Proposal 0.0.6 of an XML format to replace TDB files

Bo Sundman et al. February 13, 2024

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The current TDB format for Calphad databases has worked well for 40 years but introducing new models and features has revealed some awkward features, in particular the TYPE_DEFINITION keyword. When a change is needed it may be interesting 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 them the choice of XML is not very important except to avoid spending a year or two 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.

In section 1.1 the most important changes from previous versions of this proposal are listed and motivated. The definition of the XTDB format starts from section 2.

To avoid the confusing use of **ELEMENT** both for chemical element and the XML element I now use **TAG** for the XML element.

The proposal here is a minimal change from the TDB format intended to:

- make manually editing an XTDB file as easy as the current TDB format.
- minimize problems when using software A to read a database file written by software B.
- adding new models for different phase dependent physical properties should be simplified in the thermodynamic database.
- provide users of a database with information about the models and bibliographic information even for encrypted databases.
- improve collaboration between companies and researchers doing assessments, using and developing Calphad databases.
- software developers will be able to add tags and attributes in the database with minimal problems when the database is read by other software. Such modifications should not affect the thermodynamic data itself. Significant new features should be discussed with SGTE and integrated in the XTDB format.
- Added description how the degree for excess parameters should be interpreted, section 3.5. More opinions on this is welcome.

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 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 which develop or use Calphad databases.

If you already read an earlier version of this maybe look at the next section and the examples in the Appendix to see recent changes. Then look at points to discuss in section 5. If you find all OK or have some questions or comments send a message to bo.sundman@gmail.com to explain your points of view.

When reading the XML tag definitions from sections 2.1 to 2.9 and the corresponding notes please note what you like or dislike and send a message to to bo.sundman@gmail.com to explain your points of view.

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. Several examples are provided in the Appendices.

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.

The order of XML tags in the XTDB file is fairly free but to simplify for a human reader and editing the XTDB file a recommended order is **Defaults, DatabaseInfo** and any **AppendiXTDB** tags followed by **Element, Species** and **TPfun**s, **Phases** (with many nested tags). These will be followed by **Parameter**s, ordered by phases or by **System** and finally the **Bibliography**. The **Model** tag and other tags at the end or an a separate file.

Using the **AppendiXTDB** tag, which specifices additional files of an XTDB database, the database can be split on several files. These files must be in the same directory as the primary database file or on a subdirectory. (Note the use of "/" and "\" depend on the operating system). The **Default, DatabaseInfo** and **AppendiXTDB** 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 also with a capital letter.

1.1 Significant changes from earlier versions

1. The "DISORDERED_PART" which can occur in the TYPE_DEFINITION in TDB files for some phases, is now called **Disordered_2Part** or **Disordered_3Part**, see section 2.4. There is no need for an attribute *Subtract* to distinguish them.
2. Two complete examples added for Al-C with new unaries (from Malin Selleby) and Al-Li from (Bengt Hallsted) are included with modifications according to this version of XTDB.
3. The **AppendiXTDB** tag for using several files for a database has been added.
4. The tags **UnarySystem, BinarySystem** and **TernarySystem** have been added to facilitate organizing large databases. In the **BinarySystem** tag a software specific attribute can provide commands for calculating the phase diagram of the system.
5. The **Parameter** or **TPfun** tags can appear anywhere but is recommended to include those tags in the relevant **UnarySystem, BinarySystem** or **TernarySystem** tag. It is not an error to have a **Parameter** for another system inside a **xSystem** tag.

1.2 UPPER and lower case, abbreviations and some more

In a TDB file UPPER and lower case letters was treated as identical. The XML tags and attributes are case sensitive. But I propose that in the attribute values, for example element, species and phase names, the UPPER and lower case letters will be considered as identical.

The characters "(" and ")" are not allowed in the *Id* attribute of **Species** or **Phase** tags in order to simplify the parsing the *Id* attribute of the **Parameter** tag and to simplify interpreting commands in the user interface of the software. It can be a bit complicated to set a condition for the fraction of a species of a phase when both the phase name and species name can contain parenthesis using a command line user i/f.

It is forbidden to abbreviate species *Id*, the species have a separate attribute for its stoichiometric formula and thus rather short names are recommended for the name of a species.

Abbreviation of phase names is allowed and this is a reason to forbid the use of parentheses in phase names. An abbreviation using only a left or right parenthesis will create problems when parsing the XTDB file or in a user interface. The attribute *CrystalStructure* can be used to provide further information about the phase.

The current 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 (if there are no other phases which fit).

1.3 The XTDB file and some more

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 be 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 this document some examples with 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 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.

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

- Comments can be added anywhere in the XML file starting with "<!—" and ending with "—>". There must not be any forbidden characters inside the comment.
- Free text can be added inside a tag after its attributes and a ">" character. In such a case the tag must then be terminated by a "/TagName>" on a separate line. No forbidden characters are allowed in such texts.

All such comments will normally be ignored by software reading the database.

2 The XTDB 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 but many of them will appear several times in the XTDB file to provide the data. Some of the attributes are also optional, those which are mandatory have left justified !.

2.1 The system XTDB tags

The **AppendiXTDB** 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 AppendiXTDB 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 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.
	LowT	Default value of low T limit.
	HighT	Default value of high T limit.
	Bibref	Default bibliographic reference for parameters.
	Elements	VA and/or /- (the electron).
	RKorder	see section 3.5
	GlobalModel	Any model applicable to the whole system, for example EEC
DatabaseInfo		Optional tag with information about the database
	Info	Free text (excluding the characters <> &).
	Date	Last update of the database information.
AppendiXTDB		Optional tag with additional file for the XTDB database. It should contain only XTBD tags but some tags are forbidden, see above.
!	File	File name, possibly on a subdirectory.
	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 with no 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.

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 independent. 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, see section 3.1.1.
!	Stoichiometry	One or more element *Id* each followed by an unsigned real or two integers separated by a "/" representing the stoichiometric ratio, see section 3.1.2. For examples see appendix A.1.
	MQMQA	For a constituent in the MQMQA model. See section 3.1.3.
	UNIQUAC	For a constituent in the UNIQUAC model. See section 3.1.4.

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** should be detected by software.

See section 3.2 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 TDB 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. The name can be used in the "Expr" attribute of other functions or parameters, see section 3.2.
	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 3.2
	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 3.2.
	HighT	Omitted if the default high T limit applies.

2.4 The phase tag and some related tags

The phase tag has two "compulsory subtages" 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 section 3.3.1.
!	Configuration	Model for the configurational entropy, see section 3.3.2.
	State	G for gas phase, L for liquid phase. Needed for 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 or more 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.
Disordered_2Part		Optinal 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	Name of disordered phase, see section 3.3.3.
!	Sum	Number of sublattices, starting from the first in the ordered phase to be summed for the disordered phase constitution. All sublattices summed must have the some set of constituents. Nomally an extra sublattice is an interstitial one.
Disordered_3Part		Optional tag inside the **Phase** tag of an ordered phase. Similar to Disordered_2Part but eq. 2 below is used.
	Disordered	Name of disordered phase, see also section 3.3.3.
!	Sum	Number of sublattices, starting from the first in the ordered phase to be summed for the disordered phase constitution. All sublattices summed must have the some set of constituents. Nomally an extra sublattice is an interstitial one.

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

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

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

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

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

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 the papers by Ansara et al., J All and Comp, **247** (1997) pp 20–30 and Hallstedt et al, Calphad, **31** (2007) pp 28–37.

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 separately for each binary, ternary etc. subsystem. See also sections 2.6, 2.9, appendix A.4 and appendix D.

Tag	Attributes	Explanation
Parameter		Specifies the T, P expression of a model parameter for a set of constituents.
!	Id	As in TDB files, for example G(LIQUID,A,B:VA;2). See also the **Parameter2** tag.
	LowT	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 3.2.
	HighT	If the default high T limit applies.
!	Bibref	Bibliographic reference, unless default bibref set.

The attribute *Id* defines the parameter as in the current TDB file. It starts with a model parameter identifier (MPID), see section 3.4, followed within parenthesis by a phase name (which can be abbreviated) and one or more constituents in each sublattice of the phase. 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 3.5. If the digit is zero the semicolon and the digit can be omitted.

A wildcard, "*" see section 3.6. can be used as constituent in a sublattice indicating that the parameter is independent of the constituents in the sublattice.

The parameters are the essential parts of the database and they are generated from separate assessment of experimental and theoretical data for binary and higher order systems. Databases are collections of such assessment and database manager frequently has to 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	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 3.2.
	HighT	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 3.5
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 3.6, 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.

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 AppendiXTDB 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 basic 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.
!	Bibref	Where the model is described.
!	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.
Permutations		For FCC and BCC lattices a 4 sublattice tetrahedron model identical permutations of a parameter will be included only once in the XTDB file.
!	Id	This is used in **AmendPhase** tag. Its value can be 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 More models including 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 θ will have the additional θ described by the GEIN function in the *Expr* attribute in the **TPfun** tag, see section 3.2. 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.
!	Bibref	Where the model is described.
!	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.
Einstein		The low T vibrational model.
!	Id	This Id is used in **AmendPhase** tag.
!	Bibref	Where the model is described.
!	MPID1	Specifies the Einstein model parameter identifier (MPID) for parameters.
Liquid2state		The liquid 2-state model.
!	Id	This Id is used in **AmendPhase** tag.
!	Bibref	Where the model is described.
!	MPID1	Specifies liquid model parameter identifier (MPID) for parameters.
!	MPID2	Specifies Einstein model parameter identifier (MPID) for parameters.
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 Model tags which need additional data

Some models are related to 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 and Kohler ternary extrapolation models are most likely used together with the parameters for a specific ternary. The Muggianu ternary model is the default ternary extrapolation model. There are more models to be considered and we must take care how they can be integrated in the XTDB format.

Tag	Attributes	Explanation
ToopModel		Subset of 3 constituents for which the Toop ternary extrapolation model should be used. By default the Muggianu extrapolation is used.
!	Bibref	Where the model is described.
	Phase	Can be omitted if used inside a **Phase** tag. Otherwise the phase for which the model should be used.
!	Constituents	Specifies 3 constituents, the Toop constituent first.
KohlerModel		Subset of 3 constituents for which the Kohler ternary extrapolation model should be used. By default the Muggianu extrapolation is used.
!	Bibref	Where the model is described.
	Phase	Can be omitted if used inside a **Phase** tag. Otherwise the phase for which the model should be used.
!	Constituents	Specifies 3 constituents in any order.

Evidently one can use Toop or Kohler when there are several sublattices (in the MQMQA model) and they have normally different constituents, but maybe a sublattice should be specified?

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 normally 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 parameters for a unary system. There can be parameters for the unary also outside this tag.
!	Element	Constituent for the parameters in the system.
!	Bibref	Main bibliographic references.
BinarySystem		Encloses a set of parameters for a binary system. There can be parameters for the system outside this tag. Possibly also a software dependent attribute to calculate the system.
!	Elements	Constituents for the parameters in the system joined by hyphens.
!	Bibref	Main bibliographic references.
	CalcPD	Software specific commands to calculate the phase diagram. The software is specified in the **XTDB** tag.
TernarySystem		Encloses a set of parameters for a ternary system. There can be parameters for the system outside this tag.
!	Elements	Constituents for the parameters in the system joined by hyphens.
!	Bibref	Main bibliographic references.

Within a **BinarySystem** tag the parameters should be for the constituents in the *Elements* attribute. The parameters should have their own bibliographic reference which is needed for the database manager. Only the *Bibref* for the **BinarySystem** is listed when reading the database. Several *Bibref*s values can be given.

```
<BinarySystem Elements="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>
```

An additional feature with this tag is that the software reading the database can elucidate the subsystems which have been assessed in the database.

The software should extract the references for all parameters extracted from the database and list them if a user asks for a list of parameters (even for encrypted databases).

2.10 More elaborate or missing XML tags

The XTDB tags listed above covers all the basic modeling of thermodynamic data needed for calculations. But there are some optional directives used with the TYPE_DEFINITION keyword in the TDB file.

Some features of the TYPE_DEFINITION, which do not relate to the thermodynamic data, have may have to be replaced by software specific XML tags, for example the TYPE_DEFINITION keyword can be used to create composition sets if certain elements have been selected (for example Fe-Ti-C) or testing if certain phases should be rejected/restored.

This require 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.

Tag	Attributes	Explanation
Ifelement		Depending on the elements selected by user
!	Elements	If one (or more enclosed by parenthesis) elements in this attribute have been selected
	AndElements	And one (or more) elements in this attribute have been selected
	OrElements	Or one (or more) elements in this attribute have been selected
!	Action	software specific way to act if this clause is true.

This is an tentative tag which must be elaborated.

As 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).

3 More detalied explanation of some tags and attributes

Note that the XML tags and attributes are case sensitive whereas the names of chemical elements, species, functions, phases and other identifiers are case insensitive as in the TDB file. For example a chemical element 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.

As a devoted Fortran programmer I prefer character variables with fixed length and also because it is difficult to format nice output with very long names of functions or phase names. For a human it is also complicated to handle long names, even if they may be abbreviated.

It is important to be strict here, it is easy to misunderstand a definition if one is not very explicit.

3.1 The Species attritues

The species are used as constituents in the sublattices of phases.

3.1.1 Species Id

A species name (i.e. the *Id* attribute) 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 a **Phase, Parameter**

or any other tag or attribute.

Qusestion: Should the characters "-" and "_" be treated as identical in species ID? Charged species may not have to have an explicit charge in its *Id*.

3.1.2 Species stoichimetry

The species stoichiometry is a sequence of one or more chemical element names (case insensitive) followed by a real number specifying the 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 final stoichiometry unity can also be ignored. **No grouping using parenthesis are allowed when specifying the stoichiometry, for example use BAN2O6, not BA(N1O3)2.**

For MQMQA clusters the stoichiometry can maybe be omitted?

3.1.3 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" />

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.

3.1.4 UNIQUAC attribute

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

3.2 TPfun attributes and expression

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 cannot be abbreviated.

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). No spaces allowed in a simple term. A "complex term" is a simple term multiplied with a math function 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(θ) to calculate $1.5R\theta + 3RT\ln(1 - \exp(-\theta/T))$;

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

It is not allowed to group several terms together using parenthesis, for example "exp(1-3*T+2*T*LN(T))". The 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);" />
```

3.3 The phase tag and attributes

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

3.3.1 The phase name

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.

3.3.2 The configurational entropy model

For the configuration 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 "RKM" for a Redlich-Kister-Muggianu model with a single lattice and one site. An RKM, CEF or MQMQA model could have Toop or Kohler ternary models.

3.3.3 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.

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 pure elements as endmembers (and possibly some long range interaction parameters). In Thermo-Calc terminology this is the "NEVER" model.

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.

3.4 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. There are already some defined but there should be an extensive list of future MPIDs to avoid that different software use the same for (slightly) different things. See Appendix C.

The letter "&", frequently used for mobilities, is forbidden in XML but it can be replaced by some other character, for example "@". Using "&" seems clumsy.

An initial set of model parameter identifies (MPID) should be defined, see section 3.4 and Appendix C. At present 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 an excess model parameter defines the power used for the composition dependence in a binary Redlich-Kister polynomial. For other excess models see section 3.5.

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

3.5 Excess model parameter and degree

In the binary Redlich-Kister series for a system A-B the composition dependence depend on the difference $(x_\mathrm{A} - x_\mathrm{B})^n$, where n is the degree. The order of the elements in the 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 $(x_\mathrm{A} - x_\mathrm{C})$.

For ternary parameters Hillert has proposed (in Caphad, vol 4, (1980) pp 1-12) to have a ternary composition dependent parameter L(PHASE,A,B,C;0..3):

$$ {}^{E}G_M = x_{\rm A}x_{\rm B}x_{\rm C}(v_{\rm A}\ {}^{0}L_{\rm A,B,C} + v_{\rm B}\ {}^{1}L_{\rm A,B,C} + v_{\rm C}\ {}^{2}L_{\rm A,B,C}) \quad (4) $$

where

$$ v_{\rm A} = (1 + 2x_{\rm A} - x_{\rm B} - x_{\rm C})/3 \quad (5) $$
$$ v_{\rm B} = (1 + 2x_{\rm B} - x_{\rm C} - x_{\rm A})/3 \quad (6) $$
$$ v_{\rm C} = (1 + 2x_{\rm C} - x_{\rm A} - x_{\rm B})/3 \quad (7) $$

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.

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

$$ {}^{E}G_M = y_{1,\rm A}y_{1,\rm B}y_{2,\rm C}y_{2,\rm D}(\ {}^{0}L_{\rm A,B:C,D} + (y_{1,\rm A} - y_{1,\rm B})\ {}^{1}L_{\rm A,B,C} + (y_{2,\rm C} - y_{2,\rm D})\ {}^{2}L_{\rm A,B,C}) \quad (8) $$

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

3.6 The use of wildcards for constituents in parameters

In some parameters a wildcard, "*", is used to indicate the parameter is independent of the constituent in this sublattice. For example:

A parameter G(sigma,GA:GA:*;0)=100000;

means that the Gibbs energy of formation of "phase" with GA in first and second sublattice is independent of the constituent in the third. In OC this parameter is stored only once with an indication it does not depend on the constituent in the third sublattice. If one later finds that for example the Gibbs energy for sigma with TA in the third sublattice should be just +70000 then, in OC one can set

G(sigma,GA:GA:TA)=-30000;

because OC stores the two parameters separately and will add the latter, multiplied with the fraction of TA when calculating its contribution to the Gibbs energy. These parameters can appear any order in the database.

This may be handled differently in other software and for different properties and requires attention.

3.6.1 The EBEF model use many wildcards

This model use the same notation for parameters as in CEF, and can replace a large number of **Parameter** tags for endmember parameters by fewer **Parameter** tags, representing bond energies between pairs of constituents. The bond energy parameters specify constituents in only 2 (or 3) sublattices in phases with 3 or more sublattices and use wildcards in remaining sublattices.

Using the **Disordered_2Part** tag and the *Sum* attribute equal to the number of sublattices for a SIGMA phase the pure element parameters can be specified as G(SIGMA,CR) and just a single sublattice. An "endmember" parameter G(SIGMA,CR:FE:*:*:*) in the ordered part will then represent the bond energy between CR in first and FE in second sublattice, independent on the constituents in the other sublattices. Note that the

parameter G(SIGMA,FE:CR:*:*:*) will normally not have the same value because the sublattices have different environments.

Using such parameters (fitted for example to DFT calculated endmember energies) the number of parameters can be reduced by more than an order of magnitudes and, in addition, extrapolations can be improved!

3.6.2 An alternative notation to wildcards

To avoid using explicit wildcards one could indicate the sublattice after the constituent, i.e. to use

G(SIGMA,CR@1:FE@3) instead of G(SIGMA,CR:*:FE:*:*), where the number after the character "@" indicates the sublattice.

3.6.3 A missing wildcard in the I2SL model parameters?

An I2SL model may exist with only neutrals in the anion sublattice. For example the chemical elements C and S can be neutrals in the I2SL model and their parameters are in Thermo-Calc are written as G(I2SL,C), omitting the cation sublattice. In OpenCalphad it is written G(I2SL,*:C) which may be a bit more consistent as it indicates that the constituent on the cation sublattice is irrelevant.

Alternatively the parameter could be written G(I2SL,C@2) if the proposal above is accepted.

Note that an interaction between neutrals with a single specific cation is forbidden in the I2SL model.

3.7 CVM and the cluster site model

These should eventually be included also.

4 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 Points discussed

1. I propose *Expr* may be terminated by a ";" and anway the attribute is terminated by a double quote.
2. The GEIN function is used in the attribute *Expr* of a **Parameter** or in the *Expr* of a **TPfun**.

Normally it is used for a pure element modeled with several Einstein θ. Only one of these is selected to vary with composition, as $\ln(\theta)$, using the model parameter identifier (MPID) LNTH. There is no need for a composition dependent factor for this parameter.

3. I added an attribute RKorder to the **Defaults** to allow deviation from the alphabetrical order of the constituents in Redlich-Kister series. If set the sofware can simply switch the sign if it find the actual order is not alphabetical.

4. It is suggested that the elements should automatically by considered as species and there is no error to include them in the list of species.

5. The model parameter identifier "L" is frequently used for interaction Gibbs energies, I think this or "G" can be accepted.

   But the should it be an error to use "L" for a Gibbs energy of an endmember.

6. I have changed the **Sublattice** tag to be **Sites** and if the argument NumberOf is 1 then the nested tag **Constituents** do not need the *Sublattice* attribute, just the *List* one. I have always felt uncomforable to have phases with a single "sublattice".

7. If a **TPfun** or **Parameter** is calculated outside its defined T range the value calculated should be using the expression in the range closest below or above the actual T.

8. Check if you agree with the discussion on wildcards in section 3.6.

9. Should the hypen "-" and underscore "_" be treated as identical in names and other attributes? My proposal is that in the XTDB file one should only use underscore but for interactive use the hypen should be treated as identical to an underscore.

10. 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.

11. We should define some rules for software specific extentions of XTDB tags, for example handling selection of data.

12. We should have a list of MPID which may be software specific.

6 Summary

There are certainly many more things to take care of but I think it is more important to agree on a minimum common XML 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.

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 3.6 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>
```

For the second parameter maybe one can have

```
     <SublConst Sublattice=="1" Species="AL FE" />
```

rather than having two SublConst tags?

A.6 Models

An extended form of the **Models** should be defined a separate global library file with the **Id** and full description but the models used in an XTDB file should 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="GLOWTEIN" 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>
...
<ToopModel Phase="Liquid" Constituents="C Fe Cr" />
```

The **ToopModel** or **KohlerModel** tags can appear anywhere in the XTDB file, even within the **Phase** tag but, more likely together with all the **Parameter** tags from an assessment of the binary or ternary system in order to simplify editing a large XTDB file. Either way may be a bit complicated to handle by the calculating software reading the XTDB file.

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

Appendix B Proposal of Id and descriptions of model tags.

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

For models that are not agreed a full description of the model and its model parameter identifiers (MPIDs) should be provided in the XTDB file. Note the different software may use different model parameter identifiers (MPID) for the same property.

```
<Models>
  This is a short explanation of XTDB model tags (or "elements") and their attributes, the models for the configuration
  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 Toop and Kohler tags will normally appear together with model parameters for the binaries and has thus a phase at
  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*
    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 the (redundant) antiferromagnetic factor.
    CT is the Curie T and NT the Neel T and BMAGN the average Bohr magneton number.
  </Magnetic>
  <Einstein Id="GLOWTEIN" 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 u
    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 compressib
  </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
    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=" " means the Gibbs energy of the ordered phase is calculated a second time usin
    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 different 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 liqui
  </EEC>
  <KohlerTernary Phase=" " Constituents=" " Bibref="01Pel" >
    The symmetric Kohler model can be used for a specified ternary subsystem as described in the paper by Pelton.
    The 3 constituents, separated by a space, can be in any order.
  </KohlerTernary>
  <ToopTernary Phase=" " Constitutents=" " Bibref="01Pel" >
    The asymmetric Toop model can be used for a specified ternary subsystem as described in the paper by Pelton.
    The 3 constituents, separated by a space, must have the Toop constituent as the first one.
  </ToopTernary>
  <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 DisorderedPart mo
  </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>
```

Appendix C Proposal of initial set of Model Parameter Identifiers, MPID

The 32 model parameter identifiers, MPID, defined in OC are listed in Table 1. In OC a parameter for a disordred part of a **DisorderedPhase** use the same phase name and have fewer sublattices. Software can handle this.

When I started to develop OC I wanted to use only 4 letters for the MPID as I know that many abbreviate for example BMAGN to just BM and I do not want to allow abbreviations of MPID. But I have no strong feelings for this.

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
6	IBM	-	P	&<constituent#sublattice>;	12	Individual Bohr magneton number
7	LNTH	-	P		2	Einstein temperature
8	V0	-	-		1	Volume at T0, P0
9	VA	T	-		4	Thermal expansion
10	VB	T	P		0	Bulk modulus
11	VC	T	P		0	Alternative volume parameter
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
17	THT2	-	P		2	Smooth step function T
18	DCP2	-	P		2	Smooth step function value
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
22	LPTH	T	P		0	Lattice angle TH
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)
31	TSCH	-	P		2	Schottky anomaly T (OC)
32	CSCH	-	P		2	Schottky anomaly Cp/R. (OC)
33	NONE	T	P		0	Unused

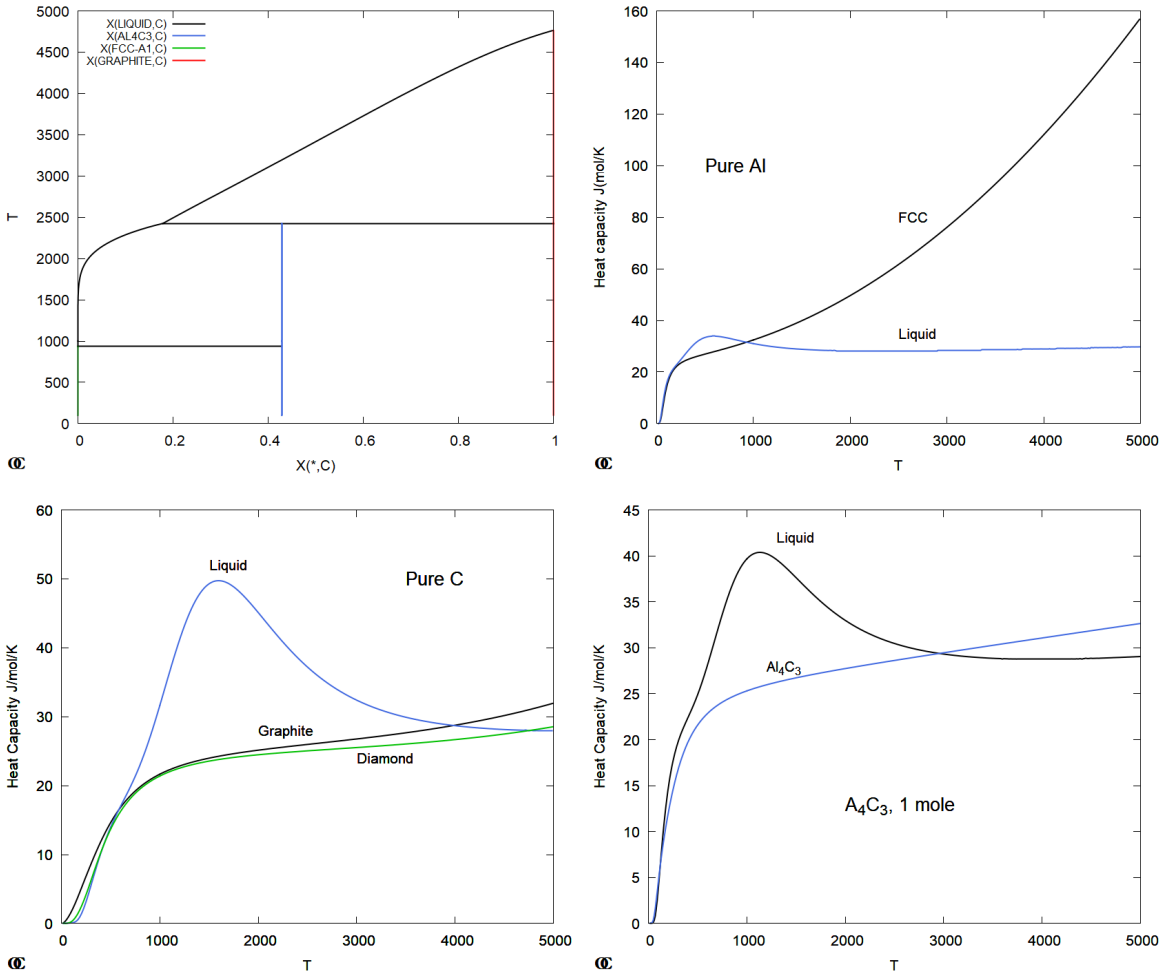
Appendix D Complete examples

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" />
  </metadata>
  <Defaults LowT="10" HighT="6000" Bibref="U.N. Known" Elements="VA /-" />
  <Element Id="AL" Refstate="FCC_A1" Mass="2.698200E+01" H298="4.577300E+03" S298="2.832200E+01" />
  <Element Id="C" Refstate="GRAPHITE" Mass="1.201100E+01" H298="1.054000E+03" S298="5.742300E+00" />
  <Species Id="VA" Stoichiometry="VA" />
  <Species Id="AL" Stoichiometry="AL" />
  <Species Id="C" Stoichiometry="C" />
  <TPfun Id="R"     Expr="8.31451;" />
  <TPfun Id="RTLNP" Expr="R*T*LN(1.0E-5)*P);" />
  <TPfun Id="G0AL4C3" Expr=" -277339-.005423368*T**2;" />
  <TPfun Id="GTSERAL" Expr=" -.001478307*T**2-7.83339395E-07*T**3;" />
  <TPfun Id="GTSERCC" Expr=" -.00029531332*T**2-3.3998492E-16*T**5;" />
  <TPfun Id="G0BCCAL" Expr=" +GHSERAL+10083;" />
  <TPfun Id="G0HCPAL" Expr=" +GHSERAL+5481;" />
  <TPfun Id="GHSERAL" Expr=" -8160+GTSERAL;" />
  <TPfun Id="GHSERCC" Expr=" -17752.213+GEGRACC+GTSERCC;" />
  <TPfun Id="G0DIACC" Expr=" -16275.202-9.1299452E-05*T**2-2.1653414E-16*T**5;" />
  <TPfun Id="GEDIACC" Expr=" +0.2318*GEIN(+813.63716)+.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" >
    <Sites NumberOf="1" Multiplicities="1" >
      <Constituents Sublattice="1" List="AL C" />
    </Sites>
    <AmendPhase Models="LIQ2STATE" />
  </Phase>
  <Phase Id="AL4C3" Configuration="CEF" State="S" >
    <Sites NumberOf="2" Multiplicities="4 3" >
      <Constituents Sublattice="1" List="AL" />
      <Constituents Sublattice="2" List="C" />
    </Sites>
    <AmendPhase Models="GLOWTEIN" />
  </Phase>
  <Phase Id="BCC_A2" Configuration="CEF" State="S" >
    <Sites NumberOf="2" Multiplicities="1 3" >
      <Constituents Sublattice="1" List="AL" />
      <Constituents Sublattice="2" List="C VA" />
    </Sites>
    <AmendPhase Models="GLOWTEIN" />
  </Phase>
  <Phase Id="DIAMOND" Configuration="CEF" State="S" >
    <Sites NumberOf="1" Multiplicities="1" >
      <Constituents Sublattice="1" List="C" />
    </Sites>
    <AmendPhase Models="GLOWTEIN" />
  </Phase>
```

```
  <Phase Id="FCC_A1" Configuration="CEF" State="S" >
    <Sites NumberOf="2" Multiplicities="1 1" >
      <Constituents Sublattice="1" List="AL" />
      <Constituents Sublattice="2" List="C VA" />
    </Sites>
    <AmendPhase Models="GLOWTEIN" />
  </Phase>
  <Phase Id="GRAPHITE" Configuration="CEF" State="S" >
    <Sites NumberOf="1" Multiplicities="1" >
      <Constituents Sublattice="1" List="C" />
    </Sites>
    <AmendPhase Models="GLOWTEIN" />
  </Phase>
  <Phase Id="HCP_A3" Configuration="CEF" State="S" >
    <Sites NumberOf="2" Multiplicities="1 0.5" >
      <Constituents Sublattice="1" List="AL" />
      <Constituents Sublattice="2" List="C VA" />
    </Sites>
    <AmendPhase Models="GLOWTEIN" />
  </Phase>
  <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" />
  <Parameter Id="LNTH(BCC_A2,AL:VA;0)"  Expr=" +LN(+233);"  Bibref="20HE" />
  <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" />
  <Parameter Id="LNTH(HCP_A3,AL:VA;0)"  Expr=" +LN(+263);"  Bibref="20HE" />
  <Parameter Id="G(HCP_A3,AL:C,VA;0)"  Expr=" 0;"  Bibref="20HE" />
  <Bibliograpy>
    <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>
```

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.

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 **DisorderedPart** 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 **DisorderedPart** 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

```
<Database version="0.0.1">
  <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? -->
  <Species Id="Va" Stoichiometry="Va1" />
  <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" >
```

```
      <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" >
<CrystalStructure Prototype="Cu" PearsonSymbol="cF4" SpaceGroup="Fm-3m" />
<CrystalStructure Prototype="AuCu" PearsonSymbol="tP4" SpaceGroup="P4/mmm" />
<CrystalStructure Prototype="AuCu3" PearsonSymbol="cP4" SpaceGroup="Pm-3m" />
    <Sites NumberOf="5" Multiplicities="0.25 0.25 0.25 0.25 1" >
      <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>
    <DisorderedPart Disordered="A1_FCC" Sum="4" Subtract="Y" />
    <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>
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<!-- 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" />
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      <Constituents Sublattice="5" List="Va" />
    </Sites>
    <DisorderedPart Disordered="A2_BCC" Sum="4" Subtract="Y" />
    <AmendPhase Models="IHJREST BCC4PERM" />
  </Phase>

  <Phase Id="HCP_A3" Configuration="CEF" State="S" >
<CrystalStructure Prototype="Mg" PearsonSymbol="hP2" SpaceGroup="P6_3/mmc" />
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    <Sites NumberOf="2" Multiplicities="1 0.5" >
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      <Constituents Sublattice="2" List="Va" />
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  </Phase>

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

  <Phase Id="AL4LI9" Configuration="CEF" State="S" >
<CrystalStructure Prototype="Al4Li9" PearsonSymbol="mC26" SpaceGroup="C2/m" />
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      <Constituents Sublattice="1" List="Al" />
      <Constituents Sublattice="2" List="Li" />
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  </Phase>
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  <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" />
  <Parameter Id="G(A2_BCC,AL:VA)"  Expr="GHSERAL+10083-4.813*T;" HighT="2900"  Bibref="91Din" />
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  <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>

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  <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>

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  <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" />
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  <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" />
  <Parameter Id="G(BCC_4SL,AL,LI:*:*:*:VA;1)"  Expr="+L1BALLI;" Bibref="07Hal" />
  <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" />

<!-- metastable -->
  <Parameter Id="G(HCP_A3,AL,LI:VA;0)"  Expr="-27000+8*T;" Bibref="98Sau2" />

  <TPfun Id="UFALLI" Expr="-3270+1.96*T;" />
  <TPfun Id="L0FALLI" Expr="+2960-1.56*T;" />
  <TPfun Id="L2FALLI" Expr="0;" />
  <TPfun Id="L2FALLI" Expr="0;" />
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  <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;" />
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  <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="GBALLI3" Expr="+2*UB1ALLI+1.5*UB2ALLI+3250;" />
  <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;" />
  <TPfun Id="LDB2ALLI" Expr="+GBAL3LI-0.5*GB2ALLI-GB32ALLI+GBALLI3+4*L2BALLI;" />

  <Bibliography>
    <Bibitem Id="91Din" Text="A.T. Dinsdale, Calphad, 15, 317-425(1991)." />
    <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 "DisorderedPart" integrated in the ordered FCC and BCC phases. Note the suffix "D" and the reduced number of sublattices for the Gibbs energy parameters in the disordered part.

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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    <Trange Expr="-11276.24+223.048446*T-38.5844296*T*LN(+T)+.018531982*T**2-5.764227E-06*T**3+74092*T**(-1);
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  <TPfun Id="GLIQAL" Expr=" +11005.029-11.841867*T+GHSERAL+7.9337E-20*T**7;" HighT="933.47" >
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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);"
    <Trange Expr="+3005.684-6.626102*T+GHSERLI;" HighT="3000" />
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  <AmendPhase Models="BCC4PERM" />
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    <Bibitem Id="98SAU2" Text="N. Saunders, COST 507, Final report round 2, 1998; Al-Li" />
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