BetaShape

A new code for improved calculations of beta spectra

The BetaShape program is available at http://www.nucleide.org/logiciels.htm

Xavier Mougeot

BetaShape vs LogFT

	LogFT	BetaShape
Range	β^-, β^+ and ε transitions	β^-, β^+ transitions. *ε transitions not treated yet.*
Calculated values	Mean energies, log *ft*, β^+/ε probabilities. No spectrum	Mean energies, log *ft*, β^-/β^+ and correlated $\overline{\nu_e}/\nu_e$ spectra, multiple transitions
Input	ENSDF files	ENSDF files, command line for individual transitions
Output	Report file, new ENSDF file. Uncertainties.	3 report files, new ENSDF file, ASCII files for single and total spectra. Uncertainties.
Structure	Fortran, 78 functions, 1 program	C++, 6 classes, 155 functions, 4 interfaced programs
Modelling	1. Analytical model, tabulated values of electron wave functions 2. Allowed and first- and second-forbidden unique transitions. Otherwise allowed. 3. Approximate Fermi function and λ_k parameters 4. Approximate finite nucleus size and screening	1. Dirac equation solved numerically 2. Extended forbiddenness (allowed and every forbidden unique). Forbidden non-unique with xi-approximation (1^{st} as allowed, 2^{nd} as first forbidden unique, etc.) 3. Exact Fermi function and λ_k parameters 4. Inherent finite nucleus size and more precise screening 5. Radiative corrections 6. Database of experimental shape factors (130)

Outlook

- **Electron capture transitions**

  An improved modelling has been developed and presented at the ICRM 2017 conference.

  1) Dirac equation solved numerically; 2) extended forbiddenness (allowed and every forbidden unique); 3) realistic shell occupation; 4) more precise overlap and exchange corrections; 5) hole effect by means of first order perturbation theory; 6) shake-up and shake-off effects.

  Improvements are on-going to speed-up the calculations before any implementation in BetaShape.

- **Atomic effects**

  High precision calculations of screening and exchange effects for allowed transitions were demonstrated to be of importance. Improvements are still necessary to speed-up the calculations before any implementation in BetaShape. These corrections have to be extended to forbidden unique transitions.

- **Nuclear structure**

  Inclusion of the nuclear structure for beta decays is in progress. This should allow the precise calculation of forbidden non-unique transitions.

About mean energies and log *ft* values

Calculated quantities in BetaShape

- **Experimental shape factors** (database of 130 transitions)
$\longrightarrow$ if existing, used to determine recommended values

X. Mougeot, Phys. Rev. C 91, 055504 (2015)

- **Mean energy** $\bar{E} = \int_0^{E_0} E \cdot N(E)\mathrm{d}E \Big/ \int_0^{E_0} N(E)\mathrm{d}E$

- **Log *ft* value**

$$\left.\begin{array}{l} ☑\ f_{\beta^-} = \int_1^{W_0} N(W)\mathrm{d}W \\ \\ ☒\ f_{\varepsilon/\beta^+} = \boldsymbol{f_\varepsilon} + \boldsymbol{f_{\beta^+}} \end{array}\right\}$$

Partial half-life: $t_i = T_{1/2}/I_\beta \qquad \longrightarrow \log ft$

provided that $f_{\beta^+} \neq 0$
and $I_{\beta^+} \neq 0$

$$\rightarrow \log ft = \log\left(\frac{f_{\beta^+}}{I_{\beta^+}} T_{1/2}\right) + \log\left(\frac{1+f_\varepsilon/f_{\beta^+}}{1+I_\varepsilon/I_{\beta^+}}\right)$$

However

$$\frac{I_\varepsilon}{I_{\beta^+}} = \frac{\lambda_\varepsilon}{\lambda_{\beta^+}} = \frac{K_{\mathrm{nuc}} \sum_x n_x C_x f_x}{K_{\mathrm{nuc}} \int_1^{W_0} N(W)\mathrm{d}W} \approx \frac{f_\varepsilon}{f_{\beta^+}}$$

C_x: lepton dynamics

K_{nuc}: nuclear structure (allowed, forbidden unique)

n_x: relative occupation number of the orbital, not accounted for in the LogFT program

For allowed and forbidden unique electron capture transitions, one has

$$\boxed{\rightarrow \log ft \approx \log\left(\frac{f_{\beta^+}}{I_{\beta^+}} T_{1/2}\right)}$$

Uncertainties

- Standard uncertainties from input parameters are propagated: Q-value, level energies, half-life, branching ratio. Calculations are performed at $E_{\max} - u(E_{\max})$, $E_{\max}$ and $E_{\max} + u(E_{\max})$.

- Asymmetric uncertainties are symmetrized. Warnings are given in the output files.

- Otherwise, the code estimates a relative uncertainty of about 60% (i.e. the uncertainty associated with a flat distribution between zero and twice the value). Warnings are given in the output files.

- Uncertainties from experimental shape factors are not accounted for. Correlations between the parameters of a shape factor are not provided in the publications and must be considered.

- This treatment of uncertainties is opened to discussion and can be changed following different recommendations.

Examples (1)

exp. built from experimental shape factor
calc. full calculation (theoretical shape factor)

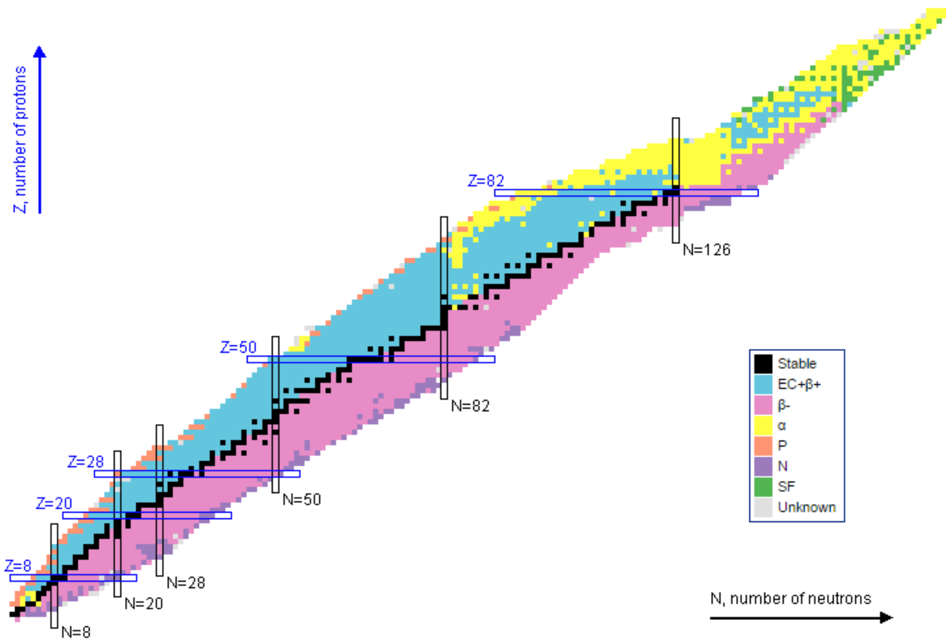
RN	BetaShape E_{mean} (keV)	BetaShape log *ft*	LogFT E_{mean} (keV)	LogFT log *ft*	Nature	Comments
^{14}C (β^-)	48.2323 (13) *49.4506 (14)*	9.0954 (22) *9.0474 (22)*	49.47	9.0400 (30)	allowed	exp. *calc.*
^{63}Ni (β^-)	17.1777 (14) *17.4817 (14)*	6.942 (6) *6.680 (6)*	17.425 (6)	6.7	allowed	exp. *calc.*
^{210}Bi (β^-)	317.56 (21) *389.88 (31)*	7.7118 (10) *8.1384 (12)*	389.00 (40)	8	1st f.nu.	exp. *calc.*
^{241}Pu (β^-)	5.096 (33) *5.209 (33)*	3.284 (8) *5.925 (8)*	5.23 (5)	5.8	1st f.nu.	exp. *calc.*
^{90}Sr (β^-)	193.6 (5) *195.5 (5)*	9.390 (6) *9.424 (6)*	195.8 (8)	9.400 (10)	1st f.u.	exp. *calc.*
^{204}Tl (β^-)	235.82 (6) *239.98 (6)*	10.2152 (15) *10.1933 (15)*	244.05 (6)	10.0980 (15)	1st f.u.	exp. *calc.*

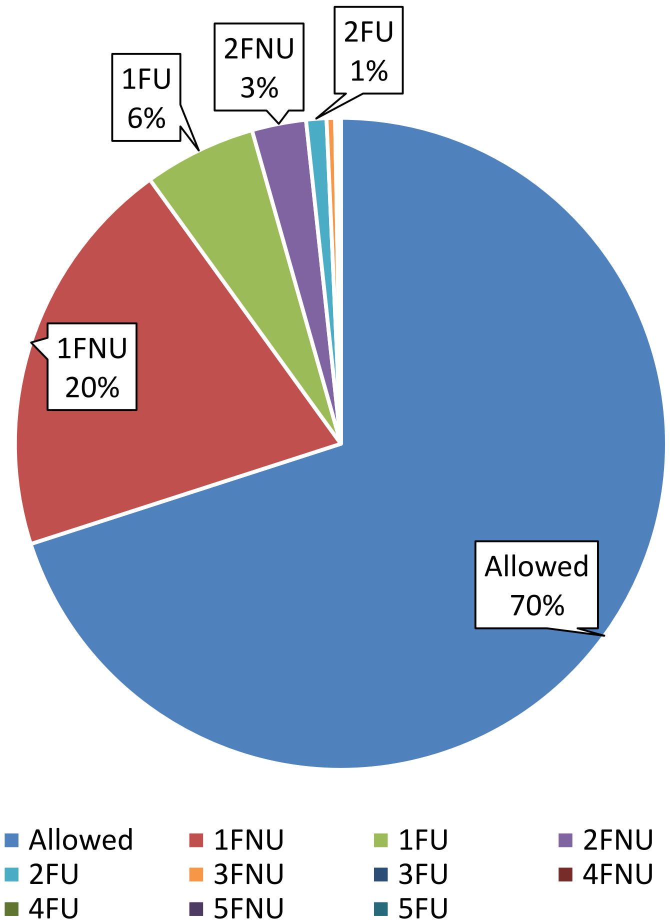
Examples (2)

exp. built from experimental shape factor
calc. full calculation (theoretical shape factor)

RN	BetaShape E_{mean} (keV)	BetaShape log *ft*	LogFT E_{mean} (keV)	LogFT log *ft*	Nature	Comments
^{36}Cl (β^-)	314.102 (29)	13.3454 (28)	251.33	13.3210 (30)	2nd f.nu.	exp.
	278.418 (19)	*13.6716 (28)*				*calc.*
^{99}Tc$_{gs}$ (β^-)	95.19 (44)	11.929 (10)	84.6 (5)	12.325 (12)	2nd f.nu.	exp.
	101.39 (49)	*12.087 (10)*				*calc.*
^{10}Be (β^-)	252.33 (26)	13.867 (18)	202.56 (25)	13.397 (18)	2nd f.u.	exp.
	252.02 (26)	*13.872 (18)*				*calc.*
^{87}Rb (β^-)	56.46 (19)	16.206 (14)	81.67 (36)	17.499 (10)	3rd f.nu.	exp.
	115.14 (43)	*17.062 (13)*				*calc.*
^{40}K (β^-)	583.982 (48)	20.5788 (14)	560.18 (5)	20.75	3rd f.u.	exp.
	583.283 (48)	*20.6006 (14)*				*calc.*
^{113}Cd$_{gs}$ (β^-)	139.83 (35)	22.931 (11)	92.6 (10)	23.127 (14)	4th f.nu.	exp.
	140.42 (40)	*22.795 (11)*				*calc.*

ENSDF database analysis

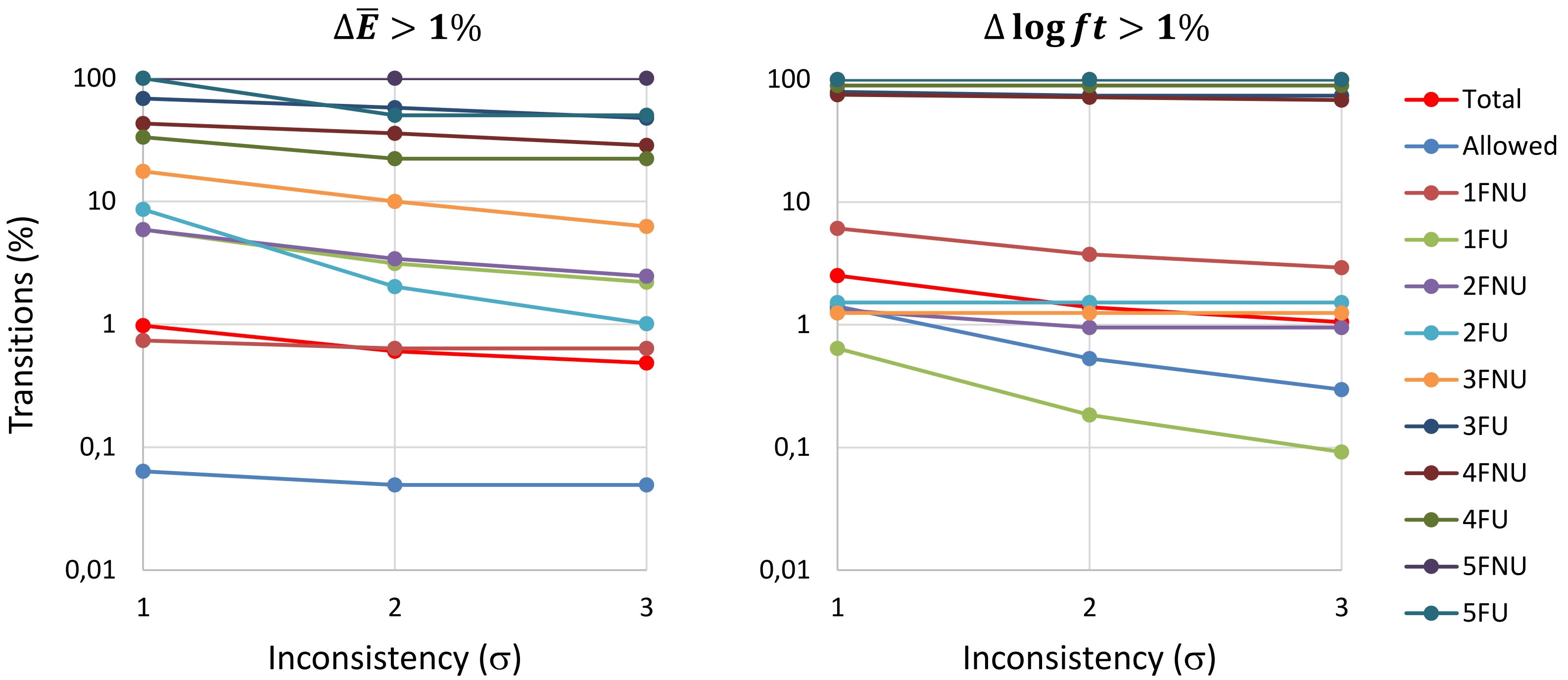




- 21 768 $\beta^{\pm}$ transitions read in ENSDF database
- 19 602 $\beta^{\pm}$ transitions with $I_\beta \geq 0$ and $E_{\max} \geq 0$ keV
- 4 529 transitions calculated as allowed due to lack of spins and parities

Study of the consistency of the results from LogFT and BetaShape at 1σ, 2σ, 3σ (68.3%, 95.4%, 99.7% C.L.) → **Validation of BetaShape**

BetaShape vs LogFT



For allowed and forbidden unique β^+/ε transitions

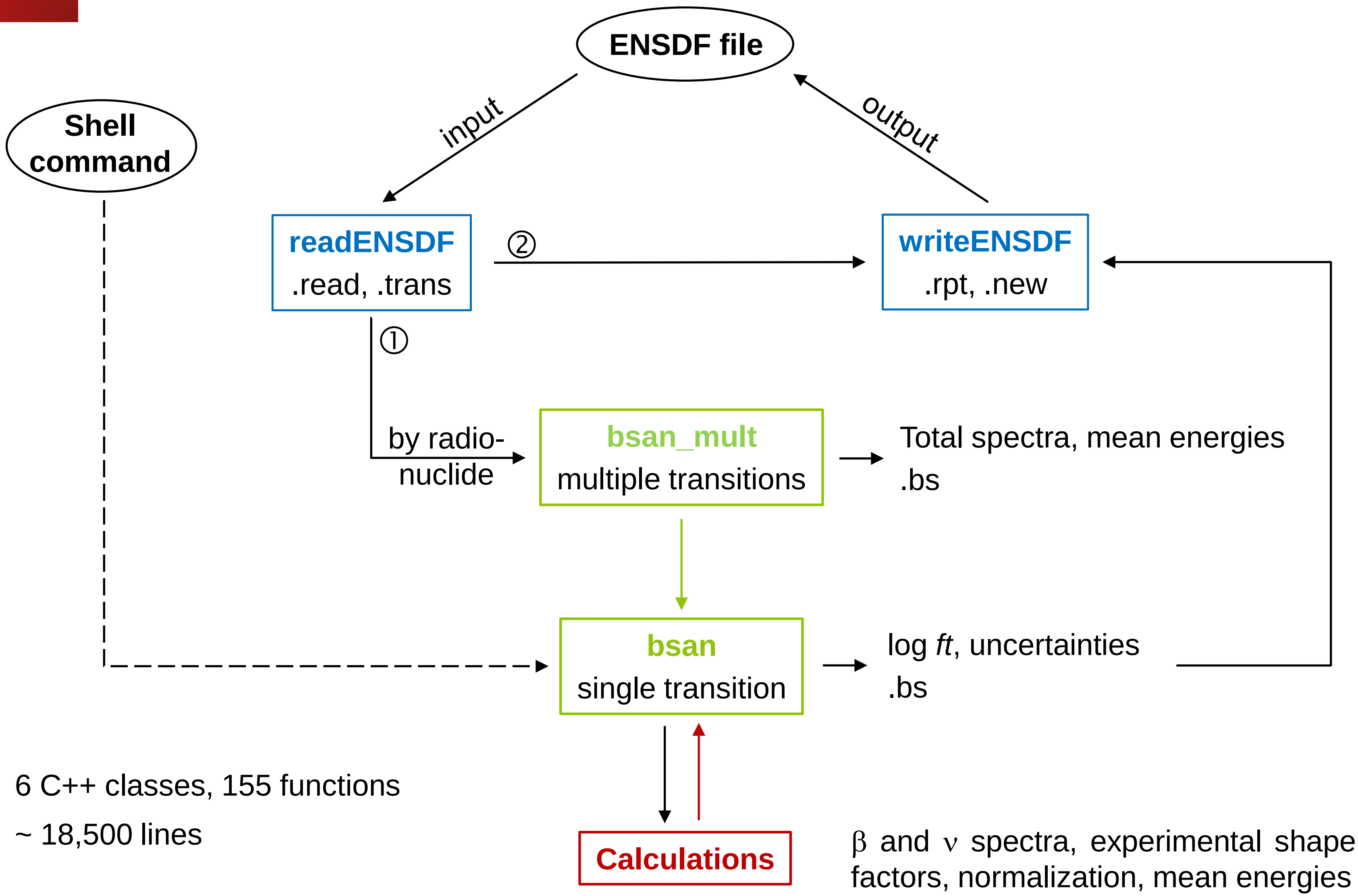
$$\boxed{\log ft \approx \log\left(\frac{f_{\beta^+}}{I_{\beta^+}} T_{1/2}\right)}\ ?$$

→ 21 of 8 506 β^+ transitions with inconsistent log *ft* at 1σ (experimental shape factors, no uncertainty on intensities, disagreement ≤ 2.5%)

This approximation leads to consistent results with LogFT for β^+/ε transitions at the precision level of current nuclear data.

Example of outputs

Structure of the BetaShape code



- 6 C++ classes, 155 functions
- ~ 18,500 lines

Output file

.bs

single transition

Transition parameters and options for calculation

Experimental shape factor

Mean energies, log *ft* values, analysis parameters

β and ν spectra

```
------------------------------------------------------------------------------------------------


BetaShape
Analytical version: 1.0 (24/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

------------------------------------------------------------------------------------------------

Parent nucleus: 39-Y-90 [2-] g.s.  --> Daughter nucleus: 40-Zr-90 [0+] g.s.
Calculation of the 1st forbidden unique transition from the beta - decay of Y-90

Bühring's screening correction is considered.

End-point energy: 2278.7 (16) keV     Energy step: 7 keV     Intensity: 0.99983 (7)

An experimental shape factor has been found: (1 - 0.0114*W) * (q^2 + l_2*p^2)
Energy range of the measurement: 60 - 2230 keV
From [1975FL07] D. Flothmann, H. J. Gils, W. Wiesner, R. Löhken, Z. Physik A 272, 219 (1975)

Input mean energy: 926.7 (8) keV
Mean energy from the calculated spectrum: 929.2 (7) keV
Mean energy from the experimental shape factor: 924.9 (7) keV

Input log ft value: 8.05
Log ft value from the calculated spectrum: log ft 9.2530 (18)   with components: log f 3.8901 (18) and log partial T1/2 5.36284 (21)
Log ft value from the experimental shape factor: log ft 9.2293 (18)   with component: log f 3.8664 (18)

Agreement of the experimental and calculated spectra in [60,2230] keV: 99.96 %
Corresponding disagreement: 3.74e-002 %
Variation of the mean energies: 4.69e-001 %

E(keV)      dN/dE calc.     unc.            dN/dE exp.      unc.
     0      3.36918e-004    4.58510e-007    3.44512e-004    4.63582e-007
     7      3.41551e-004    4.62475e-007    3.48727e-004    4.66815e-007
    14      3.46078e-004    4.66214e-007    3.53096e-004    4.70191e-007
    21      3.50499e-004    4.69728e-007    3.57618e-004    4.73710e-007
    28      3.55063e-004    4.73366e-007    3.62345e-004    4.77437e-007
    35      3.59826e-004    4.77202e-007    3.67258e-004    4.81342e-007
     ⋮                          ⋮                               ⋮
  2268      2.66793e-007    8.46140e-008    2.68018e-007    8.46841e-008
  2275      3.19957e-008    3.35393e-008    3.23681e-008    3.37721e-008
  2278.7    0.00000e+000    0.00000e+000    0.00000e+000    0.00000e+000


-------------------------
Antineutrino spectrum
-------------------------

Mean energy from the calculated spectrum: 1348.3 (14) keV
Mean energy from the experimental shape factor: 1355.0 (14) keV

E(keV)      dN/dE calc.     unc.            dN/dE exp.      unc.
     0      0.00000e+000    0.00000e+000    0.00000e+000    0.00000e+000
     7      1.19068e-007    2.85693e-010    1.15165e-007    2.79463e-010
    14      4.71474e-007    1.12839e-009    4.56103e-007    1.10402e-009
    21      1.05012e-006    2.50687e-009    1.01606e-006    2.45326e-009
    28      1.84802e-006    4.40036e-009    1.78842e-006    4.30718e-009
```

Output file

Transition parameters and options for calculation

.bs
single transition

```
------------------------------------------------------------------------------------------

BetaShape
Analytical version: 1.0 (24/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

------------------------------------------------------------------------------------------

Parent nucleus: 39-Y-90 [2-] g.s.  -->  Daughter nucleus: 40-Zr-90 [0+] g.s.
Calculation of the 1st forbidden unique transition from the beta - decay of Y-90

Bühring's screening correction is considered.

End-point energy: 2278.7 (16) keV     Energy step: 7 keV     Intensity: 0.99983 (7)

An experimental shape factor has been found: (1 - 0.0114*W) * (q^2 + l_2*p^2)
Energy range of the measurement: 60 - 2230 keV
From [1975FL07] D. Flothmann, H. J. Gils, W. Wiesner, R. Löhken, Z. Physik A 272, 219 (1975)

Input mean energy: 926.7 (8) keV
Mean energy from the calculated spectrum: 929.2 (7) keV
```


Parent nucleus: 39-Y-90 [2-] g.s. --> Daughter nucleus: 40-Zr-90 [0+] g.s.
Calculation of the 1st forbidden unique transition from the beta - decay of Y-90

Bühring's screening correction is considered.

End-point energy: 2278.7 (16) keV Energy step: 7 keV Intensity: 0.99983 (7)


```
      35     3.59826e-004     4.77202e-007     3.67258e-004     4.81342e-007
       ⋮                ⋮                             ⋮
    2268     2.66793e-007     8.46140e-008     2.68018e-007     8.46841e-008
    2275     3.19957e-008     3.35393e-008     3.23681e-008     3.37721e-008
  2278.7     0.00000e+000     0.00000e+000     0.00000e+000     0.00000e+000


------------------------
Antineutrino spectrum
------------------------

Mean energy from the calculated spectrum: 1348.3 (14) keV
Mean energy from the experimental shape factor: 1355.0 (14) keV

E(keV)      dN/dE calc.      unc.             dN/dE exp.       unc.
       0     0.00000e+000     0.00000e+000     0.00000e+000     0.00000e+000
       7     1.19068e-007     2.85693e-010     1.15165e-007     2.79463e-010
      14     4.71474e-007     1.12839e-009     4.56103e-007     1.10402e-009
      21     1.05012e-006     2.50687e-009     1.01606e-006     2.45326e-009
      28     1.84802e-006     4.40036e-009     1.78842e-006     4.30718e-009
```

Output file

.bs

single transition

Experimental shape factor

```
---------------------------------------------------------------------------------

BetaShape
Analytical version: 1.0 (24/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

---------------------------------------------------------------------------------

Parent nucleus: 39-Y-90 [2-] g.s.  -->  Daughter nucleus: 40-Zr-90 [0+] g.s.
Calculation of the 1st forbidden unique transition from the beta - decay of Y-90

Bühring's screening correction is considered.

End-point energy: 2278.7 (16) keV     Energy step: 7 keV     Intensity: 0.99983 (7)

An experimental shape factor has been found: (1 - 0.0114*W) * (q^2 + l_2*p^2)
Energy range of the measurement: 60 - 2230 keV
From [1975FL07] D. Flothmann, H. J. Gils, W. Wiesner, R. Löhken, Z. Physik A 272, 219 (1975)

Input mean energy: 926.7 (8) keV
Mean energy from the calculated spectrum: 929.2 (7) keV
Mean energy from the experimental shape factor: 924.9 (7) keV
```


An experimental shape factor has been found: (1 - 0.0114*W) * (q^2 + l_2*p^2)
Energy range of the measurement: 60 - 2230 keV
From [1975FL07] D. Flothmann, H. J. Gils, W. Wiesner, R. Löhken, Z. Physik A 272, 219 (1975)


```
E(keV)      dN/dE calc.     unc.           dN/dE exp.      unc.
     0      3.36918e-004    4.58510e-007   3.44512e-004    4.63582e-007
     7      3.41551e-004    4.62475e-007   3.48727e-004    4.66815e-007
    14      3.46078e-004    4.66214e-007   3.53096e-004    4.70191e-007
    21      3.50499e-004    4.69728e-007   3.57618e-004    4.73710e-007
    28      3.55063e-004    4.73366e-007   3.62345e-004    4.77437e-007
    35      3.59826e-004    4.77202e-007   3.67258e-004    4.81342e-007
     ⋮                          ⋮                               ⋮
  2268      2.66793e-007    8.46140e-008   2.68018e-007    8.46841e-008
  2275      3.19957e-008    3.35393e-008   3.23681e-008    3.37721e-008
  2278.7    0.00000e+000    0.00000e+000   0.00000e+000    0.00000e+000


------------------------
Antineutrino spectrum
------------------------

Mean energy from the calculated spectrum: 1348.3 (14) keV
Mean energy from the experimental shape factor: 1355.0 (14) keV

E(keV)      dN/dE calc.     unc.           dN/dE exp.      unc.
     0      0.00000e+000    0.00000e+000   0.00000e+000    0.00000e+000
     7      1.19068e-007    2.85693e-010   1.15165e-007    2.79463e-010
    14      4.71474e-007    1.12839e-009   4.56103e-007    1.10402e-009
    21      1.05012e-006    2.50687e-009   1.01606e-006    2.45326e-009
    28      1.84802e-006    4.40036e-009   1.78842e-006    4.30718e-009
```

Output file

.bs

single transition

```
--------------------------------------------------------------------------------------------


BetaShape
Analytical version: 1.0 (24/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

--------------------------------------------------------------------------------------------

Parent nucleus: 39-Y-90 [2-] g.s.  -->  Daughter nucleus: 40-Zr-90 [0+] g.s.
Calculation of the 1st forbidden unique transition from the beta - decay of Y-90

Bühring's screening correction is considered.

End-point energy: 2278.7 (16) keV     Energy step: 7 keV     Intensity: 0.99983 (7)

An experimental shape factor has been found: (1 - 0.0114*W) * (q^2 + l_2*p^2)
Energy range of the measurement: 60 - 2230 keV
From [1975FL07] D. Flothmann, H. J. Gils, W. Wiesner, R. Löhken, Z. Physik A 272, 219 (1975)

Input mean energy: 926.7 (8) keV
Mean energy from the calculated spectrum: 929.2 (7) keV
Mean energy from the experimental shape factor: 924.9 (7) keV

Input log ft value: 8.05
Log ft value from the calculated spectrum: log ft 9.2530 (18)   with components: log f 3.8901 (18) and log partial T1/2 5.36284 (21)
Log ft value from the experimental shape factor: log ft 9.2293 (18)   with component: log f 3.8664 (18)

Agreement of the experimental and calculated spectra in [60,2230] keV: 99.96 %
Corresponding disagreement: 3.74e-002 %
Variation of the mean energies: 4.69e-001 %

E(keV)      dN/dE calc.     unc.             dN/dE exp.       unc.
```

Mean energies, log *ft* values, analysis parameters


```
Input mean energy: 926.7 (8) keV
Mean energy from the calculated spectrum: 929.2 (7) keV
Mean energy from the experimental shape factor: 924.9 (7) keV

Input log ft value: 8.05
Log ft value from the calculated spectrum: log ft 9.2530 (18)   with components: log f 3.8901 (18) and log partial T1/2 5.36284 (21)
Log ft value from the experimental shape factor: log ft 9.2293 (18)   with component: log f 3.8664 (18)

Agreement of the experimental and calculated spectra in [60,2230] keV: 99.96 %
Corresponding disagreement: 3.74e-002 %
Variation of the mean energies: 4.69e-001 %
```


```
Mean energy from the calculated spectrum: 1348.3 (14) keV
Mean energy from the experimental shape factor: 1355.0 (14) keV

E(keV)      dN/dE calc.     unc.            dN/dE exp.      unc.
     0      0.00000e+000    0.00000e+000    0.00000e+000    0.00000e+000
     7      1.19068e-007    2.85693e-010    1.15165e-007    2.79463e-010
    14      4.71474e-007    1.12839e-009    4.56103e-007    1.10402e-009
    21      1.05012e-006    2.50687e-009    1.01606e-006    2.45326e-009
    28      1.84802e-006    4.40036e-009    1.78842e-006    4.30718e-009
```

Output file

```
--------------------------------------------------------------------------------------------

BetaShape
Analytical version: 1.0 (24/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

--------------------------------------------------------------------------------------------

Parent nucleus: 39-Y-90 [2-] g.s.  -->  Daughter nucleus: 40-Zr-90 [0+] g.s.
Calculation of the 1st forbidden unique transition from the beta - decay of Y-90

Bühring's screening correction is considered.
```

.bs

single transition

E (keV)	dN/dE calc.	unc.	dN/dE exp.	unc.
0	3.36918e-004	4.58510e-007	3.44512e-004	4.63582e-007
7	3.41551e-004	4.62475e-007	3.48727e-004	4.66815e-007
14	3.46078e-004	4.66214e-007	3.53096e-004	4.70191e-007
21	3.50499e-004	4.69728e-007	3.57618e-004	4.73710e-007
28	3.55063e-004	4.73366e-007	3.62345e-004	4.77437e-007
35	3.59826e-004	4.77202e-007	3.67258e-004	4.81342e-007

```
36284 (21)

Agreement of the experimental and calculated spectra in [60,2230] keV: 99.96 %
```

β and ν spectra

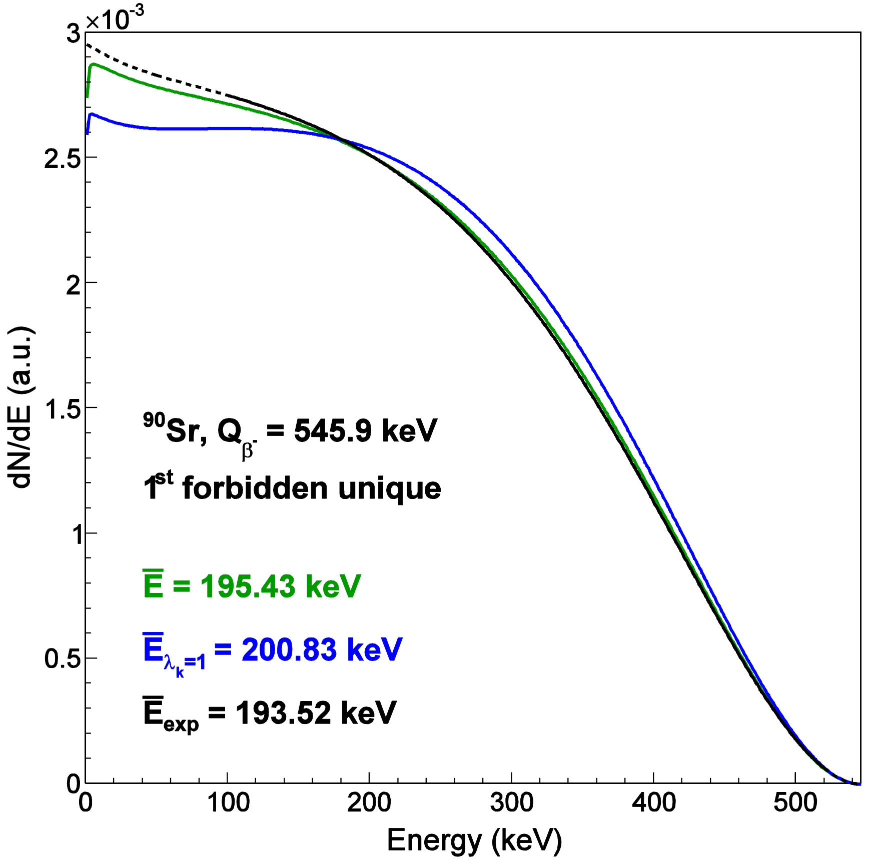
```
-------------------------
Antineutrino spectrum
-------------------------

Mean energy from the calculated spectrum: 1348.3 (14) keV
Mean energy from the experimental shape factor: 1355.0 (14) keV
```

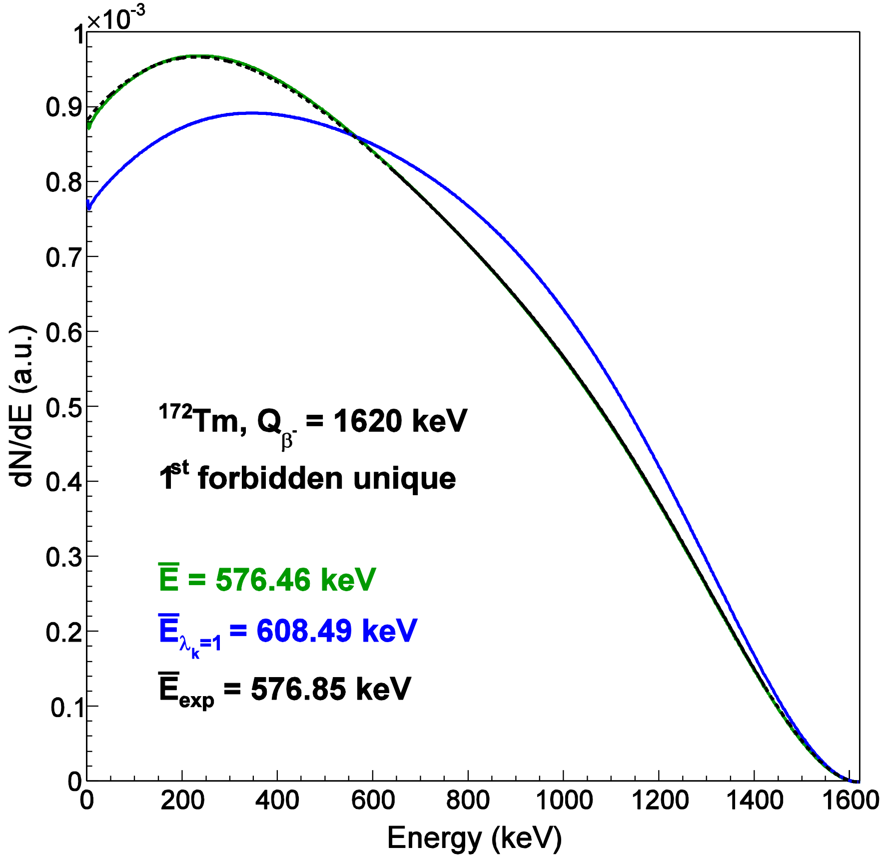
E (keV)	dN/dE calc.	unc.	dN/dE exp.	unc.
0	0.00000e+000	0.00000e+000	0.00000e+000	0.00000e+000
7	1.19068e-007	2.85693e-010	1.15165e-007	2.79463e-010
14	4.71474e-007	1.12839e-009	4.56103e-007	1.10402e-009
21	1.05012e-006	2.50687e-009	1.01606e-006	2.45326e-009
28	1.84802e-006	4.40036e-009	1.78842e-006	4.30718e-009

7	1.19068e-007	2.85693e-010	1.15165e-007	2.79463e-010
14	4.71474e-007	1.12839e-009	4.56103e-007	1.10402e-009
21	1.05012e-006	2.50687e-009	1.01606e-006	2.45326e-009
28	1.84802e-006	4.40036e-009	1.78842e-006	4.30718e-009

Examples of improved spectra

Precision of the common $\lambda_k = 1$ approximation





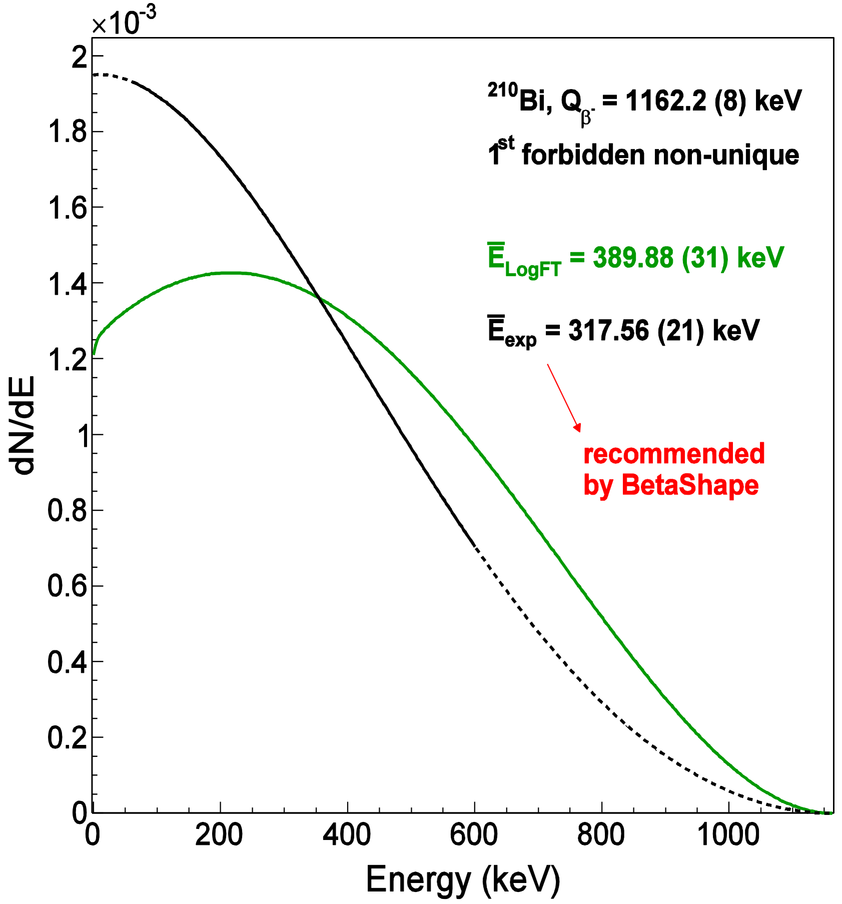
Complete $(1 - R^2) = 0.06\ \%$ and $|\Delta\bar{E}| = 0.99\ \%$

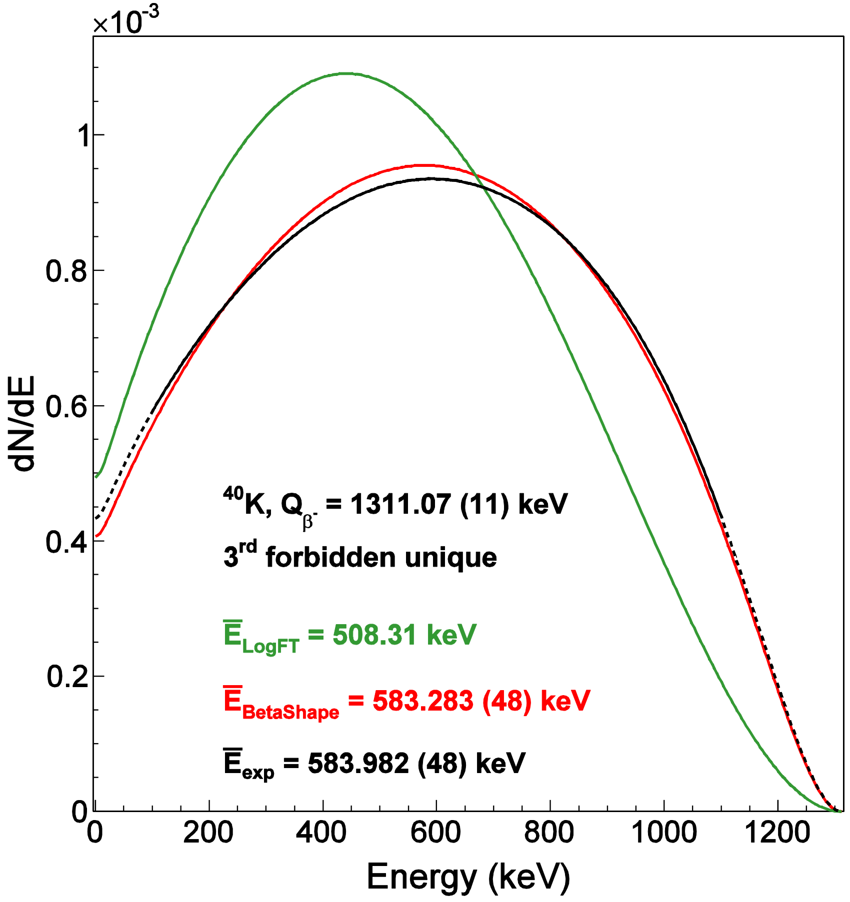
$\lambda_k = 1$ $(1 - R^2) = 0.93\ \%$ and $|\Delta\bar{E}| = 3.8\ \%$

Complete $(1 - R^2) = 0.003\ \%$ and $|\Delta\bar{E}| = 0.17\ \%$

$\lambda_k = 1$ $(1 - R^2) = 5.9\ \%$ and $|\Delta\bar{E}| = 5.5\ \%$

Examples of improved calculations





These two transitions are **calculated as allowed by the LogFT program.**