UT-BATTELLE

R-Matrix Limited Format Proposal

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R-Matrix Limited Format proposal

- File 2 (resonance region)
  - LRU = 1 (resolved-resonance region)
    - LRF = 7 (RML format)

Why is this format needed?

- **The so-called "Reich Moore format" (LRF=3) is a limited form of Reich-Moore –**
  - **One entrance channel**
  - **At most two fission channels**
  - **No charged particles**
  - **No inelastic channels**
- **New evaluations require those features**
- **The "General R-Matrix" might be used for these, but has not been implemented**

What does the format look like?
Three essential components –

1. **Particle-pairs**

Repeat as many times as needed

2. **Spin-group definitions**
   - **channels reference the particle-pairs**
3. **Resonances**
4. (Maybe other information as well)

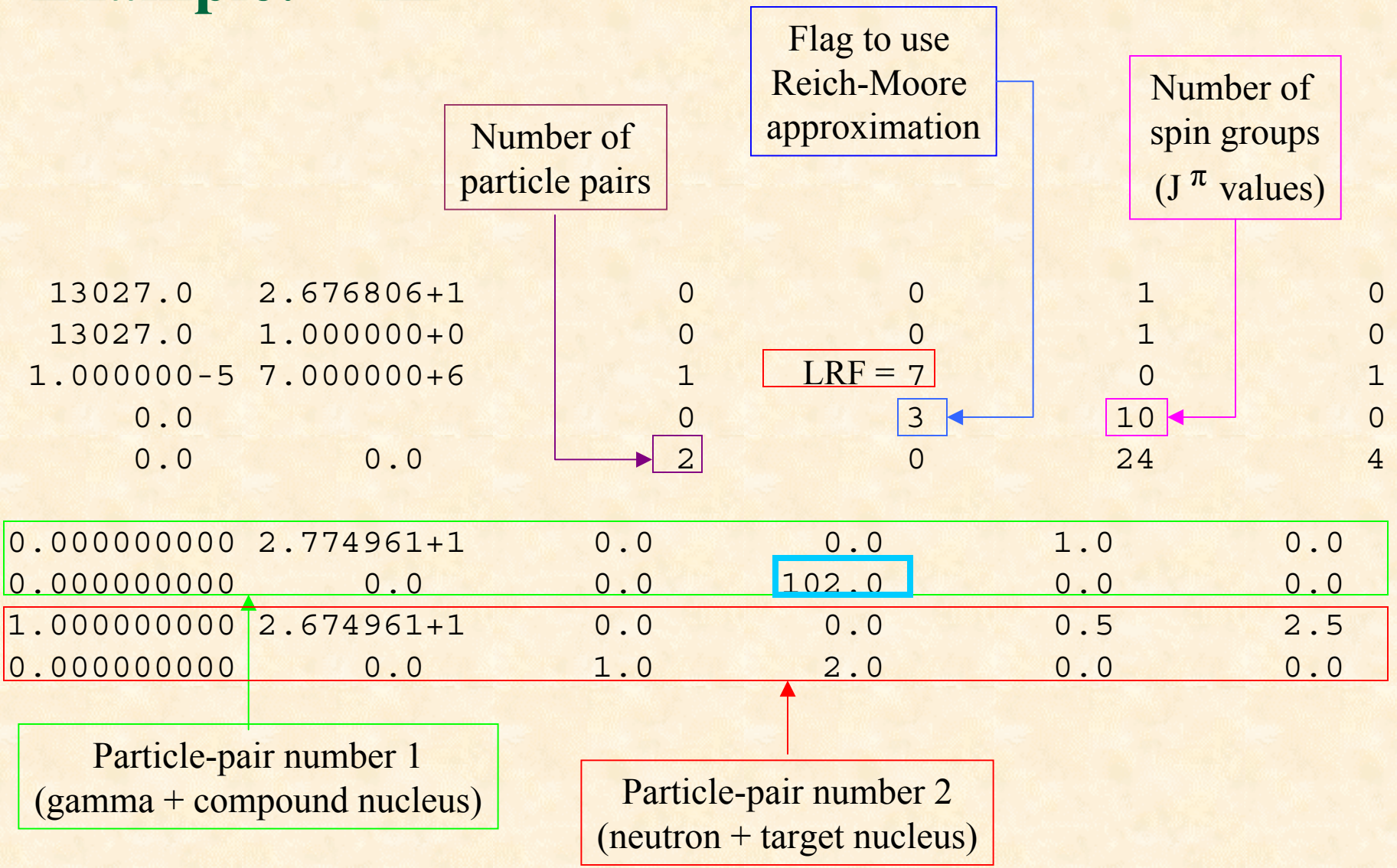
(1) Particle-pair definitions

- **Possible particle-pairs –**
  - **(1) gamma + compound nucleus (capture)**
  - **(2) neutron + target nucleus (elastic)**
  - **(3) neutron + exited target nucleus (inelastic)**
  - **(4) fission (in which case do not specify particle info)**
  - **(5) others reactions**
    - **non-eliminated gamma channels**
    - **alpha + other nucleus**
    - **etc.**

(1) Particle-pair definitions, contd.

- List of pairs includes the following –
  - Descriptors for each member of the pair
    - MT value may be sufficient
      - (e.g., fission or "eliminated" gamma)
    - mass, spin, parity, charge
    - Q-value if needed
  - Descriptors for the pair
    - Flag whether to calculate penetrabilities
    - Flag whether to calculate shift factors

Example: ^{27}Al



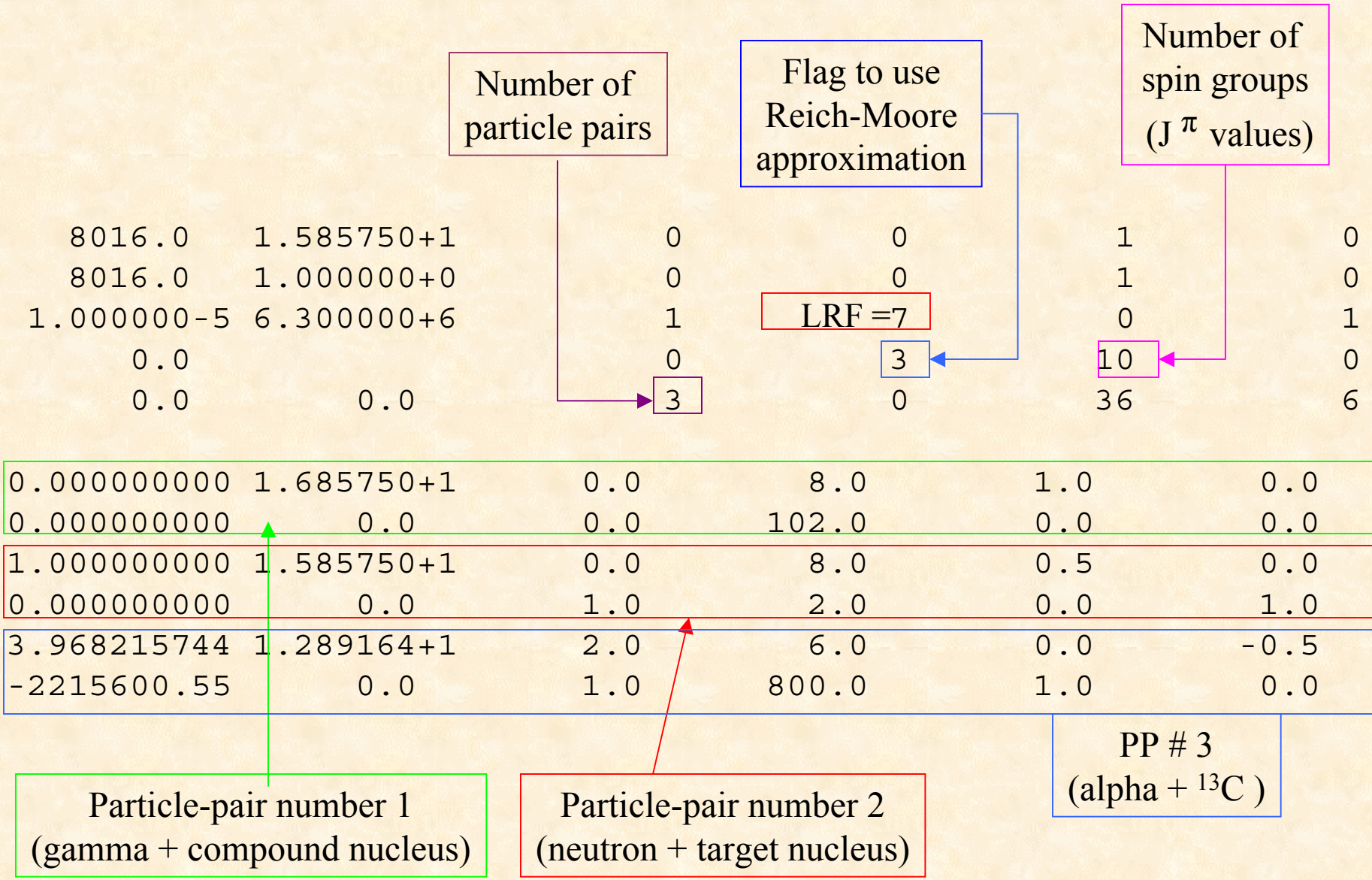
Example: ^{27}Al, revisited

```
  13027.0   2.676806+1          0          0          1          0
  13027.0   1.000000+0          0          0          1          0
1.000000-5 7.000000+6          1          7          0          1
     0.0                       0          3         10          0
     0.0         0.0           2          0         24          4

####   MA         MB          ZA          ZB          IA          IB
0.000000000 2.774961+1         0.0         0.0         1.0         0.0
0.000000000        0.0         0.0       102.0         0.0         0.0
####   Q          SHF         PNT          MT          PA          PB


####   MA         MB          ZA          ZB          IA          IB
1.000000000 2.674961+1         0.0         0.0         0.5         2.5
0.000000000        0.0         1.0         2.0         0.0         0.0
####   Q          SHF         PNT          MT          PA          PB
```

Example: ^{16}O with alpha channel




```
   8016.0    1.585750+1          0          0          1          0
   8016.0    1.000000+0          0          0          1          0
1.000000-5 6.300000+6          1          0          1          1
      0.0                       0          3         10          0
      0.0          0.0          3          0         36          6

0.000000000 1.685750+1        0.0        8.0        1.0        0.0
0.000000000       0.0         0.0      102.0        0.0        0.0
1.000000000 1.585750+1        0.0        8.0        0.5        0.0
0.000000000       0.0         1.0        2.0        0.0        1.0
3.968215744 1.289164+1        2.0        6.0        0.0       -0.5
-2215600.55       0.0         1.0      800.0        1.0        0.0
```

Example: ^{16}O with alpha channel, revisited

```
   8016.0   1.585750+1          0          0          1          0
####  Z_A   Abundance            0        LFW        NER
   8016.0   1.000000+0          0          0          1          0
#### Emin    Emax            Lru=1 => Resolved Resonance Region
####                                 Lrf=7 => R-Matrix Limited
 1.000000-5 6.300000+6          1          7          0          1
####                Flag for Reich-Moore =  3
####                             Number of J values = 10
      0.0                       0          3         10          0
####  3 pairs of particles are defined next
#### First pair is gamma & compound nucleus, 2nd is neutron, 3rd is alpha
      0.0         0.0           3          0         36          6
####   MA         MB           ZA         ZB         IA         IB
####   Q          SHF          PNT        MT         PA         PB
0.000000000 1.685750+1        0.0          8.0       1.0        0.0
0.000000000       0.0         0.0        102.0       0.0        0.0
1.000000000 1.585750+1        0.0          8.0       0.5        0.0
0.000000000       0.0         1.0          2.0       0.0        1.0
3.968215744 1.289164+1        2.0          6.0       0.0       -0.5
-2215600.55       0.0         1.0        800.0       1.0        0.0
```

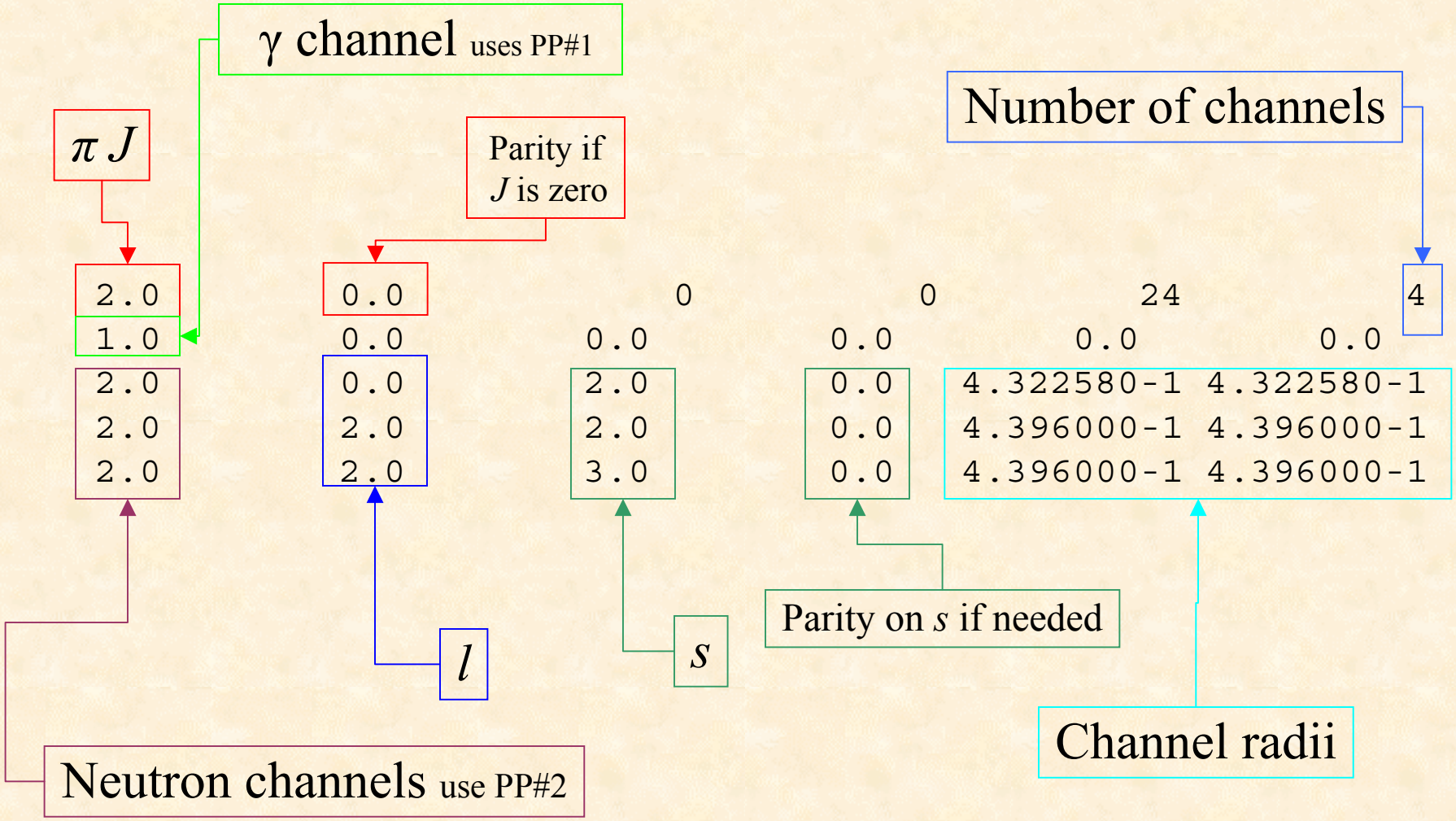
ZA and ZB are necessary here!

(2) Spin group definitions –

- **For each spin group (that is, for each compound nuclear state), define –**
  - **J^{π} and number of channels**

- **For each channel in that spin group, define –**
  - **which particle pair**
  - **orbital angular momentum l**
  - **channel spin $s = i + I$**
  - **boundary condition if needed**
  - **channel radii if needed**

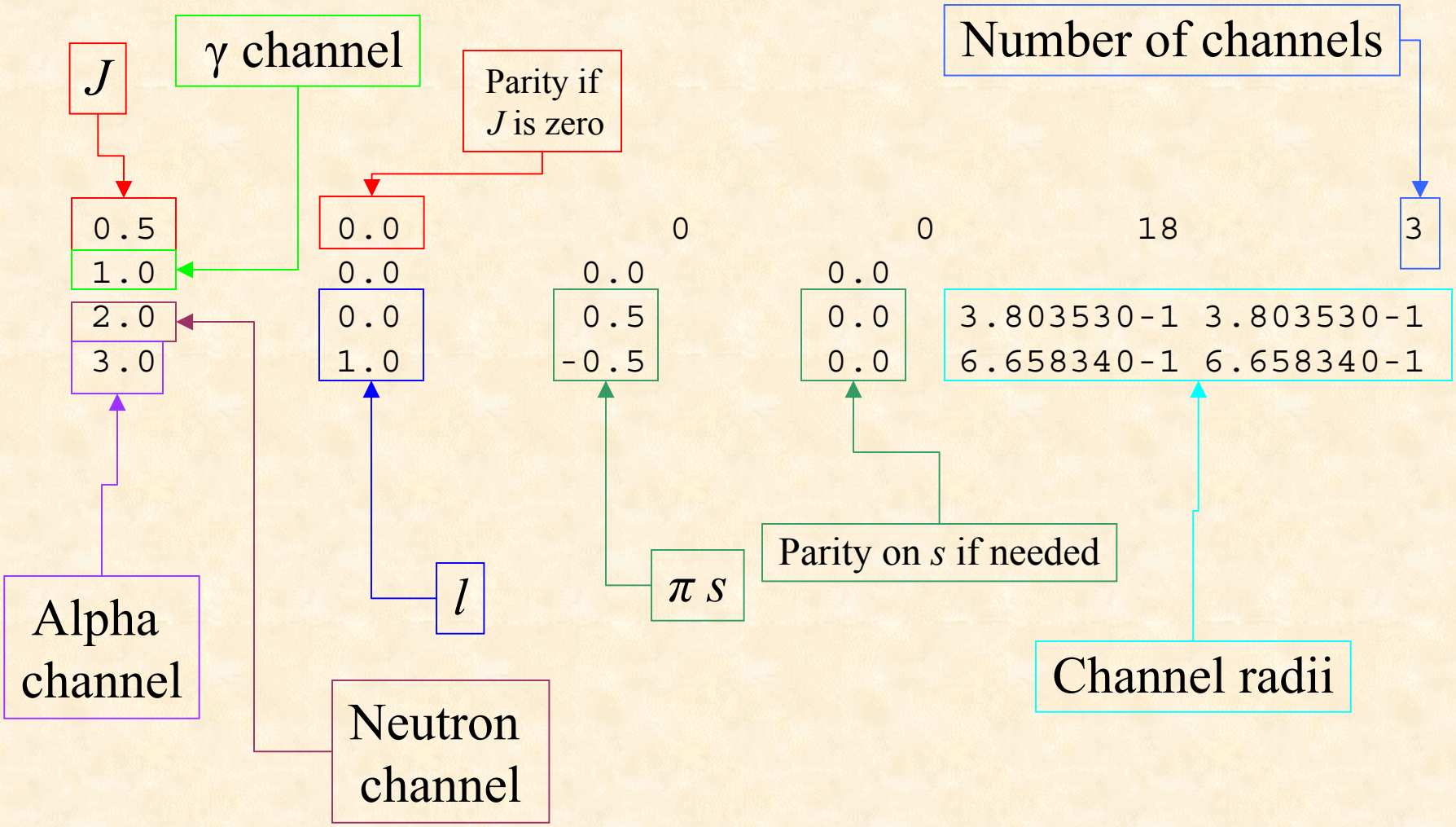
Example: ^{27}Al, continued



Example: ^{27}Al, revisited

```
####
####    Spin group is defined in the next lines
####    J     Parity                          Number of channels=  4
      2.0         0.0              0           0          24           4
####
#### First channel is gamma, 2nd, 3rd, and 4th are neutron
####  IPP         L          SCH                      APE          APT
      1.0         0.0        0.0         0.0
      2.0         0.0        2.0         0.0   4.322580-1 4.322580-1
      2.0         2.0        2.0         0.0   4.396000-1 4.396000-1
      2.0         2.0        3.0         0.0   4.396000-1 4.396000-1
```

Example: ^{16}O, continued



Example: ^{16}O, revisited

```
####
####    Spin group is defined in the next lines
####    J     Parity                          Number of channels=  3
      0.5         0.0              0          0          18           3
####
#### First channel is gamma, second is neutron, third is alpha
####  IPP         L          SCH                      APE         APT
      1.0         0.0         0.0         0.0
      2.0         0.0         0.5         0.0   3.803530-1 3.803530-1
      3.0         1.0        -0.5         0.0   6.658340-1 6.658340-1
```

(3) Resonance parameters –

- For each spin group, specify the number of resonances
- For each resonance, give –
  - Energy
  - Partial width for channel # 1
  - Partial width for channel # 2
  - Partial width for channel # 3
  - Partial width etc.
- Use more than one line per resonance, if needed
- Start each resonance on a new line

Example: ^{27}Al, continued

Number of resonances

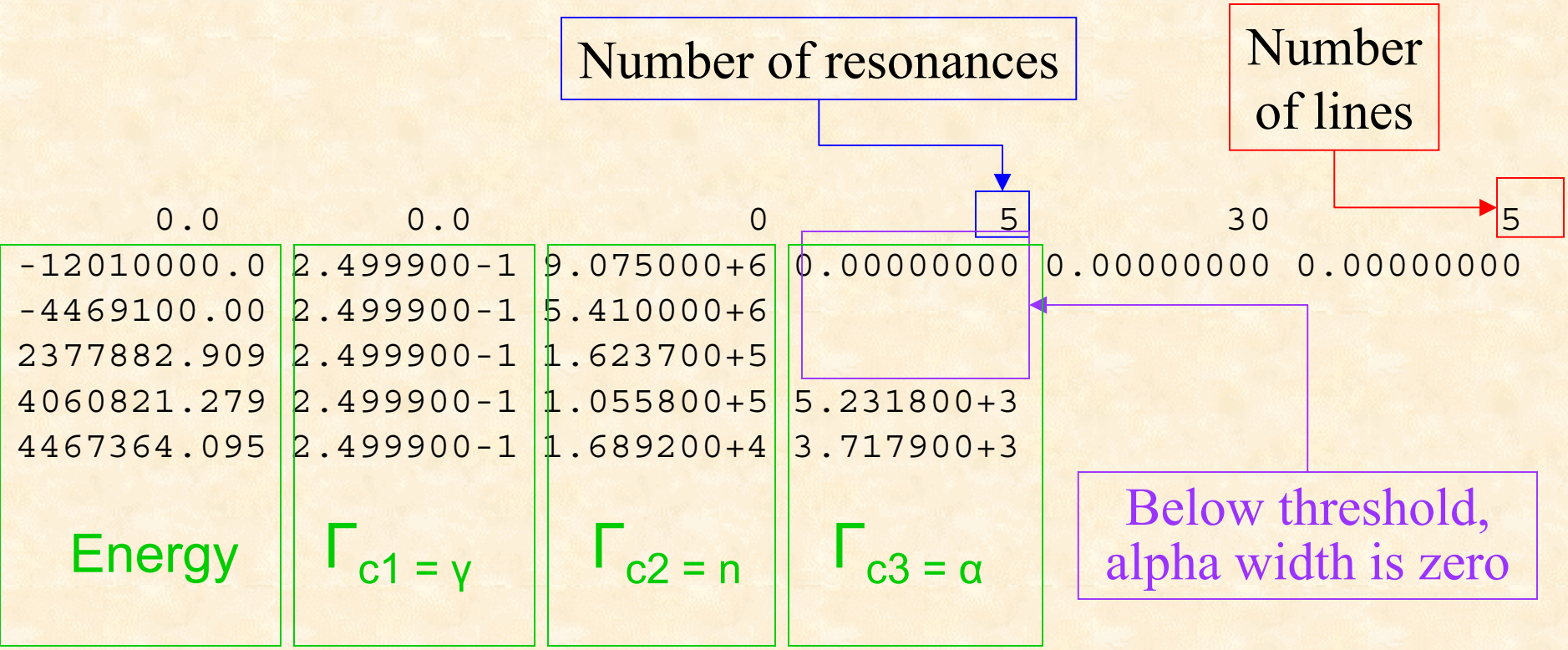
Number of lines

0.0	0.0	0	14	84	14
-4585600.00	9.967500-1	3.291200+6	1.000000-7	1.000000-7	0.000000-0
-16628.0000	1.596400+0	2.391700+1	1.000000-7	1.000000-7	
34843.96177	2.679000+0	3.306800+3	1.000000-7	1.000000-7	
203490.4383	3.416400+0	1.407000+4	1.000000-7	1.000000-7	
260781.8750	2.748000+0	1.000000-7	9.926000+1	1.000000-7	
268534.9420	8.735000-1	1.000000-7	1.000000-7	1.559100+2	
429653.4314	5.070300-1	5.693000+4	1.000000-7	1.000000-7	
490496.6226	4.909000-1	3.654800+3	1.000000-7	1.000000-7	
654609.3750	1.964000-1	1.000000-7	1.000000-7	1.615000+2	
714897.6382	2.210000+0	1.358500+3	1.000000-7	1.000000-7	
759626.1506	1.090000+0	1.000000-7	1.000000-7	1.002400+4	
822114.4650	2.210000+0	8.049000+3	1.000000-7	1.000000-7	
1120000.000	2.000000+0	1.147000+5	1.000000-7	1.000000-7	
1630000.000	2.000000+0	3.726200+4	1.000000-7	1.000000-7	
Energy	$\Gamma_{c1 = \gamma}$	Γ_{c2}	Γ_{c3}	Γ_{c4}	

Example: ^{27}Al, revisited

```
####
####    14 resonances in   14 lines
####  E_res Gamma_gam  Gamma_n1   Gamma_n2   Gamma_n3
      0.0         0.0          0         14         84          14
-4585600.00 9.967500-1 3.291200+6 1.000000-7 1.000000-7 0.000000-0
-16628.0000 1.596400+0 2.391700+1 1.000000-7 1.000000-7
34843.96177 2.679000+0 3.306800+3 1.000000-7 1.000000-7
203490.4383 3.416400+0 1.407000+4 1.000000-7 1.000000-7
260781.8750 2.748000+0 1.000000-7 9.926000+1 1.000000-7
268534.9420 8.735000-1 1.000000-7 1.000000-7 1.559100+2
429653.4314 5.070300-1 5.693000+4 1.000000-7 1.000000-7
490496.6226 4.909000-1 3.654800+3 1.000000-7 1.000000-7
654609.3750 1.964000-1 1.000000-7 1.000000-7 1.615000+2
714897.6382 2.210000+0 1.358500+3 1.000000-7 1.000000-7
759626.1506 1.090000+0 1.000000-7 1.000000-7 1.002400+4
822114.4650 2.210000+0 8.049000+3 1.000000-7 1.000000-7
1120000.000 2.000000+0 1.147000+5 1.000000-7 1.000000-7
1630000.000 2.000000+0 3.726200+4 1.000000-7 1.000000-7
```

Example: ^{16}O, continued



Example: ^{16}O, revisited

```
####
####      5 resonances in    5 lines
####   E_res Gamma_gam  Gamma_n  Gamma_alpha
       0.0         0.0             0           5          30           5
-12010000.0 2.499900-1 9.075000+6 0.00000000 0.00000000 0.00000000
-4469100.00 2.499900-1 5.410000+6
2377882.909 2.499900-1 1.623700+5
4060821.279 2.499900-1 1.055800+5 5.231800+3
4467364.095 2.499900-1 1.689200+4 3.717900+3
```

Below threshold, alpha width is zero

(2,3) Spin groups and resonance parameters –

- **Repeat as many times as needed**

(4) Optional extra stuff –

- **Background R-matrix**
- **Tabulated values for phase shifts**
- **Relativistic kinematics**

Added after posting the proposal on the web site, to accommodate Gerry Hale's EDA code

Implementation of this format?

- SAMMY can write and/or read in this format
- A stand-alone code SAMRML is available
  - Derived from cross-section-calculation portion of SAMMY
  - Experiment-related pieces were removed
    - Only one nuclide
    - No corrections for any measurement-related effects
  - "All" cross section types are generated

SAMRML

- Calculates energy-differential elastic, absorption, and reaction cross sections
  - Next version of SAMRML will also calculate angular distributions
- Calculates partial derivatives of cross sections with respect to resonance parameters
  - A later version will read File 32 (covariance matrix for the resonance parameters) and calculate covariance matrix for the cross sections

SAMRML, continued

- SAMRML can be used in two ways
  - Insert this coding directly into your processor code (after appropriate re-writes)
  - Write independent coding, use SAMRML to test results

SUMMARY

- **Evaluations are available which cannot be expressed via existing implemented formats**
  - **^{37}Cl, ^{35}Cl, ^{19}F**
- **Proposed format is sufficiently general to cover most currently-foreseen evaluations**
- **Implementation in processor codes should not be a major hurdle**
  - **SAMRML can help here**