Reactions in the new scheme

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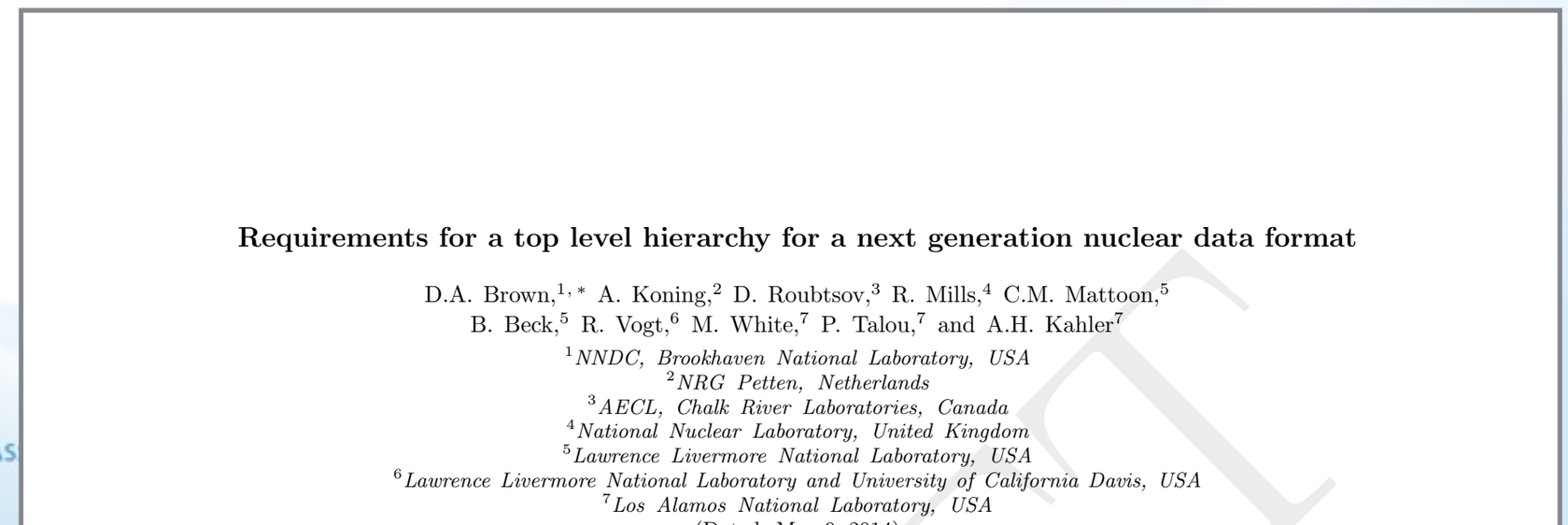
BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

I am trying to capture your view of how to arrange nuclear data

- **I will present the consensus view of required arrangement of nuclear data,**
  - presented at SG38 Meeting in Tokai, Japan, Dec. 2013
  - revised and presented at SG38 Meeting in Paris, France, Apr. 2014
  - revised again for this meeting
- **Issues dealt with already (I think)**
  - Reaction major vs. energy major
  - Documentation requirements
- **Element & attribute names are illustrative. They can be changed.**



Requirements for a top level hierarchy for a next generation nuclear data format

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[2] *NRG Petten, Netherlands*
[3] *AECL, Chalk River Laboratories, Canada*
[4] *National Nuclear Laboratory, United Kingdom*
[5] *Lawrence Livermore National Laboratory, USA*
[6] *Lawrence Livermore National Laboratory and University of California Davis, USA*
[7] *Los Alamos National Laboratory, USA*

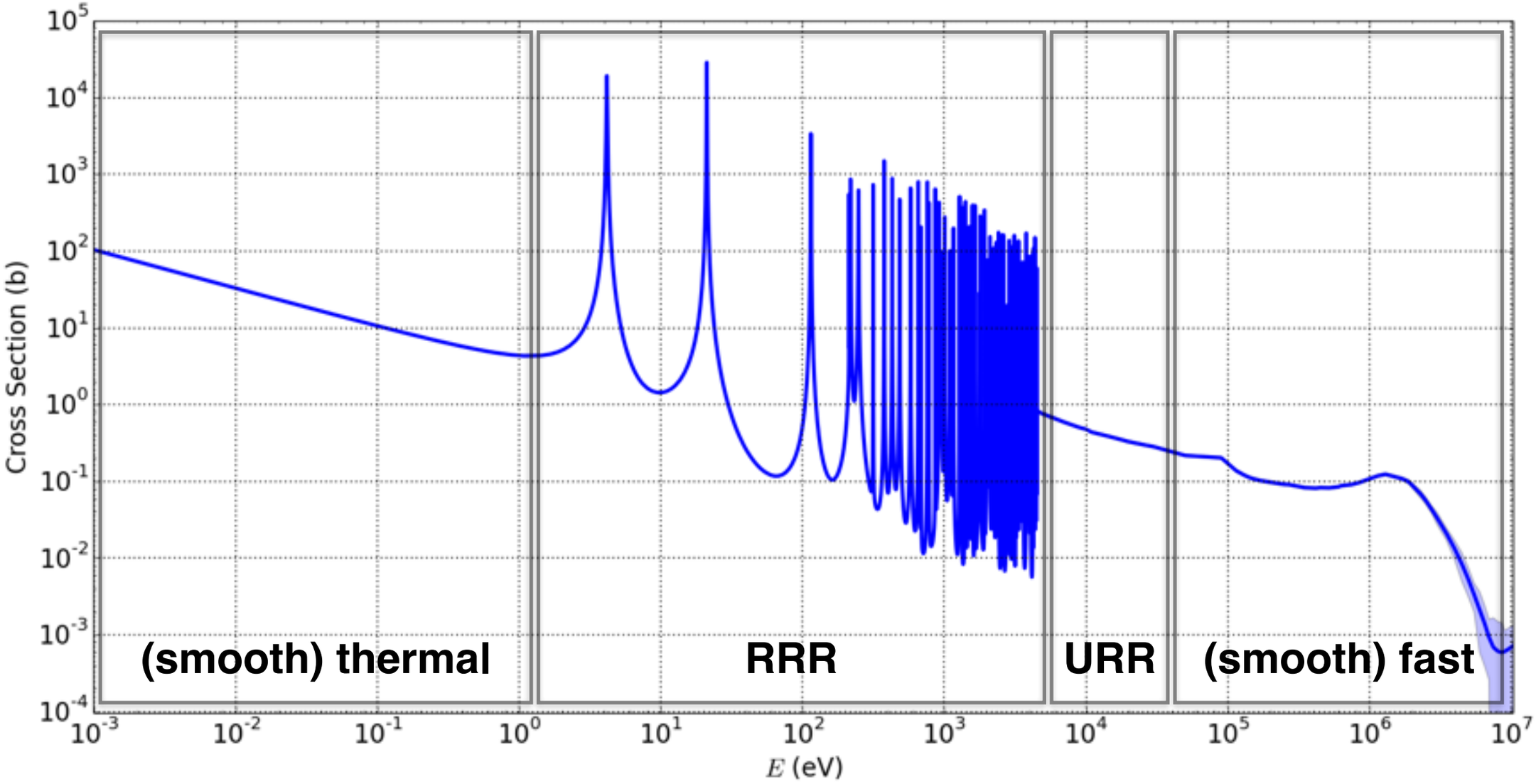
All MF's are covered

- **1 (general info.)**: <documentation>
- **2 (RR):** <resonances>
- **3 (cross sections):** <crossSection>
- **4 (n angle dist.):** a <distribution>
- **5 (n energy dist.):** a <distribution>
- **6 (energy-angle dists.):** a <distribution> (note: <dcrossSection_dOmega> for LACS)
- **7 (TSL):** <dcrossSection_dOmega_dE>
- **8 (FPY):** a <distribution>
- **8 (decay):** in <localMaterialDatabase>
- **9 (rad. decay mult.)**: a <distribution>
- **10 (prod. cross sections)**: a derived <crossSection>
- **12 (gamma yields):** continuum gammas are in <distribution> or discretes in <localMaterialDatabase>
- **13 (gamma prod. cross sections):** a derived transport data
- **14 (g angle dist.):** a <distribution>
- **15 (g energy dist.):** a <distribution>

All MF's are covered

- **26 (g-, e- dists.):** a <distribution>
- **27 (atomic scatt.):** <dcrossSection_dOmega>
- **28 (atomic relax.):** in <localMaterialDatabase>
- **30 (model param. cov.):** a <covariance> & <sensitivity>
- **31 (nubar cov.):** a <covariance>
- **32 (RR cov.):** a <covariance> & <sensitivity>
- **33 (cross section cov.):** a <covariance>
- **34 (ang. dist. cov):** a <covariance>
- **35 (energy dist. cov.):** a <covariance>
- **40 (rad. prod. cov.):** a <covariance>

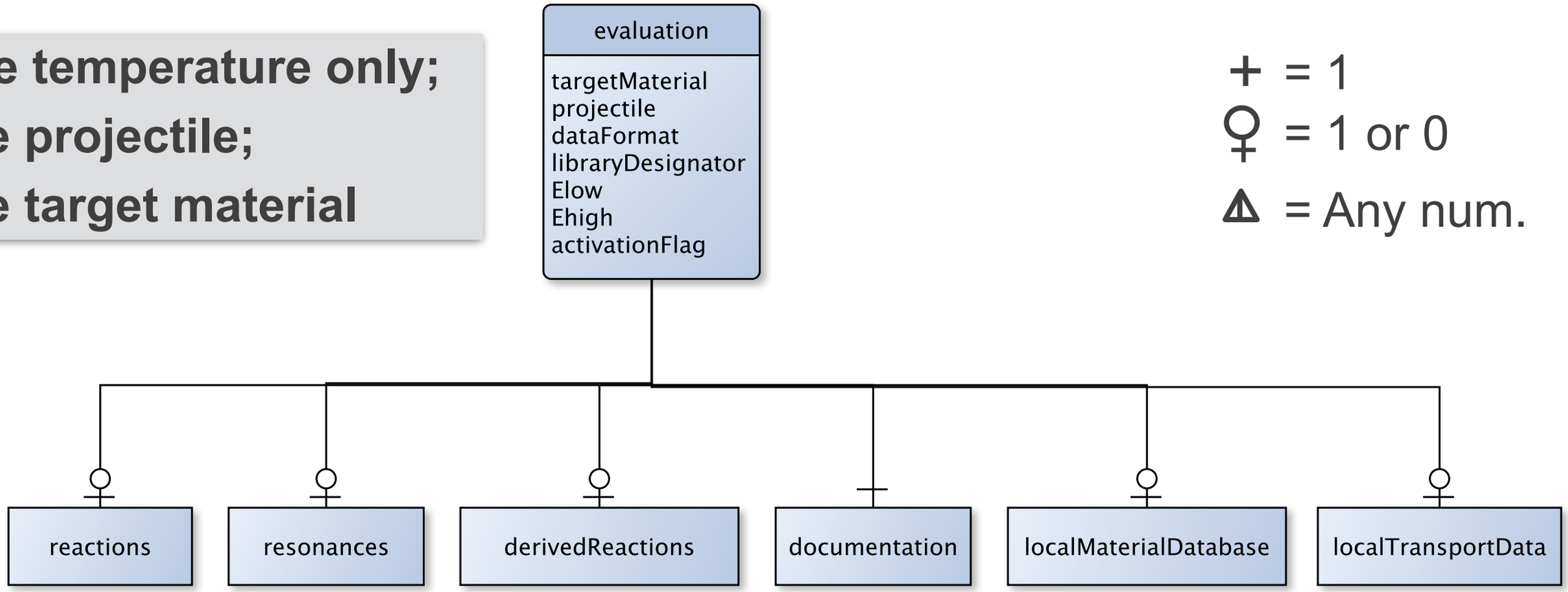
This is the most-typical use case: a neutron hitting a nucleus



- With a little planning, we can also accommodate charged particle and gamma induced reactions too
- TSL data is actually not a stretch

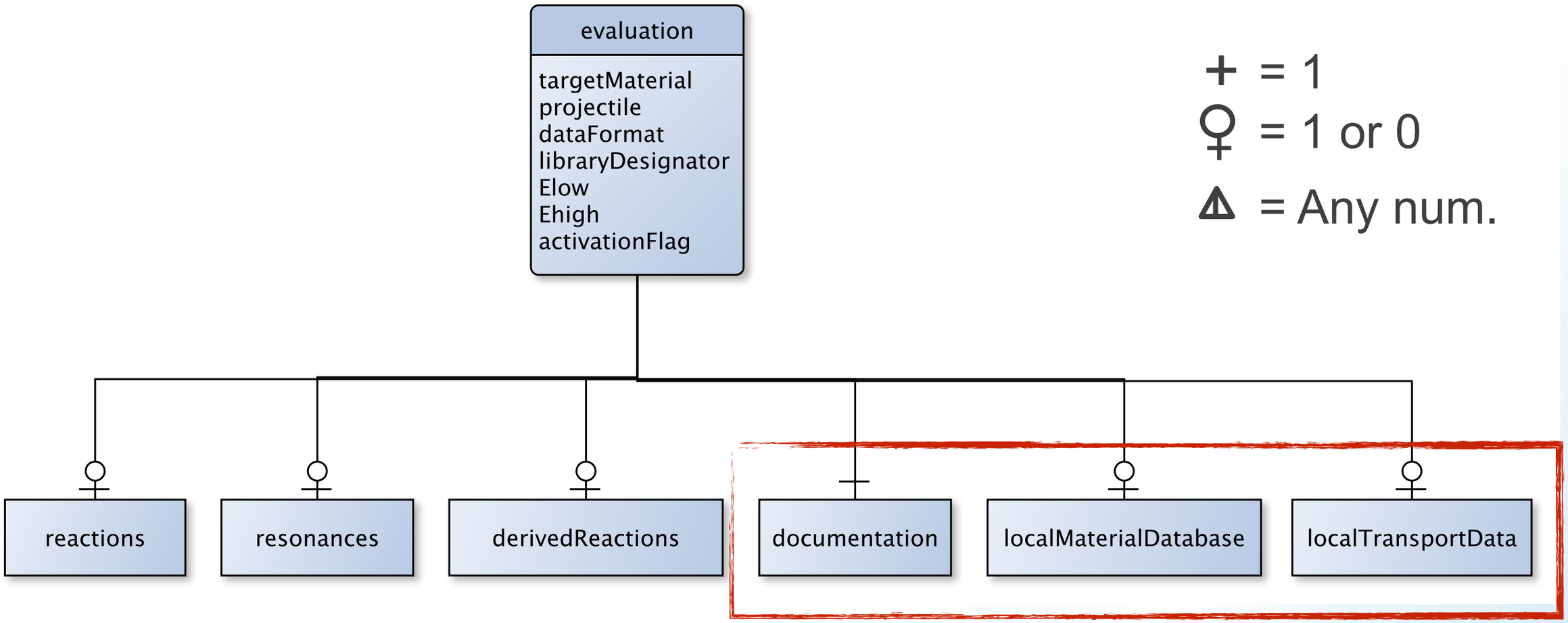
The top level: an <evaluation>

One temperature only;
one projectile;
one target material



+ = 1
♀ = 1 or 0
⧋ = Any num.

The top level: an <evaluation>, cont.



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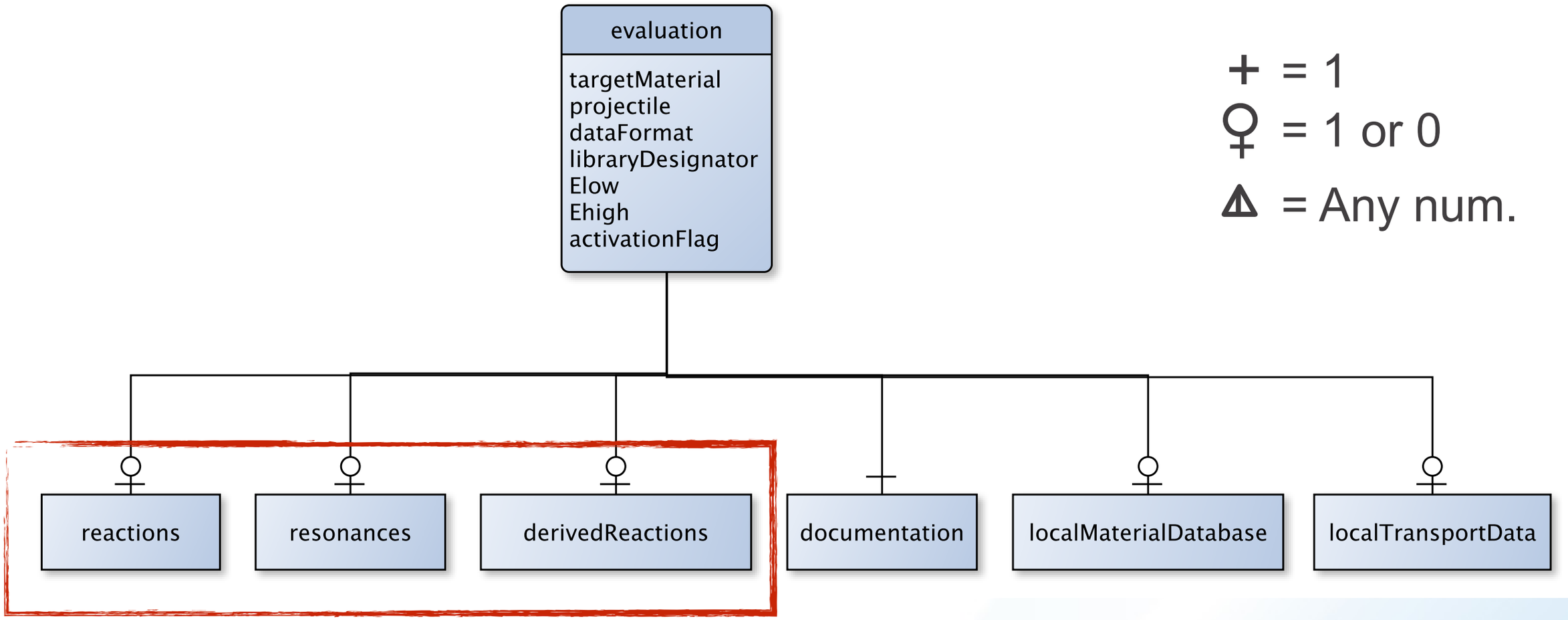
- **<localMaterialDatabase>** Fulfills need to override default material information (esp. for older evaluations) — *will discuss later this morning*
- **<localTransportData>** Data needed for transport, overriding or describing things specific for this evaluation (e.g. local group structure) — *will discuss this tomorrow afternoon*
- **<documentation>** Allowed at all levels — *thoroughly discussed in previous SG38 meetings?*

The top level: an <evaluation>, cont.



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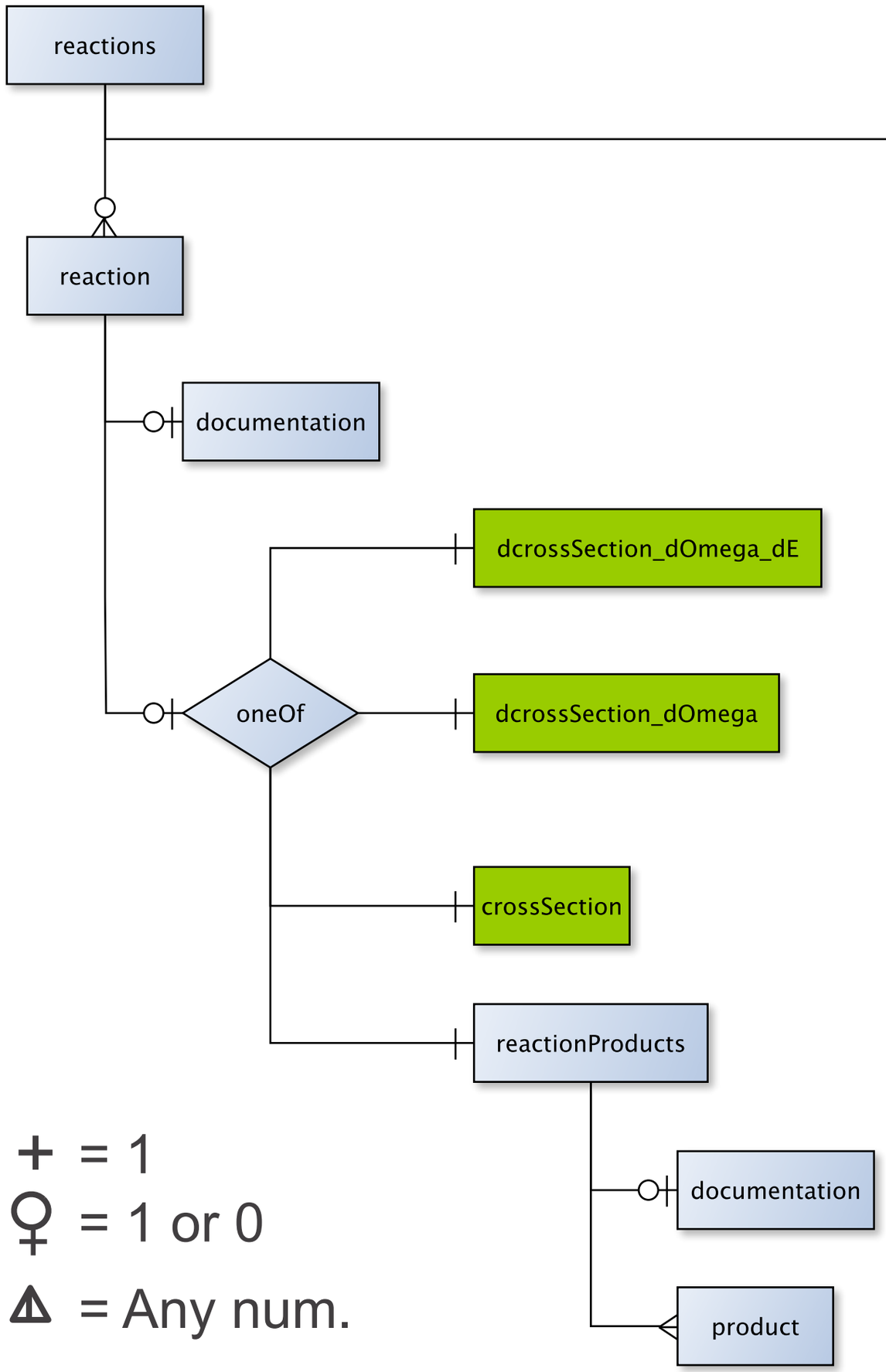
- **<reactions>** is the base of most kinds of reaction data
- **<derivedReactions>** similar to reactions, but contains reactions such as total, non-elastic, etc. which are derived from main **<reactions>**
- **<resonances>** are for anything explicitly described by the R matrix (basically ENDF MF=2, MT=151) — *will discuss this afternoon*

<reactions>



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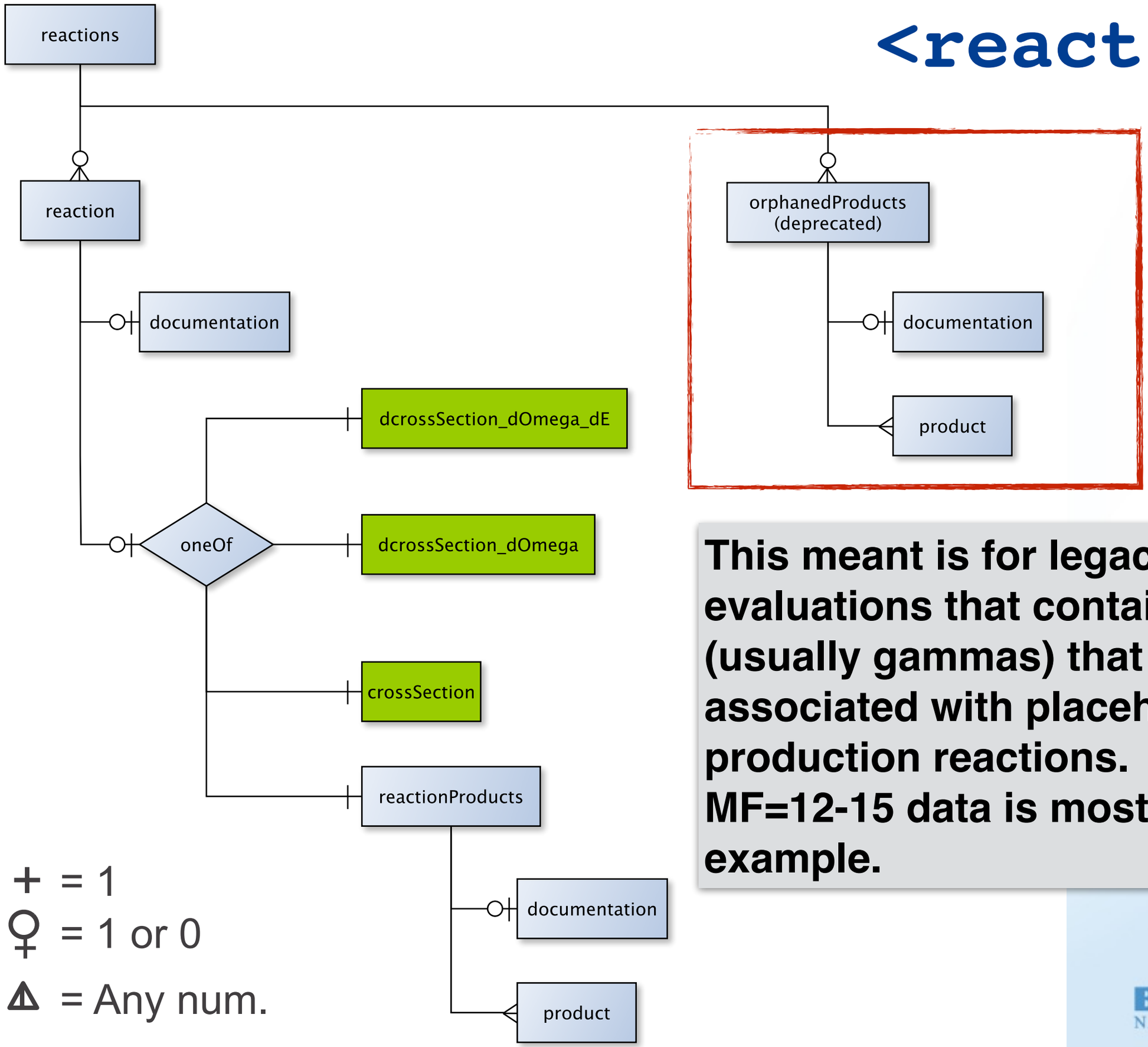
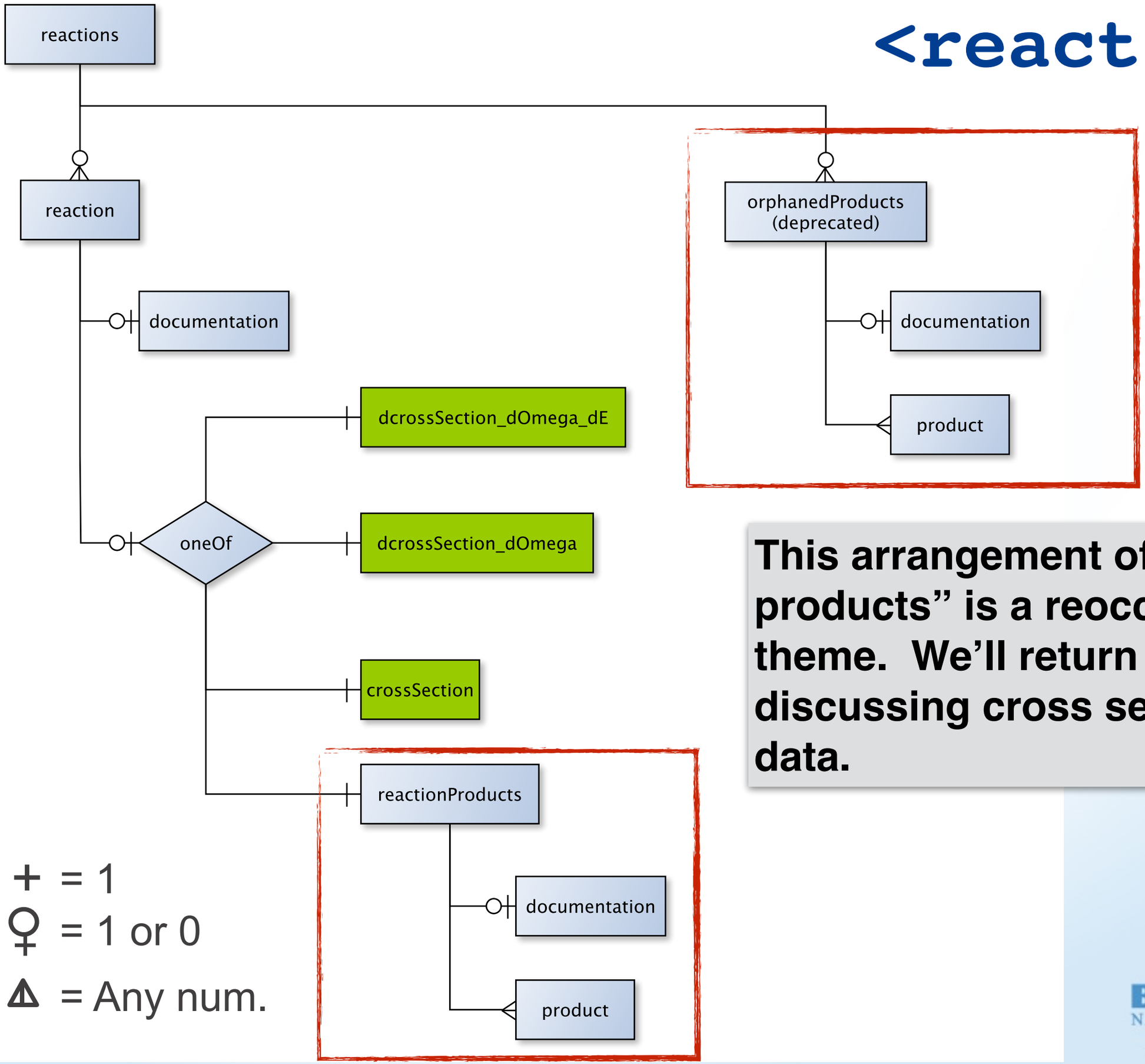
Green boxes have real data tables in them. We'll discuss low level containers & their use in the afternoon.

<reactions>



This meant is for legacy evaluations that contain products (usually gammas) that are associated with placeholder or production reactions. MT=3,4, MF=12-15 data is most common example.

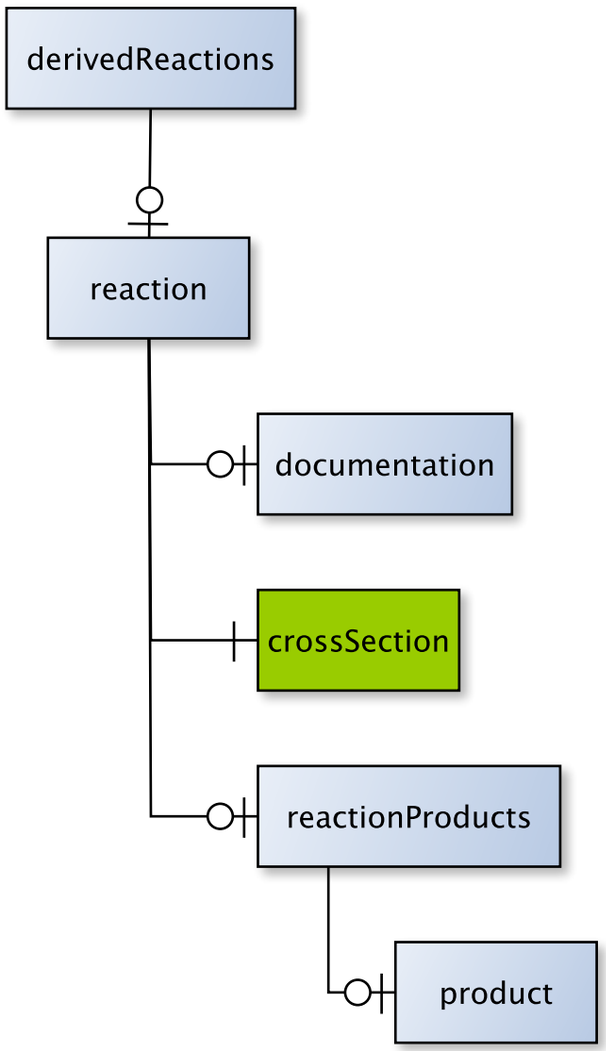
<reactions>



This arrangement of a “list of products” is a reoccurring theme. We’ll return to it after discussing cross section data.

(need better name)

An aside: <derivedReactions>



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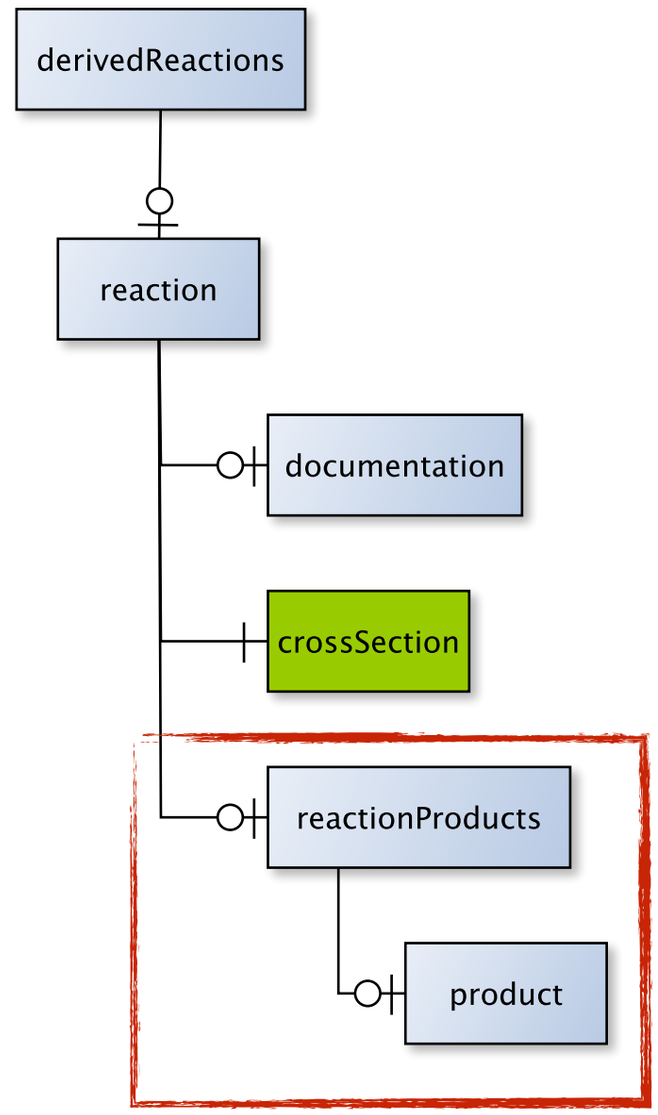
- **Typical uses:**
  - (n,tot) (MT=1) cross section is sum of all other cross sections, but often well measured.
  - total fission (MT=18) cross section is sum of first, second, … chance fission
  - Activation or particle production too
- **Having the cross section here allows us to store covariance on the cross section**
- **Sumrule must be stored in `<reaction>` element**
- **Not meant for transport!!!**
- **Allows evaluator option to store total inelastic gammas instead of using `<orphanedProducts>` (should be deprecated)**

(need better name)

An aside: <derivedReactions>



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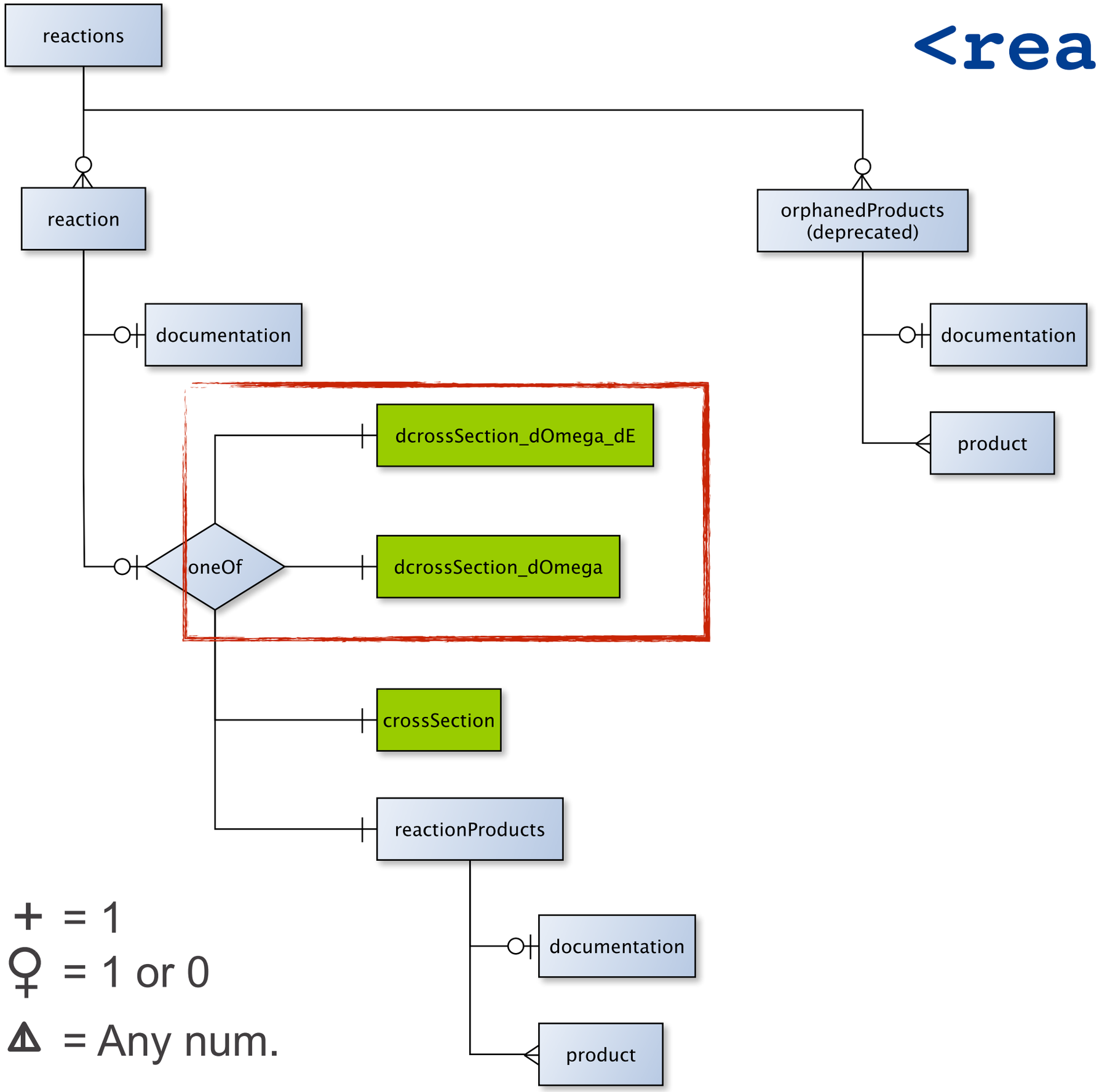
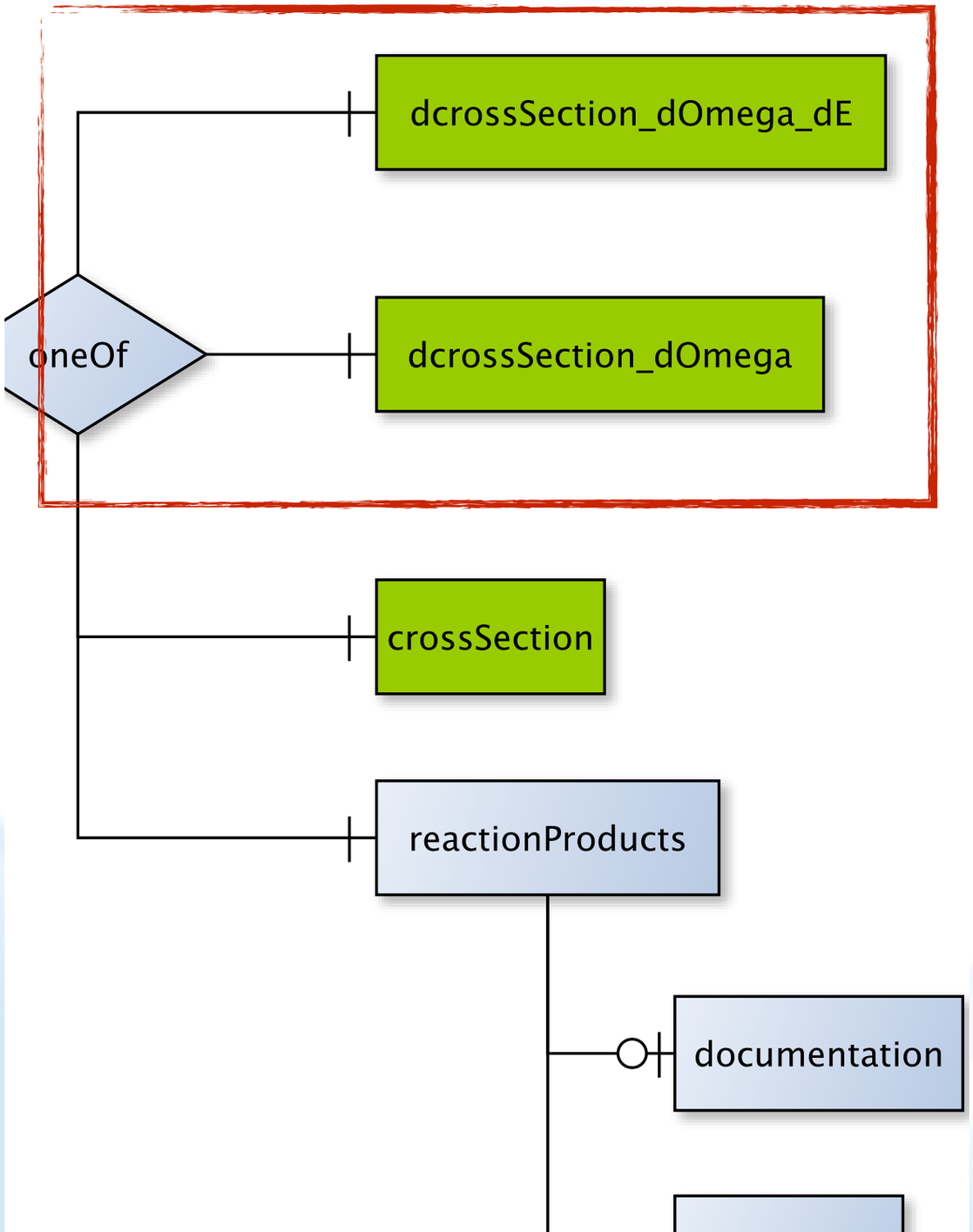
Note "list of products" again

<reactions>

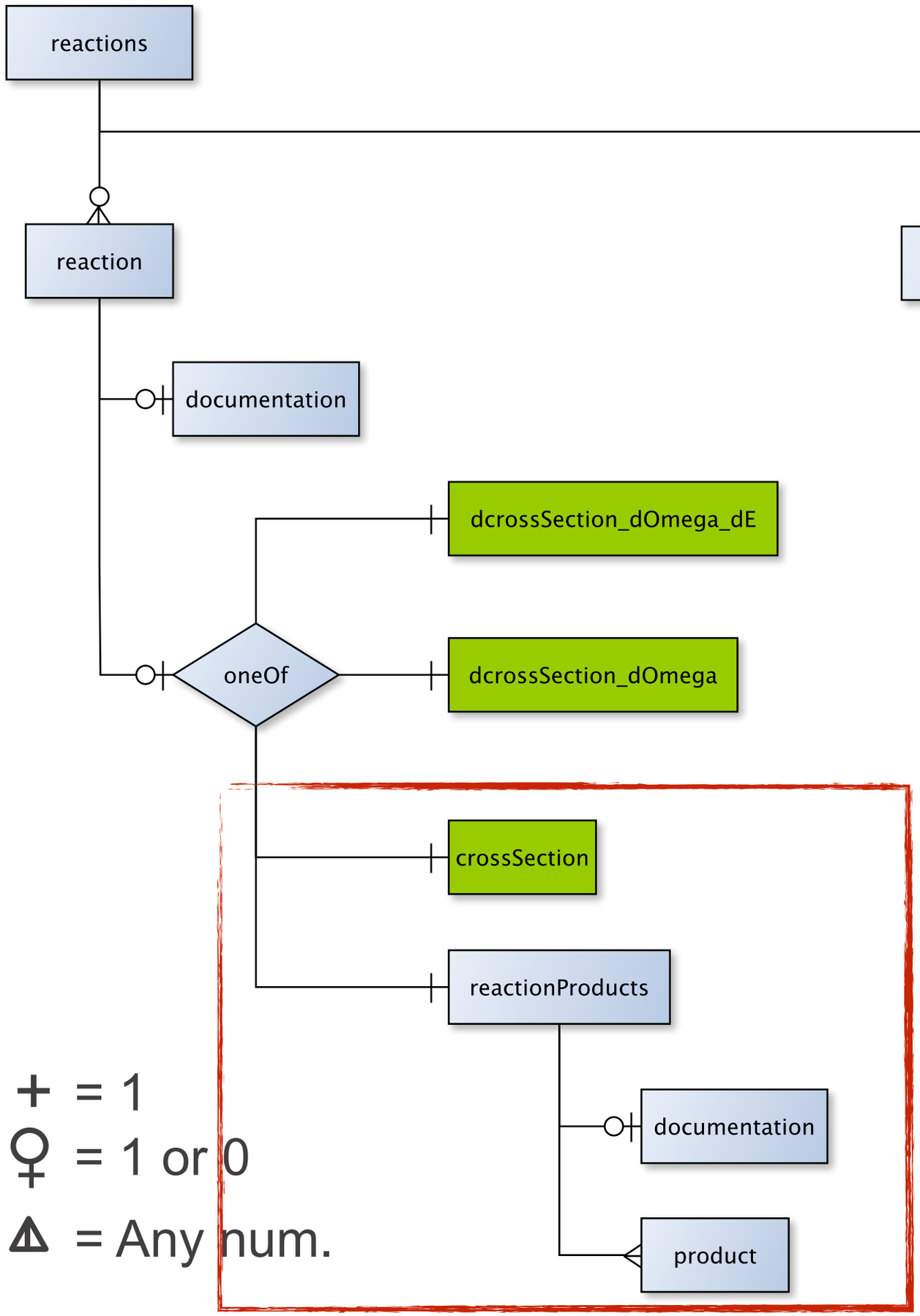


ENDF has a few special cases that require parametric or other treatment of the cross section



- **With two-body kinematics, store *dσ(E)/dΩ* as parameterized data:**
  - Atomic scattering using Klein-Nishina formula
  - Large Angle Coulomb Scattering (LACS) data
- **Without two-body kinematics, store *dσ(E)/dΩdE'* itself**
  - Thermal Scattering Law (TSL)

<reactions>



- **Two-body reactions:**

$$\frac{d\sigma(E)}{d\Omega} = \frac{1}{2\pi}\sigma(E)P(\mu|E)$$

- **Everything else:**

$$\frac{d\sigma(E)}{d\Omega dE'} = \frac{1}{2\pi}\sigma(E)P(\mu, E'|E)$$

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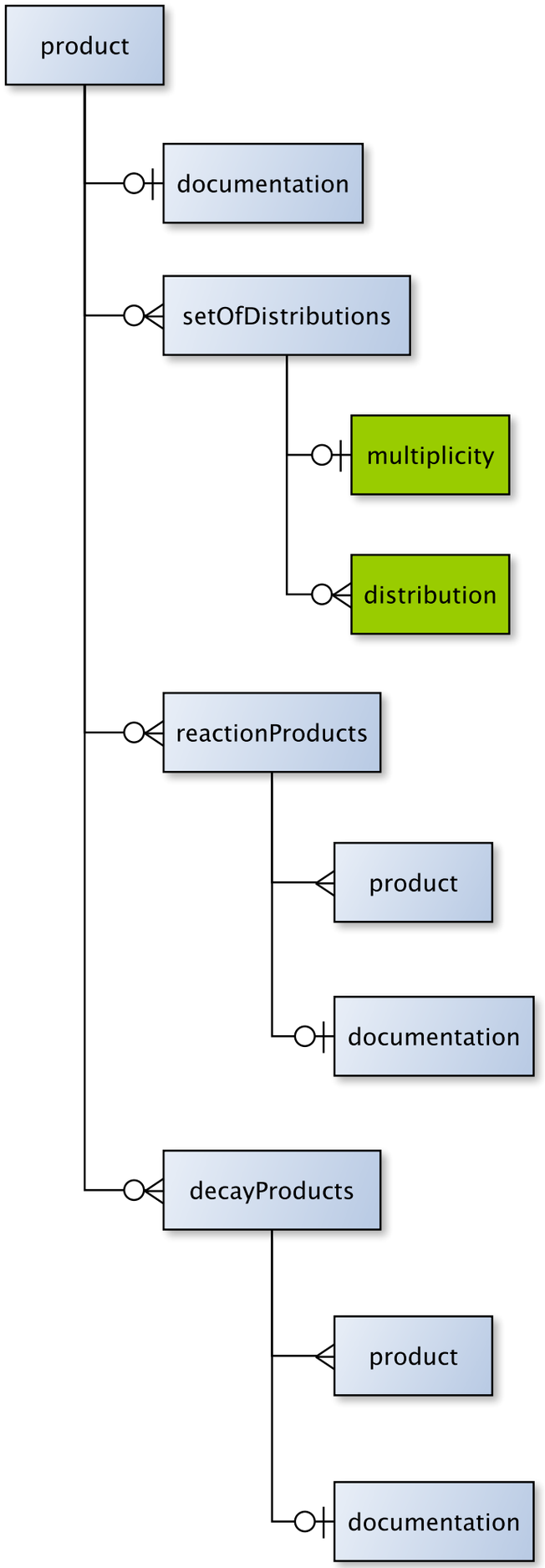
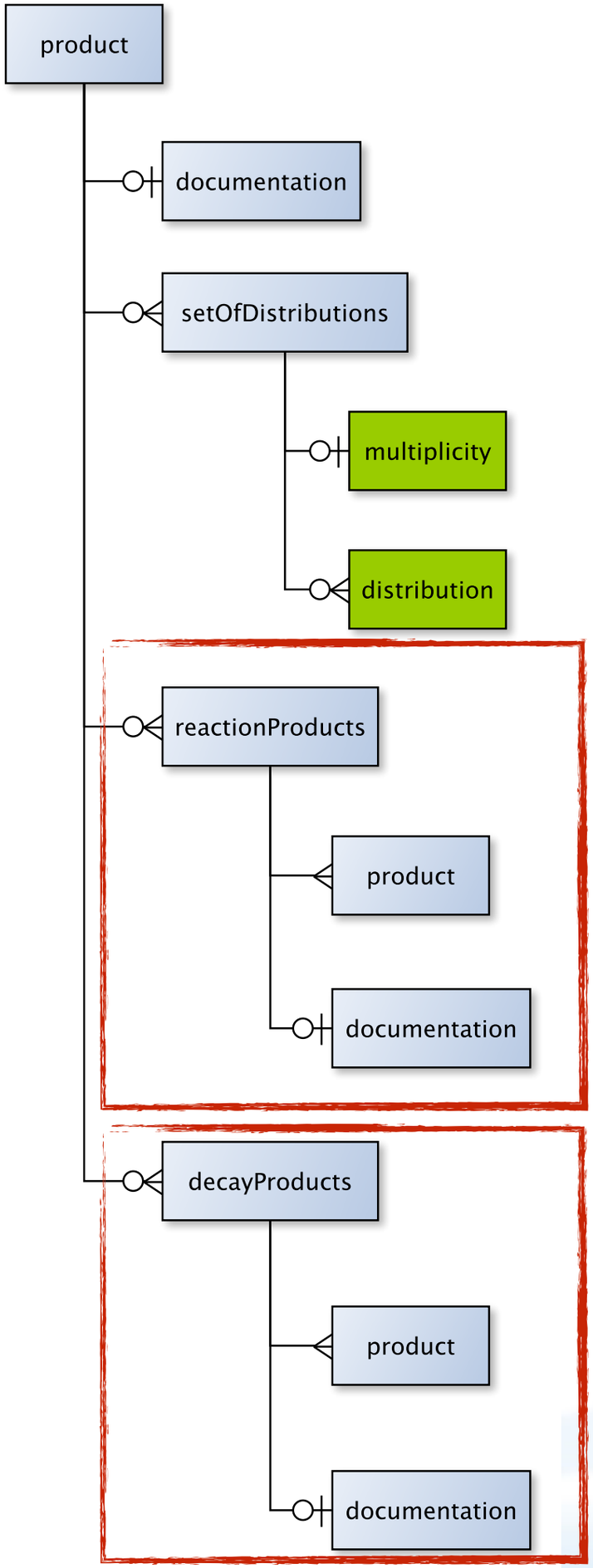
<product> element holds everything about a product

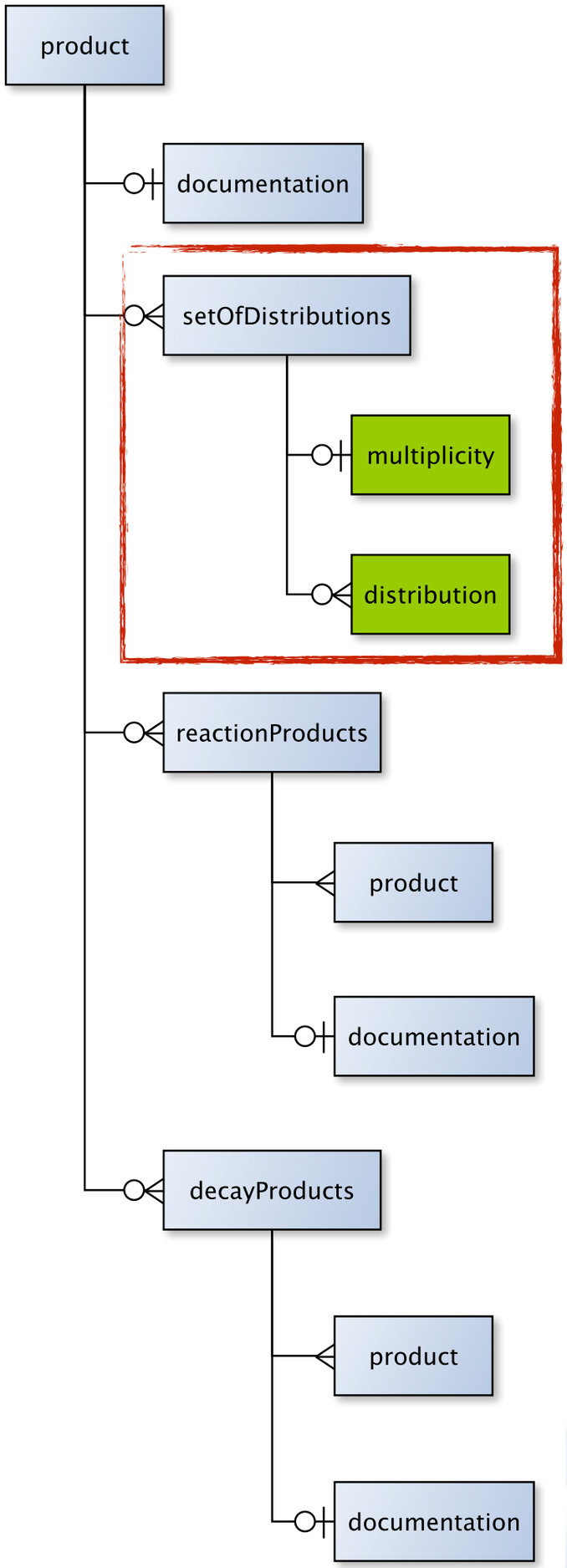


<product> element holds everything about a product



Products can break up into more reactionProducts, which have products that can breakup into more reactionProducts ….

Products that decay have decayProducts, decayProducts have more products which can have decayProducts which have products ….



<product> element holds everything about a product

- **Multiplicity**
  - may be just an `int` and be obvious (n,2n)
  - may be interpolation table (for nubar data)
  - may include P(nu|E) for fission
  - ***possibly should be moved up a level, what do you all think?***
- **Distributions are divided into components;** they are listed on the next slide

A <distribution> collects all the possible representations of an observable together

<component>	<form>	ENDF equivalent
angular	pointwise	MF4 LTT2
	Legendre	MF4 LTT1
	isotropic	MF4 LTT0
	recoil	MF6 LAW4
energy	pointwise	MF5 LF1
	Evaporation Spectrum	MF5 LF9
	Maxwellian	MF5 LF7
	Watt Spectrum	MF5 LF11
	Madland-Nix	MF5 LF12
	N-Body Phase Space	MF6 LAW6
energy-angular	Kalbach-Mann	MF6 LAW1 LANG2
angular-energy	pointwise	MF6 LAW7
uncorrelated	combination of 'angular' and 'energy'	MF4 and MF5