Light Nuclei Evaluation by Resonance Neutron Reactions

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**ABSTRACT**

It is well known that for light nuclei, by slow neutron capture, radionuclides are not produced and therefore their determination by INAA is not possible. Then for evaluation of their properties, it could be better to combine a few neutron reactions in neutron transmission experiments (methods), depending on the value of the cross-sections of selected types of reactions. One S-resonance was considered from each element in the sample composed of only five medium and heavy elements and one trace light element. Results on ⁶Li and ¹⁰B nuclei are presented and they demonstrate that the missing of one type of measurement technique could lead to errors in the data processing. Both nuclei have a very low value of capture cross-section and a very high value of (n, α) cross-section. Due to the positions of S-resonances and their reduced neutron widths, these light nuclei influence significantly the spectra and furthermore, the order of measurements can also be important.

1. Introduction

Among the nuclear analytical methods developed in the last century (such as IPAA, PGAA, PIXE, RBS, XRF, and others) instrumental neutron activation analysis (INAA) remains the most significant one. By INAA methods in a nondestructive manner, with high sensitivity and negligible matrix effects, it is possible to determine more than 75 elements for a wide range of applications in the field of technological processes, geology, medicine, environment, and life sciences, etc. (Corte & Simonits, 1989), (Sterba et al., 2008), (Verma, 2007). One of the INAA limitations consists in the determination of light elements (such as H, He, Li, Be, B, C, N, O, and Ne) because their thermal capture cross-sections are very small (Mughabghab, 2003). On the other hand, these elements could be evaluated by alternative methods, as for example, Prompt Gamma Activation Analysis (PGAA) (Révay, 2001).

In the interaction of slow neutrons with nuclei resonant state or compound nucleus states are formed. After, the compound nucleus is decaying on possible channels. For slow neutrons, these channels usually are: elastic, inelastic, capture, proton, alpha, and with less probability other channels. The presence of resonance states in neutron reactions, allows one to use other methods different from INAA based on neutron resonance analysis and transmission of the...
neutrons (Jeong-Yeon et al., 2011), (Leinweber et al., 2006). The neutron capture method can be applied very well in the case of medium and heavy nuclei due to the presence of enough number of resonances. For light nuclei, the situation is changing because the first resonant states occur from tens or hundreds of keV and for many open exit channels like capture, proton, alpha, and others the cross-sections are very low. But some light nuclei have a very high value of \( (n, \alpha) \) cross-section in comparison with other channels, which make them possible to be observed in transmission measurements (Mughabghab, 2003).

In the present study, we realized a Direct Monte Carlo simulation for the evaluation of the concentration and other properties of light nuclei from some samples, consisting of a succession of capture and total cross-section measurements in neutron resonance analysis (NRA) experiments. We have computed and analyzed the cases when a sample contains light elements (as \(^6\)Li and \(^{10}\)B) in the matrix of some medium and heavy nuclei. The \(^6\)Li and \(^{10}\)B nuclei, for thermal neutrons, have a very high value of \( (n, \alpha) \) cross-section and a very small capture cross-section (Mughabghab, 2003), (Brusegan, 2004). The present computer evaluation is a proposal for experiments on light nuclei data evaluation to the IREN - the new pulsed resonance neutron source from the FLNP.

2. Methods

Some important parameters relevant for the present research are the natural abundances of light nuclei and their neutron reaction \( Q \) – values (Table 1). Looking at the given nuclear data it is obvious that for slow and resonance neutrons there are not so many open channels for almost all light nuclei (Rosman & Taylor, 1999), (\( Q \)-value Calculator\(^1 \)). Table 1 suggests the possible nuclei and the corresponding nuclear reactions for analysis and they are: \(^6\)Li, \(^{10}\)B, \(^{17}\)O, and \(^{21}\)Ne in \( (n, \alpha) \) reaction and \(^{14}\)N in \( (n, p) \) reaction. The cross-sections of the \(^{17}\)O\((n, \alpha)\), \(^{21}\)Ne\((n, \alpha)\) and \(^{14}\)N\((n, p)\) are of order of 1 barn or lower and in relation with the low value of capture cross-section and the number of resonances in the used energy interval (up to 16 keV) make these nuclei not enough applicable for the type of analysis proposed. It is necessary to take into account other properties of the \(^{14}\)N, \(^{17}\)O, and \(^{21}\)Ne (Brusegan, 2004). As can be seen in Table 1 \(^6\)Li and \(^{10}\)B have a very high value of \( (n, \alpha) \) cross-section and very low value of capture cross-section and they are suitable for NRA. Table 1 and reference (Brusegan, 2004) suggest that by a combination of capture and transmission NRA methods \(^6\)Li and \(^{10}\)B nuclei could be precisely identified and evaluated.

Other nuclei in Table 1 have negative \( Q \)-values. Therefore, their presence can be evaluated with high energy neutrons overloading the reaction threshold. In this case, it is necessary to have intense high energy neutron sources and to prepare new types of neutron experiments. Many of these nuclei have relatively high value of nonresonant scattering cross section of order of ten barns. Nonresonant scattering cross-section is practically constant in a wide energy range and in a real experiment it acts like a background usually separated by some filters (Brusegan, 2004).

\(^1\) Available: http://www.nndc.bnl.gov/qcalc
Table 1.
Natural abundance and $Q$ neutron reactions for light nuclei

<table>
<thead>
<tr>
<th>Element</th>
<th>Nat. ab. (%)</th>
<th>$Q_p$ (keV)</th>
<th>$Q_s$ (keV)</th>
<th>$Q_{\gamma}$ (keV)</th>
<th>$Q_{\text{tot}}$ (keV)</th>
<th>$Q_\alpha$ (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^3$He</td>
<td>0.000137</td>
<td>763.7549</td>
<td>-3268.914</td>
<td>763.7568</td>
<td>0</td>
<td>20577.6</td>
</tr>
<tr>
<td>$^4$He</td>
<td>99.999863</td>
<td>-22694</td>
<td>-17589.293</td>
<td>-17589.295</td>
<td>-</td>
<td>0</td>
</tr>
<tr>
<td>$^4$Li</td>
<td>7.53</td>
<td>-2725.967</td>
<td>-2363.8</td>
<td>4783.385</td>
<td>-18675</td>
<td>4783.39</td>
</tr>
<tr>
<td>$^7$Li</td>
<td>92.41</td>
<td>10410.6</td>
<td>-7751.375</td>
<td>-3356.6</td>
<td>-24844</td>
<td>-5347</td>
</tr>
<tr>
<td>$^9$Be</td>
<td>100</td>
<td>-12824.27</td>
<td>-14663.6</td>
<td>-10438.984</td>
<td>-21613.3</td>
<td>-601.06</td>
</tr>
<tr>
<td>$^{10}$B</td>
<td>19.9</td>
<td>226.408</td>
<td>-4361.324</td>
<td>230.564</td>
<td>-15756</td>
<td>2788.99</td>
</tr>
<tr>
<td>$^{11}$B</td>
<td>80.1</td>
<td>-10723.79</td>
<td>-9003.145</td>
<td>-9558.205</td>
<td>-23146.23</td>
<td>-6632.51</td>
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<tr>
<td>$^{12}$C</td>
<td>98.93</td>
<td>-12586.55</td>
<td>-13732.334</td>
<td>-18929.225</td>
<td>-19466.566</td>
<td>-5701.25</td>
</tr>
<tr>
<td>$^{13}$C</td>
<td>1.07</td>
<td>-12654.81</td>
<td>-15308.29</td>
<td>-1241.404</td>
<td>-23908.95</td>
<td>-3835.26</td>
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<tr>
<td>$^{14}$N</td>
<td>99.632</td>
<td>625.876</td>
<td>-5325.994</td>
<td>-4015.0752</td>
<td>-17365.38</td>
<td>-158.11</td>
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<tr>
<td>$^{15}$N</td>
<td>0.368</td>
<td>-8989.359</td>
<td>-7982.864</td>
<td>-9902.064</td>
<td>-23320.63</td>
<td>-7621.06</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>99.757</td>
<td>-9638.31</td>
<td>-9902.844</td>
<td>-14478.905</td>
<td>-14616.797</td>
<td>-2215.61</td>
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<tr>
<td>$^{17}$O</td>
<td>0.038</td>
<td>-7897.8</td>
<td>-11556.87</td>
<td>-7788.735</td>
<td>-17541.857</td>
<td>1817.7</td>
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<tr>
<td>$^{18}$O</td>
<td>0.205</td>
<td>-13113.6</td>
<td>-13717.3</td>
<td>-13343.67</td>
<td>-21335.55</td>
<td>-5008.26</td>
</tr>
<tr>
<td>$^{19}$F</td>
<td>100</td>
<td>-4039.91</td>
<td>-5770.68</td>
<td>-7557.064</td>
<td>-16218.7</td>
<td>-1524.64</td>
</tr>
<tr>
<td>$^{20}$Ne</td>
<td>90.48</td>
<td>-6242.181</td>
<td>-10618.953</td>
<td>-14794.125</td>
<td>-13120.307</td>
<td>-586.72</td>
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<tr>
<td>$^{21}$Ne</td>
<td>0.27</td>
<td>-4901.08</td>
<td>-10778.773</td>
<td>-11122.875</td>
<td>-15926.55</td>
<td>696.15</td>
</tr>
<tr>
<td>$^{22}$Ne</td>
<td>9.25</td>
<td>-10035.8</td>
<td>-13041.56</td>
<td>-14885.795</td>
<td>-18682.08</td>
<td>-5713.18</td>
</tr>
</tbody>
</table>

2.1. The Resonance Neutron Capture

In the interaction of slow neutron with target nucleus a compound nucleus with a finite time of life, definite properties (like spin, parity, and others) is formed that is described by quantum states or resonant states. After a time much longer than the time necessary for neutron to pass the nucleus the compound nucleus is decaying on possible channels (Brusegan, 2004), (Oprea, 2002). If the resonant states are well defined and far away from each other (as isolated) the cross-section of emission of $x$ particle from the compound nucleus can be described by single-level Breit – Wigner formula:

$$
\sigma_{nx} = g \pi a^2 \frac{\Gamma_n \Gamma_x}{(E - E_{nx})^2 + \Gamma_{tot}^2 / 4}
$$

(1)

where $g = \frac{(2J + 1)}{(2l + 1)(2s + 1)}$, $J$, $I$, $s = \text{spin of compound nucleus, target nucleus and}$ respectively, neutron, $\lambda = \frac{\lambda}{2\pi}$ = reduced neutron wavelength, $\Gamma_n, \Gamma_x, \Gamma_{tot} = \text{neutron, x-emitted}$ particle and total widths, $\Gamma_{tot} = \Gamma_n + \Gamma_x + \Gamma_y + \Gamma_d + \Gamma_a + \Gamma_f + \Gamma_{he} + \Gamma_f + ... = \text{total width, } x = n, n', p, d, t, He^3, \alpha, f + \text{other nuclear clusters, } E_s = \text{resonance energy.}$

If the emergent particle is a gamma quanta or an alpha particle then occur the $(n, \gamma)$ process or the $(n, \alpha)$ reaction, respectively. These processes will be used further in the computer simulations.

For a better description of experimental data, generally, the neutron resonance parameters and widths from (Brusegan, 2004) are used because these parameters are usually obtained experimentally. For slow neutron processes, the neutrons with orbital momentum $l=0$ ($s$-neutrons) and $l=1$ ($p$-neutrons) play an important role. By interaction with nuclei, the $s$-neutrons will form the $S$-resonance and $p$-neutrons will form the $P$-resonance. For each of them according to (Brusegan, 2004) the widths of $s$ and $p$-neutrons, respectively, have the following parametric formula:

$$
\Gamma_s^n(E_n[eV]) = \Gamma_{tot}^p(E_n[eV]), \Gamma_s^n(E_n[eV]) = \Gamma_{tot}^p(E_n[eV])p(E_n)
$$

(2)
\[ \Gamma^S_{n0}, \Gamma^p_{ni} = \text{reduced neutron widths for } s \text{ and } p \text{ neutron, respectively, } \]
\[ p_i(E_n) = \frac{\left( \frac{R}{\lambda} \right)^2}{1 + \left( \frac{R}{\lambda} \right)^2} \]

with \( \lambda = \text{reduced neutron length} \), \( R[fm]=1.45A^{\frac{1}{3}} = \text{nucleus radius} \). The suppression factor is a result of increasing nuclear barrier height by centrifugal component which reduces the probability of the neutron passing through the barrier. Due to the suppression factor, the resonances produced by \( s \)-neutrons are large and \( p \)-neutrons are enough thin.

Two examples of one \( S \) and \( P \) isolated resonances using the Breit-Wigner single level formula, according to relations (1-3), in Figures 1 and 2 are represented. The theoretical evaluations in Figures 1 and 2 are part of the computer-simulated experiments as the \( ^{14}\text{N} \) and \( ^{35}\text{Cl} \) nuclei are used in the calculations.

Figure 1. Cross sections calculated with the formula (1) and parameters from (Brusegan, 2004); large \( S \)-resonance with energy \( E_S = 648 \text{ keV} \) in \( ^{14}\text{N}(n,\gamma)^{15}\text{N} \) reaction

Figure 2. Cross sections calculated with the formula (1) and parameters from (Brusegan, 2004); thin \( P \)-resonance with energy \( E_P = 398 \text{ eV} \) in \( ^{35}\text{Cl}(n,\gamma)^{36}\text{Cl} \) reaction
In most of the cases (spectra), there are many resonances. If the resonances are isolated (as far as one from each other) and the interference between resonances can be neglected then these conditions can be expressed as the total width of resonance which is much lower than the distance (in energy scale) between any closest resonances.

$$\Gamma_i \langle |E_i - E| \rangle$$  \(4\)

In this case, the cross-section is a sum of the contributions of all resonances.

$$\sigma = \sum_{i=1}^{N} \sigma_i$$  \(5\)

2.2. Neutron Transmission

The neutron transmission method (NT) can be used as an alternative method of light nuclei identification to neutron capture (Lampoudis et al., 2011). In the attenuated flux, there are contributions from all open channels (\(\gamma, n, p, d, t, ^3\text{He}, \alpha, \text{ions}\)). The expression of the emergent neutron intensity is:

$$T = \exp \left[ - \sum_{i=1}^{n_{\text{elem}}} n_i \sigma_i^{\text{tot}} \right]$$  \(6\)

where \(n_i\) is the concentration of \(i^{\text{th}}\) element from the target \([m^{-2}]\), \(\sigma_i^{\text{tot}}\) = the total cross-section of \(i^{\text{th}}\) element, \(n_{\text{elem}}\) = number of elements from the target.

In the simple case of the presence only of S resonances, the cross-section of the \(i^{\text{th}}\) element is:

$$\sigma_i^{\text{tot}} = \sigma_i^{\text{pot}} + \sigma_i^{\text{rec}} + \sigma_i^{\text{int \_off}} = 4\pi R_i^2 \sum S_i \frac{g_{\text{Si}}^i \pi \lambda_i^2}{\left( E - E_i \right)^2 + \left( \frac{\Gamma_{\text{Si}}^{i \text{tot}}}{2} \right)^2} + \frac{4g_{\text{Si}}^i \lambda \pi \Gamma_{\text{Si}}^{S_i} R_i \left( E - E_{\text{Si}} \right)}{\left( E - E_{\text{Si}} \right)^2 + \left( \frac{\Gamma_{\text{Si}}^{S_i}}{2} \right)^2}$$  \(7\)

where \(R_i = 1.45 A_i^{1/3} [fm]\) = the radius of the \(i^{\text{th}}\) nucleus, \(A_i\) = mass number.

The first term in (7) is the potential scattering. The second term represents the resonant interaction in different open channels \((x=n, p, d, t, ^3\text{He}, \alpha, \text{etc.})\) and the third term comes from the interference between potential and resonant neutron scattering. In many cases, the interference between resonant and potential scattering can be neglected. For slow neutrons where only neutron and capture channels are open the resonant – potential scattering interference can be observed because gives a deviation from the known \(1/\nu\) law of cross-section.

The expressions (6) and (7) in the real experiments are factors that can influence the measurements. In the NT very often the time-of-flight method is used (Pikelner, 2000). The neutron energy using this approach is extracted from the time necessary for the neutrons to get from a pulsed neutron source to a neutron detector. The energy resolution in this case by (Pikelner, 2000) is:

$$\Delta E = 2.8 \cdot 10^{-2} \frac{\Delta t}{L} E_n^{1.5}$$  \(8\)

where \(L [m]\) = neutron path from source to the detectors, \(t [\mu s]\) = time necessary of neutrons to pass the path \(L\), \(\Delta t\) = time uncertainty, \(E_n [eV]\) = neutron energy.

Another factor influencing the measurements is the Doppler broadening of the resonances due to the thermal motion of target nuclei (Frenkel, 1939), (Ygnatyuk & Popov, 2000). The correction of the cross-section caused by thermal motion depends on the physical properties of the target and has the following form:
\[ \sigma_{\text{exp}} = \sigma_{\text{th}} \psi(\alpha, \beta) \]  

where \( \sigma_{\text{exp}} \) = measured cross-section, \( \sigma_{\text{th}} \) = theoretical (expected value) of the cross-section, \( \psi(\alpha, \beta) \) = correction factors depending on \( (\alpha, \beta) \) parameters. Supposing that the target can be approximated with an ideal gas (Ygnatyuk & Popov, 2000), (Bethe & Placzek, 1937), then the correction factor is:

\[ \psi(\alpha, \beta) = \frac{1}{\alpha \sqrt{\pi}} \int_{-\infty}^{\infty} \frac{1}{1+y^2} \exp \left( \frac{\beta - y}{\beta} \right)^2 dy \]  

\( \beta = \frac{2\Delta}{\Gamma} \), \( y = \frac{E - E_0}{\Gamma} \), \( \Delta = \left( \frac{4m_s E_0 k_BT}{M} \right) \) = Doppler width

2.3. Computer Simulated Experiment

From relations (1-6) it is easy to see that in the neutron capture or other emitted particles spectra the resonance structure can be evidenced very well (Postma & Schillebeeckx, 2005). The main purpose of this work is to evaluate the possibility of determining the properties of some light nuclei (cross-section, concentration, widths and others) by a succession of resonance neutron capture and total cross-section measurements in an NT experiment using a computer-simulated experiment. In a Direct Monte-Carlo simulation, a sample containing a number of medium and heavy elements and one trace light nucleus was considered. The elements from the sample are 1 - 87Sr, 2 - 95Mo, 3 - 54Fe, 4 - 64Ni, 5 - 35Cl. With number 6 in the sample is noted the analyzed light nucleus, namely \(^6\text{Li}\) or \(^{10}\text{B}\).

By using the neutron resonance parameters (Brusegan, 2004) it was observed that the thermal cross-sections values are described mainly by the \( S \)-resonances for both nuclei and less by the \( P \)-resonances (Blatt & Weisskopf, 1979). For simplicity of the calculation, only the \( S \)-resonances for medium and heavy nuclei in a wide energy interval up to 16 keV were taken into account. One of the medium nuclei \((^{35}\text{Cl})\) has a negative resonance \( E_S = -180 \text{ eV} \). This resonance will not be seen in the spectra but it will influence the “tail” of capture and neutron spectra in the region of the incident slow neutrons. The concentrations of the light elements were chosen of the order of ppm.

In the analysis, it was considered one by one two light nuclei. First nucleus was \(^6\text{Li}\) and the second one was \(^{10}\text{B}\). Both nuclei are important in fundamental and applicative researches and have similar nuclear properties. The main properties of the \(^6\text{Li}\) and \(^{10}\text{B}\) light nuclei (Brusegan, 2004), (INDC(CCP)-262, 1986) will be used in the computer simulated experiment. For \(^6\text{Li}\) the main contribution to the cross-section is given by the negative \( S \)-resonance \( E_S = -808 \text{keV} \) with spin and parity \( J^z = (1/2)^+ \). This resonance leads to the following experimental values of neutron capture and \((n, \alpha)\) cross-section for thermal neutrons:

\( \sigma_{ny} = (0.0385 \pm 0.003) \) b (Brusegan, 2004), (Park, et al., 2006) \( \sigma_{na} = (940 \pm 4) \) b (Brusegan, 2004). As in the case of the \(^{35}\text{Cl}\) nucleus, the negative \( S \)-resonance of \(^6\text{Li}\) cannot be observed in the spectra but the high value of \((n, \alpha)\) cross-section will influence consistently the tail of the NT spectra. The \(^6\text{Li}\) nucleus has also a \( P \)-resonance with energy \( E_p = 248 \text{keV} \), spin, and parity \( J^z = (5/2)^- \) (Brusegan, 2004). In spite of the fact that the neutron capture and the \((n,\alpha)\) cross-section are very high in the vicinity of the \( P \)-resonance (calculated of the order of \( 10^5 \) b) they are decreasing very quickly due to the suppression factor - relations (2) and (3); for slow neutrons up to 16 keV their values can be neglected.
For the light nucleus $^{10}$B the following data were considered (Brusegan, 2004), (INDC(CCP)-262, 1986): one $S$-resonance with properties $E_S = 170.6 keV$, $J_S^p = (5/2)^+$, which gives the main contribution in the cross-sections for thermal neutrons, $\sigma_{ny} = (0.5 \pm 0.2) b$ and $\sigma_{na} = (3837 \pm 9) b$. Like in the case of $^6$Li the capture cross-section is much lower than $(n, \alpha)$ cross-section and $S$-resonance is far from the region of interest still this resonance will give influence especially on the NT spectra. In the table with neutron resonance parameters (Brusegan, 2004) there is also indicated another negative $S$-resonance with properties $E_S = (-946 \pm 6) keV$, $J_S^p = (7/2)^+$ but the contribution of this resonance to the cross-section is considerably lower than the contribution of the other $S$-resonance and therefore in these first calculations it was not considered.

The method proposed in this study is based mainly on the properties of the analyzed nuclei and considers that the $(n, \alpha)$ process is dominant in comparison with other possible processes. The Monte-Carlo simulated experiment was computed on the basis of the formulas presented before. The software code can be described by the following stages:

1. Theoretical data simulation;
2. Simulated experimental data for neutron resonance analysis and NT;
3. Least square methods for both types of experiments;
4. Error evaluation of simulated experimental data;
5. Extraction of necessary information;
6. Graphic representation section with export option on ASCII files for the other graphical tools.

The theoretical data are obtained using the relations (1 - 10). The simulated experimental data are based on the theoretical ones supposing that every experimental data has the corresponding standard error distributed in accordance with the Gauss Law. First, the experimental data for the capture experiment were simulated. From these data, the concentrations for heavy and medium elements were extracted. The light nuclei have a very low value of capture cross-section and therefore at this stage can be neglected. The high value of the $(n, \alpha)$ cross-section allows the light nuclei to be observable in NT spectra. From the capture experiment, the other 5 element concentrations were obtained with an error of about 10%. They will be further used in the NT simulated experiment. In this work were chosen two cases. The first case is often met in applicative researches and this is the obtaining of the trace concentration of light nucleus. The second case is interesting mainly in fundamental researches (but it can be of interest also in applicative problems) and this case is the extraction of the neutron widths of light nuclei. The neutron widths are important for cross-section evaluation and for other situations involving nuclear structure and reaction models.

3. Results and Discussion

The first case presented is the $^6$Li nucleus. The other five nuclei in the sample are medium and heavy. The $^6$Li and one medium nucleus have a negative resonance. Therefore these nuclei will not be seen in the simulated spectra (Figures 3a, 3b for NRA and Figures 3c, 3d for NT) but they will influence the “tail” of the spectra giving the possibility to extract the necessary data.

First, from the experimental simulated data, the concentration of $^6$Li nucleus was extracted. Initial, the concentration of $^6$Li nucleus in the sample is:

$$n_{Li} = 5.33 \cdot 10^{22} m^{-2}$$ (11)
After the application of the computing procedure described before, considering 1024 experimental data in a wide energy interval of incident neutrons up to 16 keV, the following value of concentration was extracted:

\[ n_{Li}^{fit} = (5.55 \pm 0.83) \times 10^{22} \text{m}^{-2} \text{ with a relative error } \varepsilon \approx 15\% \quad (12) \]

We have tested many variants. If the number of experimental data is higher the error is improved. The concentration also was varied. Therefore, by increasing the concentration the error is decreasing. Finally, if the concentration can be reduced by an order of magnitude relative to relation (12) the obtained relative error of fitted concentration can be considered still acceptable.

Another interesting case is to obtain the neutron widths for light nuclei. Let us consider the same sample composed from all six elements and the concentration of the $^6$Li nucleus is known. Applying the same procedure by simulated NRA experiment the concentrations of heavy and medium elements are obtained with an error of about 10-15%. After, these concentrations are introduced in NT simulation from where the reduced neutron width for $^6$Li nucleus corresponding to the negative S-resonance is obtained by fitting. From (Brusegan, 2004) the reference value of reduced neutron width corresponding to the negative S-resonance, $E_S = -808$ keV, is:

\[ \Gamma_{n0} = 295 eV \quad (13) \]

After NRA and NT computer simulated experiment, using 1024 data, the neutron width was extracted as:

\[ \Gamma_{n0}^{fit} = (290.72 \pm 67.71) eV \text{ with relative error } \varepsilon \approx 0.23 \quad (14) \]

In order to improve the value from (14) also some other variants such as more experimental points, another set of concentrations, other neutron energy intervals, were processed. Increasing the number of simulated experimental data the relative error (14) is improved. At the first sight, it seems interesting that the neutron width for the $^6$Li nucleus is very well extracted up to 1 keV but this is easy to explain due to the presence of negative S-resonance which is influencing the low neutron energy region.
The second case analyzed similarly with $^6$Li was $^{10}$B nucleus. Then it is possible to make the same computer simulated experiments like in the case of the $^6$Li nucleus. A sample composed of five heavy and medium nuclei and $^{10}$B trace light nucleus ($\approx$ ppm) is considered. In Figures 4a and 4b, only four elements are represented. One element, $^{35}$Cl nucleus, has a negative $S$-resonance and $^{10}$B nucleus has the $S$-resonance very far ($E_S = 170$ keV) and it is not represented in the figures. The effect of the $S$-resonance of $^{10}$B nucleus influences significantly the spectra because in Figures 4a and 4b the element number 1 is present but is not visible already in NT spectra shown in Figures 4c and 4d. In all Figures 4a-4d are represented only the cases in a wide energy interval up to 16 keV and with 1024 simulated experimental data. By the selected computer codes other situations were tested, including more experimental data, other energy intervals, and concentrations, but these cases are not represented here. In Figures 3 and 4 the results of computer simulation with 1024 experimental data are represented. Other cases were tested as well and due to the presence of $S$-resonance with the main contribution to the cross-section it will be enough to analyze the low energy part of the spectra, with less than 1024 experimental data, in order to extract the element concentration and the width.
Initially, $^{10}$B nucleus had the concentration value:

$$n_{^{10}B} = 1.53 \cdot 10^{23} \text{ m}^{-2} \quad (15)$$

After applying the NRA and NT computer experiment the concentration with an error of less than 10% was obtained:

$$n_{^{10}B}^{fit} = (1.6 \pm 0.12) \cdot 10^{23} \text{ m}^{-2} \quad (16)$$

For neutron width of $^{10}$B nucleus the reference value from (Brusegan, 2004) is:

$$\Gamma_{n^{10}B} = 296 \text{ keV} \quad (17)$$

and from the simulation procedures, the following width was obtained:

$$\Gamma_{n^{10}B}^{fit} = (304.29 \pm 73) \text{ keV} \quad , \quad \text{relative error } \varepsilon \approx 0.24 \quad (18)$$

From Table 1 isotopes with positive Q-values are $^{14}$N, $^{17}$O, and $^{21}$Ne in (n, p) and (n, $\alpha$) reactions, respectively. We have already started the computer simulation on the first two nuclei. The third nucleus will not be analyzed yet because the computer-simulated experiment at this stage is based on the knowledge of necessary widths which do not exist for the $^{21}$Ne nucleus until now in literature. In comparison with $^6$Li and $^{10}$B nuclei the $^{14}$N, $^{17}$O, and $^{21}$Ne have a much lower thermal cross-section for the corresponding reaction and in future theoretical and experimental evaluations, it will be a source of uncertainties in parameters determination. For $^{14}$N(n,p)$^{14}$C, $^{17}$O(n,$\alpha$)$^{14}$C and $^{21}$Ne(n,$\alpha$)$^{20}$O reactions the thermal cross-sections are, respectively, $\sigma_{np} = (1.81 \pm 0.5)\text{b} \quad , \quad \sigma_{n\alpha} = (0.235 \pm 0.01)\text{b} \quad \text{and} \quad \sigma_{n\alpha} < 1.5\text{b}$ (Mughabghab, 2003). For $^{14}$N and $^{17}$O using only one S-resonance the experimental data from (Koehler & Graff, 1991) and (Koehler & O’Brien, 1989), for slow neutrons, are well described by the theoretical approach developed here (Figures 5 and 6).
4. Conclusions

The computer simulation accomplished during the present work has demonstrated the possibility of evaluation of the properties of several light nuclei by a combination of nuclear analytical methods like neutron resonance capture and neutron transmission (NRA and NT). This new neutron approach methodology is based on the properties of the nuclei from the sample. Different content of the sample will necessitate analyzing the properties of nuclei for the corresponding setup and preparations of the measurements. For the simplicity of the calculations, only one $S$-resonance was considered from each element in the sample composed of only five medium and heavy elements and one trace light element. It is obvious that in the energy interval up to 16 keV the medium, and heavy nuclei have more than one resonance and the content of samples may have more heavy, medium and light nuclei. These factors are foreseen to be included in future works. The $^6\text{Li}$ and $^{10}\text{B}$ nuclei are similar in this study. Both nuclei have a very low value of capture cross-section and very high value of $(n, \alpha)$ cross-section. Due to the positions of $S$-resonances and their reduced neutron widths, these light nuclei influence significantly the spectra. In particular, from Figures 4a-4d the element number 1 (i.e. $^{87}\text{Sr}$) appear in the capture spectra (Figure 4a) but is already “covered” by the...
background in NT spectra (Figure 4d). From here it follows that performing only one type of measurements (NRA or NT) could lead to errors and the order of measurement methods can also be important.

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References


Oprea, C., Doctor of Physics Thesis, (18.09.2002). Faculty of Physics, University of Bucharest, Bucharest.


INDC(CCP)-262 (1986) *Neutron capture, Compendium*, EnergoAtomIzdat, Moscow, (in Russian)


