Resonances

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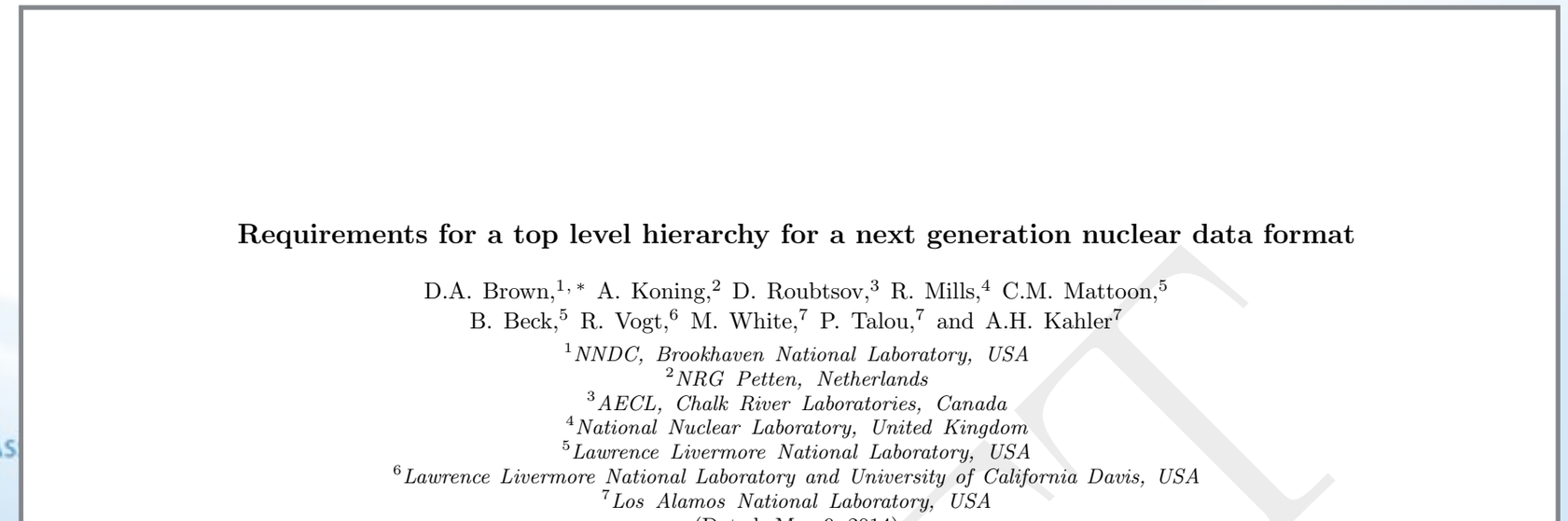
BROOKHAVEN NATIONAL LABORATORY

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
- **Element & attribute names are illustrative. They can be changed.**
- **We've tried to have a detailed discussion about the resonances, but I don't think we've really wrapped it up**



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

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[4] *National Nuclear Laboratory, United Kingdom*
[5] *Lawrence Livermore National Laboratory, USA*
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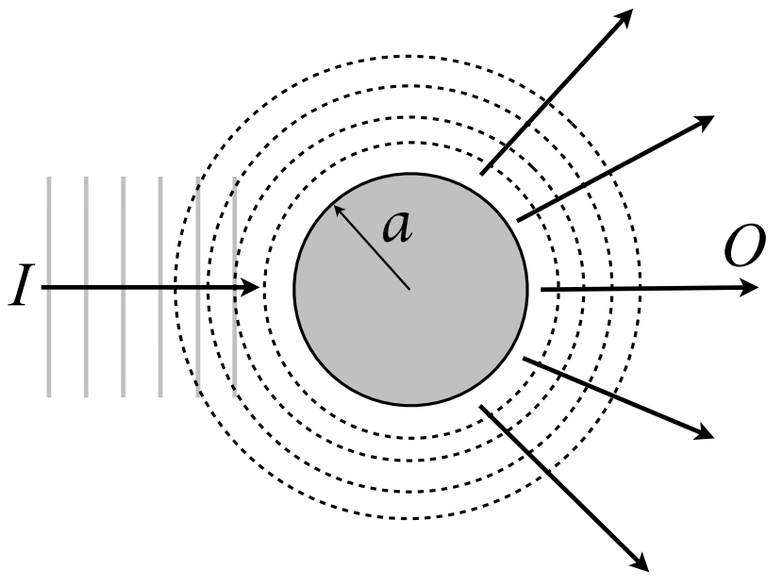
[7] *Los Alamos National Laboratory, USA*

R matrix background



$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E}$$

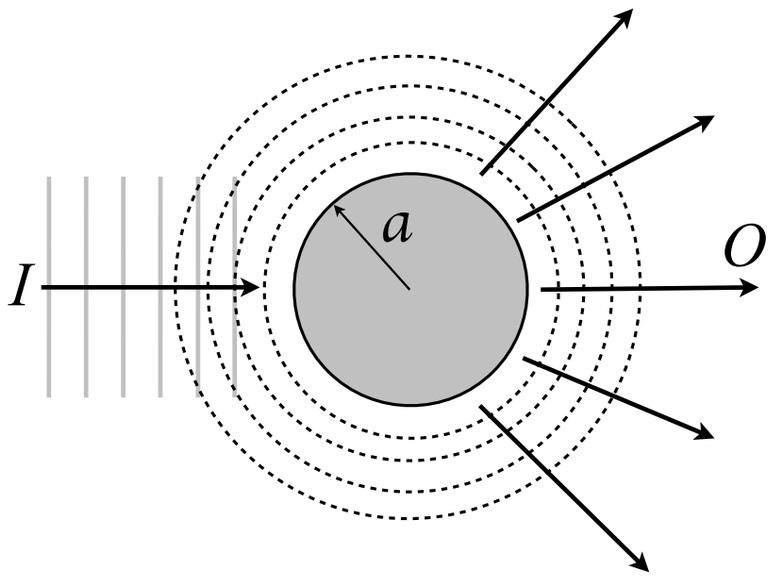
$$U_{cc'} = e^{-i(\varphi_c+\varphi_{c'})}\sqrt{P_c}\sqrt{P_{c'}} \times \{[\mathbf{1}-\mathbf{R}(\mathbf{L}-\mathbf{B})]^{-1}[\mathbf{1}-\mathbf{R}(\mathbf{L}^*-\mathbf{B})]\}_{cc'}$$

Given by the WF

Boundary parameter

- Divide the universe with a spherical box.
- Outside box, use two-particle “free” wave functions
- Somewhere inside the box is the reaction zone; we don’t care about the details. Can write those details as the Green’s function solution of Schoedinger’s equation.
- The R matrix is the Green’s function.
- **“Everything” can be written in terms of R; with it we can compute the scattering matrix U, so we have dσ/dΩ.**

R matrix background



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- "Everything" can be written in terms of R; with it we can compute the scattering matrix U:

$$\sigma_c \equiv \sum_{c'} \sigma_{cc'} = 2\pi\lambda_c^2(1-\Re U_{cc})$$

$$\sigma_{cc'} = \pi\lambda_c^2 g_c|\delta_{cc'} - U_{cc'}|^2$$

$$\frac{d\sigma_{\alpha,\alpha'}(E)}{d\Omega} = \frac{1}{k^2(2i+1)(2I+1)}\sum_{s,s'}\sum_{L=0}^{\infty} B_L(\alpha s,\alpha' s';E)P_L(\mu)$$

$U_{cc'}$ is in there, but you do NOT want to see the equation

R matrix background

- R matrix theory works for any two particles
- R matrix theory is exact
- R matrix theory is elegant

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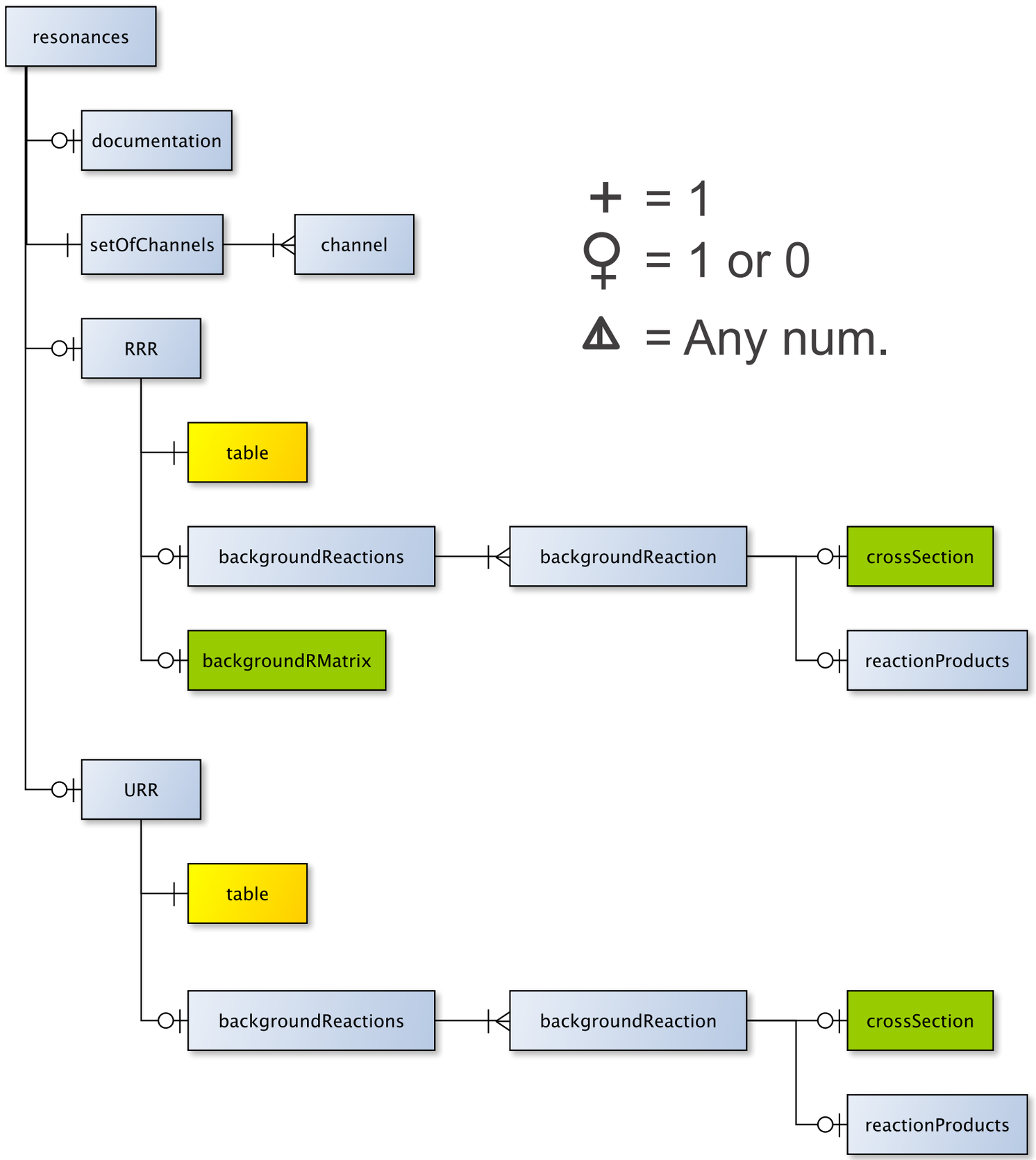
ENDF screws it up

<resonances>



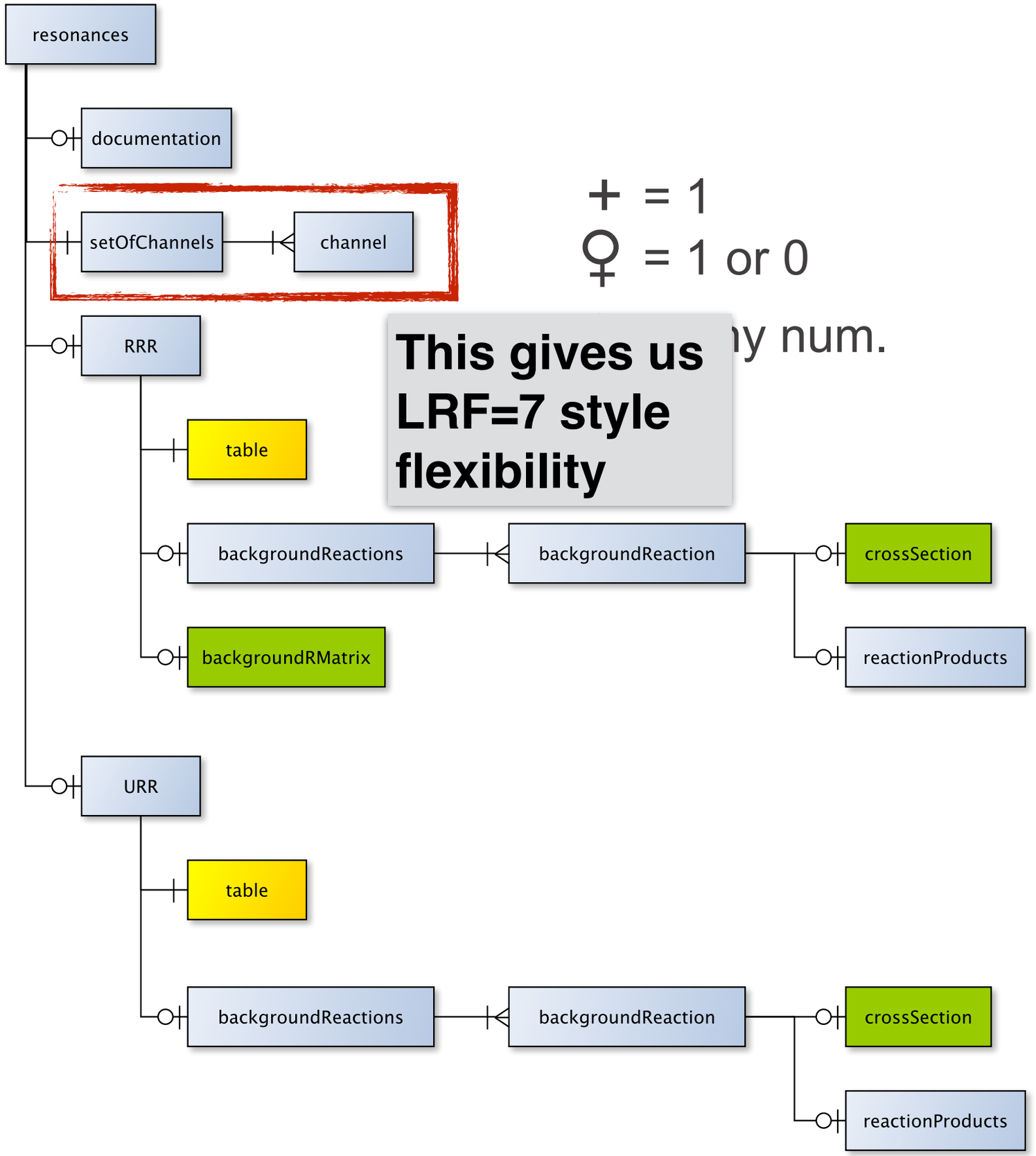
+ = 1

♀ = 1 or 0

△ = Any num.

- **Standard ENDF MF=2, MT=151 *(but improved)***
- **<setOfChannels>: the list of channels/ reactions in this element**
- **<RRR> are the resolved resonances**
- **<URR> are average resonance data**

<resonances>



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This gives us LRF=7 style flexibility

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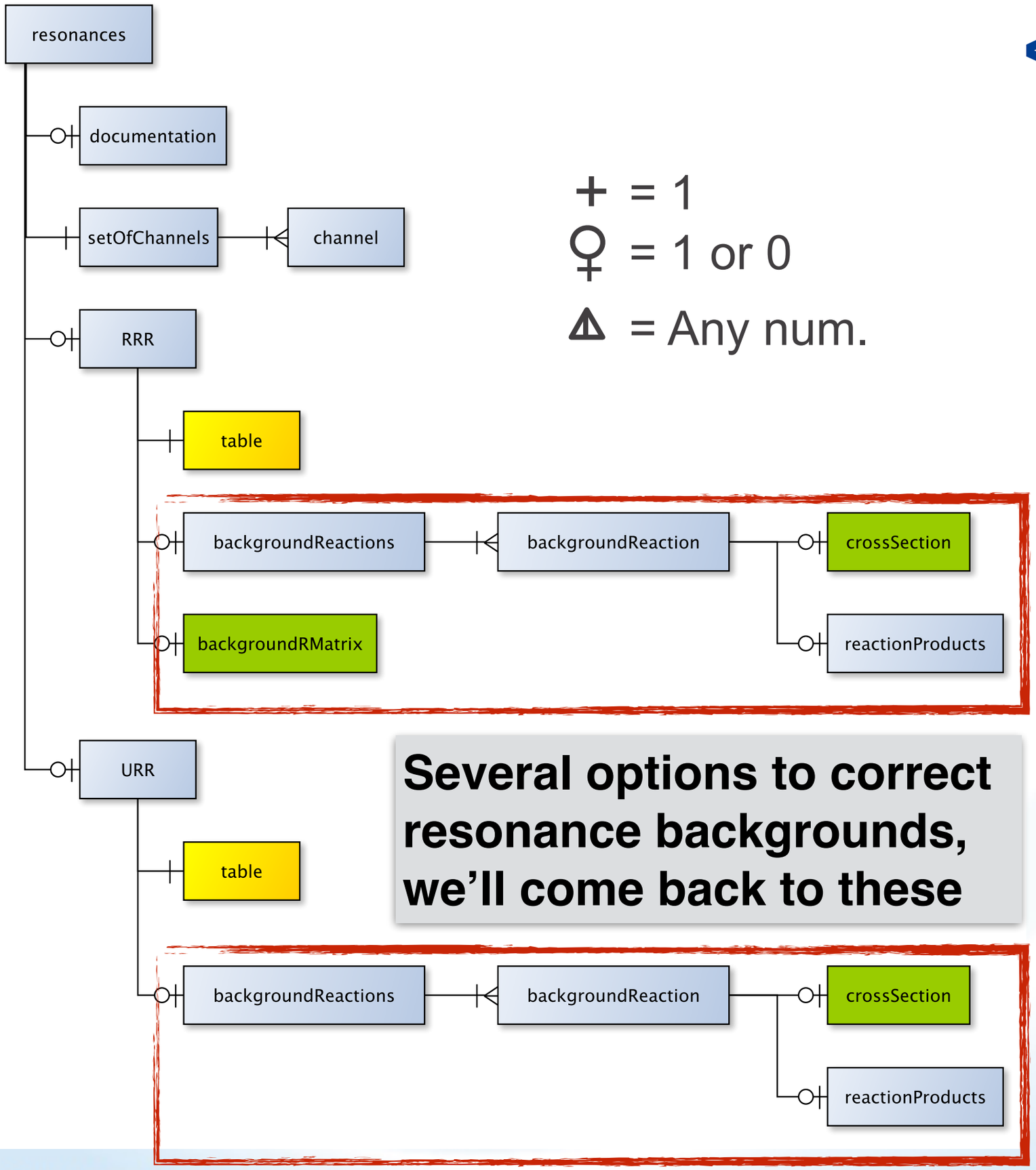
What we need for a <channel>

- **reaction designator**
  - really just the identity of the 2 particles
  - ENDF's LRF=7 has all this, but w/o particle database is quite verbose
- **relativistic/non-relativistic flag**
- **ENDF MT (if appropriate)**
- **s, l, J, Π**
- **other user-definable quantum numbers** (e.g. K)
- **boundary parameter B_c**
- **channel radius information**
- **sign of reduced width**

<resonances>



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Several options to correct resonance backgrounds, we'll come back to these

- **Standard ENDF MF=2, MT=151 *(but improved)***
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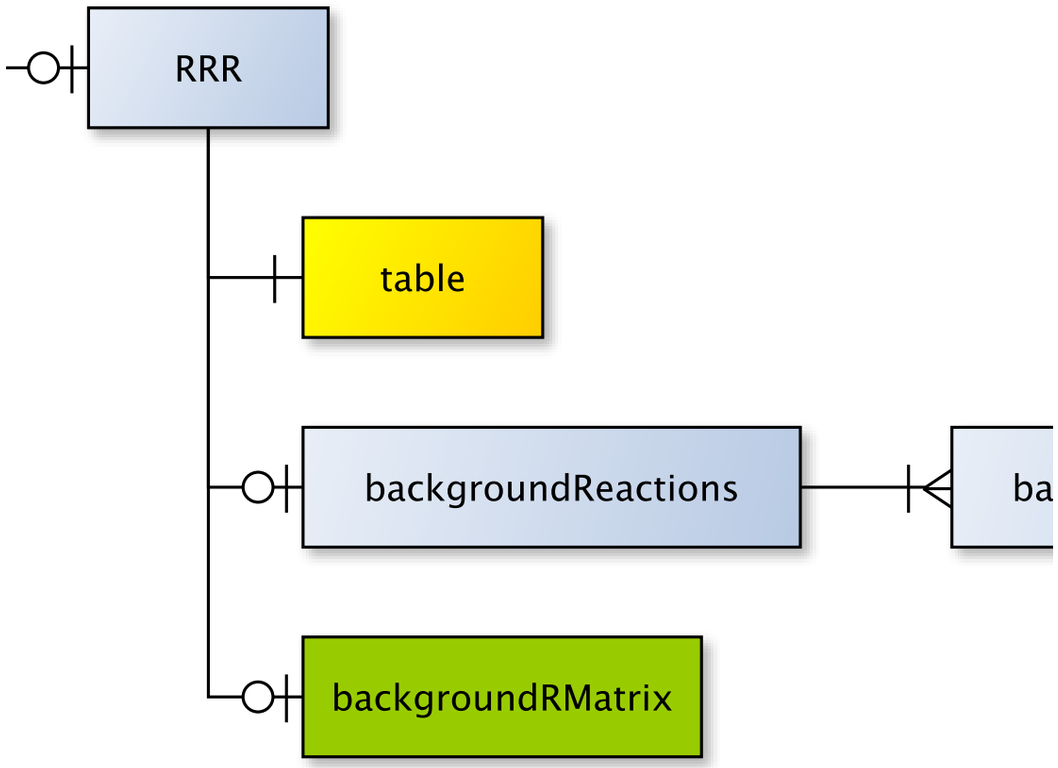
RRR, cont.



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- ENDF gives a lot of possible approximations and modifications to the R matrix; not all of these are faithful to R matrix theory
- **We will need to grandfather in all of the ENDF approximations, no matter how bad they are:**
  - ***(LRF=1)* SLBW**
  - ***(LRF=2)* ENDF-style MLBW**
  - ***(LRF=7, KLM=2)* CALENDF-style MLBW (aka MNBW) — this is a controlled R-matrix approximation**
  - ***(LRF=3)* ENDF-style Reich-Moore**
  - ***(LRF=7, KRM=3)* Reich-Moore — this is a controlled R-matrix approximation**
  - ***(LRF=7, KRM=4)* Full R-matrix**
  - ***(LRF=4)* Adler-Adler ?**
- **Do w/ attribute on <RRR>**

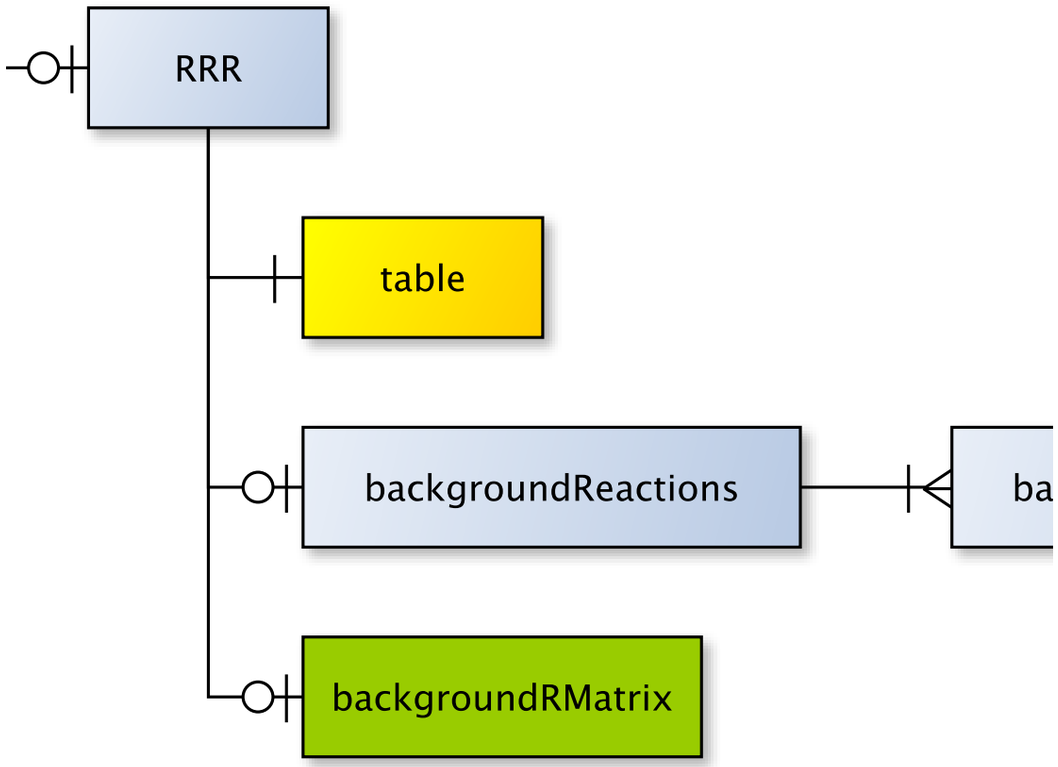
RRR

- The RRR doesn't need a complicated format, but it needs a complete one. All we need is a `<table>`:

E	Γ	Γ	Γ	Γ	...
eV	eV	eV	eV	meV	...
1.23	9.433	0	2.33E-03	7.1	...
1.46	4.833	0	2.33E-03	4.6	...
3.45	1.78	1.78	0	0	...
...	...	...	...	...	

- Columns in table must map to appropriate <channel>

RRR, cont.



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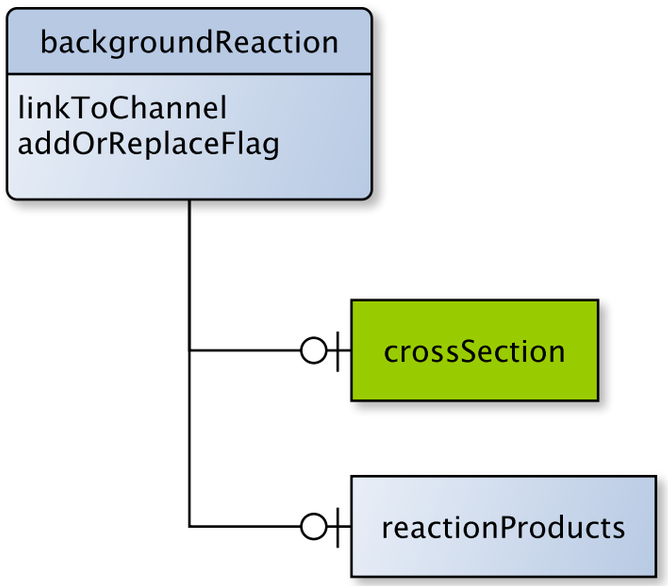
- ENDF provides a lot of tricks to help repair damage bad approximations cause
- **We will need to grandfather in all the ENDF tricks to fix the ENDF approximations, no matter how bad they are.**
- **Background R-matrix fixes:**
  - ***(KBK=0)* Dummy resonances**
  - ***(KBK=1)* Tabulated function**
  - ***(KBK=2)* SAMMY's logrithmic parameterization**
  - ***(KBK=3)* Froehner's parameterization**

Fixing the background R-matrix is not always enough



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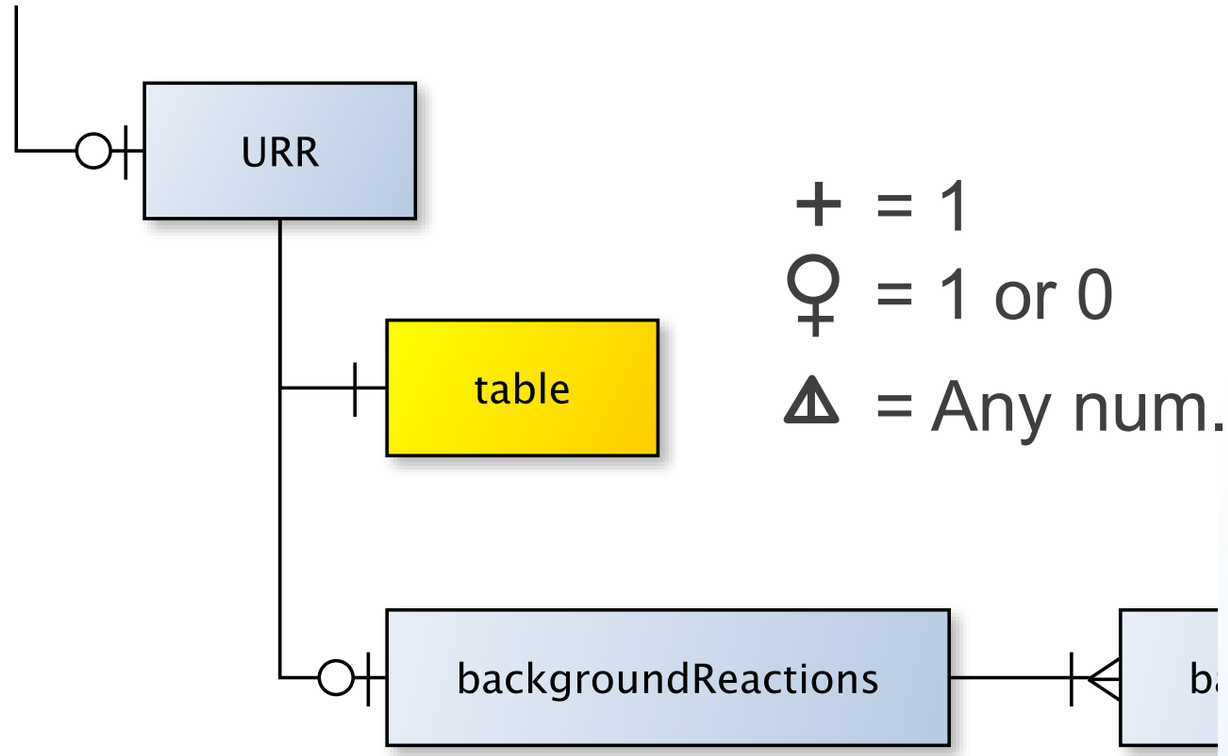
- **Background cross sections may be needed to be added to certain channels**
- **Angular distributions may need to be specified if parameterization doesn't support them or if we don't trust them**
- Better to keep this with the RRR than in the <reaction> hierarchy.

URR

- **We don't know the resonances (they are unresolved). We assume**
  - the resonance energies are distributed according to random matrix theory
  - the widths of the resonances are distributed with χ^2 distributions
- **ENDF further assumes the resonances were given in SLBW**
- **With these assumptions, can compute**
  - average cross sections
  - probability distributions for cross sections, e.g. P(σ|E) using NJOY's PURR module
- **GRUCON developers take it further… they replace all RRR with URR. Compute $P(\sigma_{tot}|E)$ and $P(\sigma_x|\sigma_{tot},E)$**

URR

- Need: degree of freedom for each channel
- Need: table with:
  - incident energy
  - average level spacing
  - average width for each channel
- Need interpolation scheme for average parameters
- Should we also put a flag for the approximation (to allow other than SLBW)?
- Need a spot for PURR probability distributions, to be covered later



Are we missing anything?