE:C;1)    298.15  550;  6000 N REF5 !
 PARAM BMAGN(BCC_A2,CR,FE:C;0) 298.15 -.85;  6000 N REF5 !

$***** HCP_A3 (Solution) ********************************************
$PHASE HCP_A3  %BC  2 1   .5 !
$ Note the C TYPE_DEF for 2nd HCP composition-set (M2C) is not necessary
$    for the (Fe,Cr)-C system.
 PHASE HCP_A3  %B   2 1   .5 !
 CONST HCP_A3  : CR,FE,
               : VA%,C :  !

 PARAM G(HCP_A3,CR:VA;0) 298.15 +GHSERCR#+4438;           6000 N REF1 !
 PARAM TC(HCP_A3,CR:VA;0)    298.15 -1109;  6000 N REF1 !
 PARAM BMAGN(HCP_A3,CR:VA;0) 298.15 -2.46;  6000 N REF1 !
 PARAM G(HCP_A3,FE:VA;0) 298.15 +GHSERFE#+GPFEHCP#
               -3705.78+12.591*T-1.15*T*LN(T)+6.4E-04*T**2; 1811 Y
                              +GHSERFE#+GPFEHCP#
               -3957.199+5.24951*T+4.9251E+30*T**(-9);      6000 N REF0 !
 PARAM G(HCP_A3,CR:C;0) 298.15 +GHSERCR#+.5*GHSERCC#
               -18504+9.4173*T-2.4997*T*LN(T)+.001386*T**2; 6000 N REF1 !
 PARAM G(HCP_A3,FE:C;0) 298.15 +GFEFCC#+.5*GHSERCC#+GPCFCC#
                               +52905-11.9075*T;          6000 N REF3 !

 PARAM L(HCP_A3,CR:C,VA;0)  298.15  +4165;  6000 N REF1 !
 PARAM L(HCP_A3,FE:C,VA;0)  298.15 -22126;  6000 N REF3 !
$PARAM L(HCP_A3,FE:C,VA;0)  298.15 -17335;  6000 N TCFE3 !
 PARAM L(HCP_A3,CR,FE:VA;0) 298.15 +10833-7.477*T; 6000 N REF4 !

$***** SIGMA (Solution) *********************************************
 PHASE SIGMA  %  3 8   4   18 !
 CONST SIGMA  : FE
              : CR
              : CR,FE :  !
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 PARAM G(SIGMA,FE:CR:CR;0)  298.15 +8*GFEFCC#+22*GHSERCR#
                               +92300-95.96*T+GPSIG1#;   6000 N REF4 !
 PARAM G(SIGMA,FE:CR:FE;0)  298.15 +8*GFEFCC#+4*GHSERCR#+18*GHSERFE#
                               +117300-95.96*T+GPSIG2#;  6000 N REF4 !

$***** CEMENTITE (Solution) ******************************************
 PHASE CEMENTITE  %  2 3   1 !
 CONST CEMENTITE  : CR,FE%
                  : C :  !

 PARAM G(CEMENTITE,CR:C;0)  298.15 +3*GHSERCR#+GHSERCC#
                                   -48000-9.2888*T; 6000 N REF2 !
 PARAM G(CEMENTITE,FE:C;0)  298.15 +GFECEM#;          6000 N REF3 !

 PARAM L(CEMENTITE,CR,FE:C;0)  298.15 +25278-17.5*T;  6000 N REF2 !

$***** M3C2 (Compound) ***********************************************
 PHASE M3C2  %  2 3   2 !
 CONST M3C2  : CR
             : C :  !

 PARAM G(M3C2,CR:C;0)  298.15 +GCRM3C2#;  6000 N REF2 !

$***** M7C3 (Solution) ***********************************************
 PHASE M7C3  %  2 7   3 !
 CONST M7C3  : CR%,FE
             : C :  !

 PARAM G(M7C3,CR:C;0)  298.15 +GCRM7C3#;          6000 N REF2 !
 PARAM G(M7C3,FE:C;0)  298.15 +7*GHSERFE#+3*GHSERCC#
                               +75000-48.2168*T; 6000 N REF2 !

 PARAM L(M7C3,CR,FE:C;0)  298.15 -4520-10*T;  6000 N REF2 !

$***** M23C6 (Solution) **********************************************
 PHASE M23C6  %  3 20   3   6 !
 CONST M23C6  : CR%,FE%
              : CR%,FE%
              : C :  !
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 PARAM G(M23C6,CR:CR:C;0)  298.15 +GCRM23C6#;           6000 N REF5 !
 PARAM G(M23C6,FE:CR:C;0)  298.15 +.1304348*GCRM23C6#
                                  +.8695652*GFEM23C6#; 6000 N REF5 !
 PARAM G(M23C6,CR:FE:C;0)  298.15 +.8695652*GCRM23C6#
                                  +.1304348*GFEM23C6#; 6000 N REF5 !
 PARAM G(M23C6,FE:FE:C;0)  298.15 +GFEM23C6#;           6000 N REF5 !

 PARAM L(M23C6,CR,FE:CR:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !
 PARAM L(M23C6,CR,FE:FE:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !

$***** GRAPHITE (Compound) ******************************************
 PHASE GRAPHITE  %  1  1.0  !
 CONST GRAPHITE  : C :  !

 PARAM G(GRAPHITE,C;0)  298.15 +GHSERCC#+GPCGRA#; 6000 N REF0 !

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$ ASSESSED_SYSTEMS information:
$    *  necessary for the BIN and TERN modules in TCC
$                     the Binary Phase Diagram module in TCW
$                 and the Equilibrium calculation routine in TCW
$---------------------------------------------------------------------------
 ASSESSED_SYSTEM
$... Binary ...
  C-FE(;P3 TMM:300/4000 *)
  C-CR(;P3 TMM:300/4000 *)
  CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
        ;P3 TMM:300/3000 STP:.6/1200/1/-2/2)
$ CR-FE(TDB -HCP ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
$       ;P3 TMM:300/3000 STP:.6/1200/1/-2/2)
$
$... Ternary ...
  C-CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
          ;P3 STP:.4/.5/1 STP:0.1/0.5/1)
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$ LIST OF REFERENCE:
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$-------------------------------------------------------------------------
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       v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
       at high temperatures.'
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