## List Ceatech

## 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	$\beta^-$ , $\beta^+$ and $\varepsilon$ transitions	$\beta^-$ , $\beta^+$ transitions. $\varepsilon$ transitions not treated yet.
Calculated values	Mean energies, log $ft$ , $\beta^+/\varepsilon$ probabilities. No spectrum	Mean energies, log <i>ft</i> , $\beta^-/\beta^+$ and correlated $\overline{v_e}/v_e$ 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	<ol> <li>Analytical model, tabulated values of electron wave functions</li> <li>Allowed and first- and second-forbidden unique transitions. Otherwise allowed.</li> <li>Approximate Fermi function and λ<sub>k</sub> parameters</li> <li>Approximate finite nucleus size and screening</li> </ol>	<ol> <li>Dirac equation solved numerically</li> <li>Extended forbiddenness (allowed and every forbidden unique). Forbidden non-unique with xiapproximation (1<sup>st</sup> as allowed, 2<sup>nd</sup> as first forbidden unique, etc.)</li> <li>Exact Fermi function and λ<sub>k</sub> parameters</li> <li>Inherent finite nucleus size and more precise screening</li> <li>Radiative corrections</li> <li>Database of experimental shape factors (130)</li> </ol>







#### 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







Experimental shape factors (database of 130 transitions)
 → if existing, used to determine recommended values

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

• Mean energy 
$$\overline{E} = \int_0^{E_0} E \cdot N(E) dE / \int_0^{E_0} N(E) dE$$

$$\begin{array}{lll} \text{Log } \textit{ft} \text{ value } & \swarrow f_{\beta^-} = \int_1^{W_0} N(W) dW \\ & \swarrow f_{\varepsilon/\beta^+} = \textit{f}_{\varepsilon} + \textit{f}_{\beta^+} \end{array} \end{array} \end{array} \text{ Partial half-life: } t_i = T_{1/2}/I_{\beta} \longrightarrow \log ft \\ & \text{ provided that } f_{\beta^+} \neq 0 \\ & \text{ and } I_{\beta^+} \neq 0 \end{array} \longrightarrow \log ft = \log \left( \frac{f_{\beta^+}}{I_{\beta^+}} T_{1/2} \right) + \log \left( \frac{1 + f_{\varepsilon}/f_{\beta^+}}{1 + I_{\varepsilon}/I_{\beta^+}} \right) \end{array}$$

However

$$\frac{I_{\varepsilon}}{I_{\beta^+}} = \frac{\lambda_{\varepsilon}}{\lambda_{\beta^+}} = \frac{K_{\text{nuc}} \sum_{x} n_x C_x f_x}{K_{\text{nuc}} \int_1^{W_0} N(W) dW} \approx \frac{f_{\varepsilon}}{f_{\beta^+}}$$

 $C_{x}$ : lepton dynamics

*K*<sub>nuc</sub>: 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

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



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







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

#### BetaShape

#### LogFT

RN	E <sub>mean</sub> (keV)	log ft	E <sub>mean</sub> (keV)	log ft	Nature	Comments
<sup>14</sup> C (β <sup>-</sup> )	48.2323 (13)	9.0954 (22)	40.47	9.0400 (30)	allowed	exp.
	49.4506 (14)	9.0474 (22)	49.47			calc.
63NI: (0-)	17.1777 (14)	6.942 (6)	47 405 (6)	6.7	allowed	exp.
<sup>ο3</sup> ΝΙ (β <sup>-</sup> )	17.4817 (14)	6.680 (6)	17.425 (6)			calc.
<sup>210</sup> Βi (β <sup>-</sup> )	317.56 (21)	7.7118 (10)	200.00 (40)	8	1 <sup>st</sup> f.nu.	exp.
	389.88 (31)	8.1384 (12)	389.00 (40)			calc.
241 Dec. (0-)	5.096 (33)	3.284 (8)		5.8	1 <sup>st</sup> f.nu.	exp.
241 <b>Pu</b> (β <sup>-</sup> )	5.209 (33)	5.925 (8)	5.23 (5)			calc.
	193.6 (5)	9.390 (6)			Act	exp.
<sup>90</sup> Sr (β⁻)	195.5 (5)	9.424 (6)	195.8 (8)	9.400 (10)	1 <sup>st</sup> I.U.	calc.
<sup>204</sup> ΤΙ (β <sup>-</sup> )	235.82 (6)	10.2152 (15)			1 <sup>st</sup> f.u.	exp.
	239.98 (6)	10.1933 (15)	244.05 (6)	10.0980 (15)		calc.







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

BetaShape

#### LogFT

RN	E <sub>mean</sub> (keV)	log ft	E <sub>mean</sub> (keV)	log ft	Nature	Comments
<sup>36</sup> Cl (β <sup>-</sup> )	314.102 (29)	13.3454 (28) 13.6716 (28)	251.33	13.3210 (30)	2 <sup>nd</sup> f.nu.	exp.
		13.07 10 (20)				
$90\mathbf{T}_{-}$	95.19 (44)	11.929 (10)	94 G (E)	10 205 (10)	2nd f pu	exp.
<sup>33</sup> IC <sub>gs</sub> (β <sup>-</sup> )	101.39 (49)	12.087 (10)	04.0 (3)	12.325 (12)	∠ <sup>™</sup> I.NU.	calc.
	252.33 (26)	13.867 (18)		40.007 (40)		exp.
<sup>10</sup> Be (β <sup>-</sup> )	252.02 (26)	13.872 (18)	202.56 (25)	13.397 (18)	2 <sup>nd</sup> f.U.	calc.
	56.46 (19)	16.206 (14)		17.499 (10)	3 <sup>rd</sup> f.nu.	exp.
°' KD (β <sup>-</sup> )	115.14 (43)	17.062 (13)	81.67 (36)			calc.
4014 (0)	583.982 (48)	20.5788 (14)				exp.
<sup>40</sup> Κ (β <sup>-</sup> )	583.283 (48)	20.6006 (14)	560.18 (5)	20.75	3 <sup>rd</sup> f.u.	calc.
<sup>113</sup> Cd <sub>gs</sub> (β <sup>-</sup> )	139.83 (35)	22.931 (11)		00.407.(44)	4+b ¢	exp.
	140.42 (40)	22.795 (11)	92.6 (10)	23.127 (14)	4 <sup>.n</sup> f.nu.	calc.





### **ENSDF** database analysis



- + 21 768  $\beta^{\pm}$  transitions read in ENSDF database
- 19 602  $\beta^{\pm}$  transitions with  $I_{\beta} \ge 0$  and  $E_{\max} \ge 0$  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  $1\sigma$ ,  $2\sigma$ ,  $3\sigma$  (68.3%, 95.4%, 99.7% C.L.)



→ Validation of BetaShape

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## BetaShape vs LogFT



For allowed and forbidden unique  $\beta^+/\varepsilon$  transitions

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

 $\rightarrow$  21 of 8 506  $\beta^+$  transitions with inconsistent log *ft* at  $1\sigma$  (experimental shape factors, no uncertainty on intensities, disagreement  $\leq$  2.5%)

This approximation leads to consistent results with LogFT for  $\beta^+/\varepsilon$  transitions at the precision level of current nuclear data.



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## **Example of outputs**









BetaShape | X. Mougeot | 12





#### Output file

376

28

1.84802e-006

4.40036e-009

1.78842e-006

Transition parameters and options for calculation

Experimental shape factor

Mean energies, log *ft* values, analysis parameters

 $\beta$  and  $\nu$  spectra

1									
2									
3	BetaShape								
4	Analytical	version: 1.0 (2	4/06/2016)						
5	Author: A. Mougeot (Xavier.Mougeotecea.ir) /FR IIST Ishorstaire Astional Henri Becguarel (INHB) Gif.sur-Yvette E-01101 France								
7	CLA, LISI,	Laboratoire Nat	Numical Periov C	01 055504. Errati	m Phys. Pey. C 92, 01	50002 (2015)			
8	Flease Cite	e: A. Mougeot, P	Mysical Review C	91, 055504; Errau	um Phys. Rev. C 92, 0	59902 (2015)	he		
9							.03		
10							single transition		
11	Parent nuc	leus: 39-Y-90 [2	-] g.s> Dau	ghter nucleus: 40-	-Zr-90 [0+] g.s.		Single hanshor		
12	Calculation	n of the 1st for	bidden unique tra	nsition from the b	oeta - decay of Y-90				
13									
14	Bühring's :	screening correc	tion is considere	d.					
15	Ford marine .		(1.C) hell Energy		T	-			
17	End-point (	energy: 22/0./ (	16) Kev Energ	y step: / kev	Incensicy: 0.99965 (	7)			
18	An experime	ental shape fact	or has been found	: (1 - 0.0114*W) *	* (g^2 + 1 2*p^2)				
19	Energy rand	ge of the measur	ement: 60 - 2230	keV					
20	From [1975]	- FL07] D. Flothma	nn, H. J. Gils, W	. Wiesner, R. Löhl	cen, Z. Physik A 272,	219 (1975)			
21							J		
22	Input mean	energy: 926.7 (	(8) keV						
23	Mean energy	y from the calcu	lated spectrum: 9	29.2 (7) keV					
24	Mean energy	y from the exper	imental shape fac	tor: 924.9 (7) ke	7				
25	Input log	ft walnes 9 05							
20	Log ft valu	ue from the calc	ulated enectrum.	log ft 9 2530 (18)	with components.	log f 3 8901	(18) and log partial $T1/2 = 36284$ (21)		
28	Log ft valu	ue from the expe	rimental shape fa	ctor: log ft 9.229	3 (18) with compone	ent: log f 3	.8664 (18)		
29	-								
30	Agreement o	of the experimen	tal and calculate	d spectra in [60,2	2230] keV: 99.96 %				
31	Correspond:	ing disagreement	: 3.74e-002 %						
32	Variation o	of the mean ener	gies: 4.69e-001 %						
33	F (Ino.17)	dN/dE colo	118.0	dN/dE own					
35	L(Kev)	3 36918e-004	4 58510e-007	3 44512e-004	4 63582e=007				
36	7	3.41551e-004	4.62475e-007	3.48727e-004	4.66815e-007				
37	14	3.46078e-004	4.66214e-007	3.53096e-004	4.70191e-007				
38	21	3.50499e-004	4.69728e-007	3.57618e-004	4.73710e-007				
39	28	3.55063e-004	4.73366e-007	3.62345e-004	4.77437e-007				
40	35	3.59826e-004	4.77202e-007	3.67258e-004	4.81342e-007				
			:		:				
359	2268	2.66793e-007	8.46140e-008	2.68018e-007	8.46841e-008				
360	2275	3.19957e-008	3.35393e-008	3.23681e-008	3.37721e-008				
361	2278.7	0.00000e+000	0.00000e+000	0.00000e+000	0.00000e+000				
362									
363									
364									
365	Antineutri	no spectrum							
366									
67	Maan		land an	949 9 (14)					
369	Mean energy	y from the calcu	iiated spectrum: 1	1340.3 (14) KeV	keV				
370	nean energ	y rrom one exper	imentar snape fac	.001. 1000.0 (14)	AC 7				
371	E (keV)	dN/dE calc.	unc.	dN/dE exp.	unc.				
372	0	0.00000e+000	0.00000e+000	0.00000e+000	0.00000e+000				
373	7	1.19068e-007	2.85693e-010	1.15165e-007	2.79463e-010				
374	14	4.71474e-007	1.12839e-009	4.56103e-007	1.10402e-009				



4.30718e-009





List Ceatech	Output file	1 2 3 4 5 6 7 8 9 10 11	<pre>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) </pre>	<mark>.bs</mark> single transition
		12 13	Calculation of the 1st forbidden unique transition from the beta - decay of Y-90	
		14 15	Bühring's screening correction is considered.	
Experimental shape factor		16 17	End-point energy: 2278.7 (16) keV Energy step: 7 keV Intensity: 0.99983 (7)	
		18 19	An experimental shape factor has been found: $(1 - 0.0114*W) * (q^2 + 1_2*p^2)$ Energy range of the measurement: 60 - 2230 keV	
		20 21	From [1975FL07] D. Flothmann, H. J. Gils, W. Wiesner, R. Löhken, Z. Physik A 272, 219 (1975)	
		22	Input mean energy: 926.7 (8) keV Mean energy from the calculated spectrum: 929.2 (7) keV	
		24	Mean energy from the experimental shape factor: 924.9 (7) keV	

An experimental shape factor has been found: (1 - 0.0114\*W) \* (q^2 + 1\_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)

34	E(keV)	dN/dE calc.	unc.	dN/dE exp.	unc.
35	0	3.36918e-004	4.58510e-007	3.44512e-004	4.63582e-007
36	7	3.41551e-004	4.62475e-007	3.48727e-004	4.66815e-007
37	14	3.46078e-004	4.66214e-007	3.53096e-004	4.70191e-007
38	21	3.50499e-004	4.69728e-007	3.57618e-004	4.73710e-007
39	28	3.55063e-004	4.73366e-007	3.62345e-004	4.77437e-007
40	35	3.59826e-004	4.77202e-007	3.67258e-004	4.81342e-007
			:		:
			1.000 ILC 007		1.000.00 00.
359	2268	2.66793e-007	8.46140e-008	2.68018e-007	8.46841e-008
360	2275	3.19957e-008	3.35393e-008	3.23681e-008	3.37721e-008
361	2278.7	0.00000e+000	0.00000e+000	0.00000e+000	0.00000e+000
362					
363					
364					
365	Antineutrino	spectrum			
366					
367					
368	Mean energy	from the calcul	ated spectrum: 13	348.3 (14) keV	
369	Mean energy	from the experi	mental shape fact	or: 1355.0 (14) k	ceV
370					
371	E(keV)	dN/dE calc.	unc.	dN/dE exp.	unc.
372	0	0.00000e+000	0.00000e+000	0.00000e+000	0.00000e+000
373	7	1.19068e-007	2.85693e-010	1.15165e-007	2.79463e-010
374	14	4.71474e-007	1.12839e-009	4.56103e-007	1.10402e-009
375	21	1.05012e-006	2.50687e-009	1.01606e-006	2.45326e-009
376	28	1.84802e-006	4.40036e-009	1.78842e-006	4.30718e-009





List CERTECH Output file	<pre>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) 9</pre>	.bs
	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	single transition
	13 14 Bühring's screening correction is considered. 15	
	16       End-point energy: 2278.7 (16) keV       Energy step: 7 keV       Intensity: 0.99983 (7)         17       Intensity: 0.99983 (7)	
	18 An experimental snape factor has been found: (1 - 0.0114*W) * (q <sup>-2</sup> + 1_2*p <sup>-2</sup> ) 19 Energy range of the measurement: 60 - 2230 keV	
	20 From [1975FL07] D. Flothmann, H. J. Gils, W. Wiesner, R. Löhken, Z. Physik A 272, 219 (1975) 21	
	22 Input mean energy: 926.7 (8) keV	
	23 Mean energy from the calculated spectrum: 929.2 (7) keV 24 Mean energy from the experimental shape factor: 924.9 (7) keV	
Mean energies log ft	25	
inicali chorgico, log it	26 Input log ft value: 8.05	
values, analysis	27 Log ft value from the calculated spectrum: log ft 9.2530 (18) with components: log f 3.8901 (1	8) and log partial T1/2 5.36284 (21)
noromotoro	Log It value from the experimental snape factor: log it 9.2293 (18) with component: log i 3.86	64 (18)
parameters	Agreement of the experimental and calculated spectra in [60,2230] keV: 99.96 %	
	31 Corresponding disagreement: 3.74e-002 %	
	32 Variation of the mean energies: 4.69e-001 %	
	33 34 E(keV) dN/dE calc. unc. dN/dE exp. unc.	
Input mean energy: 926.7 (8) keV		
Mean energy from the calculated spectru	a: 929.2 (7) keV	
Mean energy from the experimental shape	factor: 924.9 (7) keV	
the children one children out on apertanenout on ape		
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 %

> 368 Mean energy from the calculated spectrum: 1348.3 (14) keV 369 Mean energy from the experimental shape factor: 1355.0 (14) keV 371 E(keV) dN/dE calc. unc. dN/dE exp. unc. 372 0 0.00000e+000 0.00000e+000 0.00000e+000 0.00000e+000 373 7 1.19068e-007 2.85693e-010 1.15165e-007 2.79463e-010 374 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-009 375 376 28 1.84802e-006 4.40036e-009 1.78842e-006 4.30718e-009





list ceatech	utput file	<pre>1 2 3 BetaShape 4 Analytical version: 1.0 5 Author: X. Mougeot (xavi 6 CEA, LIST, Laboratoire N 7 Please cite: X. Mougeot, 8 9 10 11 Parent nucleus: 39-Y-90 12 Calculation of the 1st f 13 14 Bühring's screening corr</pre>	<pre>(24/06/2016) er.mougeot@cea.fr) Mational Henri Becquerel (LNHB), Physical Review C 91, 055504; ) [2-] g.s&gt; Daughter nucleu forbidden unique transition from rection is considered.</pre>	Gif-sur-Yvette F-91191, France Erratum Phys. Rev. C 92, 059902 (20 s: 40-Zr-90 [0+] g.s. the beta - decay of Y-90	<sup>015)</sup> .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
		30 Agreement of the experim	ental and calculated spectra in	[60,2230] keV: 99.96 %	
	Antineutrin	o spectrum			
	Mean energy Mean energy	from the calcul from the experi	ated spectrum: 13 mental shape fact	348.3 (14) keV cor: 1355.0 (14) ke	v
	E(keV)	dN/dE calc.	unc.	dN/dE exp.	unc.
$\beta$ and $\nu$ spectra	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
		373         7         1.19068e-007           374         14         4.71474e-007           375         21         1.05012e-006           376         28         1.84802e-006	7         2.85693e-010         1.15165e           7         1.12839e-009         4.56103e           5         2.50687e-009         1.01606e           5         4.40036e-009         1.78842e	-007 2.79463e-010 -007 1.10402e-009 -006 2.45326e-009 -006 4.30718e-009	





## **Examples of improved spectra**





#### Precision of the common $\lambda_k = 1$ approximation





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## **Examples of improved calculations**



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



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