

SBGN PD

Current status, future changes and
unresolved issues

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SBGN-9, Edinburgh, 30/4/13



PD Specification

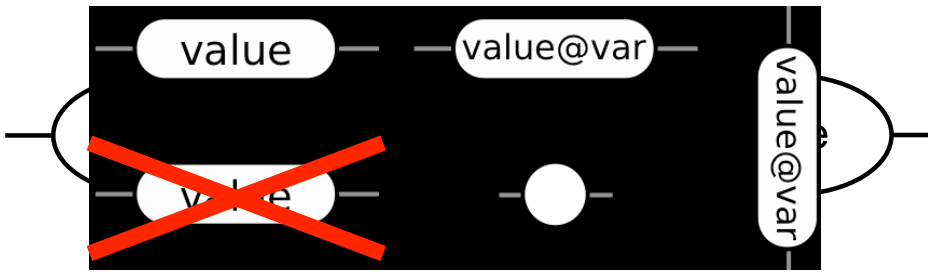
- Level 1 Version 1: Sep 2008
 - Original specification
- Level 1 Version 1.1: Sep 2009
 - Fixed inconsistencies
 - Typos
 - Clarified “ontology” of glyphs
 - Nomenclature changes for consistency with other languages
- Level 1 Version 1.2: Oct 2010
- Level 1 Version 1.3: Feb 2011
 - Minor changes of clarity
 - Document errors
- Level 1 Version 2.0 Q2 2013

What's in Version 2.0

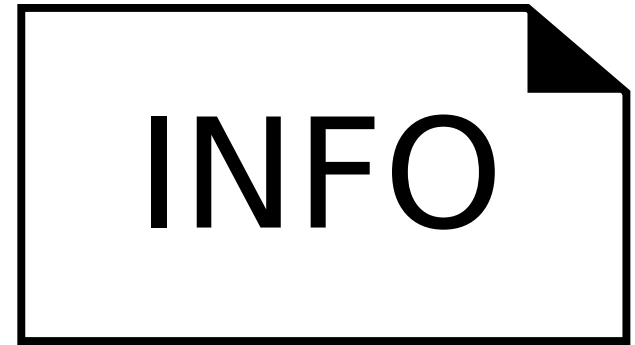
- New/Modified Glyphs
- Resolving semantic “issues”
- Enumerated rules
- Improve organisation/clarity of the spec

Resolved Issues

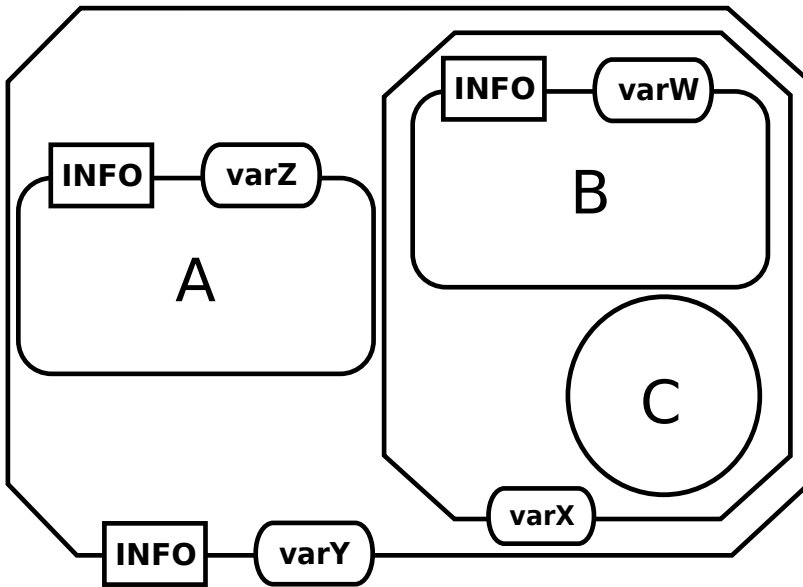
State Glyph Change



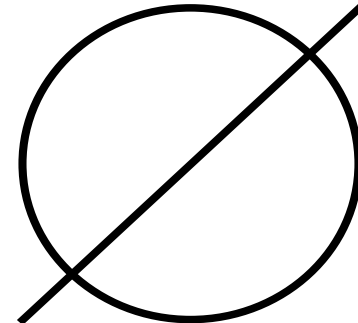
New Annotation Glyph

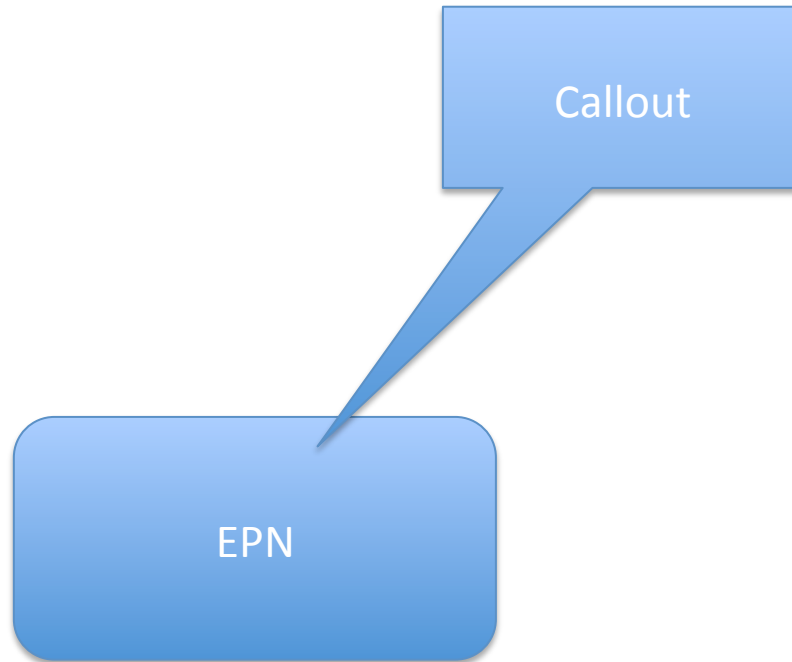


Complex Subunits are Decorators

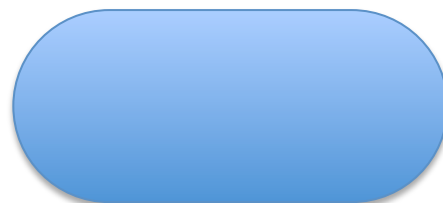
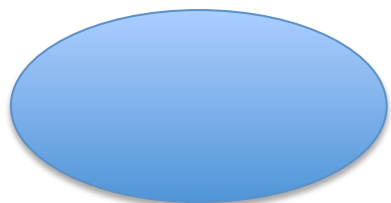


Empty Set



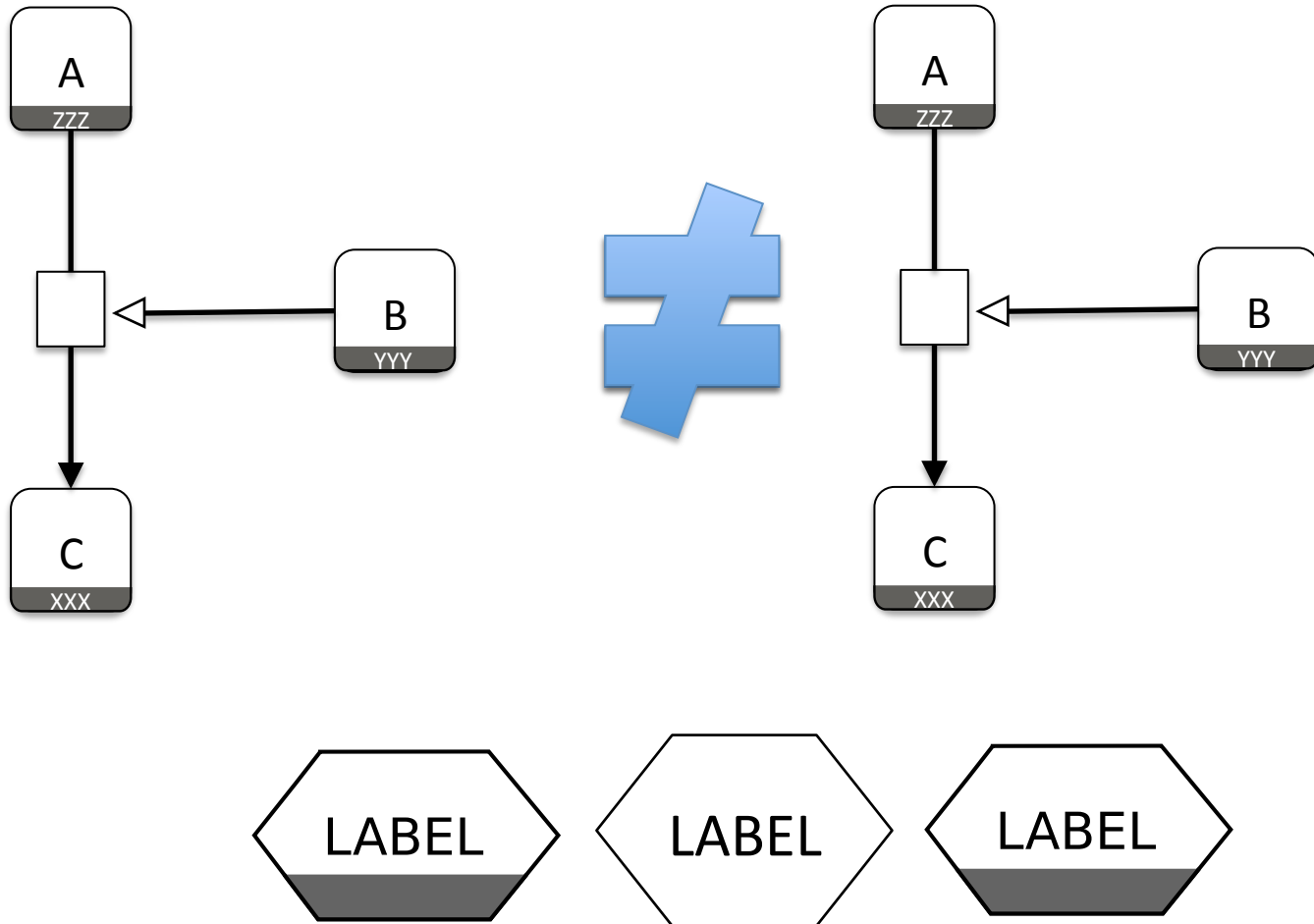


Simple Chemical



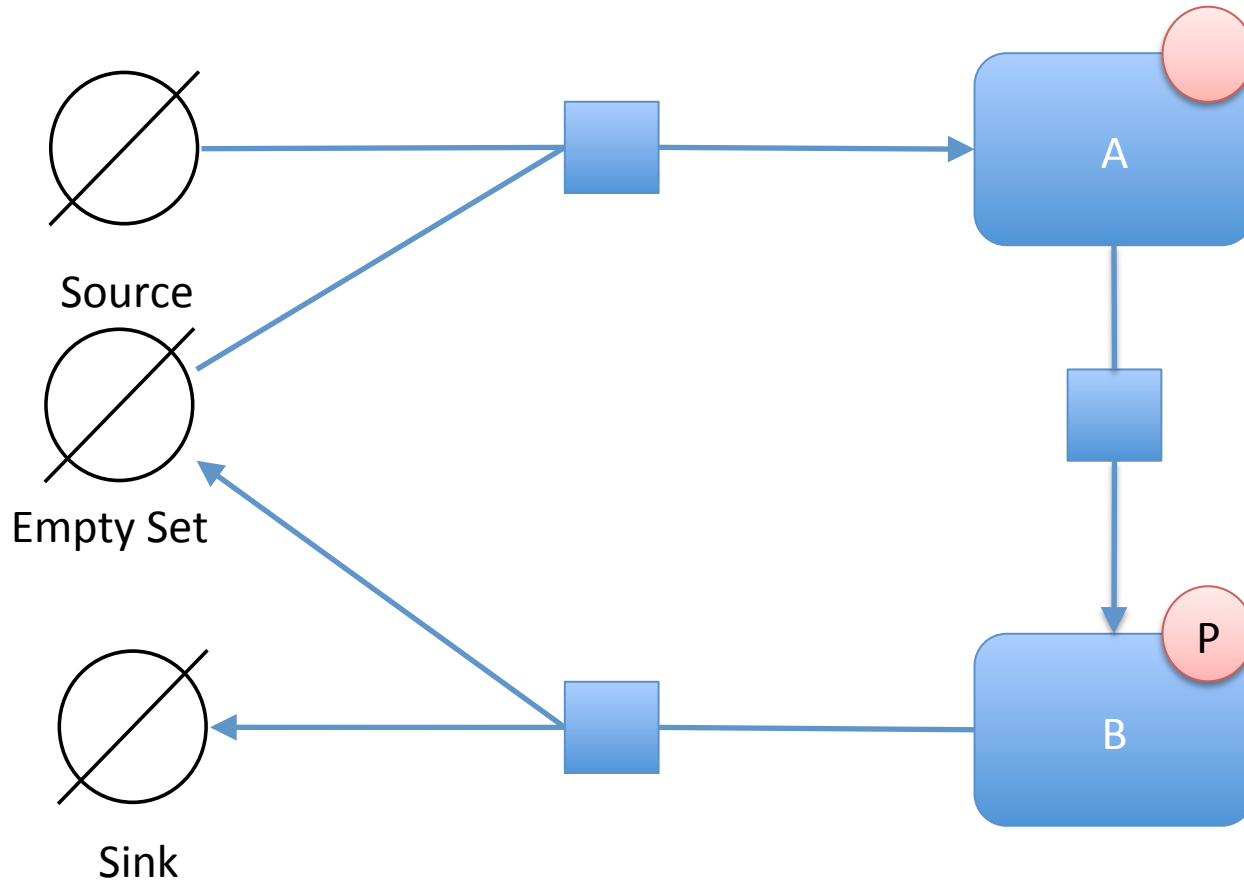
Level 1 Version 2.0: Semantics

Process Duplication

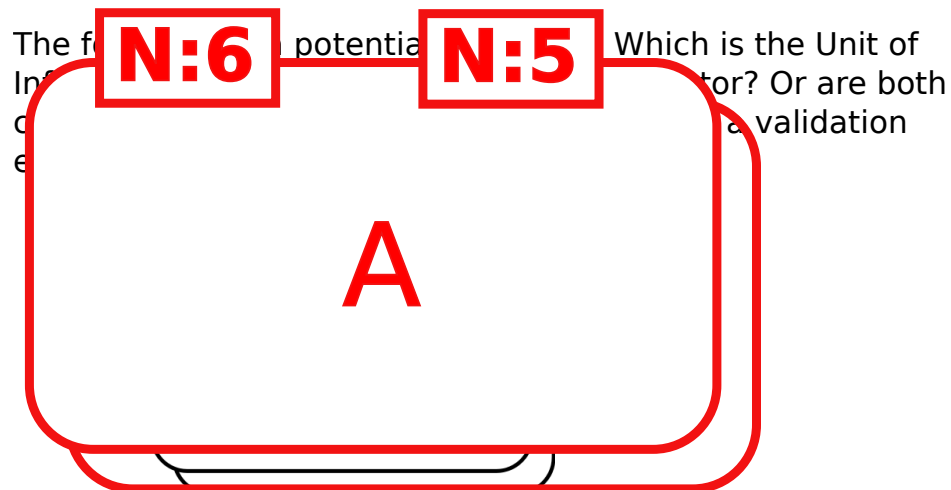
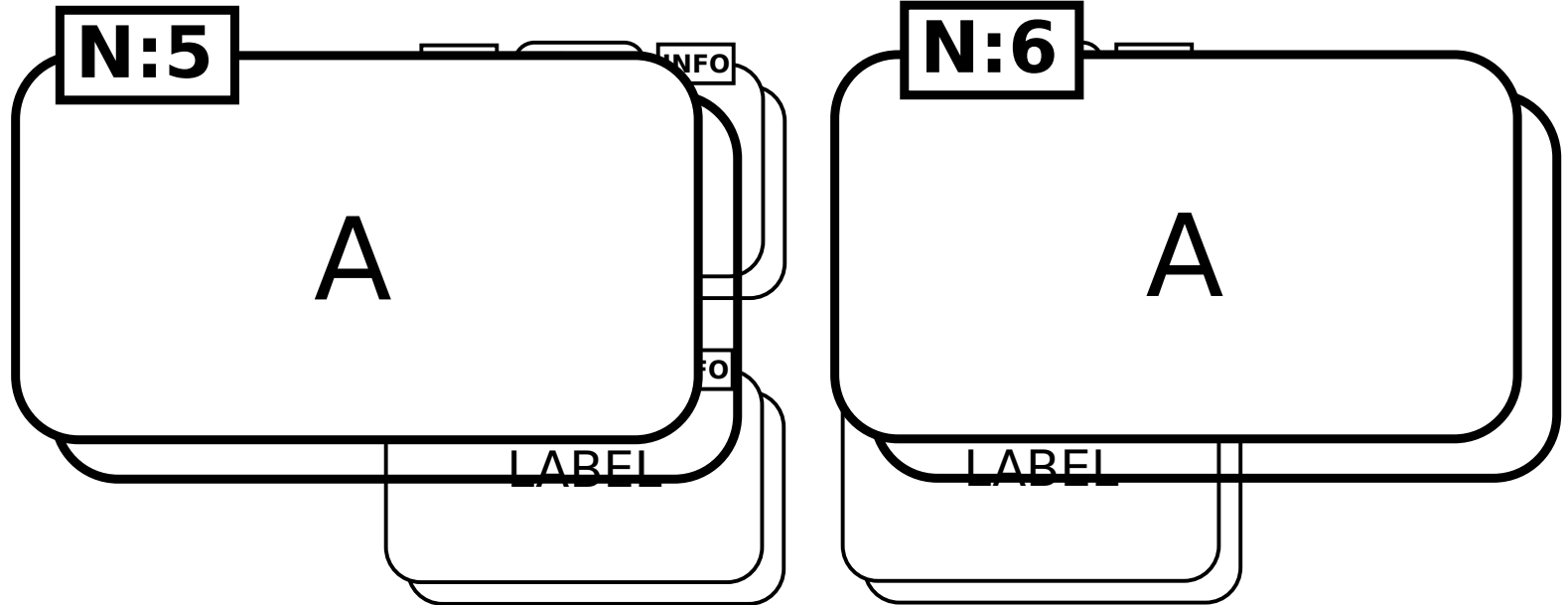


Level 1 Version 2.0: Semantics

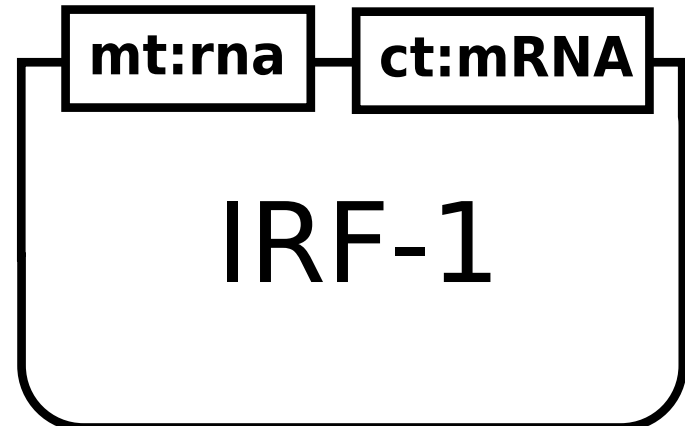
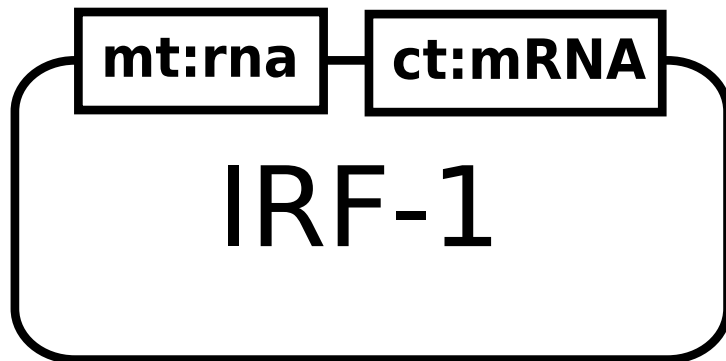
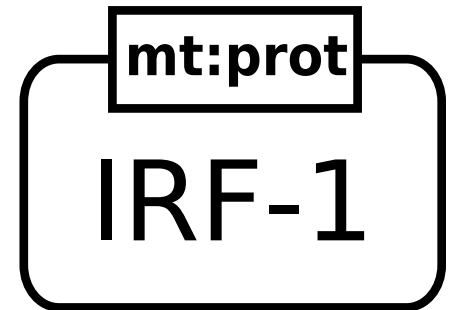
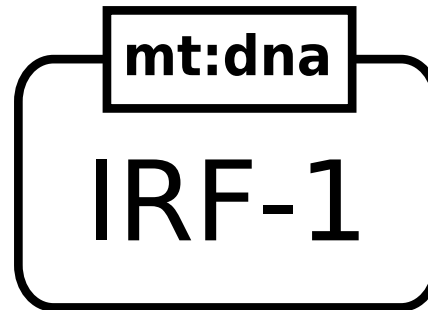
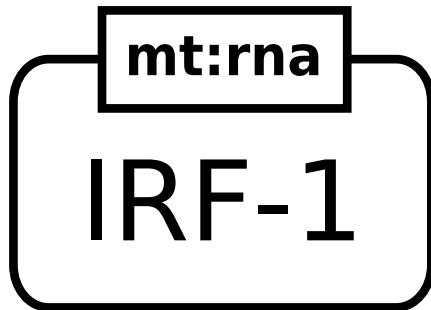
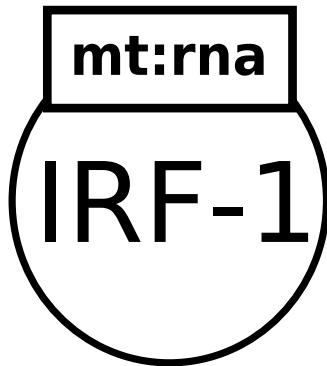
Source and Sink => Empty Set



Cardinality Glyph



Material Type



Level 1 Version 2.0: Spec

- Major rewrite
 - Based on SBML spec
 - Based on UML spec
- Aim
 - Remove ambiguities that exist in current spec
 - Remove grey areas

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Rule and Constraints

None.

Changes from Previous Version

Although not defined explicitly in the previous version, arguably this concept did exist in the language.

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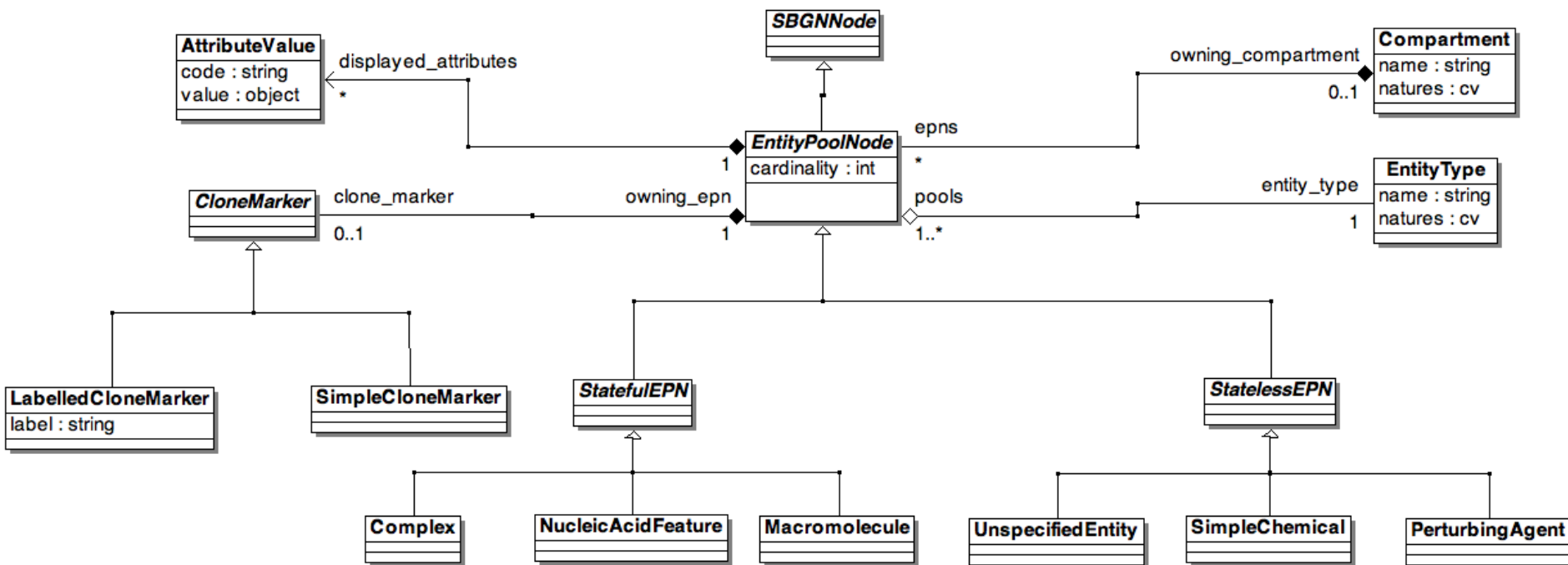
Attributes

cardinality: int (**R**) The number of copies of the entity. Must be a positive non-zero integer.

Associations

owning_compartment:Compartment (0..1) The compartment that this EPN belongs to.

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therefore distinguished from other pools with the same entity type by its cardinality, its owning_compartment and the values of its StateVariables (where appropriate). It must belong to a compartment or be associated with the map (c.f. section 5.5) and can contain a clone marker if it is cloned (see section 5.7)—note that not all EPNs can be cloned.

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Generalisation

- SBGNNNode (see section 5.5)

section 5.5) (degree > 0).

- All StateVariableDefinitions associated with the EntityType must have an associated StateVariable.

¹¹This is an alternate way of using the Unit of Information to display information, but to constrain it so that it presents attributes of the EPN not general annotation. See the AttributeValue class for more information.

¹⁰Although this concept is discussed it is not explicitly defined previously.

Rules and Constraints

- State variables do not need to be logically unique, therefore two or more StatefulEPN nodes with the same name are permitted.

Stateful entities, Old Marker changes physical changes, for example chemical modification of StatefulEPN and translation changes, which we wish to record in a Process Description map. This information is captured via the StateVariable (as can be seen in figure 5.10). The LabelCloneMarker must be used to indicated that the StatefulEPN is cloned in the previous version.

Changes from Previous Version

StatefulEPN is cloned in the previous version.

Macromolecule

Many biological processes involve *macromolecules*: biochemical substances that are built up from the equivalent linking of pseudo-identical units. Examples of macromolecules include proteins, nucleic acids (RNA, DNA) and polysaccharides (glycogen, cellulose, starch, etc.). Attempting to define a separate glyph for all of these different molecules would lead to an explosion of symbols in SBGN, so instead, SBGN Process Description Level 1 defines only one glyph for all macromolecules. The same glyph is to be used for a protein, a nucleic acid, a complex sugar, and so on. The exact nature of a particular macromolecule in a map is then clarified using its label and decorations, as will become clear below.

Generalisation

- StatefulEPN (see section 5.5)

Generalisation

Attributes

- EntityPoolNode (see section 5.5)

No additional attributes.

Attributes Associations

No additional attributes.
No additional associations.

Associations Constraints

No additional StateVariable constraints. The state variables that belong to this class.

Notation

There are two glyphs associated with Macromolecule. The first *Macromolecule monomer* is used when cardinality = 1 and the second *Macromolecule multimer* is used when cardinality > 1.

Glyph: *Macromolecule monomer*

SBO Term: SBO:0000245 ! macromolecule

Container: A macromolecule is represented by a rectangular container with rounded corners, as illustrated in Figure 5.17.

Label: A *macromolecule* is identified by a label placed in an unbordered box containing a string of characters. The characters can be distributed on several lines to improve readability, although this is not mandatory. The label box must be attached to the center of the container. The label may spill outside of the container.

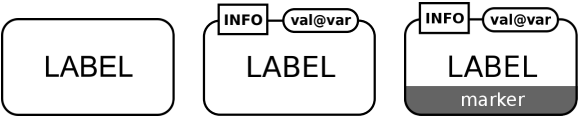


Figure 5.17: The Process Description glyph for *macromolecule*, shown plain and unadorned on the left, and with an additional state variable and a unit of information in the middle and the cloned form on the right.

Glyph: *Macromolecule multimer*

SBO Term: SBO:0000420 ! multimer of macromolecules

Container: A *multimer* is represented by two identical containers shifted horizontally and vertically and stacked one on top of the other. Figure 5.18 illustrates the glyph.

Label: As monomer

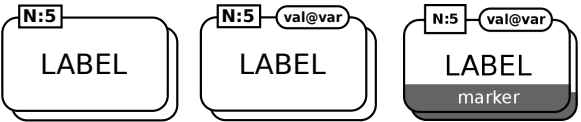


Figure 5.18: The Process Description glyph for *macromolecule multimer*, shown plain and unadorned on the left, and with an additional state variable and a unit of information in the right and the cloned form on the right.

Usage Examples In this section, we provide examples of Entity Pool Node representations drawn using the SBGN Process Description Level 1 glyphs described above.

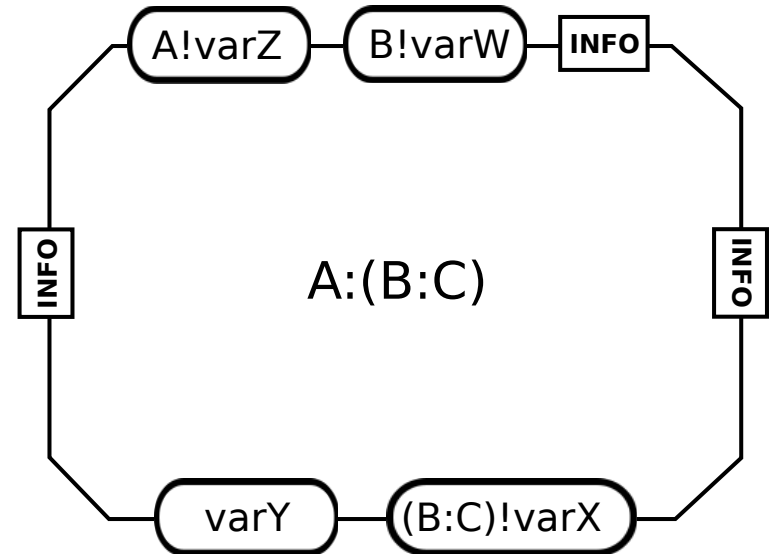
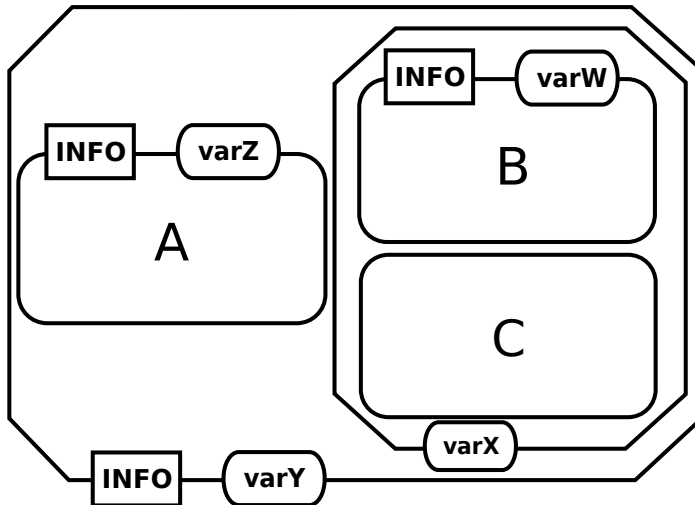
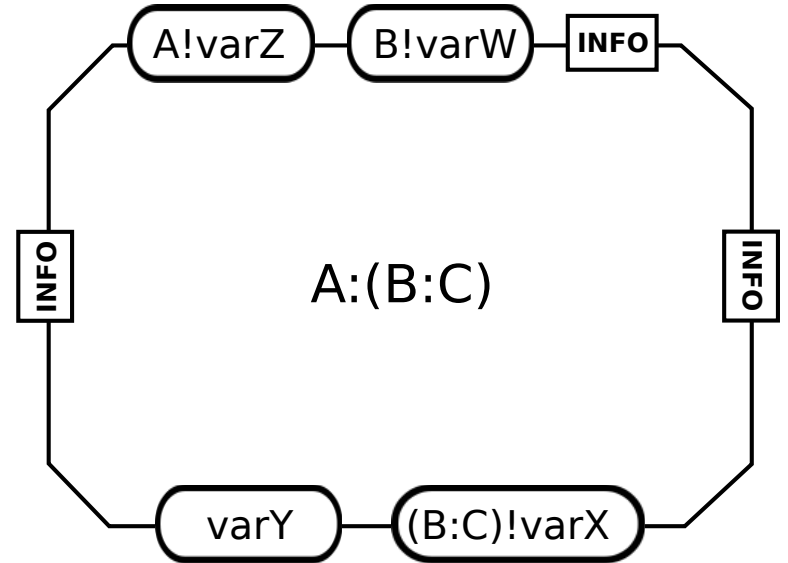
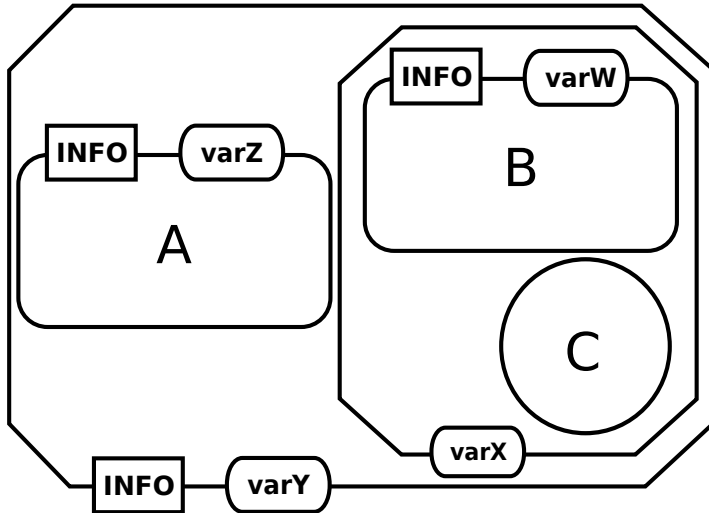
Figure 5.19 represents calcium/calmodulin kinase II, with phosphorylation on the sites threonine 286 and 306, as well as catalytic and autoinhibitory domains. Note the use of *units of information* and *state variables*.

Worked Examples: Help

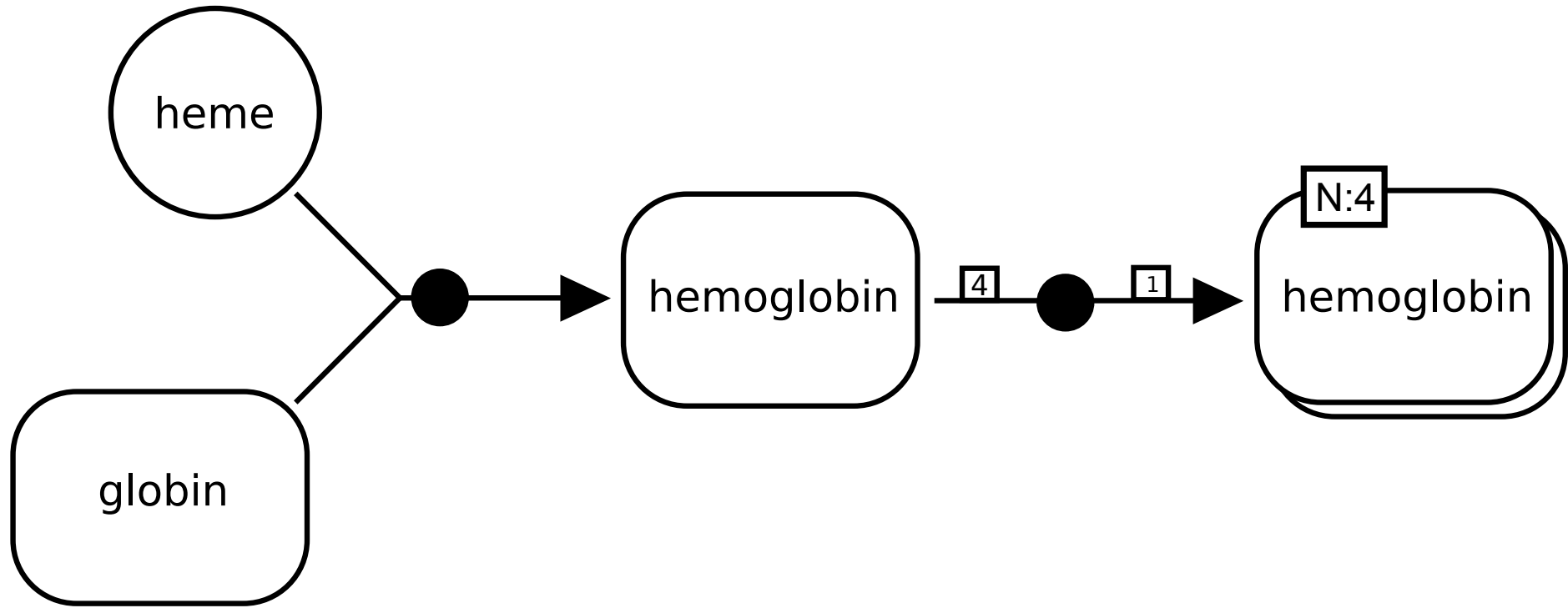
- Metabolism
- Signalling – states, complexes, multimers
- Compartments, perturbation and phenotypes
- Gene regulation. Poss transport between compartments
- Submap usage

Unresolved Issues

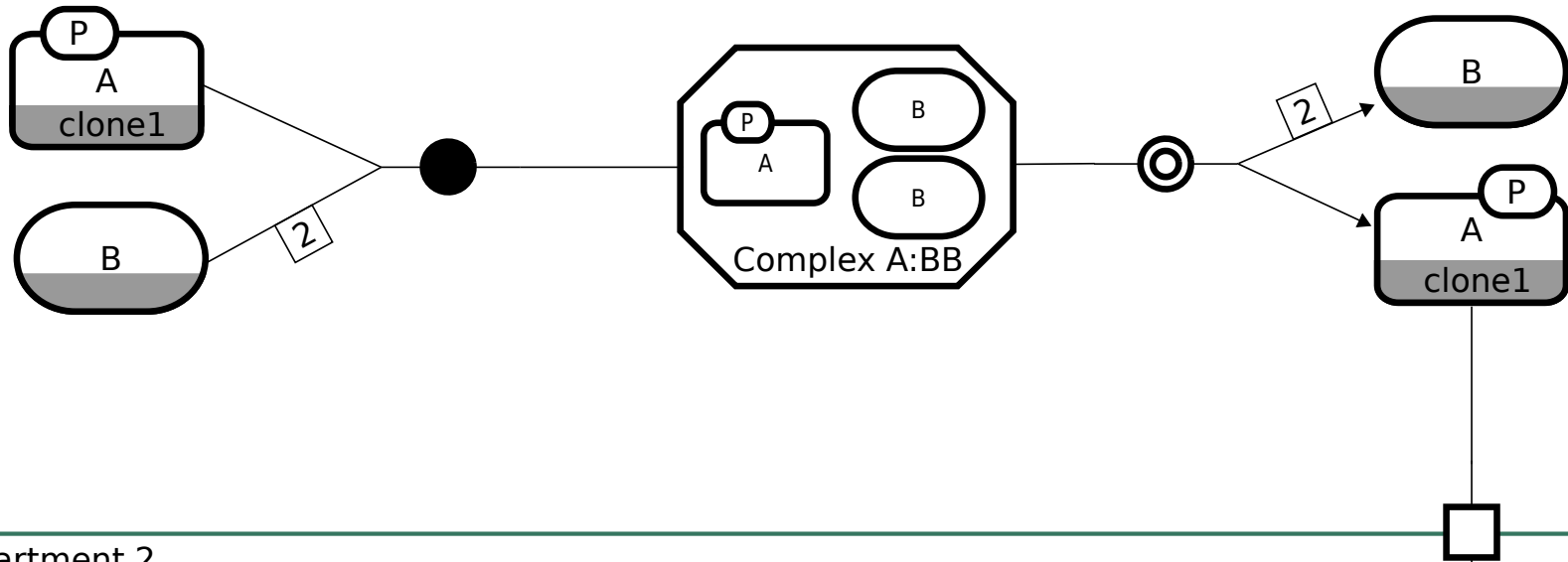
Complex Identity



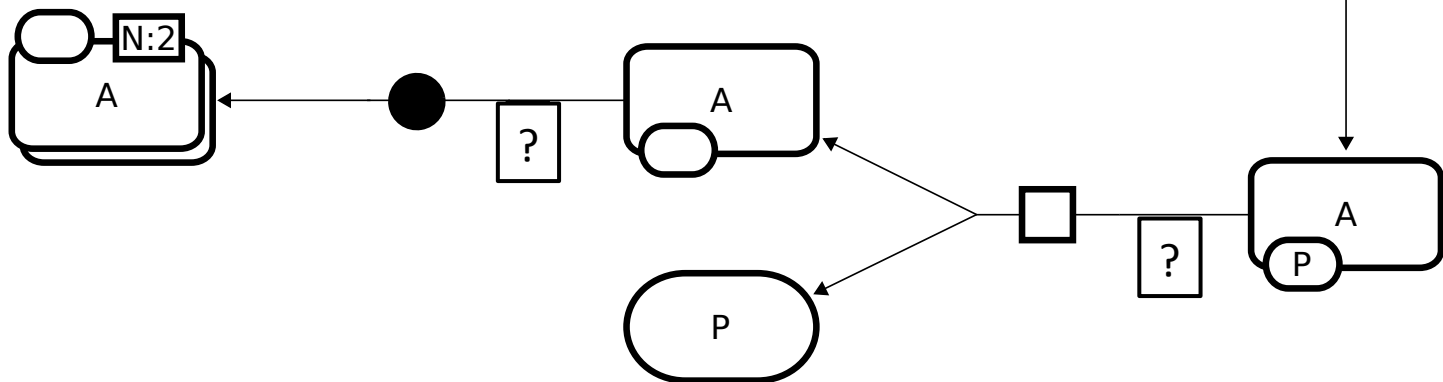
Stoichiometry

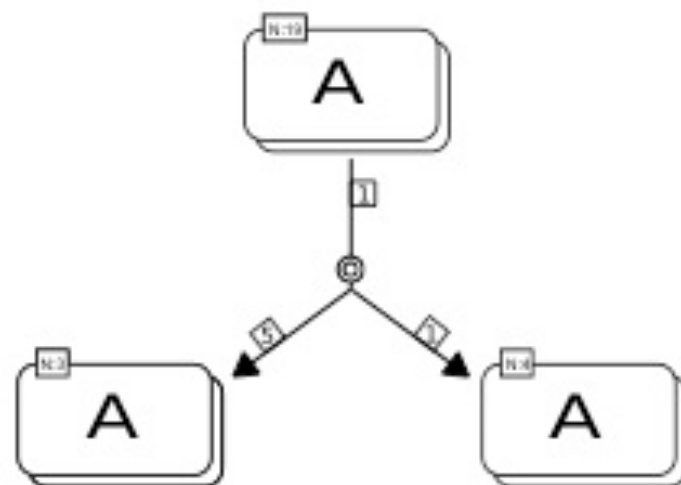
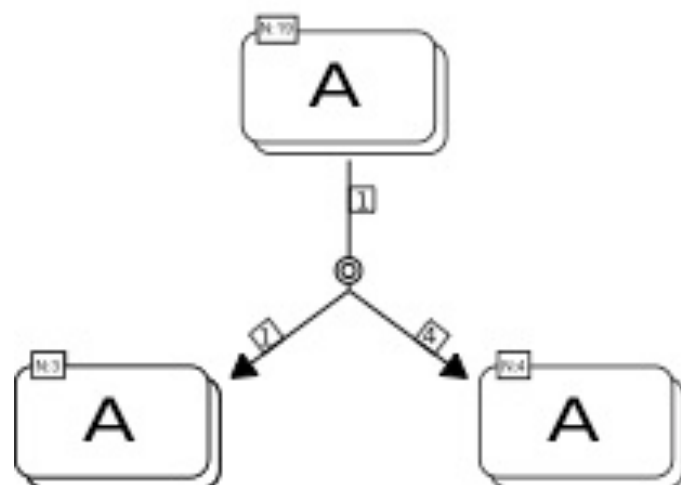
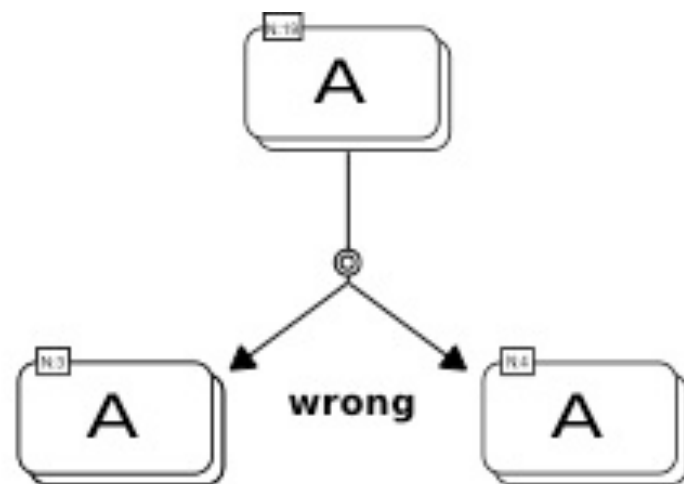


Compartment 1

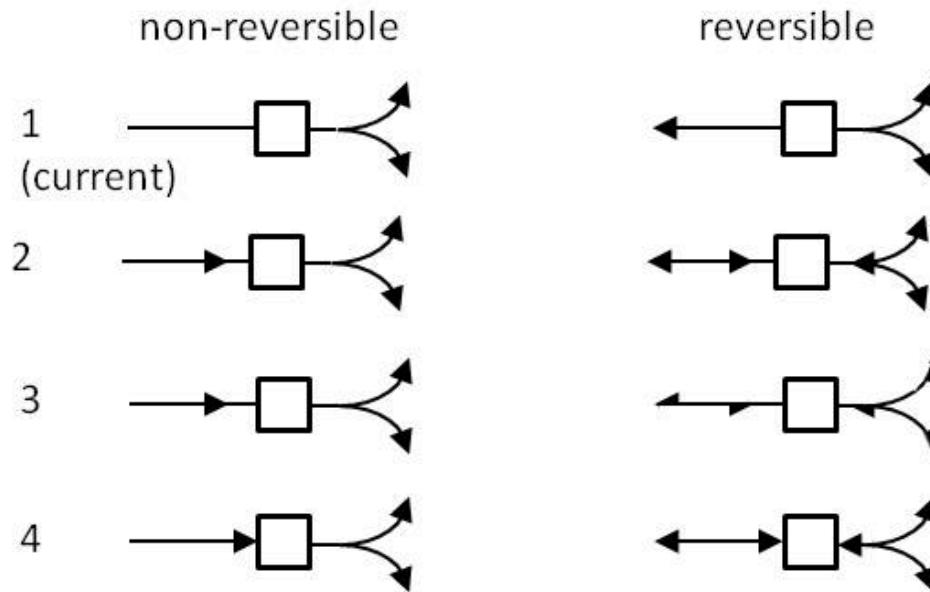


Compartment 2

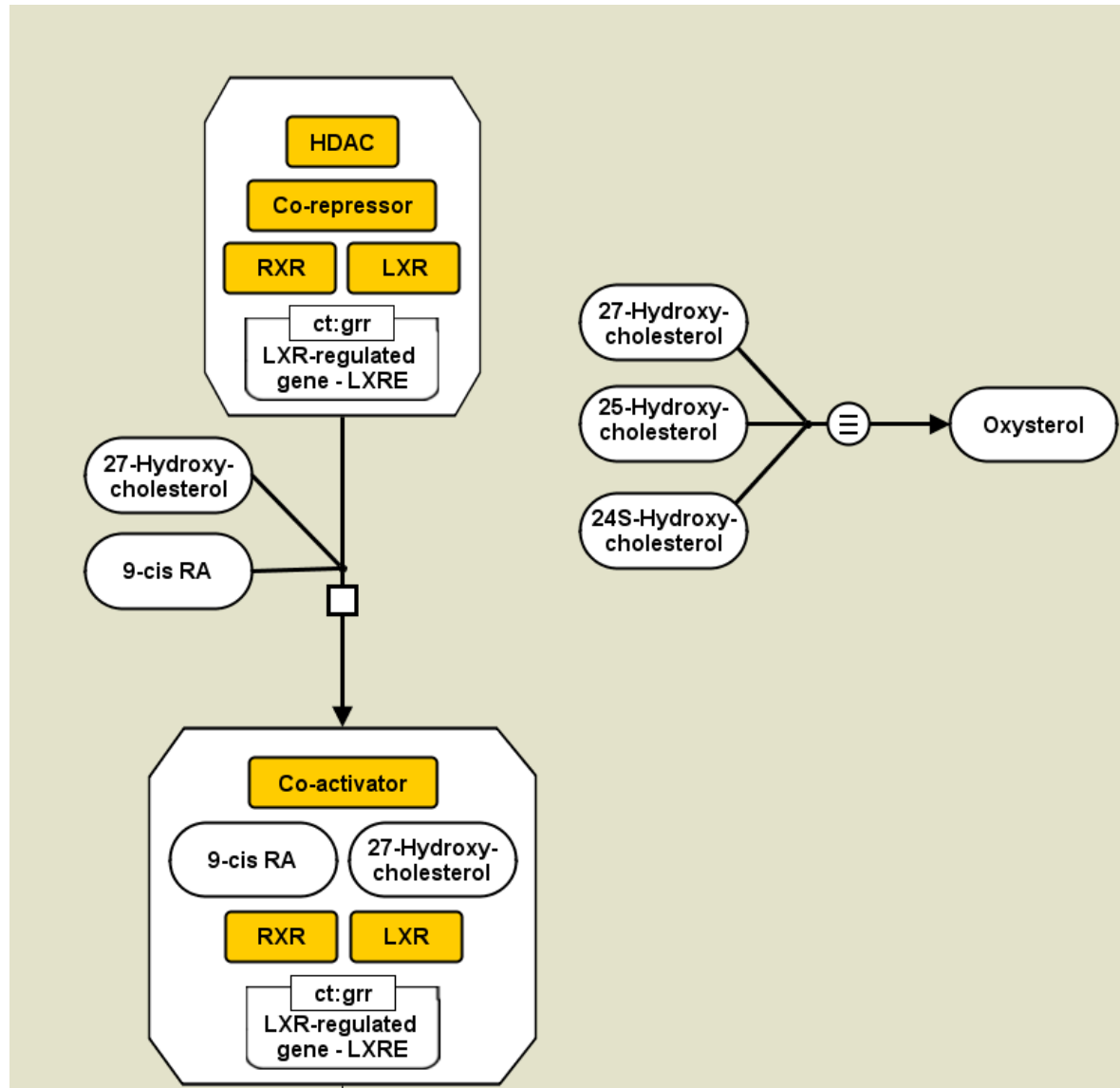




For Discussion: Reversible Arcs



Generics



Generics: outcomes

- New glyph?
- Looks like it works
- Experimental proposal?
- Tool support?

Road Map for PD

- Level 1 Version 2.0
 - Draft for Review: Q2 2013
 - RFC: 2-3 Weeks
 - Release Q3 2013

Acknowledgements

- SBGN Editors
 - Tobias Czauderna
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 - Nicolas Le Novère
 - Huaiyu Mi
 - Emek Demir
- SBGN Community