

# Coincidence Summing Corrections in GESPECOR

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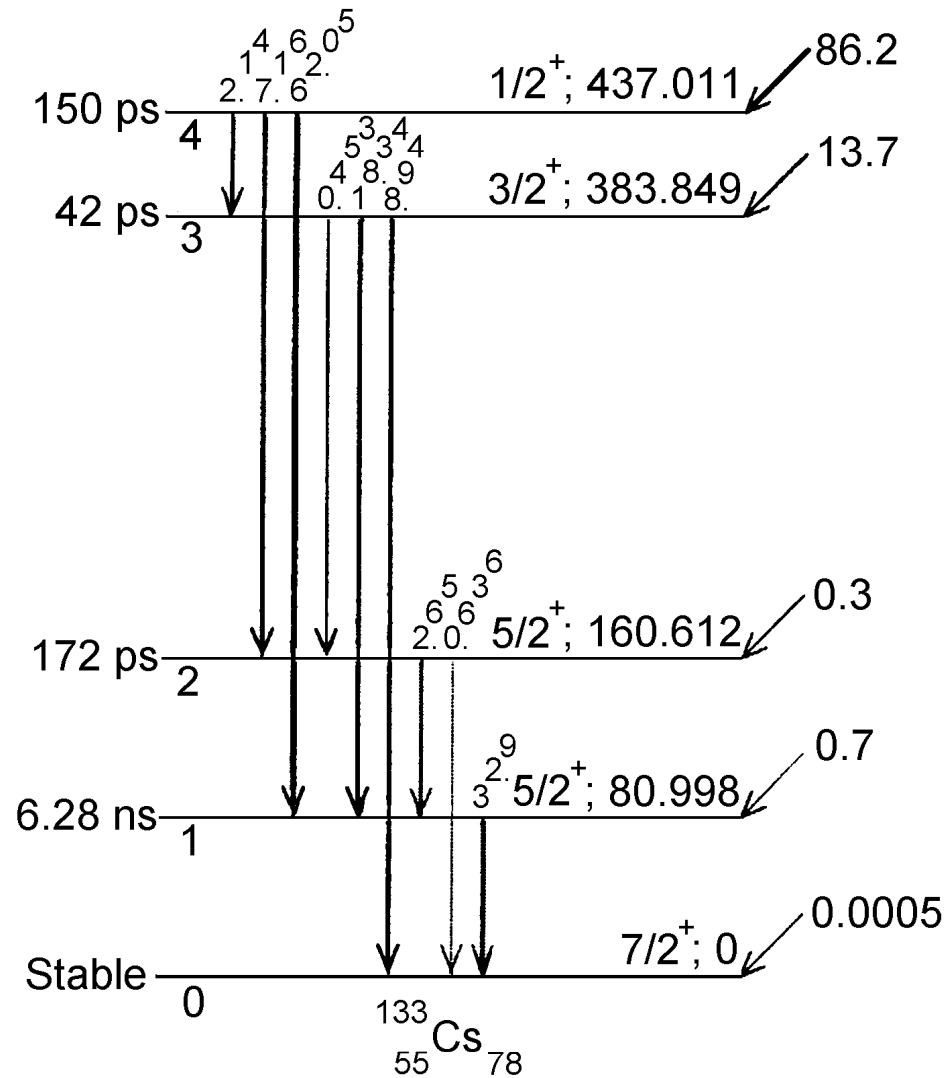
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PTB, Braunschweig

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Paris, February 23-24, 2009

## Ba-133 EC decay



| E (keV)  | I <sub>γ</sub> (per 100 Dis) |
|----------|------------------------------|
| 53.1622  | 2.14±0.03                    |
| 79.6142  | 2.65 ±0.05                   |
| 80.9979  | 32.9 ±0.3                    |
| 160.6121 | 0.638 ±0.004                 |
| 223.2368 | 0.453 ±0.003                 |
| 276.3989 | 7.16 ±0.05                   |
| 302.8508 | 18.34 ±0.13                  |
| 356.0129 | 62.05 ±0.19                  |
| 383.8485 | 8.94 ±0.06                   |

Data source: Nucleide

## Ex: 302 keV peak

But: 302 keV photon is emitted together with other radiations!

- 1  $K\alpha(\text{EC4})\text{-}53\text{-}302\text{-}81$
- 2  $K\alpha(\text{EC4})\text{-}53\text{-}302\text{-}K\alpha(81)$
- 3  $K\alpha(\text{EC4})\text{-}53\text{-}302\text{-}K\beta(81)$
- 4  $K\alpha(\text{EC4})\text{-}53\text{-}302\text{-}other(81)$  (other => no signal in detector)
- 5  $K\alpha(\text{EC4})\text{-}K\alpha(53)\text{-}302\text{-}81$
- 6  $K\alpha(\text{EC4})\text{-}K\alpha(53)\text{-}302\text{-}K\alpha(81)$

And so on, ending with

- 48  $other(\text{EC4})\text{-}other(53)\text{-}302\text{-}other(81)$

Other decay paths start by feeding the 383 keV level (EC3):

- 49  $K\alpha(\text{EC3})\text{-}302\text{-}81$
- 50, 51, 52, 53, 54, 55, 56, 57, 58, 59
- 60  $other(\text{EC3})\text{-}302\text{-}other(81)$

Each combination  $i$  has a specific **joint emission probability**  $p_i$

$$p(302) = p_1 + p_2 + p_3 + \dots + p_{60}$$

Each combination has a specific probability to contribute to the count-rate in the 302 keV peak, e.g. combination (1)

$$K\alpha(\text{EC4})-53-302-81 \Rightarrow \varepsilon_i = [1 - \mu(K\alpha)][1 - \mu(53)] \varepsilon(302) [1 - \mu(81)]$$

$\mu(E)$  = total detection efficiency for photons of energy  $E$

$\varepsilon_i < \varepsilon(302) \Rightarrow$  **coincidence losses from the 302 keV peak**

Additional complication – angular correlation of photons

Apparent efficiency for 302 keV peak of Ba-133 would be:

$$\varepsilon(302, \text{Ba-133}) = (p_1 \varepsilon_1 + p_2 \varepsilon_2 + p_3 \varepsilon_3 + \dots + p_{60} \varepsilon_{60}) / p(302)$$

Note that any secondary photon (e.g. 53 keV) is included in several terms, in each through  $\mu(53)$

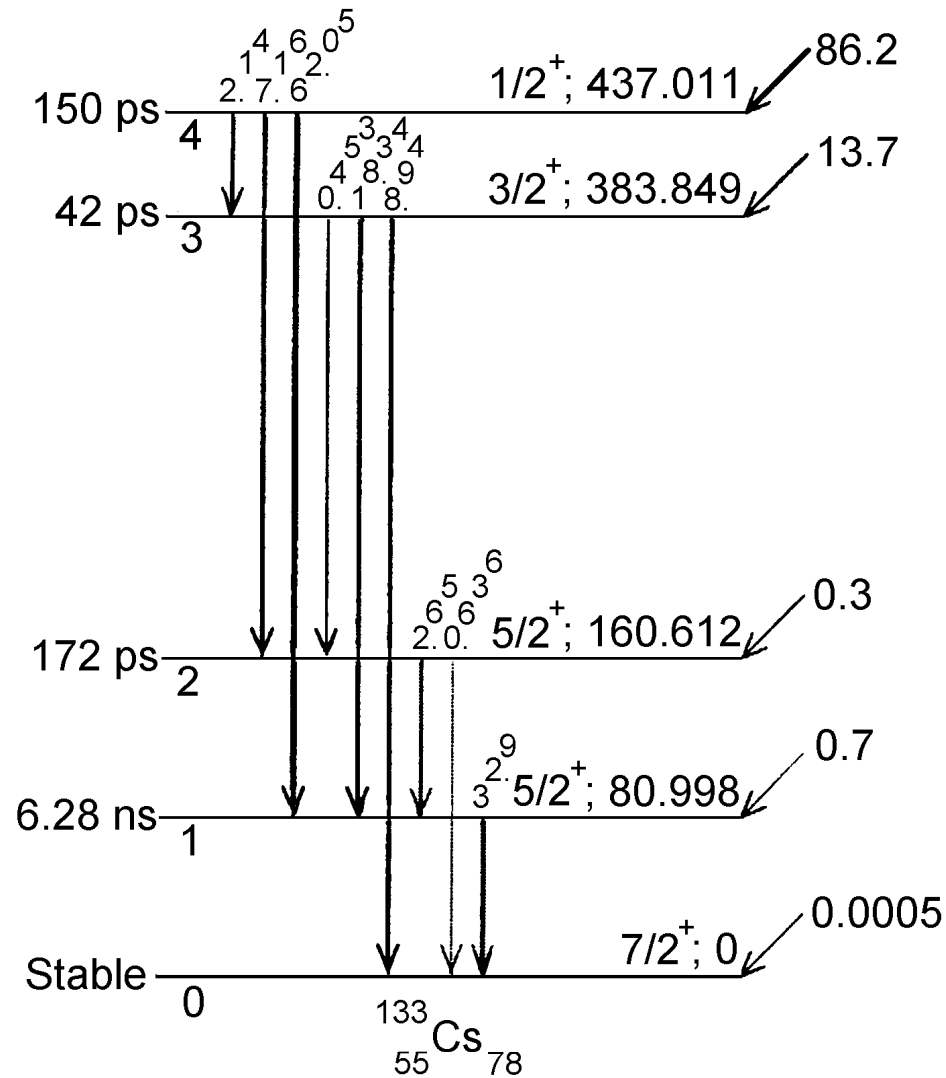
⇒ It is better to use hierarchically ordered groups, by transforming the above expression:

$$\begin{aligned} \varepsilon(302, \text{Ba-133}) = & \varepsilon(302) [1 - p_{302, K\alpha} \mu(K\alpha) - p_{302, K\beta} \mu(K\beta) - \dots \\ & p_{302, 81} \mu(81) + p_{302, K\alpha, K\beta} \mu(K\alpha) \mu(K\beta) + \dots p_{302, 53, 81} \mu(53) \mu(81) \\ & - \dots p_{302, K\beta, 53, 81} \mu(K\beta) \mu(53) \mu(81)] \end{aligned}$$

$p_{302, K\beta, 53, 81}$  = joint emission probability of the group if the main radiation (302) has been emitted

Advantage of new decomposition: decoupling of decay scheme data evaluation from efficiency computations  
- especially important for volume sources

## Ba-133 EC decay



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Data source: Nucleide

## Sum peak contributions to the 302 keV peak:

Combinations like:

$K\alpha(\text{EC4})$ -53-223-79-81 contribute to the 302 keV peak  
with a probability  $[1-\mu(K\alpha)][1-\mu(53)] \varepsilon(223) \varepsilon(79) [1-\mu(81)]$

Other 59 similar contributions

**In the presence of coincidence summing**

$R(E) \neq \varepsilon(E) I(E) A$ , but

$R(E) = F_C \varepsilon(E) I(E) A$

$F_C$  = coincidence summing correction factor, depends on:

- decay scheme parameters
- peak and total efficiency for the set of energies of all the photons

## Computation of decay scheme parameters in GESPECOR:

Data source: DDEP (Nucleide) or ENSDF

- automatic extraction procedure and formatting in the style of KORDATEN file (initially developed by Debertain and Schotzig)
- presently about 225 nuclides

Decay scheme parameters:

- => Joint emission probabilities, hierarchically ordered, combining all the possible decay paths
- computation by a fast algorithm [Sima and Arnold, ARI 66 (2008)]
- nuclides with less than 100 levels, otherwise arbitrary decay scheme
- radiations considered: gamma photons,  $K\alpha$ ,  $K\beta$  X-rays, annihilation photons
- angular correlations can be easily incorporated
- user friendly interfaces

COINCIDENCE-SUMMING CORRECTIONS AND EFFICIENCY

Tutorial Standard M.C. Fast W.D. Peak Effy Tot. Effy Close

Detector File= **PT06.DET**

Geometry File= **M1000.geo**

Material File for the Matrix of the Sample= **Soil.mat**

Density (g/cm<sup>3</sup>)= **1.3**

Shield File= **SHWD.SHI**

Output files Selected: Available:

Decay Data Files Selected: Available: AL26\_511.ded BA333spx.ded BE7\_477.ded

Batch Calculations Current: Included:

CALCULATION: Single set Multiple sets

DETECTOR Available: Selected: **PT06.DET** PT09.DET PTWD.DET

GEOMETRY Available: Selected: **M1000.geo** MARPS.GE Mn1000.gcc

SOURCE MATRIX Selected: Available: Soil.mat Density: **1.3** Sedim.mat Soil.mat Steel.mat

SHIELD Available: Selected: **SHWD.SHI** BigSh.shi BigShstest.s cpr.shi

View File from Directory:

D:\ Devegesp nov06 GESPECOR bin

File: arngespecor.exe compfiles.exe defa.ini dexrdex\_ges.ini

DECAY DATA FILES Tutorial Settings Selected

NUCLIDE INPUT DATA ENERGY LIST: X-Ray Sum Peaks:

I-132 I-132M TE-133 I-133 XE-133 XE-133M **BA-133** TE-134 I-134 I-134M

RADIONUCLIDE: **BA-133** Decay mode: **EC**

Peak energy=

Energy interval for search= **3**

Lower limit of the relative intensity= **.001**

User defined Output Filename?

Filename= **BA.ded**

ENERGY LIST: Sorted by:  keV  (%)

| Energy (keV)       | Intensity (%) |
|--------------------|---------------|
| 6 Gamma Sum Peaks: |               |
| 437.011            | 2.52126E+01   |
| 357.397            | 2.35628E+00   |
| 134.160            | 5.31859E-01   |
| 304.235            | 1.48149E-01   |
| 132.776            | 1.20028E-02   |
| 213.774            | 7.27031E-03   |

CALCULATION Run Display Coincidence Decay Data File Print Energy List

COINCIDENCE-SUMMING CORRECTIONS AND EFFICIENCY

Tutorial Standard M.C. Fast W.D. Peak Effy Tot. Effy Close

Detector File= **PT06.DET**  
 Geometry File= **M1000.geo**  
 Material File for the Matrix of the Sample= **Soil.mat**  
 Density (g/cm<sup>3</sup>)= **1.3**  
 Shield File=

Decay Data Files

Selected: BA276.ded

Available: AL26\_511.ded, BA276.ded, BA302.ded

New View

CALCULATION:

Single set  Multiple sets

DETECTOR

Available: PT06.DET, PT09.DET, PTWD.DET

Selected: PT06.DET

GEOMETRY

Available: M1000.geo, MARPS.GE, Mn1000.gec

Selected: M1000.geo

SOURCE MATRIX

Available: Sedim.mat, Soil.mat, Steel.mat

Output files Selected:

DECAY DATA FILE

Tutorial Settings

NUCLIDE

- I-132
- I-132M
- TE-133
- I-133
- XE-133
- XE-133M
- BA-133**
- TE-134
- I-134
- I-134M

CALCULATION

Run

Text File Display

SAVE T.W.FONT PRINT

D:\Devegesp\nov06\GESPECOR\dedat\BA276.ded 27 lines beginning with line 1

```

BA-133      EC      KORDATEN VERSION: 4.1      Wed Apr 25 01:41:04 2007
Peak energy (keV): 276.399      gamma yield: 0.7160E-01
Number of secondary correlated radiations: 4
 1      79.61      0.32400E+00      0.00000      0.00000      0.00000
 2
0.34899E+00 0.92724E-01
 2      160.61      0.78005E-01      0.00000      0.00000      0.00000
 1
0.46863E-01
 3      81.00      0.32755E+00      0.00000      0.00000      0.00000
 2
0.35694E+00 0.96217E-01
 4      31.69      0.14837E+01      0.00000      0.00000      0.00000 => X-Ray
 2
0.73958E+00 0.12559E+00
Number of cases with multiple correlated gammas: 1
 2      0.11825E+00      1      3
    
```

## Computation of the efficiencies:

-Decoupled from the evaluation of the decay scheme

(a) Standard:

1. Full Monte Carlo simulation

-Variance reduction techniques

-Very important for volume sources

2. Well-type detector: combination of experimental peak efficiencies with an accurate analytical formula for the total efficiency [Sima, Nucl. Instrum. Meth. A 450 (2000)]

(b) Non-standard: application of fitted formulae for peak and total efficiency

User friendly interfaces for the detector, geometry and shield

**GESPECOR** TUTORIAL DETECTOR GEOMETRY SHIELD MATERIAL ATTENUATION COINCIDENCE EFF.TRANSFER OPTIONS INFO EXIT

---

**DETECTOR FILE** Tutorial NEW SAVE DELETE PRINT

Detector type:  HPGe  Well View

Crystal radius (cm)= 3.750  
Crystal length (cm)= 8.200

Crystal well:  
Radius (cm)= 0.8000  
Length (cm)= 5.6500

Thickness of dead layer (cm):  
Inside well= 0.00000  
Outside well= 0.05000

Dist. bottom of the crystal well - end cap bottom: 0.300

Radius of the well of the end cap: 0.500  
Length of the well of the end cap: 6.150

Available files:  
Selected: PTWD.DET

psi37.det  
PT06.DET  
PT09.DET  
PTWD.DET

Detector holder:  
Thickn. inside well= 0.00000  
Thickn. outside well= 0.10000  
Density (g/cm<sup>3</sup>)= 2.70000E+00  
Material file: al.mat

End cap:  
End cap diam. (cm)= 9.000  
Window thickn. (cm)= 0.07500  
Density (g/cm<sup>3</sup>)= 2.70000E+00  
Material file: al.mat

End cap outside the well:  
Side thickness (cm)= 0.15000  
Density (g/cm<sup>3</sup>)= 2.70000E+00  
Material file: al.mat

**Well-Type detector**

View File from Directory:

D:\  
Devegesp  
May05  
GESPECOR  
bin

File:  
DEFA.INI  
dexrdexr\_ges.ini  
DREDDRED.GES  
ENLOG.GES

### GEOMETRY FILE

Tutorial NEW SAVE DELETE PRINT

Sample geometry type:  Cylinder  Marinelli

Selected: MARPS.GEO

Available files:

- madtr5.geo
- MARPS.GEO**
- ml1.geo
- ml2.geo
- ml3.geo
- ml4.geo
- ml5.geo
- ml6.geo
- ml7.geo

Sample inner radius (cm) = 4.500

Sample inner height (cm) = 7.000

Sample outer radius (cm) = 8.000

Sample outer height (cm) = 12.600

Container walls thickness = 0.001

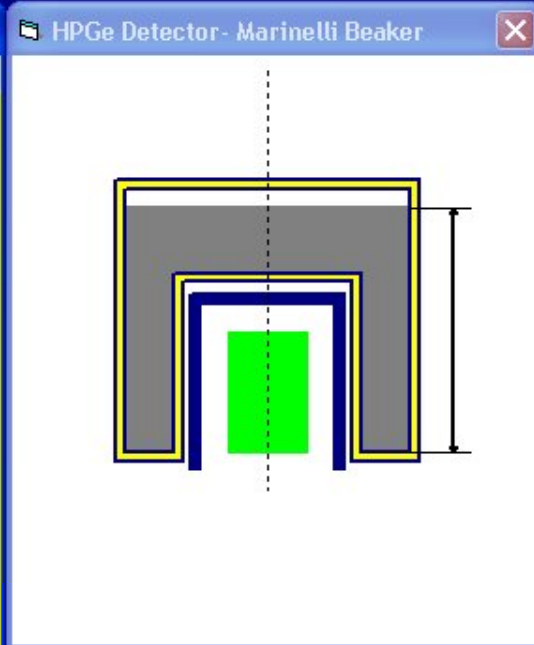
Material file: POLYPROP.mat

Density (g/cm<sup>3</sup>) = 9.00000E-01

Distance from the end cap to the container bottom = 0.001

View

Source Volume: 2.08806E+03 cm<sup>3</sup>



#### View File from Directory:



#### File:



## SHIELD FILE

Tutorial NEW SAVE DELETE PRINT

Shield inner radius (cm)= 8.000

Shield inner height (cm)= 14.6000

Shield outer radius (cm)= 8.750

Shield outer height (cm)= 15.100

Material file

cu.mat

Density (g/cm<sup>3</sup>)= 8.960Distance end cap – inner top  
of shield= 5.600

Selected:

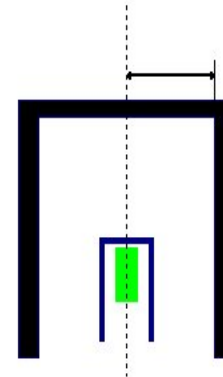
SH06.SHI

Available files:

BigSh.shi  
BigShstest.shi  
ISAA.shi  
P6Close.shi

View

## Shield Geometry



View File from Directory:

E:\  
DEVEGESP  
feb08  
GESPECOR  
bin

File:

arngespecor.exe  
compfiles.exe  
defa.ini  
dexrdexr\_ges.ini

COINCIDENCE-SUMMING CORRECTIONS AND EFFICIENCY

Tutorial Standard M.C. Fast W.D. Peak Effy Tot. Effy Close

Detector File= **DRCNF08.det**  
 Geometry File= **DRVS1b.geo**  
 Material File for the Matrix of the Sample= **Soil.mat**  
 Density (g/cm<sup>3</sup>)= **1.3**  
 Shield File=

Decay Data Files

Selected: Available:

01CO60.det  
 AG110M\_1334.det  
 AG110M\_1384.det

New View

CALCULATION:

Single set  
 Multiple sets

DETECTOR

Available:

Selected: **DRCNF08.det**

0\_icrmg.det  
 0\_icrms.det  
 000.det

GEOMETRY

Available:

Selected: **DRVS1b.geo**

0\_icrm2.geo  
 0\_icrm3.geo  
 00testC025.ge

COURSE MATRIX

Available:

AIR.MAT  
 Al.mat  
 Asse.mat

Available:

BigSh.shi  
 BigShtest.shi  
 ISAA.shi

actory:

**Text File Display**

T.W.FONT PRINT

E:\DEVEGESP\feb08\GESPECOR\results\PT06\_C100\_Soil.sco 122 lines beginning with line 1

| Nuclide | Decay | Energy  | Yield      | Fc          | Nsec | Nsum | IdealEff.   | Err. (%) |
|---------|-------|---------|------------|-------------|------|------|-------------|----------|
| EU-152  | EC    | 39.91   | 0.5856E+00 | 0.81147E+00 | 33   | 0    | 0.73909E-02 | 0.24E+00 |
| EU-152  | EC    | 121.78  | 0.2841E+00 | 0.85632E+00 | 29   | 0    | 0.83615E-01 | 0.11E+00 |
| EU-152  | BETA- | 344.28  | 0.2659E+00 | 0.90573E+00 | 17   | 0    | 0.46982E-01 | 0.24E+00 |
| EU-152  | EC    | 1408.01 | 0.2085E+00 | 0.91752E+00 | 2    | 8    | 0.16617E-01 | 0.20E+00 |
| EU-152  | EC    | 45.70   | 0.1476E+00 | 0.81482E+00 | 33   | 0    | 0.16797E-01 | 0.18E+00 |
| EU-152  | EC    | 964.08  | 0.1450E+00 | 0.89569E+00 | 6    | 2    | 0.21909E-01 | 0.37E+00 |
| EU-152  | EC    | 1112.08 | 0.1341E+00 | 0.93083E+00 | 4    | 2    | 0.19716E-01 | 0.25E+00 |
| EU-152  | BETA- | 778.90  | 0.1297E+00 | 0.86419E+00 | 3    | 1    | 0.25373E-01 | 0.25E+00 |
| EU-152  | EC    | 1085.84 | 0.1013E+00 | 0.10400E+01 | 5    | 2    | 0.20233E-01 | 0.32E+00 |
| EU-152  | EC    | 244.70  | 0.7550E-01 | 0.80686E+00 | 22   | 0    | 0.61154E-01 | 0.14E+00 |
| EU-152  | EC    | 867.38  | 0.4243E-01 | 0.78138E+00 | 5    | 0    | 0.23602E-01 | 0.23E+00 |
| EU-152  | EC    | 443.96  | 0.2800E-01 | 0.83342E+00 | 7    | 0    | 0.38519E-01 | 0.22E+00 |
| EU-152  | EC    | 443.96  | 0.3200E-02 | 0.76628E+00 | 12   | 0    | 0.38345E-01 | 0.14E+00 |
| EU-152  | BETA- | 411.12  | 0.2238E-01 | 0.78587E+00 | 8    | 0    | 0.40920E-01 | 0.20E+00 |
| EU-152  | BETA- | 1089.74 | 0.1730E-01 | 0.87966E+00 | 3    | 4    | 0.20009E-01 | 0.30E+00 |
| EU-152  | BETA- | 1299.14 | 0.1633E-01 | 0.86212E+00 | 2    | 6    | 0.17626E-01 | 0.27E+00 |

|         |           |           |           |           |           |
|---------|-----------|-----------|-----------|-----------|-----------|
| BA-133  | EC        | 31.692    | 0.894     | 4.53      | 0.104     |
| 0.000   | 5.000E-04 | 0.000E+00 | 0.000E+00 | STABLE    |           |
| 80.998  | 7.000E-01 | 8.800E-01 | 0.000E+00 | 6.280E-03 |           |
| 160.612 | 3.000E-01 | 7.900E-01 | 0.000E+00 | 1.720E-04 |           |
| 383.849 | 1.370E+01 | 7.734E-01 | 1.761E-01 | 4.200E-05 |           |
| 437.011 | 8.620E+01 | 6.720E-01 | 2.520E-01 | 1.500E-04 |           |
| 2 1     | 80.998    | 3.290E+01 | 1.740E+00 | 1.460E+00 | 2.200E-01 |
| 3 1     | 160.612   | 6.380E-01 | 3.100E-01 | 2.400E-01 | 5.400E-02 |
| 3 2     | 79.614    | 2.650E+00 | 1.770E+00 | 1.515E+00 | 2.040E-01 |
| 4 1     | 383.849   | 8.940E+00 | 2.030E-02 | 1.690E-02 | 2.730E-03 |
| 4 2     | 302.851   | 1.834E+01 | 4.430E-02 | 3.810E-02 | 4.960E-03 |
| 4 3     | 223.237   | 4.530E-01 | 9.950E-02 | 8.530E-02 | 1.130E-02 |
| 5 2     | 356.013   | 6.205E+01 | 2.560E-02 | 2.110E-02 | 3.510E-03 |
| 5 3     | 276.399   | 7.160E+00 | 5.690E-02 | 4.610E-02 | 8.550E-03 |
| 5 4     | 53.162    | 2.140E+00 | 6.020E+00 | 4.930E+00 | 8.600E-01 |

Evaluation of  $F_c$  is very difficult for nuclides with complex decay schemes and for volume sources

Methods developed for this purpose differ in the way in which

- evaluate the necessary decay scheme parameters
- evaluate the necessary peak and total efficiencies
- combine the decay data with the efficiency data

(1) Recursive formulae (Andreev et al, McCallum & Coote, Debertain & Schotzig, Morel et al, Jutier et al)

(2) Matrix formalism (Semkow et al, Korun et al)

(3) Generalized lists (Novkovic et al)

(4) Monte Carlo simulation of the decay paths and of detection efficiencies (Decombaz et al)

(5) Analytic evaluation of decay scheme parameters decoupled from Monte Carlo evaluation of efficiencies (Sima and Arnold)

# Computation of joint emission probability of groups of photons

Search of all the decay paths (Sima and Arnold, ARI 2008):

- the decay scheme is considered an oriented graph
- the levels are the nodes of the graph
- the transitions are the edges of the graph
- the problem of finding the decay paths is equivalent with finding the paths with specific properties in the graph
  - a fast algorithm of the breadth-first type was implemented

Joint emission probabilities can be computed for any nuclide with less than 100 levels

-radiations considered: gamma photons,  $K\alpha$ ,  $K\beta$  X-rays, annihilation photons

## Computation of the efficiencies:

Monte Carlo simulation, decoupled from the evaluation of the decay scheme

- Variance reduction techniques

Peak efficiency:

- focalized emission towards the detector

- attenuation between the emission point and detector

treated analytically

- forced first interaction in the detector

- stop at first energy loss outside detector

Total efficiency

- stop at first interaction in the detector

User friendly interfaces for the detector, geometry and shield