Evaluation process overview

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Prelude

Each radionuclide, each evaluation is specific.

The evaluation strategy always depends on the available information (measurements and theoretical predictions) and on the uncertainties.

→ Each choice should be justified in the Comments file (report of the evaluation).

The aim is built the best possible decay scheme, consistent, balanced, complete and with the lowest possible uncertainties on all the quantities of interest.

Focus is made in this presentation on the most common case.

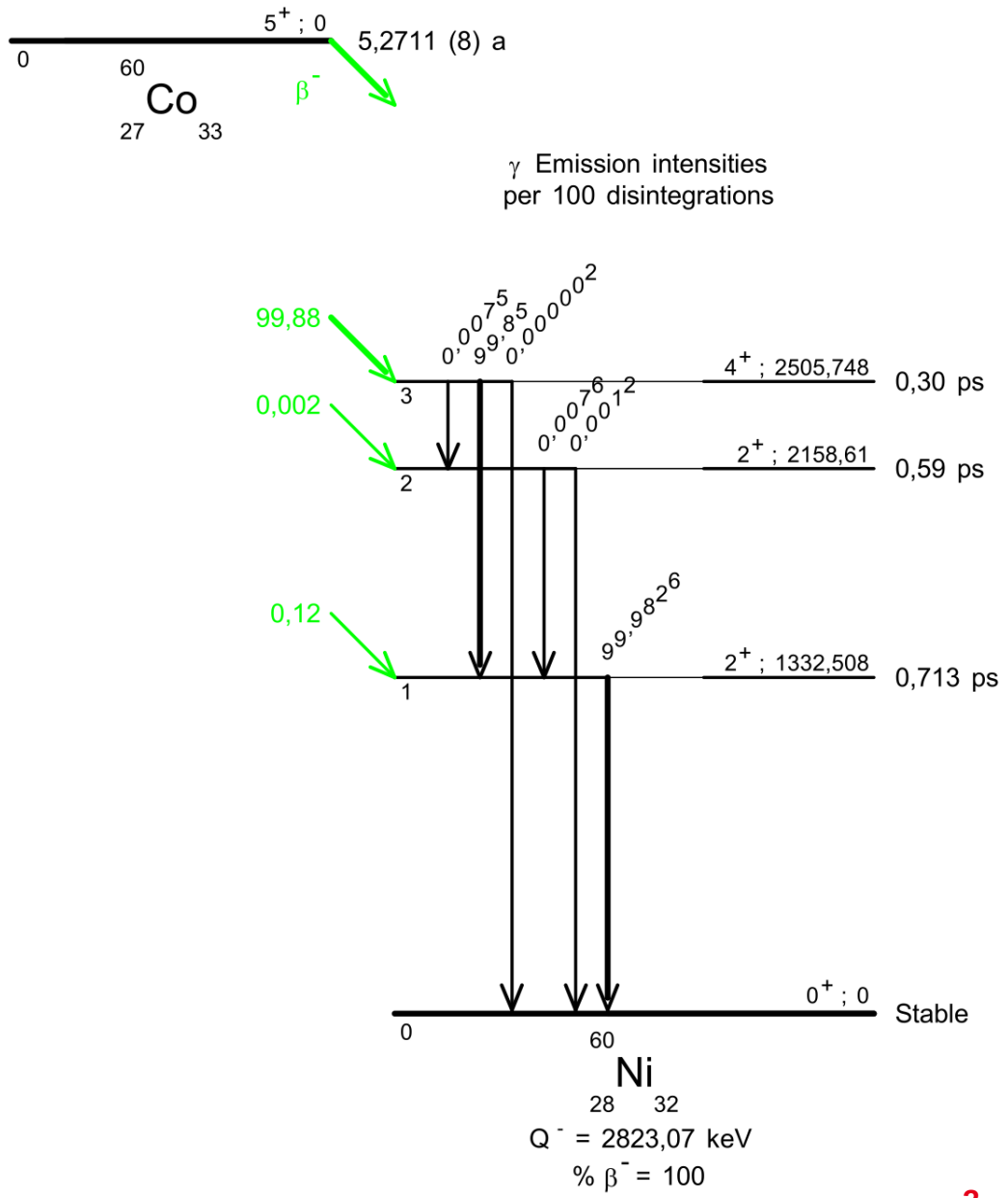
DDEP mission

Provide recommended decay data to non-specialists

- Metrology
- Nuclear Physics (detector calibration)
- Nuclear Medicine
- Nuclear Power
- Etc.

Main information of interest:

- Half-life, Q-value
- Decay scheme (alpha, beta, gamma)
- Energy and emission intensity of the decay
- Atomic data due to internal conversion
  - X-rays
  - Conversion electrons
  - Auger electron



Process

Initiation of a new evaluation

- Need from a project / collaboration
- Following a user request
- Evaluator initiative

Evaluation

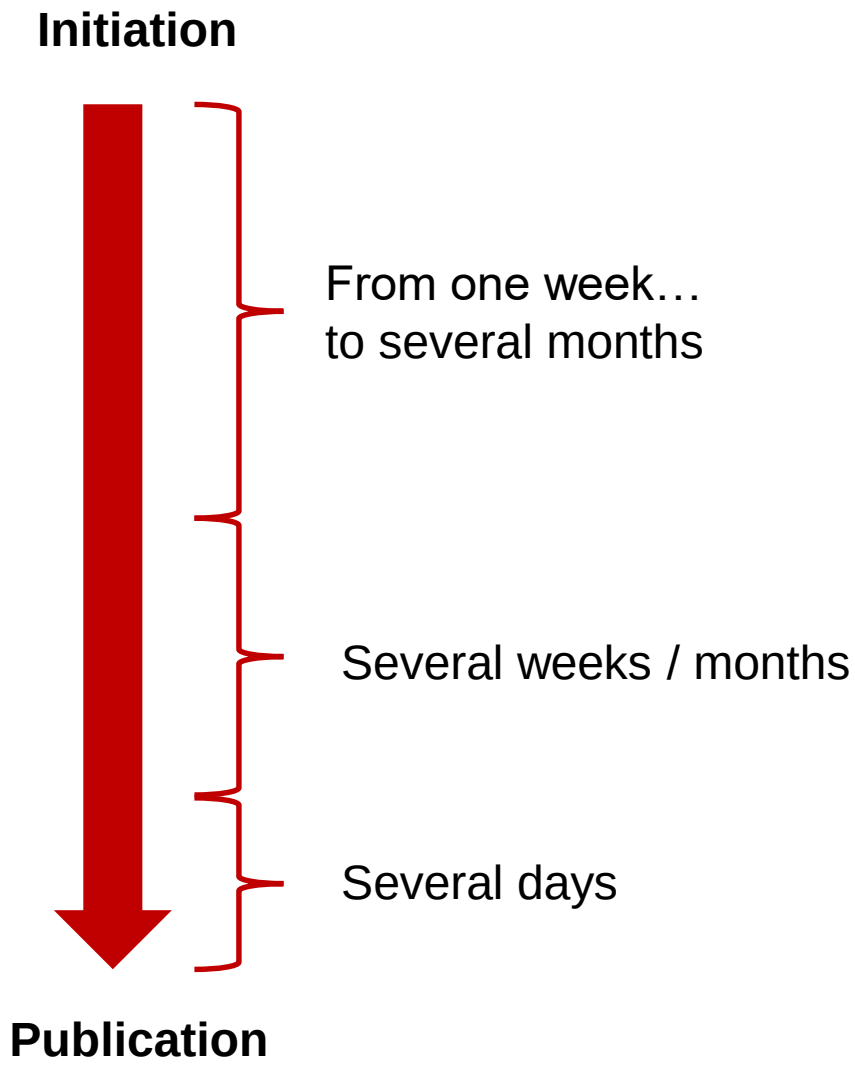
- Performed independently by 1 or 2 evaluators
- Using DDEP regulation and tools

Review process

- One DDEP reviewer is assigned
- Complete verification of the evaluation
- Discussion with evaluator until agreement

Editing and publishing

- Edited at LNHB and made available online
- Published in international journal / BIPM monography



Overview

Where to start ?

Understand the different types of data

General properties

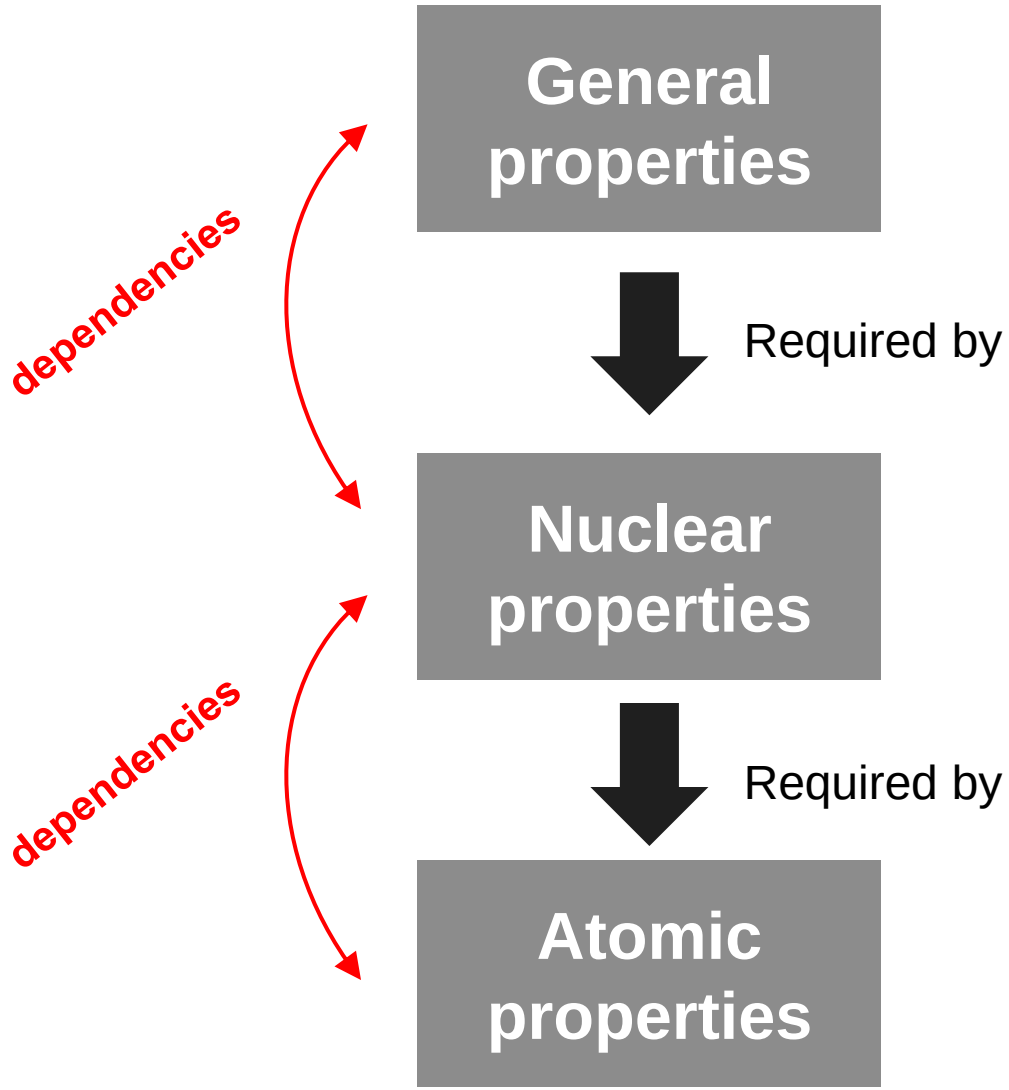
- Q-value
- Half-life
- Nuclei levels
- Decay scheme

Nuclear transitions

- Gamma transitions
- Electron transitions (IC + β-decay)
- Alpha transitions

Atomic transitions

- X-ray transitions
- Auger transitions



Definition of the nucleus

First step is obvious: Z and A that define the nucleus. Nothing else?

Physically, a metastable state has its own decay scheme, its own branching ratios, etc.

→ The decays of the nucleus ground-state and of its metastable state are different.

→ Evaluations are different, but can be linked via the available measurements.

→ **Nucleus ground state and metastable states are considered to be different nuclei.**

ENSDF evaluation focuses on nuclear structure information

→ Q-value is from ground state to ground state. Can be negative: ^{87}Sr is stable but ^{87m}Sr is not!

DDEP evaluation focuses on decay data

→ Q-value includes the level energy of the metastable state. This is the available energy for the decay.

→ Ground-state-to-ground-state Q-value is taken in the latest Atomic Mass Evaluation (2020 for the moment). Except if new, more precise measurements are available.

Levels

DDEP do not evaluate reaction data
→ ENSDF do. Level properties are usually better and can be taken as such.

However, **if level properties come dominantly from decay data, one should evaluate them**. GTOL code is useful.

- Level sequence from the ground state to the Q-value energy. Only levels that play a role in the decay scheme.
- Energies and uncertainties. Can be established from γ-ray energies.
- Spins and parities. If not well known, several possibilities.
- Half-lives and uncertainties.

Adopted levels	Sb129	Sn129M
Create levels from ENSDF file	Level Energy	Half-life
J 11/2 - π Sn129M Parent Level: 0	4074 *27*	6,96 min *0,09*
J 13/2 - π Sb129 Level: 5	1911,11 *0,05*	
J 15/2 - π Sb129 Level: 4	1860,97 *0,05*	2,2 µs *0,2*
J 19/2 - π Sb129 Level: 3	1851,22 *0,06*	17,4 min *0,3*
J 9/2 + π Sb129 Level: 2	1161,35 *0,04*	
J 11/2 + π Sb129 Level: 1	1128,56 *0,04*	
J 7/2 + π Sb129 Level: 0	0 	4,362 h *0,025*

Half-life

Table 1 – Measured half-life values of the ground state of ^{129}Sn.

References	$T_{1/2}$ (min)	Comments
1962HA16	57.6 (31)	Not used, out of range
1967BI15	2.5	Not used, no uncertainty
1972IZ01	2.52 (12)	
1974FO06	2.50 (27)	Recalculated, but no systematic uncertainty
1974GR29	2.25 (5)	Recalculated, but no systematic uncertainty
1980DE35	2.16 (4)	No detail, no systematic uncertainty
1982HU09	2.4 (1)	
1987STZO	2.5	Not used, no uncertainty
Recommended	**2.23 (5)**	Weighted mean, external uncertainty

→ Each choice should be justified in the Comments file (report of the evaluation).

Half-life

Table 2 – Measured half-life values of the 35-keV level of ^{129}Sn.

References	$T_{1/2}$ (min)	Comments
1962DR01	6.2 (12)	Na(I)Tl
1962HA16	8.8 (6)	Beta counter, not used
1967BI15	7.5 (1)	Beta counter, not used
1974FO06	7.3 (2)	Ge(Li)
1974GR29	8.9 (6)	Beta counter, not used
1980DE35	6.7 (4)	Ge(Li)
1982HU09	6.9 (1)	Ge(Li)
Recommended	**6.96 (9)**	Weighted mean, internal uncertainty

→ Each choice should be justified in the Comments file (report of the evaluation).

Gamma-ray emission intensities

These intensities are usually measured relative to a dominant peak

→ Renormalizing consistently all the peaks at the same reference.

→ Identifying the initial and final levels.

→ Summing all intensities to the ground state (if no metastable state of long half-life in the decay scheme). That gives the normalization factor from which absolute intensities are deduced.

Sometimes, absolute intensities have been measured

→ Requires first an accurate measurement of the sample activity.

→ Usually performed by metrology laboratories.

→ If at least one peak emission intensity is absolute, it must be used as a normalization factor.

Gamma transition probabilities

How to go from γ-ray emission intensities to γ transition probabilities?

Needs to include conversion electrons and pair creation

$$P_g = I_\gamma + I_{ce} + I_{e\pm}$$

→ **Internal conversion coefficients α_i and α_π, from BrIcc code.**

For a given sub shell, $\alpha_i = I_{ce\,i}\,/I_\gamma$. One deduces the useful relations: $\alpha_T = \alpha_K + \alpha_L + \alpha_M + \cdots$

$$I_{ce} = \frac{\alpha_T}{1+\alpha_T} P_g \qquad I_\gamma = \frac{P_g}{1+\alpha_T} \qquad I_{ce\,i} = \frac{\alpha_i}{1+\alpha_T} P_g$$

ICC calculation requires multipolarity and mixing ratio δ.

Example:

- Mixed multipolarity (y%) M1 + (x%) E2
- Mixing ratio defined by δ^2 = E2/M1, i.e. the probability ratio of E2 transition to M1 transition.

$L = \lvert J_i - J_f \rvert$	$\pi_f/\pi_i = -1$		$\pi_f/\pi_i = +1$	
	Transition	Possible mixture	Transition	Possible mixture
0 $(0 \to 0)$	Forbidden		Forbidden	
0 $(1/2 \to 1/2)$	E1		M1	
0 $(1 \to 1)$	E1	M2	M1	E2
1	E1	M2	M1	E2
2	M2	E3	E2	M3
3	E3	M4	M3	E4
4	M4	E5	E4	M5
even L $(J_i$ or $J_f = 0)$	ML		EL	
odd L $(J_i$ or $J_f = 0)$	EL		ML	

Contribution of atomic data

Internal conversion creates atomic vacancies

→ There exists a link between multipolarities and mixing ratios, and atomic emission intensities.

Sometimes, multipolarity and mixing ratio not well known, but atomic emission intensity was measured (usually for the dominant K shell).

→ **It is then possible to adjust the multipolarity and the mixing ratio to retrieve the atomic emission intensity.**

✓ Can be done by hand or with BrIccMixing code.

✓ Decay data are then more consistent.

Branching ratios

Gamma transition imbalance gives the branching ratios

→ For each level, look at gamma transitions coming in and going out.

→ If more goes out than comes in, the level must be fed in an another way.

→ The difference thus determines the branching ratio.

Usually, γ-ray measurements are the most accurate

→ It is therefore the best method to establish the decay scheme.

One can also have accurate measurements of α or β intensities

→ They can then be used, in part or totally, to establish the decay scheme.

→ Case by case.

Beta transitions and electron captures

For these transitions, DDEP provides the following information

- Transition nature, deduced from spin and parity change between initial and final nuclear levels.
- Transition energy.
- log *ft* value.
- $\beta^{\pm}$: mean energy of the beta spectrum.
- ε: capture probabilities of the sub shells.
- ε/β^{+}: competition between ε and β^{+} if transition energy > 2 m_e → Branch splitting

All these quantities are calculated, using the BetaShape code (current version is 2.4 from June 2024).

Annihilation radiation emission

Internal pair creation and β^{+} transitions → Emission of the 511-keV photon from positron annihilation.

$$I_{\gamma}(511\ \mathrm{keV}) = 2 \times \left(\sum I_{\gamma\pm} + \sum P_{\beta+} \right)$$

without annihilation-in-flight process, which do depend on the material.

Atomic emissions

Atomic vacancies are created by internal conversion and electron capture

→ Probabilities are given by the BrIcc and BetaShape codes, respectively, for all sub shells.

Transition energies and probabilities are from tabulations (see previous presentation).

EMISSION code

→ Used to calculate the atomic emission intensities based on transition energies and intensities, and on vacancy creation probabilities.

→ Provides detailed information for X-rays and Auger electrons for vacancies in K, L_1, L_2 and L_3 shells.

If measurements are available, comparison to EMISSION values should be done.

XL Emissions Sb129 Sn129M

Norme: 3,1881 – 4,594 | 3,15 (8)

	Energy (keV) Min	Energy (keV) Max	Photons per disintegration x 100	Uc
XL	3,1881	4,594	3,15	0,08
L_ℓ	3,1881		0,062	0,0021
L_α	3,5959	3,6051	1,65	0,05
L_η	3,4361		0,0251	0,0009
L_β	3,8439	4,1699	1,26	0,04
L_γ	4,2294	4,594	0,161	0,005

Update ALL energies

AUGER Emissions Sb129 Sn129M

Norme : 20,966 – 22,088 | 100, | 3,47 | 0,12

	Energy keV	Relative Probability	Nb electrons per disintegration x 100	Uc
Auger K				
KLL	20,966 – 22,088	100		
KLX	24,796 – 26,357	44,7	3,47	0,12
KXY	28,6 – 30,49	5		
Auger L	2,2448 – 4,6355		36,78	0,24

Atomic emissions

Energy Conservation (5)
At. process - consumed energy

Sn129M -> Sb129

Decay rate (%): 100

Q At. (keV): 823

Uc: 6

Wording	Energy (keV)	Probability	E x P	Uc	Summation	Sum uc	relative error (%)
K Alpha 2	26,1111	6,5	169,7	2,6			
K Alpha 1	26,3594	12,14	320	4,5			
K Beta 1	29,7884	3,45	102,8	2,1			
K Beta 2	30,4466	0,715	21,8	0,7	614	6	
Auger K-L1L1	20,95	0,263	5,5	0,26			
Auger K-L1L2	21,27	0,31	6,59	0,31			
Auger K-L1L3	21,51	0,396	8,53	0,4			
Auger K-L1M1	24,85	0,0958	2,38	0,12			
Auger K-L1M2	24,98	0,0605	1,51	0,08			
Auger K-L1M3	25,03	0,0766	1,92	0,1			
Auger K-L1M4	25,26	0,00526	0,133	0,007			
Auger K-L1M5	25,27	0,00578	0,146	0,007			
Auger K-L1N1	25,64	0,02	0,512	0,026			

Energy conservation

A good method to test the consistency of the decay scheme

→ Calculation of total decay energy with uncertainty propagation.

→ To be compared to Q-value, possibly weighted by the decay process probability, e.g. 90% β^- and 10% β^+/ε.

RADLST in ENSDF

Atomic model not precise, only K and L_1 shells.

Saisinuc software in DDEP

Atomic model more precise.

Energy Conservation (3)
Nuclear Process

K40 -> Ca40

Decay rate (%)	Q (keV)	Uc	Q x decay rate		TOTAL	Total Uc	relative error (%)		Uc
89,25	1311,07	0,11	117012,9975		117010	220	0,000	±	0,188

Wording	Energy (keV)	Probability	E x P	Uc	Summation	Sum Uc	partial relative error (%)	Uc "rounded"
								0,188
b-	1311,07	89,25	117010	220	117010	220	0,00	

Asymmetric uncertainties

DDEP provide symmetric uncertainties only $m \pm \sigma$

→ Most of our users do not know how to deal with asymmetric uncertainties X^{+a}_{-b}

Why asymmetric uncertainties?

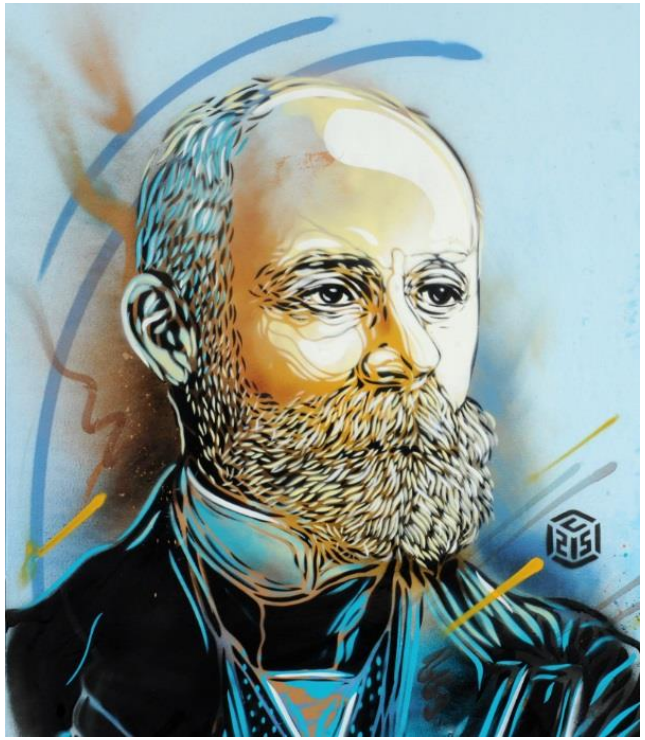
- Limitation of the measurements.
- Propagation of uncertainties
  - → Taylor expansion is valid only for linear relations/equations, for small relative uncertainties (≲10%) and neglecting correlations.
  - → Even starting with symmetric uncertainties, combination of quantities can lead to asymmetric uncertainties.

How to symmetrize asymmetric uncertainties?

Neither exact nor good method. DDEP follows the method employed for Atomic Mass Evaluations.

Median value that divides the distribution in two equal areas: $m \simeq X + 0{,}64 \times (a - b)$

Corresponding symmetric uncertainty is: $\sigma = (1 - 2/\pi) \times (a - b)^2 + a \times b$

→ **Value changed from X to m.**

Thank you for attention