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AN ACCURATE REDETERMINATION OF THE ^{118}Sn BINDING ENERGY

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1. Introduction

The use of primary γ rays from neutron capture to place levels in a nuclear level scheme is a valuable tool in nuclear structure physics. Due to the general complexity of the secondary γ-ray spectra, there is a decided advantage to measuring the primary γ-ray energy (and thus the excitation energy) to as great a precision as possible to avoid ambiguity in the assignment of the secondary γ rays. Modern Ge(Li) and intrinsic germanium detector systems make it possible to measure γ-ray energies to 10 MeV with a precision of $\lesssim 0.1$ keV relative to a standard set of energies.

In radiative capture of thermal neutrons by ^{117}Sn the primary transition on the ground state of ^{118}Sn is intense and dominates the hard part of the γ-ray spectrum. This gives the hope to measure the binding energy of neutron, B_n, with better precision than the value given in [1]: 9326.31(140) keV. If there is some peak on spectrum with high precision of position in order to achieve good energy precision one must pay attention to the standards which are used for energy calibration. For improving the energy precision of the 9326 keV transition new measurements of B_n for ^{64}Cu have been made. Result of these measurements differs from value in [1]. We used an original energy calibration procedure in which a priori information is taken into account by a Monte-Carlo simulation.

We have divided this paper as follows: the discussion about the connection between γ-ray energies and the fundamental constants (Section 2), the description of calibration procedure (Section 3), the experiments (Section 4), the results of B_n for ^{64}Cu and for ^{118}Sn (Section 5), and discussion (Section 6).

2. The connection between γ-ray energies and the fundamental constants

All of the data of energy standards may be divided in two groups: absolute energies and energies measured relative to some energy standard. The majority of the relative energies from radioactive decay have been measured relative to 412-keV ^{198}Au line. Therefore, it is convenient to use this line, the so-called "gold standard", as the standard for data evaluation. In a number of measurements of captured γ-rays this standard was used for the determination of energies to 8-9 MeV.

The most precise absolute γ-ray energies are based on γ-ray wavelength measurements made on a two axis flat crystal spectrometer. Precision γ-ray measurements

require knowledge of two quantities, the lattice spacing, d, and the diffraction angle, θ. These two quantities are combined using the Bragg condition for diffraction, $\lambda = 2d\sin(\theta)$, to obtain the wavelength, λ, of the γ ray. The conversion of the γ-ray wavelengths to energies in keV involves only the voltage-wavelength conversion factor, $E\lambda$. The values d and $E\lambda$ are in the list of the fundamental constants and the each next adjustment of these constants will result in change of the absolute energies.

In May 1972 the IUPAP Commission on Atomic Masses and Fundamental Constants established a task group to produce, recommend, and publish a consistent set of calibration standards for use in γ -ray spectroscopy. Based on the 1973 adjusted values of the fundamental constants of Cohen and Taylor [2] such a list was published in 1979 [3]. After the 1986 evaluation of the fundamental constants [4] authors of [3] published new recommended standards for γ-ray energy calibration (1999) [5].

That paper appeared in 2000 but before its publication, there was a new (1998) evaluation of the fundamental constants [6]. Now we introduce some values from this evaluation important for γ-ray spectroscopy. First of all is the electron mass, m_e, or the energy of annihilation peak: 510.998902(21) keV. In addition, d= 0.1920155845(56) nm and $E\lambda$= 1.239841857(49) $\times 10^{-6}$ eVm. We have used two the latter values, recalculated the energy of the "gold standard" in manner of [5] and determined 411.80176(12) keV. This value slightly differs from latest one, 411.80205(17) keV, published in [5].

It may be ascertained that a set of standards from radionuclides in [5] satisfies in full the needs of calibration in low part of γ-ray spectrum. The situation for γ rays from neutron capture is more complicated because first of all the lack of absolute measurements of energies of captured γ rays. These measurements go on in ILL, Grenoble, on GAMS4 spectrometer. A new value of the deuteron binding energy was reported in [7,8] based on an absolute wavelength determination of the 2.2 MeV n-p γ-ray. In the papers only the value of the absolute wavelength of this γ ray is presented. We have calculated E_γ and determined 2223.24846(41) keV. When we took a value of deuteron mass 1875.612762(75) MeV from new set of fundamental constants [6] and calculated recoil we determined the deuteron binding energy 2224.56614(41) keV which is published in [7,8]. The paper [8] concludes by describing the first crystal diffraction measurement of the 8.6 MeV ^{36}Cl binding energy. The result of this measurement will be very important for energy calibration of captured γ rays. The high capture cross section of σ = 43 b and the favorable

(about equally spaced) distribution of intense primary and secondary transitions up to 8.6 MeV make this reaction particularly promising for calibration purposes of γ-ray detectors at a reactor.

Now we want to introduce another constant which is useful in calibration of γ-spectra. The γ-ray energies E_γ are converted to transition energies E_t by adding the recoil energy; that is,

$$E_t = E_\gamma + \alpha E_\gamma^2.$$

On the other hand, one can determine E_γ from E_t by

$$E_\gamma = \frac{\sqrt{1+4\alpha E_t}-1}{2\alpha},$$

where $\alpha = C/A$. If all of the energies are in keV and A is the atomic mass, coefficient $C = 0.536772103(21) \times 10^{-6}$. The full precision of this value is not necessary, but three or four significant figures might not be sufficient.

3. The energy calibration procedure

A calibration procedure is used for finding a correspondence between the peak positions on a spectrum and the energies. Input data for the calibration procedure may be divided into four groups:

(1) In a calibration procedure, the independent variables $x_i, i = 1, 2, ..., n$, corresponding to some well-known standard quantities (the dependent variables) y_i are measured and a calibration function $y = f(x)$ is then fitted to the data. Variables x_i are the peak positions in spectrum measured and y_i are the energy standards. If y_i are independent to each other, the Least- Squares Method (LSM) is used to determine

$$f(x) = \sum_{k=0}^{p} a_k x^k,$$

where a_k correspond coefficients of the calibration polynomial (p degree) for the spectrum. In the LSM the error of each standard is sum of the error of the peak position and the error of energy in scale of positions. In result for each peak we have two errors: Δx_{is} – statistical error of position in the energy scale and Δx_{ir} – systematic error, which is determined from resulting matrix.

(2) In semiconductor γ-ray detectors there is a well-known difference in energies of any ($E_\gamma \geq 1022$ keV) full-energy peak and the corresponding single and double

escape peaks, equal to m_e or $2m_e$. Positions of these peaks are independent variables and the peak energies are correlated and there is one energy error for three such peaks.

(3) Some peaks which are known primary transitions from one isotope i have one common value B_{ni} with its error ΔB_{ni} and different values of energy levels, E_l. As a rule the error of B_n is one order greater than errors of E_l.

(4) Peaks which join groups (2) and (3). These peaks have one common B_n and triplets of transitions on levels with known E_l. Error of B_n is common for all peaks and errors of E_l are common for triplets.

For groups (2),(3),(4) it is complicated to take into account the errors of energies.

If we search in calibration procedure a value connected with position of one peak this task is simple. But if we search B_n, we can use the positions of some number of peaks, which are members of group (2), (3) or (4). In this case it is difficult to determine the error of B_n. This paper shows a way how the errors of energies in groups (2), (3) or (4) can be included and how the error of B_n can be determined.

We discuss the calibration procedure in the LSM framework. This procedure is intended to determine one value, namely B_n. In the LSM the best value of one parameter gives minimal value of the chi-square function Q and the second derivative in this point is connected with the standard deviation (SD) of the parameter. In the procedure the value of parameter is changed by steps and each value of function Q is calculated. From interpolation of all these values by parabola the values of B_n and ΔB_n are determined. In order to take into account the errors of energies, which are common for some peaks, the Monte-Carlo simulation is used. For group (2) the Gaussian simulation with SD equal to ΔE_γ is used. For each group (3) events from Gaussian distribution with mean value B_{ni} and SD equal to ΔB_{ni} are simulated. For a group (4) the same simulation as for group (3) is made. There are some triplets in the group which have the common error ΔE_l. When the full error of each peak position of triplet is calculated, the value $\sqrt{3} \times \Delta E_l$ is added.

Now we describe one event of simulation in detail. For each group (2), (3) and (4) one value from Gaussian distribution with own mean and SD is generated. For each peak of standards the energy and the full error is calculated. The errors of the values, which are generated, not enter in the calculation of the full error because they will be taken into account in the Monte-Carlo simulation. With these data 40 steps of value of B_n under the examination are made. On each step coefficients of the calibration polynomial with fixed degree p are found. The value of function Q, which is minimized, is the only one result of the step. The best value of B_n and

ΔB_n are determined in interpolation results of steps by parabola. These values are remembered.

After all simulations the analysis of the distributions of B_n and ΔB_n is made. The mean value of B_n is the final result of B_n and chi-square sum of SD of B_n and mean value of ΔB_n is the final result of ΔB_n.

$f(x)$ is not fitted directly in the procedure. In the beginning x_i are ordered and

$$f_1(x) = y_1 + \frac{y_n - y_1}{x_n - x_1}(x - x_1)$$

is calculated. Values $z_i = y_i - f_1(x_i)$ are fitted in the procedure and a calibration function $\varphi(x)$ is obtained. This gives more stable results of Q in steps.

One important remark we have to introduce now. If $f(x)$ or $\varphi(x)$ are linear functions every energy standard with small error will give small ΔB_n in result. These functions are however not linear, and a precise Bn is possible only if the standards are peaks which are close by peaks which give the value of B_n.

There are other energy calibration procedures in which a priori information is taken into account. One of these procedures is described in [9]. In the procedure the complicated function Q with different a priori information included is minimized. A self-calibration procedure is presented in [10] that enables an improvement of the precision of data through a functional relationship between variables. The main differences of our approach with these procedures are:

(1) The procedures [9,10] are devoted to improve the values of energy standards. It is not always handy because this requires the use of the covariance matrix of results.

(2) In these procedures the problem with ΔB_n when B_n is determined from positions of some number of peaks is not solved in obvious manner.

4. The experiments

The γ-ray spectrum from thermal neutron radiative capture by ^{117}Sn have been measured at the JINR IBR-2 pulsed reactor. The measurement was carried out on the exit of mirror neutron guide at the flight path 6b of IBR-2. The distance from active zone was 34 m and neutron flux on the sample was $3 \times 10^6 n/cm^2 \times s$. The sample consisted of 400 g metallic tin enriched in ^{117}Sn to 88 % . The γ rays were detected by the 72 cm^3 HPGe detector. Results of this measurement have been published in [11]. The hard part of this spectrum is shown in Fig. 1.

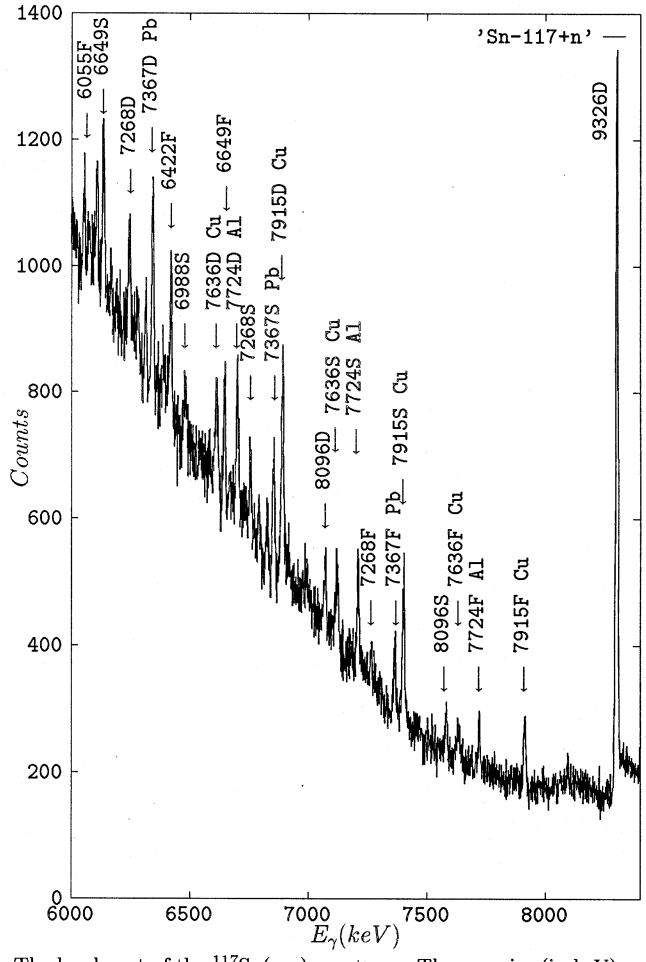

Fig. 1. The hard part of the ^{117}Sn(n,γ) spectrum. The energies (in keV) and the types of the peaks (D,S,F) are labeled. If the peak is from background capture, source nucleus is in the label.

It is seen that for energy calibration of the spectrum we can use the peaks from background capture of neutrons by Cu, Al and Pb. Peak 9326D from capture by ^{117}Sn is at the end of the spectrum and the nearest background peak is 7915F peak from ^{63}Cu(n,γ) reaction. ΔB_n for ^{64}Cu in [1] is greater than values ΔB_n for ^{28}Al and ^{208}Pb. In these circumstances it is reasonably to obtain new value of B_n for ^{64}Cu with the utmost of accuracy.

Two spectra were used for the determination of B_n for ^{64}Cu. One of these spectra was measured at the same place as the ^{117}Sn(n,γ) spectrum. Some additional experimental installation was placed in the beam and the test of background conditions was the aim of this measurement. The hard part of this spectrum is shown in Fig. 2. Peaks from capture by Cl, Al and Pb were used as the standards.

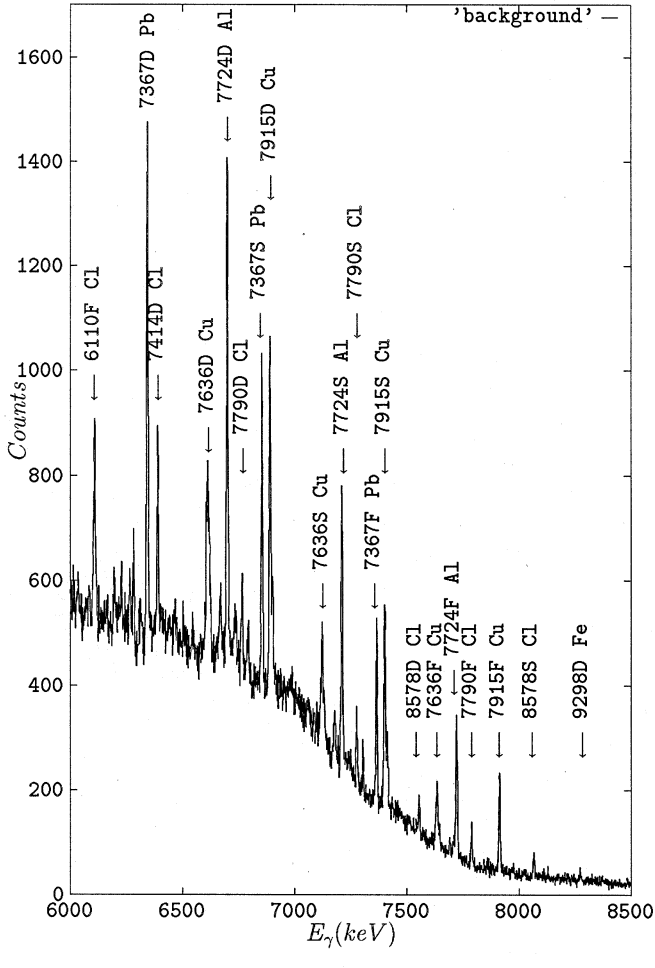

Fig. 2. The hard part of the 'background' spectrum. The labels are the same as in fig. 1.

Another spectrum was obtained at the Brookhaven High Flux Beam Reactor. The γ rays were detected with a three-crystal (Ge(Li)-NaI) pair spectrometer [12]. This measurement was devoted to the study of the ^{158}Gd(n,γ) reaction. Value

of B_n of ^{159}Gd is 5943 keV and all peaks in the spectrum with greater energy are background peaks. The hard part of this spectrum is shown in Fig. 3. As standards on this spectrum the peaks from Pb, Al and Ge were used.

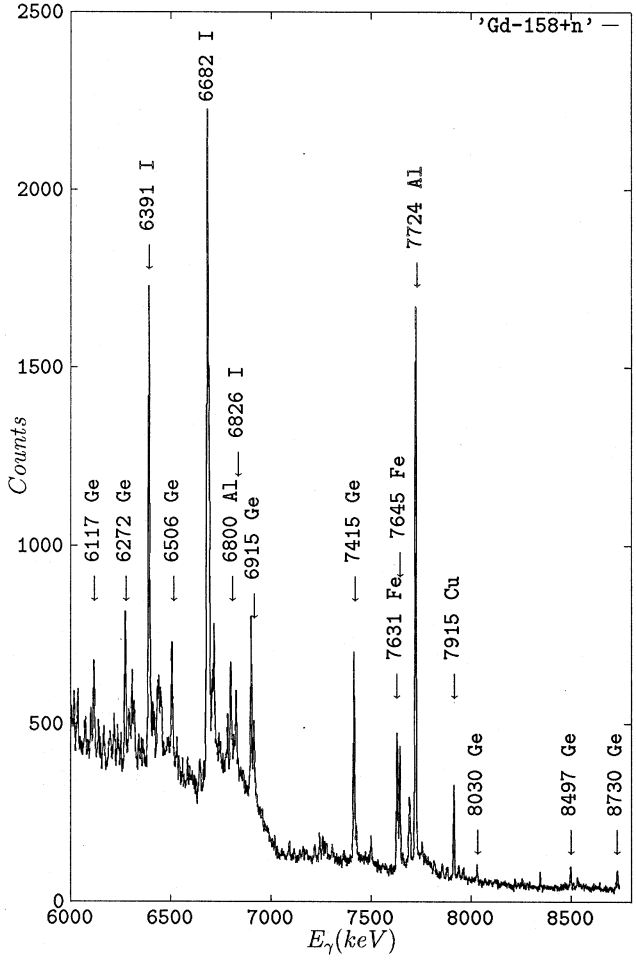

Fig. 3. The hard part of the BNL spectrum. The labels show the energy of transition and the source nucleus.

Further the next notation for the three spectra will be used:

1) - for spectrum ^{117}Sn(n,γ);

2) - for background spectrum;

3) - for BNL spectrum.

5. The results

The spectra were fitted using the FORTRAN computer code SPANAL [13]. Peak positions obtained have been used in the procedure described in section 3 for determining values of B_n. Some nuclei used as standards are shown in Table 1. Values

Table 1
Values of B_n and E_γ on the ground states of some nuclei used in this work and data for ^{118}Sn from [1]

Sample	A+1	Z	B_n (keV)	ΔB_n (keV)	E_γ (keV)	Reference
^{27}Al	28	13	7725.18	0.09	7724.036	[14]
^{35}Cl	36	17	8579.68	0.09	8578.583	[15]
^{56}Fe	57	26	7646.03	0.10	7645.480	[1]
^{63}Cu	64	29	7915.96	0.11	7915.435	[1]
^{117}Sn	118	50	9326.31	1.40	9325.914	[1]
^{207}Pb	208	82	7367.82	0.09	7367.680	[1]

of B_n were determined for ^{57}Fe, ^{64}Cu and ^{118}Sn. Energy standards in wide energy range were used for obtaining the information about non-linearity of each spectrum. Number of events 10000 was collected in each Monte Carlo simulation. All results are presented in Table 2. Results of calculation of B_n in the LSM framework with usual estimation of ΔE_γ are compared with results of the Monte-Carlo calculations. It is seen from the table that all ΔB_n determined in the Monte-Carlo simulation are somewhat greater than LSM ones.

Values of χ^2 per degree of freedom were analyzed. They are connected with degree of non-linearity of spectra. For the spectrum 1) these values are about 1.3, for the spectrum 2) - about 1.0 and for the spectrum 3) – are greater than 2. One important comment must be done in connection with this analysis. When spectra are very complicated and background peaks are used as standards there is big probability that some peaks might suffer from contribution of other backgrounds. Thus in some cases the peak 7693F from Al has an unusually large value for χ^2. This might be from contribution of 7697F peak from Ni.

Table 2

Values of B_n and E_γ on the ground states determined in this work.

Isotope	LSM		Monte-Carlo		E_γ	Spectrum
	B_n (keV)	ΔB_n (keV)	B_n (keV)	ΔB_n (keV)	(keV)	
^{57}Fe	7646.083	0.083	7646.083	0.091	7645.533	3)
^{64}Cu	7915.514	0.081	7915.514	0.092	7914.989	2)
^{64}Cu	7915.543	0.119	7915.537	0.120	7915.012	3)
^{118}Sn	9326.603	0.160	9326.602	0.169	9326.206	1) [a]
^{118}Sn	9326.620	0.130	9326.620	0.141	9326.224	1) [b]
^{118}Sn	9326.420	0.124	9326.420	0.132	9326.024	1) [c]

[a] Peak 7915F from Cu was not used.

[b] Energy of peak 7915F from Cu was taken from [1].

[c] Energy of peak 7915F from Cu was taken from this work.

Values of B_n for ^{64}Cu were determined from spectra 2) and 3). Figs. 4a and 5a show deviation of the energy calibration function from a linear function for spectrum 2) and 3). Values z_i described in sec.3 are on y axis for each peak used in calibrating procedure. Figs. 4b and 5b illustrate dependence of χ^2 from steps of B_n (see sec.3). Two values of B_n are very close to each other. Mean value 7915.52(8) keV was determined from two measurements. This value was used to obtain B_n for ^{57}Fe from the spectrum 3).

Three values of B_n for ^{118}Sn are placed in Table 2. In the first peak 7915F from Cu was not used in calibration procedure, in the second the energy of this peak was calculated from value of B_n for ^{64}Cu published in [1]. The third value of B_n was determined using our energy of peak 7915F from Cu. Fig. 6 shows data similar to Figs.4 and 5 for Cu from the third value of the ^{118}Sn calibration.

6. Discussion

As it is seen in Table 2 for better determination of B_n for ^{118}Sn from the spectrum 1) it was important to know B_n for ^{64}Cu with as great a precision as possible. We determined this value from two different spectra and have mean value 7915.52(8)

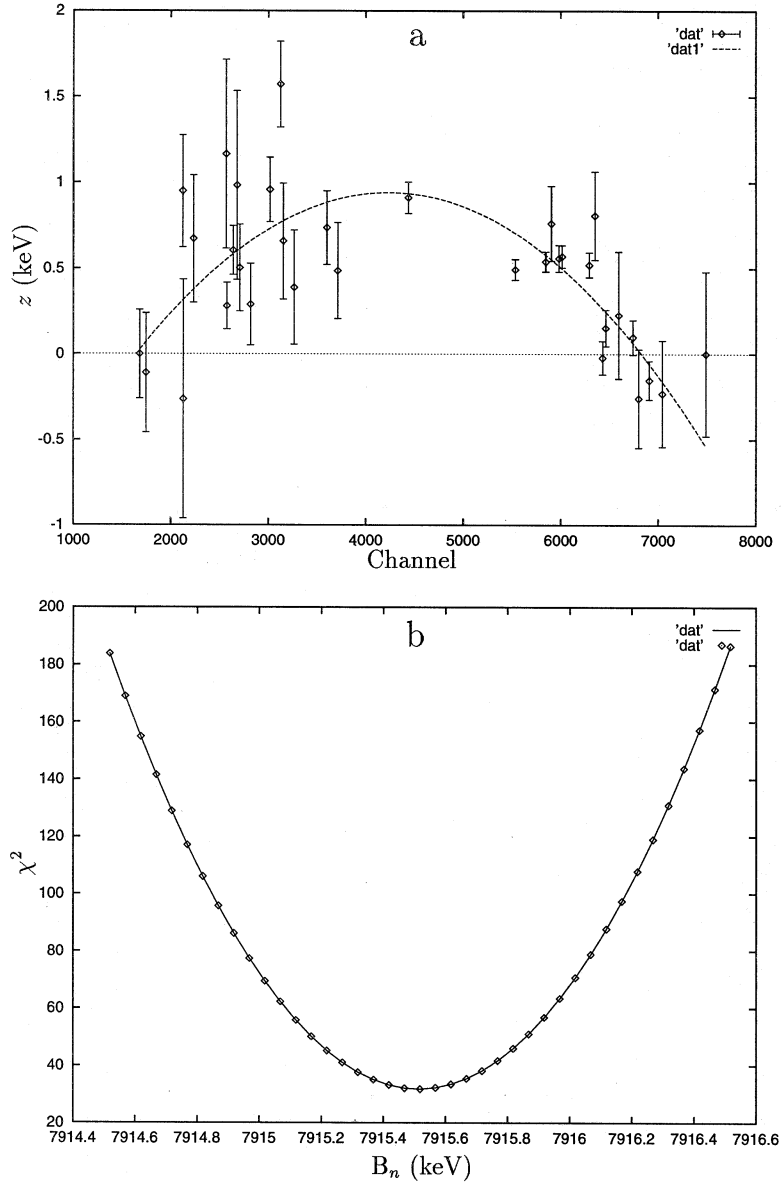

Fig. 4. Determination of B_n for ^{64}Cu from the spectrum 2) (see sec.3). (a) – Deviation of the energy calibration function from a linear function. (b) – Variation of the χ^2 as a function of B_n.

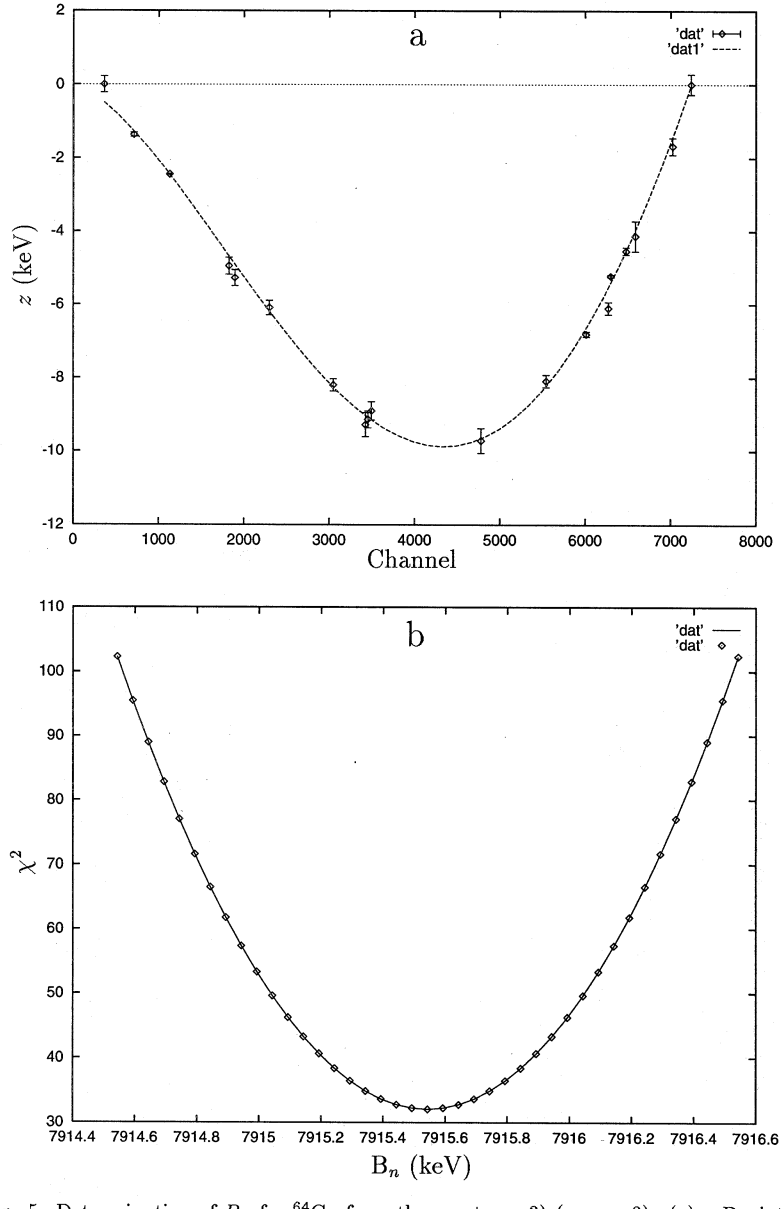

Fig. 5. Determination of B_n for ^{64}Cu from the spectrum 3) (see sec.3). (a) – Deviation of the energy calibration function from a linear function. (b) – Variation of the χ^2 as a function of B_n.

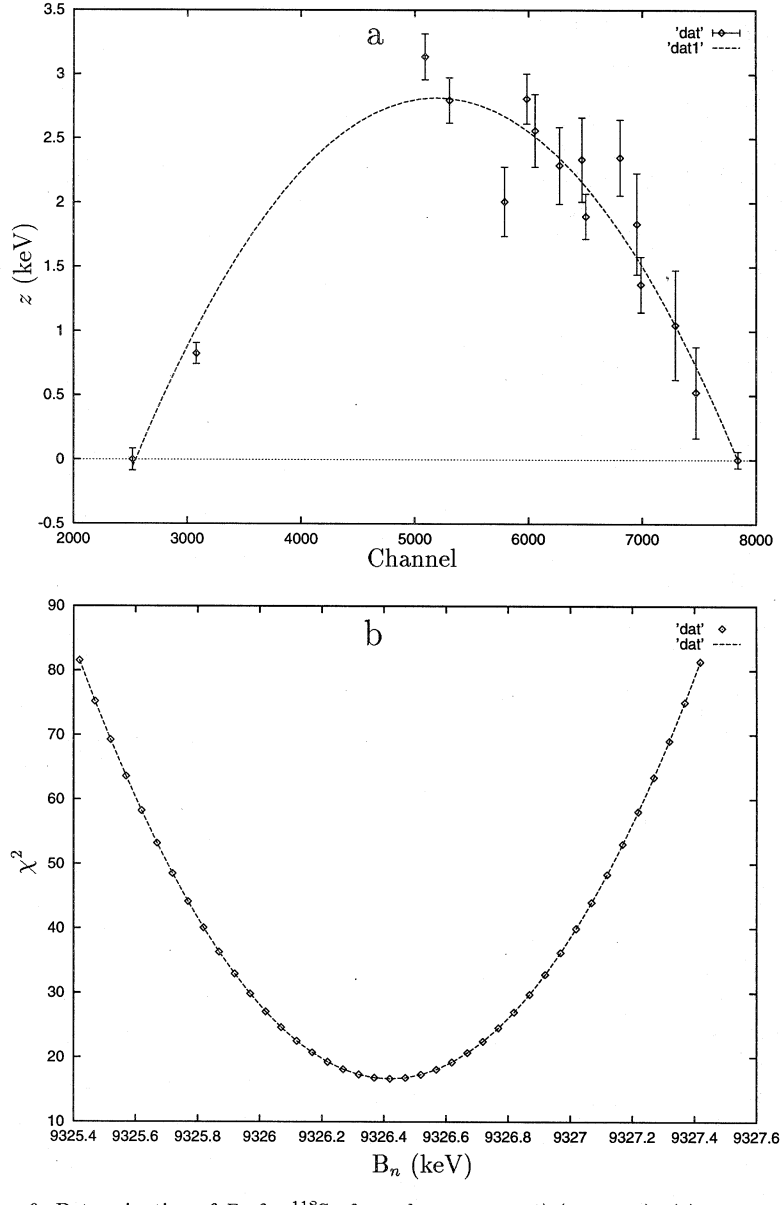

Fig. 6. Determination of B_n for ^{118}Sn from the spectrum 1) (see sec.3). (a) – Deviation of the energy calibration function from a linear function. (b) – Variation of the χ^2 as a function of B_n.

keV, which essentially differs from previous results: 7915.96(11) keV in [1] or 7916.09(12) keV in [16]. The new value obtained was used in the calibration procedure and two values of B_n were determined, namely: from the spectrum 3) for ^{57}Fe and from the spectrum 1) for ^{118}Sn. In Table 3 a comparison of values of E_γ of primary transition on the ground state of ^{57}Fe from different works is done. It is seen that our value is in good agreement with other results. Different results of B_n for ^{118}Sn are presented in Table 4. The mean value of two the most precise results of the B_n for ^{118}Sn (from [22] and our) was determined to be 9326.35(9) keV.

Table 3

A comparison of values E_γ on the ground state of ^{57}Fe

E_γ (keV)	ΔE_γ (keV)	Reference
7645.48	0.10	[1]
7645.47	0.15	[17]
7645.74	0.17	[18]
7645.58	0.10	[19]
7645.39	0.04	[20]
7645.53	0.09	This work

Table 4

A comparison of values B_n for ^{118}Sn

B_n (keV)	ΔB_n (keV)	Reference
9326.31	1.40	[1]
9326.22	0.26	[21]
9326.30	0.11	[22]
9326.60	0.20	[11] [a]
9326.42	0.13	This work

[a] Value B_n for ^{64}Cu was taken from [1].

The most surprising part of this paper is the large difference between the new result for ^{64}Cu and previous ones. We have three arguments in favor of our result. The first argument is that the two values from 2) and 3) are in good agreement from two measurements at different sites and with different instruments. The second argument is the good agreement of B_n for ^{57}Fe from spectrum 3) with previous results. The third is the value of B_n for ^{118}Sn achieved with these spectra is closer to the most precise previous B_n for ^{118}Sn from [22]. New measurements of B_n for ^{64}Cu are desirable.

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Борзаков С.Б. и др. Е3-2001-55
Новое аккуратное определение энергии связи нейтрона в ^{118}Sn

Энергия хорошо известной сильной гамма-линии из ^{198}Au, так называемый «золотой стандарт», преобразована с учетом нового уточнения фундаментальных констант. Получено значение 411,80176(12) кэВ, что на 0,29 эВ ниже, чем предыдущее значение 1999 г. Разработана калибрационная процедура для определения энергии связи нейтрона B_n из сложных (n,γ)-спектров. Использован математически простой функционал, который включает только члены, параметрами которых являются коэффициенты полинома. Априорная информация о связи между энергиями различных пиков на спектре учитывалась с помощью симуляции методом Монте-Карло. Процедура была использована для получения значения B_n для ^{118}Sn и ^{64}Cu. Спектр гамма-лучей из теплового радиационного захвата нейтронов ядром ^{117}Sn был измерен на импульсном реакторе ИБР-2. Гамма-лучи регистрировались 72 см^3 HPGe-детектором. Значение B_n для ^{64}Cu получено из двух гамма-спектров. Один спектр был измерен на реакторе ИБР-2 тем же детектором, другой спектр — парным спектрометром на Брукхэйвенском высокопоточном реакторе. Из этих двух спектров получено значение 7915,52(8) кэВ. Среднее значение двух наиболее точных величин B_n для ^{118}Sn оказалось равным 9326,35(9) кэВ. Определено значение B_n для ^{57}Fe, равное 7646,08(9) кэВ.

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Borzakov S.B. et al. E3-2001-55
An Accurate Redetermination of the ^{118}Sn Binding Energy

The energy of well-known strong γ-line from ^{198}Au, the «gold standard», has been modified in the light of new adjustments in the fundamental constants and the value of 411.80176(12) keV was determined which is 0.29 eV lower than the latest 1999 value. An energy calibration procedure for determining the neutron binding energy, B_n, from complicated (n,γ)-spectra has been developed. A mathematically simple minimization function consisting only of terms having as parameters the coefficients of the energy calibration curve (polynomial) is used. A priori information about the relationships among the energies of different peaks on the spectrum is taking into account by a Monte Carlo simulation. The procedure was used in obtaining of B_n for ^{118}Sn and ^{64}Cu. The γ-ray spectrum from thermal neutron radiative capture by ^{117}Sn has been measured on the IBR-2 pulsed reactor. γ-rays were detected by a 72 cm^3 HPGe-detector. B_n for ^{64}Cu was obtained from two γ-spectra. One spectrum was measured on the IBR-2 by the same detector. The other spectrum was measured with a pair spectrometer at the Brookhaven High Flux Beam Reactor. From these two spectra B_n for ^{64}Cu was determined equal to 7915.52(8) keV. The mean value of two the most precise results of the B_n for ^{118}Sn was determined to be 9326.35(9) keV. The B_n for ^{57}Fe was determined to be 7646.08(9) keV.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

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