Review and Update:

Multistate, *Multicomponent* and *Multicompartment Species* Package for SBML Level 3

(SBML-Multi Specification, Version 1, Release 0.1, draft Rev369)

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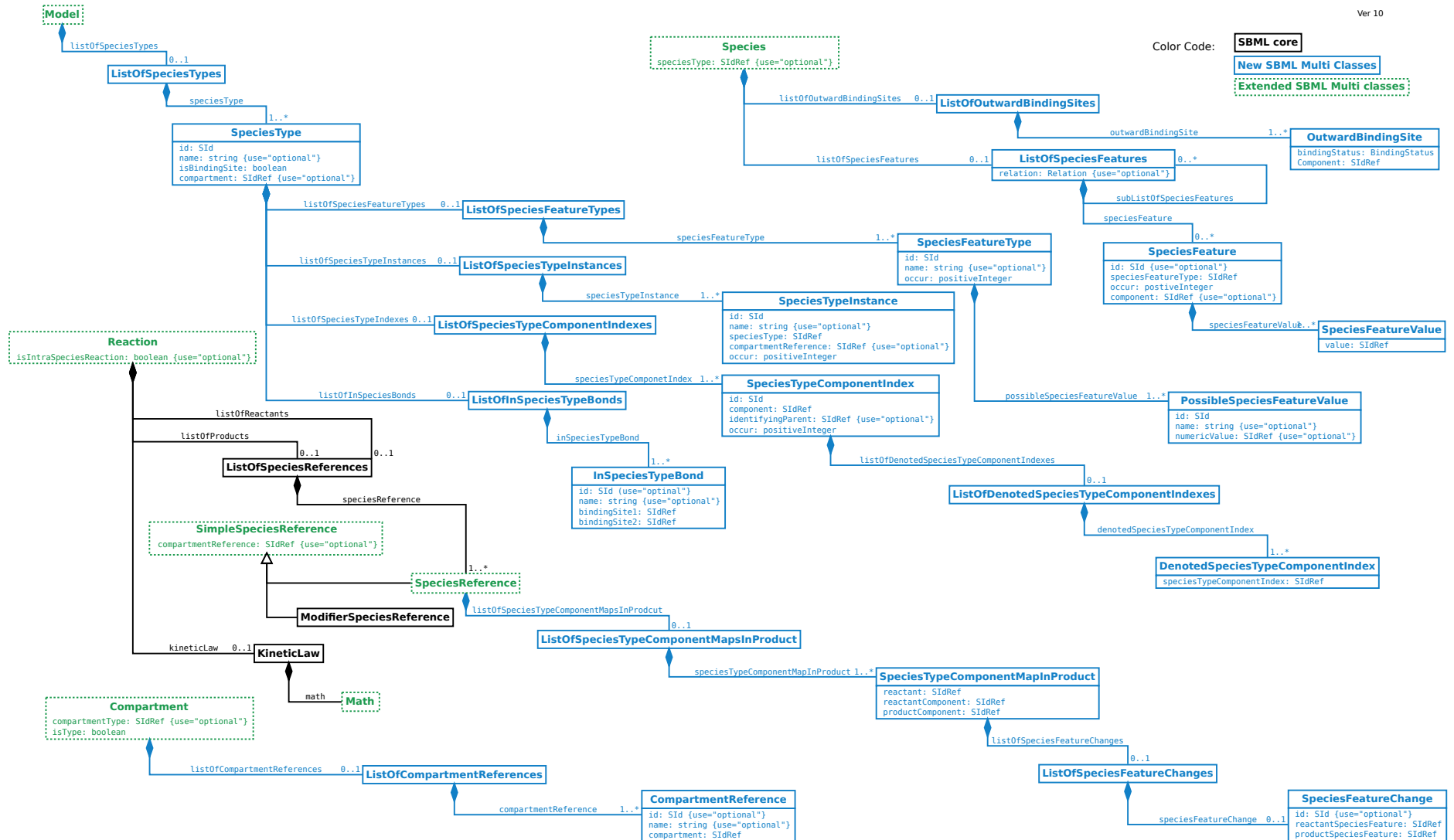
COMBINE, Paris 2013

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And all the people who contributed to the discussions on the sbml-multi list
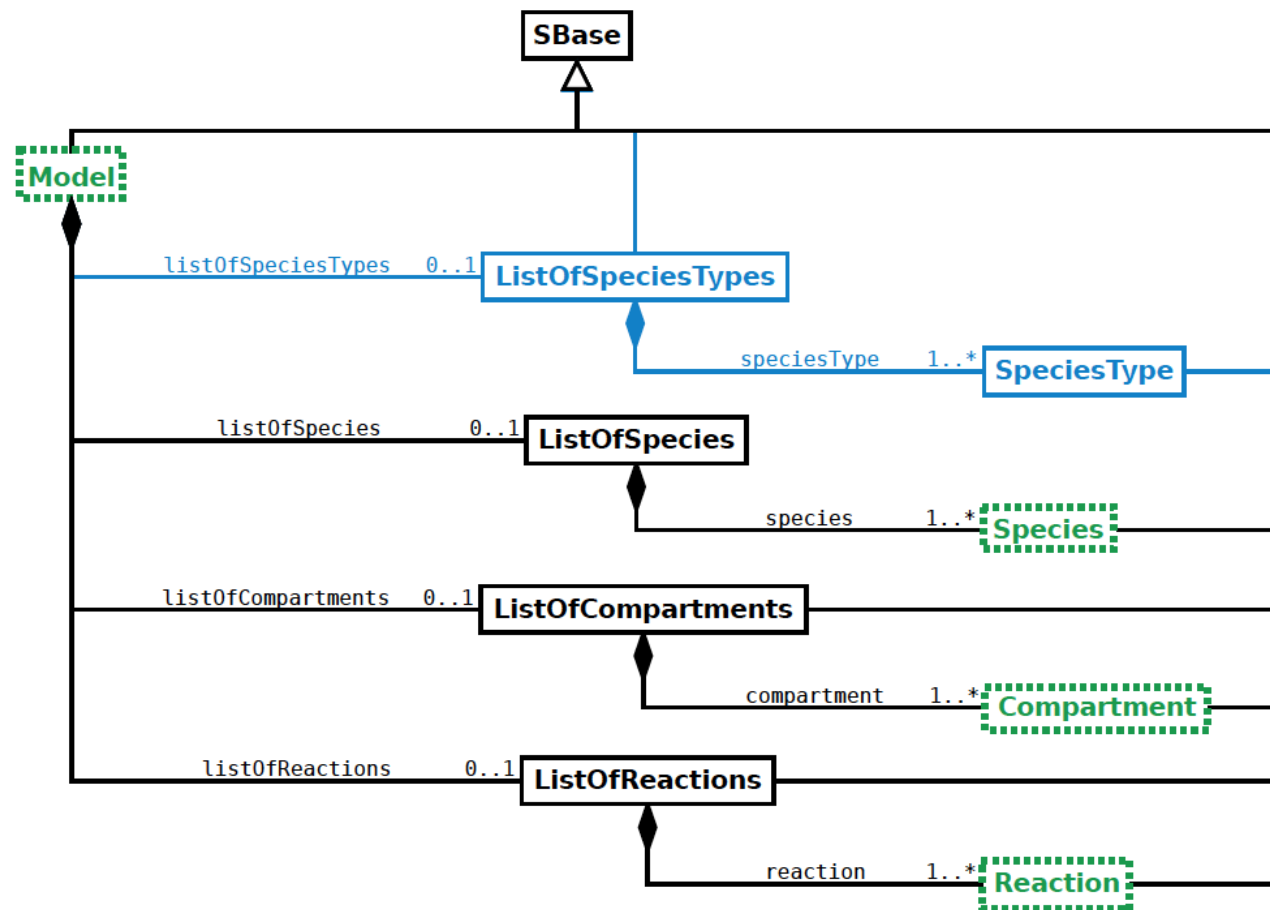
Major Development after HARMONY 2013

- New draft specification covers all features in previous proposals with detailed description of the semantics

- New **SpeciesTypeComponentIndex** replaces ~~**SpeciesTypeInstanceReference**~~

- Multiple occurrences of components and features

  - For example, a molecule may have

    - 10 binding sites of the same type.

    - 8 domains of the same "phosphorylation" type.

- Variable properties/behaviors among multiple occurrences of the same component or feature

  - For example,

    - 2 of 10 binding sites are "*unbound*", the others can be either "*bound*" or "*unbound*"

    - 3 of 8 phosphorylation domains are "phosphorylated", 1 of 8 is "*unphosphorylated*", and the other can be either.

- Optional numericValue for features
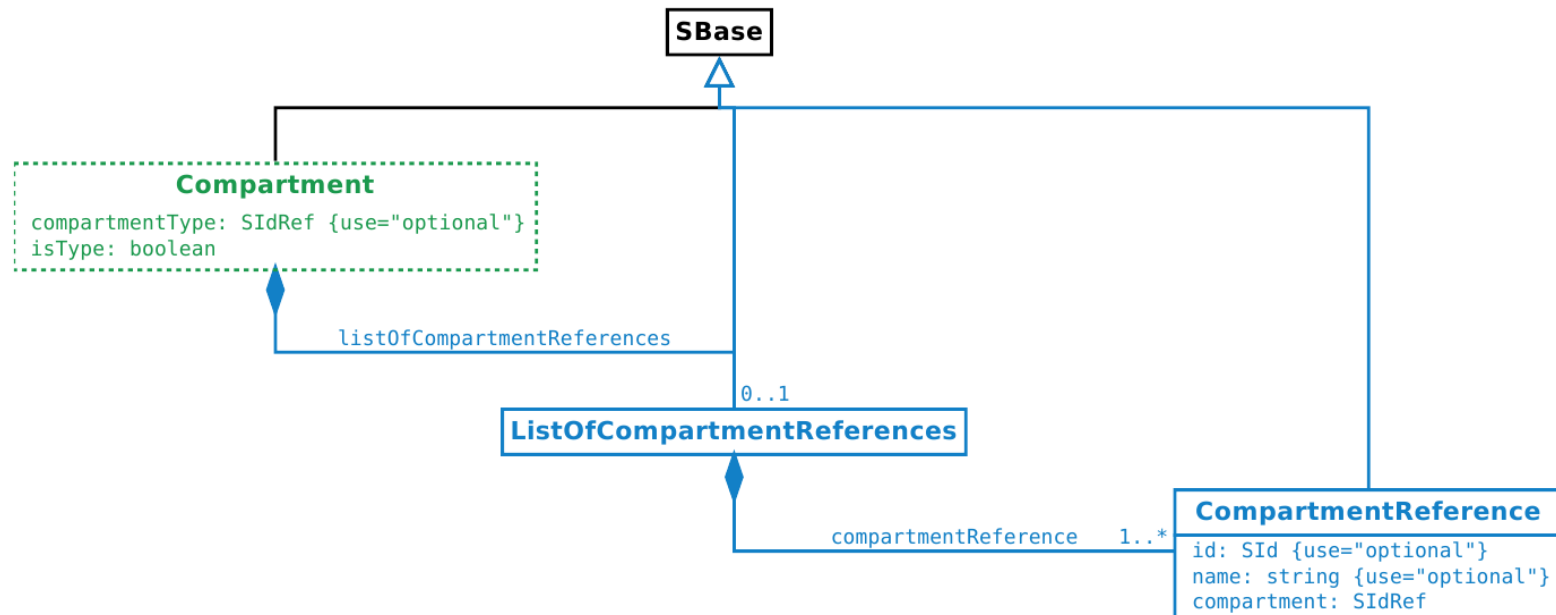
- Revised examples

"Full" UML

Ver 10

Color Code:
- **SBML core**
- **New SBML Multi Classes**
- **Extended SBML Multi classes**

Model
listOfSpeciesTypes

ListOfSpeciesTypes 0..1

speciesType

SpeciesType 1..*
- id: SId
- name: string {use="optional"}
- isBindingSite: boolean
- compartment: SIdRef {use="optional"}

Species
- speciesType: SIdRef {use="optional"}

listOfOutwardBindingSites 0..1

ListOfOutwardBindingSites

outwardBindingSite 1..*

OutwardBindingSite
- bindingStatus: BindingStatus
- Component: SIdRef

listOfSpeciesFeatures 0..1

ListOfSpeciesFeatures 0..*
- relation: Relation {use="optional"}

subListOfSpeciesFeatures

speciesFeature 0..*

SpeciesFeature
- id: SId {use="optional"}
- speciesFeatureType: SIdRef
- occur: positiveInteger
- component: SIdRef {use="optional"}

listOfSpeciesFeatureTypes 0..1

ListOfSpeciesFeatureTypes

speciesFeatureType 1..*

SpeciesFeatureType
- id: SId
- name: string {use="optional"}
- occur: positiveInteger

speciesFeatureValue 1..*

SpeciesFeatureValue
- value: SIdRef

listOfSpeciesTypeInstances 0..1

ListOfSpeciesTypeInstances

speciesTypeInstance 1..*

SpeciesTypeInstance
- id: SId
- name: string {use="optional"}
- speciesType: SIdRef
- compartmentReference: SIdRef {use="optional"}
- occur: positiveInteger

listOfSpeciesTypeIndexes 0..1

ListOfSpeciesTypeComponentIndexes

speciesTypeComponetIndex 1..*

SpeciesTypeComponentIndex
- id: SId
- component: SIdRef
- identifyingParent: SIdRef {use="optional"}
- occur: positiveInteger

possibleSpeciesFeatureValue 1..*

PossibleSpeciesFeatureValue
- id: SId
- name: string {use="optional"}
- numericValue: SIdRef {use="optional"}

Reaction
- isIntraSpeciesReaction: boolean {use="optional"}

listOfInSpeciesBonds 0..1

ListOfInSpeciesTypeBonds

inSpeciesTypeBond 1..*

InSpeciesTypeBond
- id: SId {use="optinal"}
- name: string {use="optional"}
- bindingSite1: SIdRef
- bindingSite2: SIdRef

listOfDenotedSpeciesTypeComponentIndexes 0..1

ListOfDenotedSpeciesTypeComponentIndexes

denotedSpeciesTypeComponentIndex 1..*

DenotedSpeciesTypeComponentIndex
- speciesTypeComponentIndex: SIdRef

listOfReactants
listOfProducts 0..1 0..1

ListOfSpeciesReferences

speciesReference

SimpleSpeciesReference
- compartmentReference: SIdRef {use="optional"}

1..*

SpeciesReference

ModifierSpeciesReference

kineticLaw 0..1 **KineticLaw**

math **Math**

listOfSpeciesTypeComponentMapsInProdcut 0..1

ListOfSpeciesTypeComponentMapsInProduct

speciesTypeComponentMapInProduct 1..*

SpeciesTypeComponentMapInProduct
- reactant: SIdRef
- reactantComponent: SIdRef
- productComponent: SIdRef

listOfSpeciesFeatureChanges 0..1

ListOfSpeciesFeatureChanges

speciesFeatureChange 0..1

SpeciesFeatureChange
- id: SId {use="optional"}
- reactantSpeciesFeature: SIdRef
- productSpeciesFeature: SIdRef

Compartment
- compartmentType: SIdRef {use="optional"}
- isType: boolean

listOfCompartmentReferences 0..1

ListOfCompartmentReferences

compartmentReference 1..*

CompartmentReference
- id: SId {use="optional"}
- name: string {use="optional"}
- compartment: SIdRef
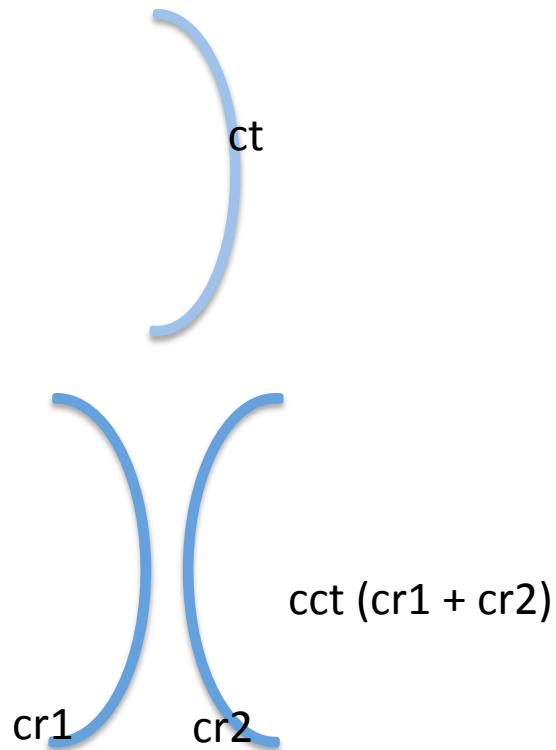
Model

Compartment

- **Compartment**
  - *compartmentType*: reference to a "*isType=true*" compartment
  - *isType*: if "*true*", can not be initialized directly.
- **CompartmentReference**
  - *compartment*: reference to a "sub" compartment

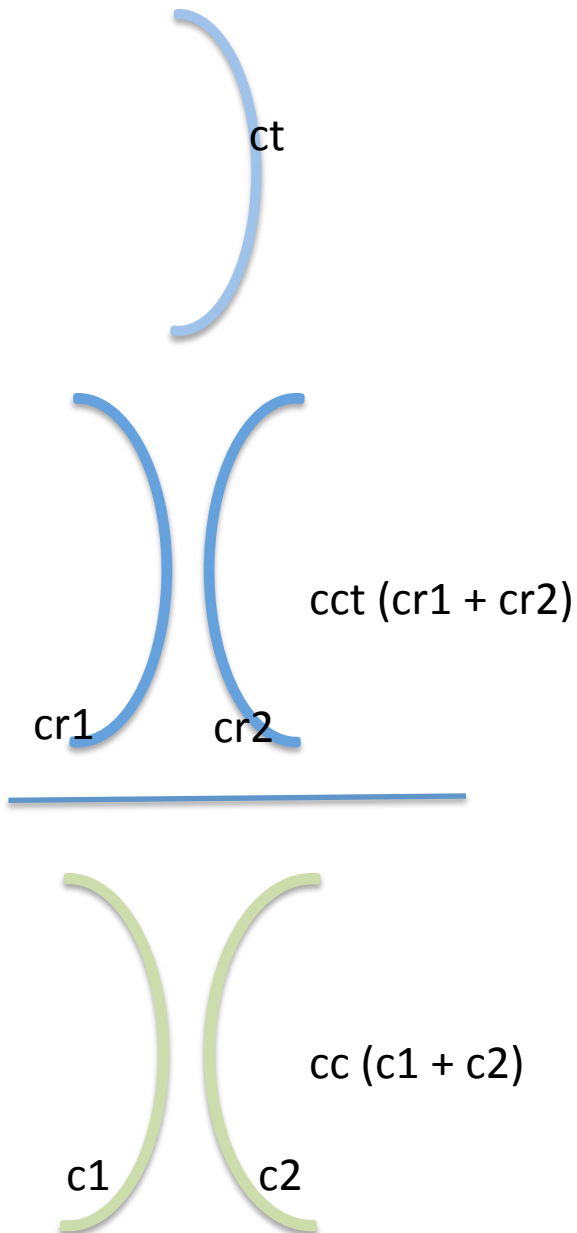# Compartment

ct

`<compartment id="ct" multi:isType="true" />`

Compartment

ct

cct (cr1 + cr2)

cr1   cr2

```
<compartment id="ct" multi:isType="true" />
<compartment id="cct" multi:isType="true">
  <multi:listOfCompartmentReferences>
    <multi:compartmentReference multi:id="cr1"
      multi:compartment="ct" />
    <multi:compartmentReference multi:id="cr2"
      multi:compartment="ct" />
  </multi:listOfCompartmentReferences>
</compartment>
```
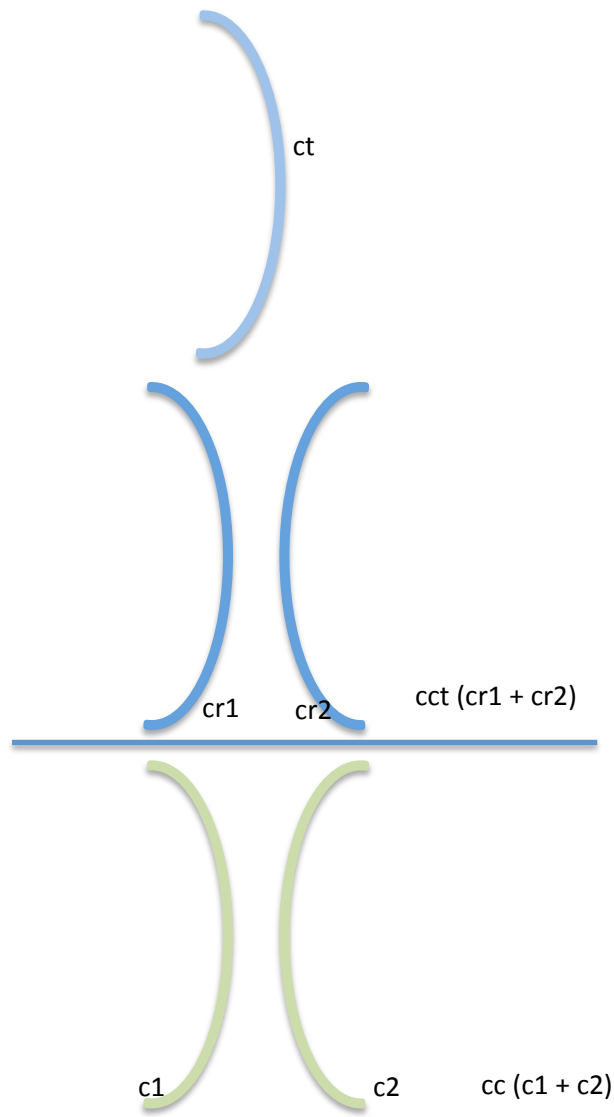
Compartment

ct

cct (cr1 + cr2)

cr1   cr2

cc (c1 + c2)

c1   c2

```
<compartment id="ct" multi:isType="true" />
<compartment id="cct" multi:isType="true">
  <multi:listOfCompartmentReferences>
    <multi:compartmentReference multi:id="cr1"
      multi:compartment="ct" />
    <multi:compartmentReference multi:id="cr2"
      multi:compartment="ct" />
  </multi:listOfCompartmentReferences>
</compartment>
<compartment id="c1" multi:isType="false"
  multi:compartmentType="ct" />
<compartment id="c2" multi:isType="false"
  multi:compartmentType="ct" />
<compartment id="cc" multi:isType="false"
  multi:compartmentType="cct">
  <multi:listOfCompartmentReferences>
    <multi:compartmentReference multi:compartment="c1" />
    <multi:compartmentReference multi:compartment="c2" />
  </multi:listOfCompartmentReferences>
</compartment>
```
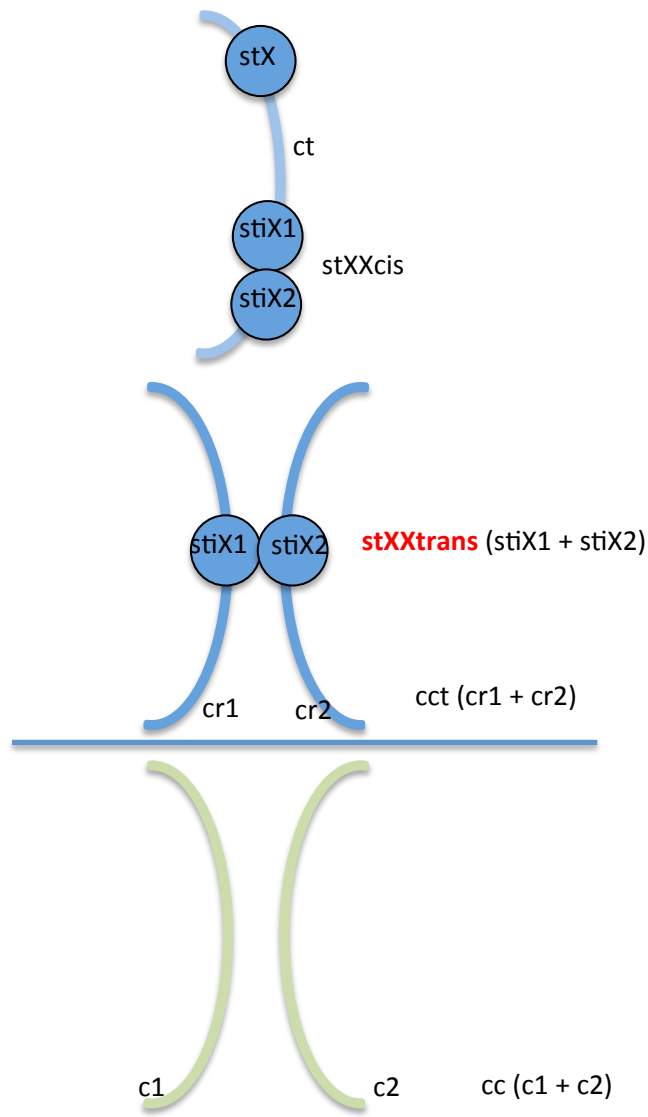
# SpeciesType

# SpeciesType, SpeciesTypeInstance, InSpeciesTypeBond and Species

**SpeciesType**

id: SId
name: string {use="optional"}
isBindingSite: boolean
compartment: SIdRef {use="optional"}

**Species**

speciesType: SIdRef {use="optional"}

listOfSpeciesTypeInstances

0..1

**ListOfSpeciesTypeInstances**

listOfSpeciesFeatureTypes

listOfSpeciesComponentIndexes

speciesTypeInstance

1..*

listOfInSpeciesTypeBonds

0..1

**SpeciesTypeInstance**

id: SId
name: string {use="optional"}
speciesType: SIdRef
compartmentReference: SIdRef {use="optional"}
occur: positiveInteger

**ListOfInSpeciesTypeBonds**

inSpeciesTypeBond

1..*

**InSpeciesTypeBond**

id: SId (use="optinal"}
name: string {use="optional"}
bindingSite1: SIdRef
bindingSite2: SIdRef

# Compartment, SpeciesType, SpeciesTypeInstance, InSpeciesTypeBond and Species

ct

cr1  cr2  cct (cr1 + cr2)

c1  c2  cc (c1 + c2)
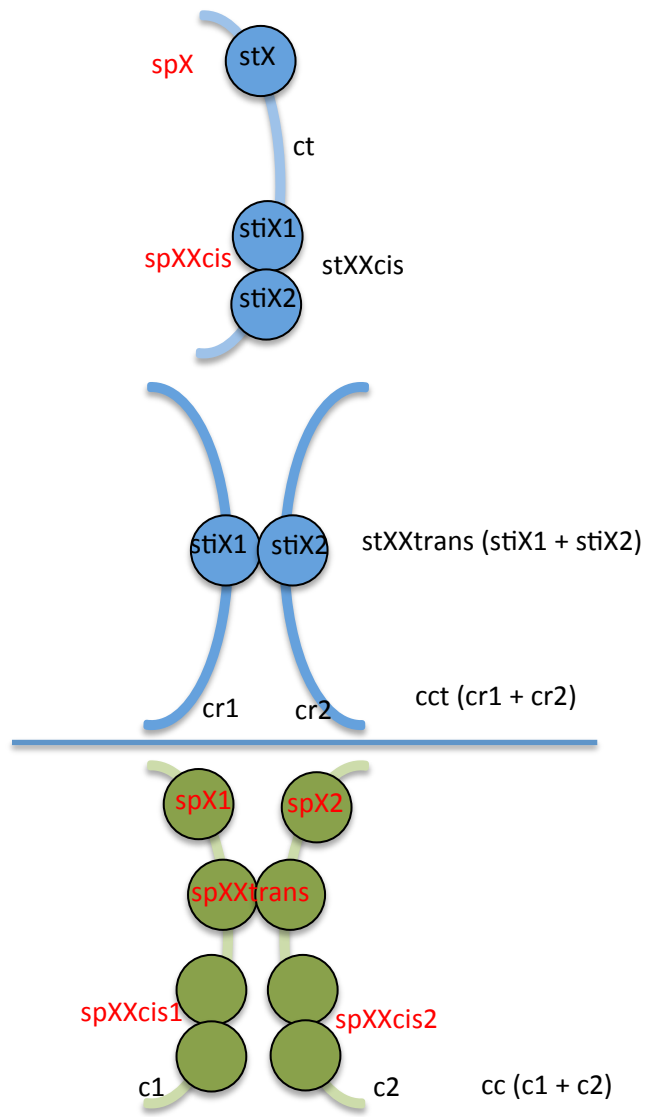
```
<compartment id="ct" multi:isType="true" />
<compartment id="cct" multi:isType="true">
  <multi:listOfCompartmentReferences>
    <multi:compartmentReference multi:id="cr1"
      multi:compartment="ct" />
    <multi:compartmentReference multi:id="cr2"
      multi:compartment="ct" />
  </multi:listOfCompartmentReferences>
</compartment>
<compartment id="c1" multi:isType="false"
  multi:compartmentType="ct" />
<compartment id="c2" multi:isType="false"
  multi:compartmentType="ct" />
<compartment id="cc" multi:isType="false"
  multi:compartmentType="cct">
  <multi:listOfCompartmentReferences>
    <multi:compartmentReference multi:compartment="c1" />
    <multi:compartmentReference multi:compartment="c2" />
  </multi:listOfCompartmentReferences>
</compartment>
```

# Compartment, SpeciesType, SpeciesTypeInstance, InSpeciesTypeBond and Species



stX

ct

stiX1

stXXcis

stiX2

cr1    cr2    cct (cr1 + cr2)

c1     c2     cc (c1 + c2)
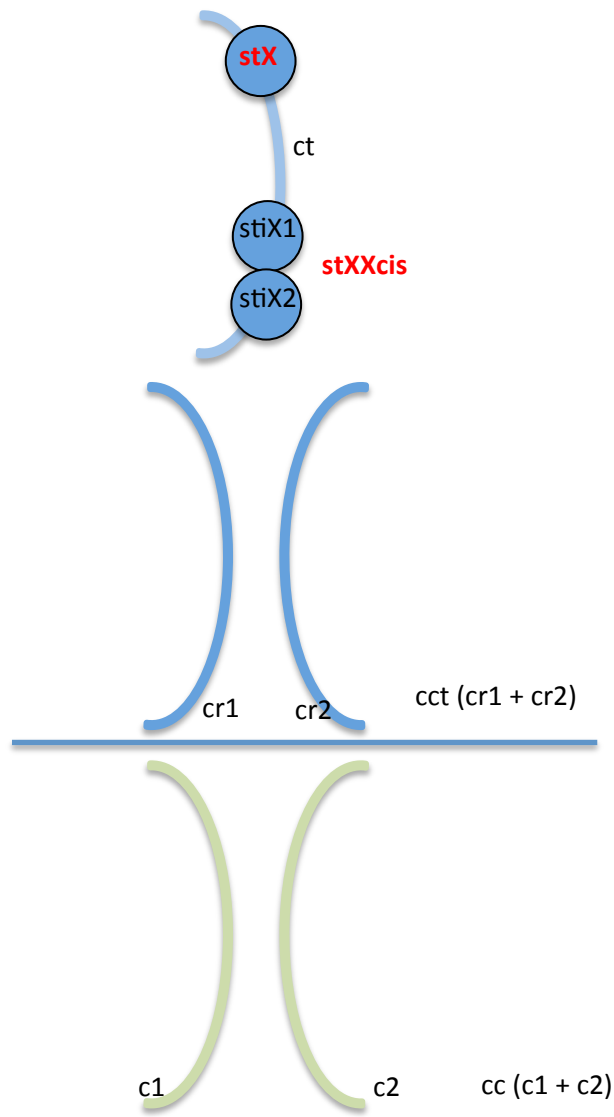
```
<multi:speciesType multi:id="stX" multi:compartment="ct"
        multi:isBindingSite="true" />


<multi:speciesType multi:id="stXXcis"
        multi:compartment="ct" multi:isBindingSite="false">
        <multi:listOfSpeciesTypeInstances>
            <multi:speciesTypeInstance multi:id="stiX1"
                multi:speciesType="stX" multi:occur="1" />
            <multi:speciesTypeInstance multi:id="stiX2"
                multi:speciesType="stX" multi:occur="1" />
        </multi:listOfSpeciesTypeInstances>
        <multi:listOfInSpeciesTypeBonds>
            <mult:inSpeciesTypeBond
                multi:bindingSite1="stiX1"
                multi:bindingSite2="stiX2" />
        </mult:listOfInSpeciesTypeBonds>
</multi:speciesType>
```

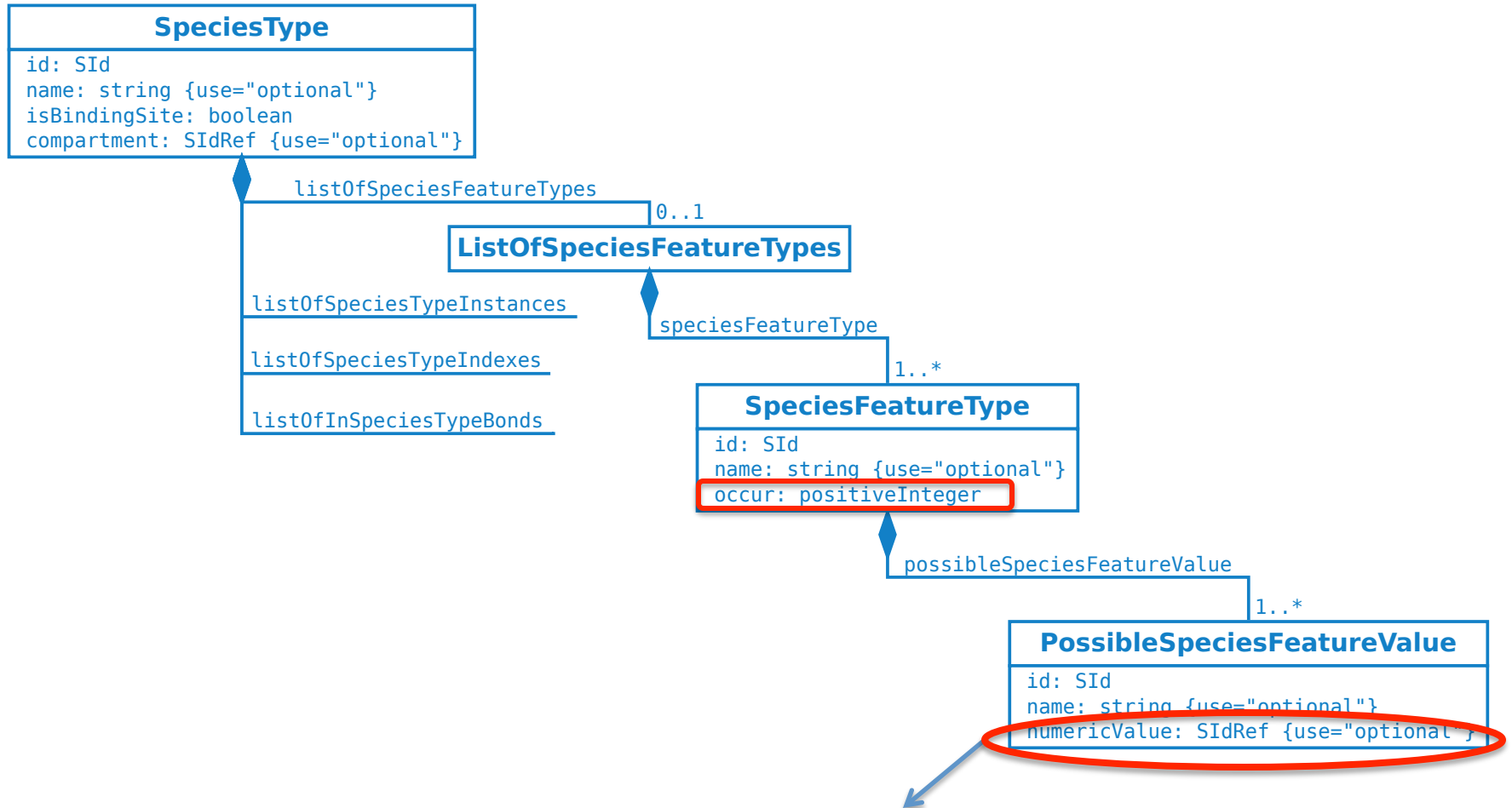# Compartment, SpeciesType, SpeciesTypeInstance, InSpeciesTypeBond and Species

stX

ct

stiX1

stXXcis

stiX2

stiX1 stiX2   **stXXtrans** (stiX1 + stiX2)

cr1   cr2   cct (cr1 + cr2)

c1   c2   cc (c1 + c2)

```
<multi:speciesType multi:id="stXXtrans"
        multi:compartment="cct" multi:isBindingSite="false">
    <multi:listOfSpeciesTypeInstances>
        <multi:speciesTypeInstance multi:id="stiX1"
                multi:speciesType="stX"
                multi:compartmentReference="cr1"
                multi:occur="1" />
        <multi:speciesTypeInstance multi:id="stiX2"
                multi:speciesType="stX"
                multi:compartmentReference="cr2"
                multi:occur="1" />
    </multi:listOfSpeciesTypeInstances>
    <multi:listOfInSpeciesTypeBonds>
        <mult:inSpeciesTypeBond multi:bindingSite1="stiX1"
                multi:bindingSite2="stiX2" />
    </multi:listOfInSpeciesTypeBonds>
</multi:speciesType>
```

Compartment, SpeciesType, SpeciesTypeInstance, InSpeciesTypeBond and Species

spX

stX

ct

stiX1

spXXcis

stiX2

stXXcis

stiX1 stiX2

stXXtrans (stiX1 + stiX2)

cr1 cr2

cct (cr1 + cr2)

spX1 spX2

spXXtrans

spXXcis1

spXXcis2

c1 c2

cc (c1 + c2)

<species id="*spX*" multi:speciesType="*stX*"
    compartment="*ct*" />

<species id="*spXXcis*" multi:speciesType="*stXXcis*"
    compartment="*ct*" />

<species id="*spX1*" multi:speciesType="*stX*"
    compartment="*c1*" />

<species id="*spX2*" multi:speciesType="*stX*"
    compartment="*c2*" />

<species id="*spXXtrans*" multi:speciesType="*stXXtrans*"
    compartment="*cc*" />

<species id="*spXXcis1*" multi:speciesType="*stXXcis*"
    compartment="*c1*" />

<species id="*spXXcis2*" multi:speciesType="*stXXcis*"
    compartment="*c2*" />

SpeciesFeatureType

SpeciesType

```
id: SId
name: string {use="optional"}
isBindingSite: boolean
compartment: SIdRef {use="optional"}
```

listOfSpeciesFeatureTypes

listOfSpeciesTypeInstances

listOfSpeciesTypeIndexes

listOfInSpeciesTypeBonds

0..1

ListOfSpeciesFeatureTypes

speciesFeatureType

1..*

SpeciesFeatureType

```
id: SId
name: string {use="optional"}
occur: positiveInteger
```

possibleSpeciesFeatureValue

1..*

PossibleSpeciesFeatureValue

```
id: SId
name: string {use="optional"}
numericValue: SIdRef {use="optional"}
```

Reference the id of a *parameter* object

SpeciesTypeComponentIndex

SpeciesType

listOfSpeciesFeatureTypes

listOfSpeciesTypeInstances

listOfInSpeciesTypeBonds

listOfSpeciesTypeComponentIndexes
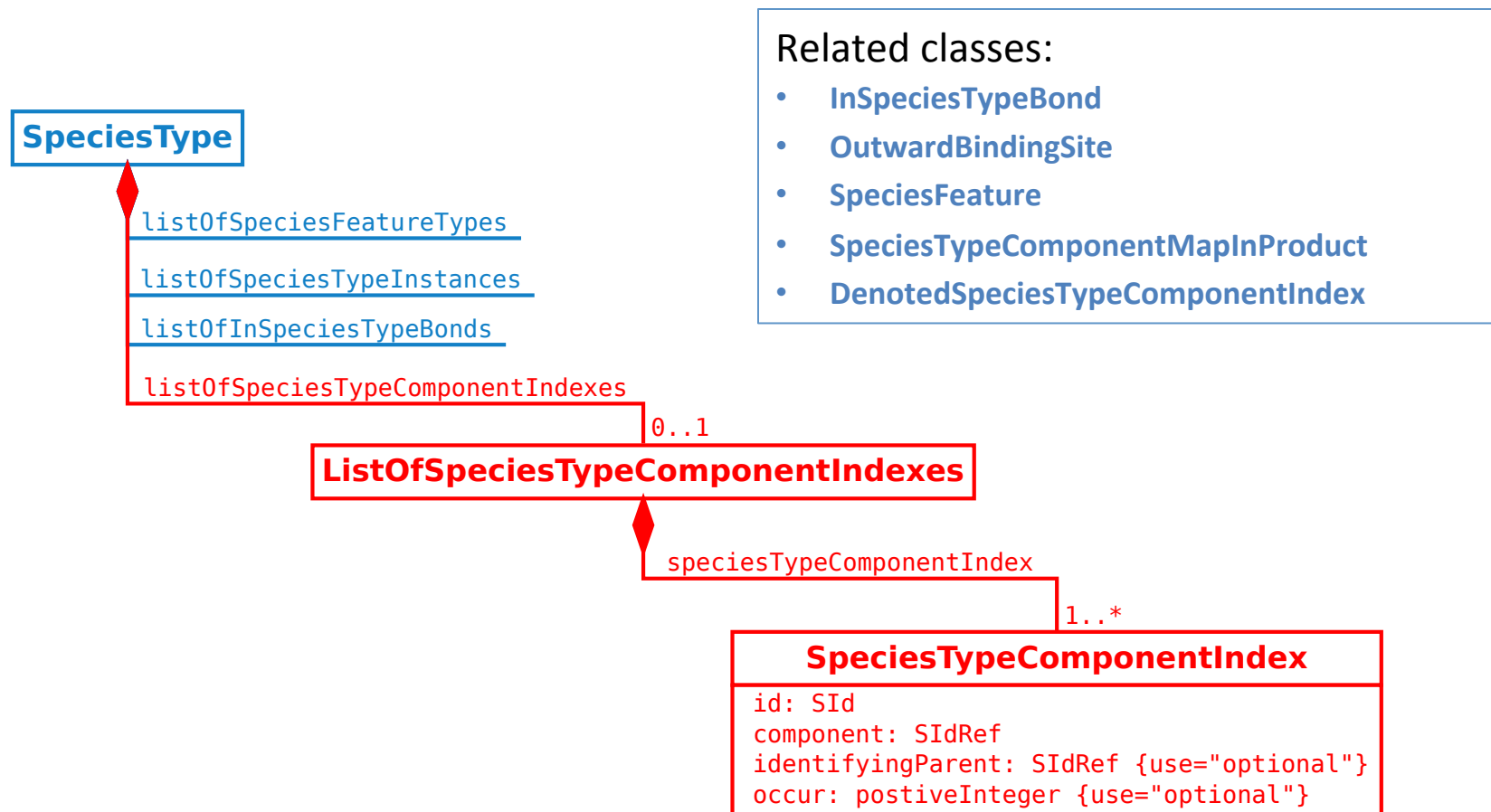
Related classes:
- **InSpeciesTypeBond**
- **OutwardBindingSite**
- **SpeciesFeature**
- **SpeciesTypeComponentMapInProduct**
- **DenotedSpeciesTypeComponentIndex**

0..1

ListOfSpeciesTypeComponentIndexes

speciesTypeComponentIndex

1..*

SpeciesTypeComponentIndex

id: SId
component: SIdRef
identifyingParent: SIdRef {use="optional"}
occur: postiveInteger {use="optional"}

SpeciesTypeComponentIndex

<multi:speciesType multi:id="stC" />
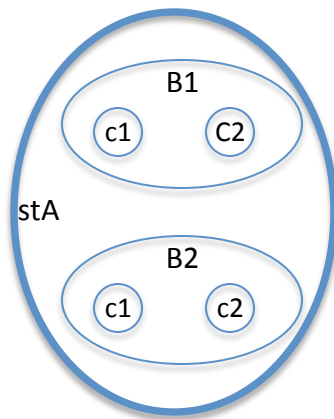
<multi:speciesType multi:id="stB">
   <multi:listOfSpeciesTypeInstances>
      <multi:speciesTypeInstance multi:id="c1"
         multi:speciesType="stC" multi:occur="1" />
     <multi:speciesTypeInstance multi:id="c2"
         multi:speciesType="stC" multi:occur="1" />
   </multi:listOfSpeciesTypeInstances>
</multi:speciesType>

<multi:speciesType multi:id="stA">
   <multi:listOfSpeciesTypeInstances>
      <multi:speciesTypeInstance multi:id="B1"
         multi:speciesType="stB" multi:occur="1" />
      <multi:speciesTypeInstance multi:id="B2"
         multi:speciesType="stB" multi:occur="1" />
   </multi:listOfSpeciesTypeInstances>
   …
</multi:speciesType>

B1
c1   C2
stA
B2
c1   c2

SpeciesTypeComponentIndex

Index: B1C1   Index: B1C2

B1

c1   C2

stA

B2

c1   c2

Index: B2C1   Index: B2C2
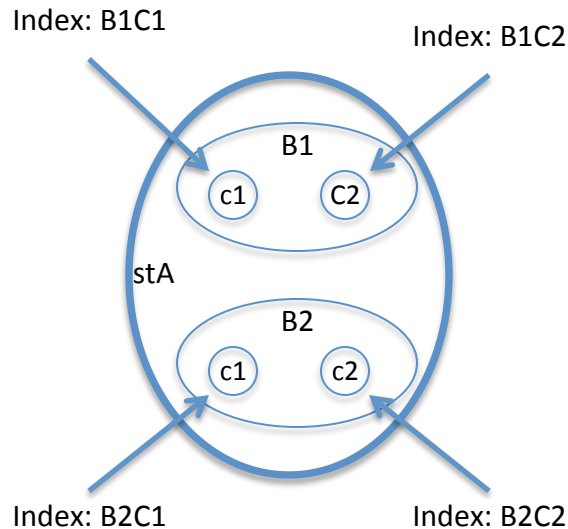
<multi:speciesType multi:id=*"stA" …>*
  <multi:listOfSpeciesTypeInstances>
    <multi:speciesTypeInstance multi:id=*"B1" …/>*
    <multi:speciesTypeInstance multi:id=*"B2" …/>*
  </multi:listOfSpeciesTypeInstances>
  <multi:listOfSpeciesTypeComponentIndexes>
    <multi:speciesTypeComponentIndex
      multi:id="B1C1" multi:component="c1"
      multi:identifyingParent="B1"" multi:occur="1" />
    <multi:speciesTypeComponentIndex
      multi:id="B1C2" multi:component="c2"
      multi:identifyingParent="B1" multi:occur="1" />
    <multi:speciesTypeComponentIndex
      multi:id="B2C1" multi:component="c1"
      multi:identifyingParent="B2" multi:occur="1" />
    <multi:speciesTypeComponentIndex
      multi:id="B2C2" multi:component="c2"
      multi:identifyingParent="B2" multi:occur="1" />
  </multi:listOfSpeciesTypeComponentIndexes>
</multi:speciesType>

Reference components of **SpeciesType** or **Species**

- Need to be able to identify a component without ambiguity
    - Define binding status of a component
    - Define feature(s) of a component
    - Identify binding sites of an **inSpeciesTypeBond**

- Components of a **SpeciesType** can be**:**
    - **SpeciesTypeInstances**
    - Some or all occurrences of a **SpeciesTypeInstance** with occur > "1"
    - The **SpeciesType** itself

- Components of **Species**
    - Components of the **speciesType** referenced by the **species**

- Components can be referenced in the following ways:
    - **SpeciesTypeInstance** id
    - or **SpeciesType** id
    - or **SpeciesTypeComponentIndex** id
      Note:
      SpeciesTypeComponentIndex has the "occur" attribute and therefore can be used for some or all occurrences of a **SpeciesTypeInstance**, for example, 2 of 5 binding sites of a speciesTypeInstance (occur="5") are unbound.

Reference components of **SpeciesType** or **Species**
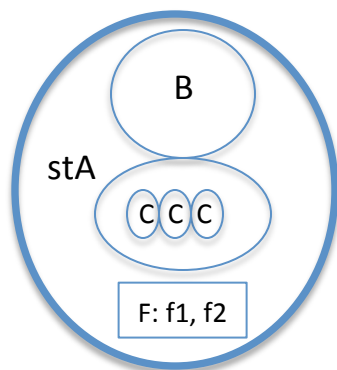
For example, components in a referencing species:

- Feature of **stA**: "f1" [speciesType]
- **B**: "unbound" [speciesTypeInstance]
- **c1** (one C): "bound" [Index]
- **c23** (two Cs): "unbound" [Index]

"**c1**" and "**c23**" are mutually exclusive!

```
<multi:speciesType multi:id="stC" multi:isBindingSite="true" />
<multi:speciesType multi:id="stB" multi:isBindingSite="true" />
<multi:speciesType multi:id="stA" multi:isBindingSite="true">
  <multi:listOfSpeciesTypeInstances>
    <multi:speciesTypeInstance multi:id="B"
        multi:speciesType="stB" multi:occur="1" />
    <multi:speciesTypeInstance multi:id="C"
        multi:speciesType="stC" multi:occur="3" />
  </multi:listOfSpeciesTypeInstances>
  <multi:listOfSpeciesFeatureTypes>
    <multi:speciesFeatureType multi:id="F" multi:occur="1" >
      <multi:possibleSpeciesFeatureValue multi:id="f1" />
      <multi:possibleSpeciesFeatureValue multi:id="f2" />
    </multi:speciesFeatureType>
  </multi:listOfSpeciesFeatureTypes>
  <multi:listOfSpeciesTypeComponentIndexes>
    <multi:speciesTypeComponent multi:id="c1"
        multi:component="C" multi:occur="1" />
    <multi:speciesTypeComponent multi:id="c23"
        multi:component="C" multi:occur="2" />
  </multi:listOfSpeciesTypeComponentIndexes>
</multi:speciesType>
```
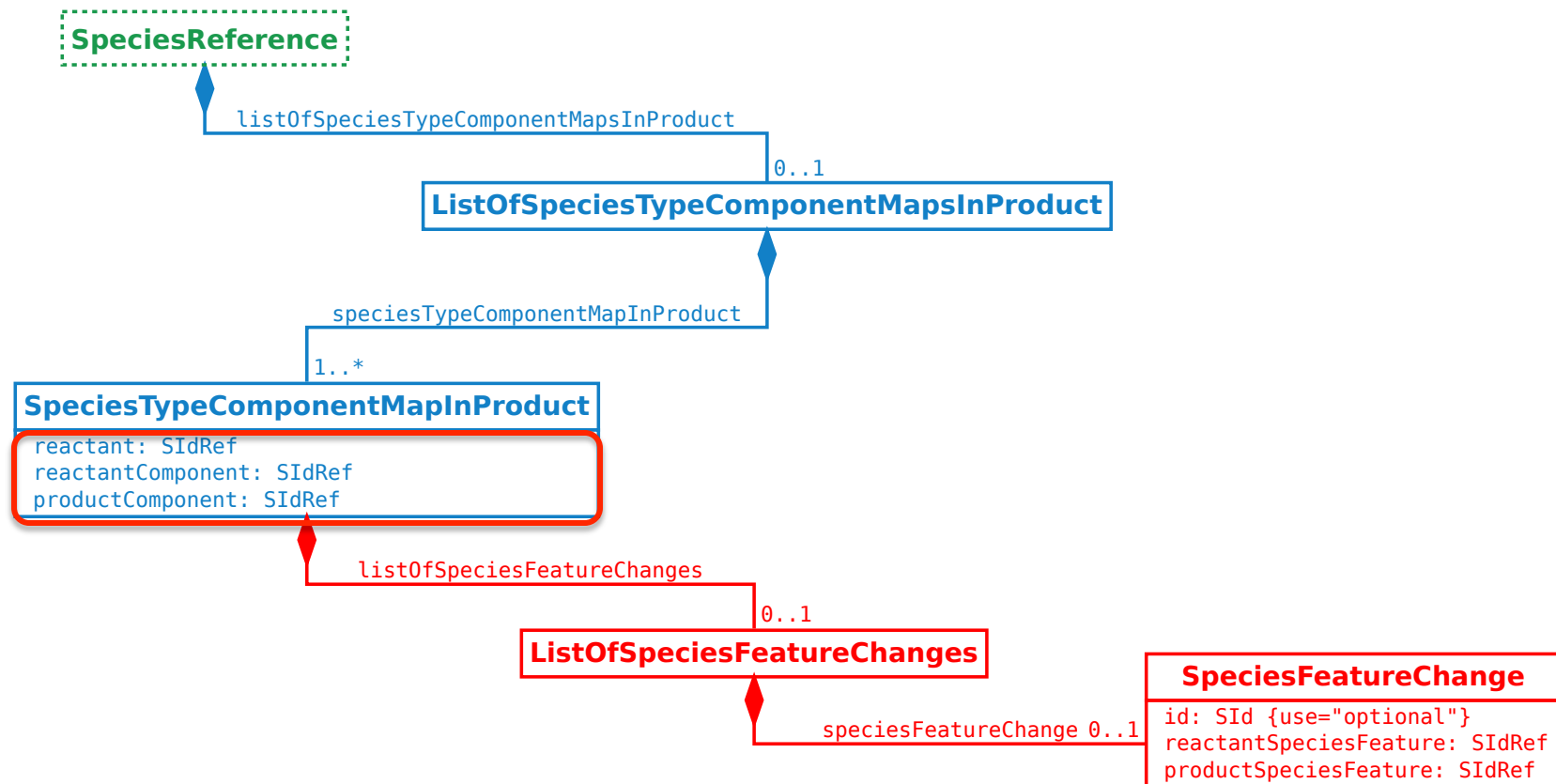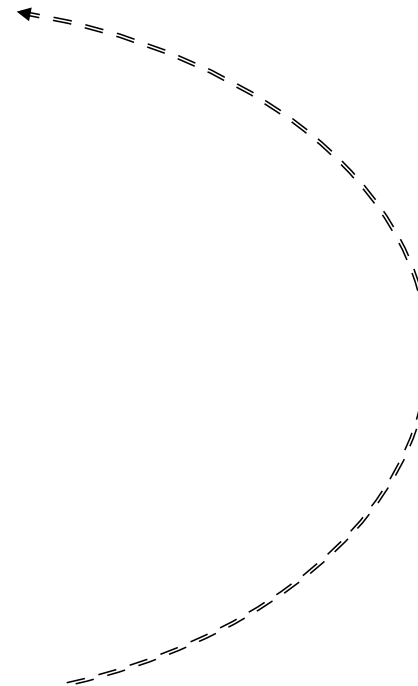
Species
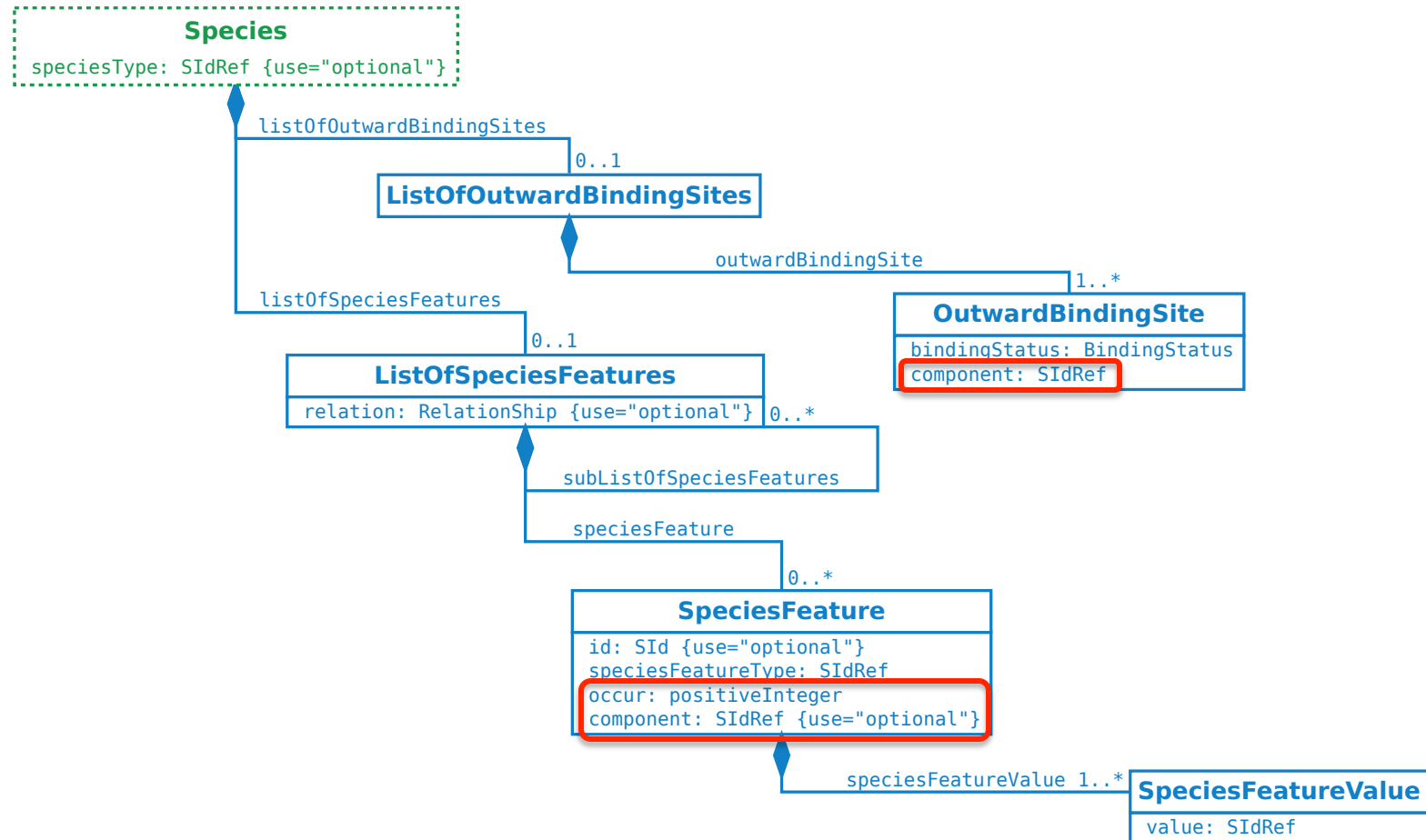
Reaction
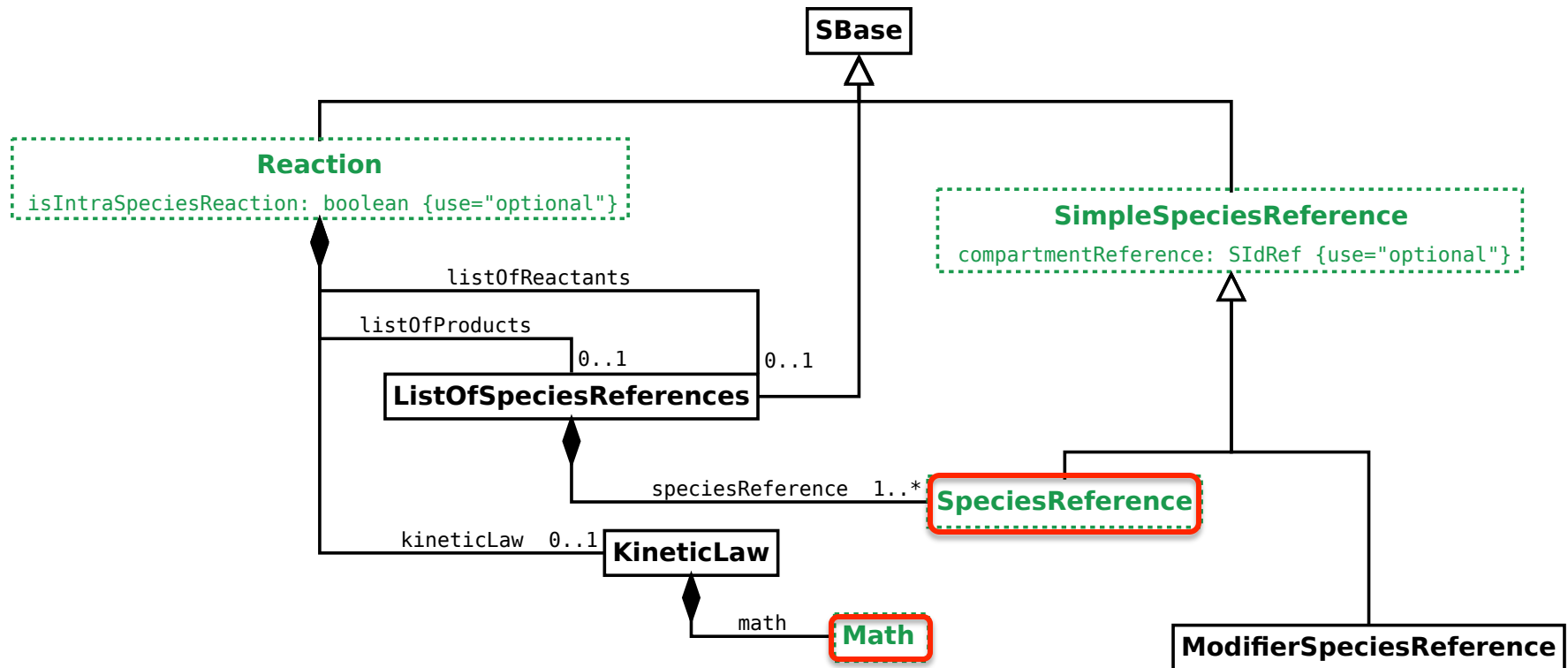
SpeciesTypeComponentMapInProduct and SpeciesFeatureChange

SpeciesReference

listOfSpeciesTypeComponentMapsInProduct

0..1

ListOfSpeciesTypeComponentMapsInProduct

speciesTypeComponentMapInProduct

1..*

SpeciesTypeComponentMapInProduct

reactant: SIdRef
reactantComponent: SIdRef
productComponent: SIdRef

listOfSpeciesFeatureChanges

0..1

ListOfSpeciesFeatureChanges

speciesFeatureChange 0..1

SpeciesFeatureChange

id: SId {use="optional"}
reactantSpeciesFeature: SIdRef
productSpeciesFeature: SIdRef

A slide from HARMONY 2013

- New **SpeciesType** class within **Model** class

  - **SpeciesFeatureType** class -- Multistate

  - **SpeciesTypeInstance** class -- Multicomponent

  - **InSpeciesTypeBond** class

-

  -

- Extended **Species** class

  - **OutwardBindingSiteReference** class

  - **SpeciesFeature** class

- Extended **Reaction** class

  - **SpeciesTypeInstanceReferenceMap** class

- Linking class: **SpeciesTypeInstanceReference**

Current version: **SpeciesTypeComponentIndex** replaces ~~**SpeciesTypeInstanceReference**~~

- New **SpeciesType** class within **Model** class

    – **SpeciesFeatureType** class -- Multistate

    – **SpeciesTypeInstance** class -- Multicomponent

    – **InSpeciesTypeBond** class

-

    –

- Extended **Species** class

    – **OutwardBindingSite** class

    – **SpeciesFeature** class

- Extended **Reaction** class

    – **SpeciesTypeComponentMapInProduct** class

- Linking class: ~~**SpeciesTypeInstanceReference**~~

SpeciesTypeComponentIndex
under **SpeciesType** class

Multiple occurrences of **SpeciesFeatureType** and **SpeciesFeature**

Use case:

- A species has 5 phosphorylation sites.
- The species has at least one unphosphorylated site
- One site can be phosphorylated in one phosphorylation reaction.

```
<multi:speciesType multi:id="stX" ...>
    <multi:listOfSpeciesFeatureTypes>
        <multi:speciesFeatureType multi:id="phosphorylation"
            multi:occur="5">
            <multi:possibleSpeciesFeatureValue
                multi:id="phosphorylated" />
            <multi:possibleSpeciesFeatureValue
                multi:id="unphosphorylated" />
        </multi:speciesFeatureType>
    </multi:listOfSpeciesFeatureTypes>
</multi:speciesType>
```

```
<species id="spX1" multi:speciesType="stX" ...>
    <multi:listOfSpeciesFeatures>
        <multi:speciesFeature multi:id="U"
            multi:speciesFeatureType="phosphorylation"
            multi:occur="1">
            <multi:speciesFeatureValue
                multi:value="unphosphorylated" />
        </multi:speciesFeature>
    </multi:listOfSpeciesFeatures>
</species>
<species id="spX2" multi:speciesType="stX" ...>
    <multi:listOfSpeciesFeatures>
        <multi:speciesFeature multi:id="P"
            multi:speciesFeatureType="phosphorylation"
            multi:occur="1">
            <multi:speciesFeatureValue
                multi:value="phosphorylated" />
        </multi:speciesFeature>
    </multi:listOfSpeciesFeatures>
</species>
```

Multiple occurrences of **SpeciesFeatureType** and **SpeciesFeature**

Use case:

- A species has 5 phosphorylation sites.

- The species has at least one unphosphorylated site

- One site can be phosphorylated in one phosphorylation reaction.

```
<reaction id="transformation" …>
    <listOfReactants>
        <speciesReference id="reactant" species="spX1" … />
    </listOfReactants>
    <listOfProducts>
        <speciesReference id="product" species="spX2" …>
            <multi:listOfSpeciesTypeComponentMapsInProduct>
                <multi:speciesTypeComponentMapInProduct  multi:reactant="reactant" multi:reactantComponent="stX"
                    multi:productComponent="stX">
                    <multi:listOfSpeciesFeatureChanges>
                        <multi:speciesFeatureChange multi:reactantSpeciesFeature="U"  multi:productSpeciesFeature="P" />
                    </multi:listOfSpeciesFeatureChanges>
                </multi:speciesTypeComponentMapInProduct>
            </multi:listOfSpeciesTypeComponentMapsInProduct>
        </speciesReference>
    </listOfProducts> …
</reaction>
```

More on the phosphorylation example

Use case:

- A species has 5 phosphorylation sites which are also binding sites.
- The species has at least one unphosphorylated site
- One site can be bound and phosphorylated in one reaction.

```
<multi:speciesType multi:id="stb" multi:isBindingSite="true">
    <multi:listOfSpeciesFeatureTypes>
        <multi:speciesFeatureType multi:id="phosphorylation"
            multi:occur="1">
            <multi:possibleSpeciesFeatureValue
                multi:id="phosphorylated" />
            <multi:possibleSpeciesFeatureValue
                multi:id="unphosphorylated" />
        </multi:speciesFeatureType>
    </multi:listOfSpeciesFeatureTypes>
</multi:speciesType>
<multi:speciesType multi:id="stX" …>
    <multi:listOfSpeciesTypeInstances>
        <multi:speciesTypeInstance
            multi:id="b"  multi:speciesType="stb"
            multi:occur="5" />
    </multi:listOfSpeciesTypeInstances>
    <multi:listOfSpeciesTypeComponentIndexes>
        <multi:speciesTypeComponentIndex
            multi:id="b1" multi:component="b" multi:occur="1" />
    </multi:listOfSpeciesTypeComponentIndexes>
</multi:speciesType>
```

```
<species id="spX1" multi:speciesType="stX" …>
    <multi:listOfSpeciesFeatures>
        <multi:speciesFeature multi:id="U"
            multi:component="b1"
            multi:speciesFeatureType="phosphorylation"
            multi:occur="1">
            <multi:speciesFeatureValue
                multi:value="unphosphorylated" />
        </multi:speciesFeature>
    </multi:listOfSpeciesFeatures>
</species>
<species id="spX2" multi:speciesType="stX" …>
    <multi:listOfSpeciesFeatures>
        <multi:speciesFeature multi:id="P"
            multi:component="b1"
            multi:speciesFeatureType="phosphorylation"
            multi:occur="1">
            <multi:speciesFeatureValue
                multi:value="phosphorylated" />
        </multi:speciesFeature>
    </multi:listOfSpeciesFeatures>
</species>
```

More on the phosphorylation example

Use case:

- A species has 5 phosphorylation sites which are also binding sites.

- The species has at least one unphosphorylated site

- One site can be bound and phosphorylated in one reaction.

```
<reaction id="transformation" …>
    <listOfReactants>
        <speciesReference id="reactant" species="spX1" … />
    </listOfReactants>
    <listOfProducts>
        <speciesReference id="product" species="spX2" …>
            <multi:listOfSpeciesTypeComponentMapsInProduct>
                <multi:speciesTypeComponentMapInProduct
                    multi:reactant="reactant" multi:reactantComponent="b1" multi:productComponent="b1">
                    <multi:listOfSpeciesFeatureChanges>
                        <multi:speciesFeatureChange multi:reactantSpeciesFeature="U" multi:productSpeciesFeature="P" />
                    </multi:listOfSpeciesFeatureChanges>
                </multi:speciesTypeComponentMapInProduct>
            </multi:listOfSpeciesTypeComponentMapsInProduct>
        </speciesReference>
    </listOfProducts>
    ...
</reaction>
```

Math: new attributes of the *ci* element

- The *speciesReference* attribute

  – Replace the ~~whichValue~~ attribute in the last version

  – Use with *species id* or speciesFeature *id*

    - Species: concentration
      individual – default
      sum – specified by representationType

    - SpeciesFeature:
      number of appearances in the species – default
      numericalValue of the feature – specified by representationType

- The *representationType* attribute

  – Use with "pattern" species and
    representationType="sum": sum of the concentrations of all mapping "fully defined" species (section 3.19)

  – Use with speciesFeature and
    representationType="numericValue": value in the parameter referenced by the *numericValue* attribute of
    possibleSpeciesFeatureValue.

Back to the phosphorylation example

Use case:

- A species has 5 phosphorylation sites.

- The species has at least one unphosphorylated site

- One site can be phosphorylated in one phosphorylation reaction.

- The reaction rate depends on the number of phosphorylated sites in the product

```
<reaction id="transformation" ...>
    <listOfReactants>
        <speciesReference id="reactant" species="spX1" ... />
    </listOfReactants>
    <listOfProducts>
        <speciesReference id="product" species="spX2" ...>

            ...
        </speciesReference>
    </listOfProducts>
    <kineticLaw>
        <math xmls="http://www.w3.org/1998/Math/MathML">
            <apply>
                <ci> k </ci>
                <ci> spX1 </ci>
                <ci multi:speciesReference="product"> P </ci>
            </apply>
        </math>
    </kineticLaw>
</reaction>
```

Alternative:
Id of possibleSpeciesFeatureValue?

"sum" of species concentration

k1 * Si / (k2 + SUM(Si))

```
<reaction id="r">
    <listOfReactants>
        <speciesReference species="Si" />
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="Pi" />
    </listOfProducts>
    <kineticLaw>
        <math xmlns="http://www.w3.org/1998/Math/MathML">
            <apply>
                <divide>
                    <apply>
                        <times />
                        <ci>Si</ci>
                        <ci>k1</ci>
                    </apply>
                    <apply>
                        <plus />
                        <ci>k2</ci>
                        <ci multi:representationType="sum">Si</ci>
                    </apply>
                </divide>
            </apply>
        </math>
        <listOfLocalParameters>
            <localParameter id="k1" ... />
            <localParameter id="k2" ... />
        </listOfLocalParameters>
    </kineticLaw>
</reaction>
```

Discussion…