LEXFOR "Sums" and EXFOR Formats "Sample"

(N. Otsuka, O. Schwerer, 2018-08-26, Memo CP-D/964)

A revised **LEXFOR Sums** is proposed as appended to this memo taking into account the following the NRDC 2018 meeting conclusions:

C19 The modifier (REACTION SF8) FCT will be used for quantities for a natural sample divided by the sum of the isotopic abundances of the target isotopes contributing to the reaction (CP-D/954=WP2018-28). When the authors give the isotopic abundances of the contributing target isotopes, they must be coded under the keyword SAMPLE.

C20 The process code (REACTION SF3) X will be used when the data set is partial for secondary energies originated from several reaction products and the secondary energies are unresolved (CP-D/954=WP2018-28).

We also propose to add the underlined part in **EXFOR Formats Chapter 7 Sample** because the isotopic abundance is not always given by the authors when RAB is used.

SAMPLE Used to give information on the structure, composition, shape, etc., of the measurement sample. 1. Must be present and must contain coded information when the data modifier RAB is coded under the keyword REACTION and the isotopic abundances adopted by the author are known. Otherwise, its presence is optional and free text or coded information, with or without free text, may be given.

Sums

Sums of 2 or more reactions can be expressed as a reaction combination using the separator `+´ (see EXFOR Formats Manual Chapter 6).

~~For mathematical correctness, certain reaction combinations require that isotopic abundances be coded in SF8:~~

~~***Example***:~~
~~Two expressions of the ^{47}Sc production cross section by neutron irradiation of a natural titanium sample at the neutron energy where only ^{47}Ti and ^{48}Ti contribute (*a*: natural isotopic abundance):~~

~~REACTION ((22-TI-47(N,P)21-SC-47,,SIG,,A)+~~
~~(22-TI-48(N,X)21-SC-47,,SIG,,A))~~
~~$a(^{47}\mathrm{Ti})\,\sigma[^{47}\mathrm{Ti}(n,p)^{47}\mathrm{Sc}] + a(^{48}\mathrm{Ti})\,\sigma[^{48}\mathrm{Ti}(n,np+pn+d)^{47}\mathrm{Sc}] = \sigma[^{nat}\mathrm{Ti}(n,x)^{47}\mathrm{Sc}]$~~

~~REACTION ((22-TI-47(N,P)21-SC-47,,SIG)+~~
~~(22-TI-48(N,X)21-SC-47,,SIG,,RAB))~~

~~$\sigma[^{47}\mathrm{Ti}(n,p)^{47}\mathrm{Sc}] + [\,a(^{48}\mathrm{Ti}) / a(^{47}\mathrm{Ti})]\,\sigma[^{48}\mathrm{Ti}(n,np+pn+d)^{47}\mathrm{Sc}] = \sigma[^{nat}\mathrm{Ti}(n,x)^{47}\mathrm{Sc}] / a(^{47}\mathrm{Ti})$~~

~~Sum Reactions~~

Sum reactions such as absorption or nuclide production, where the individual competing reactions may not be known, are not coded using the form above.

Production from Several Contributing Target Nuclides

When several target nuclides of the element may contribute to formation of a product, the author may express it by a sum of isotopic cross sections. In the following examples,

- a(A) is the isotopic abundance of the target nuclide A,
- σ(A) is the isotopic cross section for the target nuclide A,
- σ(0) is the elemental cross section (*i.e.*, production cross section for a natural sample).

Summation is taken over the all energetically possible production channels:

1. **σ(0)=a(A)σ(A) + a(B)σ(B) +...**

   This is nothing other than the elemental cross section, and should not be coded by the sum reactions.

   Example:

   `(22-TI-0(N,X)21-SC-47,,SIG)`

   Forbidden:

   ((22-TI-47(N,P)21-SC-47,,SIG,,A)+(22-TI-48(N,X)21-SC-47,,SIG,,A))

2. **σ(0)/a(A)=σ(A) + [a(B)/a(A)]σ(B) + ...**

   This is coded with a modifier RAB (multiplied by the natural isotopic abundance of the target nuclide divided by the natural isotopic abundance of the target nuclide of the first term). The isotopic abundance a(A) adopted by the author must be given under SAMPLE if known.

   Example:

   ((22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(N,X)21-SC-47,,SIG,,RAB))

3. **σ(0)/[a(A)+a(B)+...]=[a(A)σ(A) + b(B)σ(B) + ...] / [a(A) + a(B) + ...]**

   This is coded with a general quantity modifier FCT with free text explanation about the multiplier. The isotopic abundances such a(A) and a(B) adopted by the author must be given under SAMPLE if known.

   Example:

   ((22-TI-47(N,P)21-SC-47,,SIG,,FCT)+(22-TI-48(N,X)21-SC-47,,SIG,,FCT))

   Elemental cross section divided by the sum of isotopic abundances of 47Ti and 48Ti.

Sum of Unresolved Partial Quantities

When the quantity is a sum of partial quantities whose secondary energies are unresolved (*e.g.*, due to detection resolution), it is coded as an inclusive reaction quantity (*i.e.*, SF3=X).

Example:

412 keV gamma production from n+^{nat}Fe reaction originated from production of two unresolved gammas, ^{54}Fe(n,n')^{54}Fe (411.5 keV) and ^{56}Fe(n,2n)^{55}Fe (411.7 keV), is coded by

(26-FE-0(N,X)0-G-0,PAR,SIG)

rather than

(26-FE-54(N,INL)26-FE-54,PAR,SIG,G,A)+(26-FE-56(N,2N)26-FE-55,PAR,SIG,G,A)

The contributing process is explained under EN-SEC.

Example:
EN-SEC (E,G) 411.5 keV gamma of 54Fe and 411.7 keV gamma of 55Fe, unresolved

Reactions to Sums of Isomeric States

Reactions to sums of isomeric states are coded using the separator "+" in the isomer field of the reaction product; see **Isomeric States**.

Example: (…(P,X)39-Y-102-M1+M2,,SIG)

Note: If the sum of all isomeric reactions is equal to the cross section for the given nuclide, it is coded without the isomer field.

Example: (…(P,X)47-AG-109,,SIG)

Forbidden: (…(P,X)47-AG-109-G+M,,SIG)