

# XMLTDB data format documentation

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DRAFT May 19, 2023

Use color to indicate changes!

## Abstract

This is the draft definition of an XML format for thermodynamic data for Calphad applications in materials science

## 1 Introduction

During the work with the 1991 unary database [1] a database format called TDB was developed to handle the complex set of model parameters used in models for different phases. Today, almost 40 years later, it is time to take advantage of the development of computer science to revise this format using the XML, a well established markup language, explained for example in the web site [2].

During its 40 years of use the TDB databases have been extended to include other data, for example kinetic and structural, which is related to the phases in a system. The intention is that the XMLTDB should also accomodate such data. It should be simple to introduce additional model parameters related to any other property depending on the phase constitution,  $T$  and  $P$ .

The basic structure in the TDB format is:  
**keyword data !**

where the exclamation mark, “!” is the terminator, This makes it possible to transform to XML by using a mix of XML elements and attributes for the data. The transfer to XML has been straightforward but not painless as a complex set of additional features has been introduced during the time TDB files has been used. Most of the data in a TDB file can be tranferred to a tentative XMLTDB format using an UPLOAD program [3]. An example is found in Appendix D.

The XMLTDB format should contain the thermodynamic and related data but software specific directives, intended to simplify calculations using the data, should be excluded or included in a software specific XML element.

### 1.1 The Gibbs energy expression

The Calphad method to calculate phase diagrams based on modeling the Gibbs energy of each phase in a system has been described in many books and papers [4, 5, 6, 7, 9, 8, 10, 11].

The thermodynamic database provides model parameters to a thermodynamic software in order to calculate the Gibbs energy,  $G_M^\alpha$  for each phase in a system. The main objective is to calculate equilibrium state of the system by minimizing the total Gibbs energy of the system, depending on the set of external condition and the model parameters has been fitted to experimental and theoretical data in a separate assessment procedure. A more practically useful application is to provide thermodynamic information for simulating phase transformations together with kinetic data.

For each phase the Gibbs energy is expressed as:

$$G_M^\alpha = {}^{\text{srf}}G_M^\alpha - T {}^{\text{cfg}}S_M^\alpha + {}^E G_M^\alpha + f_M^\alpha \cdot {}^{\text{phy}}G_m^\alpha \quad (1)$$

where the term  ${}^{\text{srf}}G_M^\alpha$  has parameters for the surface of reference of the Gibbs energy and  ${}^E G_M^\alpha$  has parameters to describe interaction energies between constituents within the phase. The capital  $M$  used as subscript means the Gibbs energy is per mole formula unit of the phase, which may vary with the phase constitution. Each phase can have a different model, in particular for its configurational entropy,  ${}^{\text{cfg}}S_M^\alpha$ , which depend on its structure. There can be contribution from several physical models, denoted  ${}^{\text{phy}}G_m^\alpha$ , with specific model parameters. This term has subscript, “ $m$ ”, as this is normally modeled per mole of atoms and the factor  $f_M^\alpha$  is the number of atoms per formula unit of the phase.

## 1.2 Assessment of model parameters

The model parameters in the database are obtained by an assessment procedure where experimental and theoretical data are recalculated from the models using a thermodynamic software. The model parameters are varied using a least square fitting software in order to obtain the best description. Frequently conflicting information must be weighted or rejected by the scientist performing the assessment in order to obtain a satisfactory result, as discussed in many published papers and also in [7].

The assessments usually deal with binary and ternary systems where there are sufficient reliable experimental data but the main applications of the databases are to calculate multicomponent systems with up to 10-15 components. It is thus important to use models which give realistic extrapolations and the development of new models is still ongoing, inspired by the use of the database.

The assessment procedure is an integrated process involving experimental work, theoretical calculations and improved modeling by scientists. The models cannot be too complex because for example a simulation of a phase transformations for an alloy with 10-15 components requires a very large number of equilibrium calculations which typically can take weeks to perform on a high speed computer. Some model parameters must also be estimated from experience because there are no experimental data available. But the calculations are an essential tool replacing many years of experimental trial and error work in order to develop new or improved materials. This technique can be complemented, but not replaced, by recent methods inspired machine learning [13, 14].

## 2 Description of the proposed XMLTDB format

The XMLTDB format is an attempt to make a smooth transition from the TDB format to the XML in order to maintain the possibility to edit the XMLTDB file manually by scientists without particular experience of XML. The possibility to edit TDB files manually has been a great advantage for developing models and assessing experimental data using the current TDB format.

### 2.1 Short overview

This summary has the basic set of XML elements for the XMLTDB format. A detailed explanation is found in Appendix A

1. **Defaults** specify default values for some attributes in order to avoid listing irrelevant information.
2. **Models** is an optional part of the XML file with documentation and references for various models used. A separate XMLTDB model library file with all models and model parameter identifiers (MPID) will be provided. Each model has an ID which can be used when adding this model to a phase. New models will be added when tested and available in the application software.
3. **Element** specifies an element with its chemical symbol, the name of its reference phase, its molar mass, H298 and S298.
4. **Species** is an element or a molecular like aggregate of two or more elements with fixed stoichiometric ratios. A species has a name which is used when it is a constituent of a phase. A species can have an electric charge. Some species used for phases with the MQMQA [12] or UNIQUAC [15] models will have additional data such as bond fractions or volume and area needed for the configurational entropy of the phase.
5. **TPfun** has an ID and a mathematical expression in  $T$  and  $P$  and other TPfuns. Only very simple expressions are allowed as explained in Appendix A.3.
6. **Trange** is needed if a TPfun or parameter is valid in limited  $T$  range or have several ranges. Each Trange record with the upper  $T$  limit and expression. The value of the expression and its first and second derivative wrt  $T$  must be continuous when crossing a range.
7. **Phase** has a name, a configurational entropy model and all model parameters are associated with a phase. It can have one or more sublattices with different number of sites and constituents. Additional models can contribute to its Gibbs energy.
8. **Sublattices** specifies the number of sublattices of a phase and their site ratios. Optionally more crystallographic information can be provided.
9. **Constituents** has a sublattice index and a list of species as constituents in the sublattice.
10. **Amend-phase** specifies an additional model for a phase. It may have some extra model specifications.

11. **Parameter** has a model parameter identifier (MPID) specifying the type of property, a phase name and sublattice constituents. It has also a degree to indicate some additional model feature and a bibliographic reference. Finally it has a mathematical expression which may depend on  $T$  and  $P$  and include TPfun identifiers.
12. **Bibliography** contains all the bibliographic information for models and parameters.

## 2.2 Manual editing and efficient parsing

There are special parsers of XML files which work better the more detailed the data is separated in elements and attributes. However, very detailed specification of the data makes it inconvenient for editing manually which is still an important tool for scientists interested in modeling and assessment of model parameters. For example a model parameter can be described as:

```
<Parameter id="G(FCC,W:C,VA;0)" expression=" 50000+10*T;" bibref="90Gus"/>
```

which is similar to the way the parameter is listed in the TDB format or in an extended way which is simpler for an XML parser such as:

```
<Parameter mpid="G" phase="FCC" bibref="90Gus">
  <Constituentarray degree="0">
    <Site refid="1">
      <Constituent id="W"/>
    </Site>
    <Site refid="2">
      <Constituent id="C"/>
      <Constituent id="VA"/>
    </Site>
  </Constituentarray>
  <Trange expression=" 50000+10*T;" />
</Parameter>
```

and there is no question which is preferred by a scientist who is editing the XML file.

However, there is no reason not to allow both methods in the XMLTDB file, a human can without too much effort translate the extended parameter attributes to the simpler one in order to edit it and with a little effort the software using an XML parser can do the opposite.

## 2.3 Extensions and future changes in the XMLTDB format

The XMLTDB format is open to extensions and changes but they should be communicated and agreed by a governing committee, for example appointed by SGTE, in order to be universally agreed and circulated to all groups which use XMLTDB.

### 3 Application and software specifics

The TDB files are used by many different software to calculate equilibria, phase diagrams and various properties of multicomponent systems. The databases are also used for simulations of phase transformation together with mobilities and other phase dependent data stored in the TDB file.

More things to write about:

1. How to handle duplicate parameters in the XML file?
2. A wildcard parameter is independent of the constituent in one or more sublattices, how to handle wildcard parameters? In particular if there is an “overlapping” parameter with a specific constituent in the same sublattice as the parameter with a wildcard.
3. Order of RK constituents, alphabetical or as written?
4. Should the database specify miscibility gaps for example in Fe-Ti-C to have both an FCC representing austenite and an FCC representing the MC carbide? Or in Al-Ni to represent the FCC and the L1<sub>2</sub> ordered phase.
5. There is a need for a free software to check consistency of an XMLTDB file.
6. Is there an interest to develop a software to write the model parameters in an XML file as a nicely formatted a LaTeX file?
7. For the application software: is the  $f_M^\alpha$  from eq. 1 correctly implemented?
8. A property such as BMAGN is extensive but as it is inside a physical model I am not sure it should be multiplied with the  $f_M^\alpha$  defined in eq. 1.
9. UPLOAD program has not implemented
  - extracting software specific data from TDB.
  - DATA\_INFORMATION and some other TDB keywords. {colormagenta item The gas constant  $R$  has changed ... should we use the new value?
10. more?

### 4 Anything else?

### 5 Summary

The intention is that the XMLTDB format should be used for the same applications as the current TDB files and eventually replace them. It is thus important to think of all possible (and future) applications when deciding the format. We have also to consider the scientists who frequently explicitly manipulate the databases in order to develop models and software based on assessments of experimental and theoretical data.

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# Appendix A The XML elements and attributes for Calphad databases

This is a complete description of the XML format which will (hopefully) replace the current TDB format.

## A.1 Some general features

In most cases the thermodynamic data in the XMLTDB files will be the same as in the TDB files. A difference with the TDB file is that the XML elements and attributes are case sensitive and cannot be abbreviated. The data in the TDB files is case insensitive and keywords and phase names can be abbreviated.

1. All names, identifiers, symbols etc. of elements, species, phases, TPfuns in the XMLTDB file are case insensitive. All names etc. must start with a letter A-Z and may contain letters, numbers 0-9 and the underscore character “\_”. Some names, as specified below, can contain additional characters. In most cases this is the same way names are treated in TDB files.
  - (a) An element is one or two letters which are case insensitive. Fictitious elements can be used.
  - (b) A species name can in addition contain the characters “+”, “-” and “/”.
  - (c) A model parameter identifier can in the TDB file contain an ampersand “&” to specify a constituent. This is used for mobilities at present but may be extended. As “&” is reserved in XML files another letter should be used, maybe “@”?
  - (d) ?? any more special characters or exceptions?
2. Names of elements and species must not be abbreviated but frequently phase names are and it is allowed as long as they do not become ambiguous.

Species names must not be abbreviated in the XMLTDB file and thus one may have species names which are abbreviations of other species, for example C1O and C1O2. A species name is independent of its stoichiometric formula.

Phase names can be abbreviated and each part of a phase name separated by an underscore, “\_”, can be abbreviated separately. Interactive entering of a phase name should allow the hyphen, “-”, to be used instead of the underscore. For this reason it is not allowed to have phase names that are abbreviations of another phase, for example U3O8\_S and U3O8\_S2.

Model parameter identifiers (MPID), TPfun names and bibrefs must not be abbreviated.

A maximum length of names other identifiers should be decided, I propose:

- (a) Elements 2 letters.
- (b) Element reference phase: 24 characters
- (c) Species names: 24 characters.
- (d) Phase names: 24 characters
- (e) TPfun names: 16 characters



- (f) Model parameter identifiers: 8 characters (not including any constituent specifier used for mobilities etc.)
  - (g) Model identifier: 16 characters
  - (h) Bibrefs: 16 characters
3. Model parameter identifiers (MPID) are used for model parameters of a phase which depend on the constitution of the phase and frequently also on  $T$  and  $P$ .  
 The model parameter “G” for a Gibbs energy parameter. All other must be associated with a particular model. They are case insensitive. The use of “L” for excess parameter should be discouraged and be converted to “G”.  
 Some MPID contain a reference to a constituent of the phase, for example mobility data, and in the TDB file the species included in the MPID separated by an ampersand “&”. As XML uses this character for other things it is suggested this character is changed, for example to “@”.
  4. The hash character, “#”, frequently used in TDB files at the end of a function identifier, is redundant and not allowed.  
 The hash character, “#”, followed by a digit, is also used in some software to indicate composition sets of a phase.
  5. Any other use of special characters?

## A.2 Detailed explanation of all XMLTDB elements and attributes

For examples see also Appendix D.

### A.2.1 Defaults element

Some default values of particular attributes can be set here. If an attribute has the default value it can be omitted for the element. If we have for example:

```
<Defaults low_T="298.15" high_T="6000" />
```

this means that a low  $T$  limit for a TPfun element such as:

```
<TPfun id="GHSERXX" low_T="298.15" >
<Trange high_T="6000" Expression=" 10000-10*T;" />
</TPfun>
```

can be simplified to be:

```
<TPfun id="GHSERXX" Expression=" 10000-10*T;" />
```

### A.2.2 Models element

All models, except for the configurational entropy, which are used in a XMLTDB file must be taken from a general XMLTDB-models file which can optionally be included in the XMLTDB file. The XMLTDB-models file have a short description of each model and

specify the model parameter identifiers (MPID) which should be provided. Each model has a unique ID which can be needed for adding this model to a phase, sometimes with additional dat. For example:

```
<Magnetic-model id="IHJBCC" MPID1="TC" MPID2="BMAGN" anti-ferromagnetic_factor=" -1.00"
  f_below_TC=" +1-0.905299383*TAO**(-1)-0.153008346*TAO**3-.00680037095*TAO**9-.00153008346*TAO**15;"
  f_above_TC=" -.0641731208*TAO**(-5)-.00203724193*TAO**(-15)-.000427820805*TAO**(-25);" bibref="82Her" > in G=f(TAO)*LN(BETA+1) where TAO=T/TC
</Magnetic-model>
<Magnetic-model id="IHJREST" MPID1="TC" MPID2="BMAGN" anti-ferromagnetic_factor=" -3.00"
  f_below_TC=" +1-0.860338755*TAO**(-1)-0.17449124*TAO**3-.00775516624*TAO**9-.0017449124*TAO**15;"
  f_above_TC=" -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25);" bibref="82Her" > in G=f(TAO)*LN(BETA+1) where TAO=T/TC
</Magnetic-model>
<Magnetic-model id="IHJQX" MPID1="CT" MPID2="NT" MPID3="BMAGN" anti-ferromagnetic_factor=" 0.00"
  f_below_TC=" +1-0.842849633*TAO**(-1)-0.174242226*TAO**3-.00774409892*TAO**9-.00174242226*TAO**15-.000646538871*TAO**21;"
  f_above_TC=" -.0261039233*TAO**(-7)-.000870130777*TAO**(-21)-.000184262988*TAO**(-35)-6.65916411E-05*TAO**(-49);" bibref="12Xiong" > in G=f(TAO)*LN(BETA+1) whe
</Magnetic-model>
<Einstein-model id="GLOWTEIN" MPID1="LNTH" bibref="01Qing" >
  Gibbs energy due to the Einstein low T vibrational entropy model, G=1.5*R*THETA+3*R*T*LN(1-EXP(-THETA/T)).
</Einstein-model>
```

Each model defined have a unique ID which is used together with the phase element which have the model. The MPIDs specified for the model are used for the parameters describing how these parameters depend on the phase constitution and possibly  $T$  and  $P$ .

### A.2.3 Element element

The element is from the periodic chart or can be fictitious.

An element has the attributes:

- a chemical symbol, one or two letters
- the name of its reference phase
- its mass in gram/mol
- H298-H0 in J/mol
- S298 in J/mol/K

```
<Element id="FE" refstate="BCC_A2" mass="55.847" H298="4489" S298="27.2" />
```

Maybe add the English name of the element? For example that Sb is Antimony Sb?  
Maybe remove H298-H0 and S298?

The vacancy is treated as an element and be used to occupy a site in a sublattice. When calculating an equilibrium the chemical potential must be zero at equilibrium and there is no constraint on the number of vacancies.

The electron, denoted “/” can be listed among the elements but cannot exist by itself. If there is a need of a free electron it can be associated with a vacancy. At equilibrium each phases must be electrically neutral.

All attributes are mandatory.

### A.2.4 Species element

A species is an element or a molecular like aggregate of two or more elements with fixed stoichiometric ratios. A species has a name which is used when it is a constituent of a phase. A species can have an electric charge. In the future some species used for phases with the MQMQA [12] or UNIQUAC [15] models can have additional data which is not yet elaborated.

```
<Species id="C10" stoichiometry="C10" />
<Species id="O-2" stoichiometry="O/-2" />
```

One should avoid species names that could be interpreted as elements. Species are used as constituent of the phases. The stoichiometry must contain element names followed by a real number as the stoichiometric factor. Grouping using parenthesis is not allowed. A charge is specified using “/-” for a negative or “/+” for a positive ion.

Mandatory attributes are “id” and “stoichiometry”.

### A.2.5 TPfun element

Frequently some expressions are used in several model parameters and it is convenient to define them separately as functions. A TPfun has an ID and a mathematical expression in  $T$  and  $P$  which can also include other TPfuns. Only very simple expressions are allowed but can include references to other TPfun IDs. For a simple example see section A.2.1

Thermodynamic data must frequently be extrapolated over a large range of  $T$  and  $P$  and it can be necessary to breakpoint to change the expression in different regions. At such a breakpoint the values of the expressions must have identical values and well as identical first and second derivatives (representing continuous entropy and heat capacity).

To describe the expression with a limited range in  $T$  or several ranges the Trange element is used.

Mandatory attributes are “id”, optional attribute is “low\_T” (which can be ignored if same as the default “low\_T”) and “Expression” (which can be replaced by one or several “Trange” elements). For the expression see section A.3

### A.2.6 Trange element

This is part of a TPfun or Parameter element. If it has a high\_T limit different from the default it is specified together with the expression, see section A.3. Several ranges require require several Trange elements. The value of the function and its first and second derivative wrt  $T$  must be continuous when crossing a range. An example used for a TPfun element is:

```
<TPfun id="GHSERAL" >
  <Trange High_T="700" Expression="-7976.15+137.093038*T-24.3671976*T*LN(T)-.001884662*T**2" />
  <Trange High_T="933.47" Expression="-11276.24+223.048446*T-38.5844296*T*LN(T)+.018531982*T**2" />
  <Trange High_T="2900" Expression="-11278.378+188.684153*T-31.748192*T*LN(T)-1.230524E+28*T**2" />
</TPfun>
```

Mandatory attribute is “expression” and optional “high\_T”.

### A.2.7 Phase element

This is the key element of the XMLTDB file. All data are referred to a specific phase. A phase has a name, a configurational model depending on its sublattices and constituents specified by extra elements. All model parameters belong to a phase. Phases can have additional models specified. For example:

```

<Phase id="BCC_4SL" Configuration_model="CEF_3terms" state="S" >
  <Sublattices number_of="5" Ratios="0.25 0.25 0.25 0.25 3" >
    <Constituent sublattice="1" list="AL FE" />
    <Constituent sublattice="2" list="AL FE" />
    <Constituent sublattice="3" list="AL FE" />
    <Constituent sublattice="4" list="AL FE" />
    <Constituent sublattice="5" list="VA" />
  </Sublattices>
  <Amend-phase model="IHJBCC" />
  <Amend-phase model="DISFS" info="BCC_4SL A2_BCC" sum_sublattices="4" />
  <Amend-phase model="BCCPERM" info="The parameters have BCC permutations" />
</Phase>

```

where the `configuration_model` specify the Compound Energy Formalism (CEF) [19] and that the Gibbs energy has 3 terms which is associated with the disordered fraction model “DISFS” specified in section A.4.5. The state is “S” for a solid phase which is important if the Equi-Entropy Criterion (EEC) is applied at high  $T$ , see section A.4.7.

This phase has 5 sublattices where the first 4 represent an unsymetric tetrahedron in the BCC lattice, all with AL and FE as constituents. The last sublattices is for interstitials such as C or N but in this case it is empty, i.e. occupied only by VA representing the vacancy. There are 3 times as many interstitial sites as substitutional in BCC.

One amend-phase element specifies a magnetic model with “IHJBCC” and another the disordered fraction set model with “DISFS” which also specify the ordered and disordered parts of the phase. In OC this is done differently but it may be useful to have an option to extract just the disordered phase.

The “BCCPERM” model specifies that parameters which are identical when constituents are permuted on the sublattices for ordering are only listed once in the XMLTDB file.

Other configurational models used are I2SL for the partially ionic 2-sublattice model. The CEF model include the ideal model without sublattices and excess parameters and the single sublattice regular model with Redlich-Kister-Muggianu (RKM) excess parameters as special cases but only may allow configurational models as “ideal” and “RKM” for these.

Models that are less frequent in TDB files, such as the modified quasichemical model in the quadruple approximation (MQMQA) or UNIQUAC for polymeric liquids, can be used for software which has implemented them. However, they require also special species attributes, see “section A.2.4.

I do not think other binary excess models than Redlich-Kister (RK) is interesting as one can always convert them to an RK model. Ternary excess models such as Kohler [20] and Toop [21] can be interesting but one should consider Pelton’s proposal that each ternary can have a different extrapolation and implement that. See the section A.4.8.

Maybe there are other configurational models to think about for example CVM? It must be easy to add new models with new features without changing the basic XMLTDB structure.

### A.2.8 Sublattices element

This is part of the Phase element and specifies the number of sublattices and the site ratio for each. The sum of site ratios is the formula unit of the phase. Note that the number of atoms per formula units can vary with composition. Optionally more crystallographic information can be provided but it will normally be irrelevant for the thermodynamic calculations..

### A.2.9 Constituents element

This is part of the Phase element and for each sublattice there is a list of the constituents in the sublattice. The order of the sublattices must be the same as the order of sites in the “ratio” attribute of the sublattice element. The order of the sublattices is also important for the parameter element, see A.2.11.

### A.2.10 Amend-phase element

This is part of the Phase element and specifies an additional model for a phase. It may have some extra model specifications, for example in the “DISFS” model the ordered and disordered phases and the number of sublattices to be summed are included.

### A.2.11 Parameter element

This is the element which provides the actual data for the models of the phases. It has a complex identifier specifying the type of property (MPID), the phase and sublattice constituents and a degree to indicate some additional use. Finally a bibliographic reference to the paper where the parameter was published or who provided the parameter. The parameter must specify the phase because it may occur independently of the phase as a scientist manually editing an XMLTDB database may prefer to arrange all parameters for each binary or ternary system together.

The complex identifier is the same which has been used in TDB files and the phase constituents are in sublattice order, those mixing in the same sublattice are separated by a comma, “,”, and a colon, “:” separates constituents in different sublattices.

The parameter has a mathematical expression which can include TPfun element names provided this is valid for the whole default  $T$  range. If it is valid in a limited  $T$  range then one or more Trange elements are needed to specify different expressions. Examples:

```
<Parameter id="G(A2_BCC,AL:VA;0)" Bibref="91Din" >
  <Trange High_T="2900" Expression="+GALBCC;" />
</Parameter>
```

```
<Parameter id="G(BCC_4SL,AL:AL:AL:FE:VA;0)" Expression="+GD03ALFE;" Bibref="08Sun" />
<Parameter id="TC(BCC_4SL,AL:AL:AL:FE:VA;0)" Expression="-125;" Bibref="010hn" />
<Parameter id="BMAGN(BCC_4SL,AL:AL:AL:FE:VA;0)" Expression="BMALFE;" Bibref="08Sun" />
```

A parameter such as G(BCC\_4SL,AL:AL:AL:FE:VA;0) has 4 identical permutations with the Fe in different sublattices. As the “BCCPERM” model was indicated for the

BCC\_4SL phase this parameter is listed only once. If the software does not have implemented these permutations it has to generate them when reading the database.

The reason to use a complex identifier is explained in section 2.2 but in order to simplify the use of an XML parser in the software one may use the element in section A.2.12.

#### A.2.12 Parameter2 element

This element has the same information as the parameter but is split in parts in order to simplify the use of an XML parser.

```
<Parameter2 mpid="G" phase="FCC" bibref="90Gus">
  <Constituentarray degree="0">
    <Site refid="1">
      <Constituent id="W"/>
    </Site>
    <Site refid="2">
      <Constituent id="C"/>
      <Constituent id="VA"/>
    </Site>
  </Constituentarray>
  <Trange expression=" 50000+10*T;" />
</Parameter>
```

Software reading an XMLTDB file should be able to handle both forms of the parameter element.

#### A.2.13 Bibliography element

There can be bibliographic references for each parameter and possibly models for phases using bibitem elements.

#### A.2.14 Bibitem element

Inside the bibliographic element each bibliographic reference should be explicitly defined by this element, see Appendix D for an example.

### A.3 The mathematical expression

The mathematical expression used in expressions should be very simple. No grouping of terms using parenthesis is allowed and division of terms is not allowed.

- A simple term is a signed numeric value possibly multiplied with  $T$  and  $P$  raised to a power and possibly also multiplied with a TPfun symbol.
- A complex term is a simple term multiplied with the natural logarithm, LN, or the exponential, EXP, of a simple term.
- The argument of LN or EXP must be a simple term.
- Negative powers of  $T$  or  $P$  must be enclosed in parenthesis.

- As part of the Einstein low  $T$  model a function GEIN is needed which can take a simple term as argument. GEIN(X) is eq. A1 but the value of X should be the logarithm of the Einstein  $\theta$ ,  $\ln(\theta)$ , because that is what is used in the composition dependent LNTH parameter.
- In some software there are other functions allowed because they are used for kinetic models, for example ERF.

One reason to keep the expression simple is that some software needs to calculate first and second derivatives of the Gibbs energy expression with respect to  $T$  and  $P$  millions of times for each equilibrium calculation. Complex functions can be achieved by introducing several functions calling each other. There is normally no check of circular calls but such will normally lead to a crash of the calculation.

## A.4 Additional XML elements

This consists for the moment only of model elements. Each model has a descriptive element with a reference. Most models also have one or more model parameter identifiers (MPID) which are used to describe how the contribution to the Gibbs energy of the phase depend on  $T$ ,  $P$  and its constitution.

### A.4.1 There are 3 magnetic models

```
<Magnetic-model id="IHJBCC" MPID1="TC" MPID2="BMAGN" anti-ferromagnetic_factor=" -1.00"
  f_below_TC=" +1-0.905299383*TA0**(-1)-0.153008346*TA0**3-.00680037095*TA0**9-.0015300834
  f_above_TC=" -.0641731208*TA0**(-5)-.00203724193*TA0**(-15)-.000427820805*TA0**(-25);" b
</Magnetic-model>
<Magnetic-model id="IHJREST" MPID1="TC" MPID2="BMAGN" anti-ferromagnetic_factor=" -3.00"
  f_below_TC=" +1-0.860338755*TA0**(-1)-0.17449124*TA0**3-.00775516624*TA0**9-.0017449124*
  f_above_TC=" -.0426902268*TA0**(-5)-.0013552453*TA0**(-15)-.000284601512*TA0**(-25);" bi
</Magnetic-model>
<Magnetic-model id="IHJQX" MPID1="CT" MPID2="NT" MPID3="BMAGN" anti-ferromagnetic_factor="
  f_below_TC=" +1-0.842849633*TA0**(-1)-0.174242226*TA0**3-.00774409892*TA0**9-.001742422
  f_above_TC=" -.0261039233*TA0**(-7)-.000870130777*TA0**(-21)-.000184262988*TA0**(-35)-6
</Magnetic-model>
```

The functions is included only for documentation, they must be implemented in the software to be used. The MPID are slightly different and different software may actually use different names.

There is also a question of the reference state for the magnetism. Normally it is taken to be in the paramagnetic state at high  $T$ .

*Maybe some extra term needed for the IHJQX model for the reference state?*

### A.4.2 The Einstein model

This is the Einstein model which depend on the Einstein  $\theta$ . The LNTH parameter should be the natural logarithm of  $\theta$ . This adds a Gibbs energy contribution:

$$G = 1.5R\theta + 3RT \ln(1 - \exp(-\frac{\theta}{T})) \quad (\text{A1})$$

where  $\theta$  is the Einstein  $T$ . But to have a better description of the composition dependence the logarithm of  $\theta$  is used in LNTH.

```
<Einstein-model id="GLOWTEIN" MPID1="LNTH" bibref="01Qing" >
```

```
    Gibbs energy due to the Einstein low T vibrational entropy model, G=1.5*R*THETA+3*R*T*L  
</Einstein-model>
```

#### A.4.3 The Liquid 2-state model

The amorphous phase is an Einstein solid with  $\theta$  in the LNTH parameter and a G2 parameter determining the  $T$  for the transition from liquid to amorphous state. This model removes the breakpoint in the 1991 unary database when extrapolating the Gibbs energy of the liquid to low  $T$ . It does not describe the glass transition.

```
<Liquid-2state-model id="LIQ2STATE" MPID1="G2" MPID2="LNTH" bibref="14Becker" >
```

```
    Unified model for the liquid and the amorphous state treated as an Einstein solid  
</Liquid-2state-model>
```

#### A.4.4 A simple volume model

It is also possible to make many parameters dependent on  $P$  but the result may be surprising. This model was proposed by Lu et al. [16] for low  $P < 1$  GPa. Note that each phase can have a different volume model.

```
<Volume-model id="VOLOWP" MPID1="V0" MPID2="VT" MPID3="VB" bibref="05Lu" >
```

```
    The volume of a phase is described as function of T, P and its constitution.  
</Volume-model>
```

The parameter V0 is a constant representing the volume at  $T = 298.15$  and  $P = 1$  bar. VT is the thermal expansion at  $P = 1$  bar as function of  $T$ . VB represent a bulk modulus parameter which can depend on  $T$  and  $P$  and should be fitted to high pressure data.

#### A.4.5 The disordered fraction model

This model simplifies modeling of phases with ordering and order/disorder transitions. It combines the Gibbs energy of the ordered phase with another Gibbs energy without the ordering sublattices (excluding any interstitial sublattice). The interstitial sublattice must be the last and, if present, the disordered phase must also have an interstitial sublattice.

For a phase  $\alpha$  with an ordered part, ( $\alpha, \text{ord}$ ) and a disordered one, ( $\alpha, \text{dis}$ ) the Gibbs energy is calculated as

$$G_M^\alpha = G_M^{\alpha, \text{dis}}(x) - T^{\text{cfg}} S_M^{\alpha, \text{dis}} + G_M^{\alpha, \text{ord}}(y) \quad (\text{A2})$$

where the mole fractions  $x$  are calculated from the ordered fractions  $y$ . This model is denoted in the configurational\_model attribute as CEF\_2terms. The configurational entropy of the disordered phase is ignored. It is preferred for modeling phases which never disorder such as  $\sigma, \mu$ .



There is an alternative disordered model denoted as CEF\_3terms with the expression

$$G_M^\alpha = G_M^{\alpha,\text{dis}}(x) + G_M^{\alpha,\text{ord}}(y) - G_M^{\alpha,\text{ord}}(y = x) \quad (\text{A3})$$

where the ordered part is calculated twice, the second time with the mole fractions on all sublattices. When the phase is disordered the model parameters in  $G_M^{\alpha,\text{ord}}$  are eliminated. This model has been used for phases for order/disorder transformations as the parameters in the ordered phase does not affect the ordered phase but it is now discouraged as the ordered parameters may create strange phenomena. It is denoted as CEF\_3terms. In this model the disordered configurational entropy is eliminated by default.

```
<Disordered-fraction-model id="DISFS" bibref="07Hal" >
```

```
    The disordered fractions are summed over the ordered sublattices indicated at the phase  
</Disordered-fraction-model>
```

#### A.4.6 The permutation models

These model reduces the number of parameters in the database by eliminate all permutations. It must be implemented in the software. BCC and FCC has different symmetry as the tetrahedra are different.

```
<FCC-permutations id="FCCPERM" bibref="09Sun" >
```

```
    Permutations of ordered FCC parameters with the same set of elements are listed only on  
</FCC-permutations>
```

This model reduces the size of the database by avoiding storing all 24 permutations of a parameter such as G(FCC\_4SL,A:B:C:D:VA;0) of an ordered FCC phase in the database.

```
<BCC-permutations id="BCCPERM" bibref="09Sun" >
```

```
    Permutations of ordered BCC parameters with the same set of elements are listed only on  
</BCC-permutations>
```

The reduction of parameters is slightly less for BCC as the tetrahedron is not symmetric.

#### A.4.7 The EEC model

The Equi-Entropy criteria [17] means that a solid phase with higher entropy than the liquid phase must not be allowed to become stable. At a given  $T$  a solid phase can only have higher entropy than a liquid (with different composition) if the extrapolation of the Gibbs energy of the metastable solid is unphysical. The aim of this model is to remove the breakpoint in the Gibbs energy extrapolation of solid phases above their melting  $T$  and prevent the reappearance of the solid at even higher  $T$  due to an extrapolated heat capacity of the metastable solid which has no physical meaning.

It must be implemented in the software but the database should indicate if it is necessary.

```
<EEC id="EEC" bibref="20Sun" >
```

```
    Equi-Entropy Criterion means that solid phases with higher entropy than the liquid phase  
</EEC>
```

#### A.4.8 Ternary excess models

Pelton [18] has proposed a way to define the ternary excess model separately for each ternary. This could be implemented as an amend-phase option. Maybe something like:

```
<Excess-model id="Kohler" bibref="60Kohler" >
```

A ternary interaction has a Kohler excess model. The three constituents are specified at

```
</Excess-model>
```

```
<Excess-model id="Toop" bibref="65Toop" >
```

A ternary interaction has a Toop excess model. The three constituents are specified at

```
</Excess-model>
```

A phase with a Toop and Kohler model must for each ternary specify

```
<Amend-phase model="Toop" info="Fe Cr Ni" />
```

```
<Amend-phase model="Kohler" info="Mo Cr Ni" />
```

For the Toop model the first of the 3 constituents is the Toop constituent whereas for the Kohler model the order does not matter.

This is not implemented in any software as far as I know even if it might work in GES5.

## Appendix B Converting from TDB to XMLTDB format and vice versa

An UPLOAD program [3] has been developed and tested to convert various TDB files to the XMLTDB format proposed here. There are still many features to be discussed to obtain the final format.

If it is found that the final XML format is too complex for manual editing the TDB format may be kept for manual editing. But that will be a pain for the future.

## Appendix C Integration of 3rd generation models

The new unary parameters tries to make the Calphad databases more attractive to physicists and remove some of the less nice features of the 2nd generation unary, such as the break points in the Gibbs energies at the melting  $T$  of the elements.

### C.1 The low $T$ heat capacity and entropy

This concerns the Einstein model for low  $T$  vibrational energy which will also enforce the heat capacity is zero at  $T = 0$  K [22]. The Einstein heat capacity integrated to a Gibbs energy is shown in eq. A1.

The Einstein model was preferred as one anyway has to add a polynomial in  $T$  (without any powers of  $T$  less or equal to 1 and no  $\ln(T)$  term) in order to fit the deviation from the Dulong-Petit assumption that the heat capacity at high  $T$  should be  $3R$ .

The restriction that there should not be any linear term in  $T$  is to obey the 3rd law, i.e. that the entropy of a perfectly crystalline phases must be zero at  $T = 0$  K. But there is still a discussion if phases with crystalline disorder, for example magnetite which is an inverse spinel or the amorphous phase, should have  $S = 0$  at  $T = 0$  K.

There is an interesting use of the Einstein model for the lattice stabilities (introduced by Larry Kaufman in 1970 [4] and considered to be the first generation unary database) which represent a Gibbs energy difference between a stable,  $\alpha$ , and metastable,  $\beta$ , state of a pure element, and which usually have a linear  $T$  dependence, for example:

$$G_A^\beta - G_A^\alpha = \Delta H - T\Delta S \quad (C1)$$

where the linear  $T$  term can be converted to an Einstein  $\theta$  and this have zero entropy at  $T = 0$  K.

Many of the lattice stabilities were kept in the 2nd generation database and they are important to describe phase diagrams. But they violate the the 3rd law. However, one can easily convert the  $\Delta S$  to an Einstein  $\theta$  for the metastable phase using:

$$\theta^\beta = \theta^\alpha \exp\left(-\frac{\Delta S}{3R}\right) \quad (C2)$$

which will result in the same difference in Gibbs energy at finite  $T$  and that metastable phases of the pure elements also has  $S = 0$  at  $T = 0$  K.

## C.2 The magnetic model

The second part of the new unary is the magnetic model with a new expression and separate Curie and Néel  $T$  [23]. Individual Bohr magneton numbers will most likely not implemented. If the reference state for the magnetic state is selected at the paramagnetic state at high  $T$  this may give some entropy at  $T = 0$  K.

Selecting the ferro- or antiferro magnetic state at  $T = 0$  K creates other problems at high  $T$ .

## C.3 The low $T$ extrapolation of the liquid

The liquid 2-state model [24] use an Einstein solid for the low  $T$  amorphous state and a gradual transition to the stable high  $T$  liquid. As already stated the entropy of the metastable amorphous state may have nonzero entropy at  $T = 0$  K.

## C.4 The high $T$ extrapolation of the solid phase

The extrapolation of the heat capacity of the solid phases of the pure elements above their melting  $T$  is modeled with a restricted polynomial and this may extrapolate at high  $T$  to a high heat capacity and subsequently a very negative Gibbs energy of the solid. This may be so negative that the solid would become more stable than the liquid at even higher  $T$ . This was avoided in the 1991 unary by a breakpoint at the melting  $T$  and forcing the solid heat capacity to approach that of the liquid phase. But this breakpoint leads to some other problems, for example modeling compounds using the Kopp-Neumann rule [25], and should the breakpoint should be removed.

The Equi-Entropy Criterion (EEC) [17] was introduced to handle this extrapolation problem. The EEC states that at a given  $T$  a solid phase cannot be in equilibrium, i.e. be stable, together with a liquid if the solid has higher entropy than the liquid phase, even if the solid and liquid has different compositions.

The fact that the solid phase has so high entropy is due to an unphysical extrapolation of its heat capacity above its melting  $T$ . The high entropy means the solid is “mechanically unstable” but to find way to model this “instability” in multicomponent system has turned out to be very complicated whereas the entropy criteria is readily available.

## Appendix D Example of the tentative XMLTDB format

A TDB file for the system Al-Fe has been used to generate this XML file using the UPLOAD program.

### D.1 Example of the tentative XMLTDB format

The lines are very long but the essential inoformation is still readable.

```
<?xml version="1.0"?>
<?xml-model href="database.rng" schematypens="http://relaxng.org/ns/structure/1.0" type="application/xml"?>
<Database version="0.0.1">
  <metadata>
    <writer>xmldbproject test
      TDBfile="C:\Users\bosun\Documents\GitHub\XMLTDB\software\examples\AlFe-4SLBF.TDB"
      Software="Thermo-Calc"
      Date="2023-05-15"
    </writer>
  </metadata>
  <!-- Statistics elements="4" species="3" tpfuns="26" phases="9" parameters="54" bibrefs="6" -->
  <Defaults low_T=" 298.15" high_T=" 6000.00" />
  <Models>
    <Magnetic-model id="IHJBCC" MPID1="TC" MPID2="BMAGN" anti-ferromagnetic_factor=" -1.00"
      f_below_TC=" +1-0.905299383*TAO**(-1)-0.153008346*TAO**3-.00680037095*TAO**9-.00153008346*TAO**15;"
      f_above_TC=" -.0641731208*TAO**(-5)-.00203724193*TAO**(-15)-.000427820805*TAO**(-25);" bibref="82Her" > in G=f(TAO)*LN(BETA+1) where TAO=T/TC
    </Magnetic-model>
    <Magnetic-model id="IHJREST" MPID1="TC" MPID2="BMAGN" anti-ferromagnetic_factor=" -3.00"
      f_below_TC=" +1-0.860338755*TAO**(-1)-0.17449124*TAO**3-.00775516624*TAO**9-.0017449124*TAO**15;"
      f_above_TC=" -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25);" bibref="82Her" > in G=f(TAO)*LN(BETA+1) where TAO=T/TC
    </Magnetic-model>
    <Magnetic-model id="IHJQX" MPID1="CT" MPID2="NT" MPID3="BMAGN" anti-ferromagnetic_factor=" 0.00"
      f_below_TC=" +1-0.842849633*TAO**(-1)-0.174242226*TAO**3-.00774409892*TAO**9-.00174242226*TAO**15-.000646538871*TAO**21;"
      f_above_TC=" -.0261039233*TAO**(-7)-.000870130777*TAO**(-21)-.000184262988*TAO**(-35)-6.65916411E-05*TAO**(-49);" bibref="12Xiong" > in G=f(TAO)*LN(BETA+1)
    </Magnetic-model>
    <Einstein-model id="GLOWTEIN" MPID1="LNTH" bibref="01Qing" >
      Gibbs energy due to the Einstein low T vibrational entropy model, G=1.5*R*THETA+3*R*T*LN(1-EXP(-THETA/T)).
    </Einstein-model>
    <Liquid-2state-model id="LIQ2STATE" MPID1="G2" MPID2="LNTH" bibref="14Becker" >
      Unified model for the liquid and the amorphous state treated as an Einstein solid
    </Liquid-2state-model>
    <Volume-model id="VOLLOWP" MPID1="V0" MPID2="VA" MPID3="VB" bibref="05Lu" >
      The volume of a phase is described as function of T, P and its constitution.
    </Volume-model>
    <Disordered-fraction-model id="DISFS" bibref="07Hal" >
      The disordered fractions are summed over the ordered sublattices indicated at the phase. The Gibbs energy calculated 2 or 3 times as indicated by the CEF.
    </Disordered-fraction-model>
    <FCC-permutations id="FCCPERM" bibref="09Sun" >
      Permutations of ordered FCC parameters with the same set of elements are listed only once.
    </FCC-permutations>
    <BCC-permutations id="BCCPERM" bibref="09Sun" >
      Permutations of ordered BCC parameters with the same set of elements are listed only once.
    </BCC-permutations>
    <EEC id="EEC" bibref="20Sun" >
      Equi-Entropy Criterion means that solid phases with higher entropy that the liquid phase must not be stable.
    </EEC>
  </Models>
  <Element id="/" refstate="ELECTRON_GAS" mass=" 0.000000E+00" H298=" 0.000000E+00" S298=" 0.000000E+00" />
  <Element id="VA" refstate="VACUUM" mass=" 0.000000E+00" H298=" 0.000000E+00" S298=" 0.000000E+00" />
  <Element id="AL" refstate="FCC_A1" mass=" 2.698200E+01" H298=" 4.577300E+03" S298=" 2.832200E+01" />
```

```

<Element id="FE" refstate="BCC_A2" mass=" 5.584700E+01" H298=" 4.489000E+03" S298=" 2.728000E+01" />
<Species id="VA" stoichiometry="VA" />
<Species id="AL" stoichiometry="AL" />
<Species id="FE" stoichiometry="FE" />
<TPfun id="GHSERAL" >
  <Trange High_T="700" Expression=" -7976.15+137.093038*T-24.3671976*T*LN(T) -.001884662*T**2-8.77664E-07*T**3+74092*T**(-1);" />
  <Trange High_T="933.47" Expression=" -11276.24+223.048446*T-38.5844296*T*LN(T)+.018531982*T**2 -5.764227E-06*T**3+74092*T**(-1);" />
  <Trange High_T="2900" Expression=" -11278.378+188.684153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9);" />
</TPfun>
<TPfun id="GALLIQ" >
  <Trange High_T="933.47" Expression=" +11005.029-11.841867*T+7.934E-20*T**7 +GHSERAL;" />
  <Trange Expression=" +10482.382-11.253974*T+1.231E+28*T**(-9)+GHSERAL;" />
</TPfun>
<TPfun id="GALBCC" Expression="+10083-4.813*T+GHSERAL;" />
<TPfun id="GHSERFE" >
  <Trange High_T="1811" Expression=" +1225.7+124.134*T-23.5143*T*LN(T) -.00439752*T**2-5.8927E-08*T**3+77359*T**(-1);" />
  <Trange Expression=" -25383.581+299.31255*T-46*T*LN(T)+2.29603E+31*T**(-9);" />
</TPfun>
<TPfun id="GFELIQ" >
  <Trange High_T="1811" Expression=" +12040.17-6.55843*T-3.6751551E-21*T**7 +GHSERFE;" />
  <Trange Expression=" -10839.7+291.302*T-46*T*LN(T);" />
</TPfun>
<TPfun id="GFEFCC" >
  <Trange High_T="1811" Expression=" -1462.4+8.282*T-1.15*T*LN(T)+6.4E-04*T**2 +GHSERFE;" />
  <Trange Expression=" -27097.396+300.25256*T-46*T*LN(T)+2.78854E+31*T**(-9);" />
</TPfun>
<TPfun id="LFALFE0" Expression="-104700+30.65*T;" />
<TPfun id="LFALFE1" Expression="+30000-7*T;" />
<TPfun id="LFALFE2" Expression="+32200-17*T;" />
<TPfun id="UFALFE" Expression="-4000*T;" />
<TPfun id="GAL3FE" Expression="+3*UFALFE+9000;" />
<TPfun id="GAL2FE2" Expression="+4*UFALFE;" />
<TPfun id="GALFE3" Expression="+3*UFALFE-3500;" />
<TPfun id="SFALFE" Expression="+UFALFE;" />
<TPfun id="UBALFE1" Expression="-4023-1.14*T;" />
<TPfun id="UBALFE2" Expression="-1973-2*T;" />
<TPfun id="GD03ALFE" Expression="+2*UBALFE1+UBALFE2+3900;" />
<TPfun id="GB2ALFE" Expression="+4*UBALFE1;" />
<TPfun id="GB32ALFE" Expression="+2*UBALFE1+2*UBALFE2;" />
<TPfun id="GD03FEAL" Expression="+2*UBALFE1+UBALFE2-70+0.5*T;" />
<TPfun id="BMALFE" Expression="-1.36;" />
<TPfun id="BLALFE0" Expression="-0.3;" />
<TPfun id="BLALFE1" Expression="-0.8;" />
<TPfun id="BLALFE2" Expression="0.2;" />
<TPfun id="ZERO" Expression="0.0;" />
<TPfun id="UN_ASS" >
  <Trange High_T="300" Expression=" 0.0 ;" />
</TPfun>
<Phase id="LIQUID" Configuration_model="CEF" state="L" >
  <Sublattices number_of="1" Ratios="1" >
    <Constituent sublattice="1" list="AL FE" />
  </Sublattices>
</Phase>
<Phase id="A1_FCC" Configuration_model="CEF" state="S" >
  <Sublattices number_of="2" Ratios="1 1" >
    <Constituent sublattice="1" list="AL FE" />
    <Constituent sublattice="2" list="VA" />
  </Sublattices>
  <Amend-phase model="IHJREST" />
</Phase>
<Phase id="A2_BCC" Configuration_model="CEF" state="S" >
  <Sublattices number_of="2" Ratios="1 3" >
    <Constituent sublattice="1" list="AL FE" />
    <Constituent sublattice="2" list="VA" />
  </Sublattices>
  <Amend-phase model="IHJBCC" />
</Phase>
<Phase id="AL13FE4" Configuration_model="CEF" state="S" >
  <Sublattices number_of="3" Ratios="0.6275 0.235 0.1375" >
    <Constituent sublattice="1" list="AL" />
    <Constituent sublattice="2" list="FE" />
    <Constituent sublattice="3" list="AL VA" />
  </Sublattices>
</Phase>
<Phase id="AL2FE" Configuration_model="CEF" state="S" >
  <Sublattices number_of="2" Ratios="2 1" >
    <Constituent sublattice="1" list="AL" />
    <Constituent sublattice="2" list="FE" />
  </Sublattices>
</Phase>
<Phase id="AL5FE2" Configuration_model="CEF" state="S" >
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    <Constituent sublattice="1" list="AL FE" />
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    <Constituent sublattice="4" list="AL FE" />
    <Constituent sublattice="5" list="VA" />
  </Sublattices>
  <Amend-phase model="IHJBCC" />
  <Amend-phase model="DISFS" info="BCC_4SL A2_BCC sum_sublattices="4" />
  <Amend-phase model="BCCPERM" info="The parameters have BCC permutations" />
</Phase>
<Phase id="FCC_4SL" Configuration_model="CEF_3terms" state="S" >
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    <Constituent sublattice="2" list="AL FE" />
    <Constituent sublattice="3" list="AL FE" />
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    <Constituent sublattice="5" list="VA" />
  </Sublattices>
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  <Parameter id="TC(A1_FCC,FE:VA;0)" Expression="-201;" Bibref="91Din" />
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  <Parameter id="G(A2_BCC,FE:VA;0)" Expression="+GHSERFE;" Bibref="91Din" />
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  <Parameter id="G(LIQUID,AL,FE;0)" Expression="-88090+19.8*T;" Bibref="08Sun" />
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  <Parameter id="G(LIQUID,AL,FE;2)" Expression="-2000;" Bibref="08Sun" />
  <Parameter id="G(A1_FCC,AL,FE:VA;0)" Expression="+LFALFE0;" Bibref="08Sun" />
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  <Parameter id="G(AL2FE,AL:FE;0)" Expression="-104000+23*T+2*GHSERAL+CHSERFE;" Bibref="08Sun" />
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  <Parameter id="BMAGN(BCC_4SL,AL,FE:*:*:VA;2)" Expression="+BLALFE2;" Bibref="08Sun" />
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  <Parameter id="G(FCC_4SL,FE:FE:AL:VA;0)" Expression="+GAL2FE2;" Bibref="08Con" />
  <Parameter id="G(FCC_4SL,FE:FE:FE:AL:VA;0)" Expression="+GALFE3;" Bibref="08Con" />
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</Binary-parameters>

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<Bibitem ID="93Sei" Text="M Seiersten, unpublished 1993" />
<Bibitem ID="010hn" Text="I Ohnuma, unpublished 2001" />
<Bibitem ID="08Con" Text="D Connetable et al, Calphad 2008; AL-C-Fe" />
<Bibitem ID="08Sun" Text="B Sundman, to be published" />
<Bibitem ID="08Dup" Text="N Dupin, vacancies in bcc" />
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<Bibitem ID="20Sun" Text="B. Sundman, U. R. Kattner, M. Hillert, M. Selleby, J. Agren, S. Bigdeli, Q. Chen, A. Dinsdale, B. Hallstedt, A. Khvan, H. Mao and R. L. Martin, Thermodynamic modeling of the Fe-C system, Calphad, Vol 36 (2012) 1-12" />
</Bibliography>
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0 $ From database: User data 2008. 8. 1
127 $ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM A2_BCC
155 $ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM A1_FCC
</TDB-comments>
</Database>

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## D.2 The original TDB format

\$ Database file written 2008- 8-15

\$ From database: User data 2008. 8. 1

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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 AL    FCC_A1            2.6982E+01  4.5773E+03  2.8322E+01!
ELEMENT FE    BCC_A2            5.5847E+01  4.4890E+03  2.7280E+01!

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FUNCTION GHSERAL 298.15 -7976.15+137.093038*T-24.3671976*T*LN(T)
-.001884662*T**2-8.77664E-07*T**3+74092*T**(-1); 7.00000E+02 Y
-11276.24+223.048446*T-38.5844296*T*LN(T)+.018531982*T**2
-5.764227E-06*T**3+74092*T**(-1); 9.33470E+02 Y
-11278.378+188.684153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9);
2.90000E+03 N !
FUNCTION GALLIQ 298.15 +11005.029-11.841867*T+7.934E-20*T**7
+GHSERAL#; 9.33470E+02 Y
+10482.382-11.253974*T+1.231E+28*T**(-9)+GHSERAL#; 6000 N !
FUNCTION GALBCC 298.15 +10083-4.813*T+GHSERAL#; 6000 N !
FUNCTION GHSERFE 298.15 +1225.7+124.134*T-23.5143*T*LN(T)
-.00439752*T**2-5.8927E-08*T**3+77359*T**(-1); 1.81100E+03 Y
-25383.581+299.31255*T-46*T*LN(T)+2.29603E+31*T**(-9); 6000 N !
FUNCTION GFELIQ 298.15 +12040.17-6.55843*T-3.6751551E-21*T**7
+GHSERFE#; 1.81100E+03 Y
-10839.7+291.302*T-46*T*LN(T); 6000 N !
FUNCTION GFEFCC 298.15 -1462.4+8.282*T-1.15*T*LN(T)+6.4E-04*T**2
+GHSERFE#; 1.81100E+03 Y
-27097.396+300.25256*T-46*T*LN(T)+2.78854E+31*T**(-9); 6000 N !
FUNCTION LFALFEO 298.15 -104700+30.65*T; 6000 N !
FUNCTION LFALFE1 298.15 +30000-7*T; 6000 N !
FUNCTION LFALFE2 298.15 +32200-17*T; 6000 N !

```

```

FUNCTION UFALFE      298.15 -4000+T;  6000    N !
FUNCTION GAL3FE      298.15 +3*UFALFE#+9000;  6000    N !
FUNCTION GAL2FE2     298.15 +4*UFALFE#;  6000    N !
FUNCTION GALFE3      298.15 +3*UFALFE#-3500;  6000    N !
FUNCTION SFALFE      298.15 +UFALFE#;  6000    N !
FUNCTION UBALFE1     298.15 -4023-1.14*T;  6000    N !
FUNCTION UBALFE2     298.15 -1973-2*T;  6000    N !
FUNCTION GD03ALFE    298.15 +2*UBALFE1#+UBALFE2#+3900;      6000    N !
FUNCTION GB2ALFE     298.15 +4*UBALFE1#;  6000    N !
FUNCTION GB32ALFE    298.15 +2*UBALFE1#+2*UBALFE2#;  6000    N !
FUNCTION GD03FEAL    298.15 +2*UBALFE1#+UBALFE2#-70+0.5*T; 6000    N !
FUNCTION BMALFE      298.15 -1.36; 6000 N !
FUNCTION BLALFE0     298.15 -0.3; 6000 N !
FUNCTION BLALFE1     298.15 -0.8; 6000 N !
FUNCTION BLALFE2     298.15 0.2; 6000 N !
FUNCTION ZERO        298.15 0.0; 6000.00 N !
FUNCTION UN_ASS      298.15 0.0 ; 3.00000E+02 N !

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TYPE_DEFINITION % SEQ *!
DEFINE_SYSTEM_DEFAULT ELEMENT 2 !
DEFAULT_COMMAND DEF_SYS_ELEMENT VA /- !

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TYPE_DEFINITION X GES AMEND_PHASE_DESCRIPTION BCC_4SL DIS_PART A2_BCC,,,!
TYPE_DEFINITION Y GES AMEND_PHASE_DESCRIPTION FCC_4SL DIS_PART A1_FCC,,,!

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PHASE LIQUID:L % 1 1.0 !
  CONSTITUENT LIQUID:L :AL,FE : !

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PARAMETER G(LIQUID,AL;0) 298.15 +GALLIQ#;  6000    N 91Din !
PARAMETER G(LIQUID,FE;0) 298.15 +GFELIQ#;  6000    N 91Din !
PARAMETER G(LIQUID,AL,FE;0) 298.15 -88090+19.8*T;  6000    N 08Sun !
PARAMETER G(LIQUID,AL,FE;1) 298.15 -3800+3*T;  6000    N 08Sun !
PARAMETER G(LIQUID,AL,FE;2) 298.15 -2000;  6000    N 08Sun !

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TYPE_DEFINITION F GES A_P_D @ MAGNETIC -3.0 2.80000E-01 !
PHASE A1_FCC %F 2 1 1 !
  CONSTITUENT A1_FCC :AL,FE : VA : !

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PARAMETER G(A1_FCC,AL:VA;0) 298.15 +GHSERAL#;  6000    N 91Din !
PARAMETER G(A1_FCC,FE:VA;0) 298.15 +GFEFCC#;  6000    N 91Din !
PARAMETER TC(A1_FCC,FE:VA;0) 298.15 -201;  6000    N 91Din !
PARAMETER BMAGN(A1_FCC,FE:VA;0) 298.15 -2.1;  6000    N 91Din !
PARAMETER G(A1_FCC,AL,FE:VA;0) 298.15 +LFALFE0#;  6000    N 08Sun !
PARAMETER G(A1_FCC,AL,FE:VA;1) 298.15 +LFALFE1#;  6000    N 08Sun !
PARAMETER G(A1_FCC,AL,FE:VA;2) 298.15 +LFALFE2#;  6000    N 08Sun !

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TYPE\_DEFINITION B GES A\_P\_D @ MAGNETIC -1.0 4.00000E-01 !

PHASE A2\_BCC %B 2 1 3 !

CONSTITUENT A2\_BCC :AL,FE : VA : !

PARAMETER G(A2\_BCC,AL:VA;0) 298.15 +GALBCC#; 2.90000E+03 N 91Din !

PARAMETER G(A2\_BCC,FE:VA;0) 298.15 +GHSERFE#; 6000 N 91Din !

PARAMETER TC(A2\_BCC,FE:VA;0) 298.15 1043; 6000 N 91Din !

PARAMETER BMAGN(A2\_BCC,FE:VA;0) 298.15 2.22; 6000 N 91Din !

PARAMETER G(A2\_BCC,AL,FE:VA;0) 298.15 -122960+32\*T; 6000 N 93Sei !

PARAMETER G(A2\_BCC,AL,FE:VA;1) 298.15 2945.2; 6000 N 93Sei !

PARAMETER TC(A2\_BCC,AL,FE:VA;0) 298.15 -438; 6000 N 010hn !

PARAMETER TC(A2\_BCC,AL,FE:VA;1) 298.15 -1720; 6000 N 010hn !

PHASE AL13FE4 % 3 .6275 .235 .1375 !

CONSTITUENT AL13FE4 :AL : FE : AL,VA : !

PARAMETER G(AL13FE4,AL:FE:AL;0) 298.15 -30680+7.4\*T+.765\*GHSERAL#  
+.235\*GHSERFE#; 6000 N 08Sun !

PARAMETER G(AL13FE4,AL:FE:VA;0) 298.15 -28100+7.4\*T+.6275\*GHSERAL#  
+.235\*GHSERFE#; 6000 N 08Sun !

PHASE AL2FE % 2 2 1 !

CONSTITUENT AL2FE :AL : FE : !

PARAMETER G(AL2FE,AL:FE;0) 298.15 -104000+23\*T+2\*GHSERAL#+GHSERFE#;  
6000 N 08Sun !

PHASE AL5FE2 % 2 5 2 !

CONSTITUENT AL5FE2 :AL : FE : !

PARAMETER G(AL5FE2,AL:FE;0) 298.15 -235600+54\*T+5\*GHSERAL#  
+2\*GHSERFE#; 6000 N 08Sun !

PHASE AL8FE5\_D82 % 2 8 5 !

CONSTITUENT AL8FE5\_D82 :AL,FE : AL,FE : !

PARAMETER G(AL8FE5\_D82,AL:AL;0) 298.15 +13\*GALBCC#; 6000 N 08Sun !

PARAMETER G(AL8FE5\_D82,FE:AL;0) 298.15 +200000+36\*T+5\*GALBCC#  
+8\*GHSERFE#; 6000 N 08Sun !

PARAMETER G(AL8FE5\_D82,AL:FE;0) 298.15 -394000+36\*T+8\*GALBCC#  
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 PARAMETER G(AL8FE5\_D82,FE:FE;0) 298.15 +13\*GHSEFE#+13000; 6000 N 08Sun !  
 PARAMETER G(AL8FE5\_D82,AL:AL,FE;0) 298.15 -100000; 6000 N 08Sun !  
 PARAMETER G(AL8FE5\_D82,AL,FE:FE;0) 298.15 -174000; 6000 N 08Sun !

\$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM A2\_BCC

PHASE BCC\_4SL:B %BX 5 .25 .25 .25 .25 3 !

CONSTITUENT BCC\_4SL:B :AL,FE : AL,FE : AL,FE : AL,FE : VA : !

PARAMETER G(BCC\_4SL,AL:AL:AL:FE:VA;0) 298.15 +GD03ALFE#; 6000 N 08Sun !  
 PARAMETER TC(BCC\_4SL,AL:AL:AL:FE:VA;0) 298.15 -125; 6000 N 010hn !  
 PARAMETER BMAGN(BCC\_4SL,AL:AL:AL:FE:VA;0) 298.15 BMALFE; 6000 N 08Sun !

PARAMETER G(BCC\_4SL,AL:AL:FE:FE:VA;0) 298.15 +GB2ALFE#; 6000 N 08Sun !  
 PARAMETER TC(BCC\_4SL,AL:AL:FE:FE:VA;0) 298.15 -250; 6000 N 010hn !  
 PARAMETER BMAGN(BCC\_4SL,AL:AL:FE:FE:VA;0) 298.15 2\*BMALFE; 6000 N 08Sun !

PARAMETER G(BCC\_4SL,AL:FE:AL:FE:VA;0) 298.15 +GB32ALFE#; 6000 N 08Sun !  
 PARAMETER TC(BCC\_4SL,AL:FE:AL:FE:VA;0) 298.15 -125; 6000 N 010hn !  
 PARAMETER BMAGN(BCC\_4SL,AL:FE:AL:FE:VA;0) 298.15 BMALFE; 6000 N 08Sun !

PARAMETER G(BCC\_4SL,AL:FE:FE:FE:VA;0) 298.15 +GD03FEAL#; 6000 N 08Sun !  
 PARAMETER TC(BCC\_4SL,AL:FE:FE:FE:VA;0) 298.15 -125; 6000 N 010hn !  
 PARAMETER BMAGN(BCC\_4SL,AL:FE:FE:FE:VA;0) 298.15 BMALFE; 6000 N 08Sun !

PARAMETER G(BCC\_4SL,AL,FE:\*\*\*\*:VA;1) 298.15 -634+0.68\*T; 6000 N 08Sun !  
 PARAMETER G(BCC\_4SL,AL,FE:\*\*\*\*:VA;2) 298.15 -190; 6000 N 08Sun !  
 PARAMETER TC(BCC\_4SL,AL,FE:\*\*\*\*:VA;0) 298.15 +125; 6000 N 010hn !  
 PARAMETER BMAGN(BCC\_4SL,AL,FE:\*\*\*\*:VA;0) 298.15 BLALFE0; 6000 N 08Sun !  
 PARAMETER BMAGN(BCC\_4SL,AL,FE:\*\*\*\*:VA;1) 298.15 BLALFE1; 6000 N 08Sun !  
 PARAMETER BMAGN(BCC\_4SL,AL,FE:\*\*\*\*:VA;2) 298.15 BLALFE2; 6000 N 08Sun !

\$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM A1\_FCC

PHASE FCC\_4SL:F %FY 5 .25 .25 .25 .25 1 !

CONSTITUENT FCC\_4SL:F :AL,FE : AL,FE : AL,FE : AL,FE : VA : !

PARAMETER G(FCC\_4SL,AL:AL:AL:AL:VA;0) 298.15 +ZERO#; 6000 N 08Con !  
 PARAMETER G(FCC\_4SL,FE:AL:AL:AL:VA;0) 298.15 +GAL3FE#; 6000 N 08Con !  
 PARAMETER G(FCC\_4SL,FE:FE:AL:AL:VA;0) 298.15 +GAL2FE2#; 6000 N 08Con !  
 PARAMETER G(FCC\_4SL,FE:FE:FE:AL:VA;0) 298.15 +GALFE3#; 6000 N 08Con !  
 PARAMETER G(FCC\_4SL,FE:FE:FE:FE:VA;0) 298.15 +ZERO#; 6000 N 08Con !  
 PARAMETER G(FCC\_4SL,AL,FE:AL,FE:\*\*\*\*:VA;0) 298.15 +SFALFE#; 6000 N 08Con !

ASSESSED\_SYSTEM AL-FE(TDB -A2\_B2 -A2\_VA -BCC\_VA -B2\_BCC  
;G5 C\_S:BCC\_4/AL:AL:FE:FE:VA: C\_S:BCC\_4/AL:FE:FE:FE:VA:  
;P3 TMM:300/3000 STP:0.99/1400/-1 STP:0.77/600/1 STP:0.45/500/1 )  
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#### LIST\_OF\_REFERENCES

NUMBER SOURCE

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01Ohn 'I Ohnuma, unpublished 2001'  
08Con 'D Connetable et al, Calphad 2008; AL-C-Fe'  
08Sun 'B Sundman, to be published'  
08Dup 'N Dupin, vacancies in bcc'  
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