

A summary of the XML tags and attributes

A complete and maybe updated version is available at <https://github.com/sundmanbo/XTDB>. Tagnames are **bold** and names of attributes are in *italics*. Attributes which are mandatory are indicated by a !M to the left. Some explanations at the end.

Table 1: Global tags

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

Table 2: The Element and Species tags

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

Table 3: The phase tag. All data belong to a phase.

Tag	Attributes	Explanation
Phase		All thermodynamic data is part of a phase.
!M	Id	Phase name, special rules apply.
!M	Configuration	Model for the configurational entropy.
	State	Needed if EEC is used.
CrystalStructure		Optional inside a Phase tag.
	Prototype	Prototype phase
	StrukturBericht	For example A3, B2, C14, D0_3 etc.
	PearsonSymbol	For example hR21 cI2.
	SpaceGroup	For example 127, 166.
Sublattices		Only once inside a Phase tag.
!M	NumberOf	Number of sublattices, an integer value > 0 .
!M	Multiplicities	One real value > 0 for each sublattice.
Constituents		Only inside the Sublattices tag.
	Sublattice	Can be omitted if only one sublattice.
	WyckoffPosition	Optional specification.
!M	List	Species <i>Id</i> separated by a space.
AmendPhase		Optional tag inside a Phase tag to specify a contribution from a physical model.
	Models	One or more model <i>Ids</i> , separated by a space. There can be an DisorderedPart tag inside this tag.

Table 4: The function tag. Use the **Trange** tag if several T ranges, no provision for breakpoints in P .

Tag	Attributes	Explanation
TPfun		Defines a T, P expression to be used in parameters or other functions.
!M	Id	The <i>Id</i> can be used in the <i>Expr</i> attribute of other functions or parameters.
	LowT	Can be omitted if the default low T limit applies.
!M	Expr	Simple mathematical expression, possibly terminated by “;”.
	HighT	Can be omitted if the default high T limit applies.
Trange		Only inside a TPfun or Parameter tag for an expression with several T ranges. The function and its first and second derivative must be continuous.
!M	Expr	Simple mathematical expression possibly terminated by “;”.
	HighT	Can be omitted if the default high T limit applies.

Table 5: The parameter tag. These tags the central part of an XTDB database. The very compact form used in TDB files is retained.

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

Table 6: The bibliography for parameters

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

Table 7: The tags for current TDB models

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

Table 8: The tags for the new unary database

Tag	Attributes	Explanation
Einstein		The low T vibrational model.
!M	Id	This Id is used in AmendPhase tag.
!M	MPID1	Specifies the MPID for the Einstein θ .
!M	Bibref	Where the model is described.
Liquid2state		The liquid 2-state model.
!M	Id	This Id is used in AmendPhase tag.
!M	MPID1	Specifies the MPID for the 2-state transition energy.
!M	MPID2	Specifies the MPID for the Einstein θ for the low T extrapolation.
!M	Bibref	Where the model is described.
EEC		Specifies that the Equi-entropy model applies to the whole database.
!M	Id	has the value EEC.
!M	Bibref	Where the model is described.

Table 9: Miscellaneous tags

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

Table 10: Summary of all tags

Tag	Use
XTDB	Must start an XTDB file.
Defaults	Optional default values.
DatabaseInfo	Optional database information.
AppendXTDB	Optional extra XTDB files for a large database.
Element	Element data.
Species	Species data. Species are constituents of phases.
Phase	Phase data, constituents and models.
CrystalStructure	Optional inside a Phase tag.
Sublattices	Only once inside a Phase tag.
Constituents	Only inside a Sublattices tag.
AmendPhase	Only once inside a Phase tag.
TPfun	Specifies Id and expression.
Trange	Inside a TPfun tag.
Parameter	Parameter identification and expression.
Bibliography	Surrounds parameter bibliograpy.
Bibitem	Bibliographic reference for a Parameter .
ModelDescriptions	Surrounds model definition tags.
Magnetic	Specifies Id and MPID for a magnetic model for a phase.
Permutation	Specifies Id for a permutation model for a phase.
DisorderedPart	Optional specification of a phase with a disordred part.
Einstein	Specifies Id and MPID for the Einstein model.
Liquid2State	Specifies Id and MPID for the Liquid 2-state model.
EEC	Specifies Id for the Equal Entropi Criterium model.
TernaryXpol	Specifies a extrapolation model for a ternary.
BinarySystem	Optional specification for an assessed binary.