# Proposal 0.1.2 of an XML format to replace TDB files

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## 1 Background

Within the Calphad comminity the databases with model parameters are important and can often be used by several different software as well as edited manually. The most frequent format for such database is called TDB and was created by the Scientif Group Thermodata Europe (SGTE) while working on the unary databse for 78 elements which was published 1991 [2]. It has been used for more than 40 years but it has limitations, in particular when adding new new models and features.

It is high time to change from this format and to adopt an accepted Markup Language as XML or JSON. The XML has been selected for a new XTDB format as it has been around for a long time and is slightly more explicit. There are many Markup Languages but as it is easy to convert between any of them and thus the choice of XML is not very critical except to avoid spending several years to discuss this choice.

XML is flexible and extendable each software may add their own flavour in a controlled way. It will be simpler to use an XTDB file by different softwares as one can easily indicate what is software specific rather than try to modify or extend the TDB format.

To avoid the confusing use of **element** both for chemical element and the XML element the word **tag** will be used for the XML element.

### 1.1 Objectives

The TDB format is well established and used by both students assessing model parameters as well as database managers and researches trying to develop new materials based on thermodynamic calculations. This proposal proposes a minimal change from the current TDB format but will simplify future extensions. The new format, called XTDB, will be used for:

- manually editing of an XTDB file should be as easy as the current TDB format also for non-experts.
- minimize problems when using software A to read a database file written by software B.
- simplify adding features and new models for different phase dependent physical properties in the thermodynamic database.
- provide users of a database with information about the models and bibliographic references, even for encrypted databases.
- improve collaboration between users and researchers dealing with Calphad databases.
- simplify for software developers to add tags and attributes in software and databases. Such modifications should be discussed between developers and users and eventually integrated in the XTDB format.

Some software has already introduced features in the TDB file which may have been fully implemented in diffent software. Some of these are discussed in section C.3.

This XTDB definition may require minor modifications in the XML format already adoped in some software. Commercial companies providing encrypted databases to customers can use whatever format they prefer for such databases. But they should provide a facility to read and write unencrypted databases in the XTDB format.

## 1.2 The XTDB file and some more

The characters used in an XTDB file are restricted to the classical ASCII character set.

The XTDB file is divided into lines (terminated by LF (Line Feed or newline as preferred by UNIX dialects) or CRLF (Carriage Return and Line Feed as preferred by Windows)). A line should not exceed 2000 characters.

All attributes of an XML tag should fit within a line of 2000 characters and only one XML tag per line in order to be easily readable by humans. Tags nested within an XML tag may extend over several lines and the end of such a tag should appear on a separate line.

The attribute *List* of the **Constituent** tag for a gas phase in a big system may exceed 2000 characters but several **Constituent** tags can be used for the a phase.

In the examples some long tags have been separated into several line in order to be readable.

A software reading the XTBD file should ignore XML tags and attributes it does not support, preferably with a warning to the user.

An XML tag starts with "<TagName" and ends with "/>" or a longer "/TagName>" on a separte line if it contains nested tags. A tag have attributes separated by one or more spaces. An attribute name ends with an equal sign, "=" and its value is given within double quotes, """, for example Id="FE".

The XML TagName and its attributes cannot be abbreviated and are case sensitive.

The characters "<", ">" and "&" are forbidden everywhere except when used for the XML itself. One should avoid using double quotes, " "" and the equal sign "=" except when required by XML itself.

Values of attributes are separated by one or more spaces.

Database managers may be interested to add more or less temporary comments inside the database and there are two simple methods

Comments in the XML file can be added anywhere starting with "<!—" and ending with "—>". There must not be any forbidden characters inside the comment. All such comments will normally be ignored by software reading the database.

If you are not familiar with XML there are plenty of information online. In brief XML has "tags" with "attributes". The tags and attributes proposed for the XTDB format are listed in section 2 below and the attributes are explained for each tag. Several examples are provided in the text and the Appendix D has some complete XTDB files.

In this document a tag is usually in **bold** when refereced in the text and an attribute in *italics*. But I have not been totally consequent. All values of the *Id* attributes are case insensitive as they are in the TDB file. Except for phase names the value of an *Id* cannot be abbreviated when used.

An XML parser is convenient for reading XML files but to simplify the life for all the the humans reading and editing the XTDB file it is strongly recommended that the attributes to an XML tag are provided in the order listed for each tag below. Software specific attributes can be added to a tag but should come at the end.

## 1.3 How this document can be read

The following proposal is for a common definition of an XTDB file format based on XML. It can hopefully become an SGTE standard acceptable by all software groups which develop or use Calphad databases.

In section 2 all proposed tags are listed with a short explanation. In section 3 a more detailed explation are given of some tags and attributes and in section 4 some additional reflexions are listed. In the Appendix A there are several examples of tags and attributes, in Appendix B an extensive list of model tags and attributes. In Appendix C some explanations how particular thermodynamic model features can be integrated in the XTDB format including the use of wildcards and the EBEF? In Appendix D a full XTDB file for the binary Al-C and Al-Li are listed and finally in Appendix F an attempt to document recent changes in this proposal from earlier versions.

A software can easily extract randomly arranged tags from an XTDB files but for a a human reader and manual editing the XTDB file the recommended order is **Defaults, DatabaseInfo** and any **AppendXTDB** tags followed by **Element, Species** and **Phases** (with many nested tags).

The main part are the **TPfuns** and **Parameter**s, ordered by phases or by **BinarySystem** and finally the **Bibliography**. The **Model** tag and other tags at the end or an a separate file.

Using the **AppendXTDB** tag, which specifices additional files of an XTDB database, the database can be split on several files. The **Default, DatabaseInfo** and **AppendXTDB** tags and all **Element, Species** and **Phase** tags must be present in the primary XTDB file.

With a few exceptions a tag or attribute starts with a capital letter and if it consists of two or more parts, such as *NumberOf*, the second part is joined without hyphen or underscore but starts with a capital letter.

# 2 The XTDB-v0.1.2 tags and attributes with short explanations

All proposed tags for the XTDB file are listed here. Further explanations of the attributes can be found in section 3.

Some tags are optional and many of them will appear several times in the XTDB file to provide the data.

An exclamation marek "!" is indicated for the mandatory attributes of a tag.

## 2.1 The system XTDB tags

The **AppendXTDB** tag makes it possible to separate a large XTDB database on several files. There are some restrictions which types of tags can be used in such files, for example the tags for **Element, Species, Phase** are not allowed in AppendXTDB files.

| Tag | Attributes | Explanation |
|---|---|---|
| XTDB | | Containing XML tags for an XTDB database. |
| ! | Version | Version of XTDB for this file. |
| | Software | Name of software generating the database. |
| ! | Date | Year/month/day the database was written or last edited |
| ! | Signature | Name/email of person or organisation generating the database. |
| Defaults | | Optional tag to provide default values of attributes in different XML tags and some other things. Some software, as specified XTDB tag, may have some "mandatory" defaults. |
| | LowT | Default value of low $T$ limit. |
| | HighT | Default value of high $T$ limit. |
| | Bibref | Default bibliographic reference for parameters. |
| | Elements | For example "VA" and/or "/-" (the electron). |
| | RKorder | see section C.1 |
| | TernaryXpol | see section 2.8.3 |
| | GlobalModel | Any model applicable to the whole database, for example EEC [8] |
| 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 file for the XTDB database. It should contain only XTBD tags but some tags are forbidden, see above. Typically the file with the Model tag appears in this tag. |
| ! | File | File name, preferably the whole path. |
| | Description | Optional information about the file. |

Note that in this and later tables the exclamation mark at the far left side of some attributes means they are mandatory.

## 2.2 The element and species tags

All constituents of the phases must be specified as **Species** and the species are aggregates of one or more **Element** with fixed stoichiometric ratios. The vacancy, denoted "VA", is considered an element which must have activity 1 at equilibrium but cannot have a fixed amount. The electron "/-" is considered as an element and can be used as a fixed charge on a **Species**. A phase with charged species must have an extra internal condition that the phase is electrically neutral at equilibrium.

There are some strong feelinga about upper and lower case for elements and sometimes phases. As elements are only used to specify the stoichiometry of species that is not a very big thing. The species *Id* are case insensitive and the species are the constituents of the phases.

Species and phase names are used when setting conditions for a calculation and the users may not have a very sophisticated understanding when to use upper or lower case. The elements are automatically also entered as species with a case insensitive *Id*.

An iron species with positive charge have the stoichiometry "FE/+2".

One can create a species for an electron using the stoichiometry "VA/–1", or a species for a "hole" with stochiometry "VA/+1"

| Tag | Attributes | Explanation |
|---|---|---|
| Element | | Specifies a chemical element in the database. The vacancy is denoted "VA" and the electron "/-". |
| ! | Id | Chemical element symbol, one or two latters, for example FE, H. The symbol is case insensitive, see section 3.1. Fictitious element names can be used. |
| | Refstate | Name of the reference phase, for example GAS. The database may not have any data for this phase. |
| ! | Mass | Mass in g/mol |
| | H298 | Enthalpy difference between 0 and 298.15 K in the reference state. Not used in equilibrium calculations. |
| | S298 | Entropy difference between 0 and 298.15 K in the reference state. Not used in equilibrium calculations |
| Species | | Specifies a molecular like aggregate used as constituent of phases. The elements, except the electron, are also species but may be specified explicitly as such. |
| ! | Id | Species name max 24 letters and some special characters, see section 3.2. |
| ! | Stoichiometry | One or more element *Id* each followed by an unsigned real or two integers separated by a "/" representing the stoichiometric ratio, see section 3.2.1. For examples see appendix A.1. |
| | MQMQA | For a constituent in the MQMQA model. See section 3.2.2. |
| | UNIQUAC | For a constituent in the UNIQUAC model. See section 3.2.3. |

## 2.3 The function and temperature range tags

The *Id* of other **TPfun**s can be used inside the attribute *Expr* of a **Tpfun**, **Parameter** and **Parameter2** tags. Infinite loops by circular calls of **TPfun** is left for the software to detect.

See section 3.3 for the restrictions of the mathenatical expresson in the *Expr* attribute and Appendix A.2 and others for examples.

There is no way at present to handle several pressure ranges in the XTDB file. For high $P$ a separate model for the volume should be used.

The value of a function, as well as its first and second derivatives with respect to $T$ and $P$, must be continuous across an interval of $T$ range. Breakpoints will normally occur only for **TPfun** of pure element data and those in the unary 1991 have been checked.

| Tag | Attributes | Explanation |
|---|---|---|
| TPfun | | Defines a $T, P$ expression to be used in parameters or other functions. |
| ! | Id | Function name, max 16 characters, see section 3.1. The name is used in the "Expr" attribute of other functions or parameters, see section 3.3. |
| | LowT | Can be omitted if the default low $T$ limit applies. |
| ! | Expr | Simple mathematical expression terminated by ;. Use the **Trange** tag if several ranges. See section 3.3 |
| | HighT | Omitted the default high $T$ limit applies. |
| Trange | | Only inside a **TPfun** or **Parameter** tag for an expression with several $T$ ranges. |
| ! | Expr | Simple mathematical expression terminated by ;. See section 3.3. |
| | HighT | Omitted if the default high $T$ limit applies. |

## 2.4 The phase tag and some related tags

The phase tag has two "compulsory subtags" i.e. **Sublattices** and **Constituents** and several optional ones depending on the model of the phase.

| Tag | Attributes | Explanation |
|---|---|---|
| Phase | | All thermodynamic data is part of a phase. |
| ! | Id | Phase name, see sections 3.1 and 3.4.1. |
| ! | Configuration | Model for the configurational entropy, see section 3.4.2. |
| | State | G for gas phase, L for liquid phase. Only needed for the liquid if EEC is used. |
| Sublattices | | Only once inside a **Phase** tag. |
| ! | NumberOf | Number of sublattices, an integer value 1 - ?. |
| ! | Multiplicities | Sites on each sublattice, as many reals as sublattices separated by a space. For an example see Appendix A.3 |
| CrystalStructure | | Optional tag inside a **Phase** tag. |
| | Prototype | Prototype phase. |
| | PearsonSymbol | Specification. |
| | SpaceGroup | Specification. |
| | CommonName | Specification. |
| Constituents | | One for each sublattice inside a **Phase** tag. |
| | Sublattice | Omitted if only one sublattice. |
| ! | List | Species *Id* in the sublattice, separated by a space, see Appendix A.3. |
| AmendPhase | | Optional tag inside a **Phase** tag to specify for example a contribution due to a magnetic model. |
| | Model | One or more models *Id*s, separated by a space, for this phase. See section 2.8 and A.3. |
| Disordered_2Part | | Optional tag inside the **Phase** tag of an ordered phase. The Gibbs energies of the ordered and disordered parts of a phase (with identical constituents but different number of sublattices) are added according to eqs. 1 below. See also section 2.4. The configurational Gibbs energy is calculated for the ordered part only. |
| | Disordered | Optional name of the disordered phase, see section 3.4.3. |
| ! | Sum | Number of sublattices, starting from the first sublattice in the ordered phase to be summed for the disordered phase constitution. All sublattices summed must have the some set of constituents. Optionally an extra interstitial sublattice can be present. |
| Disordered_3Part | | Optional tag inside the **Phase** tag of an ordered phase. Similar to Disordered_2Part but eq. 2 below is used. |
| | Disordered | Optional name of the disordered phase, see also section 3.4.3. |
| ! | Sum | Number of sublattices, starting from the first sublattice in the ordered phase to be summed for the disordered phase constitution. All sublattices summed must have the some set of constituents. Optionally an interstitial sublattice can be present. |

For a phase with the **Disordered_2Part** tag the Gibbs energy (excluding the configurational entropy) is calculated as:

$$G_M \quad = \quad {}^{\mathrm{dis}}G_M(x) + {}^{\mathrm{ord}}G_M(y) \tag{1}$$

where $x$ is averaged values of $y$ for some (or all) sublattices in the ordered phase.

For **Disordered_3Part** the Gibbs energy equation is:

$$G_M \quad = \quad {}^{\mathrm{dis}}G_M(x) + {}^{\mathrm{ord}}G_M(y) - {}^{\mathrm{ord}}G_M(y = x) \tag{2}$$

where in the last term the sublattice fractions of the ordered phase are replaced by the disordered fractions. This means that parameters in the ordered part will have no contribution to the Gibbs energy when the phase is disordered. For details see [3] and [5]

A phase with very long list of constituents (for example GAS) can have several **Constituent** tags for the same sublattice.

## 2.5 The parameter tag

All thermodynamic data, and possibly kinetic and other physical phase dependent properties, are defined by the parameter tags. They can be arranged inside a phase tag or for all phases in a **BinarySystem** tag, see 2.9, or individually. See also sections 2.6, Appendix A.4, C and D.

| Tag | Attributes | Explanation |
|---|---|---|
| Parameter | | Specifies the $T, P$ expression of a model parameter for a set of constituents. |
| ! | Id | As in a TDB files, for example G(LIQUID,A,B:VA;2). See also the **Parameter2** tag. |
| | LowT | Can be omitted if the default low $T$ limit applies. |
| ! | Expr | Simple mathematical expression terminated by ;. If several ranges use a **Trange** tag. See section 2.3 and 3.3. |
| | HighT | Can be omitted if the default high $T$ limit applies. |
| ! | Bibref | Bibliographic reference, unless the default bibref is set. |

The attribute *Id* defines the parameter as in the current TDB file. It starts with a model parameter identifier (MPID), see Appendix B.1, followed within parenthesis by a phase name (which can be abbreviated) and one or more constituents in each sublattice of the phase in the order of the sublattices.

Constituents in the same sublattice, i.e. for interaction parameters, are separated by a comma, ",", and a colon, ":", is used to separate constitents in different sublattices. The order of sublattices and their constituents are as defined by the **Phase** tag.

After the constituents in the last sublattice a semicolon, ";" followed by a single digit, 0-9, can be used to indicate a degree. This degree can have different meanings in different models but is normally used for the power in a Redlich-Kister series, see section C.1. If the digit is zero the semicolon and the digit can be omitted.

An asterisk "*", also known as wildcard, see section C.3. can be used as constituent in a sublattice indicating that the parameter is independent of the constituents in the sublattice. The wildcard is an important feature of some models, see section C.6.

The parameters are the essential parts of the database and more examples can be found in Appendix C. They are generated from separate assessment of experimental and theoretical data for binary and higher order systems. One aim of this XTDB format is to provide a simple and unified way to publish and report such assessments. Databases are collections of such assessment and database manager may have to add or modify some parameters for compatibility with other systems. In addition to the bibliographic reference a database manager is encouraged to add comments of such actions within the **Parameter** tag in order to pass on information to the next manager of the database.

## 2.6 The elaborate parameter tag

An alternative more elaborated XML tag can be used for parameters which may be preferred by software. It is straightforward to convert from one to another. It must have a subtag, **Constarray** with one or more tags **SublConst** for each constituent in each sublattice.

| Tag | Attributes | Explanation |
|---|---|---|
| Parameter2 | | A more detailed parameter tag preferred by software. |
| | Id | As in TDB file, for example G(LIQUID,A,B:VA;2). See also the **Parameter** tag. |
| ! | MPID | Model parameter identifier, for example G or TC. |
| ! | Phase | Can be omitted inside a phase tag, otherwise the phase name. |
| | LowT | Can be omitted if the default low $T$ limit applies. |
| ! | Expr | Simple mathematical expression terminated by ;. If several ranges use a **Trange** tag. See section 2.3 and 3.3. |
| | HighT | Can be omitted if the default high $T$ limit applies. |
| ! | Bibref | Bibliographic reference. |
| ConstArray | | Only inside a **Parameter2** tag. Encloses the SublConst tags. |
| | Degree | Can be omitted if zero. See section C.1 |
| SublConst | | Only inside a **ConstArray** tag. |
| ! | Sublattice | Sublattice of constituent. |
| ! | Species | A constituent *Id*. |

The **Parameter2** tag may be preferred by software but for manual editing **Parameter** is simpler, see the appendix A.4. Both tags can be used in the XTDB file and software can easily convert between them.

If the *Id* attribute is present in a **Parameter2** tag the software should check that this *Id* is identical to the long form and report an error if not.

A wildcard, "*", see section C.3, can be used as constituent in a sublattice indicating that the parameter is independent of the constituent in the sublattice.

## 2.7 Bibliography for parameters and models.

For each parameter there must be a bibliographic reference. This can be the same for all parameters from the same source. The models also have a reference which should indicate a paper where the model is explained, see Appendix A.6.

| Tag | Attributes | Explanation |
|---|---|---|
| Bibliography | | Contains bibliographic references |
| Bibitem | | Only inside a **Bibliography** tag. |
| ! | Id | Used as value in the *bibref* attribute for a parameter or model, normally a paper or a comment by the database manager. |
| ! | Text | Reference to a paper or comment. |
| | DOI | DOI of paper where the parameter was assesses. |

## 2.8 The model tags

The XML tags for generally accepted models can be on a separate file and the model *Id* attribute is the important and used in the **AmendPhase** tag for each phase which has the model. Most models have one or more model parameter identifiers (MPID) as attributes and these are used in the **Parameter** tag for the phases. See also the Appendix B. Models must be explained in a model tag with an appropriate bibliographic reference. Typically the **Model** tag is in an AppendXTDB file.

| Tag | Attributes | Explanation |
|---|---|---|
| Models | | Contains model tags usually with an *Id* attribute used in **AmendPhase** tags inside **Phase** tahs. The models usually specify one or more model parameter identifiers (MPID) needed by the model. Some models, such as **Disordered_2Part**, must be included as tags within the **Phase** tag. |

### 2.8.1 Some frequently used model tags

The XML tags listed here should be defined inside a library of **Model** tags and its *Id* attribute is used in the **AmendPhase** tag. The models normally specify one or more model parameter identifiers (MPIDs) used in parameters needed for the model. Additional text outside the attributes can be added describing the model.

| Tag | Attributes | Explanation |
|---|---|---|
| Magnetic | | There are several magnetic models. |
| ! | Id | This is used in **AmendPhase** tag. |
| | Aff | Antiferromagnetic factor (-1, -3 or 0). It is redundant but kept for compatibility with TDB file. |
| ! | MPID1 | Specifies a magnetic model parameter identifier (MPID) for parameters. |
| ! | MPID2 | Specifies a magnetic model parameter identifier (MPID) for parameters. |
| ! | MPID3 | Specifies a magnetic model parameter identifier (MPID) for parameters. |
| ! | Bibref | Where the model is described. |
| Permutations | | For FCC, HCP and BCC lattices a 4 sublattice tetrahedron model identical permutations of a parameter will be included only once in the XTDB file. See section C.4.1. |
| ! | Id | This is used in **AmendPhase** tag. At present its value can be either FCC4PERM or BCC4PERM. |
| ! | Bibref | Where the model is explained. |

The **Permutations** tag means that a parameter which can have permutation of its constituents on idetical sites is stored only once in the database. For example in an FCC ordered phase a parameter

G(FCC_4LS,FE:AL:AL:AL:VA)

has 4 identical permutations such as G(FCC,AL:FE:AL:AL:VA) etc. 3 of which are not included in the database. Thus the size of the database can be reduced but it requires that the software calculates automatcally the contribution from all 4 permutations of the constituents of indentical sides. This can be quite complicated and instead the software may create all possible permutations and store them individually when reading the database. For a multicomponent system this can be quite a lot. See Appendix B for an example of model tags.

### 2.8.2 Models tags for new unary models

After long discussions the unary group has decided to use a single composition dependent Einstein parameter for each phase and element in the new unary database. An element with its heat capacity fitted using several Einstein $\theta$ will have the additional $\theta$ described by the GEIN function in the *Expr* attribute in the **Parameter** or **TPfun** tag, see section 3.3. See also the Al-C example in Appendix D.1.

New **Model** tags may be developed and included in the XTDB file in order to specify new MPIDs for parameters.

| Tag | Attributes | Explanation |
|---|---|---|
| Volume | | Specifies the model for volume of a phase. |
| ! | Id | This is used in the **AmendPhase** tag. |
| ! | MPID1 | Specifies a volume model parameter identifier (MPID) for parameters. |
| ! | MPID2 | Specifies volume model parameter identifier (MPID) for parameters. |
| ! | MPID3 | Specifies volume model parameter identifier (MPID) for parameters. |
| ! | Bibref | Where the model is described. |
| Einstein | | The low $T$ vibrational model. |
| ! | Id | This Id is used in **AmendPhase** tag. |
| ! | MPID1 | Specifies the Einstein model parameter identifier (MPID) for parameters. |
| ! | Bibref | Where the model is described. |
| Liquid2state | | The liquid 2-state model. |
| ! | Id | This Id is used in **AmendPhase** tag. |
| ! | MPID1 | Specifies liquid model parameter identifier (MPID) for parameters. |
| ! | MPID2 | Specifies Einstein model parameter identifier (MPID) for parameters. |
| ! | Bibref | Where the model is described. |
| EEC | | Specifies that the Equi-entropy model applies to the database. This must be implemented in the software. The liquid **Phase** tag must also have the *State* attribute equal to L. |
| ! | Id | has the value EEC. |
| ! | Bibref | Where the model is described. |

### 2.8.3 Ternary extrapolation methods

Some models are concern a subset of the constituents of a phase and they must be specified explicitly and cannot be included in the **AmendPhase** tag for the phase because they include additional information. The **Disordered_2Part** and **Disordered_3Part** models are explained together with the **Phase** tag.

The Toop, Kohler and Muggianu ternary extrapolation methods are most likely specified together with the parameters for a specific ternary. The Muggianu method is often the default ternary extrapolation model but there are other extrapolation methods to be considered and they must be integrated in the XTDB format.

| Tag | Attributes | Explanation |
|---|---|---|
| TernaryXpol | | One or more subsets of 3 constituents for which do not use the default extrapolation method of the binary compositions inside a ternary subsystem. |
| | Phase | Can be omitted if used inside a **Phase** tag. Normally this tag will appear close to the **Parameter** for which the extrapolation should be used. |
| ! | Constituents | Specifies 3 constituents of the phase sepated by spaces. |
| ! | Xmode | See below. |

Examples:

```
<TernaryXpol Phase=‘‘Liquid’’ Constituents=‘‘Fe Mn Mo’’ Xmode="KKK" />
<TernaryXpol Phase=‘‘Liquid’’ Constituents=‘‘Si Fe Mn’’ Xmode="T1T1M" />
```

Where the first ternary extrapolates use the Kohler extrapolation for all binaries. In the second the first binary, Si-Fe use Toop extrapolation with Si, the first constituent, as Toop element. The second binary, Si-Mn has also Si, the first constituent as Toop elemet and the third binary, Fe-Mn use the Muggianu extrapolation method. The *Cmode* attribute is a bit particular and explained in Appendix C.2.

## 2.9 Organizing the data and software specific attributes

Each parameter in the database has a bibliography attribute and normally a software reading the database lists the relevant bibliograpic data after extracting the data from the database or it can be listed from inside the software for calculations. The references is an important feature to assure a reliable database is used. However, the number of references for a multicomponent system with 1000 or more parameters from many assessments can be very long.

Additionally, the database manager often arranges the model parameter per system to simplify updates and this habit has resulted in introducing a new tag in the XTDB format, missing in the TDB files. This arrangement in the XTDB file has no influence on the way the software handles the parameter.

| Tag | Attributes | Explanation |
|---|---|---|
| UnarySystem | | Encloses a set of **Parameter** tags for the unary data. There can be parameters for the unary also outside this tag. |
| ! | Elements | Constituent for the parameters in the system. |
| ! | Bibref | Main bibliographic references. |
| BinarySystem | | Encloses a set of **Parameter** tags for different phases of a binary system. There can be parameters for the binary outside this tag. It may have a software dependent attribute to calculate the binary. |
| ! | Species | Two constituents for the parameters separated by spaces. |
| ! | Bibref | Main bibliographic references. |
| | CalcDia | Software specific commands to calculate the binary phase diagram. The software is specified in the **XTDB** tag. |
| TernarySystem | | Encloses a set of **Parameters** tags for different phases for a ternary system. There can be parameters for the system outside this tag. |
| ! | Species | Constituents for the parameters in the system joined by hyphens. |
| ! | Bibref | Main bibliographic references. |
| | CalcDia | Software specific commands to calculate some particular ternary diagram for the system. |

Inside a **BinarySystem** tag the **Parameter** tags for all phases assessed for the constituents in the *Species* attribute can be included. The parameters should have their own bibliographic reference. The *Bibref* for the **BinarySystem** and **TernarySystem** cab be listed when reading the database informing the user which assessed systems that are in the database.

```
<BinarySystem Species="C Co" Bibref="88FER1 97KUS 06MAR" >
  <Parameter Id="G(LIQUID,C,CO;0)"  Expr=" -107940.6+24.956*T;"  Bibref="87FER1" />
  <Parameter Id="G(LIQUID,C,CO;1)"  Expr=" -9805.5;"  Bibref="87FER1" />
  <Parameter Id="G2(B2_BCC,CO:C;0)"  Expr=" +GHSERCO+3*GHSERCC+247373.5-33.574*T;"  Bibref="88FER1" />
  <Parameter Id="G(BCC_A2,CO:C;0)"  Expr=" +GHSERCO+3*GHSERCC+247373.5-33.574*T;"  Bibref="88FER1" />
  <Parameter Id="G(CBCC_A12,CO:C;0)"  Expr=" +UN_ASS;"  Bibref="Default" />
  <Parameter Id="G(CEMENTITE_D011,CO:C;0)"  Expr=" +3*GHSERCO+GHSERCC-1567+3.963*T;"  Bibref="88FER1" />
  <Parameter Id="G(CR3C2_D510,CO:C;0)"  Expr=" +63920+794.135*T-132.57*T*LN(+T)-2.35E-05*T**2
            +1296100*T**(-1);"  Bibref="14KAP" />
  <Parameter Id="G(CUB_A13,CO:C;0)"  Expr=" +UN_ASS;"  Bibref="Default" />
  <Parameter Id="G2(FCC_4SL,CO:C;0)"  Expr=" +GHSERCO+GHSERCC+50463.8-6.849*T;"  Bibref="89FER1" />
  <Parameter Id="G(FCC_A1,CO:C;0)"  Expr=" +GHSERCO+GHSERCC+50463.8-6.849*T;"  Bibref="89FER1" />
  <Parameter Id="G(HCP_A3,CO:C;0)"  Expr=" +GHSERCO+0.5*GHSERCC+22916.5-2.855*T;"  Bibref="87FER1" />
  <Parameter Id="G(M23C6_D84,CO:CO:C;0)"  Expr=" +GCO23C6;"  Bibref="97KUS" />
  <Parameter Id="G(M7C3_D101,CO:C;0)"  Expr=" -5706.9+1408.9*T-249.28*T*LN(+T)+956820*T**(-1);"
            Bibref="06MAR" />
</BinarySystem>
```

In the *CalcDia* attribute there can be software specific instructions how to calculate a phase diagram or some other diagram. This tag can provide a user which systems are assessed in the database even for an encrypted database.

### 2.10 Adding new XML tags or attributes

The XTDB tags listed above is intened to cover all the basic modeling of thermodynamic data needed for calculations. But this set of basic XTDB tags must not prevent the development of new models and there will be new tags and attributes added in the future. But such additions can, with some care, be integrated in XTDB files without corrupting the data and information already established.

There may be a need for conditional tag in the XTDB file. Maybe this can be implemented in a software independent way, but temporarily this can be handled by software specific tags, for example if certain actions should be taken depending on the user selection of elements ot species.

| Tag | Attributes | Explanation |
|---|---|---|
| IfSpecies | | Depending on the species selected by user |
| ! | Species | If one (or more enclosed by parenthesis) species in this attribute have been selected |
| | AndSpecies | And one (or more) species in this attribute have been selected |
| | OrSpecies | Or one (or more) species in this attribute have been selected |
| ! | Do | software specific way to act if this clause is true. |

This is an tentative tag which has to be elaborated.

An example of the use of this clause consider that if Fe and Ti and C have been selected then the software should automatically create two composition sets for the FCC phase to describe the cubic carbide (maybe with a slightly modified name). The same may be useful to provide for an ordered $L1_2$ phase when reading data for the Al-Ni system from an XTDB file.

## 3 Further explanation of some tags and attributes

Note that the XML tags and attributes are case sensitive whereas the names i.e. *Id* of species, functions, phases and other identifiers are **case insensitive** as in the TDB file. For example a chemical species written FE, Fe, fe and fE is the same element. Thus CO is Cobalt and to specify the stoichiometry of carbonmonoxide one must use C1O.

Presenting information and results for a user still have limitation imposed by the size of th computer screen or peper width and it is difficult to format nice output with very long names of functions or species or phases. For a human it is also complicated to handle long names, even if they may be abbreviated.

### 3.1 About UPPER and lower characters, abbreviations and forbidden characters

In an TDB file UPPER and lower case letters are treated as identical. In XML the tags and attributes are case sensitive. In this proposal all letters A-Z of the attributes, for example the name of elements, species and phases, the UPPER and lower case letters will be considered as identical.

In particular the characters "(" and ")" are not allowed in the *Id* attribute of **Species, Phase** or **TPfun** tags. This is necessary to simplify the parsing the *Id* attribute of the **Parameter** tag and to simplify interpreting commands in the user interface of the software. The allowed characters are explained the the sections 2.2 and 2.4.

In some software using a command line user i/f one can use a command:

```
set condition y(gas,co2)=0.1
```

in order to specify that the gas phase should have the constituent fraction of $CO_2$ equal to 0.1. It could be complicated if both the phase name and species name can contain parenthesis and be abbreviated.

It is not allowed to abbreviate **Species** *Id* and **TPfun** *Id*. Note that the species *Id* is normally not its stoichiometric formula and rather short names are recommended for complex molecules. In particular "(" and ")" are not allowed in **Species** Id and **Tpfun** *Id*.

Abbreviation of **Phase** *Id* is allowed because it must be used in all the **Parameters** tags. Phase identification can be very complex with StructurBerict, Pearson symbols etc and these can be provided in separate attributes such as *CrystalStructure*. But to identify the phase in a parameter in the XTDB file it is the *Id* The rule for abbreviation is that any part of a phase name starting with an underscore can be abbreviated separately, thus two phases MONOCLINIC_A and MONOCLINIC_B can be abbreviated as M_A and M_B.

## 3.2 The Species and its attributes

The species are the constituents in the sublattices of phases. A species name (i.e. the *Id* attribute) is **case insensitive** and must start with letter A-Z and can contain letters, digits and the special characters "_", "/", "-" and "+". It must not be abbreviated when used as constituent in tags and attributes such as **Phase, Parameter** etc.

### 3.2.1 Species stoichimetry

The species stoichiometry is a sequence of one or more chemical element names, each followed by a real number specifying its stoichiometric ratio. Following the TDB standard a chemical element with a two letter name does not need a stoichiometric ratio equal to unity, for example MGO for MG1O1. A stoichiometry of unity at the end can also be ignored. **No grouping using parenthesis are allowed when specifying the stoichiometry, for example use AL2S3O12, not Al2(S1O4)3.** It may not be very elegant but nice formatting is for humans not for computers.

### 3.2.2 MQMQA attribute

The *MQMQA* attribute should contain two or more chemical element names separated a comma or a sublattice separator ":" and followed by equal number of unsigned reals representing the bond fractions, For example:

<Species Id="CSLA/F" MQMQA="CS,LA:F 9.0 6.0 4.0" />

For MQMQA clusters the stoichiometry can maybe be omitted? See also Appendix A.1. According to the MQMQA model the cluster stoichometry is calculated as 2.0 divided by the bond fractions. The MQMQA species (or cluster) is always electrically neutral. For MQMQA species that are endmembers (with one species in each sublattice) a real representing the SNN/FNN ratio, usually 2.4, must be supplied.

### 3.2.3 UNIQUAC attribute

For species in the UNIQUAC model. Contains two reals representing area and volume of the species in that order but in unspecified units.

## 3.3 Expr attribute of TPfun and Parameter

The *Id* attribute of a **TPfun** must start with a letter A-Z and may contain letters, digits and the special character "_". It must not be longer than 16 characters. It must not be abbreviated when used in other tags.

When used in an *Expr* attribute it does not have to be terminated by the hash character "#" as in current TDB files.

The mathematical expressions for $T$ and $P$ used in the *Expr* attribute in **TPfun, Trange** and **Parameter** are the same as in TDB files. It is very restricted because some software must calculate first and and second derivatives with respect to $T, P$ (and constitution). A more extended mathematical expression could be allowed for expressions which are not used for database parameters. In OC it is allowed to enter more complex expressions for post processing in batch/macro files but they are not included in the database but used in macro/batch files.

In the 1990 definition of the TDB file the type of expression allowed consists of "simple terms" such as:

[signed real number] * [**TPfun Id** ] ** [power] *T** [power] *P**[power]

where [power] is an integer (a negative power must be within parenthesis, a positive must not). No spaces allowed in a simple term. A "complex term" is a simple term multiplied with a math function (EXP, LN or GEIN) of a simple term, such as:

[simple term] *LN( [simple term] )

An *Expr* attribute in **TPfun, Trange** or **Parameter** consists one or more complex terms. A positive sign of the first term can be omitted.

The following general math functions are allowed in OC:
exp(), ln(), log(), erf(). Note that log() and ln() is the same and erf() is the error function. The number of math functions can be discussed and extended.

For the unary project the following math function can be used in the *Expr* attribute:

GEIN($\theta$) to calculate $1.5R\theta + 3RT\ln(1 - \exp(-\theta/T))$;

where the argument of GEIN should be a fitted Einstein temparature, $\theta$. In the corresponding LNTH parameter one will also use the value of $\theta$ although the software will vary the logarithm of $\theta$ with the composition as this is more reasonable physically that vary $\theta$ itself.

It is not allowed to group several terms together using parenthesis, for example "exp(5.7-3*T+2*T*LN(T))". The complex expression after "exp" must be entered as a separate **TPfun** and then used as the agrument of the exponential function. For example a square root of $T$ is entered as two **TPfun**://

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

For thermodynamic parameters the expressions are usually quite simple but for other physical properties it may be interesting to allow more elaborate expressions. However, separating a complex expression into several parts may be useful for tracing its origin and can simplify updating and calculations.

## 3.4 The phase tag and attributes

All data in the XTDB database is part of a phase. The model of a phase is a simplification of the real structure.

### 3.4.1 The phase Id

A phase name must start with a letter A-Z and have no more than 24 characters. It can contain letters, numbers and the special character "_". **The characters "(" and ")" must not be used in phase names.**

Some phases which appear in different systems with different names for example CaO (lime) and MgO (periclase) are modeled as the same phase in the database because they can form (at least theoretically) a continuous solution. Thus a more structure related phase Id is preferred in the database, for example "halite". More specific information about the phase can be provided using the **CrystalStructure** tag but it will not cover all cases for which a phase may be stable.

A phase name may be abbreviated in parameters and some other cases and thus each phase name must be unique and not an abbreviation of another phase. One must not have a phase Al2O3 and another Al2O3_BIS. Phase names has to be considered carefully when adding new assessments to a database.

### 3.4.2 The configurational entropy model

For the configurational entropy model we have CEF, I2SL, MQMQA, UNIQUAC and maybe some more. Maybe also "IDEAL" could be used when there are ideal mixing and no interactions (as in ideal gas) and maybe "REGULAR" for a phase with ideal mixing in a single lattice with one site and some excess parameters.

### 3.4.3 Using several fraction variables

The phase with a **Disordered_2Part** or **Disordered_3part** tag can have an optional attribute specifying a phase with the parameters for the disordered phase (with a different number of sublattices). The constituents of this phase on its first sublattice must be the same as in the ordered phase with this tag. A second sublattice in the disordered phase may be for interstitals, corresponding to the last sublattice in the ordered phase. This means the software must calculate a separate set of fraction variables from the ordered phase by summing the first *Sum* sublattices of the ordered phase.

$$y_i^{1,\mathrm{dis}} = \sum_{s=1}^{Sum} a_s y_i^{(s),\mathrm{ord}} \tag{3}$$

where $y_i^{(s)\mathrm{ord}}$ is the constituent fraction of $i$ on sublattice $s$ in the ordered phase and $y_i^{\mathrm{dis},1}$ the fraction of $i$ in the first sublattice of the disordered phase. $a_s$ is the number of sites on sublattice $s$ in the ordered phase.

A "disordered" phase may have an additional sublattice for interstitial constituents.

If the attribute *Disordered* is specified in the **Disordered_2Part** or **Disordered_3Part** tag, the phase specified should be hidden by the software from the list of phases as its parameters are actually a part of the ordered phase. In some software, for example OC, the disordered parameters are listed together with the ordered phase, just having a reduced number of sublattices as indicated by the attribute *Sum*.

Calculating a **Disordered_3Part** model works the same way and the idea with subtracting the "ordered" part calculated using the disordered set of fractions was to allow separate assessments of the ordered and disordered phases.

For phases which never disorder, for example the sigma phase, one can also have a "disordered" part with a single sublattice containing the species representing elements as endmembers (and possibly some long range interaction parameters). In Thermo-Calc terminology this is the "NEVER" model. See also the section for EBEF C.6.

If the attribute *Disordered* is not set the parameters for the disordered part will have the same phase as those for the ordered part in the **Parameter** tag but a reduced number of sublattices.

Parameters in the ordered part of a phase with **Disordered_3Part** or **Disordered_2Part** have constituents in as many sublattices as defined for the phase. In the disordered part the number of sublattices is given by the attributes *NumberOf* for the phase subtracted by (*Sum*+1) in the **Disordered_xPart** tag. Thus for a BCC phase with 5 sublattice a parameter tag:

```
<Parameter Id="G(BCC_4SL,FE:FE:AL:AL:VA)" Expr="-3*UBCCFEAL" Bibitem="09Sun" />
```

indicates a parameter in the ordered BCC phase with 4 sublattices for ordering whereas a parameter for the same phase but only 2 sublattices:

```
<Parameter Id="G(BCC_4SL,FE:VA)" Expr="GHSERFE" Bibitem="91Din" />
```

indicares a parameter in the disordered BCC phase because the value of *Sum* is 4 in this case. Alternatively all parameters in the disordered part can be entered as a separate phase specified by the *Disordered* attribute.

See also the section on wildcards C.3 when dealing with phases witn many sublattices.

It is unfortunate we did not start to use XML 20 years ago, we could have avoided some of these complications.

### 3.5 The use of the Parameter tag

An XTDB database will consist mainly of **Parameter** tags, defined in 2.5, and expanations of its use depend very much on the models used are are detailed explainations can be found in Appendix C

## 4 A few more points

1. The GEIN function can be used in the attribute *Expr* of a **Parameter** or a **TPfun**.

   If a pure element modeled with several Einstein $\theta$ only with different weight factors (the sum of which is unity), one of these, normally that with the highest weight, is selected to vary with composition, as $\ln(\theta)$, using the model parameter identifier LNTH. A GEIN function is needed also for the selected $\theta$ with (weight-1.0) as factor.

2. The ternary extrapolation method revised. An attribute *TernaryXpol* added to the **Defaults**.

3. The **Elements** should automatically by considered as species but there is no error to include them also in the list of species.

4. The model parameter identifier "L" can be used for interaction Gibbs energies.

5. If a **TPfun** or **Parameter** is calculated outside its defined $T$ range the value calculated should use the expression in the range closest below or above the actual $T$.

6. The use of wildcards have not been defined outside users of Thermo-Calc and OpenCalphad. The definition is found section C.3.

7. Based on the XTDB format one may create additional facilities for example a program to list the parameters in a nice format for publishing using LaTeX or Word. Papers publishing assessments should provide them in the XTDB format as supplementary material.

8. We should agree on a list of MPID and how to handle software specific MPIDs. There will be several MPID which kinetic and other properties which does not concern the thermodynamic data but they should anyway be included as MPIDs.

9. The formal XTDB definition should be written as an XML file. Who can do that?

### 4.1 Error handling

One of the reasons developing a new format for thermodynamic databases was that TDB files generated by one software could not be read by another software without some sophistacated editing. The reason was normally obscure but could often be fixed by moving some lines around or adding a comma or semicolon.

With the XTDB format this should be less of a problem but any software designed to read an XTDB file should have some error handling facilities. Typical problems could be

- Models which are not implemented.
- Software specific MPID or abbreviations of some MPID.

As always the software should try to report where the error occured before crashing to allow a user to handle the problem.

## 5 Summary

There are certainly many more things to take care of but I think it is more important to agree very soon on a minimum common XTDB format which can make the thermodynamic databases more useful both for experimentalists, assessments, database maintenance and thermodynamic software, in particular for the development of new models and applications.

We can take one step at a time but be careful to to set limits for future extensions. Many different kinds of physical data for materials will probably be added to this XTDB format.

## References


[1] Mats Hillert, Caphad, **4**, (1980), pp 1–12

[2] A Dindsdale, Calphad, **15**, (1991), 317–425

[3] Ibrahim. Ansara, Nathalie Dupin, Hans Leo Lukas and Bo Sundman, J All and Comp, **247** (1997) pp 20–30

[4] B Sundman, S G Fries and A Oates, (1998) Calphad

[5] Bengt Hallstedt, Nathalie Dupin, Mats Hillert, Lars Höglund, Hans Leo Lukas, Julius C. Shuster and Nuri Solak, Calphad, **31** (2007) pp 28–37.

[6] Arthur D Pelton, Calphad **25** (2001) pp 319–328

[7] Nathalie Dupin, Ursula R Kattner, Bo Sundman, Mauro Palumbo and Suzana G Fries, J Res NIST, **123**, (2018) doi:10.6028/jres.123.020

[8] Bo Sundman, Ursula R. Kattner, Mats Hillert, Malin Selleby, John Ågren, Sedigheh Bigdeli, Qing Chen, Alan Dinsdale, Bengt Hallstedt, Alexandra Khvan, Huahai Mao, Richard Otis, Calphad, **68** (2020) 101737

Some features listed above have not been implemented in the examples.

# Appendix A Some examples

In the OC software I have now implemented a command to write an XTDB file (maybe not exactly identical to this definition as I am modifying details). In this Appendix I enclude som exmples.

Developing routines to read an XTDB file is more complicated and I prefer to wait until there is a general agreement on the XTB format.

## A.1 Chemical elements and species.

The way to define MQMQA constituents and stoichiometry is tentative.

```
  <Element Id="/-" Refstate="ELECTRON_GAS" Mass="  0.000000E+00" />
  <Element Id="VA" Refstate="VACUUM" Mass="  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" />
  <Species Id="AL2FE" Stoichiometry="AL2/3FE1/3" />
  ...
  <Species Id="LA/F" Stoichiometry="LA1/3F1" MQMQA="LA:F 6.0 2.0 2.4" />
  <Species Id="LACS/F" MQMQA="LA,CS:F 9.0 6.0 4.0" />
```

The stoichiometry of the MQMQA species is calculated from the bond ratios according to the model. The *MQMQA* attribute for an "endmember" also include a factor, SNN/FNN, needed in the configurational entropy expression.

Note that **species names must not be abbreviated as constituents in phases or parameters** and thus one can have species names which are abbreviations of another species name. For example "C1O" and "C1O2".

## A.2 Defaults, TPfun and Trange

Using default $T$ limits the function are not much more complex than in the TDB file.

```
  <Defaults LowT="298.15" HighT="6000" Bibref="U.N.Known" Elements="VA /-" />
...
  <TPfun Id="GHSERAL"  >
    <Trange HighT="700" Expr=" -7976.15+137.093038*T-24.3671976*T*LN(T)-.001884662*T**2-8.77664E-07*T**3+74092*T**(-1);"
    <Trange HighT="933.47" Expr=" -11276.24+223.048446*T-38.5844296*T*LN(T)+.018531982*T**2  -5.764227E-06*T**3+74092*T**
    <Trange HighT="2900" Expr=" -11278.378+188.684153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9);" />
  </TPfun>
...
  <TPfun Id="LFALFE0"  Expr="-104700+30.65*T;" />
  <TPfun Id="LFALFE1"  Expr="+30000-7*T;" />
  <TPfun Id="LFALFE2"  Expr="+32200-17*T;" />
  <TPfun Id="UFALFE"  Expr="-4000+T;" />
```

```
  <TPfun Id="GAL3FE"  Expr="+3*UFALFE+9000;" />
  <TPfun Id="GAL2FE2"  Expr="+4*UFALFE;" />
...
  <TPfun Id="G0SERCC"  Expr=" -17752.213+GTSERCC;" />
  <TPfun Id="GEINGRACC"  Expr=" -0.5159523*GEIN(+7.57725)+0.121519*GEIN(+6.10479)+0.3496843*GEIN(+6.8533)
        +.0388463*GEIN(+5.26269)+.005840323*GEIN(+4.166667);" />
```

## A.3 Phase

Entering phases in the XTDB file is a bit more complex but we have get rid of the TYPE_DEFINITION. It is not so nice to use CEF for the liquid, that is why I think RKM might be a nice option for a liquid model without sublattices and maybe **Sublattices** can be omitted?

```
 <Phase Id="LIQUID" Configuration="RKM" state="L" >
    <Sites NumberOf="1"  Multiplicities="1" >
      <Constituents List="AL C" />
    </Sites>
    <AmendPhase Model="LIQ2STATE" />
  </Phase>
...
  <Phase Id="A2_BCC" Configuration="CEF" state="S" >
    <Sites NumberOf="2"  Multiplicities="1  3" >
      <Constituents Sublattice="1" List="AL FE" />
      <Constituents Sublattice="2" List="VA" />
    </Sites>
    <AmendPhase Model="IHJBCC" />
  </Phase>
...
  <Phase Id="AL8FE5_D82" Configuration="CEF" state="S" >
    <Sites NumberOf="2"  Multiplicities="8  5" >
      <Constituents Sublattice="1" List="AL FE" />
      <Constituents Sublattice="2" List="AL FE" />
    </Sites>
  </Phase>
...
  <Phase Id="BCC_4SL" Configuration="CEF" state="S" >
    <Sites NumberOf="5"  Multiplicities="0.25  0.25  0.25  0.25  3" >
      <Constituents Sublattice="1" List="AL FE" />
      <Constituents Sublattice="2" List="AL FE" />
      <Constituents Sublattice="3" List="AL FE" />
      <Constituents Sublattice="4" List="AL FE" />
      <Constituents Sublattice="5" List="VA" />
    </Sites>
    <Disordered_3Part Disordered="A2_BCC" Sum="4" Bibref="09Sun" />
    <AmendPhase Model="IHJBCC BCC4Perm" />
  </Phase>
...
  <Phase Id="SIGMA" Configuration="CEF" State="S" >
    <Sites NumberOf="5" Multiplicities="2 4 8 8 8" >
      <Constituents Sublattice="1" List="MO RE" />
      <Constituents Sublattice="2" List="MO RE" />
      <Constituents Sublattice="3" List="MO RE" />
      <Constituents Sublattice="4" List="MO RE" />
      <Constituents Sublattice="5" List="MO RE" />
    </Sites>
```

```
    <Disordered_2Part Sum="5" />
  </Phase>
```

Abbreviation of phase names is allowed and thus one cannot have a phase with a name which is an abbreviation of another phase name. Phase names can be abbreviated for each part separated by an underscore, "_". A phase name "AL_X" is thus an abbreviation of "AL2_X".

## A.4 The Parameter tag

```
    <Parameter Id="G(A2_BCC,FE:VA;0)"   Expr="+GHSERFE;" Bibref="91Din" />
    <Parameter Id="TC(A2_BCC,FE:VA;0)"   Expr="1043;" Bibref="91Din" />
    <Parameter Id="BMAGN(A2_BCC,FE:VA;0)"   Expr="2.22;" Bibref="91Din" />
    <Parameter Id="G(AL8FE5_D82,AL:AL;0)"   Expr="+13*GALBCC;" Bibref="08Sun" />
...
    <Parameter Id="G(BCC_4SL,AL:AL:FE:FE:VA;0)"   Expr="+GB2ALFE;" Bibref="08Sun" />
    <Parameter id="G(BCC_4SL,AL,FE:*:*:*:VA;1)"   Expr="-634+0.68*T;" Bibref="08Sun" />
```

In the last parameter above the "wildcard" or asterisk, "*", is used for species in three of the sublattices and it means that the parameter is independent of the constituents in these sublattices. See the discussion in section C.3 how this is treated.

## A.5 The Parameter2 tag

Using the **Parameter2** tag the last two parameters above are:

```
    <Parameter2 Id="G(BCC_4SL,AL:AL:FE:FE:VA;0)" Expr="+GB2ALFE;" Bibref="08Sun" MPID="G" Phase="BCC_4SL" >
       <ConstArray Degree="0">
           <SublConst Sublattice=="1" Species="AL" />
           <SublConst Sublattice=="2" Species="AL" />
           <SublConst Sublattice=="3" Species="FE" />
           <SublConst Sublattice=="4" Species="FE" />
           <SublConst Sublattice=="5" Species="VA" />
       </ConstArray>
    /Parameter2>
...
    <Parameter2 id="G(BCC_4SL,AL,FE:*:*:*:VA;1)" Expr="-634+0.68*T;" Bibref="08Sun" MPID="G" Phase="BCC_4SL" >
       <ConstArray Degree="1">
           <SublConst Sublattice=="1" Species="AL" />
           <SublConst Sublattice=="1" Species="FE" />
           <SublConst Sublattice=="2" Species="*" />
           <SublConst Sublattice=="3" Species="*" />
           <SublConst Sublattice=="4" Species="*" />
           <SublConst Sublattice=="5" Species="VA" />
       </ConstArray>
    /Parameter2>
```

TCSAB worry that the XTDB format will increase the size of their databases which are already very big. This kind of parameter record will make them much bigger.

## A.6 Models

An extended form of the **Models** tag including references should be provided by SGTE as general **AppendXTDB** file with the tags for all generally accepted models including *Id* and all *MIPID* and detailed description. But the models used in an XTDB file can also appear in a short form as below.

```
<Models>
  <Magnetic Id="IHJBCC"  MPID1="TC" MPID2="BMAGN" Bibref="82Her" />
  <Magnetic Id="IHJREST"  MPID1="TC" MPID2="BMAGN" Bibref="82Her" />
  <Einstein Id="GEIN" MPID1="LNTH" bibref="01Che" />
  <Liquid2state Id="LIQ2STATE" MPID1="G2"  MPID2="LNTH" bibref="14Becker" >
     <!-- Unified model for the liquid and the amorphous state treated as an Einstein solid -->
  </Liquid2state>
  <Volume Id="VOLOWP" MPID1="V0"  MPID2="VA" MPID3="VB" bibref="05Lu" />
...
</Models>
...
<TernaryXpol Phase="Liquid" Constituents"Si Fe Cr" Xmode=T1T1K" />
```

The **TernaryXpol** tag can appear anywhere in the XTDB file, even within the **Phase** tag but, most likely together with the **Parameter** tags from an assessment of a ternary system in order to simplify editing a large XTDB file.

The **Disordered_2Part** or **Disordered_3Part** in section A.3 must appear within a **Phase** tag for the ordered phase.

# Appendix B An attempt to summarize model tags and MPIDs.

For the agreed models these are not needed explicitly in the database.

For models that are not trivial an extended description of the model and its model parameter identifiers (MPIDs) should be provided as an **AppendXTDB**.

```
<Models>
<!-- This is a short explanation of XTDB model tags and their attributes, the models for except for
the configurational entropy.
The AmendPhase tag (nested inside a Phase tag) is used to specify some additional models for the phase
by using the attribute "Id" specified for most of the models below.
In these model tags there are model parameter identifiers (MPID) describing the dependence on composition, T and P.
A Disordered_2Part or Disordered_3Part tag must be nested inside the Phase tag as it has additional information.
The TenaryXpol tag will normally appear together with model parameters for the binaries and has thus a phase attribute.
The EEC tag is global for the whole database if included.
Some model tags and MPIDs are tentative and some attributes of the tags are optional. -->
<Magnetic Id="IHJBCC" MPID1="TC" MPID2="BMAGN" 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 G=f(TAO)*LN(BMAGN+1) where TAO=T/TC.  Aff is the antiferromagnetic factor.
  TC is a combined Curie/Neel T and BMAGN the average Bohr magneton number. -->
</Magnetic>
<Magnetic Id="IHJREST"  MPID1="TC" MPID2="BMAGN" 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 G=f(TAO)*LN(BMAGN+1) where TAO=T/TC.  Aff is the antiferromagnetic factor.
  TC is a combined Curie/Neel T and BMAGN the average Bohr magneton number. -->
</Magnetic>
<Magnetic Id="IHJQX" MPID1="CT" MPID2="NT" MPID3="BMAGN" Aff=" 0.00" Bibref="01Che 12Xio" >
  <!-- 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);
  in G=f(TAO)*LN(BMAGN+1) where TAO=T/CT or T/NT.  Aff is a (redundant) antiferromagnetic factor.
  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" >
  <-- 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. -->
</Einstein>
<Liquid2state Id="LIQ2STATE" MPID1="G2"  MPID2="LNTH" Bibref="88Agr 13Bec" >
  <!-- Unified model for the liquid and the amorphous state which is treated as an Einstein solid.
  The G2 parameter describes the stable liquid and the transition to the amorphous state and
  LNTH is the logarithm of the Einstein THETA for the amorphous phase. -->
</Liquid2state>
```

continued on next page

```
<Volume Id="VOLOWP" MPID1="V0"  MPID2="VA" MPID3="VB" Bibref="05Lu" >
  <!-- The volume of a phase as function of T, moderate P and constitution via the model parameters:
  V0 is the volume at the reference state, VA is the integrated thermal expansion and VB is the isothermal
  compressibilty at 1 bar. -->
</Volume>
<Disordered_2Part Disordered=" " Sum=" " 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. -->
</Disordered_2Part>
<Disordered_3Part Disordered=" " Sum=" "
  <!-- In this model the Gibbs energy of the ordered phase is calculated a second time using the disordered fractions
  and subtracted.
  Some software has no special disordered phase but all parameters are stored in the ordered one and
  the parameters for the disordered phase has and fewer number of sublattices. -->
</Disordered_3Part>
<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. -->
</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. -->
</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=" " Xmode=" "  Bibref="01Pel" >
   <!-- The ternary extrapolation of the binary parameters is modified.
   The following Types are recognized: Muggianu, Kohler, Toop and ToopM -->
</TernaryXpol>
<EBEF Id="EBEF" Bibref="18Dup" >
   <!-- The Effective Bond Energy Formalism for phases with multiple sublattices using wildcards, "*", in the
   parameters for sublattices with irrelevant constituents.
   The parameters may also use the short form "constituent@sublattice" in order to specify only the constituents
   in sublattices without wildcards.  It also requires the Disordered_2Part model. -->
</EBEF>
</Models>
<Bibliography>
  <Bibitem Id="82Her" Text="S. Hertzman and B. Sundman, A Thermodynamic analysis of the Fe-Cr system,' Calphad, Vol 6 (
  <Bibitem Id="88Agr" Text="J. Agren, Thermodynmaics of supercooled liquids and their glass transition, Phys Chem Liq,
  <Bibitem Id="97Ans" Text="I. Ansara, N. Dupin, H. L. Lukas and B. Sundman, Thermodynamic assessment of the Al-Ni syst
  <Bibitem Id="01Che" Text="Q. Chen and B. Sundman, Modeling of Thermodynamic Properties for BCC, FCC, Liquid and Amorp
  <Bibitem Id="01Pel" Text="A. D. Pelton, A General Geometric Thermodynamic Model for Multicomponent  solutions, Calpha
  <Bibitem Id="05Lu" Text="X.-G. Lu, M. Selleby B. Sundman, Implementation of a new model for pressure dependence of co
  <Bibitem Id="07Hal" Text="B. Hallstedt, N. Dupin, M. Hillert, L. Hoglund, H. L. Lukas, J. C. Schuster and N. Solak, C
  <Bibitem Id="09Sun" Text="B. Sundman, I. Ohnuma, N. Dupin, U. R. Kattner and S. G. Fries, An assessment of the entire
  <Bibitem Id="12Xio" Text="W. Xiong, Q. Chen, P. A. Korzhavyi and M. Selleby, An improved magnetic model for thermodyn
  <Bibitem Id="13Bec" Text="C. A. Becker, J. Agren, M. Baricco, Q Chen, S. A. Decterov, U. R. Kattner, J. H. Perepezko,
  <Bibitem Id="18Dup" Text="N. Dupin, U. R. Kattner, B. Sundman, M. Palumbo and S. G. Fries, Implementation of an Effec
  <Bibitem Id="20Sun" Text="B. Sundman, U. R. Kattner, M. Hillert, M. Selleby, J. Agren, S. Bigdeli, Q. Chen, A. Dinsda
</Bibliography>
```

## B.1 Model parameter identifier, MPID

An MPID must start with a letter A-Z and contain letters and digits and not exceed 8 charactes. It cannot be abbreviated. In OpenCalphad some are defined, see Appendix B.1 but there should be a reserved list also for future MPIDs to avoid that different software use the same for different things.

The letter "&", frequently used for mobility parameters, is forbidden in XML but it can be replaced by some other character, using "&" seems clumsy. The special character "#" is already used by software to identify composition sets, i.e. miscibility gaps or order/disorder sets of a phase or sublattice number.

At present the MPID "G" is the Gibbs energy, TC Curie $T$, BMAGN the Bohr magneton number etc. An MPID must not be abbreviated in a parameter. Different software may use different MPID if they are well defined.

The degree in a binary excess model parameter defines the power used for the composition dependence in a binary Redlich-Kister polynomial. For higher order excess models see section C.1.

The model parameter identifier "L" is frequently used for interaction Gibbs energies, this or "G" can be accepted. But the should be an error to use "L" for a Gibbs energy of an endmember.

Some of the model parameter identifiers used in OC are listed in Table 1. In OC a parameter for a disordred part of a **Disordered_2Phase** or **Disordered_3Part** use the same phase name and simply has fewer sublattices.

Table 1: Current set of model parameter identifiers in OC. For each parameter it is indicated if it can depend on $T$, $P$ or have an extra constituent specification. Most of them have no associated code.

| Indx | Ident | T | P | Specification | Status | Note |
|---|---|---|---|---|---|---|
| 1 | G | T | P | | 0 | Gibbs Energy |
| 2 | TC | - | P | | 2 | Combined Curie/Neel T |
| 3 | BMAG | - | - | | 1 | Average Bohr magneton number |
| 4 | CTA | - | P | | 2 | Curie temperature |
| 5 | NTA | - | P | | 2 | Neel temperature |
| 7 | LNTH | - | P | | 2 | Einstein temperature |
| 8 | VO | - | - | | 1 | Volume at TO, PO |
| 9 | VA | T | - | | 4 | Thermal expansion |
| 10 | VB | T | P | | 0 | Bulk modulus |
| 12 | VS | T | P | | 0 | Diffusion volume parameter |
| 13 | MQ | T | P | &<constituent#sublattice>; | 10 | Mobility activation energy |
| 14 | MF | T | P | &<constituent#sublattice>; | 10 | RT*ln(mobility freq.fact.) |
| 15 | MG | T | P | &<constituent#sublattice>; | 10 | Magnetic mobility factor |
| 16 | G2 | T | P | | 0 | Liquid two state parameter |
| 19 | LPX | T | P | | 0 | Lattice param X axis |
| 20 | LPY | T | P | | 0 | Lattice param Y axis |
| 21 | LPZ | T | P | | 0 | Lattice param Z axis |
| 23 | EC11 | T | P | | 0 | Elastic const C11 |
| 24 | EC12 | T | P | | 0 | Elastic const C12 |
| 25 | EC44 | T | P | | 0 | Elastic const C44 |
| 26 | UQT | T | P | &<constituent#sublattice>; | 10 | UNIQUAC residual parameter (OC) |
| 27 | RHO | T | P | | 0 | Electric resistivity |
| 28 | VISC | T | P | | 0 | Viscosity |
| 29 | LAMB | T | P | | 0 | Thermal conductivity |
| 30 | HMVA | T | P | | 0 | Enthalpy of vacancy formation (MatCalc) |

# Appendix C The Parameter tag and how it relates to models

A **Parameter** *Id* attribute defined in section 2.5 starts with a model parameter identifier, MPID, see Appendix B.1. Then follows an opening paramthesis, "(", and a **Phase** *Id* and a comma and the constituents as a list of **Species***Id* separated by commas, "," or colon ":" depedning on the model for the phase and the composition dependence of the parameter. After the last constituent there is either just a closeing parenthesis, ")", or a semicolon, ";", followed by a single digit, called the degree, and a closing parenthesis. Below is an example of a reciprocal parameter in FCC_4SL:

```
<Parameter Id="G(FCC_4SL,Au,Cu:Au:Au,Cu:Cu;0)" Expr="..." Bibref="..." />
```

The reason for this rather complex parameter name is to specify the position of the model parameter in a sometimes quite complex mathematical model. In most cases the MPID refers to a Gibbs energy but there are MPID representing magnetic properties, mobilities, Einsten $\theta$ etc. In the explanation below how the **Parameter** *Id* referes to the mathermatical model for the phase will only use the Gibbs energy MPID but all properties represented by different MPID can have the same composition dependence.

The $T$ and $P$ dependence is described by the *Expr* attribute explained in section 3.3.

## C.1 Excess model parameters and degree

There has been a large number of excess parameters models proposed during (and even before) the 50 years of Calphad development. Most of them can be converted between each other or are obsolete. The excess parameter represent an bond energy between two or more different elements which are present in the same sublattice. If there are several sublattices this energy also depends on the surroundings, i.e. one must specify the constituents on all sublattices for the parameter.

There are also parameters which take into accound the simultaneous mixing of two or more elements on two or more sublattices. In fact the CEF model allows simultaneous interaction of all constituents on all sublattices. Recently that has been explored to handle interactions on intermetallic phases with many sublattices, see section C.6, using also the wildcard feature in C.3.

### C.1.1 The binary Redlich-Kister model

Only the Redlich-Kister binary excess model is allowed. Any other binary excess moldel can always be transformed into a Redlich-Kister model. A phase can have different ternary extrapolation methods, see section 2.8.3. The parameters for a Redlich-Kister expression for interaction on a sublattice $s$:

$$\Delta\, {}^{\mathrm{RK}}G_{\mathrm{AB}} \quad = \quad y_{s,\mathrm{A}} y_{s,\mathrm{B}} \sum_{\nu=0}^{n} (y_{s,\mathrm{A}} - y_{s,\mathrm{B}})^{\nu} \cdot \; {}^{\nu}L_{\mathrm{A,B}} \tag{C1}$$

where $\nu$ is known as the degree. Normally $\nu \leq 3$ and the parameters would be in the XTDB file:

```
<Parameter Id="G(LIQUID,A,B;0)" Expr="..." Bibref="..." />
<Parameter Id="G(LIQUID,A,B;1)" Expr="..." Bibref="..." />
<Parameter Id="G(LIQUID,A,B;2)" Expr="..." Bibref="..." />
```

In the binary Redlich-Kister series for a system A-B the composition dependence depend on the difference $(y_{s,\mathrm{A}} - y_{s,\mathrm{B}})^n$, in sublattice $s$ and $n$ is known as the degree. The order of the species in the fraction difference is by default alphabetical but there is a *RKorder* attribute in the **Defaults** tag to change the default and use the "actual" order the constituents are specified in the model parameter, for example L(liquid,C,A;1) would mean to use the difference $(x_{\mathrm{C}} - x_{\mathrm{A}})$ and not $(x_{\mathrm{A}} - x_{\mathrm{C}})$.

### C.1.2 The ternary excess model

For ternary parameters Hillert [1] has proposed a symmetric ternary composition dependent parameter L(PHASE,A,B,C;0..3):

$$\Delta^{\rm H3}G_{\rm ABC} = x_{\rm A}x_{\rm B}x_{\rm C}(v_{\rm A}\ {}^0L_{\rm A,B,C} + v_{\rm B}\ {}^1L_{\rm A,B,C} + v_{\rm C}\ {}^2L_{\rm A,B,C}) \quad \text{(C2)}$$

where

$$v_{\rm A} = (1 + 2x_{\rm A} - x_{\rm B} - x_{\rm C})/3 \quad \text{(C3)}$$
$$v_{\rm B} = (1 + 2x_{\rm B} - x_{\rm C} - x_{\rm A})/3 \quad \text{(C4)}$$
$$v_{\rm C} = (1 + 2x_{\rm C} - x_{\rm A} - x_{\rm B})/3 \quad \text{(C5)}$$

where the advantage of using $v$ is that the sum of them is always unity and thus avoids any unintended skewness when extrapolating to higher order system. In TC and OC a single ternary parameter with zero degree means no composition dependence, and in order to have a composition dependence parameters for all 3 degrees must be given even if one or two of them are zero.

```
<Parameter Id="G(LIQUID,A,B,C;0)" Expr="..." Bibref="..." />
<Parameter Id="G(LIQUID,A,B,C;1)" Expr="..." Bibref="..." />
<Parameter Id="G(LIQUID,A,B,C;2)" Expr="..." Bibref="..." />
```

### C.1.3 The reciprocal model for phases with sublattices

In the sublattice model one can have independent binary and ternary excess interaction on each sublattice. One can also have simultaneous interaction on two or more sublattices, and the so-called reciprocal parameter signifies interaction with two constituents on two sublattices. This parameter has an important physical significance for the thermodynamics and can approximate short range ordering [4].

$$\Delta^{\rm reci}G_{\rm AB:CD} = y_{1,\rm A}y_{1,\rm B}y_{2,\rm C}y_{2,\rm D}L_{\rm A,B:C,D} \quad \text{(C6)}$$

There is also a composition dependence proposed for reciprocal parameters such as L(PHASE,A,B:C,D;0..3) which I think is:

$$\Delta^{\rm reci}G_{\rm AB:CD} = y_{1,\rm A}y_{1,\rm B}y_{2,\rm C}y_{2,\rm D}(\ {}^0L_{\rm A,B:C,D} + (y_{1,\rm A} - y_{1,\rm B})\ {}^1L_{\rm A,B,C} + (y_{2,\rm C} - y_{2,\rm D})\ {}^2L_{\rm A,B,C}) \quad \text{(C7)}$$

```
<Parameter Id="G(BCC_A2,A,B:C,D;0)" Expr="..." Bibref="..." />
<Parameter Id="G(BCC_A2,A,B:C,D;1)" Expr="..." Bibref="..." />
<Parameter Id="G(BCC_A2,A,B:C,C;2)" Expr="..." Bibref="..." />
```

If the degree is zero the semicolon and degree can be omitted.

## C.2 Ternary extrapolation methods

In the Muggianu exgrapolation method the binary compositions are used inside the ternary system without any modifications, see Fig. C1 a). For the Kohler and Toop methods the compositions used for the binay contribution must be adjusted according to the extrapolation method. The method to handle differebt kinds of ternary extrapolations have been explained by Pelton [6] but they are rarely used. At present it is not possible to have different ternary extrapolations on different sublattices. For more details see Appendix C.2.

The ternary extrapolation in a multicomponent system can be different for each ternary combination. In some software one groups the constituents in different groups and if all 3 are in the same group the software

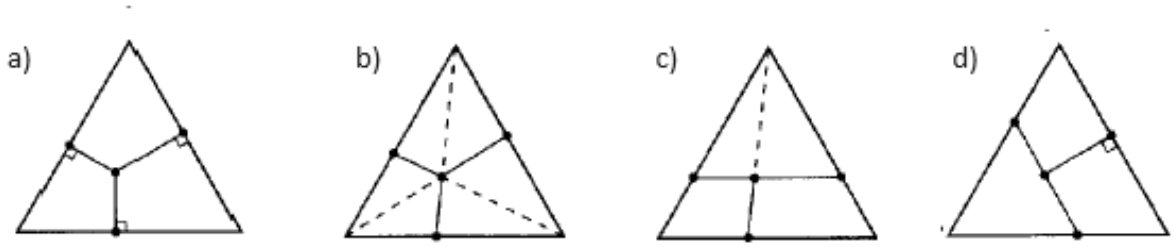


Figure C1: Various ternary extrapolation methods, the Muggianu in a), the Kohler in b), the Toop together with Kohler in c) and Toop together with Muggianu in d). More complex extrapolations can be defined if necessary.

use Kohler extrapolation, if one is different from the other two that constituent is considered as Toop element and use a Toop extrapolation of the binaries with that constituent and Kohler for the binary without the Toop element.

In the XTDB there are no groups but for each ternary comination of constituents one can specify the extrapolation of each ternary

```
<TernaryXpol Phase="LIQUID" Constituents="Fe Cr Ni" Xmode="MMM" />
<TernaryXpol Phase="LIQUID" Constituents="Fe Si Ni" Xmode="T2KT2" />
```

In the *Xmode* attribute the letters K, M and T are usef for Kohler, Muggianu and Toop extrapolation. The letters are in the order of the constituents forming the binaries: 1-2, 1-3 and 2-3. For a Toop extrapolation from a binary one must identify the Toop constituent by its order in the *Constituents* attribute.

A more compact way can be found, for example to use only numbers and for each binary use 0 if it extrapolates as Muggianu or the index of the ternary constituent if it extrapolates as Kohler or if the binary extrapolates as Toop use the constituent index of the Toop constituent. Thus "321" means all 3 binaries extrapolates as Kohler. If a binary extrapolates as Toop its constituent index is used for the binary, thus "222" means the same as "T2KT2" above.

## C.3 The use of wildcards for constituents in parameters

In some parameters a asterisk, "*", also known as wildcard is used to indicate the parameter is independent of the constituent in this sublattice. For example if one has:

```
<Parameter Id="G(C14,A,B:*)" Expr="-10000" Bibref="someone" />
<Parameter Id="G(C14,A,B:C)" Expr="+30000" Bibref="someone" />
<Parameter Id="G(C14,A,B:D)" Expr="-20000" Bibref="someone" />
```

When reading such a set of parameters from a database some software just added the wildcard parameters to the other two. That is mathematically correct but for more complex cases with wildcards in several sublattices it will be wrong. The parameter with the wildcard must be kept as a an individual parameter, independent of the constituents in that sublattice. The reason for this is explained in the sections C.4 and C.6.

## C.4 Modeling order/disorder transitions

Phases with very simple lattices such as BCC, FCC and HCP can have order/disorder transitions which are important for their properties and must be modeled correctly. The ordering means that a set of sites which have identical constitution in the disordered phase can tranform to a state with different constitutions on "identical" sublattices, for example BCC_A2/B2/$D0_3$/B32 or FCC_A1/$L1_2$/$L1_0$. Such order/disorder transition in multicomponent systems can be correctly calculated using sublattices with approximate Short Range Ordering (SRO) using a reciprocal parameter explained in section C.1.3. This means one must use models with 2 or 4 sublattices which, in the disordered state, are identical. To simplify the modeling of such phases the **Disordorderd_2Part** and **Disordorderd_3Part** tags were developed.

The Gibbs energy description of the disordered phase, ${}^{\rm dis}G_M$ in eq. 1 include all the endmember parameters for the constituents. If the disordered phase is stable for a significant composition and temperature ranges there can be parameters describing this in ${}^{\rm dis}G_M$. In ${}^{\rm ord}G_M$ all endmembers with the same constituent in all sublattices are zero because those values are in ${}^{\rm dis}G_M$. The endmember parameters in ${}^{\rm ord}G_M$ has two or more different constituents and represent the bond energy between constituents on different sublattices.

These phases can use the **Disordered_3Part** model if the disordered phase can be assessed independently from the ordered one. But there are still a large number of endmembers to assess for the ordered part and many of them represent identical configurations. This lead the the permutation model described in the next section.

### C.4.1 Permutation of parameters in ordered phases

Using 4 sublattices to decribe the ordered FCC phase means that many of the parameters are identical, for example

$$G^{\rm FCC}_{\rm A:A:A:B} = G^{\rm FCC}_{\rm A:A:B:A} = G^{\rm FCC}_{\rm A:B:A:A} = G^{\rm FCC}_{\rm B:A:A:A} \quad \text{(C8)}$$

$$G^{\rm FCC}_{\rm A:A:B:B} = G^{\rm FCC}_{\rm A:B:B:A} = G^{\rm FCC}_{\rm B:B:A:A} = G^{\rm FCC}_{\rm B:A:A:B} = G^{\rm FCC}_{\rm B:A:B:A} == G^{\rm FCC}_{\rm A:B:B:A} \quad \text{(C9)}$$

because the B atom has exactly the same environment independent of which of the 4 sublattices it occupies. This initiated the permutation feature in Thermo-Calc and OC which simplifies significantly developing models for ordered phases and in the XTDB file there will be just one parameter for each permutation:

The other 3 or 6 permutations will be generated by the software. Sometimes $u_{\rm AB}$ is quite similar when $x_{\rm AB}$ is 0.25, 0.5 or 0.75 which simplifies the assessment.

Even more interesting is that the interaction beteen two constituents in the ordered state is fairly independent of the surrondings, even in multicomponent systems. This suggested the use of the wildcard for such parameters:

```
<Parameter Id="L(FCC_4SL,A,B:*:*:*)" Expr="..." Bibref="someone" />
```

which will also be permuted on all 4 sublattices. In this case it is obvious that it would be totally wrong if the software did not treat this parameter as independent of any other parameter.

## C.5 Modeling multicomponent phases with many sublattices

Binary systems with intermetallics can be well described using the sublattice model but require often DFT calculations for their endmembers as they are frequently stable only in a small composition range. These phases use the **Disordered_2Part** model.

But such binary intermetallics extrapolate badly to ternary and higher order system because there is a large number of endmembers with 3 or more different constituents and, contrary to the phases which can totally

disorder, there are no symmetry criteria to reduce them. Using interaction parameters is also meaningless because each sublattice represent only a small change in the overall composition.

This lead to the Effective Bond Enegery Formalism [7] which represent a totally new view of the parameters in the sublattice model.

## C.6 The EBEF model use many wildcards

In an intermetallic phase with many sublattices using the **Disordered_2Part** model means that all the ordered endmember enegies represent bond energies within the intermetallic phase itself. The "lattice stability" between the stable phase of the constituent and the intermetallic is in the endmember for the disordered part. In the ordered part all endmembers with all constituents same will be zero. The ordered endmembers with 2 or more different constituents are quite similar to interaction parameters but they are strongly related to the crystalline lattice.

For a binary system one can by DFT calculations obtain a set of endmember energies representing a specific constituent in each sublattice. These DFT values can be fitted to a another set of endmembers energies where all but two of the sublattices have wildcards and the other two have different constituents. Several of these wildcard endmembers have similar overall compositions and one has to be careful that the new set of "wildcard"-endmember energies reproduces the sublattice occupancies for the original DFT calculations.

The extrapolation from binaries to ternaries of such "wildcard" endmembers is very good as shown by Dupin [7]. The reason for this is that fitting the "wildcard" endmembers create an "average" of the bond energies, originally calculated with a fixed constituent in each sublattice, which becomes related to the overall composition rather than the constitution.

This model use the same notation for parameters as in CEF, and require fewer **Parameter** tags. In a binary $\sigma$ phase with 5 sublattices one has 32 endmembers but there are only 20 endmember with pairs (as the sites are different the pair energy is not the same switching the sites of the constituents)

```
<Parameter Id="G(sigma,FE:CR:*:*:*) Expr="..." Bibref="someone" />
<Parameter Id="G(sigma,CR:FE:*:*:*) Expr="..." Bibref="someone" />
```

These endmembers can be compared with the excess Gibbs energies for an ordered FCC or BCC when such a parameter has wildcards in the sublattices without the interaction in section C.4.1. But they cannot be permuted because the sublattices are not identical.

## C.7 Simplified wildcard notation

The EBEF model may increase drastically the parameters with wildcards and if there are more wildcards then actual constituents one could consider using:

```
<Parameter Id="G(sigma,FE@1:CR@2) Expr="..." Bibref="someone" />
<Parameter Id="G(sigma,CR@1:FE@2) Expr="..." Bibref="someone" />
```

This may be useful also gor the I2SL model which may exist with only neutrals in the anion sublattice. For example the species C and S can be neutrals in the 2nd sublattice of the I2SL model without any cation. Fir example the parameter for pure liquid C could be

```
<Parameter Id="G(LIQUID,C@2) Expr="..." Bibref="someone" />
```

## C.8 CVM and the cluster site model

Parameters and equations for these models should be included in the XTDB format also.

# Appendix D Complete examples

## D.1 The Al-C system with new unary models

```
<Database version="0.0.3">
  <metadata>
    <writer Software="OpenCalphad  6.068" Date="2023-10-26" />
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  <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(+813.63716)+.01148*GEIN(+345.35022)-0.236743*GEIN(+1601.4467);" />
  <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(+1953.2502)+0.121519*GEIN(+447.96926)+0.3496843*GEIN(+947.01605)
     +.0388463*GEIN(+192.65039)+.005840323*GEIN(+64.463356);" />
  <Phase Id="LIQUID" Configuration="CEF" State="L" >
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  </Phase>
  <Phase Id="AL4C3" Configuration="CEF" State="S" >
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    </Sites>
    <AmendPhase Models="GEIN" />
  </Phase>
  <Phase Id="BCC_A2" Configuration="CEF" State="S" >
    <Sites NumberOf="2" Multiplicities="1 3" >
      <Constituents Sublattice="1" List="AL" />
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    <AmendPhase Models="GEIN" />
  </Phase>
  <Phase Id="DIAMOND" Configuration="CEF" State="S" >
    <Sites NumberOf="1" Multiplicities="1" >
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    </Sites>
    <AmendPhase Models="GEIN" />
  </Phase>
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  <Phase Id="FCC_A1" Configuration="CEF" State="S" >
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      <Constituents Sublattice="2" List="C VA" />
    </Sites>
    <AmendPhase Models="GEIN" />
  </Phase>
  <Phase Id="GRAPHITE" Configuration="CEF" State="S" >
    <Sites NumberOf="1" Multiplicities="1" >
      <Constituents Sublattice="1" List="C" />
    </Sites>
    <AmendPhase Models="GEIN" />
  </Phase>
  <Phase Id="HCP_A3" Configuration="CEF" State="S" >
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    <AmendPhase Models="GEIN" />
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  <Parameter Id="G(LIQUID,AL;0)"  Expr=" +G0LIQAL;"  Bibref="20HE" />
  <Parameter Id="LNTH(LIQUID,AL;0)"  Expr=" +LN(+254);"  Bibref="20HE" />
  <Parameter Id="G2(LIQUID,AL;0)"  Expr=" +13398-R*T-0.16597*T*LN(+T);"  Bibref="20HE" />
  <Parameter Id="G(LIQUID,C;0)"  Expr=" +G0LIQCC;"  Bibref="20HE" />
  <Parameter Id="LNTH(LIQUID,C;0)"  Expr=" +LN(+1400);"  Bibref="20HE" />
  <Parameter Id="G2(LIQUID,C;0)"  Expr=" +59147-49.61*T+2.9806*T*LN(+T);"  Bibref="20HE" />
  <Parameter Id="G(LIQUID,AL,C;0)"  Expr=" +20994-22*T;"  Bibref="20HE" />
  <Parameter Id="G(AL4C3,AL:C;0)"  Expr=" +G0AL4C3-3.08*GEIN(+401)+3.08*GEIN(+1077);"  Bibref="20HE" />
  <Parameter Id="LNTH(AL4C3,AL:C;0)"  Expr=" +LN(+401);"  Bibref="20HE" />
  <Parameter Id="G(BCC_A2,AL:C;0)"  Expr=" +GTSERAL+3*GTSERCC+1006844;"  Bibref="20HE" />
  <Parameter Id="LNTH(BCC_A2,AL:C;0)"  Expr=" +LN(+863);"  Bibref="20HE" />
  <Parameter Id="G(BCC_A2,AL:VA;0)"  Expr=" +G0BCCAL;"  Bibref="20HE" />
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  <Parameter Id="G(BCC_A2,AL:C,VA;0)"  Expr=" -819896+14*T;"  Bibref="20HE" />
  <Parameter Id="G(DIAMOND,C;0)"  Expr=" +G0DIACC+GEDIACC;"  Bibref="20HE" />
  <Parameter Id="LNTH(DIAMOND,C;0)"  Expr=" +LN(+1601.4467);"  Bibref="20HE" />
  <Parameter Id="G(FCC_A1,AL:C;0)"  Expr=" +GTSERAL+GTSERCC+57338;"  Bibref="20HE" />
  <Parameter Id="LNTH(FCC_A1,AL:C;0)"  Expr=" +LN(+549);"  Bibref="20HE" />
  <Parameter Id="G(FCC_A1,AL:VA;0)"  Expr=" +GHSERAL;"  Bibref="20HE" />
  <Parameter Id="LNTH(FCC_A1,AL:VA;0)"  Expr=" +LN(+283);"  Bibref="20HE" />
  <Parameter Id="G(FCC_A1,AL:C,VA;0)"  Expr=" -70345;"  Bibref="20HE" />
  <Parameter Id="G(GRAPHITE,C;0)"  Expr=" +GHSERCC;"  Bibref="20HE" />
  <Parameter Id="LNTH(GRAPHITE,C;0)"  Expr=" +LN(+1953.2502);"  Bibref="20HE" />
  <Parameter Id="G(HCP_A3,AL:C;0)"  Expr=" +GTSERAL+0.5*GTSERCC+2176775;"  Bibref="20HE" />
  <Parameter Id="LNTH(HCP_A3,AL:C;0)"  Expr=" +LN(+452);"  Bibref="20HE" />
  <Parameter Id="G(HCP_A3,AL:VA;0)"  Expr=" +G0HCPAL;"  Bibref="20HE" />
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  <Parameter Id="G(HCP_A3,AL:C,VA;0)"  Expr=" 0;"  Bibref="20HE" />
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    <Bibitem Id="20HE" Text="Zhangting He, Bartek Kaplan, Huahai Mao and Malin Selleby, Calphad Vol 72, (2021) 102250" />
    <Bibitem Id="Default" Text="U.N. Known" />
  </Bibliograpy>
</Database>
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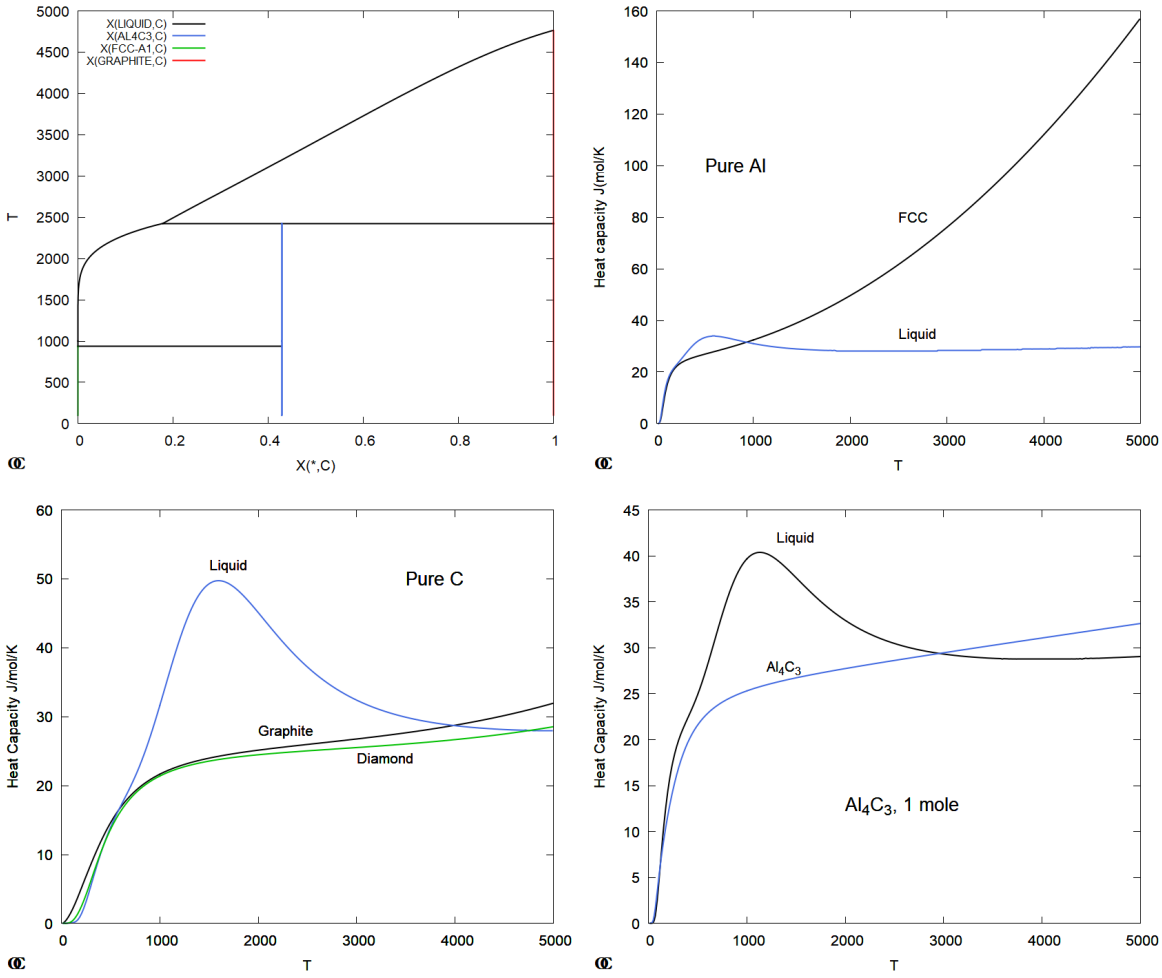
Calculated phase diagram and heat capacity curves from the assessment of Zhangting He at al for Al-C using the new unary models.




It is nice to be able to extrapolate the heat capacity down to $T = 0$ K but I propose we set the low $T$ limit at 10 K. The rapidly increasing heat capacity for the extrapolated metastable FCC phase requires the EEC model to prevent the FCC to become stable at high $T$.

Adding thermal vacancies to model the increase of the heat capacity of FCC-Al just before melting may supress the increase of the extrapolated heat capacity but reguires some extra parameters.

Alternatively one can introduce a break point in $T$ when the solid is assumed no longer to be mechanically stable.

## D.2 The Al-Li system with separated disordered FCC and BCC phases and with these integrated in the ordered phases

The first version in section D.2.1 has been generated using a TDB file where the disordered part of the 4 sublattice FCC and BCC phases has been described by separate phases A1_FCC and A2_BCC. In the **Disordered_3Part** tag this is indicated by the *Disordered* attribute. This is the way this feature is implemented in TC. The **CrystalStructure** tag has no direct influence on the thermodynamic calculations but if provided should be stored internally and be provided as information to an application software and written on any XTDB file generated by the software.

The second version in section D.2.2 has been generated by OC and in OC there are no A1_FCC or A2_BCC phases because they are integrated as "disordered parts" of the ordered phases. Thus the **Disordered_3Part** tag in the XTDB file has no no attribute *Disordered* and the parameters have a suffix "D" and no sublattices for the ordering.

Both XTDB files have the same information but reflect the way the different software handle the disordered part. There should be problem using slightly different ways to provide the thermodynamic data on the XTDB files. Each software can read the data and use its own way to store the data and it should also implement ways to write XTDB files in such a way that other software can read them. It is important that the software developers document their XTDB format to allow other software to read their database files.

### D.2.1 The Al-Li system with ordering and crystal structures

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  <XTDB Version="0.0.3" Software="Manual" Date="2023.10.10" Signature="Bengt Hallstedt" />
  <Defaults LowT="298.15" HighT="6000" Elements="Va" />
  <DatabaseInfo>
    Database for Al-Li from B. Hallstedt and O. Kim 2007.
B. Hallstedt, O. Kim, Int. J. Mater. Res., 98, 961-69(2007)
Including 4-SL ordering models for fcc and bcc.

    Dataset created 2009.06.07 by Bengt Hallstedt.
    2016.10.22: Condensed version using option F and B.
    2020.12.20: Modified for use with GES6.
    2023.04.11: Corrected number of interstitial sites in BCC_4SL.
  </DatabaseInfo>

  <Element Id="Va" Refstate="Vacuum" Mass="0.0" H298="0.0" S298="0.0" />
  <Element Id="Al" Refstate="FCC_A1" Mass="26.98154" H298="4540.00" S298="28.30" />
  <Element Id="Li" Refstate="BCC_A2" Mass="6.941" H298="4632.00" S298="29.12" />

<!-- Do we really need these? -->
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  <Species Id="Al" Stoichiometry="Al1" />
  <Species Id="Li" Stoichiometry="Li1" />

  <TPfun Id="ZERO"      Expr="0.0;" />
  <TPfun Id="UN_ASS"    Expr="0.0;" />
  <TPfun Id="R"         Expr="8.31451;" />

  <Phase Id="LIQUID" Configuration="CEF" State="L" >
    <Sites NumberOf="1" Multiplicities="1" >
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```
      <Constituents List="Al Li" />
    </Sites>
  </Phase>

<!-- I have added crystal structure information with suggested element and attributes -->
<!-- FCC_A1 does not order -->
  <Phase Id="FCC_A1" Configuration="CEF" State="S" >
<CrystalStructure Prototype="Cu" PearsonSymbol="cF4" SpaceGroup="Fm-3m" />
<CrystalStructure Prototype="NaCl" PearsonSymbol="cF8" SpaceGroup="Fm-3m" />
    <Sites NumberOf="2" Multiplicities="1 1" >
      <Constituents Sublattice="1" List="Al Li" />
      <Constituents Sublattice="2" List="Va" />
    </Sites>
    <AmendPhase Models="IHJFCC" />
  </Phase>

<!-- Disordered part of FCC_4SL, identical to FCC_A1 -->
  <Phase Id="A1_FCC" Configuration="CEF" State="S" >
<CrystalStructure Prototype="Cu" PearsonSymbol="cF4" SpaceGroup="Fm-3m" />
<CrystalStructure Prototype="NaCl" PearsonSymbol="cF8" SpaceGroup="Fm-3m" />
    <Sites NumberOf="2" Multiplicities="1 1" >
      <Constituents Sublattice="1" List="Al Li" />
      <Constituents Sublattice="2" List="Va" />
    </Sites>
    <AmendPhase Models="IHJFCC" />
  </Phase>

  <Phase Id="FCC_4SL" Configuration="CEF" State="S" >
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<CrystalStructure Prototype="AuCu3" PearsonSymbol="cP4" SpaceGroup="Pm-3m" />
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      <Constituents Sublattice="2" List="Al Li" />
      <Constituents Sublattice="3" List="Al Li" />
      <Constituents Sublattice="4" List="Al Li" />
      <Constituents Sublattice="5" List="Va" />
    </Sites>
    <Disordered_3Part Disordered="A1_FCC" Sum="4" />
    <AmendPhase Models="IHJREST FCC4PERM" />
  </Phase>

<!-- BCC_A2 does not order -->
  <Phase Id="BCC_A2" Configuration="CEF" State="S" >
<CrystalStructure Prototype="W" PearsonSymbol="cI2" SpaceGroup="Im-3m" />
    <Sites NumberOf="2" Multiplicities="1 3" >
      <Constituents Sublattice="1" List="Al Li" />
      <Constituents Sublattice="2" List="Va" />
    </Sites>
    <AmendPhase Models="IHJBCC" />
  </Phase>
```

```
<!-- Disordered part of BCC_4SL, identical to BCC_A2 -->
  <Phase Id="A2_BCC" Configuration="CEF" State="S" >
<CrystalStructure Prototype="W" PearsonSymbol="cI2" SpaceGroup="Im-3m" />
    <Sites NumberOf="2" Multiplicities="1 3" >
      <Constituents Sublattice="1" List="Al Li" />
      <Constituents Sublattice="2" List="Va" />
    </Sites>
    <AmendPhase Models="IHJBCC" />
  </Phase>

  <Phase Id="BCC_4SL" Configuration="CEF" State="S" >
<CrystalStructure Prototype="W" PearsonSymbol="cI2" SpaceGroup="Im-3m" />
<CrystalStructure Prototype="CsCl" PearsonSymbol="cP2" SpaceGroup="Pm-3m" />
<CrystalStructure Prototype="NaTl" PearsonSymbol="cF16" SpaceGroup="Fd-3m" />
<CrystalStructure Prototype="AlFe3" PearsonSymbol="cF16" SpaceGroup="Fm-3m" />
<CrystalStructure Prototype="AlCu2Mn" PearsonSymbol="cF16" SpaceGroup="Fm-3m" />
    <Sites NumberOf="5" Multiplicities="0.25 0.25 0.25 0.25 3" >
      <Constituents Sublattice="1" List="Al Li" />
      <Constituents Sublattice="2" List="Al Li" />
      <Constituents Sublattice="3" List="Al Li" />
      <Constituents Sublattice="4" List="Al Li" />
      <Constituents Sublattice="5" List="Va" />
    </Sites>
    <Disordered_3Part Disordered="A2_BCC" Sum="4" />
    <AmendPhase Models="IHJREST BCC4PERM" />
  </Phase>

  <Phase Id="HCP_A3" Configuration="CEF" State="S" >
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<CrystalStructure Prototype="NiAs" PearsonSymbol="hP4" SpaceGroup="P6_3/mmc" />
    <Sites NumberOf="2" Multiplicities="1 0.5" >
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      <Constituents Sublattice="2" List="Va" />
    </Sites>
    <AmendPhase Models="IHJREST" />
  </Phase>

  <Phase Id="AL2LI3" Configuration="CEF" State="S" >
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    <Sites NumberOf="2" Multiplicities="2 3" >
      <Constituents Sublattice="1" List="Al" />
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  </Phase>

  <Phase Id="AL4LI9" Configuration="CEF" State="S" >
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      <Constituents Sublattice="1" List="Al" />
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    </Sites>
  </Phase>
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<!-- Unary Al -->
  <Parameter Id="G(FCC_A1,AL:VA)"  Expr="GHSERAL;" HighT="2900"  Bibref="91Din" />
  <Parameter Id="G(A1_FCC,AL:VA)"  Expr="GHSERAL;" HighT="2900"  Bibref="91Din" />
  <Parameter Id="G(BCC_A2,AL:VA)"  Expr="GHSERAL+10083-4.813*T;" HighT="2900"  Bibref="91Din" />
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  <Parameter Id="G(LIQUID,AL)"  Expr="GLIQAL;" HighT="2900"  Bibref="91Din" />

  <TPfun Id="GHSERAL" Expr="-7976.15+137.093038*T-24.3671976*T*LN(T)-0.001884662*T**2-8.77664E-07*T**3+74092*
    <Trange Expr="-11276.24+223.048446*T-38.5844296*T*LN(T)+0.018531982*T**2 -5.764227E-06*T**3+74092*T**(-1)
    <Trange Expr="-11278.361+188.684136*T-31.748192*T*LN(T)-1.230622E+28*T**(-9);" HighT="2900" />
  </TPfun>

  <TPfun Id="GLIQAL" Expr="+11005.045-11.84185*T+GHSERAL+7.9337E-20*T**7;" HighT="933.47" >
     <Trange Expr="-795.991+177.430209*T-31.748192*T*LN(T);" HighT="2900" />
  </TPfun>

<!-- Unary Li -->
  <Parameter Id="G(BCC_A2,LI:VA)"  LowT="200" Expr="GHSERLI;" HighT="3000"  Bibref="91Din" />
  <Parameter Id="G(A2_BCC,LI:VA)"  LowT="200" Expr="GHSERLI;" HighT="3000"  Bibref="91Din" />
  <Parameter Id="G(FCC_A1,LI:VA)"  LowT="200" Expr="GHSERLI-108+1.3*T;" HighT="3000"  Bibref="91Din" />
  <Parameter Id="G(A1_FCC,LI:VA)"  LowT="200" Expr="GHSERLI-108+1.3*T;" HighT="3000"  Bibref="91Din" />
  <Parameter Id="G(HCP_A3,AL:VA)"  LowT="200" Expr="GHSERLI-154+2*T;" HighT="3000"  Bibref="91Din" />
  <Parameter Id="G(LIQUID,LI)"  LowT="200" Expr="GLIQLI;" HighT="3000"  Bibref="91Din" />

  <TPfun Id="GHSERLI" Expr="-10583.817+217.637482*T-38.940488*T*LN(T)+0.035466931*T**2-1.9869816E-05*T**3+159
    <Trange Expr="-559579.123+10547.8799*T-1702.88865*T*LN(T)+2.25832944*T**2-5.71066077E-04*T**3+33885874*T*
    <Trange Expr="-9062.994+179.278285*T-31.2283718*T*LN(T)+0.002633221*T**2-4.38058E-07*T**3-102387*T**(-1);
  </TPfun>

  <TPfun Id="GLIQLI" Expr="+2700.205-5.795621*T+GHSERLI;" HighT="250" >
    <Trange Expr="+12015.027-362.187078*T+61.6104424*T*LN(T)-0.182426463*T**2+6.3955671E-05*T**3-559968*T**(-
    <Trange Expr="-6057.31+172.652183*T-31.2283718*T*LN(T)+0.002633221*T**2-4.38058E-07*T**3-102387*T**(-1);"
    <Trange Expr="+3005.684-6.626102*T+GHSERLI;" HighT="3000" />
  </TPfun>

<!-- Binary Al-Li -->
  <Parameter Id="G(LIQUID,AL,LI;0)"  Expr="-44200+20.6*T;" Bibref="07Hal" />
  <Parameter Id="G(LIQUID,AL,LI;1)"  Expr="+13600-5.3*T;" Bibref="07Hal" />
  <Parameter Id="G(LIQUID,AL,LI;2)"  Expr="+14200;" Bibref="07Hal" />
  <Parameter Id="G(LIQUID,AL,LI;3)"  Expr="-12100;" Bibref="07Hal" />
  <Parameter Id="G(LIQUID,AL,LI;4)"  Expr="-7100;" Bibref="07Hal" />

  <Parameter Id="G(FCC_A1,AL,LI:VA;0)"  Expr="+LDF0ALLI;" Bibref="07Hal" />
  <Parameter Id="G(FCC_A1,AL,LI:VA;1)"  Expr="+LDF1ALLI;" Bibref="07Hal" />
  <Parameter Id="G(FCC_A1,AL,LI:VA;2)"  Expr="+LDF2ALLI;" Bibref="07Hal" />

  <Parameter Id="G(A1_FCC,AL,LI:VA;0)"  Expr="+LDF0ALLI;" Bibref="07Hal" />
  <Parameter Id="G(A1_FCC,AL,LI:VA;1)"  Expr="+LDF1ALLI;" Bibref="07Hal" />
  <Parameter Id="G(A1_FCC,AL,LI:VA;2)"  Expr="+LDF2ALLI;" Bibref="07Hal" />
```

```
  <Parameter Id="G(BCC_A2,AL,LI:VA;0)"  Expr="+LDB0ALLI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_A2,AL,LI:VA;1)"  Expr="+LDB1ALLI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_A2,AL,LI:VA;2)"  Expr="+LDB2ALLI;" Bibref="07Hal" />

  <Parameter Id="G(A2_BCC,AL,LI:VA;0)"  Expr="+LDB0ALLI;" Bibref="07Hal" />
  <Parameter Id="G(A2_BCC,AL,LI:VA;1)"  Expr="+LDB1ALLI;" Bibref="07Hal" />
  <Parameter Id="G(A2_BCC,AL,LI:VA;2)"  Expr="+LDB2ALLI;" Bibref="07Hal" />

  <Parameter Id="G(FCC_4SL,AL:AL:AL:LI:VA)"  Expr="+GFAL3LI;" Bibref="07Hal" />
  <Parameter Id="G(FCC_4SL,AL:AL:LI:LI:VA)"  Expr="+GFALLI2;" Bibref="07Hal" />
  <Parameter Id="G(FCC_4SL,AL:LI:LI:LI:VA)"  Expr="+GFALLI3;" Bibref="07Hal" />
  <Parameter Id="G(FCC_4SL,AL,LI:*:*:*:VA;0)"  Expr="+L0FALLI;" Bibref="07Hal" />
  <Parameter Id="G(FCC_4SL,AL,LI:*:*:*:VA;1)"  Expr="+L1FALLI;" Bibref="07Hal" />
  <Parameter Id="G(FCC_4SL,AL,LI:*:*:*:VA;2)"  Expr="+L2FALLI;" Bibref="07Hal" />
  <Parameter Id="G(FCC_4SL,AL,LI:AL,LI:*:*:VA;0)"  Expr="+SFALLI;" Bibref="07Hal" />

  <Parameter Id="G(BCC_4SL,AL:AL:AL:LI:VA)"  Expr="+GBAL3LI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_4SL,AL:AL:LI:LI:VA)"  Expr="+GB2ALLI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_4SL,AL:LI:AL:LI:VA)"  Expr="+GB2ALLI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_4SL,AL:LI:LI:LI:VA)"  Expr="+GBALLI3;" Bibref="07Hal" />
  <Parameter Id="G(BCC_4SL,AL,LI:*:*:*:VA;0)"  Expr="+L0BALLI;" Bibref="07Hal" />
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  <Parameter Id="G(BCC_4SL,AL,LI:*:*:*:VA;2)"  Expr="+L2BALLI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_4SL,AL,LI:AL,LI:*:*:VA;0)"  Expr="+SB1ALLI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_4SL,AL,LI:*:AL,LI:*:VA;0)"  Expr="+SB2ALLI;" Bibref="07Hal"  />

  <Parameter Id="G(AL2LI3,AL:LI)"  Expr="+2*GHSERAL+3*GHSERLI-93990+34.5*T;" Bibref="07Hal" />
  <Parameter Id="G(AL4LI),AL:LI)"  Expr="+4*GHSERAL+9*GHSERLI-193780+71.7*T;" Bibref="07Hal" />

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  <TPfun Id="L2FALLI" Expr="0;" />
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  <TPfun Id="GFAL2LI2" Expr="+4*UFALLI;" />
  <TPfun Id="GFALLI3" Expr="+3*UFALLI+4900;" />
  <TPfun Id="SFALLI" Expr="+UFALLI;" />
  <TPfun Id="LDF0ALLI" Expr="+GFAL3LI+1.5*GFAL2LI2+GFALLI3+1.5*SFALLI+4*L0FALLI;" />
  <TPfun Id="LDF1ALLI" Expr="+2*GFAL3LI-2*GFALLI3+4*L1FALLI;" />
  <TPfun Id="LDF2ALLI" Expr="+GFAL3LI-1.5*GFAL2LI2+GFALLI3-1.5*SFALLI+4*L2FALLI;" />

  <TPfun Id="UB1ALLI" Expr="-3360+1.8*T;" />
  <TPfun Id="UB2ALLI" Expr="-4230+1.86*T;" />
  <TPfun Id="L0BALLI" Expr="0;" />
  <TPfun Id="L2BALLI" Expr="0;" />
  <TPfun Id="L2BALLI" Expr="0;" />
  <TPfun Id="GBAL3LI" Expr="+2*UB1ALLI+1.5*UB2ALLI+3700;" />
  <TPfun Id="GB2ALLI" Expr="+4*UB1ALLI;" />
  <TPfun Id="GB32ALLI" Expr="+2*UB1ALLI+3*UB2ALLI;" />
```

```
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  <TPfun Id="SB1ALLI" Expr="+15000;" />
  <TPfun Id="SB2ALLI" Expr="+15000;" />
  <TPfun Id="LDB0ALLI" Expr="+GBAL3LI+0.5*GB2ALLI+GB32ALLI+GBALLI3+4*L0BALLI;" />
  <TPfun Id="LDB1ALLI" Expr="+2*GBAL3LI-2*GBALLI3+4*L1BALLI;" />
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    <Bibitem Id="98Sau2" Text="N. Saunders, COST 507, Final report round 2, 1998; Al-Li" />
    <Bibitem Id="07Hal" Text="B. Hallstedt, O. Kim, Int. J. Mater. Res., 98, 961-69(2007); Al-Li" />
  </Bibliography>

</Database>
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### D.2.2 The Al-Li system with the disordered parameters integrated in the ordered phases

This XTDB file for Al-Ni is generated from OC with the "Disordered_3Part" integrated in the ordered FCC and BCC phases. The parameters for the disordered phas have fewer sublattices for the Gibbs energy parameters.

In this listing all **TPfun** tags are in the beginning, the **CrystalStructure** tag is missing and the parameters for all phases listed together at the end. The list of parameters has been edited manually and may contain some errors.

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  </TPfun>
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    <Trange Expr="-9062.994+179.278285*T-31.2283718*T*LN(+T)+.002633221*T**2-4.38058E-07*T**3-102387*T**(-1);
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    <Trange Expr="-6057.31+172.652183*T-31.2283718*T*LN(+T)+.002633221*T**2-4.38058E-07*T**3-102387*T**(-1);"
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<TPfun Id="LDF2ALLI" Expr=" +GFAL3LI-1.5*GFAL2LI2+GFALLI3-1.5*SFALLI+4*L2FALLI;" />
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  <Parameter Id="G(L102_FCC,AL:LI:LI:LI:VA;0)"  Expr=" +GFALLI3;"  Bibref="07HAL" />
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# Appendix E Some highlights and significant changes from earlier versions

1. The implementation of **Disordered_3Part** and **Disordered_2Part** described in sedction 3.4.3 may need attention in the software.
2. The implementation of wildcards, in parameters as described in section C.3 may need attention in the software.
3. The mathematical expression used for the *Expr* attribute in the tags **TPfun, Parameter** and **Parameter2** must be as simple as in the current TDB files, see section 3.3.
4. The **Toop** and **Kohler** tags are integrated in a new **TernaryXpol** tag as there are several ternary extrapolations explained in the paper by Pelton [6].