Available online at www.sciencedirect.com
ScienceDirect
Nuclear Data Sheets 118 (2014) 250–253
Nuclear Data Sheets
www.elsevier.com/locate/nds

R-matrix Analysis for n$+^{16}$O Cross-sections up to $E_n = 6.0$ MeV with Covariances

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Neutron cross sections are analyzed for ^{16}O up to 6.0 MeV. We focus on giving the covariance and estimation of (n,α) cross sections for which all the world nuclear data libraries still have problems in the quantification. This work demonstrates a multi-channel R-matrix analysis for ^{17}O system: ^{16}O+n and ^{13}C+α. Resulting cross sections are independent of the systematic uncertainty of measurements. Also, obtained covariance data mirror both experimental and theoretical knowledge.

I. INTRODUCTION

Oxygen is one of the most important materials in nuclear applications such as reactors, in the form of water and oxide. Therefore, both experimental and theoretical studies have been devoted to know the accurate neutron cross sections for ^{16}O over the years. Nowadays, those in the world nuclear data libraries are believed to be reasonable. This is not necessarily wrong for major reactions, however, a big difference still remains among measured ^{16}O(n,α)^{13}C and/or the inverse reaction cross sections, which makes us difficult to quantify the values. In reality, the difference exceeds 30%, which is large enough to affect criticality benchmark calculations [1]. This problem is recognized in the world as listed in CIELO [2]. Also, there are increasing demands for giving uncertainties in evaluated data to estimate the margin of integral calculations. To respond to such request, the covariance data of ^{16}O are given in ENDF/B-VII.1 [3] and JENDL-4.0 [4]. However they are estimated by a simple way, roughly inferred from experimental information. This situation is also true for many other light nuclei.

The purpose of this study is to estimate the neutron cross sections for ^{16}O with covariance. Multi-channel R-matrix analyses are carried out for the ^{17}O system - ^{16}O+n and ^{13}C+α up to $E_n = 6.0$ MeV, in which we demonstrate two different approaches. This study is still on-going to resolve discrepancies in the experimental data available. We report our data analysis method and preliminary results.

II. R-MATRIX ANALYSIS

A. Models and Codes

A multi-channel R-matrix code AMUR was developed based on the formalism of Wigner-Eisenbud [5]. As long as we have enough information on the nuclear structure, the theory gives exact solutions without any approximations. The code was written with an object oriented framework (assembly of C^{++} classes rather than code). It is designed to calculate cross sections not only for the neutron but also the charged-particle reactions. The photon channel is not included in the current version, since the neutron radiative capture cross sections on light elements are very small.

The code also has functions of the parameter search with the generalized least-square method based on Bayes' theorem. Therefore, values of R-matrix parameter can be deduced from experimental cross sections with covariance. Both the statistical and systematic uncertainties can be considered in the fitting procedure. We minimize the Peelle's Pertinent Puzzle (PPP) effect by analyzing data in the logarithmic space. This is an option of the Box-Cox method [6]. The covariance of cross sections is obtained by propagating those for model parameters. The above methods are identical to those in the SOK codes [7].

B. Analysis for ^{17}O System

1. Channels Considered

The (n,α) reaction opens at $E_n = 2.36$ MeV, and the other reactions are still closed up to $E_n \sim 6.0$ MeV. Therefore, we include two partitions, n$+^{16}$O$_{\rm g.s.}$ and $\alpha+^{13}$C$_{\rm g.s.}$ in our R-matrix analysis. For the level assign-

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http://dx.doi.org/10.1016/j.nds.2014.04.050
0090-3752/2014 Published by Elsevier B.V.

ments of the compound nucleus ^{17}O, we followed those in the latest version of ENSDF except for a few cases. We include the levels of $J^{\pi} = 1/2^{\pm}, 3/2^{\pm}, 5/2^{\pm}$ and $7/2^{\pm}$, which can be excited by the incoming partial waves of $l = 0$ to 4.

2. Model Parameters

The model parameters to be searched for are the channel radius r_c for each partition and the reduced width amplitude γ_c for each resonance. The energy eigenvalues E_λ (level energies of ^{17}O) are also treated as free parameters. In addition, the background contributions from the negative and the distant levels are given as parameters.

3. Experimental Cross-sections

Table I lists the experimental cross sections preliminarily used in the model parameter search. The data of total cross sections are reported in many literatures. Most of them were measured by the time-of-flight method and given with a high energy-resolution that is enough to separate the resonances except in the higher energy region. We tentatively selected three sets of those measurements which complement the energy range of our interests, although we have confirmed that other experimental data do not disagree with the ones we used.

Because experimental data of (n,α) cross sections are limited, we decided to analyze measured cross sections of the inverse reaction ^{13}C(α,n)^{16}O. The experimental data of Harissopulos *et al.* [11] are the most recent and given with a high energy resolution over the corresponded neutron energy range. The data are essential to deduce the parameter values for the alpha-particle channels. They also help us to determine the energy eigenvalues and γ_c values for neutrons since resonances in the total cross sections data become unresolved as the energy increases.

TABLE I. Experimental cross sections preliminarily used in the parameter search.

Reaction	Author	(year)	Range adopted
O(n,tot)	Schrack *et al.* [8]	(1972)	0.50 - 6.2 MeV
	Perey *et al.* [9]	(1972)	0.50 - 6.2 MeV
^{16}O(n,tot)	Ohkubo [10]	(1984)	0.79 - 935.0 keV
^{13}C(α,n)^{16}O	Harissopulos *et al.* [11]	(2005)	0.77 - 4.6 MeV

4. Fitting Scheme

All the model parameters were deduced through the simultaneous analysis of those experimental data mentioned above. In the fitting procedure, calculated cross sections are broadened by the energy resolution of each experimental data set (we assume a reasonable resolution if the information is not available from the literatures). We first carried out the analysis without considering systematic uncertainty of measurements. The obtained parameters are used as initial values to be given for more in-depth study as described in the next paragraph.

One of our interests is to find a suitable way for the parameter search in the R-matrix analysis. It is also very relevant to estimate the covariance data. In this study, we demonstrate two different approaches in order to deal with the systematic uncertainty of experimental data as follows.

- Case-1 : Reasonable values of systematic uncertainty are inferred from literatures, and these values are fixed in the fitting procedure. In this work, 10% is assumed for total cross sections, and 50% for ^{13}C(α,n)^{16}O cross sections, so as to cover the differences among almost all the measured cross sections. This approach may be the same as that is normally used in the nuclear data evaluation.

- Case-2 : A renormalization factor is introduced for each measurement, and it is treated as a free parameter together with the model parameters. Once normalizations are obtained, experimental data are scaled by this value. Then, Case-1 is performed to obtain the final results. This might be equivalent to the data fitting procedure in the EDA code [12].

III. RESULTS AND DISCUSSIONS

A. Case-1

Resulting total cross sections are plotted with uncertainty in Fig. 1. Through the R-matrix analysis, we successfully fitted the experimental data, and obtained the model parameters with covariance. It should be noted that uncertainty of the cross sections is on average 0.5% even though we assumed 10% systematic uncertainty for the experimental data. This is also true even if we assumed different values.

The ^{13}C(α,n)^{16}O cross sections obtained are shown in Fig. 2. We successfully reproduced experimental data of total cross sections, however, present ^{13}C(α,n)^{16}O cross sections are systematically larger than the measured values of Harissopulos *et al.* by a factor of ~ 1.5. It is mainly due to the value of channel radius for the α+^{13}C system that changed from 4.92 fm (the initial value) to 5.20 fm. This value should be determined uniquely so as to be consistent with the total cross sections. Fig. 3 illustrates the obtained ^{16}O(n,α) cross section with uncertainty. Present uncertainty is on average 3% even though we assumed large systematic uncertainty of 50% for the experimental data on ^{13}C(α,n)^{16}O.

Due to the unitarity imposed on the all reaction channels considered, the systematic uncertainties in the experimental data tend to have small impact on our R-matrix