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# SigmaCalc recent development and present status of the evaluated cross-sections for IBA

A.F. Gurbich

*Institute for Physics and Power Engineering, Bondarenko Sq. 1, Obninsk 249032, Russia*
*National Research Nuclear University MEPhI, Kashirskoe Shosse 31, Moscow 115409, Russia*

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ABSTRACT

A new version of the SigmaCalc Internet site (http://sigmacalc.iate.obninsk.ru) intended to provide evaluated differential cross-sections for spectra simulation is presented. Results of the revision of previously evaluated cross-sections and new evaluations including data for PIGE were made available to the IBA community through a simple interface. New SigmaCalc features allow users to compare evaluated differential cross-sections with the available results of the cross-section measurements taken on-the-fly from the IBANDL database and to validate them against benchmarks. The current status of the evaluated cross-sections for IBA is discussed.



## 1. Introduction

The Ion Beam Analysis (IBA) methods depend on the available cross-section data. These data are needed while planning experiments and in order to derive element concentrations through computer simulation of measured spectra. A cross-section evaluation is the process of analyzing experimentally measured cross sections, combining them with the predictions of nuclear model calculations, and attempting to extract their true values [1]. In other words the givens are different sets of (generally inconsistent) experimental data measured at sparse points on energy and angle and the task is to find the most accurate possible smooth curves of $d\sigma/d\Omega(E,\theta)$. It was shown in numerous papers that the evaluation of the cross sections by combining a large number of different data sets in the framework of the theoretical model makes it possible to calculate excitation functions for analytical purposes for any scattering angle, with a reliability exceeding that of any individual measurement. The methodology of the evaluation of the cross-sections relevant to IBA and some results previously obtained can be found in [2] and [3] respectively.

SigmaCalc is the name of the Internet site. It was developed as an interface to the evaluated cross-sections in order to provide IBA practitioners with access to the evaluated data. Initially it was hosted by Surrey University, UK and then by the IAEA while this was technically possible. After a hacker attack in 2012 the SigmaCalc site was shut down along with other nuclear data services located at the IAEA NDS server [4] and after a long period of outage it was moved first back to Surrey University and then to the server of the Institute for Nuclear Power Engineering in Obninsk, Russia, (http://sigmacalc.iate.obninsk.ru) where it is currently hosted.

In the new 2.0 version of SigmaCalc the results of the evaluations performed during the SigmaCalc outage as well as the evaluations recently made including the cross-sections for PIGE were added. Many corrections were made in the previously evaluated cross-sections following feedback from the SigmaCalc users and the results of benchmarks, i.e. integral experiments which consisted of measurements of charged-particle spectra from well characterized uniform thick targets followed by standard simulations using microscopic cross-sections. The idea of benchmarking is to verify the validity of the data for the purpose they are intended for through their use in a typical application. A database of the available benchmarks was incorporated into SigmaCalc and a feature was developed to compare spectra simulated using the evaluated cross-sections against benchmarks.

In order to provide users with the possibility to compare evaluated differential cross-sections with the available results of the cross-section measurements the presentation of the calculated cross-sections was modified to combine them with experimental data taken on-the-fly from IBANDL (https://www-nds.iaea.org/exfor/ibandl.htm).

## 2. Presentation of the evaluated cross-sections

The calculations at the SigmaCalc server are made using a number of codes corresponding to various nuclear reaction models with the parameters fixed by the evaluation procedure. Naturally the

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0168-583X/

calculations take some time but this time normally does not exceed ~10 s. The SigmaCalc output formats are versatile. There is a possibility to choose units for energy and cross-sections as well as to obtain a standard file in the R33 format [5].[1] In the last case the file with the evaluated cross-sections is presented in a table along with the experimental data downloaded from the IBANDL database which is currently maintained by the IAEA NDS staff and is located at a cloud server (Fig. 1). As far as the data are taken directly from IBANDL in response for each individual request a complete set of the experimental data available in the database at the moment of the request is automatically made available to a user. Since a visual inspection continues to be important, the estimation of the agreement between different data sets using the SigmaCalc graphics module was made more sophisticated, with various options allowing the user to manipulate the image.

For the sake of traceability of changes made in the evaluated files the "Version" entry of the R33 format was used to indicate the date of the last revision of the evaluation of a given cross-section. One of the reasons for revisions is appearance of new experimental data. Naturally all the experimental data available by the moment the revision was accomplished were taken into account. As a rule the references to all the sources of experimental information used in the evaluation can be found following the link "About/Cross-sections/ReactionName" in the SigmaCalc front page.

In order to provide the integration of SigmaCalc into IBANDL it was configured to send results of calculations (as R33 files) in response to external calls. In principle for the available evaluated cross-sections both SigmaCalc and IBANDL interfaces could provide a user with an access to the same data sets. In practice updates of the links to SigmaCalc are made in IBANDL with a significant delay and currently there are several evaluated cross-sections which are already for a long time unavailable through IBANDL. On the other hand the IAEA distributes a so called SigmaCalc archive which contains a combination of obsolete and new files downloaded from different versions of SigmaCalc. Users should be cautioned that the obsolete files from the SigmaCalc version 1.6 cannot be regarded as a reliable source of the evaluated data.

For PIGE the IBANDL data are of three different sorts – differential cross-sections in mb/sr, total cross-sections in mb, and yield in number of gamma quanta emitted in a unit solid angle per 1 μC. In order to provide the comparison the calculated data are converted on-the-fly as needed.

## 3. Validation of the evaluated cross-sections

The cross-section validation can be described very simply as the comparison of calculations utilizing a set of evaluated nuclear data, with the results of measurements in a benchmark experiment [6]. In order for an experiment to be classified as a benchmark, it must satisfy a basic criterion: the measurements must be performed in a system that facilitates simple computational modeling and the results of the measurements must be reliably established and documented. Also uncertainties introduced in modeling must not be allowed to mask the errors that may be contained in the nuclear data. Benchmark experiments provide the reference for the validation of basic nuclear data in various fields (see e.g. [6] where 5 different cases are described). In the case of the IBA related cross-section such an experiment consists in the measurement of a spectrum from a uniform thick target. If the simulation of a bulk sample spectrum fits, then the cross-section is valid. If the simulation does not fit, this does not necessarily mean that the cross-section is incorrect. The discrepancy

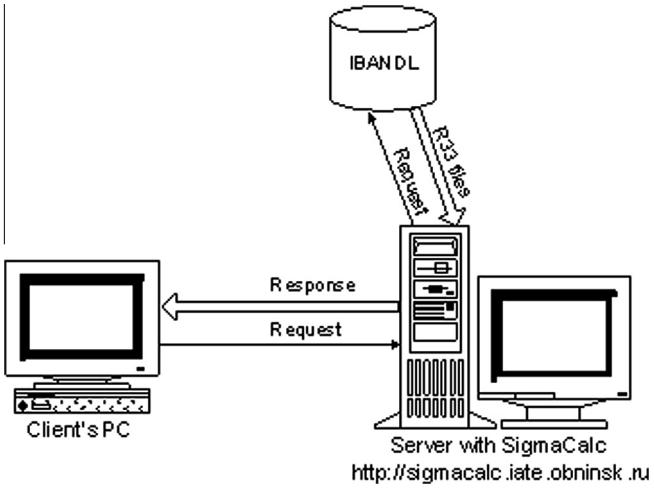


**Fig. 1.** Access to experimental data through SigmaCalc.

may be caused by the inappropriate target quality, mistakes in the accelerator energy calibration, the inaccuracy of the stopping power data and the energy loss straggling model used in the calculations, problems in taking into account such effects as multiple and plural scattering, pulse pile-up etc. Thus the validation failure may indicate more complex problems than the inaccurate cross-section and the benchmark results should be interpreted with a corresponding care. It should be stressed that a proper design of the benchmark is not a trivial task. The detailed consideration of the problems inherent in the benchmark experiment can be found elsewhere [7].

The importance of benchmarking has been recognized by the IBA community and nowadays the works in which this concept is employed are not rare in the literature (see e.g. [8–10]). Benchmarking is an important step in the evaluation methodology which provides an evaluator with a feedback for the next iteration of the cross-section evaluation. On the other hand the benchmark results enable an IBA practitioner to judge to what extent the agreement between simulated and measured spectra can be expected with the use of a given evaluated cross-section. In order to facilitate such a comparison a feature intended for a visual inspection of the validity of the cross-sections for spectra simulation was developed in SigmaCalc. A format which resembles the R33 format used for IBA relevant cross-section files was accepted for files with benchmark spectra. In addition to the spectra themselves the files contain the experimental information needed for the spectra simulation (see Appendix A).

The evaluated cross-section data constitute an array of points $(E_i,\sigma_i)$. Taking into account that the points are dense enough on energy for the cross-section to be smoothed by the spreading caused by a spectroscopy system resolution the energy spectrum for a uniform thick target is constructed in a following way.

First the energy $E_i$ is assigned to be equal to the energy $E_1$ which a projectile of the initial energy $E_0$ penetrating a sample possesses at the depth $x_i$, where the interaction characterized by the cross-section $\sigma_i$ occurs. Then the depth $x_i$ and the corresponding energy $E_{3i}$ registered by a detector are calculated. In order to speed up the calculations stopping power was approximated by a following function

$$S(E) = S_0 E^{-\alpha},$$

which is valid well above the stopping power maximum that is typical for EBS. The use is made of possibility to integrate this function analytically. The corresponding formulas are as follows:

[1] The R33 format description including its extension to accommodate PIGE data can be found at https://www-nds.iaea.org/exfor/x4guide/R33/.

$$x_i = -\int_{E_0}^{E_{1i}} S^{-1}(E)dE = -\int_{E_0}^{E_{1i}} S_0 E^{\alpha} dE = \frac{E_0^{\alpha+1}}{S_0(\alpha+1)} - \frac{E_{1i}^{\alpha+1}}{S_0(\alpha+1)},$$

$$\frac{x_i}{\cos\theta} = -\int_{E_{2i}}^{E_{3i}} S^{-1}(E)dE = \frac{E_{2i}^{\alpha+1}}{S_0(\alpha+1)} - \frac{E_{3i}^{\alpha+1}}{S_0(\alpha+1)},$$

$$E_{3i} = \left[E_{2i}^{\alpha+1} - \frac{x_i}{\cos\theta} S_0(\alpha+1)\right]^{\frac{1}{\alpha+1}} = \left\{[kE_{i1}]^{\alpha+1} - \frac{x_i}{\cos\theta} S_0(\alpha+1)\right\}^{\frac{1}{\alpha+1}},$$

where $\theta$ is a scattering angle, $E_2$ is the energy of the outgoing particle immediately after an interaction, and $k$ is a kinematical factor.

The interaction yield $Y_1(E_{1i})$ at the depth $x_i$ is obtained by a convolution of the cross-section with the beam spreading function which is assumed to be represented by Bohr's straggling theory:

$$Y_1(E_{1i}) = \frac{C}{s_{1i}\sqrt{2\pi}} \int e^{-\frac{(E-E_{1i})^2}{2s_{1i}^2}} \sigma(E)dE,$$

where

$$s_{1i}^2[\mathrm{keV}^2] = 0.26 Z_p^2 Z_t x_i [10^{18}\mathrm{at/cm}^2]$$

with $Z_p$ and $Z_t$ standing for the charges of the projectile and the target nucleus respectively, and $C$ is atomic concentration.

The yield of the registered particles $Y_3(E_{3i})$ is calculated as a convolution of the yield $Y_1(E_{1i})$ with the Gaussian spreading function, the variance $s_{2i}^2$ including both straggling on the way out and the detector resolution:

$$Y_3(E_{3i}) = \frac{1}{s_{2i}\sqrt{2\pi}} \int e^{-\frac{(E-E_{3i})^2}{2s_{2i}^2}} Y_1(E)dE.$$

The yield per a MCA channel of width $\Delta E_3$ is

$$\Delta Y_3(E_{3i}) = Q\Omega Y_3(E_{3i}) \frac{\Delta E_3}{dE_{3i}/dx},$$

where $Q$ and $\Omega$ are the number of projectiles and the detector solid angle respectively, and

$$\frac{dE_{3i}}{dx} = \left[(kE_{1i})^{\alpha+1} - \frac{x_i}{\cos\theta} S_0(\alpha+1)\right]^{-\frac{\alpha}{\alpha+1}} \left(-k^{\alpha+1} - \frac{1}{\cos\theta}\right) S_0.$$

The stopping power approximation used in the calculations is accurate up to tenths of percent in the energy range of interest as can be seen from Fig. 2. It is worth noting that the discrepancy between different systematics of the stopping power data is much greater.

As far as a single-element target can be fabricated only in rare favorable cases composite targets are as a rule used in benchmark experiments. Accordingly calculations are made for all the target elements and a sum of the spectra along with partial ones is displayed in the plot for a comparison with the measured spectrum. A typical SigmaCalc output for the benchmark [8] of the $^{32}S(pp_0)^{32}S$ cross-section with a $MoS_2$ target is presented in Fig. 3. Since SigmaCalc plots are intended for the validation of particular cross-sections rather than for analytical purposes the simulation is truncated at the high energy edge of the spectrum corresponding to the validated cross-section. The comparison between the simulations obtained with SigmaCalc and with a new version of SIMNRA [11] is demonstrated in Fig. 4. Due to secondary effects such as multiple and plural scattering which are not taken into account in the calculations the comparison between simulated and measured spectra has significant importance mainly in a relatively narrow region near the high energy edge of the spectrum. It should be noted that in the region of resonances significant differences between different simulation codes were found in the "Intercomparison" exercise [12]. It is a safe assumption that additional efforts were applied by the code developers in order to overcome the

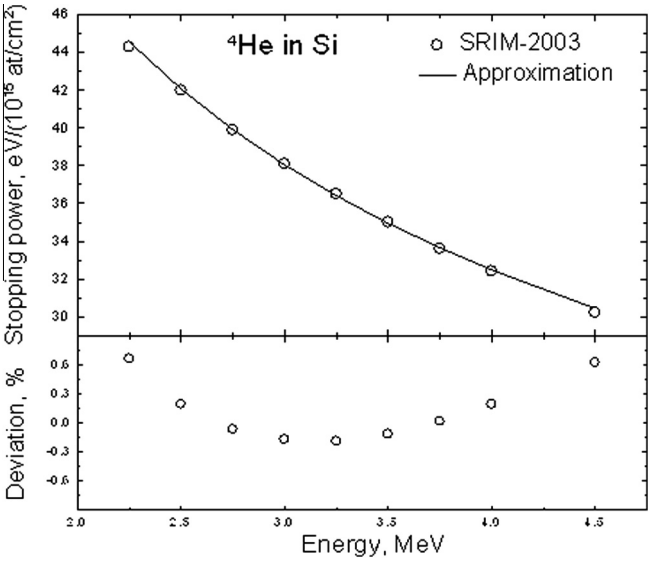


**Fig. 2.** Stopping power approximation.

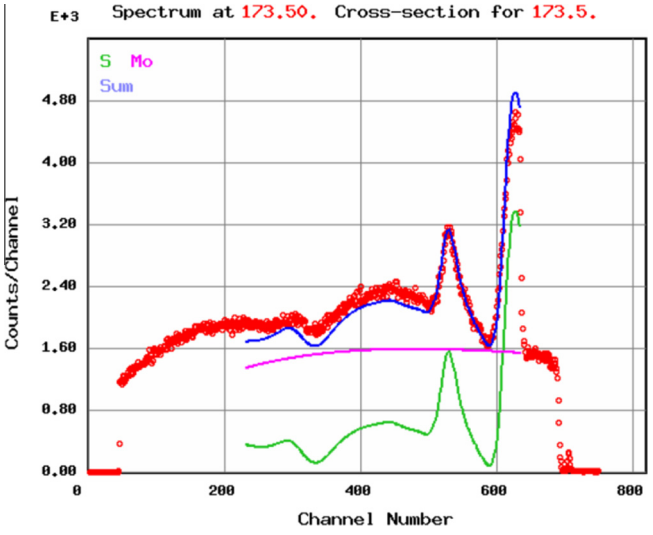


**Fig. 3.** Validation of the cross-section from SigmaCalc 2.0 against a spectrum from $MoS_2$ measured at 3538 keV [8].

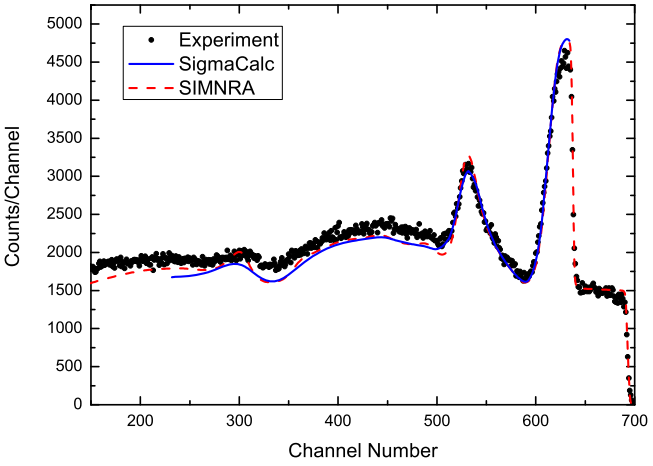


**Fig. 4.** Comparison of the simulations of the spectrum shown in Fig. 3 by SigmaCalc and by SIMNRA 6.86.

revealed problem. If they succeeded then the small discrepancies between the SigmaCalc and SIMNRA simulations seen in Fig. 4 will be similar in the case of the SigmaCalc comparison with new versions of the other codes studied in [12]. The work is under way to understand the origin of the discrepancies.

## 4. Present status of the evaluated cross-sections

The analysis of the IBANDL statistics shows that more than 90% of retrievals are for 15 cross sections related to 7 elements. All of them have been already evaluated (see Table 1) and some were validated through benchmarks. However the process of the evaluation is dynamic and it is possible that further cross-section measurements undertaken at a higher level of experimental accuracy and/or benchmark experiments give rise to the revision of the present data. Besides, the extension of the evaluation at higher energies is needed in many cases.

It should be pointed out that there are many cases where new experimental information is critically needed for the evaluation. For example there are problems even in the most wanted for EBS cross-sections such as $^{16}O(\alpha,\alpha)^{16}O$ and $^{12}C(\alpha,\alpha)^{12}C$ at elevated energies. In the case of NRA there are significant discrepancies between the available data sets for $^{16}O(d,\alpha)^{14}N$, $^{18}O(p,\alpha)^{15}N$, and a number of others. The corresponding evaluated cross-sections are pending for a revision dependent on the availability of new experimental data.

Although the cross-sections for boron are absent in the list of the most often retrieved data from IBANDL boron is a very important technological element and the quantitative determination of the boron depth distribution in both heavy and light matrices is of great scientific and technological importance. As far as EBS methods are concerned, the elastic backscattering of protons on boron as well as on other light nuclei has some advantages over the EBS with alphas because of larger probing depths and better sensitivity due to the nuclear cross section enhancement. Until recently the evaluation of the corresponding cross-sections was hampered by serious discrepancies between the available experimental data. Now that the benchmark experiment [9] resolved the conflict between the different experimental datasets the evaluation of the proton elastic scattering cross-sections for boron isotopes is one of the priorities in the future development of SigmaCalc.

There is also need in the evaluated cross-sections for NRA with $^3$He ions as projectiles. Preliminary calculations show that the theoretical approach is feasible also in this case however the available experimental information is currently insufficient for the evaluation.

As for PIGE methodologically the way of the cross-section evaluation is clear [24], and the evaluated cross-sections for $^{23}$Na(p,

**Table 1**
Evaluated cross-sections.

| Isotope | Projectile | Reaction | Evaluated to (MeV) | Reference | Last revision |
|---|---|---|---|---|---|
| $^{1}$H | α | Recoil | 12.0 | [13] | 09-12-2014 |
| $^{4}$He | p | Elastic | 3.0 | [3] | 09-12-2014 |
| $^{9}$Be | α | Elastic | 4.0 | – | 07-06-2015 |
| $^{12}$C | p | Elastic | 7.0 | [14–15] | 07-01-2015 |
| | α | Elastic | 7.2 | [16–18] | 13-01-2012 |
| | d | Elastic | 2.0 | [3] | 31-07-2008 |
| | d | $(d,p_0)$ | 1.9 | [19] | 26-01-2014 |
| $^{13}$C | p | Elastic | 2.5 | [20] | 18-11-2013 |
| $^{14}$N | p | Elastic | 5.0 | [21–22] | 10-09-2010 |
| | α | Elastic | 4.6 | [23] | 11-09-2014 |
| | d | $(d,p_0)$ | 2.05 | – | 01-02-2010 |
| | d | $(d,\alpha_{0,1})$ | 2.2 | – | 23-03-2010 |
| $^{16}$O | p | Elastic | 4.1 | [24] | 12-08-2001 |
| | α | Elastic | 6.9 | [3] | 03-09-2014 |
| | d | Elastic | 1.98 | – | 04-08-2008 |
| | d | $(d,p_{0,1})$ | 1.98 | – | 06-06-2013 |
| | d | $(d,\alpha_0)$ | 1.98 | – | 26-04-2010 |
| $^{18}$O | p | $(p,\alpha)$ | 1.0 | – | 09-10-2014 |
| $^{19}$F | p | Elastic | 1.75 | [3] | 12-11-2013 |
| | α | Elastic | 3.7 | – | 02-12-2010 |
| $^{20}$Ne | p | Elastic | 2.7 | [3] | 23-10-2008 |
| | α | Elastic | 4.0 | – | 08-10-2014 |
| $^{23}$Na | p | Elastic | 1.48 | [3] | 12-11-2013 |
| | p | $(p,p_1\gamma)$ | 2.4 | [25] | 01-09-2013 |
| $^{24}$Mg | p | Elastic | 2.7 | [26] | 28-05-2013 |
| $^{nat}$Mg | p | Elastic | 2.7 | [26] | 28-05-2013 |
| $^{27}$Al | p | Elastic | 1.82 | [27] | 12-11-2013 |
| | p | $(p,p_1\gamma)$ | 3.0 | – | 16-03-2014 |
| $^{28}$Si | p | Elastic | 3.5 | [28–29] | 05-06-2013 |
| | α | Elastic | 5.2 | [6] | 26-03-2013 |
| $^{nat}$Si | p | Elastic | 3.5 | [28–29] | 05-06-2013 |
| | α | Elastic | 5.2 | [10] | 26-03-2013 |
| $^{31}$P | p | Elastic | 2.0 | [3] | 11-11-2013 |
| $^{32}$S | p | Elastic | 3.5 | [3] | 29-10-2013 |
| $^{40}$Ar | p | Elastic | 2.8 | [3] | 17-02-2011 |
| $^{nat}$K | p | Elastic | 2.5 | [3] | 12-11-2013 |
| $^{nat}$Ca | p | Elastic | 2.9 | [3] | 06-06-2013 |
| $^{48}$Ti | p | Elastic | 2.5 | [3] | 29-05-2013 |
| $^{nat}$Ti | p | Elastic | 2.5 | [3] | 29-05-2013 |
| $^{52}$Cr | p | Elastic | 4.2 | – | 24-11-2013 |
| $^{nat}$Cr | p | Elastic | 4.2 | – | 24-11-2013 |
| $^{56}$Fe | p | Elastic | 3.3 | – | 13-05-2010 |
| $^{nat}$Fe | p | Elastic | 3.3 | – | 13-05-2010 |

$p_1\gamma)^{23}$Na and $^{27}$Al(p,$p_1\gamma)^{27}$Al are already presented in SigmaCalc, however lack of a sufficient body of consistent experimental data makes the evaluation of the PIGE data problematic. Unfortunately unreasonably large discrepancies are typical for the PIGE related experimental data (see IBANDL).

Currently evaluated cross sections are supplied without information about their uncertainty. While attempting to determine the uncertainty one is faced with the problem of systematic errors inherent in the experimental data. The classical statistical theory does not consider systematic errors. It is implied that these errors should be somehow eliminated before the methods of statistics are applied. Within the framework of a separate work the systematic error cannot be revealed in principle. However, the evaluated cross section is based on the results of several measurements and this makes it possible to determine the corresponding covariance matrix for the experimental data followed by the analysis of the errors. Such an analysis has become standard practice for neutron cross-section data, and an attempt was made to extend it to the cross-sections used in IBA [18]. Whereas the applied approach is formally robust the obtained results seem to underestimate the uncertainty.

It should be noted that the current IBA simulation codes, widely used by the IBA community, do not take into account the uncertainties in the input data and so the efforts to assign uncertainties to the evaluated cross-sections will be useless in a practical sense unless the codes applied for the IBA spectra simulation are modified to take the cross-section uncertainties into account.

## 5. Conclusions

After of about a year and a half of outage SigmaCalc was made again available to the community. It currently provides the majority of the most wanted cross-sections for EBS and NRA. Though a significant step in establishing a firm basis for analytical work has been made, the needs in the evaluated nuclear data for the ion beam analysis are not yet completely satisfied. The work remains to increase the number of the nuclei for which the evaluation was performed, to extend the energy range where the evaluation was made as well as to evaluate the cross-sections of the nuclear reactions induced by $^3$He ions. Carefully designed benchmarks and/or new measurements are needed in order to resolve problems in some important cases. The development of SigmaCalc continues with the ultimate goal to provide the IBA community with a comprehensive source of the evaluated cross-sections which should eventually substitute experimental cross-sections still used for spectra simulations.

## Acknowledgements

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## Appendix A. Format of benchmark files

The files containing benchmark spectra have the “bnm” name extension and are stored in SigmaCalc in the ASCII format resembling the R33 one:

*Comment: The same as in the R33 format*
*Source: The same as in the R33 format*
*Target: Target chemical formula (may include HTML tags)*
*Theta: The same as in the R33 format.*
*FWHM: Detector resolution (keV)*
*ChannelWidth: MCA channel width (keV)*
*Offset: MCA zero channel offset (keV)*
*Energy: The same as in the R33 format.*
*QOmega: Number of projectiles multiplied by detector solid angle in $10^{12}$ particles × sr*
*Stopping: $S_0$ α stopping power approximation parameters as defined in the text*
*Straggling: Straggling correction factor*
*Element1: Chemical symbol Atomic number Atomic mass Number of atoms per molecule Straggling correction factor*
*Element2: The same as Element1*
. . .
*ElementN: The same as Element1*
*Data:*
*Channel number Counts/Channel*
. . .
*EndData:*

An example:

*Comment: This is an example of a ∗.bnm file.*
*Source: V. Paneta et al. Nucl. Instr. Meth. B328 (2014) 1.*
*Target: MoS<sub>2</sub>*
*Theta: 173.5*
*FWHM: 15*
*ChannelWidth: 4.915*
*Offset: -19.9*
*Energy: 3538*
*QOmega: 0.0515*
*Stopping: 12.056 0.6664*
*Element1: S 16 32 2 1.0*
*Element2: Mo 42 95 1 1.0*
*Data:*
1.0 0.0
2.0 0.0
3.0 0.0
. . ..
*EndData:*

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