Proposal 0.0.3 of an XML format to replace TDB files

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Background

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 and as it is easy to convert between any generally accepted markup language, the XML has been selected for a new XTDB format as it is slightly more explicit.

As 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.

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 one 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.
- Provide better facilities to handle new models and features added by the different softwares using Calphad databases.
- Provide users of a database with information about the sources of data and parameters even for encrypted databases.
- Software 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.

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 allow users to read and write unencrypted databases in the XTDB format.

You are encouraged to ask anyone you think can contribute to defining the new database format to have a look at this and provide their comments.

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 if anything changed. Then look at points to discuss in section 3. 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.

If you read the XML tag definitions in sections 1.2 to 1.12 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 the sections below and the attributes are explaines and may have a "note". If the note is "+" the attribute is compulsory, "–" if optional. A letter A-Z in the note referes to details explained in section 1.13.

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 in the TDB file. Except for phase names the value of an *Id* cannot be abbreviated when used in other attributes.

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

As a rule 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. A major change is to use the tag **DisorderedPart** for the TDB model "DISORDERED_PART", which can occur in the TYPE_DEFINITION in TDB files. I have previously called it SplitPhase.
2. The **Constituent** tsg inside the **Parameter2** tag changed to **SublConst** to avoid confusing with the **Constituents** tag used inside the **Phase** tag.
3. The FCC4PERM and BCC4PERM are merged as variants of the **Permutations** tag.
4. Should the characters "-" and "_" be treated as identical in names and other attributes?
5. I have never liked the use of "sublattices" when a phase has just a single set of sites so now I propose:

```
 <Phase Id="LIQUID" Configuration="RKM" State="L" >
    <Sites NumberOf="1"  Multiplicities="1" >
      <Constituents List="AL C" />
    </Sites>
    <AmendPhase model="LIQ2STATE" />
  </Phase>
...
  <Phase id="BCC_A2" Configuration="CEF" State="S" >
    <Sites NumberOf="2"  Multiplicites="1  3" >
      <Constituents Sublattice="1" List="AL FE" />
```

```
    <Constituents Sublattice="2" List="VA" />
  </Sites>
  <AmendPhase Model="IHJBCC" />
</Phase>
```

6. There can be an advantage to group several parameters in a subsystem for unaries, binaries etc., see section 1.9. This is probably normal practice for a database manager but may simplify also handling the references.

7. Two complete examples added for Al-C with new unaries from Malin and Al-Li from Bengt with a suggestion for a CrystalStructure tag.

8. I have tried to update every part of this text when there has been suggestions I find interesting and useful but there can be inconsistencies between different parts of this text.

9. A late modificateion: **the characters "(" and ")" must not be used in phase names in the XTDB file.**

1.2 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.

Only one XML tag per line in order to be easily readable by humans. But an XML tag may extend over several lines, including nested tags.

All attributes of an XML tag should fit within a line (2000 characters). The attribute *List* of the **Constituent** tag for a gas phase in a big system may exceed this but then severeal **Constituent** tags can be used for the gas phase.

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 <Tag_name and ends with /> or /Tag_name> if it contains nested tags. An attribute_name ends with "=" and its value is given within double quotes, """, for example Id="FE".

The letters <, > and & are forbidden everywhere except when used for the XML itself. One should avoid using double quites, """ and the equal sign "=" outside and inside attributes values.

Comments can be added anywhere in the XML file starting with <!— and ending with —> and with no forbidden characters inside.

Comments can also be added inside a tag (outside the attributes), but avoid using any forbidden characters.

1.3 The system XTDB tags

Tag	Attributes	Note	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			Provides default values of attributes in other XML tags.
	LowT	–	Default value of low T limit.
	HighT	–	Default value of high T limit.
	Bibref	–	Default bibliographic reference.
	Elements	–	VA and/or /- (the electron).
	Model	–	Any model applicable for the system, for example EEC
DatabaseInfo			Free text (excluding <> &).
	Date	–	Last update.

1.4 The element and species tags

Tag	Attributes	Note	Explanation
Element			Specifies a chemical element in the database. The vacancy is denoted "VA" and the electron "/-".
	Id	+	Chemical element symbol, for example FE, H
	Refstate	+	Name of a phase, for example GAS
	Mass	+	Mass in g/mol
	H298	–	Enthalpy difference between 0 and 298.15 K in reference state.
	S298	–	Entropy difference between 0 and 298.15 K in reference state.
Species			Specifies a molecular like aggregate used as constituent of phases. The elements, except the electron, are also species.
	Id	A	Species name max 24 letters. For note see 1.13.
	Stoichiometry	B	One or more element *Id* each followed by an unsigned real representing the stoichiometric ratio. For note see 1.13. See also appendix A.1.
	MQMQA	C	For a constituent in the MQMQA model. For note see 1.13.
	UNIQUAC	D	For a constituent in the UNIQUAC model. For note see 1.13.

Should the elements automatically be considered as species?

1.5 The function and temperature range tags

There is at present no way to handle several pressure ranges. The value of a function, as well as its first and second derivative with respect to T, must be continuous across an interval of T range. Breakpoints occur mainly for pure element data and those in the unary 1991 have been checked.

Tag	Attributes	Note	Explanation
TPfun			Defines a T, P expression to be used in parameters or other functions.
	Id	E	Function name, max 16 characters. The name can be used in the "Expr" attribute of other functions or parameters. For note see 1.13.
	LowT	–	If the default low T limit applies.
	Expr	+	Simple mathematical expression terminated by ;. Use the **Trange** tag if several ranges. See section 1.14
	HighT	–	If 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 1.14.
	HighT	–	If the default high T limit applies.

The *Id* of other **TPfun**s can be used inside the *Expr* of a **Tpfun**, **Parameter** and **Parameter2** tags.

See section 1.14 for the restrictions of the mathenatical expresson in the *Expr* attribute and Appendix A.2 and others for examples.

1.6 The phase tag and some related tags

Normally the software requires information of sublattices, constituents and models for the phase in order to create the appropriate data structure for a phase.

Some software may not have an explicit disordered phase but arrange all **Parameter** tags for the ordered and disordered phase within the same phase. A phase with very long list of constituents (i.e. GAS) can have several **Constituent** tags for the same sublattice.

Tag	Attributes	Note	Explanation
Phase			All data belongs to a phase.
	Id	F	Phase name, see 1.13 note F.
	Configuration	G	Model for the configurational entropy. For note see 1.13.
	State	–	G for gas phase, L for liquid phase. Needed if EEC is used.
Sites			Only inside a **Phase** tag.
	NumberOf	+	Number of sublattices, an integer value 1-10
	Multiplicities	+	Sites on each sublattice, as many reals as sublattices separated by a space.
CrystalStructure			Only inside a **Phase** tag.
	Prototype	-	Prototype phase.
	PearsonSymbol	-	Specification.
	SpaceGroup	-	Specification.
Constituents			Only inside a **Phase** tag.
	Sublattice	-	Needed if several sublattices.
	List	+	Species *Id*, separated by a space, in the sublattice.
AmendPhase			Only inside a **Phase** tag.
	Model	+	List of models *Id*s, separated by a space, for this phase, see section 1.11.
DisorderedPart		H	Only inside the **Phase** tag of the 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 or 2 below. If the attribute *Subtract*="Y", the Gibbs energy of the ordered phase is calculated a second time with the disordered fractions and subtracted. The configurational Gibbs energy is calculated only for the ordered phase.
	Disordered	I	Name of disordered phase, see also 1.13.
	Sum	+	Number of sublattices in the ordered phase to be summed for the disordered phase constitution. All sublattices summed must have the some set of constituents.
	Subtract	-	Must be Y if eq. 2 is to be used.

For a phase with the **DisorderedPart** tag and without the *Subtract* attribute, 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. With *Subtract*=Y 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.

1.7 The simple parameter tag

All thermodynamic data are defined by the parameter tags. They can be arranged inside a phase tag or separately for each binary, ternary etc. subsystem. See also section 1.8 and appendix A.4.

Tag	Attributes	Note	Explanation
Parameter			Specifies the T, P expression of a model parameter for a set of constituents.
	Id	+	As in TDB file, 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 1.5.
	HighT	–	If the default high T limit applies.
	Bibref	+	Bibliographic reference.

The attribute *Id* defines the parameter as in the current TDB file. It starts with a model parameter identifier (MPID), see section 1.16, 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. If the digit is zero the semicolon and the digit can be omitted.

A wildcard, "*", can be used as constituent in a sublattice indicating that the parameter is independent of the constituents in the sublattice. See also section 1.15.

For some reason which I have forgotten it is not allowed to have a parameter for an interaction between a wildcard and a specific constituent, for example G(FCC,VA,*:VA) which would represent an interaction $y_{\mathrm{Va}}(1 - y_{\mathrm{Va}})$ is not allowed.

1.8 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.

Tag	Attributes	Note	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	J	Model parameter identifier, for example G or TC. For note see 1.13.
	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 1.5.
	HighT	–	If the default high T limit applies.
	Bibref	+	Bibliographic reference.
ConstArray			Only inside a **parameter2** tag. Encloses the SublConst tags.
	Degree	K	Can be omitted if zero, for note see 1.13.
SublConst			Only inside a **ConstArray** tag.
	Sublattice	+	Sublattice of constituent.
	Species	+	Name of a constituent (or two or more for an excess parameter?).

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, "*", can be used as constituent in a sublattice indicating that the parameter is independent of the constituent in the sublattice, see section 1.15.

1.9 Organizing the data

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	Note	Explanation
System			Encloses a set of parameters for a particular system such unary, binary or higher order.
	Elements	+	Elements for the parameters in the system joined by hyphens.
	Bibref	+	Main bibliographic references.

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

```
<System 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="GD(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="GD(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" />
</System>
```

In the example above from OC the model parameter identifier “GD” is a Gibbs energy parameter with suffix “D” used in OC for the disordered part of the ordered B2_BCC and FCC_4SL phases. Other software may create separate phases for the disordered parts.

An additional feature with this tag is that the software reading the database can elucidate the subsystems which have not 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).

1.10 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	Note	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
	Date	–	Date when the bibref tag was created
	Sign	–	Signature of the one adding the reference

1.11 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 model has one or more model parameter identifiers (MPID) as attributes and these are used in the **Parameter** tag. See also the Appendix B. Software specific models must be explained in a model tag with an appropriate bibliographic reference.

Tag	Attributes	Note	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. Other models, such as **DisorderedPart**, must be included as tags within the **Phase** tag.

1.11.1 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	Note	Explanation
Magnetic			There are several magnetic models.
	Id	+	This is used in **AmendPhase** tag.
	Aff	+	Antiferromagnetic factor (-1, -3 or 0). This is actually redundant but kept for compatibility with the 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 described.

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.

1.11.2 More models including new unary models

There is also a new magnetic model. Other new **Model** tags may be included in the XTDB file in order to specify new MPIDs.

Tag	Attributes	Note	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.

After long discussions the unary group has decided to use a single composition dependent Einstein parameter for each unary. Those elements with their 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 1.14. See also the Al-C example in Appendix D.1.

1.11.3 Model tags which need additional data

These 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 **DisorderedPart** model is explained together with the **Phase** tag. The Toop and Kohler ternary extrapolation models are most likely specified together with the parameters for a specific ternary. The Muggianu ternary model is the default 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	Note	Explanation
DisorderedPart			This is explained together with the **Phase** tag, see 1.6, because it requires additional data.
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). But they have normally different constituents, but maybe a sublattice should be specified?

1.12 Software specific XML tags and some others

The TYPE_DEFINITION keyword in the TDB file is replaced in this XML format by **AmendPhase, DisorderedPart** and some other tags and attributes. But some features of the TYPE_DEFINITION, which do not relate to the thermodynamic data, have to be replaced by software specific XML tags.

The ASSESSED_SYSTEM is an nice feature and I propose we keep such a possibility also in the XTDB file.

I think it would also be interesting for users to have an XML tag **UnAssBinary**, especially for encrypted databases, in order to indicate composition regions where the user should be careful using calculated results.

The current TYPE_DEFINITION keyword is sometimes used to create composition sets if certain elements have been selected or testing if certain phases should be rejected/restored. We should think about how this can be implemented.

Tag	Attributes	Note	Explanation
AssessedSystem			Contains **Binary** and **ternary** tags assessed model parameters. The former tag can have software dependent commands to calculate the phase diagram.
	Software	+	Software used for testing.
Binary			Inside an **AssessedSystem** or **UnAssedBinary** tag it specifies a binary system.
	System	+	Two elements joined by a hyphen.
	Commands	-	Software dependent character string to calculate the phase diagram.
Ternary			Specification of a ternary system.
	System	+	Three or more species seprated by hyphens.
UnAssessedBinary			Indication of missing binary assessments. Contains **Binary** elements without any commands.

Examples:

```
<AssessedSystem Software="TC">
  <Binary System="AG-I" Commands="TDB -* +GAS +LIQUID +FCC_A1 +AGI_S1 +AGI_S2 +I2_S ;P3 TMM:200/2500 STP:.2
  <Binary System="AG-O" Commands="TDB -* +GAS +LIQUID +FCC_A1 +AG2O ;P3 TMM:200/2500 STP:.2/1500/1" />
  <Binary System="CR-MO" Commands="TDB -* +GAS +LIQUID +BCC_A2  ;G5 C_S:BCC_A2/MO:VA MAJ:BCC_A2/CR:VA   ;P3
  <Ternary System="Cr-Fe-Ni" />
</AssessedSystem>

<UnAssessedBinary>
   <Binary System="Mo-S Cr-Sm Pt-Gd Fe-H" />
</UnAssessedBinary>
```

1.13 Notes

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.

A: 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.

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

B: 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 parenthesis are allowed.

For MQMQA clusters the stoichiometry can maybe be omitted?

C: 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 6.0 divided by the bond fractions. The MQMQA cluster is always electrically neutral. For endmember clusters (with one species in each sublattice) a real representing the SNN/FNN ratio, usually 2.4, must be supplied.

D: For species in the UNIQUAC model. Contains two reals representing volume and area of the species in m^3 and m^2 in that order.

E: The **TPfun** attribute *Id* 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 "#".

F: 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.

A phase name may be abbreviated in parameters and some other cases and thus a phase name must be unique and not an abbreviation of another phase. This has to be observed when adding new assessments to a database.

G: For the configuration model we have CEF, I2SL, MQMQA, UNIQUAC and maybe some more. Maybe also "IDEAL" when there are ideal mixing and no interactions and "RKM" for a Redlich-Kister-Muggianu model with a single lattice and one site? An RKM or CEF model could have some Toop or Kohler ternaries.

H: The disordered phase within a **DisorderedPart** can be omitted if the parameters for the disordered phase are provided within the ordered phase. In OC a suffix "D" is added after the MPID name and the parameters has the appropriate reduced number of sublattices.

For example GD(SIGMA,CR) can be used as *Id* in a **Parameter** tag for the lattice stability of Cr in SIGMA if the SIGMA phase is modelled with 3 or more sublattices and has the **DisorderedPart** tag. This avoids the need for a meaningless disordered DIS_SIGMA phase.

I: A BCC or FCC phase with a disordered part (i.e. a **DisorderedPart** model) with the attribute Subtract="Y" will have the "ordered" part calculated using the disordered set of fractions and subtracted in order to allow the use of the disordered phase separately.

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. In this case the attribute *Subtract* can be omitted or given any other value than Y.

J: An initial set of model parameter identifies (MPID) should be defined, see section 1.16 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?

K: The degree can be omitted if zero.

1.14 The mathematical expression used in Expr

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 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 extended.

The following math function is needed in *Expr* attributes for the unary project:

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

where the argument of GEIN should be the logarithm of θ. It is not allowed to group several terms together using parenthesis, for example 5*(1+3*T+2*T*LN(T)). Either one can multiply all coefficients with 5 or enter the expression within parentesis as a **TPfun** and then multiply this with 5.

A square root of T is entered as two **TPfun**://

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

1.15 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.

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

1.15.1 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 **DisorderedPart** tag without a *Subtract* attribute and the *Sum* attribute equal to the number of sublattices for a SIGMA phase the pure element parameters can be specified as GD(SIGMA,CR) using the suffix D 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:*:*:*) has not 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!

1.15.2 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.

1.15.3 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.

1.16 Model parameter identifiers, 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 unnecessary and quite clumsy.

1.17 CVM and the cluster site model

These should eventually be included also.

2 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.

3 Points to discuss

1. Should mathematical expressions be terminated by a ";"? It is not necessary because there is a final double quote of the expression but it may be nice to keep as an option.

2. The GEIN function is used in the **Parameter** for a pure element modeled with several Einstein θ. Only one of these is selected to vary with composition using the LNTH model parameter identifier (MPID).

3. Should the sign of Redlich-Kister terms depend on the alphabetrical order of the constituents or as the order the constituents are written in the parameter **Id**? Currently the TDB file use alphabetical.

4. Should the element be automatically considered as species and not included in the list of species?

5. If there in an ordered FCC phase in the database and this phase has a tag **DisorderedPart** with the attribute *Subtract*="Y" then the disordered part is a complete description of the disordered FCC. Is may be interesting to allow a user to extract just the disordered FCC parameters? For a multicomponent system calculations with the ordered FCC may be significantly longer.

   Note that a phase with the tag **DisorderedPart** but without the attribute *Subtract*="Y", the disordered phase will normally not thave parameters describing a realistic disordered phase.

6. The model parameter identifier "L" is frequently usde for interaction Gibbs energies, personally I use G for all such parameters. Should that be accepted? Or can "L" be used for all Gibbs energy parameters?

7. I have changed the **Sublattice** tag to be **Sites** and if the argument NumberOf is 1 then the following tag **Constituents** do not need the "Sublattice" argument, just a list of species. I have always felt uncomforable to have phases with a single "sublattice".

8. If a **TPfun** or **Parameter** is calculated outside its defined T range a flag should be set which can be tested by the user or application software but no error termination of the calculation. The calculated value should be that using the expression in the range closesed below or above the actual T.

4 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 have to 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>
    <DisorderedPart Disordered="A2_BCC" Subtract="Y" 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>
    <DisorderedPart 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 1.15 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 **DisorderedPart** in example 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 DisorderedPart 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 Einstein THETA is the exponential of the parameter LNTH.
  </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>
  <DisorderedPart Disordered=" " Subtract=" " 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.
    If Subtract="Y" the Gibbs energy of the ordered phase is calculated a second time using the disordered fractions an
    Some software has no special disordered phase but all parameters are stored in the ordered one and
    the parameters for the disordered phase has a suffix "D" (and different number of sublattices).
  </DisorderedPart>
  <Permutations Id="FCC4Perm" Bibref="09Sun" >
    An FCC phase with 4 sublattices for the ordered tetrahedron use this model to indicate that parameters
    with permutations of the same set of constituents on identical sublattices are included only once.
  </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 but the MPID has a suffix "D" and there are fewer sublattices.

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 string 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

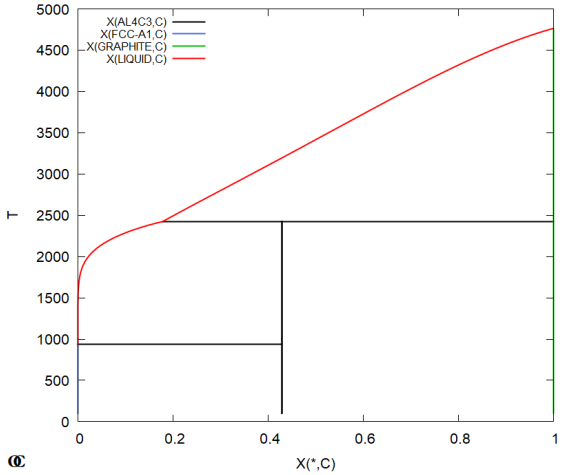
Appendix D Complete examples

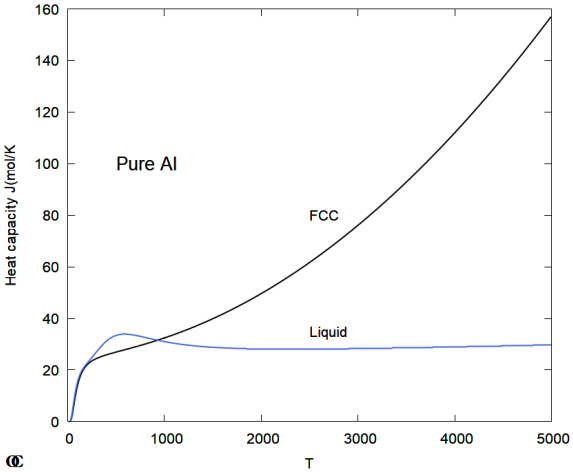
D.1 The Al-C system with new unary models

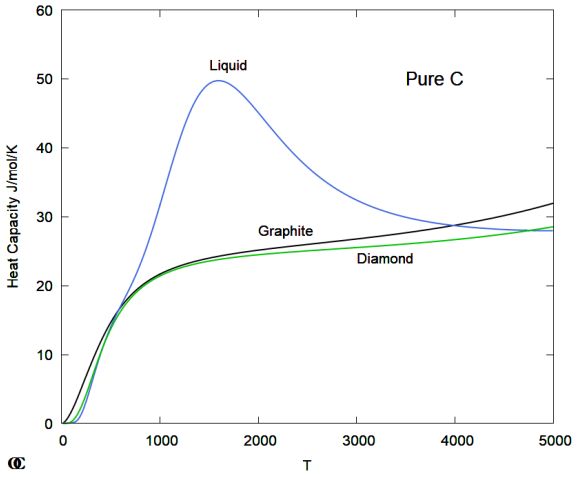
```
<?xml version="1.0"?>
<?xml-model href="database.rng" schematypens="http://relaxng.org/ns/structure/1.0" type="application/xml"?>
<Database version="0.0.3">
  <metadata>
    <writer Software="OpenCalphad  6.067" Date="2023-10-13" />
  </metadata>
  <Defaults LowT="10" HighT="6000" Bibref="U.N. Known" 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=" +G0SERAL+10083;" />
  <TPfun Id="GHHCPAL" Expr=" +G0HCPAL;" />
  <TPfun Id="GHSERAL" Expr=" +G0SERAL;" />
  <TPfun Id="GHSERCC" Expr=" +G0SERCC+GEGRACC;" />
  <TPfun Id="G0DIACC" Expr=" -16275.202-9.1299452E-05*T**2-2.1653414E-16*T**5;" />
  <TPfun Id="GEDIACC" Expr=" +0.2318*GEIN(+6.70196)+.01148*GEIN(+5.84456)-0.236743*GEIN(+7.37838);" />
  <TPfun Id="G0LIQAL" Expr=" -209-3.777*T-.00045*T**2;" />
  <TPfun Id="G0LIQCC" Expr=" +63887-8.2*T-.0004185*T**2;" />
  <TPfun Id="G0SERAL" Expr=" -8160+GTSERAL;" />
  <TPfun Id="G0HCPAL" Expr=" +G0SERAL+5481;" />
  <TPfun Id="G0SERCC" Expr=" -17752.213-.00029531332*T**2-3.3998492E-16*T**5;" />
  <TPfun Id="GEGRACC" Expr=" -0.5159523*GEIN(+7.57725)+0.121519*GEIN(+6.10479)+0.3496843*GEIN(+6.8533)
          +.0388463*GEIN(+5.26269)+.005840323*GEIN(+4.166667);" />
  <Phase Id="AL4C3" Configuration="CEF" State="S" >
    <Sites NumberOf="2" Multiplicities="4 3" >
      <Constituents Sublattice="1" List="AL" />
      <Constituents Sublattice="2" List="C" />
    </Sites>
  </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" />
```

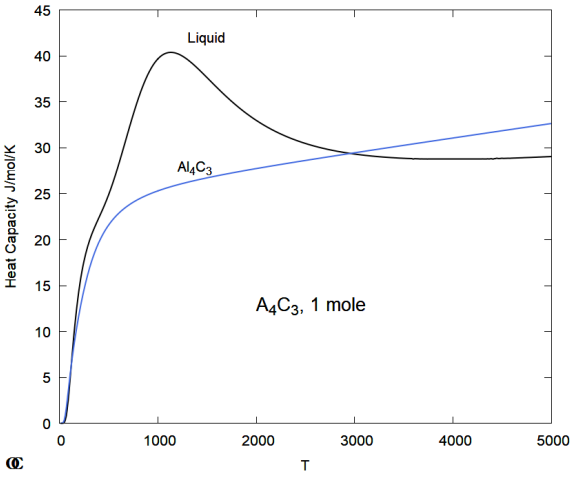
```
      <Constituents Sublattice="2" List="C VA" />
    </Sites>
    <AmendPhase Models="GLOWTEIN" />
  </Phase>
  <Phase Id="GRAPHITE" Configuration="CEF" State="S" >
    <Sites NumberOf="1" Multiplicities="1" >
      <Constituents Sublattice="1" List="C" />
    </Sites>
    <AmendPhase Models="GLOWTEIN" />
  </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>
  <Phase Id="LIQUID" Configuration="CEF" State="S" >
    <Sites NumberOf="1" Multiplicities="1" >
      <Constituents Sublattice="1" List="AL C" />
    </Sites>
    <AmendPhase Models="LIQ2STATE" />
  </Phase>
  <Parameter Id="G(AL4C3,AL:C;0)"  Expr=" +G0AL4C3+3.92*GEIN(+5.994)+3.08*GEIN(+6.98193);"  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=" +6.76041;"  Bibref="20HE" />
  <Parameter Id="G(BCC_A2,AL:VA;0)"  Expr=" +G0BCCAL;"  Bibref="20HE" />
  <Parameter Id="LNTH(BCC_A2,AL:VA;0)"  Expr=" +5.45194;"  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=" +7.37838;"  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=" +6.3081;"  Bibref="20HE" />
  <Parameter Id="G(FCC_A1,AL:VA;0)"  Expr=" +GHSERAL;"  Bibref="20HE" />
  <Parameter Id="LNTH(FCC_A1,AL:VA;0)"  Expr=" +5.64545;"  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=" +7.57725;"  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=" +6.11268;"  Bibref="20HE" />
  <Parameter Id="G(HCP_A3,AL:VA;0)"  Expr=" +GHHCPAL;"  Bibref="20HE" />
  <Parameter Id="LNTH(HCP_A3,AL:VA;0)"  Expr=" +5.57215;"  Bibref="20HE" />
  <Parameter Id="G(HCP_A3,AL:C,VA;0)"  Expr=" 0;"  Bibref="20HE" />
  <Parameter Id="G(LIQUID,AL;0)"  Expr=" +G0LIQAL;"  Bibref="20HE" />
  <Parameter Id="LNTH(LIQUID,AL;0)"  Expr=" +5.53733;"  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=" +7.24423;"  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" />
  <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









D.2 The Al-Li system with ordering and crystal structures

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<?xml-model href="database.rng" schematypens="http://relaxng.org/ns/structure/1.0" type="application/xml"?>
<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 Sublattice="1" 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>

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

  <Phase Id="BCC_4SL" Configuration="CEF" State="S" >
<CrystalStructure Prototype="W" PearsonSymbol="cI2" SpaceGroup="Im-3m" />
<CrystalStructure Prototype="CsCl" PearsonSymbol="cP2" SpaceGroup="Pm-3m" />
<CrystalStructure Prototype="NaTl" PearsonSymbol="cF16" SpaceGroup="Fd-3m" />
<CrystalStructure Prototype="AlFe3" PearsonSymbol="cF16" SpaceGroup="Fm-3m" />
<CrystalStructure Prototype="AlCu2Mn" PearsonSymbol="cF16" SpaceGroup="Fm-3m" />
    <Sites NumberOf="5" Multiplicities="0.25 0.25 0.25 0.25 3" >
      <Constituents Sublattice="1" List="Al Li" />
      <Constituents Sublattice="2" List="Al Li" />
```

```
      <Constituents Sublattice="3" List="Al Li" />
      <Constituents Sublattice="4" List="Al Li" />
      <Constituents Sublattice="5" List="Va" />
    </Sites>
    <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" />
<CrystalStructure Prototype="NiAs" PearsonSymbol="hP4" SpaceGroup="P6_3/mmc" />
    <Sites NumberOf="2" Multiplicities="1 0.5" >
      <Constituents Sublattice="1" List="Al Li" />
      <Constituents Sublattice="2" List="Va" />
    </Sites>
    <AmendPhase Models="IHJREST" />
  </Phase>

  <Phase Id="AL2LI3" Configuration="CEF" State="S" >
<CrystalStructure Prototype="Al2Li3" PearsonSymbol="hR5" SpaceGroup="R-3m" />
    <Sites NumberOf="2" Multiplicities="2 3" >
      <Constituents Sublattice="1" List="Al" />
      <Constituents Sublattice="2" List="Li" />
    </Sites>
  </Phase>

  <Phase Id="AL4LI9" Configuration="CEF" State="S" >
<CrystalStructure Prototype="Al4Li9" PearsonSymbol="mC26" SpaceGroup="C2/m" />
    <Sites NumberOf="2" Multiplicities="4 9" >
      <Constituents Sublattice="1" List="Al" />
      <Constituents Sublattice="2" List="Li" />
    </Sites>
  </Phase>

<!-- Unary Al -->
  <Parameter Id="G(FCC_A1,AL:VA)"  Expr="GHSERAL;" HighT="2900"  Bibref="91Din" />
  <Parameter Id="G(A1_FCC,AL:VA)"  Expr="GHSERAL;" HighT="2900"  Bibref="91Din" />
  <Parameter Id="G(BCC_A2,AL:VA)"  Expr="GHSERAL+10083-4.813*T;" HighT="2900"  Bibref="91Din" />
  <Parameter Id="G(A2_BCC,AL:VA)"  Expr="GHSERAL+10083-4.813*T;" HighT="2900"  Bibref="91Din" />
  <Parameter Id="G(HCP_A3,AL:VA)"  Expr="GHSERAL+5481-1.8*T;" HighT="2900"  Bibref="91Din" />
  <Parameter Id="G(LIQUID,AL)"  Expr="GLIQAL;" HighT="2900"  Bibref="91Din" />

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

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

<!-- Unary Li -->
```

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

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

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

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

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

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

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

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

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

  <Parameter Id="G(BCC_4SL,AL:AL:AL:LI:VA)"  Expr="+GBAL3LI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_4SL,AL:AL:LI:LI:VA)"  Expr="+GB2ALLI;" Bibref="07Hal" />
  <Parameter Id="G(BCC_4SL,AL:LI:AL:LI:VA)"  Expr="+GB2ALLI;" Bibref="07Hal" />
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  <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;" />
  <TPfun Id="GFAL3LI" Expr="+3*UFALLI+1750-4.7*T;" />
  <TPfun Id="GFAL2LI2" Expr="+4*UFALLI;" />
  <TPfun Id="GFALLI3" Expr="+3*UFALLI+4900;" />
  <TPfun Id="SFALLI" Expr="+UFALLI;" />
  <TPfun Id="LDF0ALLI" Expr="+GFAL3LI+1.5*GFAL2LI2+GFALLI3+1.5*SFALLI+4*L0FALLI;" />
  <TPfun Id="LDF1ALLI" Expr="+2*GFAL3LI-2*GFALLI3+4*L1FALLI;" />
  <TPfun Id="LDF2ALLI" Expr="+GFAL3LI-1.5*GFAL2LI2+GFALLI3-1.5*SFALLI+4*L2FALLI;" />

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