# XTDB, an XML based format for Calphad databases

Bo Sundman[a], Fabio Miani[b], Axel van de Walle[c], Bengt Hallstedt[d], Ursula R Kattner[e], Florian Tang[f], Taichi Abe[g], Reza Naraghi[h], Erwin Povoden-Karadeniz[i], Aurelie Jacob[i], Shuanglin Chen[j], Richard Otis[k], Kazuhisa Shobu[l], Malin Selleby[m], Alexander Pisch[n]

[a] *OpenCalphad, 9 Allée de l'Acerma, 91190 Gif sur Yvette, France*
[b] *DPIA, University of Udine, Via delle Scienze 208, 33100 Udine, Italy*
[c] *School of Engineering, Brown University, Providence, RI 02912, USA*
[d] *IWM, RWTH Aachen University, Augustinerbach 4, 52062 Aachen, Germany*
[e] *MSE, NIST, 100 Bureau Drive, Stop 8555, Gaithersburg, MD 20899, USA*
[f] *GTT-Technologies, 52134 Herzogenrath, Germany*
[g] *NIMS, Sengen, Tsukuba, Japan*
[h] *Thermo-Calc Software AB, Råsundavägen 18, 169 67 Solna, Sweden*
[i] *TU Wien, Getreidemarkt 9, 1060 Vienna, Austria*
[j] *CompuTherm, Yellowstone Dr., Madison, WI 53719, USA*
[k] *California Institute of Technology, Pasadena, CA 91109 USA*
[l] *RICT, Inc. 674-18, Tashiro-hoka, Tosu, Saga, 841-0016, Japan.*
[m] *MSE, KTH Royal Institute of Technology, Brinellvägen 23, 100 44 Stockholm, Sweden*
[n] *SIMAP, 1130, Rue de la Piscine, 38402 Saint-Martin d'Hères, France*

**Abstract**

The Calphad method uses models which depend on assessed parameters to describe the thermodynamic properties of materials. These model parameters are assessed by researchers and students using experimental and theoretical data on binary and ternary systems which can be merged to multicomponent databases and used to calculate properties and simulate processes for a wide range of materials.

There are several different software using the Calphad method for calculations and they can use slightly different models and database formats. This

*Email address:* bo.sundman@gmail.com (Bo Sundman)

paper will give a short background to the current state of database development and proposes a new format based on the eXtensive Markup Language (XML) as a unified database format. This change is particularly important as several new models for the pure elements are currently introduced in the Calphad databases.

*Keywords:*
Computational Thermodynamics, Calphad, Models, Model parameters, Databases, XML

---

## 1. Introduction

The development of software to calculate thermodynamic properties of alloys and other materials has been centered around the Calphad organization formed in 1973 [1] and the use of the lattice stabilities for the pure elements proposed by Kaufman [2]. These lattice stabilites made it possible to share and combine assessment of binary and ternary systems made by researchers all over the world.

The SGTE unary database published 1991 [3] represented a major improvement as this database including heat capacity data and a separate magnetic model[4, 5] using the Curie temperature and Bohr magneton number which can be the composition dependent. This unary database transformed Calphad to a general tool for computational thermodynamics and together with kinetic models and data, it could be applied to all kinds of simulations of phase transformation and processes. The SGTE database proposed a simple database format, called TDB (short for Thermodynamic DataBase) which with slight variations has been adopted by several software. During the last

45 years several 1000 binary and ternary systems have been assessed based on experimental and theoretical data using the Calphad models. These assessments have been integrated in several large databases, both commercial and freely available. With these databases reliable calculations can be made for multicomponent alloys, nuclear materials and other systems, simplifying the development of new materials and better processes.

The introduction of more complex models, integration of DFT data and additional materials properties have increased the interest in thermodynamic calculations [6, 7, 8, 9, 10, 11, 12, 13] and the TDB format is now past its "best before" date. In this paper a new XTDB format is proposed using the eXtended Markup Language (XML). It keeps the simplicity of manual editing of the TDB format and provides a consistent way to include new features, models and complex properties as discussed in [14, 15, 16].

## 2. The Gibbs energy and the organization of this paper

When there are references in this text to the XTDB format a tag name is written in **bold** and an attribute is written in *italics* and a short summary of the XTDB format is in Appendix A. In Appendix B there are examples of XTDB tags including the whole Al-C database and in Appendix C, an example of the **ModelDescriptions** tag with a number of physical models together their composition dependent parameter identifiers. For those not familiar with XML an introduction can be found at [17].

An XTDB database can be written and used by different software and the **ModelDescriptions** tag specifies the models that are used in a particular database. This tag is provided by the software generating the database and

if another software is reading the database it can check if a model extracted from the XTDB file is actually implemented.

### *2.1. The Gibbs energy expression*

The reason to put efforts into creating databases with models for the Gibbs energy of materials is that during a process or transformation a system always tries to reach its equilibrium state and the equilibrium is at a minimum of the Gibbs energy at constant $T, P$ and overall composition, $N_i$:

$$G = G(T, P, N_i) \tag{1}$$

where $T$ is the absolute temperature, $P$ the pressure and $N_i$ the number of moles of component $i$.

An essential feature of the Calphad method is that each phase in a system is modeled independently and its Gibbs energy depends on $T, P$ and the fractions of the constituents of the phase. Depending on the software using the database a user may calculate the set of stable phases and other properties of a system for a very wide range of external conditions.

### *2.2. The external variables*

Sometimes one is more interested in the activity of a component or the heat that is added or removed. All of these properties are available in the Calphad modeling as partial derivatives of the Gibbs energy:

$$dG = \left(\frac{\partial G}{\partial T}\right)_{P,N_i} dT + \left(\frac{\partial G}{\partial P}\right)_{T,N_i} dP + \sum_i \left(\frac{\partial G}{\partial N_i}\right)_{T,P,N_{j\neq i}} dN_i \tag{2}$$

where the variables that must be kept constant for each partial derivative are indicated. With simple mathematical transformations, see for example [18],

it is possible to use eq. 2 to calculate how the local equilibria in a system respond to changes in the external conditions of a process. In particular the heat capacity, $C_P$, and the chemical potential, $\mu_i$, of each component $i$:

$$C_P = -T \left( \frac{\partial^2 G}{\partial T^2} \right)_{P,N_i} \tag{3}$$

$$\mu_i = \left( \frac{\partial G}{\partial N_i} \right)_{T,P,N_{j \neq i}} \tag{4}$$

are essential for equilibrium calculations and kinetic simulations.

*2.3. The internal variables*

In Calphad the Gibbs energy of a system uses Gibbs energy models for each phase, $\alpha$, with different sets of constituents, which can be elements or chemical species or ions, and each with its own set of model parameters:

$$G = \sum_{\alpha} \aleph^{\alpha} \, G_M^{\alpha}(T, P, y_{s,i}^{\alpha}) \tag{5}$$

$$G_M^{\alpha} = \sum_{I} \Pi_{I_s}(y_{s,i}^{\alpha}) \; {}^{\circ}G_I^{\alpha}(T,P) - T \; {}^{\text{cfg}}S_M^{\alpha}(y_{s,i}^{\alpha}) + {}^{E}G_M^{\alpha}(T, P, y_{s,i}^{\alpha}) + {}^{\text{phy}}G_M^{\alpha}(T, P, y_{s,i}^{\alpha}) \tag{6}$$

where $\aleph^{\alpha}$ is the number of moles formula unit of $\alpha$ and $G_M^{\alpha}$ is the Gibbs energy of $\alpha$ per mole formula unit as a function of $T, P$ and $y_{s,i}^{\alpha}$ which denote the fraction of constituent $i$ on sublattice $s$. The number of constituents in a phase can be much larger than the number of components of the system. In the term $\Pi_I(y_{s,i}^{\alpha}) \; {}^{\circ}G_I^{\alpha}$ the $I$ indicates an endmember of $\alpha$ representing a possible "compound" with fixed composition and $\Pi_I(y_{s,i}^{\alpha})$ is the probability of the compound I and ${}^{\circ}G_I^{\alpha}$ its Gibbs energy. In a solution it is the contribution from this endmember to the total Gibbs energy of the phase.

${}^{\rm cfg}S_M^\alpha(y_{s,i}^\alpha)$ is the configurational entropy and ${}^{E}G_M^\alpha(T,P,y_{s,i}^\alpha)$ the contributions from interactions of the constituents mixing on the same sublattice of the phase. If a single endmember represents the constitution of the $\alpha$ phase then ${}^{\rm cfg}S_M^\alpha = {}^{E}G_M^\alpha = 0$.

The term ${}^{\rm phy}G_M^\alpha(T,P,y_{s,i}^\alpha)$ is the contribution from various physical models, for example magnetism. This contribution can also be split into a sum of the contributions to each endmember and excess terms. Most physical models have parameters which depend on the constitution and sometimes also $T$ and $P$. They are discussed in section 4.6. If the phase has charged constituents there is an extra condition for equilibrium that the phase is electrically neutral. From now on we will only deal with expressions for a single phase and the phase superscript is omitted.

Already in the 1991 unary database a separate contribution from magnetic properties was introduced, ${}^{\rm phy}G_M$, which has been essential to calculate for steels and other magnetic materials. The introduction of model parameters for physical properties such as the Curie temperature and the Bohr magneton number has greatly improved simulations of such materials.

The mixing depends on the model of the phase which in the simplest case assumes that all constituents mix on a single sublattice. Alternatively, there can be two or more sublattices each with a specific set of constituents, for example interstitial solutions. This affects the configurational entropy as well as all the model parameters used to describe the Gibbs energy and its contributions from various physical models. The sublattices describe Long Range Ordering (LRO) where the constituents mix randomly in each sublattice but some models take Short Range Ordering (SRO) into account by adding con-

stituents representing clusters to modify the configurational entropy.

*2.4. The configurational entropy*

The random mixing of constituents $y_{s,i}$ on one or more sublattices $s$ is;

$$
\begin{aligned}
{}^{\text{cfg}}S_M &= \sum_s a_s \sum_i y_{s,i} \ln(y_{s,i}) && (7)\\
\sum_i y_{s,i} &= 1 && (8)\\
M &= \sum_s a_s && (9)
\end{aligned}
$$

where $a_s$ is the number of sites on sublattice $s$ and $y_{s,i}$ is the fraction of constituent $i$ on sublattice $s$. The sum of the sites is equal to the formula unit, $M$, of the phase.

There are many different ways to include SRO in the configurational entropy, see for example [19, 20, 21, 22]. There are no parameters in the database for the configurational entropy model, the database only provides the set of clusters in the phase and possibly a Gibbs energy of formation of the clusters. A method to approximate SRO in crystalline phases by using reciprocal excess parameters was derived in [23] and is discussed in [24].

## 3. The content of a Calphad database

Selecting data for a system from the database a user normally specifies the elements in the system and all phases that can exist with these elements are extracted by the software from the database together with their model parameters. But this can be software and application dependent.

The major part of the current TDB as well as an XTDB database are model parameters and their representation in the database as discussed in section 4.6.

*3.1. Elements, species, vacancies and electrons*

The elements are the basic part of the XTDB format and they are defined as shown in Appendix A.2. The vacancy, denoted VA, is included among the chemical elements because the vacancy is needed to model interstitial solutions and defects in different phases use the vacancy. This may seem to violate the Gibbs phase rule:

$$f = n + 2 - p \tag{10}$$

where $f$ is the degrees of freedom in a system with $n$ real elements (or components) and $p$ is the number of stable phases. But the vacancy must have its chemical potential equal to zero at equilibrium and thus it will not change this rule.

Several models for the liquid [20, 25] also include vacancies, with or without a charge, as an essential model constituent. The electron is never treated as a constituent by itself but a charged vacancy can be used as a free electron or hole to model semiconductors. As each phase must be electrically neutral there is no degree of freedom added by the ions.

In the TDB file the chemical species, including the vacancy and charged species as cations and anions are introduced directly after the elements as shown in Appendix A.2. It would be possible eliminate the **Species** tag in the XTDB file and instead define the constituents separately for each phase. However, the XTDB tags needed for entering a phase, as explained in

section 3.2 and Appendix A.3, is already quite complex and in this proposal all constituents of a phase have separate **Species** tags independent of the **Phase** tag.

A species has fixed stoichiometry and in some models additional properties which must be provided as attributes in the **Species** tag.

*3.2. The phase, its constituents and models*

The XTDB tags defining a phase are in Appendix A.3. The phase tag itself has only 3 attributes, *Id* is the name of the phase, *Configuration* specifies how the configurational entropy should be calculated and the *State* which is needed if the EEC model, see section 4.5, is used for the database.

There are 3 standard values for the *Configuration*:

- CEF, the abbreviation for Compound Energy Formalism, covers all models with random mixing on one or more sublattices [26],
- MQMQA is used for liquid with the Modified Quasichemical model in the Quadruplet Approximation [20],
- I2SL is used for liquids with the Ionic 2-sublattice liquid model [25] with variable site ratios.

At present there are no other established models for the configurational entropy for using XTDB databases.

Nested inside the phase tag one must have a **Sublattices** tag even if there is only one (or no) sublattices. In this tag the attributes *NumberOf* specifies the number of sublattices and *Multiplicities* the number of sites on each, i.e.

the value of $a_s$ in eq. 9, which defines the formula unit of the phase. The values of the model parameters must be for one formula unit of the phase.

Within the **Sublattices** tag, there must be a **Constituents** tag for each sublattice. It has two attributes, *Sublattice* which can be omitted if there is only one, and *List* with a list of all constituents (already entered as **Species**), which can be present in the sublattice and separated by a space.

If the phase has some physical contributions, see eq. 6, those must be specified using the **AmendPhase** tag. The *Id*s of several models can be included in its *Models* attribute, separated by a space. There can also be a **DisorderedPart** tag if the phase has two separate sets of fraction variables. See section 3.6.

A solid phase can optionally have a **CrystalStructure** tag but using Calphad models the crystallographic designation of the phase may change with its constitution. Pure Fe as austenite can have the attribute *StructurBericht* A1 but the thermodynamic model for the same phase may be stable as ordered with *StructurBericht* $L1_2$ in Fe-Pt system or as a carbide with the *StructurBericht* B1 in the Fe-Ti-C system. The software may use the constitution of the phase to indicate this after an equilibrium calculation.

### *3.3. Contribution from the physical models*

In the TDB files the way to specify physical contributions was varied. The XTDB format has a **ModelDescriptions** tag, where all models used in the database are defined. The current models are listed with very short explanations in Appendix C. Each model has an *Id* attribute and possibly one or more model parameter identifiers (MPID) for parameters describing the composition dependence of the contribution. All models are not implemented

in all software. In for example:

```
<Phase Id="FCC_4SL" ...  >
  ...
  <Amen dPhase Models="IHJQX GEIN FCC4PERM" >
    <DisorderedPart Sum="4" Subtract="Y" />
  </AmendPhase>
</Phase>
```

the *Models* attribute specifies that the FCC_4SL phase has the magnetic model IHJQX, the Einstein low $T$ heat capacity model, explained in section 3.4, and a permutation of the parameters on the 4 sublattices for ordering explained in section 3.8. The **DisorderedPart** tag is explained in section 3.6 with examples in Appendix B.

*3.4. The Einstein low T extrapolation model*

The Einstein model is used to extrapolate the Gibbs energy of a solid phase of an element down to $T = 0$ K. The integrated Einstein heat capacity equation per mole atoms is:

$$ {}^{\mathrm{Ein}}G_m(\theta) = 1.5R\theta + 3RT\ln(1-\exp(-\theta/T)) \quad (11) $$

$$ {}^{\mathrm{Ein}}G_M^{\alpha} = \aleph^{\alpha}\ {}^{\mathrm{Ein}}G_m(\theta) \quad (12) $$

where $\theta$ is the assessed Einstein temperature. Eq. 12, including the number of moles of atoms per formula unit, $\aleph^{\alpha}$ of the $\alpha$ phase, is used in eq. 6. The value of $\ln(\theta)$ (called LNTH below) is used as composition dependent variable in the Einstein MPID parameter because it is considered more appropriate physically.

Sometimes the heat capacity of an element is fitted using several Einstein $\theta$, each with a different weight factor (the sum of which is unity), but only one of them can be composition dependent using the LNTH parameter. Thus the software must implement eq. 11 as a function called GEIN with $\theta$ as argument, for use in the *Expr* attribute, see section 4.7. The contributions from all $\theta$ are included in the Gibbs energy parameter for the endmember using GEIN functions with their assessed weight factors as shown below for the GRAPHITE phase in the assessment of Al-C by [27].

```
<TPfun Id="GEGRACC" Expr=" -0.5159523*GEIN(1953.3)+
     0.121519*GEIN(448)+0.3496843*GEIN(947)+.0388463*GEIN(192.7)+
     .005840323*GEIN(64.5);" />
<TPfun Id="GTSERCC" Expr="-.00029531332*T**2-3.3998492E-16*T**5;"/>
<TPfun Id="GHSERCC" Expr="-17752.213+GEGRACC+GTSERCC;" />
<Parameter Id="G(GRAPHITE,C;0)" Expr="GHSERCC;" Bibref="21HE" />
<Parameter Id="LNTH(GRAPH,C;0)" Expr="LN(1953.3);" Bibref="21HE" />
```

where the **TPfun** tag with the *Id* attribute GEGRACC together with the LNTH parameter is the contribution from the Einstein model using 5 different $\theta$. The **TPfun**s GTSERCC and GHSERCC are the contribution at high $T$ and the enthalpy at $T = 0$ K respectively. One of the $\theta$ is selected to vary with the composition using the LNTH parameter and its GEIN function is included in GEGRACC multiplied with the factor (weight factor -1.0). The whole Al-C assessment is in Appendix B.1.

*3.5. The liquid 2-state model*

The Gibbs energy of the liquid phase for an element is extrapolated below its melting $T$ using the liquid 2 state model, proposed by [28, 29]. The Gibbs energy expression for the liquid is:

$$G_M^{\rm Liq} \;=\; G_M^{\rm am} - RT\ln\left(1+\exp(-\frac{\Delta G_M}{RT})\right) \qquad (13)$$

where $G_M^{\rm am}$ describes the metastable amorphous state at low $T$ using an Einstein model together with the Gibbs energy parameter, "G", as a polynomial in $T$ with no heat capacity contribution at $T = 0$ K. The $\Delta G_M$ parameter, divided by $RT$ in eq. 13, describes the transition to the stable liquid and the stable liquid above the melting $T$.

The MPID1 attribute *GD* in the **Liquid2State** tag is the $\Delta G_M$ expression, see Appendix C, and the "G" parameter describes the low $T$ amorphous state. The $\Delta G_M$ polynomial, as included in to the $\ln(1-\exp(f(T)))$ term, must not have any heat capacity contribution at $T = 0$ K, see [27, 29].

*3.6. Using two Gibbs energy functions for a phase*

For phases with many sublattices it is possible to use two separate sets of parameters for the Gibbs energy. This may significantly reduce the number of model parameters, see section 3.7 and 3.9. It can be used for phases such as FCC, BCC and HCP, which can be both ordered and disordered, and for phases which are always ordered such as $\sigma, \mu$ etc. It is indicated by a **DisorderedPart** tag inside the **AmendPhase** tag of the ordered **Phase** tag.

The **DisorderedPart** tag has 3 attributes, the *Sum* which specifies the number of sublattices, $n$, in the ordered phase to be summed to obtain the

fractions of the disordered phase as:

$$x_i^{\text{dis}} = \frac{\sum_{s=1}^{n} a_s \sum_i y_{s,i}}{\sum_{s=1}^{n} a_s} \tag{14}$$

where $s$ represent the sublattices to be summed and $y_{s,i}$ are the site fraction of $i$ on the sublattice $s$. All ordered sublattices should have the same constituents but there can be a final interstitial sublattice in both the ordered and disordered part. It is not necessary that the sublattices which are summed are crystallographically identical, a $\sigma$ phase can also have a disordered part, in particular when using EBEF discussed in section 3.9. The software is responsible to ensure the number of atoms in the ordered and disordered parts are the same.

In the disordered part the Gibbs energies of the endmembers, ${}^{\circ}G_i$, provide a surface of reference relative to the stable state of the elements $i$. Thus all parameters in the ordered part become a kind of excess Gibbs energy parameters relative to this surface. For a phase with the **DisorderedPart** tag the Gibbs energy is calculated by one of these 2 equations:

$$G_M = {}^{\text{dis}}G_M(x) + {}^{\text{ord}}G_M(y) \tag{15}$$

$$G_M = {}^{\text{dis}}G_M(x) + {}^{\text{ord}}G_M(y) - {}^{\text{ord}}G_M(y = x) \tag{16}$$

where $x$ are averaged values of $y$ according to eq. 14. The configurational Gibbs energy is calculated for the ordered part only. Eq. 15 is mainly used for phases with many sublattices which never disorder for example TCP phases.

In order to use eq. 16 one must specify the attribute *Subtract*="Y" in the **DisorderedPart** tag and it is used for phases with order/disorder transitions such as FCC, BCC and HCP when the model parameters for the disordered

phase, including disordered excess parameters, have been assessed separately. Subtracting ${}^{\mathrm{ord}}G_M(y=x)$ means that the model parameters of the ordered phase will not affect the disordered state. But there are many relations between the parameters to be considered using this, for details see [14, 30].

The third attribute is *Disordered* which can indicate the *Id* of the disordered phase if those parameters are entered in a separate phase. The parameters for the disordered phase can also be part of the ordered one, using parameters with fewer sublattices, see Appendix B.4.

### *3.7. The use of wildcards as constituents*

It is possible to use parameters that does not specify the constituent in one or more of the sublattices. An extreme case is to use a parameter G(C14_Laves,*) which will add the value of the parameter to the Gibbs energy of the C14_Laves phase at all compositions. In a simulation a positive value of such a parameter can be considered as a nucleation threshold.

In some compounds which are stable in a limited composition range but may dissolve many elements an excess parameter G(C14_Laves,A,B:*) can be a useful approximation of the interaction between A and B independent of the constituent in the second sublattice.

The implementation of the wildcard parameter has sometimes been misunderstood. It is wrong if the software replaces the wildcard in the parameter with the actual constituents in the sublattice with the wildcard. Instead any parameter with an explicit constituent in the sublattice with the wildcard. should be added to the wildcard parameter. For example:

```
<Parameter Id="L(C14,A,B:C)" Expr="-7000" />
<Parameter Id="L(C14,A,B:*)" Expr="5000" />
```

should have their contribution to the Gibbs energy calculated as:

$$\Delta G = y_{1,\mathrm{A}} y_{1,\mathrm{B}} L_{\mathrm{A,B:*}} + y_{1,\mathrm{A}} y_{1,\mathrm{B}} y_{2,\mathrm{C}} L_{\mathrm{A,B:C}} \quad (17)$$

where the two parameters are totally independent and can be modified separately. Even if C is the only constituent in the 2nd sublattice both parameters should be extracted from the database.

*3.8. Permutations of parameters in some ordered phases*

When modeling ordering in phases with crystallographically identical sublattices such as $\mathrm{L1_2}$ and $\mathrm{L1_0}$ ordering in FCC, the endmember G(FCC,A:B:B:B) has 4 permutations of the constituent A on the 4 sublattices which must have identical Gibbs energy. Using the **DisorderedPart** tag and the endmembers in the disordered part to represent the Gibbs energy relative to the stable state of the constituents, the endmembers in the ordered part are related just to the bonds between the constituents. If the AB bond, $u_{\mathrm{AB}}$ is independent of composition one has:

$$\begin{aligned} G(FCC, A:A:A:B) &= 3u_{\mathrm{AB}} \\ G(FCC, A:A:B:B) &= 4u_{\mathrm{AB}} \\ G(FCC, A:B:B:B) &= 3u_{\mathrm{AB}} \end{aligned} \quad (18)$$

By specifying FCC4PERM in the *Models* attribute of the **AmendPhase** tag the permutations of a parameter G(FCC,A:A:A:B) need to be included

only once in the XTDB file. It is the software which must take care of calculating these parameters with the 3 or 4 different sets of fractions, either by an internal loop or by storing the parameter at the 4 appropriate positions in its data structure. See also Appendix B.4

An excess parameters, such as G(FCC,A,B:*:*:*) must also be permuted by the software for all identical sublattices when read from the database. Such a parameter assumes that the interaction between A and B in a sublattice is independent of the constituents on the other 3 sublattices which is reasonable even if the wildcard represents a third element. The reciprocal parameter, G(FCC,A,B:A,B:*:*), with 6 permutations is of particular interest because it can approximate the SRO contribution to the phase, see [24].

How the permutations are implemented in the software is not discussed here. Either the software stores the parameter explicitly for all possible permutations or stores the parameter only once and uses an internal loop to multiply the parameter with all relevant constituent fractions in the sublattices. The latter is recommended as it makes it easier to change the expression of the parameter. The BCC4PERM permutation is more complicated for the software as the tetrahedron is not symmetrical.

### *3.9. The EBEF model*

The wildcard feature has been further explored by Dupin [15] improving the modeling of intermetallic phases with many sublattices. Again combining the **DisorderedPart** feature described in section 3.6, the Gibbs energy of the ordered part of such phases is independent of the reference states of the elements. In a $\sigma$ phase with 5 sublattices an endmember parameter G(SIGMA,A:B:*:*:*) thus represent the bond energy between

constituent A in sublattice 1 and constituent B in sublattice 2, independent of the constituents in the other sublattices. As the sublattices are not crystallographically identical (as in an ordered FCC phase) an endmember G(SIGMA,B:A:*:*;*) will not have the same value. Using the notation $E^{st}_{\mathrm{A:B}}$ for a parameter with constituent A in sublattice $s$ and constituent B in sublattice $t$, we can describe the energy to exchange of A and B in any pair of sublattices as:

$$\Delta G^{\sigma}_{\mathrm{A,B}} \quad = \quad \sum_{s=1}^{4}\sum_{t=s+1}^{5} y_{s,\mathrm{A}}y_{t,\mathrm{B}}E^{s,t}_{\mathrm{A,B}} + y_{s,\mathrm{B}}y_{t,\mathrm{A}}E^{s,t}_{\mathrm{B,A}} \tag{19}$$

where the $E^{s,t}_{\mathrm{A,B}}$ can be fitted to DFT calculations for all combinations of endmembers in all 5 sublattices. This set of $E^{st}_{\mathrm{A,B}}$ is similar to an excess parameter $L_{\mathrm{A,B}}$ in a phase with a single sublattice and very good results have been found when extrapolating such parameters, evaluated in binary systems, to higher order systems. An example can be found in Appendix B.2.

Using model parameters such as G(SIGMA,A:B*:*:*) it is essential that the software treats them as eq. 17, i.e. independent of the fractions in the sublattices with wildcards.

### *3.10. Composition dependence of excess parameters*

This section applies to all kinds of excess parameters for the different physical models, not just the Gibbs energy parameters. In a binary system the composition dependence of the constituent fractions can be expressed in different ways. Most frequently used is the so called Redlich-Kister model, which for a substitutional model is:

$$^{\mathrm{bin}}G_{\mathrm{AB}} \quad = \quad x_{\mathrm{A}}x_{\mathrm{B}}\sum_{\nu=0}^{n}(x_{\mathrm{A}}-x_{\mathrm{B}})^{\nu}\cdot\ {}^{\nu}L_{\mathrm{AB}} \tag{20}$$

where ${}^{\nu}L_{\mathrm{AB}}$ can be a function of $T$. There are also other series expansions but they can always be transformed to a RK polynomial. Thus the XTDB file will only support the RK binary excess expression. However, some software calculate the difference $x_{\mathrm{A}} - x_{\mathrm{B}}$ in the alphabetical order, some in the order the constituents are listed in the parameter. This may require the software to change the sign of the parameters with odd powers. The composition dependent Redlich-Kister parameters have the degree specified after a semicolon in the *Id* attribute in the **Parameter** tag, see section 4.6.

*3.10.1. Ternary excess parameters*

Parameters for ternary extrapolations can be composition dependent according to the suggestion in [31]. The ternary composition dependence for a parameter $L_{1,2,3:*}$ implemented in TDB files as:

$$ {}^{\mathrm{ter}}G_{1,2,3} = y_1 y_2 y_3 (v_1 \cdot {}^{0}L_{1,2,3:*} + v_2 \cdot {}^{1}L_{1,2,3:*} + v_3 \cdot {}^{2}L_{1,2,3:*}) \quad (21) $$

where 1, 2, 3 are constituents in alphabetical order. The values of $v_i$ are:

$$ \begin{aligned} v_1 &= (1 + 2y_1 - y_2 - y_3)/3 \\ v_2 &= (1 + 2y_2 - y_3 - y_1)/3 \qquad (22) \\ v_3 &= (1 + 2y_3 - y_1 - y_2)/3 \\ v_1 + v_2 + v_3 &= 1 \qquad (23) \end{aligned} $$

where eq. 23 ensures the contribution is symmetrical in higher order systems. When implemented in the TDB format 40 years ago there was an inconsistency with the degrees of the parameter. A single ${}^{0}L_{1,2,3:*}$ was assumed to be composition independent and in order to have a composition dependent

ternary parameter one must specify all 3 parameters with indices 0, 1 and 2 even if one of the parameters is zero.

This will be modified in the XTDB by including an ${}^{0}L_{1,2,3:*}$ which is composition independent and use 1, 2, 3 for the composition dependent parameters, i.e.:

$$\begin{aligned} {}^{\rm ter}G_{1,2,3} &= y_1y_2y_3(\ {}^{0}L_{1,2,3:*} + \\ &\quad v_1\cdot\ {}^{1}L_{1,2,3:*} + v_2\cdot\ {}^{2}L_{1,2,3:*} + v_3\cdot\ {}^{3}L_{1,2,3:*}) \end{aligned} \tag{24}$$

It is not possible to make such a change reading a TDB files because there are so many old TDB files that cannot be changed consistently. But in the XTDB files this change can be made automatically by any software converting a TDB file to XTDB. There is no need for any special information in the XTDB file.

*3.10.2. Reciprocal excess parameters*

The reciprocal parameters with simultaneous interaction in two sublattices are important for an approximate SRO contribution as shown in [23] but they rarely have a higher order composition dependence. For a reciprocal parameter there is a composition dependence using the degree 0, 1 and 2:

$$\begin{aligned} \Delta G &= y_{1,\rm A}y_{1,\rm B}y_{2,\rm C}y_{2,\rm D}(\ {}^{0}L_{\rm A,B:C,D} + \\ &\quad (y_{1,\rm A}-y_{1\rm B})\cdot\ {}^{1}L_{\rm A,B:C,D} + (y_{2,\rm C}-y_{2,\rm D})\cdot\ {}^{2}L_{\rm A,B:C,D}) \end{aligned} \tag{25}$$

with the constituents in alphabetical order.

*3.11. Ternary extrapolation methods*

In ternary systems the composition dependence of the binary excess parameters can be extrapolated in different ways. Three methods are used and

explained in [31, 32] and there is a **TernaryXpol** tag that can specify the extrapolation method for each case. For example:

```
<TernaryXpol Phase="FCC" Constituents="Fe Cr Si" Xpol="KT3T3" />
```

the Xpol attribute has one letter for the extrapolation method for each binary, K and M mean Kohler or Mugganu, T means Toop and one must indicate also indicate the Toop constituent: 1, 2 or 3. The binaries are in the order of the element listed in the *Constituent* attribute. In the example above this means that the binaries Fe-Cr is Kohler, Fe-Si is Toop with Si as Toop element and Cr-Si is Toop also with Si as Toop element.

## 4. Some explanations related to Appendix A

The summary of XTDB in Appendix A is short and some additional information is provided here.

### *4.1. Names, texts and Upper and lower case*

The XML itself is case sensitive. The tags and attributes in XTDB must be written exactly as defined in Appendix A. New tags and attributes can be added when needed to handle new features.

For the data provided in the attributes the thermodynamic software is free to handle names and other texts. In the TDB format upper and lower case was treated as equivalent and XTDB will follow the same rule. Except for the cases listed below, any *Id* must start with a letter A-Z and contain only letters, numbers 0-9 and the underscore character, "_".

The length of *Id*s for species, phases, functions, etc. in the TDB files have been quite restricted. In XTDB there will be no restriction but a recommendation not to exceed 24 characters for any *Id*. But a software reading an XTDB file is allowed to modify any *Id* according to its own rules and such changes of the *Id* relative to the XTDB file should be displayed to the user while reading the database. Such changes should be saved in a way that the user can at any time obtain the original and modified *Id*s.

### *4.2. The MQMQA and UNIQUAC constituents*

The constituents needed to calculate the configurational entropy and Gibbs energy for the MQMQA model are provided as in the FactSage DAT file and must be specified in the *MQMQA* attribute of the **Species** tag. Also for the UNIQUAC model [33] for orgainic liquids each **Species** has an attribute *UNIQUAC* which defines the area and volume needed for its configurational entropy expression. Information for this is provided in the full XTDB documentation available at [34].

### *4.3. AppendXTDB files*

The XTDB file for a large system can be very big. The set of model parameters for a $\sigma$ phase with 5 sublattices and 10 constituents in each is $10^5$. There are models such as the EBEF, explained in section 3.9, which can reduce this significantly but a single file for a database may still be difficult to manage. A way to handle this is to use the **AppendXTDB** tag. Such a tag is allowed only in the primary XTDB file and the primary XTDB file should also include all **Defaults, DatabaseInfo, AppendXTDB, Element, Species, Phase** tags and their subtags. But all or parts of the **Tp-**

**fun, Trange, Parameter, ModelDescriptions** and **Bibliography** tags can be on separate **AppendXTDB** files.

*4.4. The phase and species* Id

As explained in section 4.1 upper and lower case are the same in phase *Id*. In a species *Id* the characters "/", "+" and "-" are also allowed.

Any parenthesis "(" and ")", comma "," , colon ":" and semicolon ";" are forbidden as they are used to separate the various parts of the model parameters as explained in section 4.6.

*4.5. The equi-entropy criterion, EEC*

The equi-entropy criterion [35] was proposed as a method to avoid artifact breakpoints in the extrapolated Gibbs energy of solid phases. It means the software, while calculating an equilibrium, should prevent any solid phase from becoming stable if it has higher entropy than a liquid phase at the same $T$, irrespectively of the composition of the phases. When EEC is applicable, the database must indicate if a phase represent a liquid or a solid phase in the *State* attribute.

*4.6. The model parameters*

The major part of a Calphad database is the model parameters. In the XTDB file they are written in the same compact way as in the TDB file. The parameters use the *Id*s for model parameter identifiers (MPID) in the **ModelDescriptions** tag, see Appendix A.7, the *Id* of the **Phase** and the *Id*s of the constituent **Species**. For example:

- G(LIQUID,FE+2:VA;0) is the endmember of Fe in the I2SL model.

- TC(FCC_4SL,FE:AL:AL:AL:VA;0) is the endmember of the Curie T in a 4 sublattice ordering model of the FCC phase with interstitials.

- BMAGN(BCC_A2,CR,FE:VA;1) is a first order Redlich-Kister term for the Bohr magneton in the BCC phase. The value after the semicolon indicates the power $\nu$ used for parameter in eq. 20 in section 3.10.

- G(SIGMA,MO:CR:*:*:*) is an EBEF parameter representing one half of the bond energy parameter for Cr-Mo in a 5 sublattice model of the $\sigma$ phase, see Appendix B.2.

- LNTH(AL4C3,AL:C) is the logarithm of the Einstein $\theta$ in the $Al_4C_3$ phase, see Appendix B.1.

The **Parameter** tag for XTDB has an *Id* attribute using the same simple notation as in TDB to define: 1) the MPID, 2) the phase, 3) the composition dependence and 4) the degree of a parameter. The first part of the *Id*, before the parenthesis, is the MPID. For parameters in the Gibbs energy expression ${}^{\circ}G_I$ a simple G is used as MPID. For parameters used in the ${}^{E}G_M$ one can use G or L as MPID.

In the other examples above TC is the Curie temperature and BMAGN is the Bohr magneton number in the IHJREST magnetic model, see Appendix A.7. LNTH is the MPID for the logarithm of the Einstein $\theta$, explaned in section 3.4.

After the MPID, and within parenthesis, first the phase *Id* (which can be abbreviated, see section 4.1), followed by the *Id*s of the constituents in the sublattices in the order defined in the **Phase** tag. The constituents in different sublattices are separated by a colon, ":". When two or more

constituents mix on the same sublattice they are separated by a comma ",". For a binary Redlich-Kister parameters the order of the mixing constituents may be important, see section 3.10.

Before the closing parenthesis of the *Id* in the **Parameter** tag there can be a semicolon, ";", followed by a digit. The meaning of this digit depends on the model.

As the *Id* of a **Parameter** tag contains the phase *Id* these can be arranged in the XTDB file as the database manager prefers (but after the **Phase** tags). Some may prefer to have the parameters for all phases for a binary or ternary system together to simplify updates.

### *4.7. The* Expr *attribute in TPfun and Parameter tags*

Many endmember parameters include an expression depending on the data for the pure elements and to avoid repeating this one can use the **TPfun** tag for an expression including the $T$ and $P$ as variables, and use the *Id* of these **TPfun**s in the *Expr* attribute of other **TPfun** or **Parameter** tags.

The *Expr* attribute in **TPfun, Trange** and **Parameters** must be very simple. Below are some rules:

A "simple term" in *Exp* is a signed real or integer value possibly multiplied with an integer power of T and P. A negative power must be enclosed by parenthesis. Examples:

12000 -5*T**2 3.1416E12*T**(-9) 4*T*P

A simple term can be used as argument of EXP, LN or LOG function (both LN and LOG are the natural logarithm) or it can be muliplied with the *Id* of a **TPfun**. There is also the special GEIN function, defined by eq. 11 in section 4.6, which is needed when a phase has been fitted with

several Einstein $\theta$, only one of which can be used as composition dependent in the LNTH parameter, see Appendix B.1.

Multiplying several simple terms enclosed by parenthesis with another term is not allowed in *Expr* and neither is division. To handle such cases and for example $\sqrt{T}$, one can combine **TPfun**s:

```
<TPfun Id="LNT" Expr="LN(T);" />
<Tpfun Id="SQRT" Expr="EXP(0.5*LNT);" />
```

but `Expr="EXP(0.5*LN(T));"` is not allowed.

If the **Trange** tag is used the expression as well as its first and second derivatives with respect to $T$ and $P$, must be continuous across the breakpoint. Otherwise the breakpoint represents a phase transition.

## 5. Summary

The XTDB format proposed here is very similar to the TDB format which has been used for more then 30 years to develop large multicomponent databases for Calphad applications. It has also been sufficiently flexible to handle many new models and may even have stimulated some of them. XTDB does not provide any facilities for internal verification, such features require a much more complex splitting of the data. For maintaining large commercial databases such verification is important but not for students and scientists editing small databases and manipulate models as part of an assessment. The XTDB format will make it easier to integrate Calphad databases with other types of materials databases and software.

Software for verifying the TDB database files are used by the commercial providers of thermodynamic databases and such software can also accomodate the XTDB database format. A well cocumented and easily expandable thermodynamic database format will be greatly appreciated by all scientists working with thermodynamic assessments, modeling and applications. A future project is the development of an ML based format for experimental and DFT data for use in assessments for Calphad databases.

## Acknowledgments

The authors are grateful for creative discussion with Nathalie Dupin. Economic support from Stiftelsen för Tillämpad Termodynamik (STT) and the Scientific Group Thermodata Europe (SGTE) are gratefully acknowledged.

## References

[1] P. J. Spencer, *A brief history of CALPHAD*, Calphad, **32**, (2008), doi.org:10.1016/j.calphad.2007.10.001

[2] L. Kaufman and H. Bernstein *Computer Calculation of Phase Diagrams. With Special Reference to Refractory Metals* (1970) Academic Press NY

[3] A. Dinsdale, *SGTE Data for pure elements*, Calphad, **15** (1991), doi:10.1016/0364-5916(91)90030-N

[4] G. Inden, *The role of magentism in the calculation of phase diagrams*, Physica, **103B**, doi:10.1016/0378-4363(81)91004-4

[5] S. Hertzman and B. Sundman, *A thermodynamic analysis of the Fe-Cr system*, **6**, 1982, doi:10.1016/0364-5916(82)90018-9

[6] M. Hillert, *Phase equilibria, Phase diagrams and Phase transitions* 2nd Ed. (2008) Cambridge Univ Press doi:10.1017/CBO9780511812781

[7] H. L. Lukas, S. G. Fries and B. Sundman, *Computational Thermodynamics, the Calphad method*, (2007) Cambridge Univ Press doi:10.1017/CBO9780511804137

[8] P.E.A Turchi, I. Abrikosov, B. Burton, S.G. Fries, G. Grimvall, L. Kaufman, P. Korzhavyi, V. R. Manga, M. Ohno, A. Pisch, A. Scott. W Zhang, *Interface between quantum-mechanical-based approaches, experiments and Calphad methodology*, Calphad, **31**, 2007, doi.org:10.1016/j.calphad.2006.02.009

[9] A. D. Pelton *Phase Diagrams and Thermodynamic Modeling of Solutions*, Elsevier, (2019) doi.org:10.1016/C2013-0-19504-9

[10] R. Schmid-Fetzer, *Phase Diagrams, the beginning of Wisdom*, J. Phase Equil. Diff, (2014) **35**, doi:10.1007/s11669-014-0343-5

[11] A. van de Walle and M. Asta, *High-throughput calculations in the context of alloy design* MRS Bulletin **44** (2019) doi:10.1557/mrs.2019.71

[12] C. Guéneau, M. Asta, B. Sundman *Comprehensive Nuclear Materials* 2nd Ed, Vol 1, (2020) doi:10.1016/B978-0-12-803581-8.12054-5

[13] Z. He, Q. Chen, M. Selleby *Third Generation Calphad for Key Elements*, J Phase Equil Diffus, **45**, (2024) doi:10.1007/s11669-024-01166-z

[14] B. Hallstedt, N. Dupin, M. Hillert, Lars Höglund, H. L. Lukas, J. Schuster and N. Solak *Thermodynamic models for crystalline phases. Composition dependent models for volume, bulk modulus and thermal expansion*, Calphad, **31** (2++7) pp 28-37 doi:10.1016/j.calphad.2006.02.008

[15] N. Dupin, U. R. Kattner, B. Sundman, M. Palumbo, and S. G. Fries, S. G., *Implementation of an effective bond energy formalism in the multicomponent calphad approach*, J Res. NIST, **123**, (2018), doi:10.6028/jres.123.020

[16] B. Bocklund, R. Otis, A. Eqorov, A. Obaied, I. Roslyakova, Z.-K. Liu, *ESPEI for efficient thermodynamic database development, modification and uncertainity quantification: application to Cu-Mg*, MRS Commun, 9 (2019), doi:10.1557/mrt.2019.59

[17] https://www.w3schools.com/xml/

[18] B. Sundman, X-G. Lu and H. Ohtani *The implementation of an algorithm to calculate thermodynamic equilibria for multicomponent systems with non-ideal phases in a free software*, Calphad **101** (2015), doi:10.1016/j.commatsci.2015.01.029 0927-0256

[19] R. Kikuchi *A theory of cooperative phenomana*, Phys. Rev **81** (1951) pp 988–1003 doi:10.1103/PhysRev.81.988

[20] A. Pelton, P Chartrand and G. Eriksson, *The modified quasi-chemical model: Part IV. Two-sublattice quadruplet approximation*, Met. Trans A **32A** (2001) doi:10.1007/s11661-001-0230-7

[21] E. Kremer *Associated solution model rebuilt* Calphad **77** (2022) 102408, doi:10.1016/j.calphad.2022.102408

[22] C.-L. Fu , R. P. Gorrey and B.-C. Zhou *A cluster-based computational thermodynamics framework with intrinsic chemical short-range order*, Acta Mater, **277** (2024) 1201388 doi:10.1016/j.actamat.2024.120138

[23] B. Sundman, S. G. Fries and W. A. Oates *A thermodynamic assessment of the Au–Cu system*, Calphad, **22**, (1998) pp 335-354, doi:10.1016/S0364-5916(98)00034-0

[24] B. Sundman, N. Dupin, M. H. F. Sluiter, S. G. Fries, C. Guéneau, B. Hallstedt, U. R. Kattner and M. Selleby *The legacy of "The Regular Solution Model for Stoichiometric Phases and Ionic Melts"*, J Phase Equilib Diffus, **45**, doi:10.1007/s11669-024-01163-2

[25] M. Hillert, B. Jansson, B. Sundman, J. Ågren, *A two-sublattice model for molten solutions with different tendency for ionization*, Metall. Trans. A **16A**, (1985), pp 261–266, doi:10.1007/BF02816052

[26] M. Hillert, *The compound energy formalism* J Alloys and Comp, **320**, (2001), pp 161–176, doi:10.1016/S0925-8388(00)01481-X

[27] Z. He, B. Kaplan, H. Mao, M. Selleby *The third generation Calphad description of Al-C including revision of pure Al and C.*, Calphad **72** (2021) doi:10.1016/j.calphad.2021.102250

[28] J. Ågren, *Thermodynmaics of supercooled liquids and their glass transition*, Phys Chem Liq, **18** (1988), doi:10.1080/00319108808078586.

[29] C. A. Becker, J. Agren, M. Baricco, Q Chen, S. A. Decterov, U. R. Kattner, J. H. Perepezko, G. R. Pottlacher and M. Selleby, *Thermodynamic modelling of liquids*, Phys Stat Sol B (2013), doi:10.1002/pssb.201350149

[30] I. Ansara, T. G. Chart, A. Fernández Guillermet, P. C. Hayes, U. R. Kattner, D. G. Pettifor, N. Saunders, K.Zeng, *Thermodynamic modelling of selected topologically close-packed intermetallic compounds*, Calphad, **21**, (1997), doi:10.1016/S0364-5916(97)00021-7

[31] M. Hillert, *Empirical methods of predicting and representing thermodynamic properties of ternary solution phases*, Calphad **4** pp 1–12, doi:10.1016/0364-5916(80)90016-4

[32] A. Pelton, *A general "geometric" thermodynamic model for multicomponent solutions*, Calphad **25** (2001) pp 319–328 doi:10.1016/S0364-5916(01)00052-9

[33] J Li, B. Sundman, J. G. M. Winkelman, A. I. Vakis, F. Picchioni, *Implementation of the UNIQUAC model in the OpenCalphad software*, Fluid Phase Eq., **507**, (2020), doi:10.1016/j.fluid.2019.112398

[34] https://github.com/sundmanbo/XTDB/

[35] B. Sundman, U. R. Kattner, M. Hillert,M. Selleby, J. Ågren, S. Bigdeli, Q. Chen, A. Dinsdale, B. Hallstedt, A. Khvan, H. Mao, and

R. Otis, *A method for handling the extrapolation of solid crystalline phases to temperatures far above their melting point*, Calphad, **68** (2020), 101737 doi:10.1016/j.calphad.2020.101737

## Appendix A. A summary of the XML tags and attributes

A complete version is available at [34]. Attributes which are mandatory are indicated by a !M to the left.

*Appendix A.1. Global tags*

| Tag | Attributes | Note |
|---|---|---|
| XTDB | | Containing XML tags for an XTDB database. |
| !M | Version | Version of XTDB used for this database. |
| !M | Software | Name of software generating the database. |
| !M | Date | Year/month/day the database was written or last edited |
| !M | Signature | person or organisation generating the database. |
| Defaults | | Optional tag to provide default values of attributes in different XML tags and some other things. |
| | LowT | Default value of low $T$ limit. |
| | HighT | Default value of high $T$ limit. |
| | Elements | For example "VA" (vacancy) and "/-" (the electron). |
| | GlobalModel | Any model applicable to the whole database. |
| DatabaseInfo | | Optional tag with information about the database |
| | Info | Free text (excluding the characters <> & ). |
| | Date | Last update of the database information. |
| AppendXTDB | | Optional tag with additional files for the XTDB database. It should contain XTBD tags see section 4.3. |
| | Models | The **ModelDescriptions** tag, see section 3.3. |
| | Parameters | With mainly **Parameter** tags. |
| | TPfuns | With some or all **TPfun** tags. |
| | Bibliography | With bibliographic tags. |
| | Misc | Whatever the database manager needs. |

*Appendix A.2. The Element and Species tags*

| Tag | Attributes | Explanation |
|---|---|---|
| Element | | Specifies a chemical element in the database. In addition the vacancy, denoted "VA", and the electron, 'denoted '/-", are included to handle defects and ions. |
| !M | Id | Chemical element symbol, one or two letters, for example FE, H. The Id is case insensitive, see section 4.1. |
| | Refstate | Name of the reference phase for the element. |
| !M | Mass | Mass in g/mol |
| | H298 | Enthalpy difference between 0 and 298.15 K in the reference state. |
| | S298 | Entropy difference between 0 and 298.15 K in the reference state. |
| Species | | Specifies a chemical species used as a constituent of phases. The elements, except the electron, are also species. |
| !M | Id | Species name, see section 4.1. |
| !M | Stoichiometry | One or more element *Id* each followed by an unsigned real or two integers separated by a "/" representing the stoichiometric ratio. A "/-" or "/+" followed by a digit means a negative or positive electric charge. If no digit 1 is assumed. See section 4.1. |
| | MQMQA | For a constituent in the MQMQA model. See section 4.2. |
| | UNIQUAC | For a constituent in the UNIQUAC model. See section 4.2. |

*Appendix A.3. The phase tags*

| Tag | Attributes | Explanation |
|---|---|---|
| Phase | | All thermodynamic data is part of a phase. |
| !M | Id | Phase name, see sections 4.1 and 4.4. |
| !M | Configuration | Model for the configurational entropy, see section 2.4. |
| | State | see section 4.5. |
| CrystalStructure | | Optional inside a **Phase** tag. |
| | Prototype | Prototype phase |
| | StrukturBericht | For example A3, B2, C14, D0_3 etc. |
| | PearsonSymbol | For example hR21 cI2. |
| | SpaceGroup | For example 127, 166. |
| Sublattices | | Only once inside a **Phase** tag. |
| !M | NumberOf | Number of sublattices, an integer value $> 0$. |
| !M | Multiplicities | One real value$> 0$ for each sublattice, See Appendix B.1 |
| Constituents | | Only inside the **Sublattices** tag. |
| | Sublattice | Can be omitted if only one sublattice. |
| | WyckoffPosition | Optinonal specification. |
| !M | List | Species *Id* separated by a space, see section 3.2. |
| AmendPhase | | Optional tag inside a **Phase** tag to specify a contrinution from a physical model, see section 3.3, Appendix C and Appendix B.1. |
| | Models | One or more model *Id*s, separated by a space, for this phase. There can also be an **DisorderedPart** tag inside this tag. |

*Appendix A.4. The function tag*

| Tag | Attributes | Explanation |
|---|---|---|
| TPfun | | Defines a $T, P$ expression to be used in parameters or other functions. |
| !M | Id | The *Id* can be used in the *Expr* attribute of other functions or parameters, see section 4.1. |
| | LowT | Can be omitted if the default low $T$ limit applies. |
| !M | Expr | Simple mathematical expression terminated by ;. See section 4.7. Use the **Trange** tag if several ranges. |
| | HighT | Can be omitted the default high $T$ limit applies. |
| Trange | | Only inside a **TPfun** or **Parameter** tag for an expression with several $T$ ranges. The function and its first and second derivative must be continous. |
| !M | Expr | Simple mathematical expression terminated by ;. See section 4.7. |
| | HighT | Can be omitted if the default high $T$ limit applies. |

There is no provision for breakpoints in $P$. Separate models are needed for pressure dependence above a few MPa.

*Appendix A.5. The parameter tag*

The model parameters are the central part of an XTDB database. In the example here the very compact form used in TDB files is retained.

| Tag | Attributes | Explanation |
|---|---|---|
| Parameter | | Specifies the $T, P$ expression of a model parameter for a set of constituents. |
| !M | Id | As in a TDB file, See section 4.6 |
| | LowT | Can be omitted if the default low $T$ limit applies. |
| !M | Expr | Simple mathematical expression terminated by ;. If several ranges use a **Trange** tag. See section 4.7. |
| | HighT | Can be omitted if the default high $T$ limit applies. |
| !M | Bibref | Bibliographic reference. |

*Appendix A.6. The bibliography for parameters*

| Tag | Attributes | Explanation |
|---|---|---|
| Bibliography | | Contains bibliographic references. There are no attributes. |
| Bibitem | | Only inside a **Bibliography** tag. |
| !M | Id | Used as value in the *bibref* attribute for a parameter or model, normally a paper or a comment by the database manager. |
| !M | Text | Reference to a paper or comment. |
| | DOI | DOI of paper where the parameter was assessed. |

*Appendix A.7. The tags for current models*

| Tag | Attributes | Explanation |
|---|---|---|
| ModelDescriptions | | Contains model tags usually with an *Id* attribute used in **AmendPhase** tags inside a **Phase** tag. Most models have one or more model parameter identifiers (MPID). |
| !M | Software | Name of software using these models. |
| Magnetic | | There are several magnetic models. See section Appendix C. |
| !M | Id | This is used in *Models* attribute of the **AmendPhase** tag. There are 3 variants: IHJBCC, IHJREST and IHJQX, |
| | Aff | The antiferromagnetic factor (-1, -3 or 0). |
| !M | MPID1 | Specifies the Bohr magneton number MPID |
| !M | MPID2 | Specifies a Curie or combined Curie/Neel temperature MPID |
| | MPID3 | Specifies a Neel temperature MPID for IHJQX |
| !M | Bibref | Where the model is described. |
| Permutations | | For FCC, HCP and BCC lattices a 4 sublattice tetrahedron model, See section 3.8. |
| !M | Id | This is used in the *Models* attribute of the **AmendPhase** tag. Its can be either FCC4PERM or BCC4PERM. |
| !M | Bibref | Where the model is explained. |
| DisorderedPart | | Optional tag inside the **AmendPhase** tag of an ordered phase with or without order/disorder. See section 3.6. |
| | Disordered | Optional attribute with the *Id* of the disordered phase. |
| !M | Sum | Number of sublattices in the ordered phase in eq. 14. |
| | Subtract | Must be specified if eq. 16 in section 3.6 should be used. |
| !M | Bibref | Where the model is described. |

*Appendix A.8. The tags for the new unary database*

| Tag | Attributes | Explanation |
|---|---|---|
| Einstein | | The low $T$ vibrational model, see section 3.4. |
| !M | Id | This Id is used in **AmendPhase** tag. |
| !M | MPID1 | Specifies the MPID for the Einstein $\theta$. |
| !M | Bibref | Where the model is described. |
| Liquid2state | | The liquid 2-state model, see section 3.5. |
| !M | Id | This Id is used in **AmendPhase** tag. |
| !M | MPID1 | Specifies the MPID for the 2-state transition energy. |
| !M | MPID2 | Specifies the MPID for the Einstein $\theta$ for the low $T$ extrapolation. |
| !M | Bibref | Where the model is described. |
| EEC | | Specifies that the Equi-entropy model applies to the whole database. See section 4.5. The liquid **Phase** tag must also have the *State* attribute equal to L. |
| !M | Id | has the value EEC. |
| !M | Bibref | Where the model is described. |

*Appendix A.9. Miscellaneous tags*

| Tag | Attributes | Explanation |
|---|---|---|
| TernaryXpol | | The extrapolation method for a ternary. See section 3.11. |
| !M | Phase | The *Id* of a phase. |
| !M | Constituents | The *Id*s of 3 **Species** that are constituents of the phase. |
| !M | Xpol | The type of extrapolations, for example KKK if the Kohler method is used for all 3 binaries. |
| !M | Bibref | Where the model is described. |
| BinarySystem | | Optional tag for a database manager to surround a set of model parameters for a binary system. It can be used to list which assessed systems that are present in the database. |
| !M | System | The *Id*s of the two elements inside the tag. |
| | CalcDia | Software dependent way to calculate the binary system |

## Appendix B. Examples of XTDB files

*Appendix B.1. A complete Al-C database*

```
<XTDB version="0.1.5">
<Defaults LowT="10" HighT="6000" Elements="VA /-" />
<Element Id="AL" Refstate="FCC_A1" Mass="26.982" H298="4577.3" S298="28.322" />
<Element Id="C" Refstate="GRAPHITE" Mass="12.011" H298="1054" S298="5.7423" />
<Species Id="VA" Stoichiometry="VA" />
<Species Id="AL" Stoichiometry="AL" />
<Species Id="C" Stoichiometry="C" />
<Phase Id="LIQUID" Configuration="CEF" State="L" >
  <Sublattices NumberOf="1" Multiplicities="1" >
    <Constituents Sublattice="1" List="AL C" />
  </Sublattices>
 <AmendPhase Models="LIQ2STATE" />
</Phase>
<Phase Id="AL4C3" Configuration="CEF" State="S" >
  <Crystallography PearsonSymbol="hR21" SpaceGroup="166" Prototype="Al4C3" />
  <Sublattices NumberOf="2" Multiplicities="4 3" >
    <Constituents Sublattice="1" List="AL" />
    <Constituents Sublattice="2" List="C" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<Phase Id="BCC_A2" Configuration="CEF" State="S" >
  <Crystallography Structurbericht="A2" PearsonSymbol="cI2" Prototype="W" />
  <Sublattices NumberOf="2" Multiplicities="1 3" >
```

```
    <Constituents Sublattice="1" List="AL" />
    <Constituents Sublattice="2" List="C VA" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<Phase Id="DIAMOND" Configuration="CEF" State="S" >
  <Crystallography StructurBerict="A4" PearsonSymbol="cF8" Prototype="C" />
  <Sublattices NumberOf="1" Multiplicities="1" >
    <Constituents Sublattice="1" List="C" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<Phase Id="FCC_A1" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="A1" PearsonSymbol="cF4" Prototype="Cu" />
  <Sublattices NumberOf="2" Multiplicities="1 1" >
    <Constituents Sublattice="1" List="AL" />
    <Constituents Sublattice="2" List="C VA" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<Phase Id="GRAPHITE" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="A9" PearsonSymbol="hP4"  Prototype="C" />
  <Sublattices NumberOf="1" Multiplicities="1" >
    <Constituents Sublattice="1" List="C" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
```

```
<Phase Id="HCP_A3" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="A3" PearsonSymbol="hP2" Prototype="Mg" />
  <Sublattices NumberOf="2" Multiplicities="1 0.5" >
    <Constituents Sublattice="1" List="AL" />
    <Constituents Sublattice="2" List="C VA" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<TPfun Id="R"     Expr="8.31451;" />
<TPfun Id="RTLNP" Expr="R*T*LN(1.0E-5)*P);" />
<TPfun Id="G0AL4C3" Expr=" -277339-.005423368*T**2;" />
<TPfun Id="GTSERAL" Expr=" -.001478307*T**2-7.83339395E-07*T**3;" />
<TPfun Id="GTSERCC" Expr=" -.00029531332*T**2-3.3998492E-16*T**5;" />
<TPfun Id="G0BCCAL" Expr=" +GHSERAL+10083;" />
<TPfun Id="G0HCPAL" Expr=" +GHSERAL+5481;" />
<TPfun Id="GHSERAL" Expr=" -8160+GTSERAL;" />
<TPfun Id="GHSERCC" Expr=" -17752.213+GEGRACC+GTSERCC;" />
<TPfun Id="G0DIACC" Expr=" -16275.202-9.1299452E-05*T**2-2.1653414E-16*T**5;" />
<TPfun Id="GEDIACC" Expr=" +0.2318*GEIN(+813.6)+.01148*GEIN(+345.4)
       -0.236743*GEIN(+1601.4);" />
<TPfun Id="G0LIQAL" Expr=" -209-3.777*T-.00045*T**2;" />
<TPfun Id="G0LIQCC" Expr=" +63887-8.2*T-.0004185*T**2;" />
<TPfun Id="GEGRACC" Expr=" -0.5159523*GEIN(+1953.3)+0.121519*GEIN(+448)
       +0.3496843*GEIN(+947)+.0388463*GEIN(+192.7)+.005840323*GEIN(+64.5);" />
<Parameter Id="G(LIQUID,AL;0)" Expr=" +G0LIQAL;" Bibref="21HE" />
<Parameter Id="LNTH(LIQUID,AL;0)" Expr=" +LN(+254);" Bibref="21HE" />
<Parameter Id="GD(LIQUID,AL;0)" Expr=" +13398-R*T-0.16597*T*LN(+T);" Bibref="21HE" />
```

<Parameter Id="G(LIQUID,C;0)" Expr=" +GOLIQCC;" Bibref="21HE" />

<Parameter Id="LNTH(LIQUID,C;0)" Expr=" +LN(+1400);" Bibref="21HE" />

<Parameter Id="GD(LIQUID,C;0)" Expr=" +59147-49.61*T+2.9806*T*LN(+T);" Bibref="21HE" />

<Parameter Id="G(LIQUID,AL,C;0)" Expr=" +20994-22*T;" Bibref="21HE" />

<Parameter Id="G(AL4C3,AL:C;0)" Expr=" +GOAL4C3-3.08*GEIN(+401)+3.08*GEIN(+1077);" Bibref

<Parameter Id="LNTH(AL4C3,AL:C;0)" Expr=" +LN(+401);" Bibref="21HE" />

<Parameter Id="G(BCC_A2,AL:C;0)" Expr=" +GTSERAL+3*GTSERCC+1006844;" Bibref="21HE" />

<Parameter Id="LNTH(BCC_A2,AL:C;0)" Expr=" +LN(+863);" Bibref="21HE" />

<Parameter Id="G(BCC_A2,AL:VA;0)" Expr=" +GOBCCAL;" Bibref="21HE" />

<Parameter Id="LNTH(BCC_A2,AL:VA;0)" Expr=" +LN(+233);" Bibref="21HE" />

<Parameter Id="G(BCC_A2,AL:C,VA;0)" Expr=" -819896+14*T;" Bibref="21HE" />

<Parameter Id="G(DIAMOND,C;0)" Expr=" +GODIACC+GEDIACC;" Bibref="21HE" />

<Parameter Id="LNTH(DIAMOND,C;0)" Expr=" +LN(+1601.4);" Bibref="21HE" />

<Parameter Id="G(FCC_A1,AL:C;0)" Expr=" +GTSERAL+GTSERCC+57338;" Bibref="21HE" />

<Parameter Id="LNTH(FCC_A1,AL:C;0)" Expr=" +LN(+549);" Bibref="21HE" />

<Parameter Id="G(FCC_A1,AL:VA;0)" Expr=" +GHSERAL;" Bibref="21HE" />

<Parameter Id="LNTH(FCC_A1,AL:VA;0)" Expr=" +LN(+283);" Bibref="21HE" />

<Parameter Id="G(FCC_A1,AL:C,VA;0)" Expr=" -70345;" Bibref="21HE" />

<Parameter Id="G(GRAPHITE,C;0)" Expr=" +GHSERCC;" Bibref="21HE" />

<Parameter Id="LNTH(GRAPHITE,C;0)" Expr=" +LN(+1953.3);" Bibref="21HE" />

<Parameter Id="G(HCP_A3,AL:C;0)" Expr=" +GTSERAL+0.5*GTSERCC+2176775;" Bibref="21HE" />

<Parameter Id="LNTH(HCP_A3,AL:C;0)" Expr=" +LN(+452);" Bibref="21HE" />

<Parameter Id="G(HCP_A3,AL:VA;0)" Expr=" +GOHCPAL;" Bibref="21HE" />

<Parameter Id="LNTH(HCP_A3,AL:VA;0)" Expr=" +LN(+263);" Bibref="21HE" />

<Parameter Id="G(HCP_A3,AL:C,VA;0)" Expr=" 0;" Bibref="21HE" />

<Bibliography>

<Bibitem Id="21HE" Text="Z. He, B. Kaplan, H. Mao, M. Selleby, Calphad (2021) 102250" />

```
</Bibliography>
</XTDB>
```

*Appendix B.2. A σ phase with EBEF and DisorderedPart*

```
<Element Id="AL" Refstate="FCC_A1" Mass="26.982" H298="4577.3" S298="28.322" />
<Element Id="Cr" Refstate="BCC_A2" Mass="51.996" H298="4050" S298="23.56" />
<Element Id="FE" Refstate="BCC_A2" Mass="55.847" H298="4489" S298="27.28" />

<Phase Id="SIGMA" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="D8_b" PearsonSymbol="tP30" SpaceGroup="P4_2/mnm" />
  <Sublattices NumberOf="5" Multiplicities="2 4 8 8 8" >
    <Constituents Sublattice="1" List="AL CR FE" />
    <Constituents Sublattice="2" List="AL CR FE" />
    <Constituents Sublattice="3" List="AL CR FE" />
    <Constituents Sublattice="4" List="AL CR FE" />
    <Constituents Sublattice="5" List="AL CR FE" />
  </Sublattices>
  <AmendPhase > <!-- EBEF is used for the parameters -->
    <DisorderedPart Sum="5" />
  </AmendPhase>
</Phase>

<!-- Endmember parameters are in the disordered part. They are for a single atom and
     should be multiplied by 30 (the sum of the multiplicities) by the software. -->

<Parameter Id="G(SIGMA,AL;0)" Expr=" +GSIGMA_AL;" Bibref="SGTE2025"/>
<Parameter Id="G(SIGMA,CR;0)" Expr=" +GSIGMA_CR;" Bibref="SGTE2025"/>
```

```
<Parameter Id="G(SIGMA,FE;0)" Expr=" +GSIGMA_FE;" Bibref="SGTE2025"/>

<!-- Below the 20 EBEF excess endmember parameters for the ordered part of Al-Cr.
     Without wildcards there are 32 endmembers.  The * can represent any element -->

<Parameter Id="G(SIGMA,AL:CR:*:*:*;0)" Expr=" SIGMA_X_AL1CR2;" />
<Parameter Id="G(SIGMA,AL:*:CR:*:*;0)" Expr=" SIGMA_X_AL1CR3;" />
<Parameter Id="G(SIGMA,AL:*:*:CR:*;0)" Expr=" SIGMA_X_AL1CR4;" />
<Parameter Id="G(SIGMA,AL:*:*:*:CR;0)" Expr=" SIGMA_X_AL1CR5;" />
<Parameter Id="G(SIGMA,*:AL:CR:*:*;0)" Expr=" SIGMA_X_AL2CR3;" />
<Parameter Id="G(SIGMA,*:AL:*:CR:*;0)" Expr=" SIGMA_X_AL2CR4;" />
<Parameter Id="G(SIGMA,*:AL:*:*:CR;0)" Expr=" SIGMA_X_AL2CR5;" />
<Parameter Id="G(SIGMA,*:*:AL:CR:*;0)" Expr=" SIGMA_X_AL3CR4;" />
<Parameter Id="G(SIGMA,*:*:AL:*:CR;0)" Expr=" SIGMA_X_AL3CR5;" />
<Parameter Id="G(SIGMA,*:*:*:AL:CR;0)" Expr=" SIGMA_X_AL4CR5;" />
<Parameter Id="G(SIGMA,CR:AL:*:*:*;0)" Expr=" SIGMA_X_CR1AL2;" />
<Parameter Id="G(SIGMA,CR:*:AL:*:*;0)" Expr=" SIGMA_X_CR1AL3;" />
<Parameter Id="G(SIGMA,CR:*:*:AL:*;0)" Expr=" SIGMA_X_CR1AL4;" />
<Parameter Id="G(SIGMA,CR:*:*:*:AL;0)" Expr=" SIGMA_X_CR1AL5;" />
<Parameter Id="G(SIGMA,*:CR:AL:*:*;0)" Expr=" SIGMA_X_CR2AL3;" />
<Parameter Id="G(SIGMA,*:CR:*:AL:*;0)" Expr=" SIGMA_X_CR2AL4;" />
<Parameter Id="G(SIGMA,*:CR:*:*:AL;0)" Expr=" SIGMA_X_CR2AL5;" />
<Parameter Id="G(SIGMA,*:*:CR:AL:*;0)" Expr=" SIGMA_X_CR3AL4;" />
<Parameter Id="G(SIGMA,*:*:CR:*:AL;0)" Expr=" SIGMA_X_CR3AL5;" />
<Parameter Id="G(SIGMA,*:*:*:CR:AL;0)" Expr=" SIGMA_X_CR4AL5;" />

<!-- There are also 20 EBEF endmember parameters for Al-Fe and Cr-Fe -->
```

```
<Parameter Id="G(SIGMA,AL:FE:*:*:*;0)" Expr=" SIGMA_X_AL1FE2;" />

<Parameter Id="G(SIGMA,CR:FE:*:*:*;0)" Expr=" SIGMA_X_CR1FE2;" />
```

The **TPfun**s SIGMA_X_AsBt can be fitted to DFT calculated endmembers. In a ternary EBEF there are 63 parameters, without wildcards there are $3^5 = 243$ endmembers.

*Appendix B.3. A σ phase with EBEF and DisorderedPart*

Below is a suggestion of a future possibility for a shorter notation.

```
<Element Id="AL" Refstate="FCC_A1" Mass="26.982" H298="4577.3" S298="28.322" />
<Element Id="Cr" Refstate="BCC_A2" Mass="51.996" H298="4050" S298="23.56" />
<Element Id="FE" Refstate="BCC_A2" Mass="55.847" H298="4489" S298="27.28" />

<Phase Id="SIGMA" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="D8_b" PearsonSymbol="tP30" SpaceGroup="P4_2/mnm" />
  <Sublattices NumberOf="5" Multiplicities="2 4 8 8 8" >
    <Constituents Sublattice="1" Wyckoff="2a" List="AL CR FE" />
    <Constituents Sublattice="2" Wyckoff="4f" List="AL CR FE" />
    <Constituents Sublattice="3" Wyckoff="8i1" List="AL CR FE" />
    <Constituents Sublattice="4" Wyckoff="8i2" List="AL CR FE" />
    <Constituents Sublattice="5" Wyckoff="8j" List="AL CR FE" />
  </Sublattices>
  <AmendPhase > Models="EBEF"  <!-- EBEF notation is used for the parameters -->
    <DisorderedPart Sum="5" />
```

```
  </AmendPhase>
</Phase>

<!-- Endmember parameters in the disordered part as in~\ref{sc:sigma-ebef.}
     The notation below use @ character indicate the sublattice of the constituent
     in the ordered part.  -->

<Parameter Id="G(SIGMA,AL@1:CR@2)" Expr=" SIGMA_X_AL1CR2;" />
<Parameter Id="G(SIGMA,AL@1:CR@3)" Expr=" SIGMA_X_AL1CR3;" />
<Parameter Id="G(SIGMA,AL@1:CR@4)" Expr=" SIGMA_X_AL1CR4;" />
<Parameter Id="G(SIGMA,AL@1:CR@5)" Expr=" SIGMA_X_AL1CR5;" />
<Parameter Id="G(SIGMA,AL@2:CR@3)" Expr=" SIGMA_X_AL2CR3;" />
<Parameter Id="G(SIGMA,AL@2:CR@4)" Expr=" SIGMA_X_AL2CR4;" />
```

*Appendix B.4. An FCC phase with wildcards and DisorderedPart*

```
<Element Id="AL" Refstate="FCC_A1" Mass="26.982" H298="4577.3" S298="28.322" />
<Element Id="Cr" Refstate="BCC_A2" Mass="51.996" H298="4050" S298="23.56" />
<Element Id="FE" Refstate="BCC_A2" Mass="55.847" H298="4489" S298="27.28" />
<Element Id="C"  Refstate="GRAPHITE" Mass="12.011" H298="1054" S298="5.7423" />

<Phase Id="FCC_4SL" Configuration="CEF" State="S" >
  <Sublattices NumberOf="5" Multiplicities="0.25 0.25 0.25 0.25 1" >
    <Constituents Sublattice="1" List="AL CR FE" />
    <Constituents Sublattice="2" List="AL CR FE" />
    <Constituents Sublattice="3" List="AL CR FE" />
    <Constituents Sublattice="4" List="AL CR FE" />
```

```
    <Constituents Sublattice="5" List="Va C" />
  </Sublattices>
  <AmendPhase Models="IHJREST GEIN FCC4PERM" >
    <DisorderedPart Sum="4" Subtract="N" />
  </AmendPhase>
</Phase>

<!-- The first 4 sublattices are for L1_2 and L1_0 ordering.
     Endmember parameters in the disordered part with no ordering.
     There can also be excess parameters to describe the disordered state.
     The disordered parameters are for the same phase, but have fewer sublattices. -->
<Parameter Id="G(FCC_4SL,AL:VA;0)" Expr=" +GHSERAL;" Bibref="21HE" />
<Parameter Id="LNTH(FCC_4SL,AL:VA;0)" Expr=" +LN(+283);" Bibref="21HE" />
<Parameter Id="G(FCC_4SL,AL:C;0)" Expr=" +GTSERAL+GTSERCC+57338;" Bibref="21HE" />
<Parameter Id="LNTH(FCC_4SL,AL:C;0)" Expr=" +LN(+549);" Bibref="21HE" />
<Parameter Id="G(FCC_4SL,CR:VA;0)" Expr=" +GFCC_CR;" Bibref="SGTE2025"/>
<Parameter Id="G(FCC_4SL,FE:VA;0)" Expr=" +GFCC_FE;" Bibref="SGTE2025"/>

<!-- Some excess parameters to descrive the stable disordered phase -->
<Parameter Id="G(FCC_4SL,AL:C,VA;0)" Expr=" -70345;" Bibref="21HE" />
<Parameter Id="G(FCC_4SL,AL,CR:VA;0)" Expr=" GFCC_X_ALCR0;" />
<Parameter Id="G(FCC_4SL,AL,CR:VA;1)" Expr=" GFCC_X_ALCR1;" />

<!-- Some examples of parameters in the ordered part of the FCC phase.
     A parameter G(FCC_4SL,AL:AL:AL:CR:VA;0) is permuted 4 times.
     A parameter G(FCC_4SL,AL:AL:CR:CR:VA;0) is permuted 6 times.  -->
<Parameter Id="G(FCC_4SL,AL:AL:AL:CR:VA;0)" Expr=" GFCC_AL3CR1;" />
```

```
<Parameter Id="G(FCC_4SL,AL:AL:CR:CR:VA;0)" Expr=" GFCC_AL2CR2;" />
<Parameter Id="G(FCC_4SL,AL:CR:CR:CR:VA;0)" Expr=" GFCC_AL1CR3;" />
<Parameter Id="G(FCC_4SL,AL:AL:AL:FE:VA;0)" Expr=" GFCC_AL3FE1;" />

<!-- An excess parameters with wildcards using the assumption that the AL-CR
     interaction is independent of the constituents on the other sublattices.
     This parameter is also permuted 4 times. -->
<Parameter Id="G(FCC_4SL,AL,CR:*:*:*:VA;0)" Expr=" GFCC_XO_ALCR;" />

<!-- This parameter approximate SRO both in ordered and disordered,
     it is permuted 6 times.  -->
<Parameter Id="G(FCC_4SL,AL,CR:AL,CR:*:*:VA;0)" Expr=" GFCC_SRO_ALCR;" />
```

## Appendix C. A tentative ModelDescriptions tag

This defines the physical models and their model parameter identifiers (MPID) used in the XTDB file. Each software can have its own version.

```
<ModelDescriptions Software="OpenCalphad" >
<!-- This is a short explanation of XTDB model tags and their attributes in OC. -->
<Magnetic Id="IHJBCC" MPID1="BMAGN" MPID2="TC" Aff=" -1.00" Bibref="82Her" >
 <!-- f_below_TC= +1-0.905299383*TAO**(-1)-0.153008346*TAO**3-.00680037095*TAO**9
                 -.00153008346*TAO**15; and
    f_above_TC= -.0641731208*TAO**(-5)-.00203724193*TAO**(-15)-.000427820805*TAO**(-25);
 in Gmagn=f(TAO)*LN(BMAGN+1) where TAO=T/TC.  Aff is the antiferromagnetic factor.
 For BCC phase.  TC is a combined Curie/Neel T and BMAGN the Bohr magneton number. -->
</Magnetic>
<Magnetic Id="IHJREST"  MPID1="BMAGN" MPID2="TC" Aff=" -3.00" Bibref="82Her" >
 <!-- f_below_TC= +1-0.860338755*TAO**(-1)-0.17449124*TAO**3-.00775516624*TAO**9
                -.0017449124*TAO**15; and
    f_above_TC= -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25);
 in Gmagn=f(TAO)*LN(BMAGN+1) where TAO=T/TC.  For non-bcc phases. -->
</Magnetic>
<Magnetic Id="IHJQX" MPID1="BMAGN" MPID2="CT" MPID3="NT" Aff="0" Bibref="01Che 12Xio" >
 <!-- f_below_TC= +1-0.842849633*TAO**(-1)-0.174242226*TAO**3-.00774409892*TAO**9
               -.00174242226*TAO**15-.000646538871*TAO**21; and
    f_above_TC= -.0261039233*TAO**(-7)-.000870130777*TAO**(-21)-.000184262988*TAO**(-35)
               -6.65916411E-05*TAO**(-49);
 in Gmagn=f(TAO)*LN(BMAGN+1) where TAO=T/CT or T/NT.  Aff is redundant.
 CT is the Curie T and NT the Neel T and BMAGN the average Bohr magneton number. -->
</Magnetic>
```

```
<Einstein Id="GEIN" MPID1="LNTH" Bibref="01Che 21He" >
  <!-- The Gibbs energy due to the Einstein low T vibrational model,
           G=1.5*R*THETA+3*R*T*LN(1-EXP(-THETA/T)).
   The value used for LNTH should be ln(THETA) as this varies with composition
   in a more physically reasonable way.  When there are multiple THETA the argument
   of the GEIN functions should be THETA itself as it is a constant. -->
</Einstein>
<Liquid2state Id="LIQ2STATE" MPID1="GD"  MPID2="LNTH" Bibref="88Agr 13Bec" >
  <!-- Unified model for the liquid and the amorphous state treated as an Einstein solid
    The GD parameter describes the stable liquid and the transition to the amorphous
    state.  LNTH is the logarithm of the Einstein THETA of the amorphous phase. -->
  </Liquid2state>
<DisorderedPart Disordered=" " Sum=" " Subtract=" " Bibref="97Ans 07Hal" >
  <!-- This tag is nested inside the ordered phase tag.  The disordered fractions are
    averaged over the number of ordered sublattices indicated by Sum.  The Gibbs energy
    is calculated separately for the ordered and disordered model parameters and added
    but the configurational Gibbs energy is calculated only for the ordered phase.  If
    the Subtract="Y" is included the Gibbs energy of the ordered phas is calculated
    a second time as disordered and subtracted -->
</DisorderedPart>
<Permutations Id="FCC4Perm" Bibref="09Sun" >
  <!-- An FCC phase with 4 sublattices for the ordered tetrahedron use this model to
      indicate that parameters with permutations of the same set of constituents on
      identical sublattices are included only once in the database. -->
</Permutations>
<Permutations Id="BCC4Perm" Bibref="09Sun" >
  <!-- A BCC phase with 4 sublattices for the ordered asymmetric tetrahedron use this
```

```
     model to indicate that parameters with permutations of the same set of constituents
     on identical sublattices are included only once in the database. -->
</Permutations>
<EEC Id="EEC" Bibref="20Sun" >
  <!-- The Equi-Entropy Criterion means that the software must ensure that solid phases
     with higher entropy than  the liquid phase must not be stable. -->
</EEC>
<TernaryXpol Phase=" " Constituents=" " Xpol=" "  Bibref="01Pel" >
  <!-- The ternary extrapolation of the binary parameters is specified. -->
</TernaryXpol>
<EBEF Id="EBEF" Bibref="18Dup" >
   <!-- The Effective Bond Energy Formalism for phases with multiple sublattices using
     wildcards, "*".  It also requires the DisorderedPart tag. -->
</EBEF>
<Bibliography> <!-- for the models -->
  <Bibitem Id="82Her" Text="S. Hertzman and B. Sundman, A Thermodynamic analysis of the
    Fe-Cr system,' Calphad, Vol 6 (1982) pp 67-80" />
  <Bibitem Id="88Agr" Text="J. Agren, Thermodynmaics of supercooled liquids and their
     glass transition, Phys Chem Liq, Vol 18 (1988) pp 123-139" />
  <Bibitem Id="97Ans" Text="I. Ansara, N. Dupin, H. L. Lukas, B. Sundman, Thermodynamic
     assessment of the Al-Ni system, J All and Comp, Vol 247 (1997) pp 20-30" />
  <Bibitem Id="01Che" Text="Q. Chen and B. Sundman, Modeling of Thermodynamic Properties
     for BCC, FCC, Liquid and Amorphous Iron, J Phase Eq, Vol 22 (2001) pp 631-644" />
  <Bibitem Id="01Pel" Text="A. D. Pelton, A General Geometric Thermodynamic Model for
     Multicomponent  solutions, Calphad, Vol 25 (2001) pp 319-328" />
  <Bibitem Id="07Hal" Text="B. Hallstedt, N. Dupin, M. Hillert, L. Hoglund, H. L. Lukas,
     J. C. Schuster and N. Solak, Calphad, Vol 31 (2007) pp 28-37" />
```

```
  <Bibitem Id="09Sun" Text="B. Sundman, I. Ohnuma, N. Dupin, U. R. Kattner, S. G. Fries,
     An assessment of the Al-Fe system, Acta Mater, Vol 57 (2009) pp 2896-2908" />
  <Bibitem Id="12Xio" Text="W. Xiong, Q. Chen, P. A. Korzhavyi, M. Selleby, An improved
     magnetic model for thermodynamic modeling, Calphad, Vol 39 (2012) pp 11-20" />
  <Bibitem Id="13Bec" Text="C. A. Becker, J. Agren, M. Baricco, Q Chen, S. A. Decterov,
     U. R. Kattner, J. H. Perepezko, G. R. Pottlacher and M. Selleby, Thermodynamic
      modelling of liquids, Phys Stat Sol B (2013) pp 1-20" />
  <Bibitem Id="18Dup" Text="N. Dupin, U. R. Kattner, B. Sundman, M. Palumbo, S. G. Fries,
     Implementation of an Effective Bond Energy Formalism, J Res NIST, (2018) 123020" />
  <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. Otis,
      A method for handling extrapolation of solids, Calphad, Vol 68 (2020) 101737" />
  <Bibitem Id="21He" Text="Z. He, B. Kaplan, H. Mao, M. Selleby, The third generation
      Calphad description of Al-C including revision of pure Al and C, Calphad,
      Vol 72 (2021) 102250" />
  </Bibliography>
</ModelDescriptions>
```