Excitation Functions for (n, p), (n, α) and (n, 2n)Reactions on Stable Bromine Isotopes up to 20 MeV

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Abstract-The excitation functions of (n,p), (n,α) and (n,2n) reactions for stable isotopes of bromine are calculated using EMPIRE-3.0 β 1 and TALYS-1.2 codes from threshold to 20 MeV within the framework of Hauser- Feshbach statistical model with preequilibrium effects. Recently, parity dependent nuclear level density (NLD) option has been incorporated in both codes. In the present work, the newly incorporated NLD option has been adopted for the calculations of the excitation functions for stable bromine isotopes. A reasonably good agreement between the calculated and experimental data validates the parity dependent NLD option in both codes.

Keywords- Excitation Function; Pre-Equilibrium Model; Compound Nucleus Model; Cross-Sections; Parity Dependent Nuclear Level Density

I. INTRODUCTION

Bromine isotopes are produced as fission products in the fast reactors and therefore precise knowledge of neutron cross section is quite essential in reactor technology. The present situation of (n, p), (n, α) and (n, 2n) reaction cross-section data on bromine isotopes from threshold to 20 MeV is still scanty and discrepant because of difficulty in preparing a monoenergetic neutron source for activation experiments in this energy region (except~ 14 MeV). Recently, Zhao et al. [1] measured these cross-sections with good accuracy by making use of HPGe detectors. However, no theoretical calculations were performed by them. At present, the theoretical understanding of nuclear reaction model is refined to the extent that with appropriate parameterization, nuclear models can be used to predict experimental data in energy region where data are not available or discrepant. In the present work, two recent and versatile nuclear reaction codes – EMPIRE-3.0 B1 (ARCOLE) given by Herman et al. [2] and TALYS-1.2 given by Koning et al. [3] – have been used to calculate (n,p), (n,α) and (n,2n) reactions cross sections for stable bromine isotopes from threshold to 20 MeV. In both codes, some of the input parameters used are different from the default parameters like nuclear level density option and pre-equilibrium models. The calculated values are compared with the existing experimental data (IAEA-EXFOR [4] database) as well as with evaluated data files (ENDF/B-VII.0 [5], JEFF-3.1 [6], JENDL-4.0 [7]). The main purpose of this work is to check the predictive power of nuclear model calculations on the excitation functions with parity dependent NLD option which is recently implemented in EMPIRE and TALYS codes; and to understand the equilibrium (CN) and pre-equilibrium (PE) components over the neutron energy from reaction threshold to 20 MeV.

II. NUCLEAR MODEL CALCULATIONS

TALYS and EMPIRE are computer code system for the prediction and analysis of nuclear reactions with two main purposes: firstly it can be used as a nuclear physics tool, confronting nuclear models with experiment; and secondly, as a nuclear data tool, predicting nuclear data where no experimental data exist. The theoretical calculations have been performed within the framework of Hauser-Feshbach statistical model with per-equilibrium effects by invoking suitable options in both codes. The required inputs like nuclear masses, discrete energy levels and level densities of the nuclides involved in the calculations have been taken from the latest RIPL-3 [8]. Both codes include various nuclear models, designed for calculations of cross-sections in a broad range of energies and incident particles.

Before running the EMPIRE and TALYS code, we have to optimize the input file. Nuclear level density, pre-equilibrium emission and optical model potential play an important role in determining the neutron induced reaction cross-sections. The optical potential for neutrons and protons used in both codes are the global parameterization of Koning and Delaroche [9]. For α - particle in the exit channel, optical model potential of Avrigeanu et al. [10] and Watanabe [11] have been used in EMPIRE and TALYS codes, respectively. The cross-sections are calculated by using full featured Hauser-Feshbach statistical model [12] with pre-equilibrium effects by invoking suitable options in both codes, i.e., DEGAS for exciton model of Betak and Oblozinsky, [13] for (n, p) (n,2n) reactions and PCROSS for cluster emission [14] for (n, α) reaction in EMPIRE code; Exciton Model given by Betak and Dobes [15] for (n, p) (n,2n) reactions and Kalbach systematic for cluster emission Kalbach [16] with the particle-hole state density has been adopted for (n, α) reactions in TALYS code. The nuclear structure inputs like nuclear masses, discrete energy levels and level densities of the nuclides involved in the calculations are taken from the latest compilation available in RIPL-3. In both codes, we have used the recent parity dependent NLD options in our calculations. In our earlier publication [17], we have studied the effect of different NLD (nuclear level density) options in predicting excitation functions of (n, p) reactions.

III. RESULTS AND DISCUSSIONS

The computed cross-sections based on EMPIRE and TALYS together with experimental data (EXFOR data library) and evaluated data files (ENDF/B-VII.0, JEFF-3.1, JENDL-4.0) for (n, p), (n, α) and (n, 2n) reactions on ⁷⁹Br and ⁸¹Br stable isotopes from threshold to 20 MeV are shown in Figs. 1-8. For all cases, microscopic parity dependent within the Hartee - Fock-Bogolyubov (HFB) plus combinatorial method has been used and pre-equilibrium effects have also been taken into account.

The excitation curves for ${}^{79}\text{Br}(n, p){}^{79\text{m}}\text{Se}$ based on both codes are given in Fig. 1. Few experimental data are available for this reaction. Our values do agree with the available experimental data measured with d-D neutron in the energy range of 2-6 MeV.



Fig. 1 Excitation function of ⁷⁹Br(n, p)^{79m}Se reaction calculated by EMPIRE-3.0 and TALYS-1.2 along with experimental data.





Fig. 2 Excitation function of ⁸¹Br(n, p)^{81g}Se reaction calculated by EMPIRE-3.0 and TALYS-1.2 along with experimental data

Fig. 3 Excitation function of ⁸¹Br(n, p)^{81m}Se reaction calculated by EMPIRE-3.0 and TALYS-1.2 alongwith experimental data. The dark solid line, short dashed line represents the total (CN+PE) and compound nucleus (CN) contributions, respectively by EMPIRE-3.0. Similarly light solid line, short dotted line represents the total (CN+PE) and compound nucleus (CN) contributions, respectively by TALYS-1.2

Our calculation with HFB parity dependent NLD option & pre-equilibrium effects does not match with the recent (Zhao et al.) values for 81 Br(n, p) ${}^{81g, m}$ Se [Figs. 2 and 3]. It is worth noting that ${}_{m}(7/2^{+})/{}_{g}(1/2^{-})$ must increases with E_{n} because with the increase of the neutron energy, higher angular moment start taking part, and the probability of population of a high spin state will be larger than that of a low spin state. However, the values reported by Zhao et al. are not in accordance with the present study results.

Zhao et al. detected 828.75 keV γ ray (I_{γ} = 0.28%) for determining ⁸¹Br(n, p)^{81g}Se reaction cross- section. However, metastable state of ⁸¹Se de-excites to the ground state by emitting gamma ray (E γ = 103.06, I γ = 13%).

The results of the calculation based on both codes for (n, α) , i.e., ⁷⁹Br $(n, \alpha)^{76}$ As, ⁸¹Br $(n, \alpha)^{78}$ Asreactions, are plotted in Figs. 4 and 5. It is evident that the evaluated data file results differ among themselves. In (n, α) , reaction pre-equilibrium plays a very important role as evident from the Figures. The values of cross-section become much higher when we take into account pre-equilibrium alpha particle emission by invoking Iwamoto-Harada models, i.e., PCROSS (which includes a pre-equilibrium mechanism for clusters in the incoming and outgoing channels) option in EMPIRE and Kalbach systematic for cluster emission which is based on the assumption of equidistant level spacing and is corrected for the effect of Pauli exclusion principle and for the finite depth of potential well in TALYS. The evaluated values of cross-sections are in reasonable agreement with the recent experimental values reported by Zhao et al.



Fig. 4 Excitation function of ⁷⁹Br(n,α)⁷⁶As reaction calculated by EMPIRE-3.0 and TALYS-1.2 along with experimental data



Fig. 5 Excitation function of 81 Br(n, α)⁷⁸As reaction calculated by EMPIRE-3.0 and TALYS-1.2 along with experimental data and evaluated data. The dark solid line, short dashed line represents the total (CN+PE) and compound nucleus (CN) contributions, respectively by EMPIRE-3.0. Similarly light solid line, short dotted line represents the total (CN+PE) and compound nucleus (CN) contributions, respectively by TALYS-1.2

For ⁷⁹Br(n, 2n)⁷⁸Br reactions (Fig. 6), most of the experimental data are between 13-15 MeV. Zhao et al. recently measured this cross-section at $E_n = 13.5$ MeV and 14.6 MeV. All other data files are close to each other. Our calculated values (based on EMPIRE and TALYS) are in good agreement with experimental data and evaluated data files.



Fig. 6 Excitation function of ⁷⁹Br(n, 2n)⁷⁸Br reaction calculated by EMPIRE-3.0 and TALYS-1.2 along with experimental data and evaluated data Similarly, our calculated values based on both codes do represent a general trend and support recent measurement of Zhao et al. for ⁸¹Br(n, 2n)^{80g}Br. It is interesting to note that the degree of matching between the theoretical and experimental values is improved when pre-equilibrium effects are taken into account because the pre-equilibrium process hardens the spectra of the first neutron leading to less excitation (as shown in Figs. 7 and 8) energy of CN for the emission of the second neutron and thus cross-section for (n, 2n) reaction is diminished.



Fig. 7 Excitation function of ⁸¹Br(n, 2n)^{80g}Br reaction calculated by EMPIRE-3.0 and TALYS-1.2 along with experimental data



Fig. 8 Excitation function of ⁸¹Br(n, 2n)^{80m}Br reaction calculated by EMPIRE-3.0 and TALYS-1.2 along with experimental data. The dark solid line, short dashed line represents the total (CN+PE) and compound nucleus (CN) contributions, respectively by EMPIRE-3.0. Similarly light solid line and short dotted line represent the total (CN+PE) and compound nucleus (CN) contributions, respectively by TALYS-1.2.

IV. CONCLUSIONS

The present work on the (n, p), (n, α) and (n, 2n) reaction cross-section for stable isotopes of Bromine is thus significant in the context of the scanty and /or discrepant nuclear data base available for these isotopes. The results of the present study reveal that parity dependent NLD option which has been incorporated in both codes recently, is quite suitable in predicting the cross-section for (n, p), (n, α) and (n, 2n) reaction in MeV region.

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