The definition of XTDB format version 0.1.6

as proposed by

Scientific group Thermodata Europe (SGTE)

April 6, 2025

Based on paper submitted to Calphad [2]

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1 Introduction

This is the official document defining the XTDB format, last update April 6, 2025. It is based on a format called TDB used since when SGTE developed the 1991 unary database [1]. This unpublished document is available at https://gtihub.com/sundmanbo/XTDB.

All changes of XTDB after versions 0.1.6 are listed in Appendix E

The following text is a the current version of the XTDB format published [2] and is based on the eXtesible Markup Language (XML) [3]. It is intended for thermodynamic databases based on Calphad models and recommended by the Scientific Group Thermodata Europe (SGTE) [4] for use by software in all kinds of applications requiring thermodynamic data for materials and processes.

1.1 How this document is organized

In section 2 all proposed XTDB tags (or elements), and their attributes are listed with a short explanation. In section 3 a more detailed explation are given of some tags and attributes and section 4 there is a list of things to consider. In this document a tag name will be written in **bold** and an attribute name will be written in *italics*.

An XTDB file must use the ASCII character set. The length of a tag and its attributes (excluding nested tags) must not exceed 2000 characters.

In the Appendix A there are several examples of tags and attributes, in Appendix B an extensive list of model tags and their attributes. Each software can have its own **ModelDescription** tag. In Appendix C there aee explanations how some thermodynamic models, such as EBEF in have been integrated in the XTDB format using wildcard feature.

In Appendix D the complete XTDB file for the binary Al-C and Al-Li are listed and in Appendix E all changes and additions to this proposal from earlier versions will be listed.

There is no schema defined for XTDB but it is expected that organisations maintaining large databases for thermodynamic applications will develop their own software based on an XML schema for internal verification of the databases and such software will be able to read XTDB files as well as generate subsets using the XTDB format.

1.2 The basic structure of an XTDB file

The arrangement of tags in the XTDB file is free but for a a human reader and for manual editing of the XTDB file the recommended order is **DatabaseInfo, Defaults** and any **AppendXTDB** tags followed by **Element,**

Species and **Phases** (with many nested tags).

The main part of the XTDB databas are the **Parameter** and **TPfun** tags, which can be ordered by the phases or by the systems. For maintaing a database it may be convenient to keep parameters inside **BinarySystem** tags. The **TernaryXpol** tags should be together binary parameters.

The **Model** tag should appear before any **Phase** or **Parameter** tags and the **Bibliography** at the end or both in a separate**AppendXTBD** file. The **AppendXTDB** tag, which specifices additional files of an XTDB database, allows the database to be split on several files. The **Defaults, DatabaseInfo** and **AppendXTDB** tags and all **Element, Species** and **Phase** tags must be present in the primary XTDB file.

2 The XTDB tags and attributes with short explanations

XML is case sensitive. In XTDB the name of a tag or attribute starts with a capital letter. If it consists of two or more parts, such as **DisorderedPart**, the second part is joined without hyphen or underscore but starts with a capital letter.

The data in an XTDB attribute is case insensitive, i.e. upper and lower case are treated as identical. Many tags have in *Id* attribute which is used in other tags. Its value is case insensitive and there are restrictions on which characters that can be used in an *Id*. See section 3.1.

All tags and their attributes for the XTDB are listed here. Longer explanations of the attributes can be found in section 3. Some tags are optional and many of them will appear several times in the XTDB file to provide the data. An exclamation marek "!M" is indicated for the mandatory attributes of a tag.

2.1 The Gibbs energy function

The XTDB file should be able to describe all data needed to calculate the Gibbs energy for system with several phases using this expression:

$$G \;=\; \sum_{\alpha} \aleph^{\alpha}\; G_M^{\alpha}(T,P,y_{s,i}^{\alpha}) \tag{1}$$

$$G_M^{\alpha} \;=\; \sum_{I} \Pi_{I_s}(y_{s,i}^{\alpha})\; {}^{\circ}G_I^{\alpha}(T,P) - T\; {}^{\mathrm{cfg}}S_M^{\alpha}(y_{s,i}^{\alpha}) +$$
$$ {}^{E}G_M^{\alpha}(T,P,y_{s,i}^{\alpha}) + {}^{\mathrm{phy}}G_M^{\alpha}(T,P,y_{s,i}^{\alpha}) \tag{2}$$

where $\aleph^{\alpha}$ is the number of moles formula unit of α and G_M^{α} is the Gibbs energy of α per mole formula unit as a function of T, P and the constituent fraction i in sublattice s, $y_{s,i}^{\alpha}$. The number of constituents in a phase can be much larger than the number of components of the system. In the term $\Pi_{I_s}(y_{s,i}^{\alpha})\; {}^{\circ}G_I^{\alpha}$ the I indicates an endmember of α representing a possible "compound" with fixed composition, $\Pi_I(y_{s,i}^{\alpha})$ is the probability of the compound I and ${}^{\circ}G_I^{\alpha}$ its Gibbs energy. In a solution it is the contribution from this endmember to the total Gibbs energy of the phase. ${}^{\mathrm{cfg}}S_M^{\alpha}(y_{s,i}^{\alpha})$ is the configurational entropy and ${}^{E}G_M^{\alpha}(T,P,y_{s,i}^{\alpha})$ the contributions from interactions of the constituents mixing on the same sublattice of the phase. If a single endmember represents the constitution of the α phase then ${}^{\mathrm{cfg}}S_M^{\alpha} = {}^{E}G_M^{\alpha} = 0$.

The term ${}^{\mathrm{phy}}G_M^{\alpha}(T,P,y_i^{\alpha})$ is the contribution from various physical models, for example magnetism. This contribution can also be split into a sum of the contributions to each endmember and excess terms. Most physical models have parameters which depend on the constitution and sometimes also T and P. They are discussed in section 2.7. If the phase has charged constituents there is an extra condition for equilibrium that the phase is electrically neutral.

2.2   Thermodynamic software using the XTDB

The TDB file has been used by several thermodynamic softwares but with various flavours making it difficult to exchange databases. It is the hope that the XTDB format will make it easier to handle slight differences between such software and extend the number of models used more easily. In particular the set of new models introduced in the new unary database which will extend the Calphad modeling down to $T = 0$ K. It is expected that the use of TDB files will continue in parallel for many years.

Each software will have its own **Modeldescripton** tags, in particular using different *MPID* attributes for the parameters but any now model should be communication with other software developers to make it easier to handle new models in different software.

2.2.1   Software modifications of names, *Id*

In the TDB file there were strict limits on the length of names (i.e. *Id*) for different things. In the XTDB file there are no such restrictions but it is recommended not to use more than 24 characters in any *Id*. However, a software reading an XTDB file may adjust the length of any *Id* according to its own preference (and the XTDB standard). Such changes should be displayed when reading the XTDB file and saved in a way the user can retrieve a list of all *Id*s changed.

2.2.2   Reading the XTDB file

There are several ways of extracting the information from the XTDB file into a thermodynamic software. Using an XML software tool this will most likely make the whole database available for querys from the thermodynamic software but some software may prefer to read the XTDB file itself and will probably have to read and rewind some or all files several times in order to extract the data for a thermodynamic system selected by a user.

2.3 The basic XTDB tags

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

In this and later tables the "!M" mark at the far left side of an attributes means it is mandatory.

Tag	Attributes	Explanation
XTDB		Containing XML tags for an XTDB database.
!M	Version	Version of XTDB for this file.
!M	Software	Name of software generating the database.
!M	Date	Year/month/day the database was written or last edited
!M	Signature	Name/email of person or organisation generating the database.
Defaults		Optional tag to provide default values of attributes in different XML tags and some other things. Some software, as specified in the XTDB tag, may have some "mandatory" defaults set in the **Models** tag by the software specified in the **XTDB** tag.
	LowT	Default value of low T limit for **TPfun** or **Parameter** tags.
	HighT	Default value of high T limit for **TPfun** or **Parameter** tags.
	Bibref	Default bibliographic reference a parameter.
	Elements	For example "VA" or "/-" (the electron).
	RKorder	see section C.1
	TernaryXpol	see section 2.10
	GlobalModel	Any model applicable to the whole database, for example EEC [11]
DatabaseInfo		Optional tag with information about the database
	Info	Free text (excluding the characters <> &).
	Date	Last update of the database information.
AppendXTDB		Optional tag with additional file for the XTDB database. It should contain XTBD tags but some tags are forbidden, see above.
	Models	File with **ModelDescription** tag.
	Parameters	File with mainly **Parameter** tags.
	TPfuns	File with mainly **TPfun** tags which may have to be rewinded and read several times.
	Bibliography	File with bibliographic tags.
	Miscellaneous	File with whatever the database manager needs.

These tags and the **Element, Species** and **Phases** with its nested tags must be on the primary XTDB file.

2.4   The element and species tags

A XTDB database contains data releted to its **Element** tags. The *Id* attributes of the **Element** and the **Species** tags are used in the **Constituent** tags for the **Phase** tags in the database, as explaind in section 2.6.

A **Species** tag define a chemical species based on the elements, possibly including an electric charge,

Both **Elements** and **Species** can be used as constituents of phases by including their *Id* attribute in *List* attribute the **Constituents** tag of a **Phase** tag.

The vacancy, denoted "VA", is considered an element which must have activity equal to unity at equilibrium but cannot have a fixed amount. The electron, denoted"/-", is not considered as an element but can be used as a fixed charge on a **Species**. A phase with charged species must have an extra internal software condition that the phase is electrically neutral at equilibrium.

Tag	Attributes	Explanation
Element		Specifies a chemical element in the database. In addition the vacancy, denoted "VA", and the electron, 'denoted '/-", are included to handle defects and ions.
!M	Id	Chemical element symbol, one or two latters, for example FE, H. The symbol is case insensitive, see section 3.1. Fictitious element names can be used.
	Refstate	Name of the reference phase, for example GAS. The database may not have any data for this phase.
!M	Mass	Mass in g/mol
	H298	Enthalpy difference between 0 and 298.15 K in the reference state.
	S298	Entropy difference between 0 and 298.15 K in the reference state.
Species		Specifies a chemical species used as a constituent of phases. The elements, except the electron, are also species.
!M	Id	Species name, see below.
!M	Stoichiometry	One or more element *Id*s each followed by an stoichiometric factor, see section 3.2 and Appendix A.1.
	MQMQA	For a constituent in the MQMQA model. See section 3.2.1.
	UNIQUAC	For a constituent in the UNIQUAC model. See section 3.2.2.

There are strong feelinga about upper and lower case for elements and sometimes also for phases. But in the old TDB file they were case insensitive and this has been kept for the XTDB file.

The *Id* attribute of a **Species** must start with a letter A-Z and can contain letters, digits 0-9, the special characters plus, "+", minus, "-" and the slash "/". The *Id* must not be abbreviated when used in the *List* attribute of a **Constituents** tag or in the *Id* of a **Parameter** tag or in any other tag.

The *Id* of a **Species** is important because as constituents of a phase they can be used by the thermodynamic software when setting conditions for a equilibrium calculation or for listing and plotting results. The elements are automatically entered as species with a case insensitive *Id*.

An ion, for example an iron species with positive charge can 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". It is recommended that the *Id* of an ion includes "+" or "-" but it is not necessary.

In some software the constituents are defined for each phase separately and have no separate identification but in other software the species name, i.e. *Id* can be used for setting conditions and used when listing and plotting. The XTDB format must not limit this facility.

2.5   The function and temperature range tags

The thermodynamic model parameters are usually simple mathematical expressions but many of them contain common parts refering to the same element. In order to avoid adding numbers or repeating the same numbers many times one can enter a mathematical expression as a **TPfun** tag and use the *Id* of this **TPfun** inside the *Expr* attribute of several **Parameter** tag or other **Tpfun** tags. It also avoid a lot of problems if the reference data for an element is changed.

Tag	Attributes	Explanation
TPfun		Defines a T, P expression to be used in parameters or other functions.
!M	Id	Function name, section 3.1. The name can be used in the *Expr* attribute of other functions or parameters, see section 3.11.1.
	LowT	Can be omitted if the default low T limit applies.
!M	Expr	Simple mathematical expression terminated by ;. Use the **Trange** tag if several ranges. See section 3.11.1
	HighT	Can be omitted the default high T limit applies.
Trange		Only inside a **TPfun** or **Parameter** tag for an expression with several T ranges.
!M	Expr	Simple mathematical expression terminated by ;. See section 3.11.1.
	HighT	Can be omitted if the default high T limit applies.

The *Id* attribute of a **TPfun** must start with a letter A-Z and can consist of letters, digits 0-9 and the underscore characteter, "_".

See section 3.11.1 for the restrictions of the mathenatical expresson in the *Expr* attribute and Appendix A.2 and others for examples. There is no way at present to handle several pressure ranges in the XTDB file. For high P a separate model for the volume should be used.

The value of a function, as well as its first and second derivatives with respect to T and P, must be continuous across an interval of T range. Breakpoints will normally occur only for **TPfun** of pure element data and those in the unary 1991 [1] have been checked. Using the *Id* of a **TPfun** tag inside another **TPfun** may create infinite loops by circular calls but is left for the software to detect this.

2.6 The phase tag and its nested tags

The phase tag has two "compulsory subtags" i.e. **Sublattices** and **Constituents**.

Tag	Attributes	Explanation
Phase		All thermodynamic data is part of a phase.
!M	Id	Phase name, see sections 3.1 and 3.10.1.
!M	Configuration	Model for the configurational entropy, see section 3.10.2.
	State	G for gas phase, L for liquid phase. Only needed for the liquid if EEC is used.
CrystalStructure		Optional tag inside a **Phase** tag.
	Prototype	Prototype phase
	StructurBericht	For example A3, B2, C14, D0_3 etc.
	PearsonSymbol	Specification.
	SpaceGroup	Specification.
Sublattices		Only once inside a **Phase** tag.
!M	NumberOf	Number of sublattices, an integer value.
!M	Multiplicities	Sites on each sublattice, as many reals as sublattices separated by a space. For an example see Appendix A.3
Constituents		Only inside the **Sublattices** tag.
	Sublattice	Cam be omitted if only one sublattice.
	WyckoffPosition	Optional idenificaton of the sublattice
!M	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. The **DisorderedPhase** tag, see 2.9, can also be nested.
	Models	One or more models *Id*s, separated by a space, for this phase. See section 2.9, Appendices A.3 and B.

The **Phase** tag is important because all parameters with data belongs to a phase and its constituents. The *Id* attribute must start with a letter A-Z and contain only letters, digits 0-9 and the underscore character. It can be abbreviated for example when used in the *Id* of a parameter. See section 2.7.

A phase with very long list of constituents (for example the gas) can have several **Constituents** tags. A solution phase may have several different structure designations depending on its composition and constitutions. Pure Au has *StructurBericht* A1 but alloyed with Cu it can be ordered with *StructurBericht* L1$_2$ or L1$_0$. Some software may provide information of the constitution as an suffix.

The *WyckoffPosition* attribute can simplify relating the sublattice to data from DFT calculatiions. It will normally be ignored by the thermodynamic software.

2.7 The parameter tag

All thermodynamic data, and possibly kinetic and other physical phase dependent properties, are defined by the parameter tags. They should be arranged after the **Phase** tags or inside a **BinarySystem** tag, see 2.11. They can have nested **Trange** tags. See examples in Appendix A.4, C and D.

Tag	Attributes	Explanation
Parameter		Specifies the T, P expression of a model parameter for a set of constituents.
!M	Id	As in a TDB files, for example G(LIQUID,A,B:VA;2),
	LowT	Can be omitted if the default low T limit applies.
!M	Expr	Simple mathematical expression terminated by ;. If several ranges use a **Trange** tag. See section 2.5 and 3.11.1.
	HighT	Can be omitted if the default high T limit applies.
!M	Bibref	Bibliographic reference.

The attribute *Id* defines the parameter as in the current TDB file. It starts with a model parameter identifier (MPID), defined by a **ModelDescription** tag, see Appendix B.1. For a Gibbs energy parameter "G" is used for an endmember and "G" or "L" for an excess parameter.

The MPID is followed, within parenthesis, by a phase name (which can be abbreviated) and one or more constituents in each sublattice of the phase in the order of the sublattices and a final optional degree.

The constituents are given in the order of the sublattices defined by the phase tag, separated by a colon, ":". Constituents in the same sublattice, i.e. for interaction parameters, are separated by a comma, ",". The order of sublattices and their constituents are as defined by the **Phase** tag, see section 2.6.

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

An asterisk "*", also known as wildcard, see section C.3. can be used as constituent in a sublattice indicating that the parameter is independent of the constituents in the sublattice. The wildcard is an important feature of some models, see section C.7.

The parameters constitute the major part of the database and several examples can be found in Appendix C. They are generated from separate assessment of experimental and theoretical data for binary and higher order systems.

One aim of this XTDB format is to provide a simple and unified way to publish and report parameters from such assessments. Databases are collections of such assessment and database managers integrate separate assessment, sometimes with modifications, with other systems. In addition to the bibliographic reference the database managers are encouraged to add comments within the **Parameter** tag in order to pass on information to the next manager of the database.

2.8   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.

It is important to inform the users that thermodynamic databases are not not created by computers or appear from thin air.

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

2.9   The ModelDescription tag

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. Models must be explained in a model tag with an appropriate bibliographic reference. Typically the **ModelDescription** tag is in an AppendXTDB file, for an example see Appendix B. The **ModelDescription** tag and currently used model tags are listed here. The models have an *Id* and normally some attributes, *MPIDi* which specify one or more MPID used in parameters needed for the model. Additional comments outside the attributes can be added describing the model.

The models below represent models used for a lomg time.

Tag	Attributes	Explanation
ModelDescription		Surrounds model tags usually with an *Id* attribute used in the *Models* attribute of a **AmendPhase** tag inside **Phase** tags.
		A model usually specify one or more model parameter identifiers (MPID) needed by the model. Some models, such as **DisorderedPart** must be included a tag within the **AmendPhase** tag.
	Software	Name of software generating this tag. Each software may have its own version of model parameter identifiers and may also have some unique models.
Magnetic		There are several magnetic models.
!M	Id	This is used in *Models* attribute of the **AmendPhase** tag. There are currently 3 variants: IHJBCC, IHJREST and IHJQX explained in Appendix B.
	Aff	The antiferromagnetic factor (-1, -3 or 0). It is redundant but kept for compatibility with TDB file.
!M	MPID1	Specifies the Bohr magnetion number identifier (MPID) for parameters.
!M	MPID2	Specifies the Cure or combined Curie/Neel temperature identifier (MPID) for parameters.
	MPID3	Specifies the Neel temperature in IHJQX model identifier (MPID) for parameters.
!M	Bibref	Where the model is described.
Permutations		For FCC, HCP and BCC lattices a 4 sublattice tetrahedron model, identical permutations of a parameter will be included only once in the XTDB file. See section C.5.
!M	Id	This is used in the *Models* attribute of the **AmendPhase** tag. Its can be either FCC4PERM or BCC4PERM. There are no MPID.
!M	Bibref	Where the model is explained.
DisorderedPart		Optional tag inside the **AmendPhase** tag of an ordered phase with or without order/disorder transions. The Gibbs energies of the ordered and disordered parts of a phase are added as described in section 3.4. The configurational Gibbs energy is calculated for the ordered part only.
	Disordered	Optional attribute with the *Id* of the disordered phase, Some software have the parameters for the ordered and disordered part using the same phase *Id*.
!M	Sum	Number of sublattices, starting from the first sublattice in the ordered phase to be summed for the disordered phase constitution. Optionally an extra interstitial sublattice can be present.
	Subtract	In order to use eq. 6 in section 2.9 the the constituents on the ordering sublattices must be identical and this attribute must be included with the value Y. See also section 2.6.

New **ModelDescription** tags can be developed and included in the XTDB file in order to specify new MPIDs for parameters. Some of the tags below represent models needed for the new unary database.

Tag	Attributes	Explanation
Einstein		The low T vibrational model, see section 3.6.
!M	Id	This Id is used in **AmendPhase** tag.
!M	MPID1	Specifies the Einstein model parameter identifier (MPID) for parameters.
!M	Bibref	Where the model is described.
Liquid2state		The liquid 2-state model, see section 3.8,
!M	Id	This Id is used in **AmendPhase** tag.
!M	MPID1	Specifies liquid model parameter identifier (MPID) for parameters.
!M	MPID2	Specifies Einstein model parameter identifier (MPID) for parameters.
!M	Bibref	Where the model is described.
EEC		Specifies that the Equi-entropy model applies to the database. See section 3.9. The liquid **Phase** tag must also have the *State* attribute equal to L.
!M	Id	has the value EEC.
!M	Bibref	Where the model is described.

2.10 Ternary extrapolation methods

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

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

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

Examples:

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

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

2.11 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 bibliographic 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 the user the database is reliable and to inform the users that thermodynamic databases are not not created by AI or appear from thin air. The number of references for a multicomponent system with 1000 or more parameters from many assessments is very impressive.

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

Tag	Attributes	Explanation
BinarySystem		Encloses a set of **Parameter** tags for different phases of a binary system. There can be parameters for the binary outside this tag. It may have a software dependent attribute to calculate the binary.
!M	Species	Two constituents for the parameters separated by spaces.
!	Bibref	Main bibliographic references.
	CalcDia	Software specific commands to calculate the binary phase diagram. The software is specified in the **XTDB** tag.

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

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

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

2.12 Adding new XML tags or attributes

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

A new tag or attribute should only use letters A-Z, numbers 0-9. The first letter should be capital and any following words should also be captial as in *NumberOf* or **DisorderedPart**.

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

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

This is just a suggestion which has to be elaborated.

3 Further explanation of XTDB tags and attributes

Some additional explanation of the XTDB format is listed here. This text is still preliminary and may be correted and changed.

3.1 About characters and abbreviateion of *Id*

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

The limited set of characters allowed in *Id* are listed for each case. The characters "(" and ")" and colon ":" and semicolon ":" and comma "," are not allowed in the *Id* attribute of **Element, Species, Phase** or **TPfun** tags.

It is not allowed to abbreviate **Species** *Id* and **TPfun** *Id* when used in other tags. Note that the species *Id* is normally not its stoichiometric formula and rather short *Id* are recommended for complex molecules.

Abbreviation of **Phase** *Id* is allowed because there may be many variants of almost the same phase. Each part between the underscore characted can be abbreviated separately, thus two phases MONOCLINIC_A and MONOCLINIC_B can be abbreviated as M_A and M_B.

3.2 Species stoichiometry and properties

The species stoichiometry is a sequence of one or more chemical element names, each followed by a real number specifying its stoichiometric ratio. Following the TDB standard a chemical element with a two letter name does not need a stoichiometric ratio equal to unity, for example MGO for MG1O1. A stoichiometry of unity at the end can also be omitted. Stoichiometric fractions can be specified as AlO3/2 or by real numbers such as AlO1.5. But avoid numbers such as 0.333333, use 1/3.

No grouping using parenthesis are allowed when specifying the stoichiometry, for example use AL2S3O12, not Al2(S1O4)3. It may not be very elegant but computers do not bother about nice formatting.

3.2.1 MQMQA attribute

This is special for the constituents of the MQMQA phase. These constituents represent clusters, also known as "quads", with electrically neutral constituents with one or two cations and one or two anions. The constituents of an MQMQA liquid in a FactSage DAT file, known as quadruplets or "quads" are defined as in the example below:

```
    1   1   5   5   6.00000000      6.00000000      6.00000000      6.00000000
    2   2   5   5   6.00000000      6.00000000      3.00000000      3.00000000
    3   3   5   5   6.00000000      6.00000000      2.00000000      2.00000000
    4   4   5   5   6.00000000      6.00000000      2.00000000      2.00000000
    1   2   5   5   3.00000000      6.00000000      3.00000000      3.00000000
    1   3   5   5   3.00000000      6.00000000      2.40000000      2.40000000
    1   4   5   5   3.00000000      6.00000000      2.40000000      2.40000000
    2   3   5   5   4.00000000      3.00000000      1.33333333      1.33333333
    2   4   5   5   4.00000000      6.00000000      2.00000000      2.00000000
    3   4   5   5   6.00000000      6.00000000      2.00000000      2.00000000
```

For the meaning of the values in this table please see the FactSage documentation or the detailed documentation of the implementation of MQMQA in the Thermochmica software [12]. The intital 4 numbers refer to the different elements, the other are related to the bonds between the elements. There is a software to convert DAT files to XTDB files.

In the XTDB file this table will be writted as below:

```
<Species Id="NA/CL" MQMQA="NA/CL 6 6 2.4" />
<Species Id="MG/CL" MQMQA="MG/CL 6 3 2.4" />
<Species Id="U/CL" MQMQA="U/CL 6 2 2.4" />
<Species Id="PU/CL" MQMQA="PU/CL 6 2 2.4" />
<Species Id="NAMG/CL" MQMQA="NA,MG/CL 3 6 3" />
<Species Id="NAU/CL" MQMQA="NA,U/CL 3 6 2.4" />
<Species Id="NAPU/CL" MQMQA="NA,PU/CL 3 6 2.4" />
<Species Id="MGU/CL" MQMQA="MG,U/CL 4 3 1.3333333" />
<Species Id="MGPU/CL" MQMQA="MG,PU/CL 4 6 2" />
<Species Id="UPU/CL" MQMQA="U,PU/CL 6 6 2" />
```

Where the element numbers have been replaced by the *Id*s of their chemical symbols. One can omitt the stoichiometry as it can be calculated from the MQMQA attribute. The *Id* attribute does not have to refer to the elements but the *MQMQA* attribute must follow some strict rules. The slash, "/" is used to separate cations from the anions, and if there are two cations or anions they must be seapared by a comma, ",". After this there must be as many integers or reals as there are ions and they must be in the order of the ions separated by a space. For "quads" with a single ion in each sublattice, i.e. an "endmember", there must be an FCC/SNN factor at the end, usually 2.4, i.e. there are 3 numbers.

The quads are electrically neutral, an element with several valencies will occur in several quads with different bonds.

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. See also Appendix A.1.

For MQMQA clusters the stoichiometry can maybe be omitted as it can be calculated from the data in the *MQMQA* attribute.

The *Id* attribute is used as constituent of the phase and it does not have to be related to the actual elements in the species. To conform with the normal use of the MQMQA model one can use a slash, "/" to separate the two sublattices.

In a *Stoichiometry* attrbute one can use the slash, "/", between two integers after the element *Id* to specify the stoichiometric factor or a real number. For example use 4/3 rather than 1.333333.

3.2.2 UNIQUAC attribute

This attribute is used for species with the UNIQUAC model. Each molecule is a complex species but are entered as a separate species as there are no chemical reactions between them. The UNIQUAC model calculates the configurational model using the surface area (q) and number of segments (r) of the molecules, specified in the UNIQUAC attribute.

```
    <!-- Element A is acetonitrile and B is N_Helptane -->
    <Element Id="A" />
    <Element Id="B" />
    <Species Id="ACN" Stoichiometry="A" UNIQUAC="1.72 1.87"  />
    <Species Id="N_HEP" Stoichiometry="B" UNIQUAC="4.4 5.17"  />
```

3.3 Properties per mole atom of formula unit

Note that in most physical models the Gibbs energy is defined per mole of atoms. In the Gibbs energy for the phase this must be multiplied with the number of atoms per formula unit. This in eq. 2 the value of $^{\text{phy}}G_M^\alpha$ must normally include the variable $\aleph^\alpha$:

$$^{\text{phy}}G_M^\alpha \quad = \quad \aleph^\alpha \; ^{\text{phy}}G_m \tag{3}$$

where $^{\text{phy}}G_m$ is the contribution per mole of atoms found in textbooks [16]. In earler assessment for the magnetic contribution this was frequently included in the value of the Bohr magneton number was unphysical.

3.4 Using several fraction variables

A phase with a **DisorderedPart** tag 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. The disordered phase many has an extra sublattice 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.

$$y_i^{1,\text{dis}} \quad = \quad \sum_{s=1}^{Sum} a_s y_i^{(s),\text{ord}} \tag{4}$$

where $y_i^{(s)\text{ord}}$ is the constituent fraction of i on sublattice s in the ordered phase and $y_i^{\text{dis},1}$ 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 **DisorderedPart** tag, this phase 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 the disordered parameters have the same phase name as the ordered phase, just a reduced number of sublattices as indicated by the attribute *Sum*.

Calculating a **DisorderedPart** model with the attribute *Subtract* works the same way. The reason to subtract the "ordered" part calculated with the disordered set of fractions was to allow separate assessments of the ordered and disordered phases.

For phases which never disorder, for example the sigma phase, one can also have a "disordered" part with a single sublattice containing the species representing elements as endmembers (and possibly some long range interaction parameters). In Thermo-Calc terminology this is the "NEVER" model. See also the section for EBEF C.7.

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

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

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

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

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

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

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

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

3.5   Permutations and wildcards

The permutations 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_4SL,FE:AL:AL:AL:VA)

has 3 identical permutations:

G(FCC_4SL,AL:FE:AL:AL:VA), G(FCC_4SL,AL:AL:FE:AL:VA) and G(FCC_4SL,AL:AL:AL:FE:VA)

which are not included in the database but taken care of by the software. This reduce the size of the database and avoid human errors. It requires that the software calculates automatcally the contribution from all 4 permutations of the constituents of indentical sides. There are other excess parameters with up to 24 permutations.

The wildcards, see section 2.7 is frequently used for parameters of ordered phases, see Appendix C.3, C.4 and the following sections.

For a phase with the **DisorderedPart** tag the Gibbs energy (excluding the configurational entropy) is calculated by one of these equations:

$$G_M = {}^{\mathrm{dis}}G_M(x) + {}^{\mathrm{ord}}G_M(y) \tag{5}$$
$$G_M = {}^{\mathrm{dis}}G_M(x) + {}^{\mathrm{ord}}G_M(y) - {}^{\mathrm{ord}}G_M(y = x) \tag{6}$$

where x is averaged values of y for some (or all) sublattices in the ordered phase. Eq. 5 is mainly used for phaes with many sublattices which never disorder for example intermetallic phases.

In order to use eq. 6 one must specify the attribute *Subtract* (with any value). This equation can be used for phases with order/disorder transitions such as FCC, BCC and HCP. Such phases are stable as disordered in many systems but sometimes exhitit ordering. Using eq. 6 the model parameters as ordered and disordered phase can be assessed separately because calculating the Gibbs energy of the ordered phase twice, the second time using the disordered fractions, and then subtracting means the ordered parameters will not affect the disorderd state. For details see [6] and [8]

Permutations also applies to interaction parameters, a parameter G(FCC_4SL,A,B:A:A:A) has 4 permutations and G(FCC_4SL,A,B:A,B:A:A) has 6 permutations. The latter is important to approximate the SRO in phases with order/disorder transitions.

Wildcards and permutations are often combined and in fact one often finds parameters as:

G(FCC_4SL,A,B:*:*:*) with 4 permutations and where the wildcard "*" can represent a third (or fourth) element. This is of course an approximation but it works very well. See also the EBEF model C.7.

3.6 The Einstein model and the GEIN function

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 **Parameter** or **TPfun** tag, the GEIN function is defined in eq. 7 in section 3.11.1. For multiple θ see the Al-C example in Appendix D.1.

In the 3rd generation unary project the Einsten function for the low T vibrational heat capacity has been introduced:

$$\text{GEIN}(\theta) \quad = \quad 1.5R\theta + 3RT\ln(1 - \exp(-\theta/T)) \tag{7}$$

where the argument of GEIN function should be a fitted Einstein temparature, θ in Kelvin. This θ must be allowed to vary with the composition of the phase and thus the θ was introduced as a model parameter identifier (MPID) called LNTH in OC. For physical reasons it was decided that the logarithm of θ was a more appropriate value to vary with the composition. In Appendix D.1 the whole assessment of Al-C is listed and below just the G and LNTH parameter for the diamond phase:

```
<Parameter Id="G(DIAMOND,C;0)"  Expr=" +GODIACC+GEDIACC;"  Bibref="20HE" />
<Parameter Id="LNTH(DIAMOND,C;0)"  Expr=" +LN(1601.4467);"  Bibref="20HE" />
```

However, during the assessment it was found that using several θ together with weighting factors (that summed up to unity) a better fit could be obtained. The fitted θ_i and factors f_i are in the table below:

State	f_1	θ_1	f_2	θ_2	f_3	θ_3
Fitted	0.2318	813.637	0.01148	345.35	0.763257	1601.4467
in **TPfun**	0.2318	813.637	0.01148	345.35	-0.236743	1601.4467

Multiple θ is no big surprise as the Einstein function is a simple but rather crude approximation of the low T heat capacity. But for several reasons one cannot have several LNTH parameters and thus one must select one θ to vary with the composition and the other are included in the *Expr* attribute in the **Parameter** tag for the Gibbs energy of C in the diamond phase above. In the **TPfun** GEDIACC the factor for the GEIN function of θ_3 is negative to compensate for the contribution from the LNTH parameter.

```
<TPfun Id="GEDIACC" Expr=" +0.2318*GEIN(813.637)+.01148*GEIN(345.35)-0.236743*GEIN(1601.4467);" />
```

It is recommended to use the function $\text{LN}(\theta)$ in the *Expr* of the LNTH parameter rather than its numeric value to visualize the correspondance with the arguments of the GEIN function.

3.7 The magnetic models

The magnetic contribution to the Gibbs energy was the first separate model for a physical property with composition dependent model parameters.

3.7.1 The Inden-Hillert-Jarl model

This magnetic models introduced already 50 years ago [20, 21] are still used in many databases but one should be careful about the value of the Bohr magneton number for phases with formula units larger than 1.

3.7.2 The Qing-Xiong magnetic model

In this model [23, 24] the Curie and Neel T were modeled as separate composition dependent parameters.

3.8 The 2 state liquid model

This model [25, 26] was introduced in the 3rd generation unary to handle the extrapolation of the thermodynamics of a liquid below its freezing T. It includes an Einstein model for the metastable amorphous phase and a parameter for the transition to the stable liquid.

$$G_M = G_M - RT \ln(1 + \exp(-\frac{G_M^d}{RT})) \tag{8}$$

where G_M^d is a polynomial in T describing the transition from an amorphous state with no translational degrees of freedom to the liquid state.

3.9 The equivalent entropy criterion, EEC

In the 1991 unary database a quick fix was introduced to avoid that the heat capacity of a the solid phase of an element extrapolated to very high values above its melting point. The "SGTE extrapolation" forced the heat capacity of the metastable solid to approch the heat capacity of the liquid phase. But this lead to some compounds, lcking experimental data and using the Kopp-Neumann model for thei heat capacity, to have kinks in their solid range.

A new model [11] for handling this by preventing a solid phase to be stable if its entropy is higher than that of a liquid phase at the same temperature has been introduced in the 3rd generation unary database. The solid and liquid phases do not have to have the same composition.

3.10 The phase tag and attributes

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

3.10.1 The phase Id

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

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

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

3.10.2 The configurational entropy model

For the configurational entropy model there is have

- CEF which can be used for ideal (random) mixing for sublattice models as well as substitutional models.

$$\mathrm{cfg}S_M = \sum_s a_s \sum_i y_{s,i} \ln(y_{s,i}) \tag{9}$$

$$\sum_i y_{s,o} \quad = \quad 1 \tag{10}$$

$$M \quad = \quad \sum_s a_s \tag{11}$$

where $y_{s,i}$ is the constituent fraction of i on sublattice s with a_s sites. M is the formula unit of the phase and if there are vacancies or molecules as species the number of atoms per formula unit may very with the constitution.

- I2SL is the partially ionic 2 sublattice model [17, 18] with variable ration of sites on the cation and anion sublattice.

- MQMQA is the modified quasichemical model in the quadruplet approximation [19] including an approximate short range ordering (SRO) contribution.

3.11 The TPfun and the Parameter tag

An XTDB database will consist mainly of **Parameter** tags, defined in 2.7, and expanations of its use depend very much on the models used. Some further explainations can be found in Appendix C

3.11.1 The Expr attribute of TPfun and Parameter

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

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

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

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

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

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

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

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

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

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

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

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

4 A few more points

A summary of things done and to be considered

1. 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. This XTDB definition will make it easier to collaborate and develop Calphad databases.

2. The ternary extrapolation method is a bew feature. An attribute *TernaryXpol* can be added to the **Defaults**.

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

4. All phase constituents must have a defined *Id* in a **Species** tag in order to make ot possible to use these for setting conditions, listing results and plotting.

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

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

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

8. The GEIN function can be used in the attribute *Expr* of a **Parameter** or a **TPfun**. If a pure element modeled with several Einstein θ only with different weight factors (the sum of which is unity), one of these, normally that with the highest weight, is selected to vary with composition, see section 3.6.

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

10. We should agree on a list of MPID and how to handle software specific MPIDs. However, with the **ModelDescription** tag each software may use its own MPID and each softwar may convert hem to its own preferred value.

    There may be many additional MPID for kinetic and other properties which does not concern the thermodynamic data but they should anyway have welldefined MPIDs.

11. There is no schema for the XTDB format but it is expected that those interested in a more elaborate XML/JSON etc format will provide a converter to/from the XTDB format.

12. There are certainly many more things to take care of but I think it is more important to agree now on a minimum common XTDB format which can make the thermodynamic databases more useful both for experimentalists, assessments, database maintenance and simulations using thermodynamic data as well as for the development of new models and applications.

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

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Appendix A   Some examples

Some examples are not updated to the most recent XTDB format!

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** because one can have a species name which is an 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**(-1);" />
   <Trange HighT="2900" Expr=" -11278.378+188.684153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9);" />
 </TPfun>
...
 <TPfun Id="LFALFE0"  Expr="-104700+30.65*T;" />
 <TPfun Id="LFALFE1"  Expr="+30000-7*T;" />
 <TPfun Id="LFALFE2"  Expr="+32200-17*T;" />
 <TPfun Id="UFALFE"  Expr="-4000+T;" />
 <TPfun Id="GAL3FE"  Expr="+3*UFALFE+9000;" />
```

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

A.3   Phase

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

```
 <Phase Id="LIQUID" Configuration="RKM" state="L" >
    <Sites NumberOf="1"  Multiplicities="1" >
      <Constituents List="AL C" />
    </Sites>
    <AmendPhase Model="LIQ2STATE" />
 </Phase>
...
  <Phase Id="A2_BCC" Configuration="CEF" state="S" >
    <Sites NumberOf="2"  Multiplicities="1  3" >
      <Constituents Sublattice="1" List="AL FE" />
      <Constituents Sublattice="2" List="VA" />
    </Sites>
    <AmendPhase Model="IHJBCC" />
  </Phase>
...
  <Phase Id="AL8FE5_D82" Configuration="CEF" state="S" >
    <Sites NumberOf="2"  Multiplicities="8  5" >
      <Constituents Sublattice="1" List="AL FE" />
      <Constituents Sublattice="2" List="AL FE" />
    </Sites>
  </Phase>
...
  <Phase Id="BCC_4SL" Configuration="CEF" state="S" >
    <Sites NumberOf="5"  Multiplicities="0.25  0.25  0.25  0.25  3" >
      <Constituents Sublattice="1" List="AL FE" />
      <Constituents Sublattice="2" List="AL FE" />
      <Constituents Sublattice="3" List="AL FE" />
      <Constituents Sublattice="4" List="AL FE" />
      <Constituents Sublattice="5" List="VA" />
    </Sites>
    <Disordered_3Part Disordered="A2_BCC" Sum="4" Bibref="09Sun" />
    <AmendPhase Model="IHJBCC BCC4Perm" />
  </Phase>
...
  <Phase Id="SIGMA" Configuration="CEF" State="S" >
    <Sites NumberOf="5" Multiplicities="2 4 8 8 8" >
      <Constituents Sublattice="1" List="MO RE" />
      <Constituents Sublattice="2" List="MO RE" />
      <Constituents Sublattice="3" List="MO RE" />
      <Constituents Sublattice="4" List="MO RE" />
      <Constituents Sublattice="5" List="MO RE" />
    </Sites>
    <Disordered_2Part Sum="5" />
```

```
    </Phase>
```

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

A.4   The Parameter tag

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

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

A.5   The Parameter2 tag

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

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

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

A.6   Models

An extended form of the **Models** tag including references should be provided by SGTE as general **AppendXTDB** file with the tags for all generally accepted models including *Id* and all *MIPID* and detailed

description. But the models used in an XTDB file can also appear in a short form as below.

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

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

The **DisorderedPart** section A.3 must be nested within a **Phase** tag for the ordered phase.

Appendix B   An attempt to summarize model tags and MPIDs.

The XTDB file should include an **AppendXTDB** with a link to the file defining the MPID used for models such as magnetism, low T heat capacity etc. This Appendix is such a file.

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

```
<ModelDescription>
<!-- This is a short explanation of XTDB model tags and their attributes, the models for except for
the configurational entropy.
The AmendPhase tag (nested inside a Phase tag) is used to specify some additional models for the phase
by using the attribute "Id" specified for most of the models below.
In these model tags there are model parameter identifiers (MPID) describing the dependence on composition, T and P.
A DisorderedPart tag must be inside the Phase tag as it has additional information.
The TenaryXpol tag will normally appear together with model parameters for the binaries and has thus a phase attribute.
The EEC tag is global for the whole database if included.
Some model tags and MPIDs are tentative and some attributes of the tags are optional. -->
<Magnetic Id="IHJBCC" MPID1="TC" MPID2="BMAGN" Aff=" -1.00" Bibref="82Her" >
  <!-- f_below_TC= +1-0.905299383*TAO**(-1)-0.153008346*TAO**3-.00680037095*TAO**9-.00153008346*TAO**15; and
  f_above_TC= -.0641731208*TAO**(-5)-.00203724193*TAO**(-15)-.000427820805*TAO**(-25);
  in G=f(TAO)*LN(BMAGN+1) where TAO=T/TC.  Aff is the antiferromagnetic factor.
  TC is a combined Curie/Neel T and BMAGN the average Bohr magneton number. -->
</Magnetic>
<Magnetic Id="IHJREST"  MPID1="TC" MPID2="BMAGN" Aff=" -3.00" Bibref="82Her" >
  <!-- f_below_TC= +1-0.860338755*TAO**(-1)-0.17449124*TAO**3-.00775516624*TAO**9-.0017449124*TAO**15; and
  f_above_TC= -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25);
  in G=f(TAO)*LN(BMAGN+1) where TAO=T/TC.  Aff is the antiferromagnetic factor.
  TC is a combined Curie/Neel T and BMAGN the average Bohr magneton number. -->
</Magnetic>
<Magnetic Id="IHJQX" MPID1="CT" MPID2="NT" MPID3="BMAGN" Aff=" 0.00" Bibref="01Che 12Xio" >
  <!-- f_below_TC= +1-0.842849633*TAO**(-1)-0.174242226*TAO**3-.00774409892*TAO**9-.00174242226*TAO**15
  -.000646538871*TAO**21;
  f_above_TC= -.0261039233*TAO**(-7)-.000870130777*TAO**(-21)-.000184262988*TAO**(-35)-6.65916411E-05*TAO**(-49);
  in G=f(TAO)*LN(BMAGN+1) where TAO=T/CT or T/NT.  Aff is a (redundant) antiferromagnetic factor.
  CT is the Curie T and NT the Neel T and BMAGN the average Bohr magneton number. -->
</Magnetic>
<Einstein Id="GEIN" MPID1="LNTH" Bibref="01Che" >
  <-- The Gibbs energy due to the Einstein low T vibrational model, G=1.5*R*THETA+3*R*T*LN(1-EXP(-THETA/T)).
 The value used for LNTH should be ln(THETA)
  as this varies with composition in a more physically reasonable way. -->
</Einstein>
<Liquid2state Id="LIQ2STATE" MPID1="G2"  MPID2="LNTH" Bibref="88Agr 13Bec" >
  <!-- Unified model for the liquid and the amorphous state which is treated as an Einstein solid.
  The G2 parameter describes the stable liquid and the transition to the amorphous state and
  LNTH is the logarithm of the Einstein THETA for the amorphous phase. -->
</Liquid2state>
<Volume Id="VOLOWP" MPID1="V0"  MPID2="VA" MPID3="VB" Bibref="05Lu" >
  <!-- The volume of a phase as function of T, moderate P and constitution via the model parameters:
  V0 is the volume at the reference state, VA is the integrated thermal expansion and VB is the isothermal
  compressibilty at 1 bar. -->
  </Volume>
```

```
<DisorderedPart Disordered=" " Sum=" " [Subtract=Y] Bibref="97Ans 07Hal" >
  <!-- This tag is nested inside the ordered phase tag.  The disordered fractions are averaged over the number of
  ordered sublattices indicated by Sum.
  The Gibbs energy is calculated separately for the ordered and disordered model parameters and added
  but the configurational Gibbs energy is calculated only for the ordered phase.
 If the attribute Subtract is included the Gibbs energy of the ordered phas is calculated a second time as
disordered and subtracted -->
  Some software has no special disordered phase but all parameters are stored in the ordered one and
  the parameters for the disordered phase has and fewer number of sublattices. -->
</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 liquid phase must not be stable. -->
</EEC>
<TernaryXpol Phase=" " Constituents=" " Xpol=" "  Bibref="01Pel" >
   <!-- The ternary extrapolation of the binary parameters is modified.
   The following Types are recognized: Muggianu, Kohler, Toop and ToopM -->
</TernaryXpol>
<EBEF Id="EBEF" Bibref="18Dup" >
   <!-- The Effective Bond Energy Formalism for phases with multiple sublattices using wildcards, "*", in the
   parameters for sublattices with irrelevant constituents.
   The parameters may also use the short form "constituent@sublattice" in order to specify only the constituents
   in sublattices without wildcards.  It also requires the DisorderedPart model. -->
</EBEF>
<Bibliography>
  <Bibitem Id="82Her" Text="S. Hertzman and B. Sundman, A Thermodynamic analysis of the Fe-Cr system,'
        Calphad, Vol 6 (1982) pp 67-80" />
  <Bibitem Id="88Agr" Text="J. Agren, Thermodynmaics of supercooled liquids and their glass transition,
        Phys Chem Liq, Vol 18 (1988) pp 123-139" />
  <Bibitem Id="97Ans" Text="I. Ansara, N. Dupin, H. L. Lukas and B. Sundman, Thermodynamic assessment of the Al-Ni syst
        J All and Comp, Vol 247 (1997) pp 20-30" />
  <Bibitem Id="01Che" Text="Q. Chen and B. Sundman, Modeling of Thermodynamic Properties for BCC, FCC, Liquid and Amorp
        J Phase Eq, Vol 22 (2001) pp 631-644" />
  <Bibitem Id="01Pel" Text="A. D. Pelton, A General Geometric Thermodynamic Model for Multicomponent  solutions,
        Calphad, Vol 25 (2001) pp 319-328" />
  <Bibitem Id="05Lu" Text="X.-G. Lu, M. Selleby B. Sundman, Implementation of a new model for pressure dependence
        of condensed phases in Thermo-Calc, Calphad, Vol 29 (2005) pp 49-55" />
  <Bibitem Id="07Hal" Text="B. Hallstedt, N. Dupin, M. Hillert, L. Hoglund, H. L. Lukas, J. C. Schuster and N. Solak,
        Calphad, Vol 31 (2007) pp 28-37" />
  <Bibitem Id="09Sun" Text="B. Sundman, I. Ohnuma, N. Dupin, U. R. Kattner and S. G. Fries, An assessment of the
        entire Al-Fe system including D03 ordering, Acta Mater, Vol 57 (2009) pp 2896-2908" />
  <Bibitem Id="12Xio" Text="W. Xiong, Q. Chen, P. A. Korzhavyi and M. Selleby, An improved magnetic model for thermodyn
        Calphad, Vol 39 (2012) pp 11-20" />
  <Bibitem Id="13Bec" Text="C. A. Becker, J. Agren, M. Baricco, Q Chen, S. A. Decterov, U. R. Kattner, J. H. Perepezko,
        and contributions from statistical physics, Phys Stat Sol B (2013) pp 1-20" />
  <Bibitem Id="18Dup" Text="N. Dupin, U. R. Kattner, B. Sundman, M. Palumbo and S. G. Fries, Implementation of an Effec
        Bond Energy Formalism in the Multicomponent Calphad Approach, J Res NIST, Vol 123 (2018) 123020" />
  <Bibitem Id="20Sun" Text="B. Sundman, U. R. Kattner, M. Hillert, M. Selleby, J. Agren, S. Bigdeli, Q. Chen, A. Dinsda
```

```
        B. Hallstedt, A. Khvan, H. Mao and R. Otis, A method for handling the extrapolation of solid crystalline phas
            to temperatures far above their melting point, Calphad, Vol 68 (2020) 101737" />
    </Bibliography>
    </ModelDescription>
```

B.1   Model parameter identifier, MPID

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

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

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

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

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

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

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

```
Indx Ident T P Specification            Status Note
   1 G      T P                              0 Gibbs Energy
   2 TC     - P                              2 Combined Curie/Neel T
   3 BMAG   - -                              1 Average Bohr magneton number
   4 CTA    - P                              2 Curie temperature
   5 NTA    - P                              2 Neel temperature
   7 LNTH   - P                              2 Einstein temperature
   8 V0     - -                              1 Volume at T0, P0
   9 VA     T -                              4 Thermal expansion
  10 VB     T P                              0 Bulk modulus
  12 VS     T P                              0 Diffusion volume parameter
  13 MQ     T P &<constituent#sublattice>;  10 Mobility activation energy
  14 MF     T P &<constituent#sublattice>;  10 RT*ln(mobility freq.fact.)
  15 MG     T P &<constituent#sublattice>;  10 Magnetic mobility factor
  16 G2     T P                              0 Liquid two state parameter
  19 LPX    T P                              0 Lattice param X axis
  20 LPY    T P                              0 Lattice param Y axis
  21 LPZ    T P                              0 Lattice param Z axis
  23 EC11   T P                              0 Elastic const C11
  24 EC12   T P                              0 Elastic const C12
  25 EC44   T P                              0 Elastic const C44
  26 UQT    T P &<constituent#sublattice>;  10 UNIQUAC residual parameter (OC)
  27 RHO    T P                              0 Electric resistivity
  28 VISC   T P                              0 Viscosity
  29 LAMB   T P                              0 Thermal conductivity
  30 HMVA   T P                              0 Enthalpy of vacancy formation (MatCalc)
```

Appendix C   The Parameter tag and how it relates to models

A **Parameter** attribute *Id* defined in section 2.7 starts with a model parameter identifier, MPID, see Appendix B.1. Then follows an opening paramthesis, "(", and a **Phase** *Id* and a comma and the constituents as a list of **Species***Id* separated by commas, "," or colon ":" depedning on the model for the phase and the composition dependence of the parameter. After the last constituent there is either just a closeing parenthesis, ")", or a semicolon, ";", followed by a single digit, called the degree, and a closing parenthesis. Below is an example of a reciprocal parameter in FCC_4SL:

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

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

The T and P dependence is described by the *Expr* attribute explained in section 3.11.1.

C.1 Excess model parameters and degree

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

There are also parameters which take into accound the simultaneous mixing of two or more elements on two or more sublattices. In fact the CEF model allows simultaneous interaction of all constituents on all sublattices. Recently that has been explored to handle interactions on intermetallic phases with many sublattices, see section C.7, using also the wildcard feature in C.3.

C.1.1 The binary Redlich-Kister model

Only the Redlich-Kister binary excess model is allowed. Any other binary excess moldel can always be transformed into a Redlich-Kister model. A phase can have different ternary extrapolation methods, see section 2.10. The parameters for a Redlich-Kister expression for interaction on a sublattice s:

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

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

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

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

C.1.2 The ternary excess model

For ternary parameters Hillert [5] has proposed a symmetric ternary composition dependent parameter L(PHASE,A,B,C;0..3):

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

where

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

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

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

C.1.3 The reciprocal model for phases with sublattices

In the sublattice model one can have independent binary and ternary excess interaction on each sublattice. One can also have simultaneous interaction on two or more sublattices, and the so-called reciprocal parameter signifies interaction with two constituents on two sublattices. This parameter has an important physical significance for the thermodynamics and can approximate short range ordering [7].

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

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

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

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

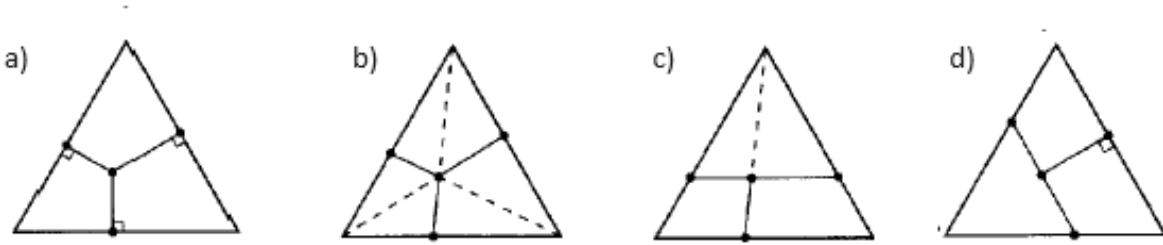## C.2 Ternary extrapolation methods

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

In the Muggianu exgrapolation method the binary compositions are used inside the ternary system without any modifications, see Fig. C1 a). For the Kohler and Toop methods the compositions used for the binay contribution must be adjusted according to the extrapolation method. The method to handle differebt kinds of ternary extrapolations have been explained by Pelton [9] but they are rarely used. At present it is not possible to have different ternary extrapolations on different sublattices. For more details see Appendix C.2.

The ternary extrapolation in a multicomponent system can be different for each ternary combination. In some software one groups the constituents in different groups and if all 3 are in the same group the software use Kohler extrapolation, if one is different from the other two that constituent is considered as Toop element and use a Toop extrapolation of the binaries with that constituent and Kohler for the binary without the Toop element.

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

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

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

Each ternary extrapolation methods must be a separate tag. If it is found necessary one could create a tag to handle several extrapolations in a more practical way.

For the attribute *Xpol* one can use only numbers if 0 is used for a Muggianu extrapolation and the index of the ternary constituent for a Kohler extrapolation and, for a Toop extrapolation the constituent index of the Toop constituent used. Thus "321" means all 3 binaries extrapolates as Kohler. If a binary extrapolates as Toop its Toop constituent index is used for the binary, thus "222" means the same as "T2KT2" above.

As a special case one can use

```
<TernaryXpol Phase=''Liquid'' Constituents=''*'' Xpol="KKK" />
```

when all ternary extrapolations are Kohler. More elaborate cases have to be implemented later, for example arranging the phase constituetns in groups and use Kohler if all 3 constituents are in the same group and Toop if there is one from a different group.

C.3   The use of wildcards for constituents in parameters

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

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

When reading such a set of parameters from a database some software just added the wildcard parameters to the other two. That is mathematically correct but this simple case but for more complex cases with wildcards in several sublattices it is wrong. The parameter with the wildcard must be kept as a an individual parameter, independent of the constituents in that sublattice. The reason for this is explained in the sections C.4 and C.7.

C.4   Modeling order/disorder transitions

Phases with very simple lattices such as BCC, FCC and HCP can have order/disorder transitions which are important for their properties and must be modeled correctly. The ordering means that a set of sites which have identical constitution in the disordered phase can tranform to a state with different constitutions on "identical" sublattices, for example BCC_A2/B2/D0$_3$/B32 or FCC_A1/L1$_2$/L1$_0$. Such order/disorder transition in multicomponent systems can be correctly calculated using sublattices with approximate Short Range Ordering (SRO) using a reciprocal parameter explained in section C.1.3. This means one must use models with 2 or 4 sublattices which, in the disordered state, are identical. To simplify the modeling of such phases the **DisordorderdPart** tag was developed.

The Gibbs energy description of the disordered phase, $^{\mathrm{dis}}G_M$ in eq. 5 include all the endmember parameters for the constituents. If the disordered phase is stable for a significant composition and temperature ranges there can be parameters describing this in $^{\mathrm{dis}}G_M$. In $^{\mathrm{ord}}G_M$ all endmembers with the same constituent in all sublattices are zero because those values are in $^{\mathrm{dis}}G_M$. The endmember parameters in $^{\mathrm{ord}}G_M$ has two or more different constituents and represent the bond energy between constituents on different sublattices.

Phases with order/disorder transition can use the **DisorderedPart** tag and *Subtract* attrubute model if the disordered phase can be assessed independently from the ordered one. But there are still a large number of

endmembers to assess for the ordered part and many of them represent identical configurations. This lead the the permutation model described in the next section.

C.5   Permutation of parameters in ordered phases

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

$$G^{\mathrm{FCC}}_{\mathrm{A:A:A:B}} = G^{\mathrm{FCC}}_{\mathrm{A:A:B:A}} \quad = \quad G^{\mathrm{FCC}}_{\mathrm{A:B:A:A}} = G^{\mathrm{FCC}}_{\mathrm{B:A:A:A}} \tag{C8}$$

$$G^{\mathrm{FCC}}_{\mathrm{A:A:B:B}} = G^{\mathrm{FCC}}_{\mathrm{A:B:B:A}} = G^{\mathrm{FCC}}_{\mathrm{B:B:A:A}} \quad = \quad G^{\mathrm{FCC}}_{\mathrm{B:A:A:B}} = G^{\mathrm{FCC}}_{\mathrm{B:A:B:A}} == G^{\mathrm{FCC}}_{\mathrm{A:B:B:A}} \tag{C9}$$

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

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

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

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

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

C.6   Modeling multicomponent phases with many sublattices

Binary systems with intermetallics can be well described using the sublattice model but require often DFT calculations for their endmembers as they are frequently stable only in a small composition range. These phases use the **DisorderedPart** model without the *Subtract* attribute.

But such binary intermetallics extrapolate badly to ternary and higher order system because there is a large number of endmembers with 3 or more different constituents and, contrary to the phases which can totally disorder, there are no symmetry criteria to reduce them. Using interaction parameters is also meaningless because each sublattice represent only a small change in the overall composition.

This lead to the Effective Bond Enegery Formalism [10] which represent a totally new view of the parameters in the sublattice model.

C.7   The EBEF model use many wildcards

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

For a binary system one can by DFT calculations obtain a set of endmember energies representing a specific constituent in each sublattice. These DFT values can be fitted to a another set of endmembers energies where all but two of the sublattices have wildcards and the other two have different constituents. Several of these

wildcard endmembers have similar overall compositions and one has to be careful that the new set of "wildcard"-endmember energies reproduces the sublattice occupancies for the original DFT calculations.

The extrapolation from binaries to ternaries of such "wildcard" endmembers is very good as shown by Dupin [10]. The reason for this is that fitting the "wildcard" endmembers create an "average" of the bond energies, originally calculated with a fixed constituent in each sublattice, which becomes related to the overall composition rather than the constitution.

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

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

These endmembers can be compared with the excess Gibbs energies for an ordered FCC or BCC when such a parameter has wildcards in the sublattices without the interaction in section C.5. But these parameters cannot be permuted because the sublattices are not identical.

C.8   Maybe a simplified wildcard notation

This is not part of this proposal but may be included in a future version. The EBEF model may increase drastically the parameters with wildcards and if there are more wildcards then actual constituents one could consider using:

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

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

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

C.9   CVM and the cluster site model

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

Appendix D Complete examples

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

```
<Database version="0.0.3">
  <metadata>
    <writer Software="OpenCalphad  6.068" Date="2023-10-26" />
  </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="GEIN" />
  </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="GEIN" />
  </Phase>
  <Phase Id="DIAMOND" Configuration="CEF" State="S" >
    <Sites NumberOf="1" Multiplicities="1" >
      <Constituents Sublattice="1" List="C" />
    </Sites>
    <AmendPhase Models="GEIN" />
  </Phase>
```
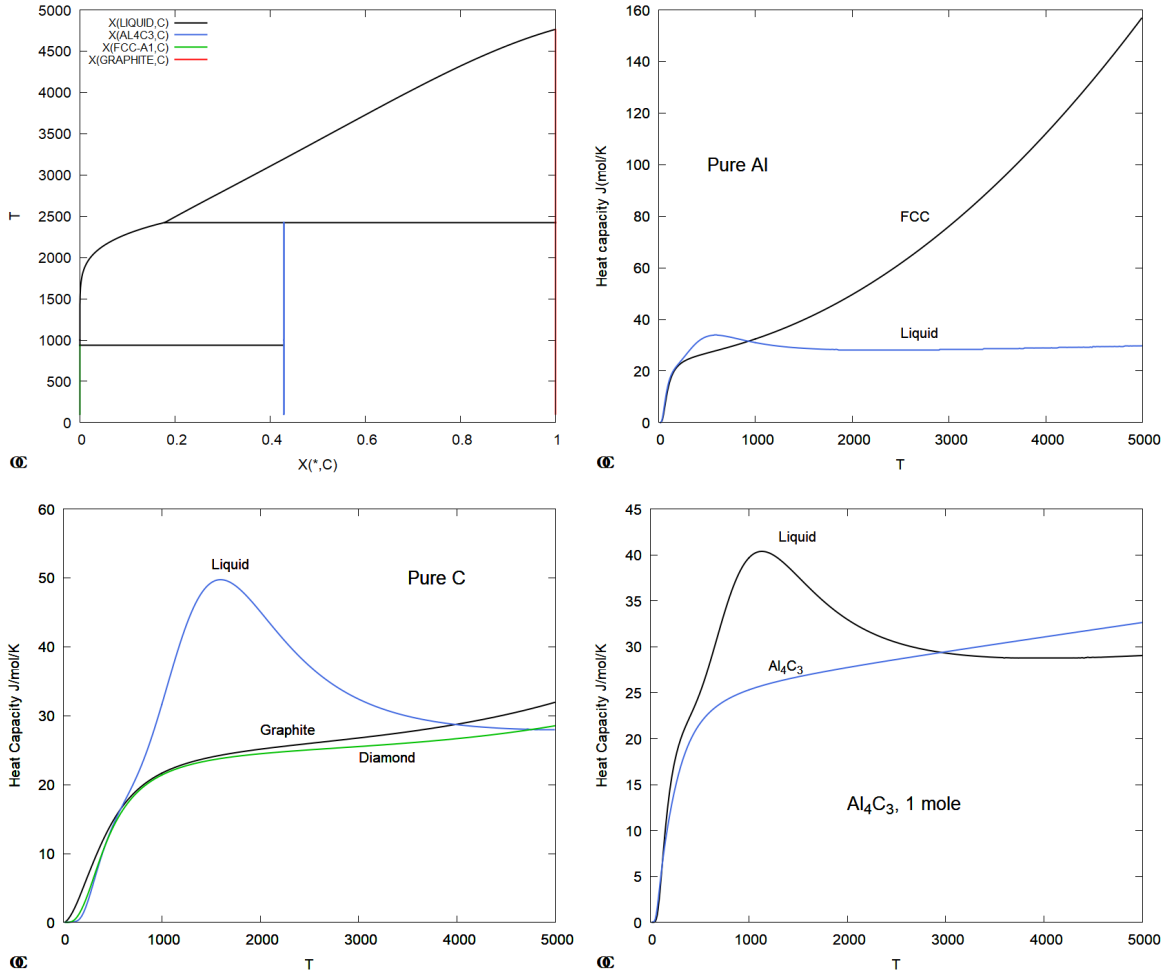
```
    <Phase Id="FCC_A1" Configuration="CEF" State="S" >
      <Sites NumberOf="2" Multiplicities="1 1" >
        <Constituents Sublattice="1" List="AL" />
        <Constituents Sublattice="2" List="C VA" />
      </Sites>
      <AmendPhase Models="GEIN" />
    </Phase>
    <Phase Id="GRAPHITE" Configuration="CEF" State="S" >
      <Sites NumberOf="1" Multiplicities="1" >
        <Constituents Sublattice="1" List="C" />
      </Sites>
      <AmendPhase Models="GEIN" />
    </Phase>
    <Phase Id="HCP_A3" Configuration="CEF" State="S" >
      <Sites NumberOf="2" Multiplicities="1 0.5" >
        <Constituents Sublattice="1" List="AL" />
        <Constituents Sublattice="2" List="C VA" />
      </Sites>
      <AmendPhase Models="GEIN" />
    </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" />
    <Bibliography>
      <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" />
    </Bibliography>
</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.

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

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

The first version in section D.2.1 has been generated using a TDB file where the disordered part of the 4 sublattice FCC and BCC phases has been described by separate phases A1_FCC and A2_BCC. In the **DisorderedPart** tag with the *Subtract* attribute 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 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" />
```

```xml
      </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>
    <Disordered_3Part Disordered="A1_FCC" Sum="4" />
    <AmendPhase Models="IHJREST FCC4PERM" />
  </Phase>

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

<!-- Disordered part of BCC_4SL, identical to BCC_A2 -->
```

```xml
  <Phase Id="A2_BCC" Configuration="CEF" State="S" >
<CrystalStructure Prototype="W" PearsonSymbol="cI2" SpaceGroup="Im-3m" />
    <Sites NumberOf="2" Multiplicities="1 3" >
      <Constituents Sublattice="1" List="Al Li" />
      <Constituents Sublattice="2" List="Va" />
    </Sites>
    <AmendPhase Models="IHJBCC" />
  </Phase>

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

  <Phase Id="HCP_A3" Configuration="CEF" State="S" >
<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" />
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    <AmendPhase Models="IHJREST" />
  </Phase>

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


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  <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" />

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

```
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    <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;" />
    <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;" />
```

```
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        <TPfun Id="SB2ALLI" Expr="+15000;" />
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        <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" parameters together with in the ordered FCC and BCC phases. The parameters for the disordered phas have one sublattices replacing the ordered sublattices.

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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  <metadata>
    <writer Software="OpenCalphad  6.067" Date="2023-10-15" />
  </metadata>
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  <Element Id="LI" Refstate="BCC_A2" Mass="6.941000E+00" H298="4.632000E+03" S298="2.912000E+01" />
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  <Species Id="LI" Stoichiometry="LI" />
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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);
    <Trange Expr="-11278.378+188.684153*T-31.748192*T*LN(+T)-1.230524E+28*T**(-9);" HighT="2900" />
  </TPfun>
  <TPfun Id="GLIQAL" Expr=" +11005.029-11.841867*T+GHSERAL+7.9337E-20*T**7;" HighT="933.47" >
    <Trange Expr="-795.996+177.430178*T-31.748192*T*LN(+T);" HighT="2900" />
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  <TPfun Id="GHSERLI" LowT="200" Expr=" -10583.817+217.637482*T-38.940488*T*LN(+T)+.035466931*T**2-1.9869816E
    <Trange Expr="-559579.123+10547.8799*T-1702.88865*T*LN(+T)+2.25832944*T**2-.000571066077*T**3+33885874*T*
    <Trange Expr="-9062.994+179.278285*T-31.2283718*T*LN(+T)+.002633221*T**2-4.38058E-07*T**3-102387*T**(-1);
  </TPfun>
  <TPfun Id="GLIQLI" LowT="200" 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)+.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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<TPfun Id="LDF1ALLI" Expr=" +2*GFAL3LI-2*GFALLI3+4*L1FALLI;" />
<TPfun Id="LDF2ALLI" Expr=" +GFAL3LI-1.5*GFAL2LI2+GFALLI3-1.5*SFALLI+4*L2FALLI;" />
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<TPfun Id="GFAL3LI" Expr=" +3*UFALLI+1750-4.7*T;" />
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</Phase>
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  <Sites NumberOf="2" Multiplicities="2 3" >
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      <AmendPhase Models="BCC4PERM" />
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      <Sites NumberOf="2" Multiplicities="1 1" >
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    </Phase>
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      <Sites NumberOf="5" Multiplicities="0.25 0.25 0.25 0.25 1" >
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    <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(AL2LI3,AL:LI;0)"  Expr=" +2*GHSERAL+3*GHSERLI-93990+34.5*T;"  Bibref="07HAL" />
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    <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" />
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    <Parameter Id="G(BD3_BCC,AL:AL:AL:LI:VA;0)"  Expr=" +GBAL3LI;"  Bibref="07HAL" />
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  <Parameter Id="G(BD3_BCC,LI:LI:AL:LI;VA;0)"  Expr=" +GBALLI3;"  Bibref="07HAL" />
  <Parameter Id="G(BD3_BCC,AL,LI:AL,LI:*:*:VA;0)"  Expr=" +SB1ALLI;"  Bibref="07HAL" />
  <Parameter Id="G(BD3_BCC,AL,LI:*:*:*:VA;0)"  Expr=" +L0BALLI;"  Bibref="07HAL" />
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    <Bibitem Id="98SAU2" Text="N. Saunders, COST 507, Final report round 2, 1998; Al-Li" />
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Appendix E Some highlights and significant changes from earlier versions

1. The definition is as in the tentative paper