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Procedure of Neutron Cross Section Evaluation in the Resonance Region and Evaluation of Iodine-129 Resonance Parameters

Soo-Youl Oh and Jonghwa Chang

Korea Atomic Energy Research Institute
P.O. Box105, Yusung, Taejon, Korea 305-600
E-mail: syoh@kaeri.re.kr

Abstract

A procedure for the evaluation of neutron cross sections in the resonance energy region has been established. The procedure is introduced herein. In the resonance region, the neutron cross sections are constructed from the resonance parameters consisting of File 2 in the ENDF-6 format, so the eventual product of the procedure is a File 2 for each nuclide under consideration. The procedure has been used for recent evaluations of 25 fission product nuclides. Among these nuclides, the evaluation results for iodine-129, which is one of the fission products important to the transmutation study, are presented. This evaluation takes account for recent measurements, thus shows differences in the evaluated thermal capture cross section, capture resonance integral, and capture cross sections in the unresolved resonance region from those of existing evaluated libraries such as the ENDF/B-VI.

1. Introduction

The energy-dependent neutron cross sections are indispensable input data for all nuclear design and analyses. The cross sections are compiled in a file, so-called the evaluated library, such as the ENDF/B of the U.S.A., JENDL of Japan, JEF of European countries, and so on. The whole energy range covered in a library is divided into two parts: the resonance energy region, which is subdivided into the resolved resonance region and unresolved region, and a higher energy region where the energy-dependent behavior of cross sections is rather smooth. For the resonance region, the cross sections are represented with resonance parameters compiled in a File 2 (Resonance Parameters) of the ENDF-6 format[1], and point-wise cross sections, *i.e.* pairs of energy and cross section value, are provided basically in File 3 (Neutron Cross Sections) for a higher energy region. The resonance parameters for each resonance consist of the resonance energy, quantum numbers such as the angular momentum of incident neutron and total resonance spin, and resonance widths (neutron, capture, fission, and other competition reaction if any). The parameterization of cross sections significantly reduces the size of a data file and the parameters themselves are important for the understanding of fundamental nuclear physics. When it is necessary, a set of point-wise cross sections in the resonance region are constructed with the aid of parameter values and a physics model such as the Single or Multi-level Breit-Wigner formula.[1, App. D]

In the resolved resonance region (RRR), because no nuclear theory has been developed for calculating the parameters from the first principle, the experiment is the only way to obtain parameters. Thus the evaluation in the resonance region is a task compiling and/or converting measured data into one recommended set of parameters for each nuclide.

For the unresolved resonance region (URR) in the present evaluation procedure, sets of ‘average’ resonance parameters are provided also in File 2. In the existing evaluated libraries, however, it is not difficult to see point-wise cross sections given in File 3, instead of resonance parameters in File 2, because the cross sections are more or less smooth in the URR. Since the URR is an extension of the RRR in fact, the parameters for the URR should have a consistency with those for the RRR. Therefore, it is required to analyze individual parameters in the RRR for providing a consistent set of URR parameters.

The reactions concerned in the resonance region are the elastic scattering, capture, and fission reaction. For some nuclides, there is the other reaction as a competition reaction, *e.g.*, the (n,α) reaction of ^{10}B. The upper energy of the URR in the present procedure is set to the energy where the first inelastic scattering channel opens.

The evaluation procedure is described first, then the evaluation results for ^{129}I, which have not been reported elsewhere, are presented in this paper.

2. Evaluation Procedure

Figs. 1 and 2 show the evaluation procedure that has been established in the Korea Atomic Energy Research Institute (KAERI). Fig. 1 shows the functional flow and Fig. 2 the computer code usage. This procedure has been used for the evaluation work of the resonance parameters of 25 fission products[2,3]. Among computer codes written in capital letters in Fig. 2, PTANAL and WRIURR are those written in KAERI. Others are available from the National Nuclear Data Center[4] of the Brookhaven National Lab., U.S.A.

For the first step of the evaluation, the information is retrieved from CINDA, the Computer Index to Nuclear Data[5], in which bibliographic information, but numeric data, is compiled for almost all activities including measurements and evaluations on the nuclide under consideration. Then, the measured resonance parameters, as well as other data such as capture cross sections in the thermal and keV energy regions, are obtained from the IAEA/NDS's EXFOR database[6] or from the literature directly. There are two famous compilations of resonance parameters; one is the BNL compilation[7] so-called "barn-book" and the other is Russia's recent one[8]. After reviewing the available measurements, numerical data of the resolved resonance parameters are prepared as an electronic file BNL325.TXT. The capture and scattering cross sections at 0.0253 eV, the bound coherent scattering length (b_{coh}), and the capture resonance integral are the quantities to be reproduced from the resolved resonance parameters. Usually, the reference thermal characteristics are adopted from the BNL compilation, but new measurements after the Compilation, if available, are taken into account.

In the second step, the orbital angular momentum (*l*) and the resonance spin (*J*) of a resonance, which have not been determined from the measurements, are determined. The Bayesian method [2,9] is applied to distinguishing *p*-wave (*l*=1) resonances from *s*-waves (*l*=0). For a resonance with a neutron width of $g\Gamma_n$, the probability that this resonance is a *p*-wave resonance is calculated from Bayes' theorem of conditional probability[9]. Rather rigorous probability density functions (pdf's) for the distributions of *s*- and *p*-wave neutron widths had been derived[10] from the χ^2 distribution proposed by Porter and Thomas[11], and those are applied to the present evaluation procedure. On the other hand, we note that the resonance spins for weak and/or high-energy resonances are seldom determined experimentally. For these resonances, a method of random assignment[2] is applied with the pdf for the *J* distribution calculated by using the Bethe formula[12] for the level density. A file ENDFA.TXT is prepared at the end of this step: this file is one of the outputs of PTANAL. Of normal, the multi-level Breit-Wigner formalism[1] is adopted in the present evaluation.

In the same step, the distribution of reduced neutron widths of the resolved resonances is fitted to a theoretical distribution to obtain the average level spacing and the neutron strength functions. This is called as the Porter-Thomas analysis in the present paper, because the Porter-Thomas distribution[11] is adopted as the theoretical distribution of reduced neutron widths. The Levenberg-Marquardt method[13] is applied to this non-linear fitting problem. The results of the analysis are used for the preparation of average resonance parameters in the URR.

In the third step, it is checked whether the current positive-energy resolved resonances produce the reference thermal cross sections and scattering lengths by using the code PSY325. If the resonance parameters fail to reproduce reference values, one or two bound level (*i.e.* negative-energy, virtual) resonances are invoked. There are systematics calculating the scattering length, thermal capture cross section, capture resonance integral, *etc*. in terms of resonance parameters.[Eqs. 12, 22, and 102 in Ref. 7, Part A] Since the summation over all positive-energy resonances in the systematics is readily obtained from the PSY325 run, one can calculate required bound level parameters that match the calculated cross sections and measured ones. However, the capture width of the bound level is usually assumed, and the potential (or effective) scattering length (R') is adjusted sometimes if no reasonable bound level has been obtained. The file ENDFR.TXT is prepared when this step is finished.

The last step is the step evaluating the average resonance parameters for the URR and appending them to the resolved resonance data file. The parameters shall reproduce measured capture cross sections in an energy region from ~keV to several tens ~ hundreds keV region. The statistical analysis of neutron widths in the second step is usually restricted to *s*-wave resonances (and *p*-wave resonances in some nuclides) due to lack of measurements of resolved, higher *l*-value resonances. Thus, the average resonance parameters for higher *l*-value resonances should be evaluated via another route. In the present evaluation procedure, parameters for up to *d*-wave (l=2) resonances are provided because contributions of $l \geq 3$ resonances to the cross section is negligible below a few hundreds keV. In evaluating the average parameters, a method of parameter adjustment based on the Bayes' theorem is applied. The general formalism for the parameter adjustment was presented in the Appendix of Ref. 3. In the present procedure, the model parameter vector consists of the neutron strength functions for *s*-, *p*-, and *d*-wave resonances, the average *s*-wave level spacing, and the average radiative widths for *s*-, *p*-, and *d*-waves. However, because the *s*-wave parameters are determined from the resolved resonances, they are more reliable, then only the parameters for *p*- and *d*-waves are subjected to adjustment in most cases. The file ENDFU.TXT that includes the unresolved region data is prepared at the end of the step. Point-wise cross sections in the unresolved region are calculated by using RECENT and SIGMA1 codes sequentially from the ENDFU.TXT file and the results are compared with the measured cross sections. If discrepancies between the calculated cross sections and measured ones are not acceptable, the unresolved parameters are further adjusted.

3. Evaluation of ^{129}I Resonance Parameters

3.1. Resolved Resonance Parameters

Iodine-129 (half life = 1.57×10^7 y) is one of the long-lived fission products subjected to the transmutation study.[14 and references therein] The neutron capture of ^{129}I, followed by β-decay of ^{130}I, yields ^{130}Xe that is a stable isotope. So the capture reaction, in an energy region of slightly harder neutron spectrum than that in a conventional light water reactor, is the major concern of the cross section evaluation for a transmutation study.

The resonance parameters of ^{129}I in ENDF/B-VI were evaluated in 1980, JENDL-3.2 in 1990, and JEF-2.2 in 1991. The resonance file in ENDF/B-VI adopted 5 resonances from the barn-book, 3rd edition, published in 1973. JENDL-3.2 and JEF-2.2 used the capture area measurement of Macklin in 1983[15] with an assumed capture width of 120 meV (JENDL-3.2) and 90 meV (JEF-2.2). Since there was no new measurement in the resonance region, Macklin's data were adopted to the present evaluation, too. Macklin's data consist of capture areas for 125 resonances in an energy region up to 3.4 keV. With the aid of old transmission measurement in ORELA for the first 5 resonances [16], the capture widths of resonances at 72.18, 96.43, and 152.69 eV were determined as 99, 82, and 91 meV meV, respectively. For the other resonances, an average capture width of 91 meV was assumed, and

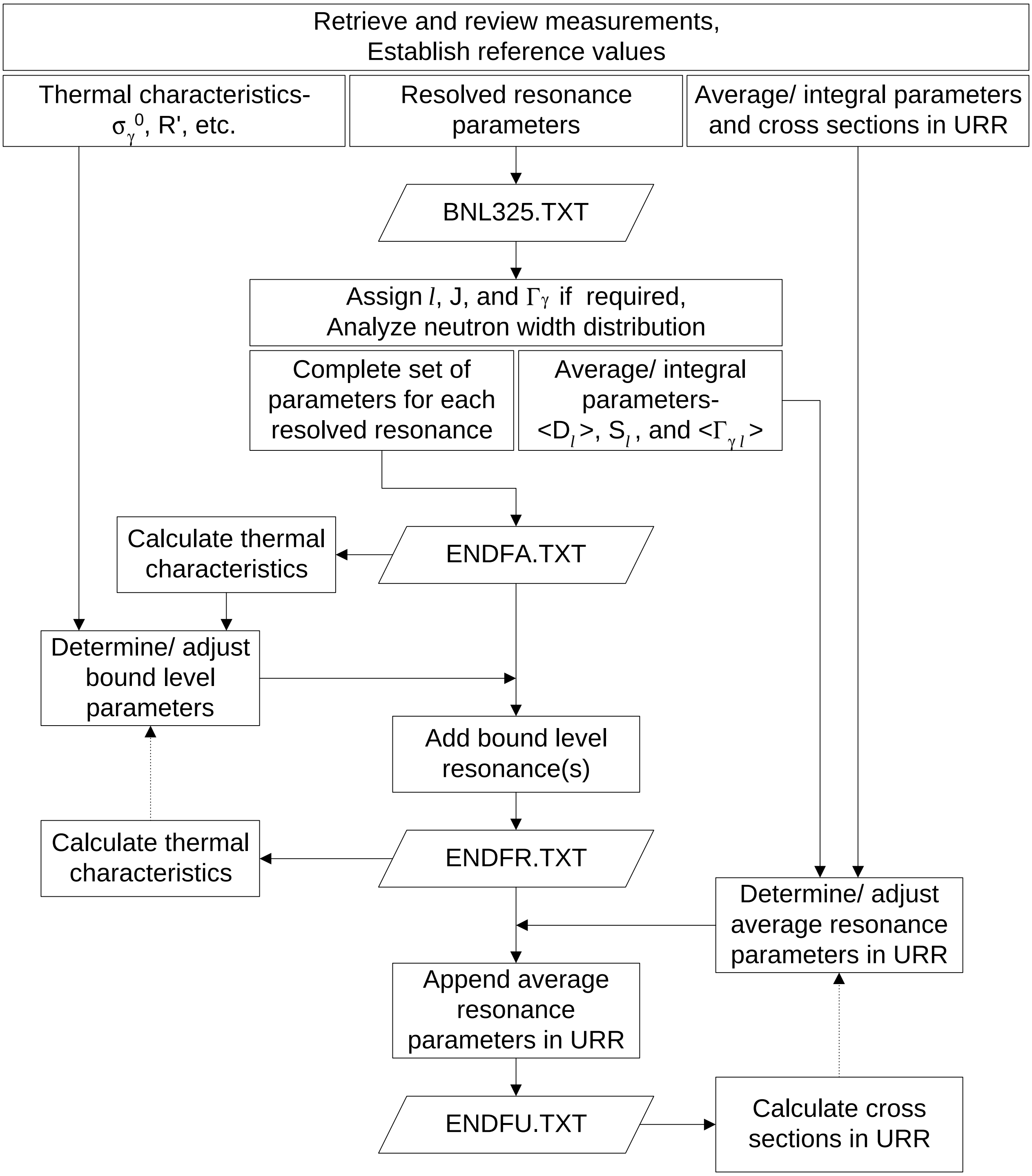

Fig. 1. Functional Flow of the Evaluation Procedure

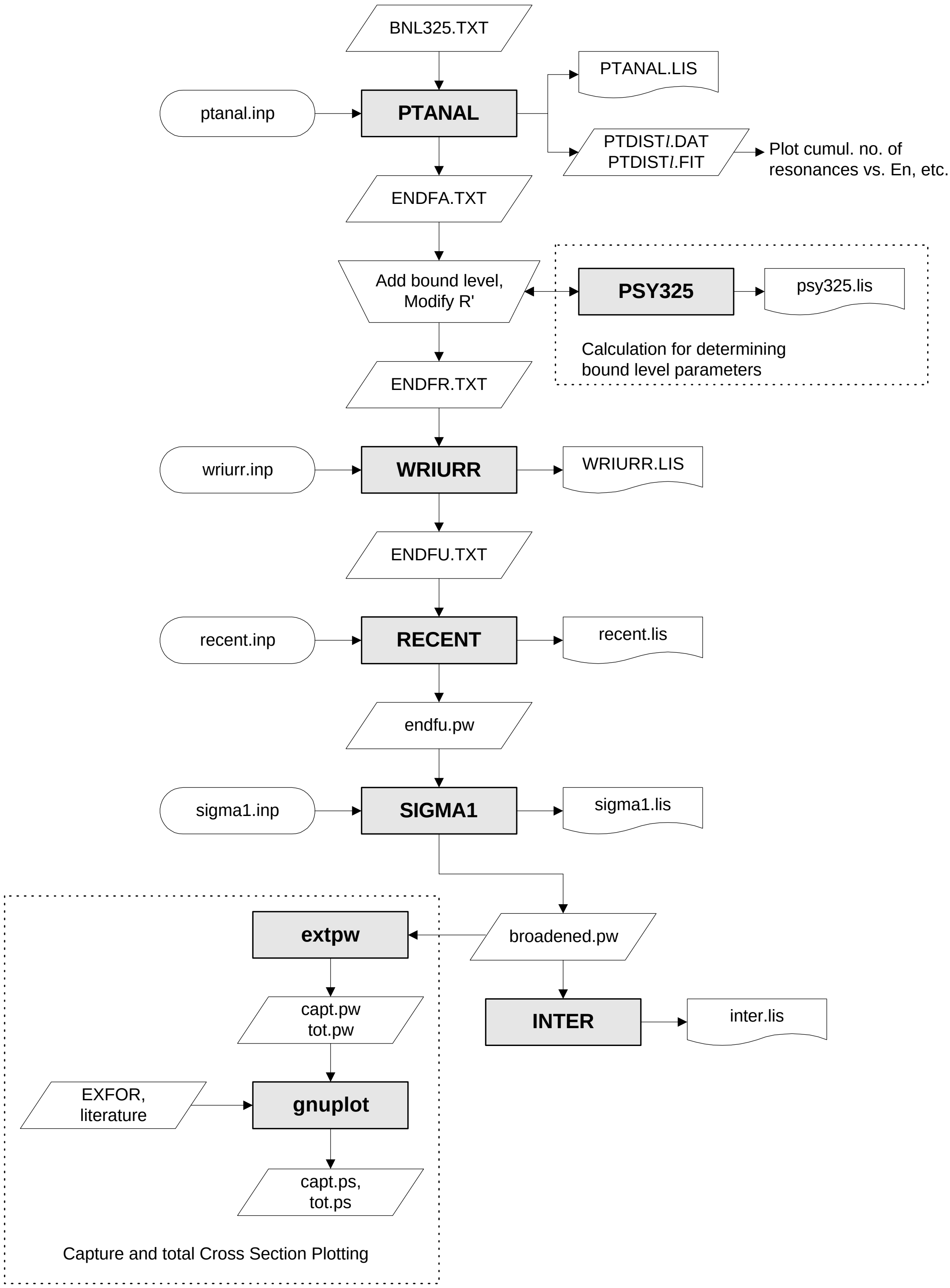

Fig. 2. Code Usage in the Evaluation Procedure

$g\Gamma_n$ values for each resonance were calculated from Macklin's capture areas. For 7 resonances, however, because of their very large capture areas, capture widths were adjusted up to 138 meV to obtain reasonable neutron widths.

The assignment of *l* values according to the Bayesian approach resulted in 105 *s*-wave and 20 *p*-wave resonances. All resonances in JENDL-3.2 and JEF-2.2 are *s*-waves.

The Porter-Thomas analysis of thus obtained neutron widths, as shown in Fig. 3 how well the analysis fits to actual data, resulted in the *s*-wave strength function $S_0 = (0.58\pm0.09)\times10^{-4}$, and the *s*-wave average level spacing $<D_0> = 27.7\pm1.4$ eV. These values are consistent with evaluated values of $S_0 = (0.50\pm0.10)\times10^{-4}$ and $<D_0> = 30\pm3$ eV in the Reference Input Parameter Library[17] within associated uncertainties. No measurement of S_0 to compare with is available for last 35 years. Meanwhile, due to insufficient number of *p*-wave resonances, the Porter-Thomas analysis for *p*-wave was not meaningful.

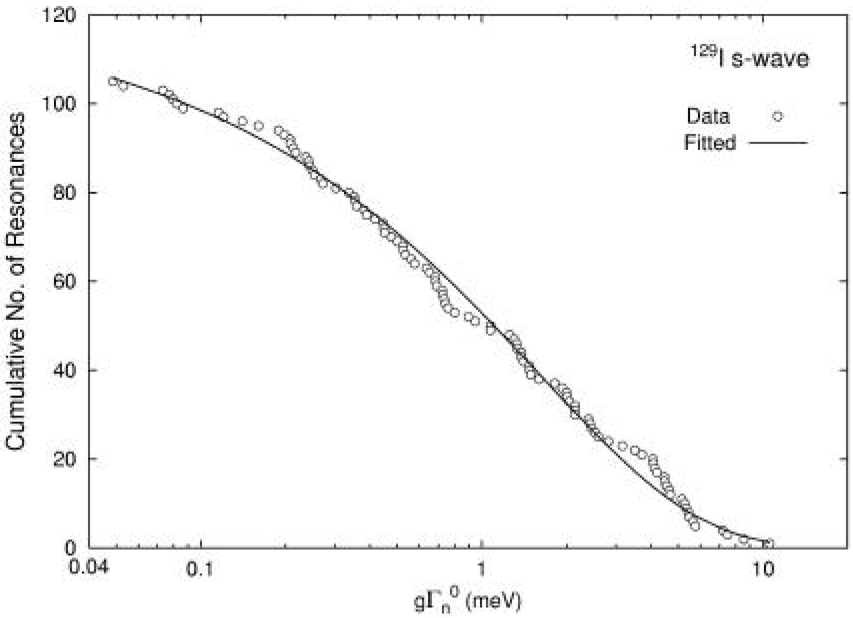

Fig. 3. Complement of the Cumulative Distribution of ^{129}I *s*-wave Neutron Reduced Widths

3.2. Thermal Characteristics

The thermal, *i.e.* 2200 m/s, capture cross section from the measurement of Nakamura et al.[18] was adopted as the reference value. To reproduce the reference thermal characteristics, one bound level resonance was invoked. The present bound level resonance parameters are as follows: resonance energy at −89.43 eV, resonance spin $J = 4$ ($l = 0$), capture width $\Gamma_\gamma = 1.58$ eV, and neutron width $\Gamma_n = 0.62$ eV. The widths look too large, but those resulted in a capture resonance integral very close to a weighted average integral of Nakamura' s and Friedmann' s[19]. On the other hand, the potential scattering length was adjusted to 5.5 fm, instead of a result from a usual systematic $R' = 1.23A^{1/3} + 0.8$ fm, where A is the atomic mass of the target divided by the neutron mass, to obtain a value of thermal total cross section close to the measured one by Block et al.[20] The thermal characteristics are summarized in Table 1. Present evaluation reproduced the thermal capture cross section of Nakamura and thermal total cross section of Block. Fig. 4 shows the capture cross sections below 100 eV. It is expected from the figure that the capture resonance integral of present evaluation lie between those from ENDF/B-VI and JENDL-3.2 or JEF-2.2.

Table 1. Thermal Characteristics of ^{129}I

Source		Capture Cross Section (b)	Scattering Cross Section (b)	Total Cross Section (b)	Capture Resonance Integral (b)
Experiment	Nakamura ' 96 [18*]	30.3±1.2			33.8±1.4
	Friedmann ' 83 [19]	33.9±1.9			30.6±1.6
	Block ' 60 [20]	31±4		35±4	
Evaluation	ENDF/B-VI**	27.2	4.57	31.8	35.6
	JENDL-3.2**	27.0	6.50	33.5	29.0
	JEF-2.2**	33.9	8.58	42.5	30.3
	Present	30.5	4.69	35.2	32.3

* Old measurements on the capture cross section are found therein.
** Data taken from JEF Report 14[21]

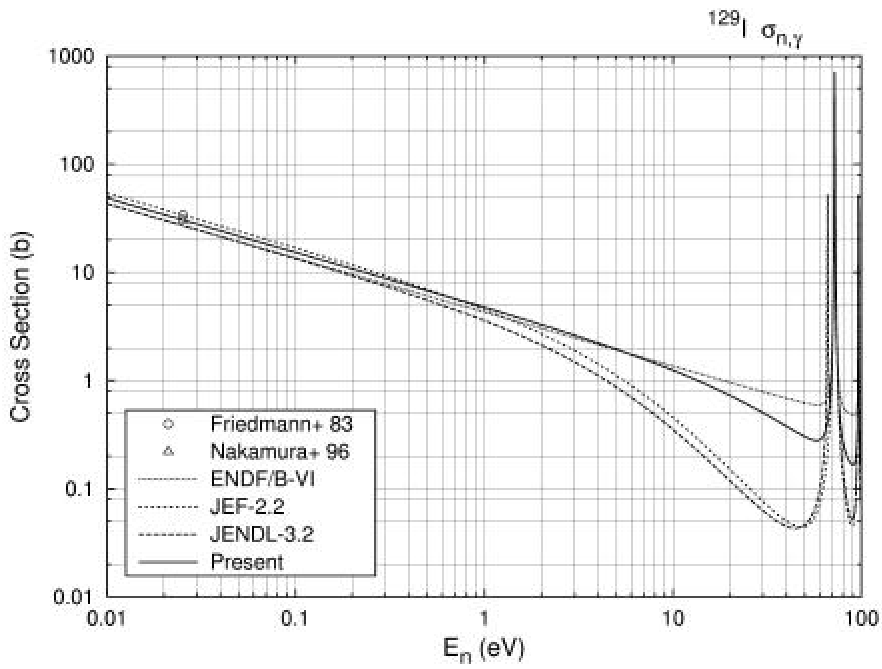

Fig. 4. Capture Cross Section of ^{129}I below 100 eV

3.3. Unresolved Resonance Parameters

The measurement of Macklin in 1983[15] is the only available measurement of ^{129}I capture cross sections in the unresolved resonance region. He reported average capture cross sections in 3 ~ 500 keV region, which was divided into 16 intervals. The average resonance parameters, as listed in Table 2, are prepared up to 28.0 keV where the first inelastic scattering channel of ^{129}I opens.

Table 2. Average Resonance Parameters for the Unresolved Resonance Region of ^{129}I

Quantity	Orbital Angular Momentum, l	JENDL-3.2	JEF-2.2	Present
Neutron Strength Function, S [10^{-4}]	0 1 2	0.53 1.33 0.89	0.52 2.08 2.00	0.58 1.50 0.58
Average Level Spacing, <D> [eV]	0 1 2	30.9 15.4 10.3	22.8 11.4 7.6	27.7 14.9 11.2
Average Capture Width, $<\Gamma_\gamma>$ [meV]	0 1 2	160 160 160	104.5 104.5 104.5	140 140 140

Notes:

1. No URR data were provided in the ENDF/B-VI. The File 3 includes cross sections for URR.
2. The strength functions of JENDL-3.2 are those at 70 keV. The average reduced neutron widths were adjusted energy by energy to reproduce Macklin' s capture cross sections.
3. JEF-2.2 provided negative background capture cross sections in File 3 to reproduce Macklin' s data.

Present evaluation adopted the values of S_0 and $<D_0>$ obtained from the analysis of resolved resonances without any adjustment. The value of S_1 was read from a graph of a deformed optical model calculation,[7, Part A, Figure 3] and S_2 was assumed to be same to S_0. It is worthy to note the average capture width. Instead of 91 meV of the resolved resonances, it was adjusted to 140 meV to reproduce Macklin' s capture cross sections. According to Macklin[15], the measured capture area suggests that the average *s*-wave capture width is not much different from that of ^{127}I, which is 136±8 meV in 2.66 to 4.02 keV region and 104±8 meV in 1.5 to 2 keV region. Fig. 5 shows capture cross sections constructed from the present resonance data as well as those in other existing libraries. It tells an improvement, especially, over ENDF/B-VI.

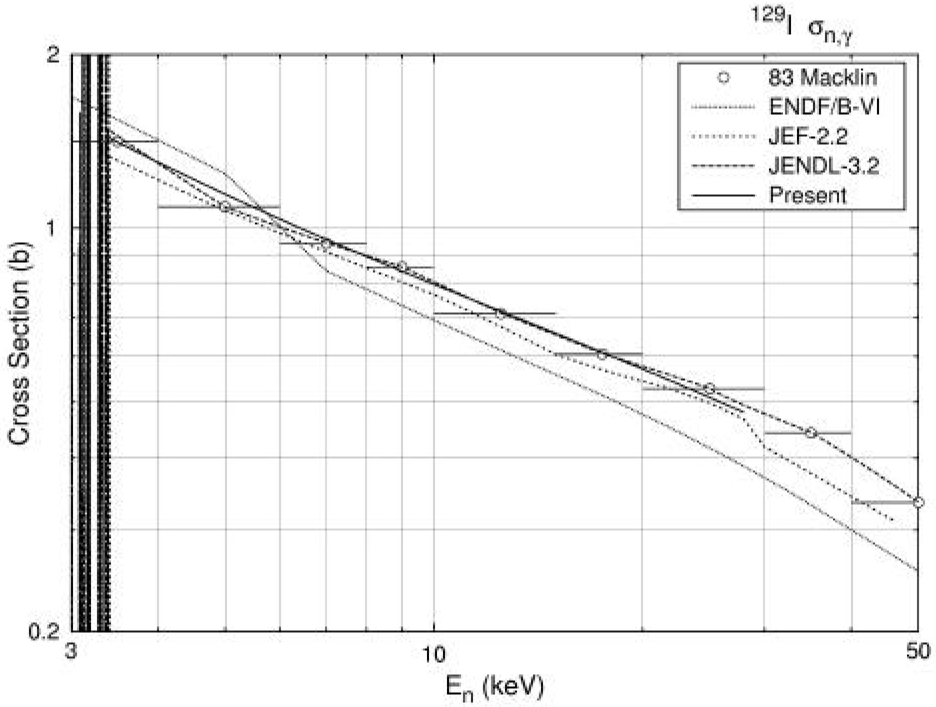

Fig. 5. Capture Cross Section of ^{129}I in the Unresolved Resonance Region

4. Remarks

The procedure for preparing the resonance parameters, *i.e.* File 2 in the ENDF-6 format, is introduced. This procedure is rather comprehensive and systematic so that an evaluator may follow the procedure for a reliable and easy evaluation. Nevertheless, the preparation of the very first parameter file BNL325.TXT is the core activity of the evaluation in the resonance region, and it requires evaluator's experience as well as careful attention to the measured parameter values. It seems that the pre-first step of the evaluation cannot be included in a more complete, formal procedure, if any.

The evaluation of ^{129}I resonance parameters took account for recent measurements, thus resulted in different cross sections from those deduced from existing evaluated libraries. It might be said that the present evaluation results in improvements over existing libraries.

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