https://doi.org/10.61092/iaea.xfh9-5z24

INDC(NDS)- 0690
Distr. IBA

IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Summary Report

Technical Meeting

Benchmarking Experiments for Ion Beam Analysis

IAEA Headquarters
Vienna, Austria

26 – 29 May 2015

Prepared by

M. Chiari
INFN Sezione di Firenze
Firenze, Italy

and

P. Dimitriou
Nuclear Data Section, IAEA
Vienna, Austria

May 2016

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from
http://www-nds.iaea.org/publications
or sent as an e-mail attachment.
Requests for hardcopy or e-mail transmittal should be directed to
NDS.Contact-Point@iaea.org
or to:
Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria

May 2016

INDC(NDS)- 0690
Distr. IBA

Summary Report

Technical Meeting

Benchmarking Experiments for Ion Beam Analysis

IAEA Headquarters
Vienna, Austria

26 – 29 May 2015

Prepared by

M. Chiari
INFN Sezione di Firenze
Firenze, Italy

and

P. Dimitriou
Nuclear Data Section, IAEA
Vienna, Austria

Abstract

A Technical Meeting was held from 26 to 29 May 2015, to discuss benchmarking experiments for validation of nuclear reaction cross-section data for Ion Beam Analysis. Participants defined the general methodology of benchmarking measurements, proposed specific guidelines for the main IBA techniques, and produced a list of priority benchmark experiments. The summaries of participants' presentations as well as the technical discussions are included in this report.

May 2016

Contents

1 Introduction

Ion beam analysis (IBA) is a family of modern analytical techniques involving the use of energetic ion beams to probe the composition of the surface layers of solids. Major areas of application include microelectronics, cultural heritage, environment, forensics, biology and materials sciences.

Although the basic physical processes underlying IBA techniques are well understood, the reliability of data interpretation is limited by poor knowledge of the physical data such as stopping powers and cross sections of the interactions of charged particles with the target ions in the solid.

The lack of reliable cross section data was recognized by the IBA community long ago and was discussed at numerous meetings and workshops. In order to address the problem the IAEA held two Coordinated Research Projects (CRP): the CRP on "Development of a Reference Database for Ion Beam Analysis" from 2005-2009 [1.1], and the CRP on a Reference Database for Particle-Induced Gamma-ray Emission spectroscopy (PIGE) from 2011- 2015 [1.2] which was concluded recently. The ultimate goal of both CRPs was to create a comprehensive and up-to-date library of recommended data of relevance to IBA. The resulting Ion Beam Analysis Nuclear Data Library is hosted on the IAEA Nuclear Data Section server (http://www-nds.iaea.org/ibandl/).

Currently IBANDL contains more than 3000 individual cross-section datasets. This includes almost all experimental differential cross-section data ever measured from the 1940's until now. Numerous evaluated theoretical cross sections are available for many cases important for practical IBA applications through the SigmaCalc website (http://sigmacalc.iate.ru/). IBANDL and SigmaCalc are heavily used by the IBA community and have largely contributed to extending the applicability of IBA methods e.g. towards higher energies, thus creating possibilities for new applications.

While knowledge of the fundamental input parameters, namely, stopping power and cross-section is often sufficient for the quantitative application of IBA methods, the requirement of traceability and quality assurance necessitates also the knowledge of the uncertainties of the used stopping power and cross-section data to estimate the total uncertainty budget of a measurement. More and more in IBA application providing all the results along with uncertainties is becoming imperative.

For well-designed experiments, the uncertainty of an IBA measurement is dominated by the uncertainty of the fundamental input data, e.g. the nuclear cross section and the stopping power, necessary for the evaluation of the measured spectra. The uncertainties of stopping-power data have been investigated for many years by statistical analyses and are well traced [1.3]. For cross sections the situation is different. Currently, evaluated SigmaCalc cross sections are not supplied with information about their uncertainty. The uncertainty of evaluated cross sections can be obtained by statistical analysis taking into account the uncertainties of the input data and their correlations. In cases where experimental data show a very large scatter or are even contradictory, performing an evaluation is not straightforward.

To address all these issues associated with the accuracy of experimental and theoretical nuclear cross-section data for IBA and benchmarking, a Consultant's meeting was held by the NDS from 11 to 13 March 2013 [1.4]. The meeting addressed various statistical approaches

and discussed benchmarking as a valuable alternative tool for validating nuclear cross-section data. Benchmarking is widely used for the validation of neutron data and such a practice could significantly improve the situation and provide insight in the uncertainties associated with nuclear data relevant to IBA.

In response to the recommendations of the above meeting [1.4], the IAEA held a Technical Meeting on Benchmarking experiments for IBA applications from 25 to 26 May 2015, at the IAEA Headquarters in Vienna. Twelve participants from eleven countries attended the meeting. Jyrki Raisanen (Finland) was elected chairman, and Massimo Chiari (Italy) rapporteur. Robin Forrest, Section Head, welcomed the participants and acknowledged the importance of their work for the IBA community, while Paraskevi Dimitriou (IAEA), the Scientific Secretary, made a brief introduction to the purpose and goals of the meeting.

The objectives and expected outputs of the meeting are described in the following section, followed by summaries of participants' presentations and the main technical points covered by the discussions. The meeting agenda and the list of participants can be found in Appendices 1 and 2, respectively. Links to the presentations are available in Appendix 4.

References

[1.1] Reference database for ion beam analysis (2005-2010), **IAEA TECDOC-1780** (December 2015); available at: https://www-nds.iaea.org/publications/tecdocs/TE-1780_web.pdf

[1.2] P. Dimitriou and A. Pedro de Jesus, Summary Report of the 3rd Research Coordination Meeting on Development of a Reference Database for Particle-Induced Gamma ray Emission (PIGE) Spectroscopy, IAEA Vienna, Austria, 7–11 April 2014, IAEA Report INDC(NDS)-0664, 2014, available at: INDC(NDS)-0664, P. Dimitriou *et al*, Development of a Reference Database for Particle-Induced Gamma-ray Emission spectroscopy, Nucl. Instrum. Methods **B 317** (2016) 33. 10.1016/j.nimb.2015.09.052; http://www-nds.iaea.org/pige/.

[1.3] J.F. Ziegler *et al*., Nucl. Instrum. Methods **B268** (2010) 1818; H. Paul, Nucl. Instrum. Methods **B273** (2012) 15.

[1.4] D. Abriola, P. Dimitriou, A. Gurbich, Summary Report of a Consultant's Meeting on Accuracy of Experimental and Theoretical Nuclear Cross-Section Data for Ion Beam Analysis and Benchmarking, IAEA Vienna, Austria, 11-13 March 2013, IAEA Report INDC(NDS)-0634, 2013, available at: INDC(NDS)-0634.

2 Objectives of the meeting

The purpose of this Technical Meeting was to lay the grounds for using benchmarking experiments to validate nuclear reaction cross sections relevant to Ion Beam Analysis. The main output is this document which can be used as a guide and reference by the community of practitioners.

The following items were addressed in detail:

- methodology of benchmarking experiments,
- guidelines for performing benchmark experiments for the various IBA techniques,
- priority list of reactions that should be considered for benchmarking,
- the need for duplicate and/or round-robin experiments, and
- dissemination.

3 Participants' Presentations

3.1 A review on the methodology of benchmarking experiments: assessment of physical and technical problems, M. Kokkoris

The implementation of all Ion Beam Analysis (IBA) depth profiling techniques critically depends on the accuracy of the available differential cross sections for the reactions involved. Unfortunately, the existing experimentally determined differential cross-section data are in many cases quite scarce and/or discrepant, thus their reliability is highly questionable. On the other hand, the evaluated cross-sections, when available, are the most reliable ones to be used in analytical studies, since they involve a critical assessment of the experimental datasets, followed by a proper tuning of the corresponding nuclear model parameters. However, it is important to point out that most of the evaluated datasets are still not adequately validated. A carefully designed benchmarking procedure (i.e. the validation of differential cross-section data via the acquisition of thick-target spectra followed by their simulation) is thus mandatory. Benchmarking can also provide the necessary feedback for the adjustment of the parameters of the nuclear model used in the evaluation process, and can help in assigning realistic uncertainties to the cross sections. Moreover, in the absence of evaluated cross sections, it can indicate recommended experimental datasets.

Recently, a dedicated effort was made to thoroughly document this procedure [1], followed by a consultant meeting organized by IAEA. In the present review an attempt was made to present the recommended steps and to critically assess the problems of the benchmarking process in the following cases: (1) In $^{nat}Si(p,p_0)$, for Ep=1.5-3.5 MeV, where channeling perturbations in crystalline wafers, if not carefully treated, can seriously affect the accuracy of the measurements, while the size of the powder used in pressurized tablets can affect the shape of resonances in the experimental thick-target yield spectra, (2) in $^{19}F(p,p_0)$ and $^{nat}B(p,p_0)$, for Ep=1.5-2.5 MeV, where, for the removal of the important underlying α-particle background, ΔE/E telescopes have been implemented, and (3) in $^{nat}O(p,p_0)$, for Ep=1.5-4 MeV, where target related effects (e.g. roughness) need to be taken into account. New results on $^{27}Al(p,p_0)$, $^{nat}C(d,d_0)$ and $^{nat}O(d,d_0)$ were also presented and discussed.

Reference

[1] V. Paneta, J.L. Colaux, A.F. Gurbich, C. Jeynes, M. Kokkoris, Nucl. Instr. Methods **B328** (2014) 1-7.

3.2 Accurate analysis using elastic backscattering together with benchmarking, Ch. Jeynes

We have recently demonstrated that Rutherford backscattering (RBS) analysis can be used as a fully traceable reference method [1,2,3]. The traceability depends on the demonstration of the very high linearity of the spectrometry system [4], and on the ability to unequivocally demonstrate the high accuracy determination of the beam energy [5].

The analytical use of non-Rutherford elastic backscattering (EBS) depends on accurate knowledge of the relevant scattering cross-sections. For traceability, it is my opinion that it is essential for evaluated cross-sections [6,7] to be used, but this is not enough since it has turned out to be remarkably difficult to properly construct an uncertainty budget for EBS. Consequently, it is currently my opinion that the uncertainty budget for any particular analysis must be constructed with the help of benchmarking spectra.

One application of such an approach was shown with the example of a primary determination of the resonance energy of the $^{16}O(\alpha,\alpha)^{16}O$ reaction near 3.04 MeV, which was determined by EBS as 3038.1 ± 1.3 keV [5] (the literature value is 3038.1 ± 2.3 keV [8]).

Benchmarking should not only be used to validate EBS cross-sections but also be used to accurately determine the position of EBS resonances. We have demonstrated that in both cases valid estimates of uncertainty can be made.

References

[1] C. Jeynes, N.P.Barradas, E. Szilágyi, Accurate determination of Quantity of Material in thin films by Rutherford backscattering spectrometry, Analytical Chemistry 84 (2012) 6061-6069; http://dx.doi.org/dx.doi.org/10.1021/ac300904c

[2] J. L. Colaux and C. Jeynes, High accuracy traceable Rutherford backscattering spectrometry of ion implanted samples, Analytical Methods **6** (2014) 120-129; http://dx.doi.org/10.1039/c3ay41398e

[3] Julien L. Colaux, Chris Jeynes, Keith C. Heasman and Russell M. Gwilliam, Certified ion implantation fluence by high accuracy RBS, Analyst **140** (2015) 3251-3261; http://dx.doi.org/10.1039/c4an02316a

[4] Julien L. Colaux and Chris Jeynes, Accurate electronics calibration for particle backscattering spectrometry, Analytical Methods **7** (2015) 3096-3104; http://dx.doi.org/10.1039/c4ay02988g

[5] J.L. Colaux, G. Terwagne, C. Jeynes, On the traceably accurate voltage calibration of electrostatic accelerators, Nucl. Instrum. and Methods **B349** (2015) 173–183; http://dx.doi.org/10.1016/j.nimb.2015.02.048

[6] D. Abriola, N.P. Barradas, I. Bogdanović-Radović, M. Chiari, A.F. Gurbich, C. Jeynes, M. Kokkoris, M. Mayer, A.R. Ramos, L. Shi, I. Vickridge, Development of a reference database for Ion Beam Analysis and future perspectives, Nucl. Instrum. and Methods **B269** (2011) 2972-2978; http://dx.doi.org/10.1016/j.nimb.2011.04.056

[7] A.F. Gurbich, Evaluated differential cross-sections for IBA, Nucl. Instrum. Methods **B268** (2010) 1703-1710.

[8] D.R. Tilley, C.M. Cheves, C.H. Kelley, S. Raman, H.R. Weller, Energy levels of light nuclei, A = 20, Nucl. Phys. A **636** (1998) 249–364.

3.3 Benchmark test measurements of elastic backscattering cross-sections measured at the Ruđer Bošković Institute (RBI), I. Bogdanović Radović

In order to examine if excitation functions for N(p,p)N and Al(p,p)Al that were measured at RBI in the energy range from 2.5 to 5 MeV can interpret properly the experimentally obtained thick target yields we performed benchmark test measurements. For N, thick BN target covered with 8 nm Au was used. To separate N(p,p)N spectrum from the background coming from $^{10}B(p,\alpha)^{10}B$, $^{11}B(p,\alpha)^{11}B$ as well as possible pile-up contributions ΔE-E telescope was used. Simulations were done using SIMNRA [1] program. The step width of the incident ions was chosen in such a way that for each point in the cross section file there was at least one sublayer in the simulation program. Contrary to the case of N, which is having only several well-separated resonances, excitation function for Al shows complex resonant structure in the measured energy range. Although energy resolution of our accelerator, target thickness as well as used energy steps (10--25 keV) were too wide to cover all details of complex excitation function for Al, we performed benchmark experiment using thick pure Al target covered with thin Au layer for the normalization purposes. This time two

simulation programs were tested SIMNRA [1] and NDF [2]. The results of our benchmark experiment for N and Al was shown and discussed.

References

[1] M. Mayer, Technical Report IPP 9/113, Max–Planck Institut fur Plasmaphysik, Garching, Germany, 1997.
[2] N.P. Barradas, C. Jeynes, R.P. Webb, Appl. Phys. Lett. **71** (1997) 291.

3.4 Nuclear reaction analysis and other IBA techniques at ANSTO, R. Siegele

At ANSTO a wide range of IBA techniques is used for quantitative analysis. These include a number of nuclear reaction techniques such as $^{16}O(p,\alpha)^{15}N$ at 846 keV as well as the intense (α,α) elastic scattering resonances for ^{12}C at 5.50-5.80 MeV and for ^{18}O at 7.30-7.65 MeV [1].

Currently a new beamline for the use of the $^{1}H(^{15}N,\alpha\gamma)^{12}C$ at 6.385 MeV for the depth profiling of Hydrogen is under development. Furthermore (p,γ) reactions are used on a regular basis to analyse specimens for fluorine and sodium.

Heavy ion ERDA is used on a regular basis for light elemental profiling in materials science [2]. Since ERDA can be used to profile a wide range of elements, some of the scattering cross sections are no longer Rutherford.

All these techniques require multiple input parameters that need careful examination in order to be reliable. An overview of the techniques used at ANSTO and evaluation of the accuracy and precision of the measurements was given. To validate these results a long-term evaluation of the analysis of data from the ANSTO beamlines was presented.

Some of the techniques that will be used on ANSTO beamlines currently under construction were also discussed.

References

[1] J.A. Davies, F.J.D. Almeida, J.S. Forster, H.K. Haugen, T.E. Jackman, and R. Siegele, Quantitative calibration of intense (α,α) elastic scattering resonances for ^{12}C at 5.50-5.80 MeV and for ^{18}O at 7.30-7.65 MeV, Nucl. Instrum. Methods **B85** (1994) 28.
[2] R. Siegele and David D. Cohen. Mapping of light elements with the ANSTO high energy heavy ion microprobe. Nucl. Instrum. Methods **B161-163** (2000) 354-358.

3.5 Proposal of a methodology to perform PIGE benchmarking experiments, A. Pedro de Jesus

The presentation started with a brief overview of the LIBPhys Laboratory, group and work. The Accelerator and Radiation Technologies Laboratory of CTN/IST has three accelerators: a 2.5 MV Van de Graaff, a 210 kV DanFisik Implanter and a 3 MV General Ionex Cockroft-Walton Tandetron. Emphasis was put on the nuclear reaction line and installed capabilities and the work done in relation to PIGE, namely: development of codes ERYA and ERYA profiling; cross section measurement of γ-producing reactions related to Li, B, F, Na, Mg, Al, P, for proton energy up to 4 MeV and Be for proton energy up to 1.7 MeV.

General considerations were made about benchmarking measurements, first in connection to cross section measurements, trying to answer the following questions: Is there enough cross

section data? What about γ angular distributions? Is there need for interlaboratory accurate "reference measurements"? The answers to these questions come from the fact that in relation to PIGE bulk analysis, systematic deviation of cross section values and other systematic uncertainties may be ruled out by adequate system calibration, while relative uncertainties (from one part of the excitation function versus another, due to experimental mistake or angular distributions) do matter! There are only a few measurements of angular distributions. If theory cannot help by evaluating cross sections and including angular distributions to convert from one angle to another, more measurements are needed.

In relation to benchmarking of standardless PIGE by accurate interlaboratory analysis of reference samples, a proposal was made comprising as a first step: known target, prepared in the same way; fixed energy of analysis; fixed energy values to measure the yield and extract yield calibration parameter; a given excitation function; a given code to perform the calculations; energy calibration of the accelerator at the same reference resonances. The known target should be easy to prepare, maybe Al (pure Al foil). As a second step every lab should perform analysis of an unknown (to the labs involved) reference target (NIST or equivalent).

3.6 Planning PIGE benchmarking experiments at CMAM, A. Zucchiatti

Great attention and efforts have been dedicated to improve the analytical performance of the PIGE technique, which is complementary to PIXE when the analysis of samples containing both medium and low Z elements (e.g. glasses) have to be characterized. So far reference to standards has been extensively used but fundamental parameters methods could be applied, like in EBS or PIXE once the production cross-sections are known with the required accuracy.

In the past three years, within the IAEA PIGE CRP, many new data have been collected on light elements from Li to Al, following a measurement strategy that required at least two laboratories measuring the same element and overlapping at least in a reasonably broad energy range. The data seem to have achieved a reasonable reproducibility below 3 MeV incoming proton energy, with explicit reference to the case of ^{19}F. However at higher energies they cannot be easily reconciled and therefore properly validated, unless carefully planned benchmark experiments are performed. At the same time it has been highlighted that the energy of sharp narrow resonances, to be used for light elements depth profiles should be confirmed with higher precision.

In this framework we show how CMAM is strengthening the controls on the operative chain that leads to the measurement of a cross section and in detail on: accelerator calibration, γ detector absolute efficiency measurement, collection of charge, thin layered targets preparation and characterization, measuring angle and aperture and environmental conditions (low residual vacuum, experimental room temperature). Accelerator calibration established with three different methods is presented and discussed. Precision absolute efficiency obtained with ±3% activity calibrated sources (^{133}Ba, ^{152}Eu, ^{137}Cs, ^{60}Co) is shown. The effect of the detector angular aperture on the accuracy of the differential cross-section measurement, either calculated from an experimental angular distribution or simulated with a Monte Carlo code is discussed and the range of acceptable apertures are shown. The problematic of absolute direct collected charge measurement and of thin targets preparation of light, highly mobile elements is finally discussed. Planning of benchmarking experiments at CMAM is duly ongoing.

3.7 Assessment of experimental PIGE cross section data in the case of the $^{12}C(d,p\gamma)^{13}C$ reaction, Á. Z. Kiss and L. Csedreki

While considerable effort has been devoted to establish benchmarking of Elastic Backscattering (EBS) and Nuclear Reaction Analysis (NRA) cross section data, in the case of Particle-Induced Gamma-ray Emission spectroscopy (PIGE) only a few benchmark measurements have been published up to now. Nevertheless compilation of published cross sections and critical assessment of the compiled data is in progress.

In this talk experimental cross section data for the $^{12}C(d,p\gamma)^{13}C$ reaction, available in literature [1-4], is assessed. Possible explanations of the observed differences are discussed. The importance of making a careful study of uncertainty budgets, accurate accelerator energy calibrations and absolute detector efficiency determinations is emphasized. On the basis of the critical assessment of experimental data, recommended total γ-ray producing cross sections for the 3089 keV γ-ray as a function of deuteron energy are given.

The critical assessment was controlled by a comparison of the thick target yields calculated from the above mentioned thin target cross sections of the 3089 keV γ-ray to literature data [5] of thick target yields measured at different deuteron energies for that γ-ray. The result of this PIGE benchmarking is presented.

References

[1] S. Tryti, T. Holtebekk and J. Rekstad, Angular distributions of protons near resonance for the reaction $^{12}C(d,p\gamma)^{13}C$ obtained by shape studies of y-ray lines, Nucl. Phys. **A201** (1973) 135-144.

[2] S. Tryti, T. Holtebekk and F. Ugletveit, Angular distributions of protons from the reaction $^{12}C(d,p\gamma)^{13}C$ obtained by shape studies of γ-ray lines, Nucl. Phys. **A251** (1975) 206-224.

[3] F. Papillon, P. Walter, Analytical use of the multiple gamma-rays from the $^{12}C(d,p)^{13}C$ nuclear reaction, Nucl. Instrum. Methods **B132** (1997) 468-480.

[4] L. Csedreki, I. Uzonyi, G.Á. Száki, Z. Szikszai, Gy. Gyürky, Á.Z. Kiss: Measurements and assessment of $^{12}C(d,p\gamma)^{13}C$ reaction cross sections in the deuteron energy range 740–2000 keV for analytical applications, Nucl. Instrum. Methods **B328** (2014) 59-64.

[5] Z. Elekes, Á.Z. Kiss, I. Biron, T. Calligaro, J. Salomon, Thick target γ-ray yields for light elements measured in the deuteron energy interval of 0.7-3.4 MeV, Nucl. Instrum. Methods **B168** (2000) 305-320.

3.8 Gamma-ray production cross sections and thick-target yields for the $^{14}N(p,p'\gamma)^{14}N$ reaction, J. Räisänen

Gamma-ray production cross sections for the $^{14}N(p,p'\gamma)^{14}N$ reaction have been determined in the energy range 3.586 MeV – 6.920 MeV using self-supporting 100 nm thick Si_3N_4 targets. Small energy steps of 5 keV were employed within regions near the main resonances. For benchmarking purposes proton induced thick-target γ-ray yields were measured at an angle of 55^o relative to the beam direction at 4.0, 4.5, 5.0, 5.5, 6.0 and 6.5 MeV using thick BN and Si_3N_4 targets, and a 50 μm thick polyimide (Kapton) foil. The Si_3N_4 membrane areal density and composition were determined by ERDA. The elemental compositions of the thick nitride targets were determined by TOF-ERDA measurements.

The measured cross section data is compared with the available literature data [1]. The present values are generally higher throughout the whole energy range. Reasonably good

agreement was found at energies up to 5 MeV, with increasing deviation at higher energies. In the present excitation curve the narrow resonances are narrower and stronger than in the literature excitation curve.

The measured thick-target yields are compared with corresponding calculated thick-target yields deduced from the present- and literature experimental excitation curves. This procedure serves as a good check for the cross section data as the thus obtained yield values should be comparable within the error limits. The use of different initial bombarding energies allows checking of the deduced excitation curve energy range by energy range, in our case within 0.5 MeV ranges. An exponential growth of the thick-target γ-ray yield as a function of proton energy was noted. The trends of the experimental and calculated values are similar. The calculated values are systematically lower than the experimental thick-target yields. The values obtained by using the cross section data of Ref. [1] are systematically the lowest; the deviation from the experimental values increases with bombarding energy. The mutual agreement of the calculated values is best at low energies. The BN target provides systematically slightly lower values than the Si_3N_4 target; otherwise all target materials provide consistent experimental values within uncertainty levels. It can be concluded that the measured yield values are systematically too high or the calculated yields are too low, i.e., the experimental cross sections are too low. Possible sources of error in the measured yield values are current integration, detection efficiency and the clearly most significant one is the stopping power correction. The stopping power values for all calculations have been taken from SRIM. The difference between the measured and calculated thick-target yields cannot be fully explained by the stopping power correction of the measured yields. To fully explain the noted difference the stopping powers for solid nitrogen should be about 40% lower than the values provided by SRIM. A more accurate treatment of the stopping power correction by using numerical methods is under way.

Reference

[1] G.W. Phillips *et al*. Phys. Rev. **C5** (1972) 297.

3.9 Benchmark test measurements of nuclear cross sections relevant for IBA at LABEC, M. Chiari

In this presentation some of the results obtained at LABEC from benchmark test experiments were shown, namely for the elastic scattering cross sections of protons on ^{19}F and ^{27}Al for proton beam energies higher than 3 MeV, including also the contribution of the inelastic scattering cross sections, i.e. $^{19}F(p,p')^{19}F$ and $^{27}Al(p,p')^{27}Al$, to the first relatively low-lying excited states, to reproduce the charged-particle spectra of the well-known uniform thick targets.

Recent measurements [1] of proton induced γ-ray emission thick target yields on some selected nuclides ($^{10,11}B$, ^{23}Na, ^{27}Al, ^{28}Si) for proton beam energies in the range between 2.5 and 4 MeV were discussed and compared to the yields obtained from the integration of differential cross sections available in the IBANDL data library, in order to validate them.

Reference

[1] M. Chiari, G. Ferraccioli, B. Melon, A. Nannini, A. Perego, L. Salvestrini, A. Lagoyannis, K. Preketes-Sigalas, Measurement of proton induced thick target γ-ray yields on B, N, Na, Al and Si from 2.5 to 4.1 MeV, Nucl. Instrum. Methods **B366** (2016) 77-82.

3.10 The bulk sample method in cross sections: measurement vs. benchmarking, N.P. Barradas

Scattering cross sections of interest to Ion beam Analysis are usually determined experimentally using thin film samples of known areal density. The detected yield can then be easily converted into a cross section value, provided that other quantities such as incident beam fluence and detector solid angle are known. The beam normally loses a modest amount of energy inside the film, and the cross section is usually considered to correspond to the average energy of the beam as it crosses the film. On the other hand, benchmarking of cross sections is very often made by measuring bulk sample spectra, and comparing the data with theoretical simulations assuming given cross sections. In recent years, however, a bulk sample method for experimental determination has been presented and applied to a number of cases. The method is based on simultaneously fitting many spectra, collected at different beam energies, treating the energy dependent cross section as a fit parameter. Bayesian inference data analysis is used to retrieve confidence limits of the cross section curves determined.

This method has received some criticism from experts in the field and from referees, but it also has been praised as leading to cross section data that does not depend on knowing a thin film areal density and thickness inhomogeneity. Some examples are presented, and the usefulness of bulk sample data for measurements vs. benchmarking purposes is discussed.

3.11 Current status of the benchmarking process, scope, complex problems and perspectives, M. Kokkoris

An attempt was made to discuss the scope and the future perspectives of the benchmarking process, and more specifically the goal for the creation of a new, dedicated library for model spectra, following the experience of the neutron physics community in the case of (n,f) reactions. New results were shown concerning evaluated data, and extensions of the evaluations, as well as comparisons with experimental datasets, were discussed and analyzed. Furthermore, complex technical and physical problems that affect the validation of microscopic differential cross-section data were presented, namely target related effects, stopping power variations, ADC channel width, integration region suitable for the validation, SSB detector dead layer effect (mainly in the case of (α,α) benchmarking spectra), and background subtraction in the case of (d,d) scattering. For this latter problem, the origin of the d-induced background was thoroughly presented for the important cases of $^{12}C(d,d_0,p_0)$ and $^{16}O(d,d_0,p_0,p_1,\alpha_0)$ reactions.

4 Technical discussions

Participants discussed the main steps involved in performing a well-designed and successful benchmark measurement. The proposed methodology and guidelines are expected to be refined and improved as a result of accumulated experience.

4.1 Benchmarking methodology

The general procedure for any benchmark measurement aimed at validating a given differential cross-section function is as follows:

- Define what has to benchmarked, considering a piecewise approach and including the acceptable accuracy level
- Perform the energy calibration of the accelerator
- Define energy steps for the specific excitation function
- Define detection angles for the specific excitation function
- Determine detector energy resolution and ADC calibration
- Determine detector absolute efficiency
- Choose a properly characterised suitable target
- Define measurement parameters such as beam intensity and measurement time
- Choose a suitable simulation code
- Define the basic input data for the simulation code, such as stopping power and cross sections
- Produce a traceable uncertainty budget
- Validation of the specific excitation function has to follow the piecewise approach and should take into account the uncertainty in the used basic input data.

Specific guidelines for the different cross sections and IBA techniques (Elastic Back-Scattering (EBS), Nuclear Reaction Analysis (NRA), Particle-Induced Gamma-ray Emission (PIGE) spectroscopy) were also discussed. It was agreed that in order to put these guidelines to the test, participants would form working groups where each group would undertake to carry out specific benchmark measurements using the proposed methodology and guidelines. The members of the groups would coordinate themselves, share and discuss their results and propose modifications if any to the set of guidelines.

4.1.1 EBS benchmarking guidelines

- Chose two suitable thick samples: polished non-crystalline simple targets with well-defined stoichiometry, easily available, the purest as possible (no contamination), not pellet (to avoid grains and voids). Examples: for silicon use fused SiO_2 (where very good stopping power is available) and amorphised silicon target; for carbon use glassy carbon; for oxygen fused SiO_2 and oxidised aluminum (maybe some other oxide with a high-Z element, but not too heavy to avoid too large Rutherford background). For nitrogen a GaN single crystal could be used, while rotating randomly during the measurement to eliminate channeling effects. The following holds for all the samples: a thin Au or Ag layer could be evaporated on the surface for normalization purposes.
- Define the energy steps; they should be chosen in order to have the resonances close to the surface, based on an a priori knowledge of the cross section. Considering the uncertainty in the straggling function, each step should not exceed a few hundreds of keV, e.g. 200-300 keV.
- Define the scattering angles; for the evaluated cross section it is not a problem, so every 20° should not be a problem. But in extending to higher energy, the angles should be chosen as close as possible to the experimental data sets. The evaluated

cross section should be the most updated one from SigmaCalc; to perform an intercomparison of results from various laboratories and in order to avoid the fact that an updated cross section file is released, it was agreed that a "frozen" file should be used, for example SigmaCalc 1.6 currently available from IBANDL. A common angle would have to be used by the labs participating in this inter-comparison.

- Accelerator energy calibration performed reasonably close in time with the benchmark experiment. The choice of the energy calibration points should be done so that extrapolation should be avoided.
- Beam to be used: protons, alphas, deuterons
- Energy calibration of the detector should be done in the proper way, taking into account pulse height defect corrections; the ADC energy bin should be chosen in such a way that at least three channels are available to fit a structure in the spectrum (actually this figure will have to be critically defined according to the specific excitation function).
- The beam intensity should be set in order to limit or reduce as much as possible dead time and pile-up effects, even if the pile-up can be now treated correctly at a few percent level.
- Statistics (i.e. counts per channel) for significant regions of the spectrum should be sufficient as reasonably achievable and adapted to the other uncertainties.
- Provide the uncertainty budget, for example using the template proposed by [4.1] J.L. Colaux and C. Jeynes, "High accuracy traceable Rutherford backscattering spectrometry of ion implanted samples", Analytical Methods 6 (2014) 120-129); the primary goal is to reach a 5% uncertainty level of the benchmark experiment; the uncertainty budget can be used to select the most critical parameters to work on and to reduce uncertainty to reach such an accuracy.
- Stopping power: SRIM 2003 or later values are recommended.

Standardised benchmark test for EBS

The working group on EBS benchmarking agreed that a preliminary benchmark test using SiO_2 and glassy carbon samples will have to be carried out in the different laboratories to allow for a calibration of the different laboratories and facilities and hence facilitate the comparisons of the different results obtained in future benchmark experiments.

The laboratories/institutes involved in the EBS working group, and the measurements they have agreed to do are listed in Table 1. The details of these common experimental procedures (beam energy, scattering angles) are to be discussed and agreed upon after this meeting.

Table 1. EBS benchmark test measurements and participants involved

Reaction	Laboratory involved
C(p,p)C	Bogdanovic, Chiari, Jeynes, Kokkoris, Pedro de Jesus, Siegele
O(p,p)O	Bogdanovic, Chiari, Jeynes, Kokkoris, Pedro de Jesus, Siegele
Si(p,p)Si	Bogdanovic, Chiari, Jeynes, Kokkoris, Pedro de Jesus
C(α,α)C	Jeynes, Kokkoris, Siegele
O(α,α)O	Jeynes, Kokkoris, Siegele
Si(α,α)Si	Jeynes, Kokkoris, Siegele

Participants also discussed the priorities for EBS benchmarking measurements, and agreed to distinguish between top priority reaction cross sections that need to be benchmarked because of (i) the importance of these reactions for EBS applications, (ii) the existence of several experimental cross-section data sets that may exhibit discrepancies, and also because (iii) SigmaCalc evaluated cross sections are available. Medium priority reactions are all the other reactions for which experimental data and evaluated data exist and can therefore be benchmarked at some point. The list of priority EBS reactions for benchmarking is given in Table 2. In this table, the energies in brackets (where available) indicate the maximum energies attainable at the given facility.

Table 2. List of priority reactions for EBS benchmarking

Reaction	Laboratory/Institute involved
Top Priority	
C(p,p)C	Bogdanovic, Chiari (4 MeV), Jeynes (4 MeV), Kokkoris, Pedro de Jesus (4 MeV), Siegele (4 MeV), Vickridge (2.2 MeV)
N(p,p)N	Jeynes, Kokkoris, Pedro de Jesus, Vickridge
O(p,p)O	Bogdanovic, Chiari, Jeynes, Kokkoris, Pedro de Jesus, Siegele
Si(p,p)Si	Bogdanovic, Chiari, Jeynes, Kokkoris, Pedro de Jesus
C(α,α)C	Jeynes (6 MeV)
O(α,α)O	Jeynes
N(α,α)N	Jeynes
Si(α,α)Si	Jeynes
Al(p,p)Al	Chiari, Jeynes, Kokkoris
^{nat}Ca(p,p)^{nat}Ca	Chiari ,Kokkoris, Jeynes
^{nat}K(p,p)^{nat}K	Chiari, Kokkoris, Jeynes
^{nat}Fe(p,p)^{nat}Fe	Kokkoris, Jeynes
Medium Priority	
C(d,d)C	Kokkoris (2 MeV), Vickridge (1.5 MeV)
O(d,d)O	Kokkoris, Vickridge
Si(d,d)Si	Kokkoris, Vickridge
^{6,7}Li(p,p)^{6,7}Li	Chiari, Jeynes, Kokkoris
^{9}Be(p,p)^{9}Be	Barradas (2.4 MeV), Jeynes
^{nat}Cl(p,p)^{nat}Cl	Jeynes, Kokkoris
^{nat}Ti(p,p)^{nat}Ti	Jeynes, Kokkoris
^{nat}V(p,p)^{nat}V	Jeynes, Kokkoris
^{nat}Cr(p,p)^{nat}Cr	Jeynes, Kokkoris
^{nat}Zn(p,p)^{nat}Zn	Jeynes, Kokkoris

4.1.2 NRA benchmarking guidelines

The methodology is the same as outlined above in Sect. 4.1.1 for EBS benchmarking. The top and medium priority reactions to be considered for benchmarking are given in Table 3, along with the groups involved. Like in Table 2, the energies in brackets indicate the maximum energies attainable at the given facility (where available).

Table 3. List of priority reactions for NRA benchmarking

Reaction	Laboratory/Institute involved
Top Priority	
$^{11}B(p,\alpha_0)^{8}Be$	Pedro de Jesus, Kokkoris
$^{12}C(d,p_0)^{13}C$	Kiss (2 MeV), Kokkoris (2 MeV), Vickridge (1.5 MeV)
$^{14}N(d,p_0)^{15}N$	Kiss, Kokkoris, Vickridge
$^{14}N(d,\alpha_0)^{12}C$	Kiss, Kokkoris, Vickridge
$^{14}N(d,\alpha_1)^{12}C$	Kiss, Kokkoris, Vickridge
$^{16}O(d,p_0)^{17}N$	Kiss, Kokkoris, Vickridge
$^{16}O(d,\alpha_0)^{14}N$	Kiss, Kokkoris
Medium Priority	
$D(^{3}He,p_0)^{4}He$	Barradas, Bogdanovic, Jeynes (1 MeV), Raisanen (1 MeV)
$^{7}Li(p,\alpha_0)^{4}He$	Kokkoris
$^{15}N(d,\alpha_0)^{13}C$	Vickridge
$^{24}Mg(d,p_0)^{25}Mg$	Kokkoris

4.1.3 PIGE benchmarking guidelines (bulk analysis)

- Chose two suitable thick samples. Examples: Al foil and a fused glass certified reference standard available from the market with low concentrations of Li, and F, Na, Al as oxides; preferably not a pellet (to avoid grains and voids). This holds for all the samples: a thin Au or Ag layer can be evaporated on the surface for normalization purposes. In some cases, like for Li, a thick pellet made of very fine grains Li_2WO_4 could be used as well. Alternatively one can use an amorphised $LiNbO_3$ thick sample. For aluminium measurements within the working group, the solution would be to purchase a 99.999% pure polished Al foil (2 mm thick), cut in small pieces and distribute to the group. The working group on PIGE will thus start with a polished Al and fused multicomponent glass.
- Define the energy steps; they should be chosen so that the measured energies are above and below relevant resonances, provided the cross section is known a priori. In case of a slowly varying cross section (as in the p+7Li case), each step should not exceed a few hundreds of keV, e.g. 200-300 keV. The benchmark should be extended up to 4 MeV proton beam energy. The same energy steps should be agreed upon and used in all the laboratories involved in the benchmarking of a specific reaction.
- Define the measurement angles. Especially in the case where the γ-ray emission is not isotropic, care should be taken not to integrate over a large angular range. In the absence of evaluated PIGE cross sections, if the cross sections to be benchmarked are measured cross sections, the central angle of the detector should be chosen as close as possible to the one of the measured cross sections.
- Accelerator energy calibration should be performed, or use existing energy calibration if it is recent to the benchmark experiment.
- Beam to be used: protons, deuterons.
- Measurement of the absolute efficiency of the γ-ray detector should be done according to the guidelines already outlined in the final report of the PIGE CRP [in preparation], i.e. by fitting the measured points using a third-degree polynomial function to describe the inverse of the γ-ray energy; a Monte Carlo calculation could be performed to corroborate the results especially for low energy γ-rays or to

extrapolate to higher γ-ray energy. At least two calibrated radioactive sources should be used in order to correct for systematics effects in the activity of each single source as given by the supplier.

- The beam intensity should be adjusted to limit or reduce as much as possible dead time and pile-up effects; one other way of reducing the impact of dead time and peak pile-up is to shorten the amplifier shaping time, especially since the resulting worsening of the energy resolution is not a problem.
- Counting statistics of the γ-ray lines (i.e. area of the peak) should be sufficient, as much as is practically possible. Particular attention should be paid to background subtraction and to reporting the relevant uncertainties in the uncertainty budget.
- Estimate the uncertainty budget, for example using the template proposed by J.L. Colaux and C. Jeynes, "High accuracy traceable Rutherford backscattering spectrometry of ion implanted samples", Analytical Methods 6 (2014) 120-129); the primary goal is to reach a 10% uncertainty level of the benchmark experiment; the uncertainty budget can be used to select the most critical parameters to improve so as to reduce the uncertainty down to the desired level.
- Stopping power: to obtain pure element γ-ray yields from the thick target yields of compound targets (e.g. multicomponent glass), corrections for the different stopping powers values are required as suggested in the "Handbook of Modern Ion Beam Materials Analysis" (2009 edition); SRIM 2003 or later values are recommended, as for EBS and NRA benchmarking.

Standardised benchmark test for PIGE

It has been agreed that a preliminary benchmark test using the polished Al sample will have to be carried out by the different laboratories/institutions to calibrate the different facilities and allow a straightforward comparison of the results in the subsequent benchmark experiments. The details of these common experimental procedures (beam energy, scattering angles) are to be discussed and agreed upon after this meeting.

A list of priority PIGE cross sections that need to be benchmarked for bulk analysis applications is given in Table 4, along with the groups that will be involved. Like in Table 2, the energies in brackets indicate the maximum energies attainable at the given facility (where available).

Table 4. Top priority γ-ray emission reactions for PIGE (bulk analysis) benchmarking

Reaction	Laboratory involved
Top Priority	
^{7}Li(p,nγ)^{7}Be, 429 keV	Bogdanovic (3 MeV), Chiari (4 MeV), Kiss (4 MeV), Kokkoris (5 MeV), Pedro de Jesus (4 MeV), Raisanen (5 MeV), Siegele (4 MeV), Zucchiatti (5 MeV)
^{7}Li(p,p'γ)^{7}Li, 478 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{19}F(p,p'γ)^{19}F, 110 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{19}F(p,p'γ)^{19}F, 197 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{23}Na(p,p'γ)^{23}Na, 441 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{27}Al(p,p'γ)^{27}Al, 844 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Zucchiatti

Reaction	Laboratory involved
^{27}Al(p,p'γ)^{27}Al, 1014 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
Medium Priority	
^{12}C(d,p'γ)^{13}C, 3089 keV	Kiss (2 MeV), Kokkoris (2 MeV)
^{14}N(d,p'γ)^{15}N, 1885 keV	Kiss, Kokkoris
^{16}O(d,p'γ)^{17}O, 871 keV	Kiss, Kokkoris
^{10}B(p,p'γ)^{10}B, 719 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{10}B(p,α'γ)^{7}Be, 429 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{11}B(p,p'γ)^{11}B, 2124 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{25}Mg(p,p'γ)^{25}Mg, 390 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{25}Mg(p,p'γ)^{25}Mg, 585 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{31}P(p,p'γ)^{31}P, 1266 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti

4.1.4 PIGE benchmarking guidelines (depth profiling)

Special considerations regarding targets and nuclear resonances are in order for benchmarking PIGE cross sections intended for depth profiling analysis:

- For F depth profiling, an implanted target, e.g. SiF into Silicon at 160 keV (F implanted down to 125 nm in Silicon, 10% maximum peak F concentration; 10^{17} F/cm^2) can be used. For the purposes of the group measurements included in the following tables, such a sample can be produced and characterized at the University of Surrey, and then distributed to the involved laboratories. If a reasonable target can be produced, e.g. TaN isotopically enriched in 15N over Silicon, also depth profiling of ^{15}N can be benchmarked.
  Resonance energies to be used: 872 keV proton energy for the p+^{19}F and 429 keV proton energy for the p+^{15}N.

For the rest the methodology is the same as for the benchmarking of PIGE cross sections for bulk analysis (see Sect. 4.1.3).

The list of priorities for benchmarking PIGE cross sections used for depth profiling is given in Table 5.

Table 5. Top priority for PIGE (depth profiling) benchmarking

Reaction	Laboratory involved
^{15}N(p,α'γ)^{12}C, E_R = 429 keV	Vickridge
^{19}F(p,p'γ)^{19}F, E_R = 872 keV	Kokkoris, Pedro de Jesus
^{19}F(p,α'γ)^{16}O, E_R = 872 keV	Kiss, Kokkoris, Pedro de Jesus

4.1.5 Targets/samples

The successful completion of the benchmarking measurements depends on the availability of the targets mentioned in the previous sections and listed in Table 6. Steps will be taken by those involved in the working groups to provide the samples. The NDS IAEA will support this effort where possible.

Table 6. List of target samples proposed for the benchmarking measurements

Sample type	Purpose
Glassy carbon	EBS, NRA benchmark
Fused SiO_2	EBS, NRA benchmark
Amorphous Silicon	EBS, NRA benchmark
GaN single crystal	NRA benchmark
Polished Al foil	PIGE for bulk analyis benchmark
Multicomponent glass	PIGE for bulk analyis benchmark
SiF implanted in Silicon	PIGE for depth profiling benchmark
TaN (enriched in ^{15}N) over Silicon	PIGE for depth profiling benchmark

4.2 Dissemination

The dissemination of the benchmark thick-target yields was discussed extensively.

It was agreed that all the charged particle benchmark spectra should be uploaded on a special section of IBANDL, which would be available from the main IBANDL web page through a link on the left-hand side menu bar.

The format of the files containing the measured spectra should be simple ASCII files with data stored in X Y columns (channel vs count/channel or energy vs yield (N_γ/sr/uC)). The file should also include information on the experimental conditions and the associated uncertainties in a comments section just as in the R33 format.

A proposal to include calculation capabilities to this section of IBANDL, to allow the user to benchmark his/her own cross-section file or any other cross-section file available on IBANDL was discussed with IAEA staff Viktor Zerkin. The idea is to enable the user to run a simple spectrum simulator through the IBANDL interface to create thick-target spectra from differential cross-section data, which then could be compared with the stored benchmark spectra. As an example, the ERYA code could be adapted to the IBANDL interface for use in benchmarking of PIGE cross sections.

A detailed description of the proposed functionality of the new benchmark data library is given in Appendix 1.

5 Recommendations

The Technical Meeting on Benchmarking experiments for IBA applications, held from 26 to 29 May at the IAEA, Vienna, covered a wide range of issues related to benchmarking differential cross-section data for IBA applications. During the four days of the meeting participants deliberated on the methodology of benchmarking, proposed the specific steps that need to be taken when benchmarking cross-section data for the various IBA techniques (EBS, NRA, PIGE), and produced a list of priority benchmarking measurements that need to be considered by the IBA experimental groups who have access to experimental facilities. The dissemination of benchmark data was also addressed and suggestions were made. A list of additional tasks assigned to participants is given in Appendix 2 while the complete list of the priority measurements is given in Appendix 3.

Participants also agreed to promote the activity of benchmarking nuclear data for IBA in the IBT Roadmap, and make it known to the broader IBA community so as to attract participation from other laboratories.

Appendix 1

Functionality of IBANDL benchmarking interface

One of the specific objectives of making benchmark spectra available on IBANDL is that users will be able to use the same file formats to do the same operations with their own data. Points (1-5) below list the specific functions of the new IBANDL web interface that need to be implemented to achieve this objective, as proposed and discussed at this meeting.

Benchmark spectra uploaded to IBANDL will have complete associated information summarized in the "Comments" field in the R33 format, together with the citation of the published paper. For acceptance as a formal benchmark, proper documentation must exist, including an evaluation of the uncertainties and conclusions of the benchmark.

Simulations will be calculated by a cut-down NDF [1] simulator from the input data provided in the thick-target spectra file together with reaction cross-sections selected by the user. NDF has modules for RBS, EBS, ERD, PIGE, Narrow Resonance Profiling (NRP) (and PIXE too), and all of these may (eventually) be available, but we will start with EBS. The user will be able to simulate single spectra of types available in the new IBANDL segment. The user will access the NDF single-spectrum simulator only through the IAEA web interface.

Benchmarks are necessarily of samples which are as simple as possible. We anticipate that only "simple" simulations will be available using the cut-down NDF, i.e. pure smooth single-layer samples. The cut-down version of NDF that will be available through the IAEA will not include the advanced features of NDF that make it so powerful in analytical applications (especially fitting, and the multi-spectrum handling features), but the basic functions necessary to do the simulations correctly, even in "simple" cases.

The following functions are deemed as desirable in order to allow the user to perform similar benchmarking operations with selected data sets or other datasets including his/her own:

1. Thick film target (benchmark) spectra will be uploaded to IBANDL and made available in dedicated tables according to the type of spectrum (EBS, NRA, PIGE etc). These data files will include, in a fixed format together with the spectrometry data, all appropriate experimental conditions, namely:
    a. Type of spectrum (EBS, ERD, NRA, PIGE thick target yield, NRP), including reaction and detected particle(s);
    b. Target composition and thickness (eg."natural abundance SiO_2, 2.2.μm");
    c. Beam and beam energy (eg. "$^1H^+$, 2235±4 keV"), with true collected charge (eg. "10±0.3 μC") together with both true collection time and dead time;
    d. (for EBS) detector energy resolution together with incident, scattering & solid angles (eg. "17.4±0.3 keV, 1.2±0.2°; 148.7±0.2°; 2.5±0.1 msr"). Pileup rejection details must be included if used. The electronics calibration is required (eg. 2.984±0.003 keV/channel -0.5±0.2 keV with detector dead layer of $550 \cdot 10^{15}$Si/cm^2);
    e. (for ERD or NRA) as for EBS, plus any extra information needed (detector foils or partial depletion etc);
    f. (for PIGE TTY) as for EBS, plus detector absolute efficiency at the specific gamma-ray energy (eg. "$3.2 \cdot 10^{-3}$, 844 keV"), together with particle incident and gamma-ray emission angles; pileup rejection details must be included if used;
    g. (for NRP) as for EBS, but detailed parameters still to be decided.

    The information listed above will be provided in the format required by the NDF simulation code which is in accordance with the IBA database format (*details to be provided by N. Barradas*)

2. The user will be able to select benchmark spectra from this dedicated table in IBANDL and compare with data simulated using selected cross-sections.
3. IBANDL will recognize the beam energy and scattering angle in the supplied spectrum, as well as the elements of the compound target and their relative abundance, and suggest a list of appropriate IBANDL cross-section functions to the user (with the recommended cross section function -where it exists -labelled appropriately), for all elements in the compound target, but should also allow other data sets to be used, including the user's own, through the function 'Add your own R33 dataset for benchmarking'.
4. The user will also be able to give IBANDL his/her own spectra (in the fixed data format) for simulation with selected cross-sections again using a function similar to 'Add your thick target spectra for simulation'.
5. In a further step to be developed at a later stage it would be useful for IBANDL to allow the user to explore the implications of the uncertainties listed in the input data.

Reference

[1] NDF – General purpose code for data analysis of Ion Beam Analysis Data, available at: http://www.itn.pt/facilities/lfi/ndf/uk_lfi_ndf.htm

Appendix 2

List of Actions agreed at the TM on Benchmarking experiments for IBA.

Perform the EBS proficiency test benchmark measurements	All concerned (see Table 1)
Determine the details of the experimental procedures (beam energy steps, measurement angle, γ-ray energies…) for the PIGE proficiency test benchmark measurements test	All concerned (see Table 1)
Perform the top priority benchmark measurements (EBS, NRA, PIGE) by the end of 2016	All concerned (see Tables 1,2,3,4)
Measure EBS N(p,p)N using a GaN single crystal rotating randomly by the end of 2016	Vickridge
Propose solutions for the multicomponent thick targets for benchmark measurements of PIGE for bulk analysis	All concerned (see Section 4.1.3)
Propose proper targets for the medium priority benchmark measurements of PIGE for bulk analysis	All concerned (see Table 4)
Propose solutions for the target with certified ^{15}N quantity and depth distribution	All concerned (see Section 4.1.4)
Produce and characterise SiF implanted in Silicon target	Jeynes
Acquire and distribute polished Al samples	Chiari
Distribute glassy carbon samples	Barradas
Distribute and characterise fused silica samples	Bogdanovic
Prepare and distribute an expected uncertainty budget for the EBS proficiency test benchmark	Jeynes
Prepare a document describing functionality of the new benchmark data library	Barradas, Kokkoris, Jeynes (coordinator), NDS IAEA

Appendix 3

Complete List of priority measurements for IBA benchmarking.

Reaction	Laboratory/Institute involved
Top Priority	
EBS	
C(p,p)C	Bogdanovic, Chiari (4 MeV), Jeynes (4 MeV), Kokkoris, Pedro de Jesus (4 MeV), Siegele (4 MeV), Vickridge (2.2 MeV)
N(p,p)N	Jeynes, Kokkoris, Pedro de Jesus, Vickridge (2.2 MeV)
O(p,p)O	Bogdanovic, Chiari, Jeynes, Kokkoris, Pedro de Jesus, Siegele
Si(p,p)Si	Bogdanovic, Chiari, Jeynes, Kokkoris, Pedro de Jesus
C(α,α)C	Jeynes (6 MeV)
O(α,α)O	Jeynes
N(α,α)N	Jeynes
Si(α,α)Si	Jeynes
Al(p,p)Al	Chiari, Jeynes, Kokkoris
^{nat}Ca(p,p)^{nat}Ca	Chiari ,Kokkoris, Jeynes
^{nat}K(p,p)^{nat}K	Chiari, Kokkoris, Jeynes
^{nat}Fe(p,p)^{nat}Fe	Kokkoris, Jeynes
NRA	
^{11}B(p,α_0)^{8}Be	Pedro de Jesus, Kokkoris
^{12}C(d,p_0)^{13}C	Kiss (2 MeV), Kokkoris (2 MeV), Vickridge (1.5 MeV)
^{14}N(d,p_0)^{15}N	Kiss, Kokkoris, Vickridge
^{14}N(d,α_0)^{12}C	Kiss, Kokkoris, Vickridge
^{14}N(d,α_1)^{12}C	Kiss, Kokkoris, Vickridge
^{16}O(d,p_0)^{17}N	Kiss, Kokkoris, Vickridge
^{16}O(d,α_0)^{4}N	Kiss, Kokkoris
PIGE Bulk Analysis	
^{7}Li(p,nγ)^{7}Be, 429 keV	Bogdanovic (3 MeV), Chiari (4 MeV), Kiss (4 MeV), Kokkoris (5 MeV), Pedro de Jesus (4 MeV), Raisanen (5 MeV), Siegele (4 MeV), Zucchiatti (5 MeV)
^{7}Li(p,p'γ)^{7}Li, 478 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{19}F(p,p'γ)^{19}F, 110 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{19}F(p,p'γ)^{19}F, 197 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{23}Na(p,p'γ)^{23}Na, 441 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{27}Al(p,p'γ)^{27}Al, 844 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Zucchiatti
^{27}Al(p,p'γ)^{27}Al, 1014 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
PIGE Depth Profiling	
^{15}N(p,α'γ)^{12}C, E_R = 429 keV	Vickridge
^{19}F(p,p'γ)^{19}F, E_R = 872 keV	Kokkoris, Pedro de Jesus
^{19}F(p,α'γ)^{16}O, E_R = 872 keV	Kiss, Kokkoris, Pedro de Jesus

Appendix 3

Reaction	Laboratory/Institute involved
Medium Priority	
EBS	
C(d,d)C	Kokkoris (2 MeV), Vickridge (1.5 MeV)
O(d,d)O	Kokkoris, Vickridge
Si(d,d)Si	Kokkoris, Vickridge
^{6,7}Li(p,p)^{6,7}Li	Chiari, Jeynes, Kokkoris
^{9}Be(p,p)^{9}Be	Barradas (2.4 MeV), Jeynes
^{nat}Cl(p,p)^{nat}Cl	Jeynes, Kokkoris
^{nat}Ti(p,p)^{nat}Ti	Jeynes, Kokkoris
^{nat}V(p,p)^{nat}V	Jeynes, Kokkoris
^{nat}Cr(p,p)^{nat}Cr	Jeynes, Kokkoris
^{nat}Zn(p,p)^{nat}Zn	Jeynes, Kokkoris
NRA	
D(^{3}He,p$_0$)^{4}He	Barradas, Bogdanovic, Jeynes (1 MeV), Raisanen (1 MeV)
^{7}Li(p,α_0)^{4}He	Kokkoris
^{15}N(d,α_0)^{13}C	Vickridge
^{24}Mg(d,p$_0$)^{25}Mg	Kokkoris
PIGE Bulk Analysis	
^{14}N(d,p'γ)^{15}N, 1885 keV	Kiss, Kokkoris
^{12}C(d,p'γ)^{13}C, 3089 keV	Kiss (2 MeV), Kokkoris (2 MeV)
^{16}O(d,p'γ)^{17}O, 871 keV	Kiss, Kokkoris
^{10}B(p,p'γ)^{10}B, 719 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{10}B(p,α'γ)^{7}Be, 429 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{11}B(p,p'γ)^{11}B, 2124 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{25}Mg(p,p'γ)^{25}Mg, 390 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{25}Mg(p,p'γ)^{25}Mg, 585 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti
^{31}P(p,p'γ)^{31}P, 1266 keV	Bogdanovic, Chiari, Kiss, Kokkoris, Pedro de Jesus, Raisanen, Siegele, Zucchiatti

[The energies in brackets indicate the maximum energies attainable at the given facility.**]**

Annex 1

IAEA Technical Meeting on
Benchmarking Experiments for Ion Beam Analysis

IAEA Headquarters, Vienna, Austria
26 – 29 May 2015
Meeting Room M0E03

Preliminary AGENDA

Tuesday, 26 May

08:30 – 09:30 **Registration (IAEA Registration Desk, Gate 1)**

09:30 – 10:00 **Opening Session**
Opening Remarks
Introduction: Objectives of meeting (P. Dimitriou)
Election of Chairman and Rapporteur
Discussion and Adoption of the Agenda (Chairman)

10:00 – 12:30 **Presentations (40' incl. discussion)**

1) A Review on the Methodology of Benchmarking Experiments: Assessment of Physical and Technical Problems, *Michael Kokkoris (NTUA)*

2) Accurate analysis using elastic backscattering together with benchmarking, *Chris Jeynes (Univ. Surrey)*

3) Benchmark test measurements of elastic backscattering cross sections measurements at RBI, *Iva Bogdanović Radović (RBI)*

4) Nuclear Reaction Analysis and other IBA techniques at ANSTO, *Rainer Siegele (ANSTO)*

12:30 – 14:00 *LUNCH*

14:00 – 18:00 **Presentations (cont'd)**

5) Proposal of a Methodology to Perform PIGE Benchmarking Experiments, *Adelaide Pedro de Jesus (FCT-Univ. Nova Lisboa)*

6) Planning PIGE Benchmarking Experiments at CMAM, *Alessandro Zucchiatti (CMAM)*

7) Assessment of experimental PIGE cross section data in the case of the $^{12}C(d,p\gamma)^{13}C$ reaction, *Arpad Kiss (ATOMKI)*

8) Gamma-ray production cross sections and thick-target yields for the $^{14}N(p,p'\gamma)^{14}N$ reaction, *Jyrki Räisänen (Univ. Helsinki)*

9) Benchmark test measurements of nuclear cross sections relevant for IBA at LABEC, *Massimo Chiari (LABEC-INFN Firenze)*

10) The bulk sample method in cross sections: measurement vs. benchmarking, *Nuno Barradas (IST-Univ. Lisboa)*

Coffee break as needed

Wednesday, 27 May

09:00 – 09:40 **Presentation (cont'd)**

11) Current Status of the Benchmarking Process, Scope, Complex Problems and Perspectives, *Michael Kokkoris (NTUA)*

09:40 – 12:30 **Round Table Discussion**

Topics to discuss:
- assess the current status of experimental and evaluated data
- outline the methodology for performing benchmarking experiments
- propose guidelines for validation of nuclear cross sections using benchmarked data (EBS, NRA, PIGE)
- produce a list of priority benchmark experiments (EBS, NRA, PIGE)
- data compilation and dissemination (IBANDL)

Coffee break as needed

12:30 – 14:00 *LUNCH*

14:00 – 17:30 **Round Table Discussion (cont')**

Coffee break as needed

19:00 ***DINNER at a restaurant in the city***

Thursday, 28 May

09:00 – 12:30 **Round Table Discussion (cont'd)**

Coffee break as needed

12:30 – 14:00 *LUNCH*

14:00 – 17:00 **Round Table Discussion (cont'd)**

17:00 – ***PIGE CRP Meeting***

Coffee break as needed

Friday, 29 May

09:00 – 13:00 **Round Table Discussion (cont'd)**

Drafting of Actions Report

1**3:00** **Closing of the Meeting**

Coffee break as needed

Annex 2

Technical Meeting on Benchmarking Experiments for Ion Beam Analysis

IAEA, Vienna, Austria
26 – 29 May 2015

List of participants

AUSTRALIA
Rainer SIEGELE
Australian Nuclear Science and Technology Organisation (ANSTO), Locked Bag 2001, Kirrawee DC NSW
Tel:+ 61 297173967
E-mail: rns@ansto.gov.au

CROATIA
Iva BOGDANOVIĆ RADOVIĆ
Institute Ruder Boskovic
Bijenicka cesta 54,
HR-10000 Zagreb
Tel: +385 (1)4571227
E-mail: iva@irb.hr

FINLAND
Jyrki RÄISÄNEN
Accelerator Laboratory, POB 43, Pietari Kalmin katu 2, University of Helsinki,
00014 Helsinki
Tel: +358919150082
E-mail: jyrki.raisanen@helsinki.fi

FRANCE
Ian VICKRIDGE
Unité de recherche 7588-CNR
Institut de NanoSciences de Paris
Campus Boucicaut; 140
rue de Lourmel,
F-75015 Paris
Tel: + 33144274647
E-mail: ian.vickridge@insp.jussieu.fr

GREECE
Michael KOKKORIS
Technical University of Athens
Department of Physics
Zografou Campus
GR-15780 Athens
Tel:
E-mail: kokkoris@central.ntua.gr

HUNGARY
Árpád Zoltán KISS
Hungarian Academy of Sciences
Institute of Nuclear Research
Bem ter 18/c, P.O. Box 51
Debrecen
Tel:+ 3652509200
E-mail: azkiss@namafia.atomki.hu

László CSEDREKI
Hungarian Academy of Sciences
Institute of Nuclear Research
Bem ter 18/c, P.O. Box 51
Debrecen
Tel:+ 3652509200
E-mail: csedreki.laszlo@atomki.mta.hu

ITALY
Massimo CHIARI
Fisica Nucleare Istituto,
Via Sansone 1Sesto Fiorentino
I-50019 Firenze
Tel: +390554572273
E-mail: chiari@fi.infn.it

PORTUGAL

Nuno PESSOA BARRADAS
Instituto Technologico Nuclear
Ministry of Science, Technology and Higher Education (MCTES)
E.N.10 Apartado 21
Sacavem
Tel: +351219946150
E-mail: nunoni@ctn.ist.utl.pt

Adelaide PEDRO DE JESUS
Fundação da Faculdade de Ciências de Lisboa
Campus Faculdade de Ciências UL,
Edifício C1, Piso 3 - Campo,
P-1749-016 Lisboa
Tel:
E-mail: maj@fct.unl.pt

SPAIN

Alessandro ZUCCHIATTI
Centro de Microanálisis de Materiales
Universidad Autónoma de Madrid
Faraday 3
28049 Madrid
Tel:
E-mail: alessandro.zucchiatti@uam.es

UNITED KINGDOM

Christopher JEYNES
Surrey Ion Beam Centre
Advanced Technology Institute
University of Surrey
GUILDFORD
Tel:
E-mail: c.jeynes@surrey.ac.uk

IAEA

Paraskevi DIMITRIOU
IAEA Nuclear Data Section
Vienna International Centre
PO Box 100
1400 Vienna
Tel: + 43-1-2600-21708
Fax:+ 43-1-26007
E-mail: p.dimitriou@iaea.org

Annex 3


J. Räisänen
FINLAND
P. Dimitriou
Scientific Officer
A. Zucchiatti
SPAIN

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. box 100
A-1400 Vienna, Austria

E-mail:
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: