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Data Evaluation of Prompt γ-rays from Neutron Capture*

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Abstract: The method of prompt γ-ray data evaluation for neutron capture and how to calculate the prompt γ-ray intensities of neutron capture have been briefly presented. The prompt γ-ray data of thermal-neutron capture of some stable nuclei for $A=1$—44 and $A>190$ have been evaluated. The ENSDF format has been adopted. The checks of intensity balance and format have been made. The examples are given to illustrate its application.

Key words: neutron; (n, γ) reaction; evaluation code; data evaluation

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1 Introduction

The energies and intensities, and their decay schemes of neutron capture (specially, thermal-neutron capture) γ-ray are one of the basic data of nuclear physics research, nuclear technology application and nuclear engineering design. Today, the technique of neutron-induced Prompt γ Activation Analysis (PGAA) is widely applied in material science, chemistry, geology, mining, archaeology, food analysis, environment, medicine, and so on. The availability of high-quality guided (or filtered) thermal and cold neutron beams at high and medium flux research reactors has greatly facilitated the advancement of the PGAA method during the 1990s.

PGAA is a non-destructive radio-analytical method, capable of rapid and simultaneous multi-element analysis involving the entire Periodic Table, from hydrogen to uranium. The inaccuracy and incompleteness of the data available for use in PGAA are significant handicap in the qualitative and quantitative analysis of complicated γ spectra. Accurate and complete neutron capture γ-ray energy and intensity data are important for PGAA. The international database for PGAA has been developed under the organization of Nuclear Data Section, IAEA. The evaluation and update of prompt γ-ray data for thermal-neutron capture is a part of the IAEA project.

The method of capture prompt γ-ray data evaluation and how to calculate the prompt γ-ray intensities of thermal-neutron capture are presented, and $^{13}C(n,\gamma)$ is taken as an example how to evaluate the prompt γ-ray data, and how to calculate the prompt γ-ray intensities of thermal-neutron capture and how to give decay schemes in the text.

2 Main Evaluation Program

Main codes of neutron capture prompt γ-ray data evaluation and their functions are listed in Table 1. These codes are mainly from International Network[1] of Nuclear Structure and Decay Data Evaluation, the ENSDF data format is adopted in data evaluation.

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Biography: Zhou Chunmei (1938—), male (Han Nationaliy), Guangdong Xingning, professor, working on nuclear data evaluations and their database developments.

Table 1 Main codes and their functions of prompt γ-ray data evaluation for neutron capture

Code name	Main functions
GTOL	Level energy calculation by fitting to γ-energies
	Intensities balance calculation & checking
LWA	Limit-weighted and un-weighted average of measured data
HSICC	Internal conversion coefficients calculation
RADLST	Energy balance calculation & checking
FMTCHK	ENSDF data format checking
PANDOR	ENSDF physics checking
ENSDAT	Drawing decay schemes & listing data tables

3 Flow Chart of Prompt Neutron Capture γ Data Evaluation

The main flow chart of neutron capture γ-ray data evaluation is given in Fig. 1. The basic characters are as follows:

(1) Measured data collection

Evaluator retrieves related references from Nuclear Science References File (NSRF). On the basis of the retrieval, all measured data are collected from journals, reports, and private communications.

(2) Measured data evaluation and recommendation of the best measured data

Gathered all related-data are analyzed and compared, treated by mathematical method (for example, limit-weighted or un-weighted average of measured data). And then, the best-measured data and decay scheme can been recommended on the basis of the measured data evaluation.

(3) Establishment of temporary data file

After recommendation of the best-measured data, the evaluated data are put into computer by hand, the temporary data file can be set up in ENSDF data format.

(4) Theoretical calculation

Format checking must be carried out for the temporary data file, and correction to old one should be done if necessary. Then, physics analysis and theoretical calculation are performed and calculation results will be put into the gapes without measured data so that recommended data become a self-consistent and complete data set.

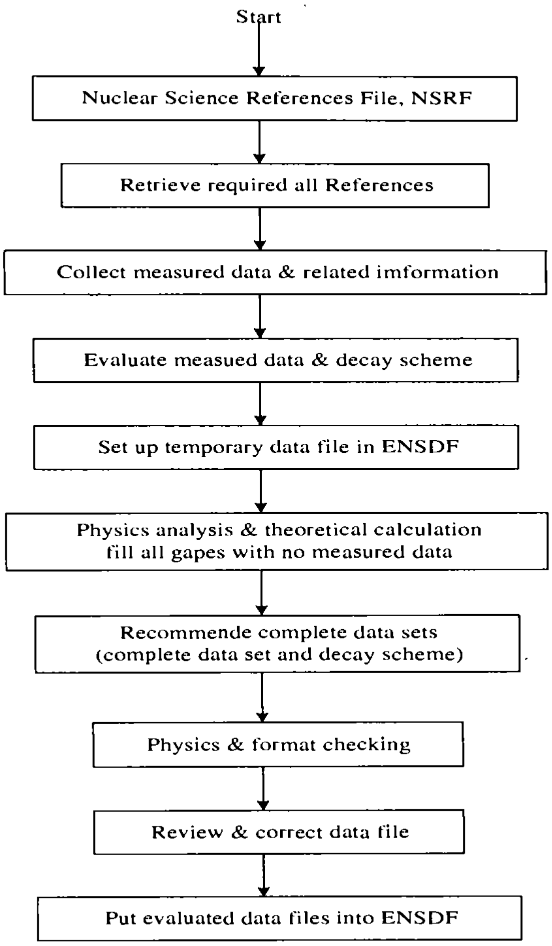

Fig. 1 Flow chart of prompt γ-ray data evaluation for neutron capture.

(5) Recommendation of complete data set

A complete data set of thermal-neutron capture prompt γ-ray data and its decay scheme is recommended as evaluated data set.

4 γ-ray Emission Intensity Calculation

In the experimental measurements, relative prompt γ-ray intensities are measured. In the practical applications, prompt γ-ray emission probabilities should be known. In general, the prompt γ-ray emission probabilities per 100 neutron captures must be given. The basic principle of the prompt γ-ray emission probability calculation is the γ transition intensity balance for each level.

Main and general methods of the thermal-neutron capture prompt γ-ray intensity calculation are summarized as follows:

4.1 Calculation from γ-ray Decaying to Ground State

If there are m γ-rays decaying to ground state, when a nuclide captures a thermal-neutron, I_k is the relative intensity for the k-th γ-ray, α_k is its total internal conversion coefficient, the equation can be written as follows,

$$N\sum_{k=1}^{m} I_k(1+\alpha_k) = 100 \ , \tag{1}$$

where N is normalization factor for γ-ray intensity per 100 neutron captures,

$$N = \frac{100}{\sum_{k=1}^{m} I_k(1+\alpha_k)} \ . \tag{2}$$

For light nuclides, the each internal conversion coefficient α_k is quite small and can be neglected, so

$$N = \frac{100}{\sum_{k=1}^{m} I_k} \ . \tag{3}$$

From Eq. (2) or (3), normalization factor N, and then, γ-ray intensities for thermal-neutron capture can be calculated.

4.2 Calculation from Primary γ-ray Decaying from Capture State

When a nuclide captures a thermal-neutron, the nuclide is de-excited from its capture state by emitting primary γ-rays. Suppose that there is n primary γ-rays, I_i is the relative intensity of i-th primary γ-ray and α_i is its total internal conversion coefficient of i-th primary γ-ray, then,

$$N\sum_{i=1}^{n} I_i(1+\alpha_i) = 100 \ , \tag{4}$$

$$N = \frac{100}{\sum_{i=1}^{n} I_i(1+\alpha_i)} \ . \tag{5}$$

And for light nuclide, Eq. (5) becomes

$$N = \frac{100}{\sum_{i=1}^{n} I_i} \ . \tag{6}$$

5 Intensity Balance Check

The most important is the physical consistent check of intensity balance for each levels.

For decay γ-ray to ground state, the Eq. (1) becomes

$$N_b\sum_{k=1}^{m} I_k(1+\alpha_k) = 100 \ , \tag{7}$$

where N_b is normalization factor for γ-ray intensities per 100 neutron captures.

For primary γ-ray from captured state, the Eq. (4) becomes as follows,

$$N_p\sum_{i=1}^{n} I_i(1+\alpha_i) = 100 \ , \tag{8}$$

where N_p is normalization factor for γ-ray intensities per 100 neutron captures. from Eqs. (7) and (8), Eq. (9) can be got as,

$$N_p\sum_{i=1}^{n} I_i(1+\alpha_i) = N_b\sum_{k=1}^{m} I_k(1+\alpha_k) \tag{9}$$

or,

$$\frac{N_p}{N_b} = \frac{\sum_{k=1}^{m} I_k(1+\alpha_k)}{\sum_{i=1}^{n} I_i(1+\alpha_i)} \ . \tag{10}$$

The normalization factors N_p and N_b for γ-ray intensities per 100 neutron captures are not exactly the same, because the measurement uncertainty exists. Therefore,

$$\frac{N_p}{N_b} \approx 1 \ , \tag{11}$$

within their uncertainty range. The Eq. (10) can be changed into

$$\frac{\sum_{i=1}^{n} I_i(1+\alpha_i)}{\sum_{k=1}^{m} I_k(1+\alpha_k)} \approx 1 \ . \tag{12}$$

or,

$$\sum_{i=1}^{n} I_i(1+\alpha_i) \approx \sum_{k=1}^{m} I_k(1+\alpha_k) \ . \tag{13}$$

The Eq. (13) is also correct within their uncertainty range. For other levels, in addition to captured state and ground state, the intensities coming into and going out the level j are the same within thier uncertainty range, as shown in Fig. 2.

$$\sum_{k=1}^{m} I_{jik}(1+\alpha_{jik}) - \sum_{i=1}^{n} I_{joi}(1+\alpha_{joi}) \approx 0 \text{ . } \quad (14)$$

In formula (14), I_{jik}, α_{jik}, I_{joi}, and α_{joi} are γ-ray relative intensities and their internal conversion coefficients for coming into and going out level J respectively.

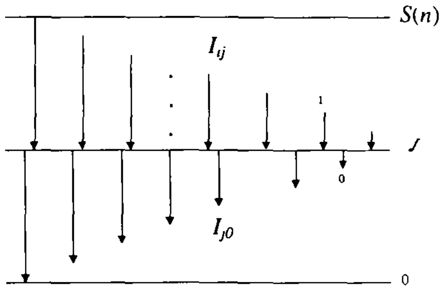

Fig. 2 Skeleton scheme of intensity balance calculation for excitation level.

6 Application

The data evaluation[2] of $^{13}C(n,\gamma)$ reaction at E=thermal is taken as an example to show its application. The evaluated level data and γ-radiation data are listed in Tables 2 and 3, respectively. The decay scheme of $^{13}C(n,\gamma)$ reaction at E=thermal is given in Fig. 3. The γ-ray intensities balance is given in Table 4. From these tables and scheme it can be seen that the evaluated data are self-consistent in physics and intensity balance.

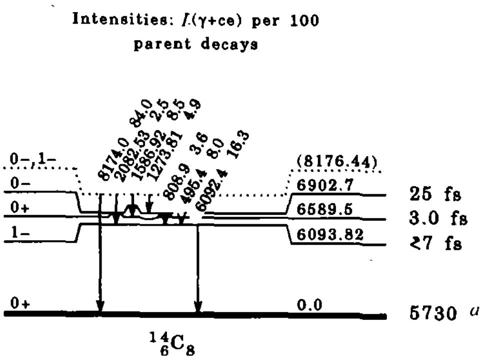

Fig. 3 Decay scheme of evaluated data for $^{13}C(n,\gamma)$ reaction E=thermal.

Table 2　^{14}C Levels listing of evaluated data for $^{13}C(n,\gamma)$ reaction E=thermal*

E(level)+	J^{π}*	$T_{1/2}$*	Comments
0.0	0^+	5 730　a　40	$\%\beta^-=100$
6 093.82　20	1^-	<7　fs	
6 589.5　3	0^+	3.0　fs　4	
6 902.7　3	0^-	25　fs　3	J^{π}: from s-wave
(8 176.44　1)	$0^-,1^-$		neutron capture

*　+ From E_γ using least-squares fit to data.

* From Ref. [3], except as noted.

Table 3　γ (^{14}C)-ray listing of evaluated data for $^{13}C(n,\gamma)$ reaction E=thermal*

E_γ+	E(level)	I_γ#@	Comments
495.4　3	6 589.5	8.0　3	
808.9　2	6 902.7	3.6　3	
1 273.81*　17	(8 176.44)	4.9　10	E_γ=1 273.92[2]
1 586.92*　18	(8 176.44)	8.5　5	E_γ=1 586.82[2]
2 082.53*　18	(8 176.44)	2.5　5	E_γ=2 082.63[2]
6 092.4　2	6 093.82	16.3　8	
8 174.0*　3	(8 176.44)	84.0　23	E_γ=8 173.92[2]

*　+ From Ref. [3], except as noted. * From level energy differences. # Intensities per 100 neutron captures from Ref. [2]. @ For intensity per 100 neutron captures.

Table 4　Intensities balance listing of evaluated data for $^{13}C(n,\gamma)$ reaction E=thermal

Level	RI			TI			NETFEEDING
	(OUT)	(IN)	(NET)	(OUT)	(IN)	(NET)	(CALC)
0.0	0.0	100.3　25	−100.3　25	0.0	100.3　25	−100.3　25	−0.3　25
6 093.82　20	16.3　8	14.1　7	2.2　11	16.3　8	14.1　7	2.2　11	2.2　11
6 589.5　3	8.0　3	8.5　5	−0.5　6	8.0　3	8.5　5	−0.5　6	−0.5　6
6 902.7　3	3.6　3	4.9　10	−1.3　11	3.6　3	4.9　10	−1.3　11	−1.3　11
8 176.44　1	100.　3	0.0	100.　3	100.　3	0.0	100.　3	100.　3

The prompt γ-ray data and their decay schemes of thermal-neutron capture for stable nuclei[4—6] ^{1}H, ^{2}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{12}C, ^{13}C, ^{14}N, ^{16}O, ^{17}O, ^{19}F, ^{20}Ne, ^{21}Ne, ^{22}Ne, ^{23}Na, ^{24}Mg, ^{25}Mg, ^{26}Mg, ^{27}Al, ^{28}Si, ^{29}Si, ^{30}Si, ^{31}P, ^{32}S, ^{33}S, ^{34}S, ^{35}Cl, ^{36}Ar, ^{36}S, ^{37}Cl, ^{39}K, ^{40}Ar, ^{40}Ca, ^{40}K, ^{41}K, ^{42}Ca, ^{43}Ca, ^{44}Ca and ones[7] of ^{193}Ir, ^{194}Pt, ^{195}Pt, ^{196}Pt, ^{197}Au, ^{207}Pb, ^{240}Pu have been evaluated by using these programs. The evaluated data have been sent to Nuclear Data Section, IAEA and used by the users. These calculation methods of γ-ray emission probabilities for neutron capture have been adopted in most data evaluations of ENSDF.

7 Discussion

In general, neutron binding energy is high, and captured state is a high excitation state and its decay scheme is quite complex. A lot of weak-intensity γ-ray are unable to be measured experimentally. Besides, measured uncertainties from background deducting and γ-spectra analysis lead to γ-ray intensity uncertainties. Strictly speaking, intensities of coming into and going out a level are unable to be exactly the same, only can be consistent within their uncertainties. The normalization factors from the primary γ-rays from captured state and the decay γ-rays to ground state are different since above reasons. In the data evaluation, normalization factor in thermal-neutron capture reaction is usually calculated from the γ-rays of decay to ground state.

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中子俘获瞬发 γ 射线数据评价*

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摘　要：简要地介绍了中子俘获瞬发 γ 射线数据及其衰变纲图的评价方法技术、主要程序及其功能、数据评价流程、强度平衡检验，以及对 $A=1-44$ 的稳定核素和 $A>190$ 的部分稳定核素的热中子俘获瞬发 γ 射线数据及其衰变纲图评价的具体应用.

关键词：中子；(n,γ)反应；评价程序；数据评价

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