As sent for publication

Appendix A. Definition of XTDB tags

Appendix B. Examples of XTDB files

Appendix B.1. A complete Al-C database

```
<XTDB version="0.1.5">
<Defaults LowT="10" HighT="6000" Elements="VA /-" />
<Element Id="AL" Refstate="FCC_A1" Mass="26.982" H298="4577.3" S298="28.322" />
<Element Id="C" Refstate="GRAPHITE" Mass="12.011" H298="1054" S298="5.7423" />
<Species Id="VA" Stoichiometry="VA" />
<Species Id="AL" Stoichiometry="AL" />
<Species Id="C" Stoichiometry="C" />
<Phase Id="LIQUID" Configuration="CEF" State="L" >
  <Sublattices NumberOf="1" Multiplicities="1" >
    <Constituents Sublattice="1" List="AL C" />
  </Sublattices>
 <AmendPhase Models="LIQ2STATE" />
</Phase>
<Phase Id="AL4C3" Configuration="CEF" State="S" >
  <Crystallography PearsonSymbol="hR21" SpaceGroup="166" Prototype="Al4C3" />
  <Sublattices NumberOf="2" Multiplicities="4 3" >
    <Constituents Sublattice="1" List="AL" />
    <Constituents Sublattice="2" List="C" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<Phase Id="BCC_A2" Configuration="CEF" State="S" >
  <Crystallography Structurbericht="A2" PearsonSymbol="cI2" Prototype="W" />
```

```
  <Sublattices NumberOf="2" Multiplicities="1 3" >
    <Constituents Sublattice="1" List="AL" />
    <Constituents Sublattice="2" List="C VA" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<Phase Id="DIAMOND" Configuration="CEF" State="S" >
  <Crystallography StructurBerict="A4" PearsonSymbol="cF8" Prototype="C" />
  <Sublattices NumberOf="1" Multiplicities="1" >
    <Constituents Sublattice="1" List="C" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<Phase Id="FCC_A1" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="A1" PearsonSymbol="cF4" Prototype="Cu" />
  <Sublattices NumberOf="2" Multiplicities="1 1" >
    <Constituents Sublattice="1" List="AL" />
    <Constituents Sublattice="2" List="C VA" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<Phase Id="GRAPHITE" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="A9" PearsonSymbol="hP4"  Prototype="C" />
  <Sublattices NumberOf="1" Multiplicities="1" >
    <Constituents Sublattice="1" List="C" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
```

```
</Phase>
<Phase Id="HCP_A3" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="A3" PearsonSymbol="hP2" Prototype="Mg" />
  <Sublattices NumberOf="2" Multiplicities="1 0.5" >
    <Constituents Sublattice="1" List="AL" />
    <Constituents Sublattice="2" List="C VA" />
  </Sublattices>
  <AmendPhase Models="GEIN" />
</Phase>
<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(+813.6)+.01148*GEIN(+345.4)
       -0.236743*GEIN(+1601.4);" />
<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(+1953.3)+0.121519*GEIN(+448)
       +0.3496843*GEIN(+947)+.0388463*GEIN(+192.7)+.005840323*GEIN(+64.5);" />
<Parameter Id="G(LIQUID,AL;0)" Expr=" +G0LIQAL;" Bibref="21HE" />
<Parameter Id="LNTH(LIQUID,AL;0)" Expr=" +LN(+254);" Bibref="21HE" />
```

<Parameter Id="GD(LIQUID,AL;0)" Expr=" +13398-R*T-0.16597*T*LN(+T);" Bibref="21HE" />

<Parameter Id="G(LIQUID,C;0)" Expr=" +G0LIQCC;" Bibref="21HE" />

<Parameter Id="LNTH(LIQUID,C;0)" Expr=" +LN(+1400);" Bibref="21HE" />

<Parameter Id="GD(LIQUID,C;0)" Expr=" +59147-49.61*T+2.9806*T*LN(+T);" Bibref="21HE" />

<Parameter Id="G(LIQUID,AL,C;0)" Expr=" +20994-22*T;" Bibref="21HE" />

<Parameter Id="G(AL4C3,AL:C;0)" Expr=" +G0AL4C3-3.08*GEIN(+401)+3.08*GEIN(+1077);" Bibref

<Parameter Id="LNTH(AL4C3,AL:C;0)" Expr=" +LN(+401);" Bibref="21HE" />

<Parameter Id="G(BCC_A2,AL:C;0)" Expr=" +GTSERAL+3*GTSERCC+1006844;" Bibref="21HE" />

<Parameter Id="LNTH(BCC_A2,AL:C;0)" Expr=" +LN(+863);" Bibref="21HE" />

<Parameter Id="G(BCC_A2,AL:VA;0)" Expr=" +G0BCCAL;" Bibref="21HE" />

<Parameter Id="LNTH(BCC_A2,AL:VA;0)" Expr=" +LN(+233);" Bibref="21HE" />

<Parameter Id="G(BCC_A2,AL:C,VA;0)" Expr=" -819896+14*T;" Bibref="21HE" />

<Parameter Id="G(DIAMOND,C;0)" Expr=" +G0DIACC+GEDIACC;" Bibref="21HE" />

<Parameter Id="LNTH(DIAMOND,C;0)" Expr=" +LN(+1601.4);" Bibref="21HE" />

<Parameter Id="G(FCC_A1,AL:C;0)" Expr=" +GTSERAL+GTSERCC+57338;" Bibref="21HE" />

<Parameter Id="LNTH(FCC_A1,AL:C;0)" Expr=" +LN(+549);" Bibref="21HE" />

<Parameter Id="G(FCC_A1,AL:VA;0)" Expr=" +GHSERAL;" Bibref="21HE" />

<Parameter Id="LNTH(FCC_A1,AL:VA;0)" Expr=" +LN(+283);" Bibref="21HE" />

<Parameter Id="G(FCC_A1,AL:C,VA;0)" Expr=" -70345;" Bibref="21HE" />

<Parameter Id="G(GRAPHITE,C;0)" Expr=" +GHSERCC;" Bibref="21HE" />

<Parameter Id="LNTH(GRAPHITE,C;0)" Expr=" +LN(+1953.3);" Bibref="21HE" />

<Parameter Id="G(HCP_A3,AL:C;0)" Expr=" +GTSERAL+0.5*GTSERCC+2176775;" Bibref="21HE" />

<Parameter Id="LNTH(HCP_A3,AL:C;0)" Expr=" +LN(+452);" Bibref="21HE" />

<Parameter Id="G(HCP_A3,AL:VA;0)" Expr=" +G0HCPAL;" Bibref="21HE" />

<Parameter Id="LNTH(HCP_A3,AL:VA;0)" Expr=" +LN(+263);" Bibref="21HE" />

<Parameter Id="G(HCP_A3,AL:C,VA;0)" Expr=" 0;" Bibref="21HE" />

<Bibliography>

```
<Bibitem Id="21HE" Text="Z. He, B. Kaplan, H. Mao, M. Selleby, Calphad (2021) 102250" />
</Bibliography>
</XTDB>
```

Appendix B.2. A σ phase with EBEF and DisorderedPart

```
<Element Id="AL" Refstate="FCC_A1" Mass="26.982" H298="4577.3" S298="28.322" />
<Element Id="Cr" Refstate="BCC_A2" Mass="51.996" H298="4050" S298="23.56" />
<Element Id="FE" Refstate="BCC_A2" Mass="55.847" H298="4489" S298="27.28" />

<Phase Id="SIGMA" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="D8_b" PearsonSymbol="tP30" SpaceGroup="P4_2/mnm" />
  <Sublattices NumberOf="5" Multiplicities="2 4 8 8 8" >
    <Constituents Sublattice="1" List="AL CR FE" />
    <Constituents Sublattice="2" List="AL CR FE" />
    <Constituents Sublattice="3" List="AL CR FE" />
    <Constituents Sublattice="4" List="AL CR FE" />
    <Constituents Sublattice="5" List="AL CR FE" />
  </Sublattices>
  <AmendPhase > <!-- EBEF is used for the parameters -->
    <DisorderedPart Sum="5" />
  </AmendPhase>
</Phase>

<!-- Endmember parameters are in the disordered part. They are for a single atom and
     should be multiplied by 30 (the sum of the multiplicities) by the software. -->

<Parameter Id="G(SIGMA,AL;0)" Expr=" +GSIGMA_AL;" Bibref="SGTE2025"/>
```

```
<Parameter Id="G(SIGMA,CR;0)" Expr=" +GSIGMA_CR;" Bibref="SGTE2025"/>
<Parameter Id="G(SIGMA,FE;0)" Expr=" +GSIGMA_FE;" Bibref="SGTE2025"/>

<!-- Below the 20 EBEF excess endmember parameters for the ordered part of Al-Cr.
     Without wildcards there are 32 endmembers.  The * can represent any element -->

<Parameter Id="G(SIGMA,AL:CR:*:*:*;0)" Expr=" SIGMA_X_AL1CR2;" />
<Parameter Id="G(SIGMA,AL:*:CR:*:*;0)" Expr=" SIGMA_X_AL1CR3;" />
<Parameter Id="G(SIGMA,AL:*:*:CR:*;0)" Expr=" SIGMA_X_AL1CR4;" />
<Parameter Id="G(SIGMA,AL:*:*:*:CR;0)" Expr=" SIGMA_X_AL1CR5;" />
<Parameter Id="G(SIGMA,*:AL:CR:*:*;0)" Expr=" SIGMA_X_AL2CR3;" />
<Parameter Id="G(SIGMA,*:AL:*:CR:*;0)" Expr=" SIGMA_X_AL2CR4;" />
<Parameter Id="G(SIGMA,*:AL:*:*:CR;0)" Expr=" SIGMA_X_AL2CR5;" />
<Parameter Id="G(SIGMA,*:*:AL:CR:*;0)" Expr=" SIGMA_X_AL3CR4;" />
<Parameter Id="G(SIGMA,*:*:AL:*:CR;0)" Expr=" SIGMA_X_AL3CR5;" />
<Parameter Id="G(SIGMA,*:*:*:AL:CR;0)" Expr=" SIGMA_X_AL4CR5;" />
<Parameter Id="G(SIGMA,CR:AL:*:*:*;0)" Expr=" SIGMA_X_CR1AL2;" />
<Parameter Id="G(SIGMA,CR:*:AL:*:*;0)" Expr=" SIGMA_X_CR1AL3;" />
<Parameter Id="G(SIGMA,CR:*:*:AL:*;0)" Expr=" SIGMA_X_CR1AL4;" />
<Parameter Id="G(SIGMA,CR:*:*:*:AL;0)" Expr=" SIGMA_X_CR1AL5;" />
<Parameter Id="G(SIGMA,*:CR:AL:*:*;0)" Expr=" SIGMA_X_CR2AL3;" />
<Parameter Id="G(SIGMA,*:CR:*:AL:*;0)" Expr=" SIGMA_X_CR2AL4;" />
<Parameter Id="G(SIGMA,*:CR:*:*:AL;0)" Expr=" SIGMA_X_CR2AL5;" />
<Parameter Id="G(SIGMA,*:*:CR:AL:*;0)" Expr=" SIGMA_X_CR3AL4;" />
<Parameter Id="G(SIGMA,*:*:CR:*:AL;0)" Expr=" SIGMA_X_CR3AL5;" />
<Parameter Id="G(SIGMA,*:*:*:CR:AL;0)" Expr=" SIGMA_X_CR4AL5;" />
```

```
<!-- There are also 20 EBEF endmember parameters for Al-Fe and Cr-Fe -->

<Parameter Id="G(SIGMA,AL:FE:*:*:*;0)" Expr=" SIGMA_X_AL1FE2;" />

<Parameter Id="G(SIGMA,CR:FE:*:*:*;0)" Expr=" SIGMA_X_CR1FE2;" />
```

The **TPfun**s SIGMA_X_AsBt can be fitted to DFT calculated endmembers. In a ternary EBEF there are 63 parameters, without wildcards there are $3^5 = 243$ endmembers.

Appendix B.3. A σ phase with EBEF and DisorderedPart

Below is a suggestion of a future possibility for a shorter notation.

```
<Element Id="AL" Refstate="FCC_A1" Mass="26.982" H298="4577.3" S298="28.322" />
<Element Id="Cr" Refstate="BCC_A2" Mass="51.996" H298="4050" S298="23.56" />
<Element Id="FE" Refstate="BCC_A2" Mass="55.847" H298="4489" S298="27.28" />

<Phase Id="SIGMA" Configuration="CEF" State="S" >
  <Crystallography StructurBericht="D8_b" PearsonSymbol="tP30" SpaceGroup="P4_2/mnm" />
  <Sublattices NumberOf="5" Multiplicities="2 4 8 8 8" >
    <Constituents Sublattice="1" Wyckoff="2a" List="AL CR FE" />
    <Constituents Sublattice="2" Wyckoff="4f" List="AL CR FE" />
    <Constituents Sublattice="3" Wyckoff="8i1" List="AL CR FE" />
    <Constituents Sublattice="4" Wyckoff="8i2" List="AL CR FE" />
    <Constituents Sublattice="5" Wyckoff="8j" List="AL CR FE" />
  </Sublattices>
  <AmendPhase > Models="EBEF"  <!-- EBEF notation is used for the parameters -->
```

```
    <DisorderedPart Sum="5" />
  </AmendPhase>
</Phase>

<!-- Endmember parameters in the disordered part as in~\ref{sc:sigma-ebef.}
     The notation below use @ character indicate the sublattice of the constituent
     in the ordered part.  -->

<Parameter Id="G(SIGMA,AL@1:CR@2)" Expr=" SIGMA_X_AL1CR2;" />
<Parameter Id="G(SIGMA,AL@1:CR@3)" Expr=" SIGMA_X_AL1CR3;" />
<Parameter Id="G(SIGMA,AL@1:CR@4)" Expr=" SIGMA_X_AL1CR4;" />
<Parameter Id="G(SIGMA,AL@1:CR@5)" Expr=" SIGMA_X_AL1CR5;" />
<Parameter Id="G(SIGMA,AL@2:CR@3)" Expr=" SIGMA_X_AL2CR3;" />
<Parameter Id="G(SIGMA,AL@2:CR@4)" Expr=" SIGMA_X_AL2CR4;" />
```

Appendix B.4. An FCC phase with wildcards and DisorderedPart

```
<Element Id="AL" Refstate="FCC_A1" Mass="26.982" H298="4577.3" S298="28.322" />
<Element Id="Cr" Refstate="BCC_A2" Mass="51.996" H298="4050" S298="23.56" />
<Element Id="FE" Refstate="BCC_A2" Mass="55.847" H298="4489" S298="27.28" />
<Element Id="C"  Refstate="GRAPHITE" Mass="12.011" H298="1054" S298="5.7423" />

<Phase Id="FCC_4SL" Configuration="CEF" State="S" >
  <Sublattices NumberOf="5" Multiplicities="0.25 0.25 0.25 0.25 1" >
    <Constituents Sublattice="1" List="AL CR FE" />
    <Constituents Sublattice="2" List="AL CR FE" />
    <Constituents Sublattice="3" List="AL CR FE" />
```

```
    <Constituents Sublattice="4" List="AL CR FE" />
    <Constituents Sublattice="5" List="Va C" />
  </Sublattices>
  <AmendPhase Models="IHJREST GEIN FCC4PERM" >
    <DisorderedPart Sum="4" Subtract="N" />
  </AmendPhase>
</Phase>

<!-- The first 4 sublattices are for L1_2 and L1_0 ordering.
     Endmember parameters in the disordered part with no ordering.
     There can also be excess parameters to describe the disordered state.
     The disordered parameters are for the same phase, but have fewer sublattices. -->
<Parameter Id="G(FCC_4SL,AL:VA;0)" Expr=" +GHSERAL;" Bibref="21HE" />
<Parameter Id="LNTH(FCC_4SL,AL:VA;0)" Expr=" +LN(+283);" Bibref="21HE" />
<Parameter Id="G(FCC_4SL,AL:C;0)" Expr=" +GTSERAL+GTSERCC+57338;" Bibref="21HE" />
<Parameter Id="LNTH(FCC_4SL,AL:C;0)" Expr=" +LN(+549);" Bibref="21HE" />
<Parameter Id="G(FCC_4SL,CR:VA;0)" Expr=" +GFCC_CR;" Bibref="SGTE2025"/>
<Parameter Id="G(FCC_4SL,FE:VA;0)" Expr=" +GFCC_FE;" Bibref="SGTE2025"/>

<!-- Some excess parameters to descrive the stable disordered phase -->
<Parameter Id="G(FCC_4SL,AL:C,VA;0)" Expr=" -70345;" Bibref="21HE" />
<Parameter Id="G(FCC_4SL,AL,CR:VA;0)" Expr=" GFCC_X_ALCR0;" />
<Parameter Id="G(FCC_4SL,AL,CR:VA;1)" Expr=" GFCC_X_ALCR1;" />

<!-- Some examples of parameters in the ordered part of the FCC phase.
     A parameter G(FCC_4SL,AL:AL:AL:CR:VA;0) is permuted 4 times.
     A parameter G(FCC_4SL,AL:AL:CR:CR:VA;0) is permuted 6 times.  -->
```

```
<Parameter Id="G(FCC_4SL,AL:AL:AL:CR:VA;0)" Expr=" GFCC_AL3CR1;" />
<Parameter Id="G(FCC_4SL,AL:AL:CR:CR:VA;0)" Expr=" GFCC_AL2CR2;" />
<Parameter Id="G(FCC_4SL,AL:CR:CR:CR:VA;0)" Expr=" GFCC_AL1CR3;" />
<Parameter Id="G(FCC_4SL,AL:AL:AL:FE:VA;0)" Expr=" GFCC_AL3FE1;" />

<!-- An excess parameters with wildcards using the assumption that the AL-CR
     interaction is independent of the constituents on the other sublattices.
     This parameter is also permuted 4 times. -->
<Parameter Id="G(FCC_4SL,AL,CR:*:*:*:VA;0)" Expr=" GFCC_XO_ALCR;" />

<!-- This parameter approximate SRO both in ordered and disordered,
     it is permuted 6 times.  -->
<Parameter Id="G(FCC_4SL,AL,CR:AL,CR:*:*:VA;0)" Expr=" GFCC_SRO_ALCR;" />
```