Nuclear decay database in fission product mass region*

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Abstract: Accurate and reliable nuclear decay databases are essential for fundamental and applied nuclear research studies. However, decay data are not usually as accurate as expected and need improvement. Hence, a new Chinese nuclear decay database in the fission product mass region (A = 66−172) based on several major national evaluated data libraries has been developed under joint efforts in the CNDC working group. A total of 2358 nuclides have been included in this decay database. Two main data formats, namely ENSDF and ENDF, have been adopted. For the total mean β and γ energies, available data from total absorption gamma ray spectroscopy measurements have been adopted. For some nuclides without experimental measurements, theoretically calculated values have been added.

Keywords: nuclear decay data, evaluation database, fission product mass region

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I. INTRODUCTION

Evaluated nuclear structure and decay data are widely used in science, industry, medicine, agriculture, etc. Thus, accurate and reliable nuclear decay databases are essential for fundamental research studies and applied techniques [1−5]. However, the collection and evaluation of nuclear decay data is not usually as simple as expected. For instance, inconsistent decay data are provided by different types of evaluated decay data libraries such as UKHEDD, UKPADD, DDEP, and IAEA [6−10].

Specifically, the decay data of fission products, actinides, and their decay products are extremely important in nuclear applications such as burn-up analysis and decay heat calculation in the nuclear industry. Besides, some hot research topics, such as the reactor antineutrino spectrum, require maximum accurate decay data of fission products to perform the summation calculation and hence obtain the spectrum. Two major decay library studies have been carried out recently aiming to improve specific decay data, in particular the Radioactive Decay Data library for JEFF-3.3 [11] and the decay data sublibrary for ENDF/B-VIII.0 [12].

The Radioactive Decay Data library of the Joint Evaluated Fission and Fusion (JEFF-3.3) project was released in 2017. It was constructed based on evaluations from specialized evaluated decay data libraries (UKHEDD, UKPADD, DDEP, IAEA, etc.), and contributions from ENSDF. It contains 3852 radionuclides and a translation of an ENSDF file into the ENDF-6 format. Data for the mean β and γ energies from total absorption gamma-ray spectroscopy (TAGS) measurements were included. The decay data sublibrary for ENDF/B-VIII.0 contains 3821 radionuclides, where each nuclide corresponds to a long-lived level, ground state, or isomer. It was constructed based on decay data available in the Evaluated Nuclear Structure Data File (ENSDF), and translated into the ENDF-6 format. Concerning those nuclei for which no decay radiation has been measured or the known decay scheme is incomplete, basic information was extracted from the latest version of the Nuclear Wallet Cards.

In China, the first nuclear decay database in the fission product mass range (A = 66−172) has been developed at China Nuclear Data Center (CNDC) in cooperation with China Nuclear Data Coordination Network. It contains approximately 2358 nuclides. On the basis of new measurements and some well-known evaluated decay data files, the decay data of these radionuclides have been reevaluated and updated. Recommended decay data characteristics, including half-lives, branching fractions, energies and emission probabilities of α, β, and γ rays, total decay energies, mean energies of electromagnetic, light, and heavy particles, and all associated uncertainties, are listed in data files with ENDF format. Two main data formats, namely ENSDF and ENDF, were adopted in this library.

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In this paper, a brief description of the evaluations, database structure, and contents of the database are provided.

II. EVALUATION PROCEDURE

A. Evaluation method and principles

For nuclear decay data evaluation research, the following procedures are generally considered: (1) Reference compilation; (2) experimental assessment; (3) statistical and theoretical calculations; (4) and data documentation. Nevertheless, it is well known that different evaluation principles lead to significantly different recommended data. Details in this regard are provided next.

Based on the NSR database [13], all available measurements are generally taken into account for an evaluation, including measurements from laboratory reports or private communications. Comprehensive examination and analysis of experimental data are conducted for each assessment, and details of any adjustment on the reported data uncertainties are provided. Then, a statistical analysis is performed to determine the "best" adopted value. If the set of adopted experimental data is proved to be inconsistent, one among the following possibilities must be considered: (1) Recommend the unweighted mean or adopt the "best" individual measurement (for instance, the one with the smallest reported uncertainty); (2) reject some measured values according to objective or subjective judgments; (3) reassess the weight of each measurement when necessary. Finally, a decay scheme is established based on the conducted evaluation.

The transition intensities for all γ-rays are calculated from the recommended emission intensities and internal conversion coefficients interpolated using the BrIcc code [14]. BrIcc is a generic tool to evaluate theoretical conversion coefficients for pure and mixed multipolarity transitions based on the "Frozen orbital" approximation. It is suitable for a wide range of applications, including nuclear structure research and data evaluations. The treatment of multipolarities, mixing ratios, and uncertainties fully complies with the procedures adopted for the ENSDF [15]. The data table calculated for the specific needs of BrIcc covers transition energies from 1 to 6000 keV. The associated atomic data are calculated from the RADLIST code [16]. The program RADLST (Radiation Listing) is designed to calculate the nuclear and atomic radiations associated with the radioactive decay of nuclei. It uses the primary input decay data in the ENSDF format and presents the calculations in a variety of forms. RADLST produces listings or computer files containing the energies and intensities for various nuclear radiations: β^-, β^+, ε, γ, conversion electrons, electron-positron pairs from internal pair formation, and α. The output is provided in terms of an ENDF-6 file containing the energies and intensities of the radiations and some additional information. The program creates MT=1, MF=451 (Comments) and MT=8, MF=457 (Decay data) sections. For a certain nuclide, (1) all decay modes of each radioactive nuclide are specified in terms of both the branching fractions and Q-values; (2) the sum of all α, β^-, β^+/electron-capture and isomeric gamma-emission probabilities must be consistent with the corresponding branching fractions; and (3) energies and emission probabilities of conversion electrons, Auger electrons, and X-rays are calculated by RADLIST code in a consistent manner.

The consistency of evaluated decay schemes is checked prior to establishing the database by comparing the effective and calculated Q-values as follows:

$$R = [(\text{effective } Q\text{-value} - \text{calculated } Q\text{-value})/ \text{effective } Q\text{-value}] * 100, \quad (1)$$

where the effective Q-value is deduced from the branching ratio of the decay mode and the Q-value resulting from evaluation [17]. The calculated Q-value is obtained from RADLIST code using the decay scheme and evaluated decay data.

Both values are obtained in two different independent manners. The effective Q-value is extracted from the atomic mass data reported by Wang *et al*. [17]. The calculated Q-value is derived from the summation of energies for all the particles emitted in the decay process, including α, β (maximum energy), neutrino, gamma, X-ray, recoil, and conversion and Auger electrons, which are calculated from the energies and emission probabilities of all particles based on the evaluated decay level scheme. Hence, the R value reflects the correction and completeness of the decay level scheme.

R value greater than 5% suggests a poorly detected decay scheme, whereas less than 5% indicates the construction of a reasonably established decay scheme [18].

For a nuclide with a reasonably established decay scheme, the total mean β and γ energies are calculated from recommended decay data using the RADLIST code. For a nuclide with no decay scheme or poorly detected decay scheme suffering from the pandemonium effect (missing β feeding the higher energy levels), the mean β and γ energies are determined from available total absorption gamma ray spectroscopy (TAGS) studies. This is the case of 57 nuclides, including ^{69}Co [19], ^{71,73}Ni [20], ^{76}Ga [21], ^{86}Br [22], ^{87}Br [23], $^{89,\,90g,\,90m}$Rb [24], ^{91}Rb [23], ^{92}Rb [25], ^{93}Rb [24], ^{93}Sr [24], ^{94}Rb [23], ^{95}Sr [24], ^{96m}Y [26], ^{98}Nb [27], ^{101,102}Zr [28], ^{102g}Tc [29], ^{103,104}Nb [30], ^{104,105}Tc [29], ^{109}Tc [28], ^{138m,139,140,141}Cs [24], ^{142}Ba [31], ^{142}Cs [31], ^{143,144,145}Ba [24], ^{143,144,145}La [24], ^{145,146,147,148}Ce [24], ^{147,148m,148g,149,151}Pr [24], ^{151,154,155}Nd [24], ^{153,154m,155,156,157}Pm [24], ^{157,158}Sm [24], and ^{158}Eu [24]. Table 1 shows typical cases which apparently exhibit the ‘pandemonium phe-

Table 1. Total mean β and γ energies from ENSDF database and TAGS measurements for some typical nuclides.

nuclide	ENSDF		TAGS	
	E_β	E_γ	E_β	E_γ
^{69}Co	2990 ± 12	0.0	3660 ± 13	1418 ± 54
^{73}Ni	1870 ± 80	1090 ± 48	2226 ± 83	3980 ± 15
^{87}Br	1650 ± 77	3340 ± 36	1144.4 ± 1.6	3941.9 ± 2.2
^{90m}Rb	1400 ± 11	3244 ± 61	1115.7 ±5.0	3769.3 ± 5.8
^{142}Cs	2920 ± 18	952 ± 26	2418 ± 73	1793 ± 47
^{144}Ba	1480 ± 56	477 ± 11	927 ± 12	785± 13
^{148m}Pr	1020 ±13	597 ± 58	674 ± 89	1492 ± 91

nomenon'.

B. Data processing methods

For single adopted data, the recommended value is directly taken from the corresponding measurement. If there are two or more adopted measurements, a weighted average value will be set as the recommended value.

The weighted average value and its uncertainty are calculated according to the following procedures [32].

Assuming that x_i and σ_i refer to individual data and their associated uncertainties, respectively, and N refers to the number of measurements, the weighted average value is then given by

$$x_w = \frac{\sum x_i w_i}{\sum w_i}, \tag{2}$$

with internal error

$$\sigma_{\text{int}} = \sqrt{\frac{1}{\sum w_i}}, \tag{3}$$

and external error

$$\sigma_{\text{ext}} = \sqrt{\sum_i \frac{(x_i - x_w)^2}{\sigma_i^2 \times (n-1)}} \times \sqrt{\frac{1}{\sum_i w_i}}. \tag{4}$$

The larger of these two uncertainties should be taken as the recommended uncertainty.

C. Data formats of the decay database

Two standard data formats, i.e., ENSDF and ENDF, were adopted in the present database. After evaluating a particular radionuclide, the recommended decay data were prepared in ENSDF format and then converted into ENDF-6 format, where the general information is stored in the data section (MF=l, MT=451), and the recommended decay data are stored within the data section (MF = 8, MT=457).

For each nuclide, the data section (MF=l, MT=451) contains the following information: (1) Radionuclide, date of evaluation, name of evaluator, date of distribution, etc.; (2) library name (CENDL-DDL1.0), material number, date type (i.e., radioactive decay data), and format type (ENDF-6); (3) detailed comments on the evaluation; (4) specific decay data not contained in the main decay data section and consistency check of the recommended data set. In the data section (MF=8, MT=457), the recommended decay data for the following characteristics are listed for each nuclide: (1) Spin and parity of the level of parent nuclide; (2) half-life of the level of the parent nuclide in second unit; (3) mean energy for γ (including X-ray) and β (or heavy) particles; (4) decay mode, decay energy (Q-values), branching fraction, and isomeric branching fraction for isomeric state; (5) energy and emission probability of γ-ray; (6) energy, emission probability, and transition type of β-particle; (7) energy, emission probability, and transition type of electron-capture; (8) energy and emission probability of α-particle; (9) energy and emission probability of delay-neutron; (10) energy and emission probability of delay-proton; (11) energy and emission probability of discrete-electron; (12) energy and emission probability of X-ray.

III. CONTENTS OF THE DECAY DATABASE

The database covers a total of 2358 nuclides in the fission product mass range (A = 66−172). The whole set of decay data and relative information is provided for each nuclide. The Q-value of total decay energies were updated using the new mass adjustment [17]. The information for beta-delayed neutron was taken from IAEA recommendations [33, 34] if the precursor exists. Some theoretical results have also been included to cover measurement-absent data.

When constructing the nuclear decay database, information extracted from well-known evaluated decay data files, such as the NUBASE [35] for evaluation of

Table 2. Consistent decay data and revised (CNDC) decay data information in the library.

Databases	NUBASE	ENSDF	DDEP	CNDC	TOTAL
Number	542	646	192	978	2358

Table 3. Comparison of the decay data in CNDC and ENSDF libraries for ^{88}Kr.

Data	Evaluated Value		Comments
$T_{1/2}$	ENSDF	2.825 ± 0.019 h	Weighted average of measured values from Wang (2.804 ± 0.015 h) [37], Ehrenberg (2.860 ±0.017 h) [38] and Clarke (2.805 ± 0.025 h) [39]
	This study	2.801 ± 0.012 h	Weighted average of measured values from Wang (2.804 ± 0.015 h) [37], Chu (2.805 ± 0.025 h) [40], Yang (2.796 ± 0.015 h) [41], Clarke (2.805 ± 0.025 h) [39]. Ehrenberg (2.860 ±0.017 h) [38] was rejected for inconsistency
$P(\beta^-$(g.s.))	ENSDF	14 ± 4 %	From Wohn [42]
	This study	14.6 ± 0.8 %	Weighted average of measured values from Dang [43], Xie [44], and decay scheme
$P(\gamma2392)$	ENSDF	34.6 ± 1.6 %	From Bunting [45] and $\Sigma(I(\gamma$+ce) to g.s.) = 86 ± 4 assuming $P(\beta$- (g.s.)) = 14 ± 4 [42]
	This study	34.8 ± 0.5 %	Weighted average of absolute measured values from Dang [43] and Xie [44]

nuclear properties, or the ENSDF [15] and DDEP [36] databases, was useful for saving time. These evaluated data could be adopted after correction based on new available measurements or different evaluation principles. A comparison of the recommended data with other databases was performed; the nuclide numbers with consistent decay data and revised data are shown in Table 2. For CNDC evaluations, a total of 978 nuclei decay were revised. A typical example of revised evaluation for the ^{88}Kr nucleus is shown in Table 3 to illustrate the process of CNDC evaluation.

IV. CONCLUSIONS

To meet the demands of the nuclear industry and fundamental research studies for nuclear decay data, a new Chinese evaluated nuclear decay database has been developed under joint efforts in the CNDC working group.

All types of decay data were reevaluated for involved nuclides according to the evaluation method and principles of the CNDC working group. For a total of 2358 nuclides in the fission product mass range (A = 66−172), a whole set of decay data is provided, including the half-life, branching fraction, total decay energy, energies of α, β, γ, and other particles, emission probabilities and mean energies, and all associated uncertainties. Data files with both ENSDF and ENDF formats are also provided. Comparing with other national decay database, the proposed database includes updated data and revised decay data for at least 978 nuclides.

Data availability statement This manuscript has no associated evaluated data or the evaluated data will not be deposited. The evaluated data will be made available upon request.

References

[1] X. Guan, J. H. Zheng, and M. Y. Zheng, Nuclear Science and Techniques **34**, 173 (2023)
[2] Z. Z. Ren, Y. W. Yang, Y. H. Chen *et al.*, Nuclear Science and Techniques **34**, 115 (2023)
[3] Q. F. Song, L. Zhu, H. Guo *et al*, Nuclear Science and Techniques **34**, 32 (2023)
[4] B. Zhang, X. B. Ma, K. Hu *et al*, Nuclear Science and Techniques **33**, 8 (2022)
[5] E. Alhassan, D. Rochman, A. Vasiliev *et al*, Nuclear Science and Techniques **33**, 50 (2022)
[6] A. L. Nichols, Applied Radiation and Isotopes **64**, 1384 (2006)
[7] M. J. Woods, S. M. Collins, Applied Radiation and Isotopes **60**, 257 (2004)
[8] V. P. Chechev, Applied Radiation and Isotopes **70**(9), 187 (2012)
[9] S. Leblond, Applied Radiation and Isotopes **206**, 111191 (2024)
[10] National Laboratory, https://www.nndc.bnl.gov/nds/
[11] M. A. Kellett, O. Bersillon, EPJ Web of Conferences **146**, 02009 (2017)
[12] D. A. Brown, M. Chadwick, R. Capote *et al.*, Nuclear Data Sheets **148**, 1 (2018)
[13] Nuclear Science References (NSR), National Nuclear Data Center, Brookhaven National Laboratory, http://www.nndc.bnl.gov/ nsr
[14] T. Kibedi, T. W. Burrows, M. B. Trzhaskovskaya *et al.*, Detectors and Associated Equipment **589**, 202 (2008)
[15] Evaluated Nuclear Structure and Decay Data (ENSDF), National Nuclear Data Center, Brookhaven National Laboratory, https://www.nndc.bnl.gov/ensdf/
[16] RADLIST, ENSDF analysis and utility programs, National Nuclear Data Center, Brookhaven National Laboratory, https://www-nds.iaea.org/public/ensdf_pgm

[17] M. Wang, W. J. Huang, F. G. Kondev *et al*., Chin. Phys. C **45**, 030003 (2021)
[18] A. L. Nichols, Detectors and Associated Equipment **369**, 516 (1996)
[19] S. Lyons, A. Spyrou, Phys. Rev. C **100**, 025806 (2019)
[20] F. Persch and D. Young, Phys. Rev. C **103**, 055808 (2021)
[21] C. Dombos, D. L. Fang, A. Spyrou *et al*., Phys. Rev. C **93**, 064317 (2016)
[22] S. Rice, A. Algora, J. L. Tain *et al*., Phys. Rev. C **96**, 014320 (2017)
[23] E. Valencia, J. L. Tain, A. Algora *et al*., Phys. Rev. C **95**, 024320 (2017)
[24] R. C. Greenwood, R. G. Helmer, M. H. Putnam *et al*., Detectors and Associated Equipment **390**, 95 (1997)
[25] A. Zakari-Issoufou, M. Fallot, A. Porta *et al*., Phys. Rev. L **115**, 102503 (2015)
[26] V. Guadilla, L. Le Meur, M. Fallot *et al*., Phys. Rev. C **106**, 014306 (2022)
[27] C. Rasco, K. P. Rykaczewski, A. Fijałkowska *et al*., Phys. Rev. C **105**, 064301 (2022)
[28] C. Dombos, A. Spyrou, F. Naqvi *et al*., Phys. Rev. C **103**, 025810 (2021)
[29] D. Jordan, A. Algora, J. L. Tain *et al*., Phys. Rev. C **87**, 044318 (2013)
[30] J. Gombas, P. A. DeYoung, A. Spyrou *et al*., Phys. Rev. C **103**, 035803 (2021)
[31] M. Wolinska-Cichocka, B. C. Rasco, K. P. Rykaczewski *et al*., Phys. Rev. C **107**, 034303 (2023)
[32] M. U. Rajput, T. D. MacMahon, Detectors and Associated Equipment **312**, 289 (1992)
[33] J. Liang, B. Singh, I. Dillmann *et al*., Nuclear Data Sheets **168**, 1 (2020)
[34] M. Birch, J. Liang, B. Singh *et al*., Nuclear Data Sheets **128**, 131 (2015)
[35] G. Kondev, M. Wang, W. J. Huang *et al*., Chin. Phys. C **45**, 030001 (2021)
[36] Decay Data Evaluation Project (DDEP), http://www.lnhb.fr/ddep_wg
[37] S. L. Wang, T. Bai, Q. Li *et al*., Applied Radiation and Isotopes **70**, 1927 (2012)
[38] B. Ehrenberg, S. Amiel, Phys. Rev. C **6**, 618 (1972)
[39] W. B. Clarke, H. G. Thode, Can. J. Phys. **42**, 213 (1964)
[40] C. Chu, G. Hu, X. Guo *et al*., J. Radioanal. Nucl. Chem. **329**, 1393(2021)
[41] Z. H. Yang, Y. Q. Ding, S. D. Zhang *et al*., Atomic Energy Science and Technology **54**, 1737 (2020)
[42] K. Wohn, M. D. Glascock, W. L. Talbert *et al*., Phys. Rev. C **13**, 2492 (1976)
[43] Y. B. Dang, D. M. Zhou, Y. Q. Ding *et al*., Atomic Energy Science and Technology **48**, 961 (2014)
[44] F. Xie, X. B. He, W. G. Jiang *et al*., Nuclear Science and Techniques **22**, 304 (2011)
[45] R. L. Bunting, W. L. Talbert, J. R. McConnell *et al*., Phys. Rev. C **13**, 1577 (1976)