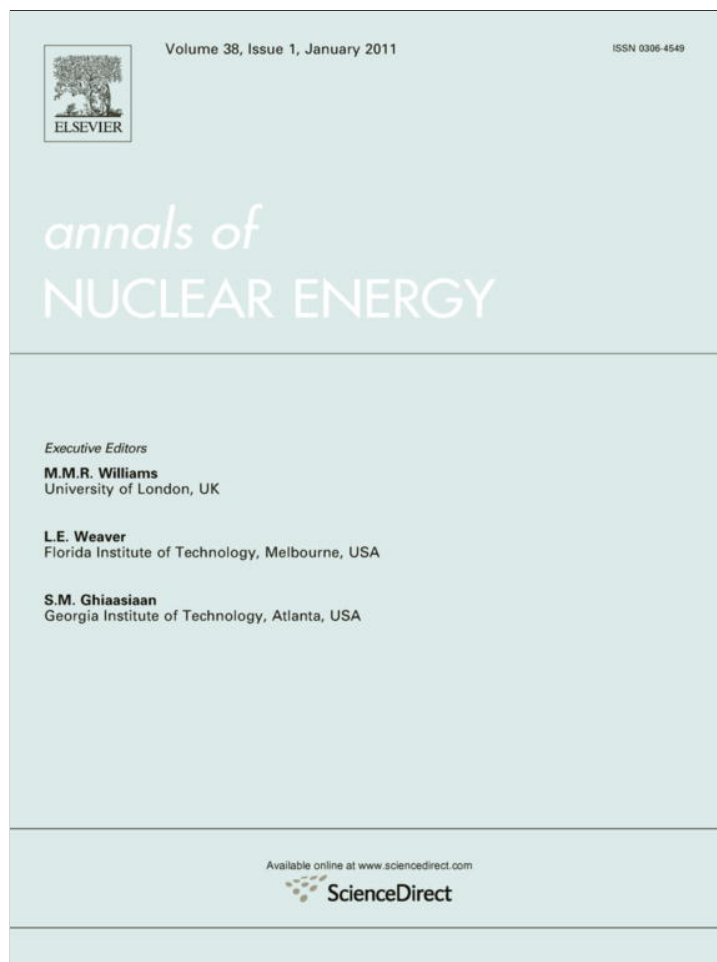


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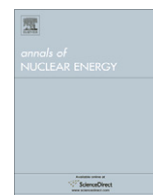
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Experimental determination of effective resonance energies for $^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$ and $^{179}\text{Hf}(n,\gamma)^{180\text{m}}\text{Hf}$ reactions

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ABSTRACT

The accuracy and precision of effective resonance energy \bar{E}_r parameter is an important point in the determination of the mass fraction of an analyte contained in the sample when NAA is used. Because the effective resonance energy \bar{E}_r is an essential parameter, which is directly introduced in the k_0 -NAA standardization method. Therefore, the effective resonance energies \bar{E}_r for the $^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$ and $^{179}\text{Hf}(n,\gamma)^{180\text{m}}\text{Hf}$ reactions were determined by cadmium ratio method using ^{55}Mn and ^{98}Mo monitors. The samples were irradiated in an isotropic neutron field of ^{241}Am -Be neutron sources. The induced activities for the radioisotopes were produced in the samples with and without a 1 mm-thick Cd shield and then measured with a p-type high pure Ge detector. The correction factors required for thermal neutron self-shielding (G_{th}) and resonance neutron self-shielding (G_{epi}) for the irradiated samples, and self absorption (F_s) and true coincidence summing (F_{coi}) effects for the measured γ -rays were taken into account. The experimental \bar{E}_r -values are found to be 49.6 ± 10.4 eV for ^{158}Gd and 17.0 ± 3.5 eV for ^{179}Hf target isotopes, respectively. The \bar{E}_r -values of ^{158}Gd and ^{179}Hf were also theoretically calculated by using the recent resonance data in the literature. Since the experimentally determined \bar{E}_r -values for the $^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$ and $^{179}\text{Hf}(n,\gamma)^{180\text{m}}\text{Hf}$ reactions are not available in literature, the present experimental results for the \bar{E}_r energies are thus compared with the present and earlier theoretical values, respectively. The presently measured \bar{E}_r value for ^{158}Gd is generally larger than those obtained \bar{E}_r values from theoretical approaches by ~ 9.1 – 16.9% . Whereas, the theoretically calculated \bar{E}_r -values for ^{179}Hf isotope deviated substantially from the presently measured value by ~ 16.9 – 37.6% . The reasons for this discrepancy are discussed in this paper.

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1. Introduction

Regarding the use of neutron capture (n,γ) reactions, one of the problems is that the users of tabulated nuclear data find the existence of discrepant values on the neutron induced reactions. These discrepant values constitute a serious drawback in connection with the choice of the “best” or more appropriate values (Segoiva et al., 2007). Some reasons for such discrepancies are: (1) use of non-consistent input data sets, (2) absence of updated input values, either related with the studied reactions or with those eventually used as standards, (3) overestimation or underestimation of the uncertainties associated to determinations, (4) incomplete information about specific convention adopted to describe the neutron flux, and (5) lack of adequate characterization of the neutron spectrum employed. In this context, the knowledge of the fundamental

nuclear parameters of Gadolinium (Gd) and Hafnium (Hf) elements are important nuclear materials, because these data are used in the radioisotope production and numerous studies related to the interaction of neutrons with matter.

Thus, Gd has exceptionally high neutron absorption cross section and therefore is used for shielding in neutron radiography and nuclear reactors. In addition, the nuclear data are important for examining the availability of Gd as a control material for fast reactors (Nishiyama et al., 2007). At present, the published experimental data are quite discrepant in different experiments, and they are not satisfactorily accurate and precise. Therefore, the new experimental data and theoretical predictions are required for the more accurate parameters and improvement of theoretical description of neutron capture reactions (Tan et al., 2004). It is also essential to produce complementary neutron-induced reaction data sets for an independent verification and to expand the boundaries of the data tables (Pritychenko et al., 2010). In addition, evaluations of nuclear-reactor system designs and fuel-cycle concepts also require neutron-capture cross sections of short-lived actinides (Scielzo et al., 2010). ^{159}Gd presents similar nuclear characteristics to ^{90}Y ,

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^{153}Sm and ^{131}I beta emitting radioisotopes, which are commonly used in medicine. Those radioisotopes with the short half-lives and high radiation dose rates have recently been used in lessening bone pain due to metastases and tumor therapy. For this reason, antitumor potential and structural characterization of ^{159}Gd is being investigated in these days, and it is reported that there is a high potential for the use of ^{159}Gd against tumor cells (Soares et al., 2010).

Similarly, Hf is one of the rare-earth isotopes with a relatively high neutron absorption cross-section in the thermal neutron energy region and is a useful absorbing material for making the control rods in thermal reactor (Nguyen et al., 2008; Shibata, 2010). The knowledge of thermal neutron cross-sections and resonance integrals of Hf is of great importance not only for design and development of nuclear reactor but also for the activation analysis and other applications concerning the interaction of neutrons with matter (Nguyen et al., 2008). In literature survey, it is seen that there are still very few measurements on the thermal neutron capture cross-sections and the resonance integrals for the particular $^{179}\text{Hf}(n,\gamma)^{180\text{m}}\text{Hf}$ reaction. Especially in the neutron epithermal energy range, the experimental works performed on natural and isotopic Hf samples are scarce. Furthermore, available data are rather old and the results given are often incomplete (Nogueira et al., 2009).

As well-known, the flux density in a thermal reactor or the moderated media from the other neutrons sources can be characterized by two components, thermal and epithermal neutron slowing down with an ideal $1/E$ distribution. Among several formalisms suggested to describe the reaction rates, a simple convention proposed by Høgdahl (1962) for $1/\nu$ nuclides is used for this purpose (El Abd, 2010):

$$R = R_{th} + R_e = G_{th}\phi_{th}\sigma_0 + G_e\phi_e I_0(\alpha)$$

where R_{th} ($=\phi_{th}\sigma_0$) is the reaction rate induced by pure thermal neutrons, R_e ($=\phi_e I_0(\alpha)$) is the reaction rate induced by epithermal neutrons, G_{th} and G_e thermal and epithermal neutron self-shielding factors, respectively. In fact, this Høgdahl formalism is valid and can also be readily used for the neutron source spectra such as (n,α) , (γ,n) radioactive sources or neutron generators even if the fast neutron spectrum of any neutron source is different from the reactor fission spectrum. Because, this formalism takes into account only two components of the moderated spectrum, i.e., the mixture of thermal and epithermal neutrons, it does not depend on the original source spectrum arising from either fission or other neutron sources. That is, it does not regard the negligible reaction rates due to fast neutron activation in the neutron field. On the other hand, basically, the k_0 -NAA method uses the concept of effective resonance energy \bar{E}_r to correct for the effect of non-ideality of the epithermal neutron flux distribution. In real neutron spectra, this behavior of the flux shape is often represented in energy range by $1/E^{1+\alpha}$ with an epithermal spectrum shape factor, α (De Corte, 2001). As well as the α -shape factor of the spectrum, the effective resonance energy (\bar{E}_r) parameter of the nuclide to be activated should be known as another essential parameter for the correction of resonance integral to thermal neutron cross section ratio, $Q_0(\alpha)$ ($=I_0(\alpha)/\sigma_0$) in a real $1/E^{1+\alpha}$ epithermal flux distribution (Moens et al., 1979; Nogueira et al., 2009). Therefore, in case of the use of inaccurate effective resonance energy (\bar{E}_r value it can give rise to more serious error on the analytical result because it is directly related to the $1/(\bar{E}_r)^\alpha$ in the $I_0(\alpha)$ definition (Simonits et al., 1984; Jovanovic et al., 1987).

In view of more accurate NAA analysis, the question arises whether the \bar{E}_r -values are susceptible to updates of experimental resonance data due to their dependencies on individual resonance energies and resonance widths. The extent of the experimental inconsistencies of \bar{E}_r -values, as well as the degree of inaccuracy

the resonance integral values require to carry out the experimental determinations on \bar{E}_r -values (Budak et al., 2008). In some cases, it is essential that the \bar{E}_r -value for an isotope should be experimentally determined when the theoretical resonance data for \bar{E}_r -values are still incomplete, obsolete, inaccurate or even not known at all (Simonits et al., 1984).

Therefore, the purpose of the present work is to determine the new experimental \bar{E}_r -values for the $^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$ and $^{179}\text{Hf}(n,\gamma)^{180\text{m}}\text{Hf}$ reactions by using reliable cadmium ratio method of which the detailed description was given in the previous studies (Budak et al., 2008; Budak et al., 2010). When the Cd-ratio method is used, the potential differences in the neutron spectrum between thermal and epithermal activation are greatly eliminated and thus resulting in more reliable and reproducible results for the \bar{E}_r -values, provided that same irradiation and counting conditions are applied to each measurement.

2. Experimental

The natural Gd element is a multi-isotopic element, which has several isotopes as ^{152}Gd (0.20%), ^{154}Gd (2.18%), ^{155}Gd (14.80%), ^{156}Gd (20.47%), ^{157}Gd (15.65%), ^{158}Gd (24.84%), and ^{160}Gd (21.86%) (Nudat, 2005). During neutron irradiation, apart from $^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$ capture reaction, the other formed radioisotopes (except ^{153}Gd) either remain stable or have a shorter half life, and they are not detected in conventional procedures (Soares et al., 2010). The natural Hf element consists of ^{174}Hf (0.16%), ^{176}Hf (5.26%), ^{177}Hf (18.60%), ^{178}Hf (27.28%), ^{179}Hf (13.62%), ^{180}Hf (35.08%) (Nudat, 2005). In these work, analytical grade natural samples of Gd and Hf was separately mixed with of Al_2O_3 powder in a higher percentage dilution in order to reduce to the neutron self-shielding effects in a large extent. Then, each of the mixtures of the samples ($\text{Gd}_2\text{O}_3 + \text{Al}_2\text{O}_3$ and $\text{HfO}_2 + \text{Al}_2\text{O}_3$) was filled in the 1 mm thick polystyrene tube of 13 mm in diameter and 6.25 mm in height. The percentages of dilution were experimentally determined in order to obtain optimum counting statistics in the measurements. Ten samples were prepared for each element. The percentage dilutions for reducing neutron self-shielding factors of the relevant samples are given in Table 1. The thermal and epithermal self-shielding factors (G_{th} and G_{epi}) for the powder mixtures filled in the polystyrene sample tubes, were calculated using the procedures for the case of the irradiations in an isotopic neutron field (Karadag et al., 2003; Karadag and Yücel, 2004, 2005). However, G_{th} and G_{epi} factors for Au and Mo-foils were calculated by the Nisle' approximation (Gilat and Gurfinkel, 1963). The required nuclear data (for instance, resonance parameters, absorption, scattering, total microscopic cross-sections, etc.) were taken from JENDL-3.3 (JENDL-3.3, 2002) and NUDAT (NuDat, 2005) online data libraries.

The irradiations were performed in isotropic neutron field, that was obtained from three ^{241}Am -Be neutron sources with having each activity of 592 GBq as described in a detail in earlier works (Karadag et al., 2003, 2007; Yücel and Karadag, 2004). The samples were irradiated in the same and fixed position of the used irradiation hole without and with 1 mm thick cylindrical Cd shield box to obtain Cd-ratio values. A set of five samples from 10 samples prepared for each element was irradiated for obtaining Cd covered-irradiation data. The remaining a set of five samples for each element was then irradiated for obtaining bare irradiation data that is not used Cd shield box. Additionally, the very thin foils of Au and Mo were also irradiated as monitor isotopes.

Some physical dimensions of the used detector-source geometry and its lead shield are given in this paper because an MCNP modeling of the counting geometry was also made for the estimation of self-absorption, F_s and true coincidence summing (TCS) corrections,

Table 1
Neutron self shielding factors for the used powder samples and foils.

Dilution of the irradiated samples	Target isotope (abundance, %)	Thermal neutron self-shielding factor including scattering ^a , G_{th}	Epithermal neutron self shielding factor ^b , G_{epi}
Al ₂ O ₃ –3.4%MnO ₂	⁵⁵ Mn (100%)	0.997	0.903
Al ₂ O ₃ –1.0%Gd ₂ O ₃	¹⁵⁸ Gd (24.84%)	0.833	0.999
Al ₂ O ₃ –1.0%HfO ₂	¹⁷⁹ Hf (13.62%)	0.998	0.947
Mo 0.025 mm-foil ^d	⁹⁸ Mo (24.13%)	0.999	0.992
Au 0.0005 mm-foil ^d	¹⁹⁷ Au (100%)	1.000	0.925 ^c

^a Calculated by Nisle' approximation, including neutron scattering effects (Gilat and Gurfinkel, 1963).

^b Calculated by approximation given in Beckurts and Wirtz (1964).

^c Technical Report No. 107 (IAEA, 1970).

^d No dilution in foils.

F_{coi} factors required for the relevant peaks. The used Ge crystal has a 82 mm diameter and a 85.5 mm length mounted in a 101.6 mm diameter Al-endcap. The detector was installed in a 10 cm thick Pb shield lined with a 1 mm thick Sn and 1.5 mm Cu thick (Canberra Model 767). The lead shield was also jacketed by a 9.5 mm steel outer housing.

The used detector is a p-type, coaxial high pure Ge detector (Canberra Model GC 11021) with a measured relative efficiency of 120.8%, an energy resolution of 1.95 keV, and a peak-to-Compton ratio of 85.7:1 at 1332.5 keV of ⁶⁰Co. It was connected to a digital spectrum analyzer (Canberra DSA-1000) with a full featured 16 K ADC/MCA analyzer, based on digital signal processing operating through a Genie-2000 gamma spectroscopy software.

The irradiated samples were counted at a distance of 10 cm from the detector in order to keep possible true coincidence (TCS) effects at a reasonably low level although the Cd-ratios cancel out the true coincidence effects on the peak areas resulting in specific activities (Yücel et al., 2007). The chosen counting periods were high enough to ensure good statistical quality of data. Background measurements were subtracted from the sample spectra. For the measurement of the activities produced in the samples, the suitable waiting times were employed, thus minimizing both dead time and pulse piling-up losses and also eliminating the possible contributions from the interfering 843.74 keV (71.8%) γ -ray emitted from ²⁷Mg (9.458 min) to the 846.77 keV (98.9%) analytical peak of ⁵⁶Mn (2.5785 h).

For the characterization of thermal flux, thermal to epithermal ratio factor (f) of the neutron irradiator unit, it was required to obtain a full-energy efficiency calibration of the Ge detector as a function of energy. To do this, the multi-nuclide standard source was used in which ²⁴¹Am, ¹⁰⁹Cd, ⁵⁷Co, ^{123m}Te, ⁵¹Cr, ¹¹³Sn, ⁸⁵Sr, ¹³⁷Cs, ⁶⁰Co and ⁸⁸Y radio nuclides spiked in the sand matrix (SiO₂, density: 1.7 ± 0.1 g cm⁻³), purchased from Isotope Products Laboratories Inc., traceable to NIST. The full-energy peak efficiencies were measured and calculated for a small cylinder tube placed at a 10 cm distance far from a 120.8% relative efficient Ge detector. In the full-energy peak efficiency calibration, the main uncertainty sources are 1.5–2% due to source activities, 0.1–1.2% due counting statistics, 0.1–1.2 due to γ -ray emission probabilities, and <1% due to systematically nature (type B uncertainties). Thus the efficiency data were fitted to a logarithmic polynomial function such as $\varepsilon = \exp(a + b \cdot \ln E + c \cdot \ln^2 E + d \cdot \ln^3 E)$ where the coefficients are found to be $a = -1.918828$, $b = 5.037222$, $c = 3.444946$, $d = 0.698902$ in the low energy region of 59–159 keV, and $a = -5.010486$, $b = -0.636695$, $c = 0.000219$, $d = 0.022974$ in the high energy region of 159–1836 keV. The MCNP calculated efficiency data were also obtained from GESPECOR Ver. 4.2 program in which both F_{coi} and F_s factors were taken into account, where F_{coi} factors calculated for a 1 mm-thick polystyrene cylinder tube of 13 mm diameter and 6.25 mm height, placed at a 10 cm distance from the 120.8% relative efficient Ge detector, and F_s factors were

estimated for the same tube geometry for SiO₂ matrix spiked with nuclides.

3. Data analysis

3.1. Experimentally determined \bar{E}_r value

The \bar{E}_r -value for the isotope is taken as an effective or average value of the energy of a single virtual resonance estimated from all the resonances of the isotope in the epithermal spectrum region. That is, a single virtual energy \bar{E}_r value has an importance because it replaces all the resonance energies lying in epithermal region, which is described by a modified $1/E^{1+\alpha}$ behavior as in Högdahl formalism (De Corte et al., 1986). However, it should be noted that the \bar{E}_r -value is very sensitive to the accuracy of the $Q_0(\alpha)$ value for the monitor used, while applying the single comparator method in the thermal activation analysis (Verheijke, 2000).

Although it is not possible to avoid entirely the error in the \bar{E}_r -value to be measured for the isotope due to an uncertainty in the $Q_0(\alpha)$ value of the monitor. Nevertheless, this can be adjusted in the determination of \bar{E}_r -values by choosing the appropriate $\bar{E}_{r,c}$ monitor isotopes whose $Q_0(\alpha)$ values and other parameters are known more accurately and even closeness to the values of the isotopes to be measured. Accordingly, ⁵⁵Mn and ⁹⁸Mo target isotopes having favorable nuclear properties were chosen as the $\bar{E}_{r,c}$ monitor in the present work. As previously described in a more detail (Yücel et al., 2007; Budak et al., 2008), these monitor isotopes have good $1/\nu$ -behaviors with Westcott-factors, $g(20^\circ\text{C}) \approx 1$ and moderate values for 2200 m s^{-1} thermal neutron cross section and resonance integral values to minimize burn-up of atoms, especially in high flux irradiations. In addition, most of the resonance captures of ⁵⁵Mn and ⁹⁸Mo occurs at a relatively higher neutron energy region, for example, the first principal resonance of ⁵⁵Mn is seen at 337 eV and that of ⁹⁸Mo is at 468 eV (JENDL 3.3., 2002), which are quite far from $1/\nu$ region, thus making their well-established effective resonance energies, as given in Table 2. In order to determine effective resonance energy for the neutron capture (n,γ) reactions of the target isotopes by the activation method using Cd-ratios of the isotopes, the description of data analysis is given briefly as follows:

As well known, the ideal $1/E$ epithermal neutron spectrum, the resonance integral cross section, I_0 , including $1/\nu$ tail of thermal neutron spectrum defined in the literature (De Corte et al., 1981) is not valid in a non-ideal, real epithermal neutron spectrum and that such a deviating epithermal neutron flux distribution can be approximated by $\Phi(E) = 1/E^{1+\alpha}$. Accordingly, a resonance integral $I_0(\alpha)$ for a real epithermal neutron spectrum characterized by α -shape factor (De Corte et al., 1979). The effective resonance energy, \bar{E}_r value as the basis firstly defined by Ryves (1969) can be estimated by the following equation (De Corte et al., 1979; Simonits et al., 1984; De Wispelaere and De Corte, 2003).

$$\frac{\ln Q_0 - 0.429}{\frac{f \cdot G_{th}}{G_{epi}(F_{Cd} R_{Cd} - 1)} - \frac{0.429}{(2\alpha + 1)E_{Cd}^2}} = \alpha \cdot \ln \bar{E}_r \quad (1)$$

In Eq. (1) above, α parameter exists in both sides of the equation. It can therefore be initially set to zero, followed by an iterative procedure until it converges to a constant value (Rajput et al., 2003; Dung and Cho, 2003). As previously shown (Budak et al., 2010), the α -shape factor was determined by using the measured Cd-ratios of monitor isotopes ^{55}Mn and ^{98}Mo , because their $Q_0(\alpha)$, \bar{E}_r -values and other essential parameters are known accurately. Thus, the extent of non-ideality of epithermal flux shape, i.e., the α -shape factor at the present sample irradiation position was determined to be $\alpha = 0.0828 \pm 0.0097$ and it was used for all irradiations.

For the determination of effective resonance energy, Eq. (1) can be written in turn for the investigated isotope (\bar{E}_r) and the chosen monitor isotopes ($\bar{E}_{r,c}$) as follows (Jovanovic et al., 1984, 1985):

$$\bar{E}_r = \left\{ (Q_0 - 0.429) / \left(\frac{f G_{th}}{(F_{Cd} R_{Cd} - 1) G_{epi}} - C_\alpha \right) \right\}^{1/\alpha} \quad (2)$$

where

$$C_\alpha = 0.429 / [(2\alpha + 1)E_{Cd}^2] \quad \text{and} \quad 0.429 = 2\sqrt{E_0/E_{Cd}}$$

where $E_0 = 0.0253$ eV and $E_{Cd} = 0.55$ eV are taken. As well-known, the division between the thermal and epithermal part of the spectrum is arbitrary and the so-called Cd cut-off energy for a 1 mm thick Cd cover, which is internationally accepted as $E_{Cd} = 0.55$ eV in Høgdahl convention in which for a small sample in a 1 mm thick Cd box, the Eq. (2) is only valid for the case of $E_{Cd} = 0.55$ eV in a non-ideal $1/E^{1+\alpha}$ epithermal distribution.

The effective resonance energy for the investigated isotope can easily be determined from the ratio of $\bar{E}_r/\bar{E}_{r,c}$ by taking into account the necessary correction factors such as neutron self-shielding factors, G_{th} and G_{epi} for both monitor (c) and investigated isotope (Jovanovic et al., 1985; Budak et al., 2008).

The Cd-ratio $R_{Cd} = A_{sp}/A_{sp}^+$ can easily be calculated from the measured specific activities of the isotope, by the following:

$$A_{sp}^- = \{N_p / (wSDCt_m)\}_{bare} \quad \text{and} \quad A_{sp}^+ = \{N_p / (wSDCt_m)\}_{Cd} \quad (3)$$

where A_{sp}^- and A_{sp}^+ are specific activities obtained after a bare and Cd-covered isotope irradiation; N_p is net number of counts under the full-energy peak collected during measuring (live) time, t_m ; w is mass of irradiated element; $S = 1 - e^{-\lambda t_{irr}}$ is saturation factor with $\lambda =$ decay constant, t_{irr} is irradiation time; $D = e^{-\lambda t_d}$ is decay factor with $t_d =$ decay time; $C = [1 - \exp(-\lambda t_r)] / \lambda t_r$ is measurement factor correcting for decay during the true time, t_r for a measurement. As seen in Table 2, cadmium transmission factors F_{Cd} for epithermal neutrons for the isotopes of interest, according to the definition of $E_{Cd} = 0.55$ eV are taken as unity but may be different from unity for some isotopes (El Nimr et al., 1981). Nuclear decay data used for the investigated isotopes, self attenuation and true coincidence summing correction factors for the measured gamma-rays are given in Table 3.

The equivalent 2200 m s^{-1} thermal and epithermal neutron fluxes at the sample irradiation position of the ^{241}Am -Be neutron irradiator were measured to be $\phi_{th} = (1.5 \pm 0.2) \times 10^4$ and $\phi_{epi} = (1.4 \pm 0.1) \times 10^3 \text{ n cm}^{-2} \text{ s}^{-1}$, respectively. The thermal to epithermal neutron flux ratio at the same position was determined to be $f = 10.42 \pm 0.31$ using ^{197}Au monitor (Yücel and Karadag, 2004). Additionally, the approaches required for the calculation of theoretical \bar{E}_r -value are briefly described in the following section to save space it, and the detailed descriptions are referred to the References (Moens et al., 1979; Jovanovic et al. 1987; Postma et al., 2001; Budak et al., 2008, 2010).

3.2. Calculation of theoretical \bar{E}_r -value

In neutron activation of the materials, the occurrence of “resonances” in total and capture cross sections in the epithermal energy range depends on strongly the neutron energy. Therefore, for the aspect of the effective resonance energy of an isotope, it can usually be utilized by the following approximate expressions. One can write:

$$\ln \bar{E}_r = \frac{\sum_i (\sigma_i \Gamma_{\gamma,i} \ln E_{r,i} / E_{r,i})}{\sum_i (\sigma_i \Gamma_{\gamma,i} / E_{r,i})} \quad (4)$$

where σ_i is partial capture cross-section \bar{E}_r is the i th resonance energy and $\Gamma_{\gamma,i}$ is the radiative width at the maximum of the i th resonance energy. It is assumed in Eq. (4) that resonance self-shielding is negligible, which certainly is the case when using sufficiently diluted samples. The latest resonance data is taken from JENDL 3.3. and JEFF 3.1., General Purpose Neutron File OECD-NEA Evaluated Data Library is used in this study. This called here the first approach and it was first used by Moens et al. (1979), but in which the neutron widths Γ_n values are neglected in Eq (4).

The second approach suggested by Jovanovic et al. (1987) is that \bar{E}_r -value can also to a good approximation be calculated by assuming its α -independence according to the term $(1\text{eV})^\alpha \equiv 1$ that are omitted.

$$\ln \bar{E}_r = \frac{\sum_i w_i \ln E_{r,i}}{\sum_i w_i} \quad (5)$$

where the weighting factor w_i is given by

$$W_i = (g \Gamma_\gamma \Gamma_n / \Gamma)_i \cdot (1/E_{r,i}^2) \quad (6)$$

where $g = (2J + 1)/2(2I + 1)$ is the statistical weight factor being I and J the spin of the target nucleus and the resonance state of the neutron captured compound nucleus, Γ_γ is the radiative width, Γ_n is the neutron width, and $\Gamma = \Gamma_\gamma + \Gamma_n$ is the total width of resonance. For the theoretical evaluation of \bar{E}_r -values via Eq. (5), the newest resonance data are taken from the available recent literature (JENDL 3.3., 2002; JEFF 3.1, 2005; ENDF/B VII.0; Mughabghab, 1984, 2006).

4. Results and discussion

The experimentally determined \bar{E}_r -values for the ^{158}Gd (n,γ) ^{159}Gd and $^{179}\text{Hf}(n,\gamma)^{180\text{m}}\text{Hf}$ reactions are given in Table 4, where the experimental results for \bar{E}_r -values for the investigated isotopes were obtained by using \bar{E}_r -values of ^{55}Mn and of ^{98}Mo monitor isotopes. It is obvious that the range of \bar{E}_r -values for the investigated isotopes of ^{158}Gd and ^{179}Hf has a good consistency between the results obtained by ^{55}Mn and ^{98}Mo , respectively. As mentioned above, both of ^{55}Mn and ^{98}Mo are suitable resonance monitors and their resonance energy range covers a wide energy range for the resonance regions of approximately between 50 and 100,00 eV. Besides this main feature, the present monitor isotopes lead to more accurate results for \bar{E}_r -values because the relevant cross sections and decay properties used in the experimental evaluation are known accurately and precisely for the monitor isotopes (^{55}Mn and ^{98}Mo). Thus this also allows us for checking the possible differences in the measured results for the \bar{E}_r -values for the $^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$ and $^{179}\text{Hf}(n,\gamma)^{180\text{m}}\text{Hf}$ reactions while using the Cd-ratios of these dual monitors (^{55}Mn and ^{98}Mo) as seen in Table 4.

The main sources of uncertainty in the experimentally determined \bar{E}_r -values given in Table 4 are mainly due to the α -shape factor (11.7%), the monitor effective resonance energy values (10.9% for ^{55}Mn and 19.9% for ^{98}Mo), and the resonance integral to thermal neutron cross section ratio, Q_0 (within range of ≈ 2.6 –6.3%).

Table 2
Nuclear data for the reactions of the monitors and investigated target isotopes.

Nuclear reaction used	Cadmium transmission factor ^{a,d,e} , F_{Cd}	Effective resonance energy ^b , \bar{E}_r (eV)	Resonance integral to thermal cross section ratio ^b , Q_0	Half-life ^c
$^{55}\text{Mn}(n,\gamma)^{56}\text{Mn}$	1.000	468 ± 51	1.053(2.6%)	2.5789(1) h
$^{98}\text{Mo}(n,\gamma)^{99}\text{Mo}(\beta^-)^{99\text{m}}\text{Tc}$	1.000	241 ± 48	53.1(6.3%)	65.94(1) h
$^{197}\text{Au}(n,\gamma)^{198}\text{Au}$	0.991	5.65 ± 0.40	15.7(1.8%)	2.695(21) d
$^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$	1.000	Studied reaction	29.9(3.1%)	18.479(4) h
$^{179}\text{Hf}(n,\gamma)^{180\text{m1}}\text{Hf}$	1.000	Studied reaction	14.4(2.4%)	5.5(1) h

^a El Nimr et al. (1981).
^b $Q_0 = I_0/\sigma_0$ with the percent standard uncertainty, s (%) (Kolotov and De Corte, 2003).
^c NNDC NuDat 2.5 database (NUDAT, 2005).
^d El Nimr and Ela-Assaly (1987).
^e El Nimr (1990).

Table 3
Self attenuation and true coincidence summing correction factors, and decay data for measured gamma-rays of interest.

Nuclear reaction	The measured gamma-ray ^a		Self absorption factor ^b		True Coincidence Summing Correction Factor ^c	Notes
	Energy (keV)	Emission probability, γ (%)	F_s (based on NIST)	F_s (based on GESPECOR)		
$^{55}\text{Mn}(n,\gamma)^{56}\text{Mn}$	846.754(20)	98.9(3)	1.0104	1.0146	0.9921	For monitor radioisotope
$^{98}\text{Mo}(n,\gamma)^{99}\text{Mo}(\beta^-)^{99\text{m}}\text{Tc}$	140.511(1)	4.52(24)	1.0062	1.0047	0.9988	$A_{sp}(\text{Mo})/A_{sp}(\text{Mo} + \text{Tc}) = 0.05992^d$ where A_{sp} is specific activities of isotope
$^{197}\text{Au}(n,\gamma)^{198}\text{Au}$	411.802(17)	95.58	1.0001	1.0019	0.9998	– For monitor radioisotope
$^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$	363.5430(18)	11.78	1.0223	1.0174	1.0000	– For radioisotope to be measured
$^{179}\text{Hf}(n,\gamma)^{180\text{m1}}\text{Hf}$	93.325(12)	17.1(3)	1.0242	1.0278	0.3046	– For radioisotope to be measured
	215.426(8)	81.3(10)	1.0272	1.0171	0.4674	
	332.275(11)	94.1(12)	1.0284	1.0142	0.4677	
	443.163(15)	81.9(12)	1.0290	1.0130	0.4698	
	500.697(13)	14.3(3)	1.0292	1.0120	0.6979	

^a NNDC NuDat 2.5 Database (NUDAT, 2005).
^b Gamma-ray self attenuation factors calculated using mass attenuation coefficients that were taken from NIST and KORDATEN Databases, respectively.
^c True coincidence summing correction factors calculated by GESPECOR Ver 4.2 software using a MCNP modeling of the present detector-source geometry.
^d Since beta branching ratio is 84.7%, the factor 0.05992 is calculated simply by $0.05992 = [0.0452/(0.8906 \times 0.847)]$ (Simonits et al., 1981).

All uncertainties are given within $\pm 1\sigma$ confidence interval. As the measurement uncertainties on the Cd-ratios are determined from the specific activities, they are generally found to be less than 2.5%. However, it is not possible to reduce the overall uncertainty of about 21% on the final results for \bar{E}_r -values of the isotopes being investigated since the magnitudes of uncertainties on the nuclear data propagated in Eq. (2). But, this argument was noted previously by Simonits et al. (1984) that about 20% uncertainty on any \bar{E}_r -value can be acceptable when it was obtained by Cd-ratio method, owing to the large uncertainty reduction in the conversion of Q_0 into $Q_0(\alpha)$.

The experimentally determined \bar{E}_r -values for the ^{158}Gd and ^{179}Hf isotopes do not appear in literature at all. Therefore, the present experimental results are compared only with the present and earlier calculated \bar{E}_r -values by using two different approaches mentioned above. Thus, the present experimental results for the \bar{E}_r -values are given in Table 5, together with the presently calculated theoretical values and old theoretical ones for \bar{E}_r -effective energies for the ^{158}Gd and ^{179}Hf isotopes.

When using the newest resonance data, the present experimental values are generally agreed with the calculated ones for \bar{E}_r -effective energies for the ^{158}Gd and ^{179}Hf isotopes within limits of the estimated uncertainty. However, the theoretical results for the \bar{E}_r -values obtained by the first approach, which suggested by

Moens et al. (1979) are not satisfactorily accurate even if the newest and most accurate neutron resonance data available in literature are used in Eq. (4). Because this Moens' approach seems to be more obsolete due to neglecting neutron widths Γ_n . Whereas the Γ_n widths of the resonances vary in the range of $\approx 10^{-3}$ to 10 eV, and they should be accounted for the \bar{E}_r -value calculation. On the other hand, the radiative gamma-ray widths Γ_γ are taken into account in Eq. (4) although they vary within the narrower energy range of ≈ 0.1 –1 eV, and are fairly constant, within one isotope, because of many γ -ray exit channels (Postma et al., 2001). Additionally, since there is no evidence that the \bar{E}_r value is dependent on the α -shape factor over the resonances (De Wispelaere and De Corte, 2003), the expanding of $\bar{E}_r^{-\alpha}$ factors in series should not be ignored for higher order terms for \bar{E}_r and α -values in the integrated Breit-Wigner expressions for all resonances as given by Moens et al. (1979) in the first approach.

As seen in Table 5, theoretically calculated \bar{E}_r values are estimated to be 41.2 eV and 45.1 eV for $^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$ reaction and they are smaller than that experimentally determined one by 9.1–16.9% for ^{158}Gd when considering two different theoretical approaches above. In case of $^{179}\text{Hf}(n,\gamma)^{180\text{m1}}\text{Hf}$ reaction, the theoretically calculated \bar{E}_r -value of 10.6 eV from the first approach (Moens' approach) deviates substantially from the measured value by about 37.6%, whereas the theoretical \bar{E}_r -value of 17.5 eV

Table 4Weighted averages of experimental effective resonance energy values for $^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$ $^{179}\text{Hf}(n,\gamma)^{180\text{m}1}\text{Hf}$ reactions.

Nuclear reactions investigated	Measured effective resonance energy values		
	Using ^{55}Mn monitor, \bar{E}_r (eV)	Using ^{98}Mo monitor, \bar{E}_r (eV)	Weighted average values for effective resonance energy, \bar{E}_r (eV)
$^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$	49.30 ± 13.5	50.00 ± 16.2	49.6 ± 10.4
$^{179}\text{Hf}(n,\gamma)^{180\text{m}1}\text{Hf}$	16.93 ± 4.64	17.17 ± 5.60	17.0 ± 3.5

Table 5Experimentally and theoretically determined effective resonance energy \bar{E}_r values for ^{158}Gd and ^{179}Hf isotopes.

Reaction	Experimentally determined effective resonance energy values Present work ^g (measured) \bar{E}_r (eV)	Theoretically calculated effective resonance energy values							
		Present work ^c [from Eq. (4)] ^a		Present work ^c [from Eq. (5)] ^d		Literature [from Eq. (4)] ^e		Literature [from Eq. (5)] ^f	
		\bar{E}_r (eV)	Deviation (%) ^b	\bar{E}_r (eV)	Deviation (%) ^b	\bar{E}_r (eV)	Deviation (%) ^b	\bar{E}_r (eV)	Deviation (%) ^b
$^{158}\text{Gd}(n,\gamma)^{159}\text{Gd}$	49.6 ± 10.4	41.2	−16.9	45.1	−9.1	45.4	−8.5	48.2 ± 3.9	−2.8
$^{179}\text{Hf}(n,\gamma)^{180\text{m}1}\text{Hf}$	17.0 ± 3.5	10.6	−37.6	17.5	2.9	–	–	16.2 ± 1.9	−4.7

^a Calculated by Eq. (4) based on the first approach (Moens et al., 1979) using newest resonance data taken from JENDL 3.3 and JEFF 3.1 data libraries.^b The percentage deviation calculated as $100 \times (\text{calculated value/experimental value} - 1)$.^c Uncertainties are not given here because no uncertainty quoted in the literature data.^d Calculated by the second approach (Jovanovic et al., 1987) based on Eq. (5), using newest resonance data taken from JENDL 3.3 and JEFF 3.1 data libraries.^e Referenced by Moens et al. (1979).^f Referenced by Jovanovic et al. (1987).^g These weighted average values are already given in Table 4.

obtained from the second Jovanovic's approach agrees very well with the experimentally determined value. The present experimental weighted average \bar{E}_r -value of 17.0 ± 3.5 eV for $^{179}\text{Hf}(n,\gamma)^{180\text{m}1}\text{Hf}$ reaction agrees with the theoretical ones calculated from the Jovanovic's approach within limits of the estimated uncertainty.

5. Conclusion

There are not available experimentally determined \bar{E}_r -values for ^{158}Gd and ^{179}Hf isotopes in survey of the literature. Hence, the present experimental \bar{E}_r -values can be used for the comparison of theoretically calculated \bar{E}_r -values for the isotopes. This also would be helpful to understand the present discrepancies in the \bar{E}_r -values determined by using the recent resonance parameter data.

This study also implies that the new resonance monitors such as ^{55}Mn and ^{98}Mo having well-known \bar{E}_r -values should be used while determining experimental \bar{E}_r -values for a variety of the isotopes. In the case of very discrepant theoretical \bar{E}_r -values, it might essentially be considered that the discrepancies between the old calculated \bar{E}_r -values and the recent ones for the \bar{E}_r -values of the isotopes are due to mostly older resonance data. This is an important point because the quantity and quality of the available resonance parameters' data are continuously improved and updated in the reliable databases. However, the second interesting point is that there is a consistency between the two known theoretical approaches used in the determination of \bar{E}_r -values.

Therefore, in practice, the experimentally determined \bar{E}_r -values might be preferred mostly in the analyses, for example, in k_0 -NAA standard method rather than use of their theoretically determined \bar{E}_r -values. If the experimental \bar{E}_r -values for the isotopes of interest are not available, it is suggested that the theoretical \bar{E}_r -values calculated from Jovanovic's approach seems to be more reasonable provided that using the recent resonance parameter data since the quantity and quality of the available data in the present literature improve continuously.

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