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**Report on the IAEA Technical Meeting on
Database of Evaluated Cross Sections for Ion Beam Applications**

IAEA Headquarters, Vienna, Austria

29 – 30 October 2003

Prepared by
I.C. Vickridge and O. Schwerer

IAEA Nuclear Data Section
Vienna, Austria

November 2003

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

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Abstract

Results of the IAEA Technical Meeting on Database of Evaluated Cross Sections for Ion Beam Applications held at the IAEA Headquarters, Vienna, Austria, 29 to 30 October 2003, are summarized in this report. The meeting discussed the nuclear data needs for ion beam analysis and produced recommendations concerning the compilation, assessment and evaluation of cross section data for ion beam analysis, as well as the related databases and their formats and their inclusion in the data collections of the IAEA Nuclear Data Section.

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MEETING SUMMARY

Background

Ion Beam Analysis denotes a suite of analytical techniques that exploit the interactions of rapid (\sim MeV) charged particles with matter to determine the composition and structure of the surface regions of solids (from \sim 0 to 100 μ m). Compositions and structures are inferred from measured quantities such as charged particle, gamma and x-ray spectra, or excitation curves, via physical models incorporating the sample structure and the basic physical processes and quantities giving rise to the observed spectra or excitation curves. The basic physical processes underlying IBA are now well understood, and the reliability of data interpretation is limited by knowledge of the physical data.

The primary quantities required are the stopping power and the cross sections of the interactions involved. Whilst work remains to be done on accurate stopping powers, the field is largely catered for by the considerable body of work of Ziegler and co-workers, embodied in the SRIM computer code. Similarly, Particle Induced X-ray Emission (PIXE) is a specific subfield of IBA for which the appropriate ionisation cross sections, fluorescent yields and photon attenuation coefficients are adequately tabulated.

The case is quite different for cross sections for nuclear reactions and non-Rutherford elastic scattering. There exists a considerable body of published data in the nuclear physics literature, much of which has been incorporated into computer-based databases over the last decade by a small number of individuals. The two principal such databases are the SigmaBase web sites and the NRABase cross section library. Examination of this unevaluated experimental data has revealed numerous discrepancies beyond the error limits reported by the authors, and ion beam analysts are faced with the dilemma of trying to decide which (if any), amongst the divergent cross section data, they should use.

Meeting Motivation

This state of affairs has been a pre-occupation of the IBA community for many years, however they have lacked the resources and coordination to make a concerted effort to improve the situation. At the same time, the Nuclear Data Section (NDS) of the IAEA has been interested in diversifying the provision of nuclear data over a wider range of activities, organising an Advisory Group Meeting (AGM) on Long Term Nuclear Data Needs in 2000. This meeting, attended by experts from a number of fields, including IBA, for which nuclear data are important, recognised the need to undertake action to improve the quality and availability of nuclear data specific for ion beam analysis. In 2002 further impetus came from a recommendation of the International Nuclear Data Committee (INDC) that a Technical Meeting be held to consider the nuclear data needs of the IBA community, and how the IAEA could play a role in meeting these needs.

Therefore, the purpose of the present Technical Meeting has been to bring together a group of IBA experts in order to consider appropriate goals and identify possible actions that could be undertaken within the framework of IAEA/NDS structures and frameworks for improving the quality and availability of nuclear data for IBA.

The deliberations held during the meeting have been guided by the Technical and Organisational Recommendations of the AGM on Long-Term Needs for Nuclear Data Development, Vienna, 28 November - 1 December 2000 (INDC(NDS)-423, May 2001). The Organisational Recommendations of the AGM had been the following:

No.	Organisational Recommendation of AGM	Action taken
1.	That the IBA community be invited to propose an IBA Nuclear Data Liaison Officer (non-IAEA funded) to provide a recognized link between the IBA community and the IAEA Nuclear Data Section and the nuclear data centre networks.	See Conclusion below
2.	That the IAEA include IBA needs in nuclear data-based training programmes.	Workshop on Nuclear Data for Materials Analysis, ICTP Trieste, May 2003
3.	That the IAEA establish a CRP on "Compilation, evaluation and measurement of Nuclear Data for IBA (with particular emphasis on applications in materials and environmental sciences)".	See Recommendation 5 below

Conclusions

In fulfilment of Organizational Recommendation #1 of the IAEA-NDS AGM, Mr. Alexander Gurbich (IPPE Obninsk, Russia) is unanimously elected by the meeting as Liaison Officer between the IBA community and NDS.

The primary role of the Liaison Officer is to serve as a recognized interface between the IBA community and NDS. Responsibilities will include overseeing the operation of the web-based collection of nuclear reaction cross sections for IBA hosted by NDS and taking pro-active action for the collection of new data for the website. The Liaison Officer is expected to be a key participant in technical meetings, and coordinated research proposals and other Agency activities related to nuclear data for IBA.

The meeting has also agreed on the following recommendations:

1	Recommended data and an assessment of their reliability should be developed for all nuclear cross sections of interest in IBA, representing the best available knowledge of the present time. These data should be made freely available to the IBA community.
2	<p>As a step towards meeting the requirements of Recommendation #1, the meeting has identified the following urgent needs of the IBA community in the field of nuclear data:</p> <p>(1) A detailed inventory of all cross sections of interest to IBA.</p> <p>(2) Critical assessment of the consistency of the available data.</p> <p>(3) On the basis of this assessment and considering the priority needs of the IBA community, further measurements and/or detailed evaluation should be undertaken.</p> <p>(4) Cross section measurements at different IBA laboratories need to be undertaken within the framework of a coordinated effort.</p> <p>(5) A coordinated effort should also be made to promote the evaluation of nuclear cross sections for IBA. The resulting evaluations should become part of the NDS collection of evaluated data libraries.</p> <p>(6) Internet-based and other tools for dissemination of evaluated cross sections are required.</p>
3	It is crucial that the NRABase and SigmaBase data collections be rapidly merged into a single database to be hosted on the Agency website. The preferred format for the cross section files is R33 (see Annex 7).
4	While the meeting recognizes the importance of the R33 format for the IBA community, it strongly recommends that all data so far not compiled in the existing databases will be compiled into EXFOR. Furthermore, data from the existing databases will be progressively included in EXFOR as resources permit. The R33 format should become an additional EXFOR computational format.
5	The establishment of an appropriate IAEA Co-ordinated Research Programme would play an important role in further progress towards a number of the goals stated above and would also fulfil Organizational Recommendation #3 of the AGM on Long Term Needs for Nuclear Data Development. The meeting recommends that IAEA supports suitable CRP proposals and, in addition, brings to bear other resources as appropriate.

Technical Meeting on
"Database of Evaluated Cross Sections for Ion Beam Applications"

IAEA Headquarters, Vienna, Austria

29 - 30 October 2003

Meeting Room A1038

Agenda

Wednesday 29 October

- 08:30 - 09:30 Registration (at Gate 1, IAEA Headquarters)
- 09:30 Opening Session
Welcome by Alan Nichols, NDS Section Head
Brief self-introduction of participants
Election of chairman and rapporteur
Review of meeting goals, adoption of Agenda
- Session 1: Brief presentations/statements by participants
(10 - 15 minutes each) and discussion
- 12:30 - 14:00 Lunch
- 14:00 - 17:30 Session 2: Discussions
- Technical recommendations of IAEA meeting on long-term data needs
 - SigmaBase, NRABase and EXFOR: experimental databases, formats
 - Future evaluated database
 - Responsibilities of liaison officer
 - Appointment of liaison officer

Thursday 30 October

- 9:00 - 12:30 Session 3: Discussions (cont.), drafting of Meeting Report
- 12:30 - 14:00 Lunch
- 14:00 - 16:30 Concluding Session: Discussion and approval of Meeting Report

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Nuclear Data in Ion Beam Analysis :
where we were, where we are, and where we should go

I. C. Vickridge, SAFIR, Groupe de Physique des Solides, Paris

Introduction.

Ion Beam Analysis (IBA) refers to a suite of analytical methods that exploit the interactions of swift (MeV energy range) massive (atomic nuclei) particles (projectiles) with matter (the target). In decreasing order of probability, the projectiles may interact with the electrons of the target atoms – leading to the so-called electronic energy loss ; through elastic collisions with the target nuclei, leading to so-called nuclear energy loss and also the methods of Rutherford Backscattering Spectrometry, non-Rutherford Elastic Backscattering Spectrometry and elastic recoil analysis ; and through nuclear reactions with the target nuclei, giving rise to the Nuclear Reaction Analysis techniques. This meeting is concerned with the data for the cross-sections of interaction between the projectile and the target nuclei – the elastic scattering and nuclear reaction cross sections – for IBA.

Evaluation of needs

It is instructive to observe how the IBA community has itself catered for its needs in nuclear reaction cross section data. At first, the data was simply collected from the nuclear physics literature, and later from the growing number of cross section measurements performed specifically for IBA, and collated into hard copies of reports or books that were used in almost every IBA lab [1-3]. However there were a number of limitations to such an approach. Firstly, none of these works included any evaluation of the measured data : they were simply collations from the published literature. In many cases, cross sections measured by different groups would vary not only in absolute value, but even in their dependencies on projectile energy and reaction angle. Different IBA practitioners had their own ideas about the reliability of different cross section data, although this was seldom published. Secondly, with the increasing use of computer

simulation and fitting codes [e.g. 4,5], the need for digital representation of cross section data became acute. Different IBA laboratories digitized their most used data in a variety of ad-hoc ways – with various levels of care and accuracy.

In recognition of the need for some kind of coordination of this dispersed and often redundant activity, and the need for IBA practitioners to have access to reliable data without necessarily having to perform their own re-evaluations of the data, a workshop was held on cross section data for IBA during the Third International Conference on Chemical Analysis (Namur, 1991) [6]. This had two results : firstly there was a proposal for an ascii data format (the R33 format) for storing and communicating experimental nuclear reaction cross sections within the IBA community [7], and secondly there were two initiatives made to set up publicly available internet sites for this data : an FTP site at Lower Hutt in New Zealand, and an HTTP site at Idaho State University. After a short time the Lower Hutt FTP site was abandoned (it became a mirror of the ISU site), and the SigmaBase was born. The Sigmabase is now the main repository of experimental IBA cross sections : it is in many ways the IBA equivalent of EXFOR. It embodies the data that the IBA community has invested its own energy into collating and archiving.

Two further important technical developments need to be mentioned. Firstly, A. Gurbich produced the NRABase, which consists of a cross section library embodied in a computer library management program. The NRABase contains not only ascii data, but also graphical representations, full references, and rather detailed notes on the cross sections that it contains. Secondly, M. Mayer produced the SIMNRA program [8], which includes a large number of nuclear reaction cross sections in the R33 format – more in fact than are now available on the Sigmabase. All of this work has occurred in parallel with and completely independently of the collation and evaluation work of the Nuclear Data Network.

An important institutional development occurred in 2001. The Nuclear Data Section of the IAEA organized a meeting on Long Term Nuclear Data Needs, to which IBA practitioners (amongst others) were invited. At this meeting, the general principle of including data used by the IBA community in EXFOR and allowing it to be accessed via an appropriate computational format (probably R33) was recognized, and it was

suggested that a Liaison Officer be named, who could coordinate efforts between the NDS and the IBA community for inclusion of IBA-related cross sections into EXFOR.

It is the purpose of the present meeting to initiate the practical application of these recommendations.

Before deciding on the practical details, I feel that it is useful to give a view of where we should be headed – even if such a vision may appear to be utopic or unrealistic for the moment.

- Ideally, all nuclear reaction cross sections for IBA will be measured and evaluated with the best possible skill available : this job needs to be done once, and to be done as well as is presently possible. We should aim not to have to re-do it before at least a generation – say 40 years (the average working life of a human scientist).
- Ideally, cross section values will be available across a sufficiently dense grid of projectile energies and reaction angles that no significant features (such as narrow resonances) will be omitted from the data.
- Ideally, all recommended cross section values (including those that will be interpolated or extrapolated on the basis of a physical model) will be within 1% of the real value
- Ideally, fully evaluated cross sections will be freely available for download to all IBA practitioners from a number of sites managed by international organisations independent of any particular nation, in format or formats used in the IBA community.

To this utopic vision, I add two considerations born of a slightly more pragmatic concern. It is clear that even with an optimistic resourcing scenario for example including support via Coordinated Research Programmes, fully evaluating IBA cross sections is likely to be a very long task. So, firstly there will need to be a prioritization of work to be done :

- Ideally, the collation and evaluation of cross sections for IBA will be performed in close collaboration with the community of IBA practitioners.

Secondly, in the meantime, IBA practitioners could benefit from improved, even if imperfect data. So :

- Ideally, recommended data, and an assessment of its reliability, for all nuclear reaction cross sections of interest in IBA, representing the best available knowledge *at the present time* should be available to the IBA community. Only where no experimental data exist and no reasonable theoretical estimate is possible should we have holes in the *presently available recommended data*

It is clear that the decisions and recommendations that will result from this meeting will be modulated by the reality of limited resources, limited theoretical knowledge, and imperfect institutional tools, however it is our job, as senior members of the IBA and Nuclear Data communities, to try and define the most effective first steps towards the goal of having the best relevant nuclear reaction data freely available to IBA practitioners.

References

- [1] *Ion beam handbook for materials analysis* Mayer, J.W. Academic Press, New York 1977.
- [2] Nuclear cross section data for surface analysis. R. A. Jarjis. Internal Report, Department of Physics, University of Manchester (1979).
- [3] *Handbook of Modern Ion Beam Materials Analysis* Ed: Joseph R. Tesmer and Michael Nastasi. (Pittsburgh, PA: Materials Research Society)
- [4] RUMP L. Doolittle Nucl. Instrum. Methods B **9** 291 (1985)
- [5] SENRAS G. Vizkelethy Nucl. Instr. Meth. B45(1990)
- [6] *A workshop on cross-section databases for IBA*. I.C. Vickridge. Nucl. Instr. and Meth. B66 (1992) 303-305.
- [7] *Proposed ASCII format for communication of reaction cross-sections in the IBA community*. I.C. Vickridge. DSIR Physical Sciences Report 33. Sept. 1991.
- [8] *Technical Report 9* Mayer M (1997) Max-Planck-Institut für Plasmaphysik 113

Contribution by A.F. GurbichOverview

To provide charged particles cross sections for IBA is the task which resembles the problem of nuclear data for other application in all respects save one. Differential cross sections rather than total ones are needed for IBA.

Accumulation of rough measured cross sections in the data base is only the first step towards establishing a reliable basis for computer assisted IBA. The analysis of the compiled data revealed numerous discrepancies in measured cross section values. These discrepancies arise from inaccuracies in the accelerator energy calibration, a cross section normalization procedure, etc. In most cases the differential cross sections are measured at one selected scattering angle and therefore they may be immediately used only in the same geometry. Fortunately in the field of the IBA interests the mechanisms of nuclear reactions are generally known and appropriate theoretical models with adjustable parameters have been developed to reproduce experimental results. Besides other advantages the extrapolation over all the range of scattering angles can be then performed on the clear physical basis. Applicability of such an approach for the evaluation of the proton and ^4He non-Rutherford elastic scattering cross sections has been demonstrated in numerous works. A good deal of the theoretical work should be done to analyze the compiled data and to produce reliable recommended cross sections.

Format issues

In 1991 the ASCII format R33 was proposed for the communication and accumulation of IBA cross section data. The propositions for its update were discussed in 2000. The R33 format was developed *ab ovo* with no relation to EXFOR. A special R33 manager was recently developed and some codes used in IBA for spectra processing were adopted to this format. So far as all the IBA related information available in EXFOR was taken from SigmaBase there is no problem of conversion from EXFOR to R33. From the practical point of view there is such a drawback in the R33 format that measurement units are not explicitly indicated.

SigmaBase

This Internet database contains about 240 data files stored in R33 and RTR formats, the R33 files being amounted roughly to 40 per cent. The database is easily accessible and has simple and convenient design. It is hosted at two servers (ISU and KFKI) which are not actually mirrors. The ISU database was last updated in 2000 while KFKI one in 1998. Those data from SigmaBase which were measured in the USA were partly incorporated into the EXFOR database due to work made by Vicky McLane in BNL. Further activity in data accumulation would be remarkably facilitated provided that new results of cross section measurements could be send by authors directly to the database i.e. the servers should be opened for everyone contribution.

NRABASE

The first version of PC-oriented data base NRABASE was developed in the end of 1994. The second version was produced in 1997 and further development of the NRABASE was made during last years. Cross sections for nuclear reactions with charged particles in the entrance and exit channels (non-Rutherford elastic scattering included) and γ -yields for some selected (p, γ) reactions have been compiled. The digitizing procedure used to retrieve data published as graphs was verified using several data sets available both as graph and tables. The accuracy of the obtained points was found to be within 3 per cent. At present the total number of data files contained in NRABASE is 232. Each of the reference is discussed in a short comment, the

attention being paid mainly to the experimental details. Digital information and comments are stored in ASCII format and graphs are in PCX or HPGL formats. The NRABASE is available from the SigmaBase Programs Archive and is distributed also on diskettes by IAEA. The total amount of the information in NRABASE is about 4 Mb.

It should be mentioned that the two major sources of the cross section data for IBA (SigmaBase and NRABASE) were developed independently of each other and they have never been compared. The task is not only to compare but to merge both the bases into a versatile database under the NDS management

SigmaCalc

To provide the IBA community with a reliable source of the nuclear data a SigmaCalc-calculator has been developed which gives the evaluated differential cross sections for any scattering angle and for energy range and elements of interest to IBA. The cross sections are calculated using nuclear reactions models fitted to the available experimental data. SigmaCalc enables the IBA scientist having no expertise in nuclear physics to perform the calculations of the required smooth curves $d\sigma(E)/d\Omega$ presented in optional units. The first version of the SigmaCalc provides data on non-Rutherford proton and ^4He -ion elastic scattering cross sections. So far as the evaluation of the cross sections is supposed to be continued it would be desirable to redesign SigmaCalc as a remote application accessible via Internet. Then new results could be easily added and become available to all the community.

Measurements

The activity in the measurements of the IBA related nuclear data seems to be based on the basis of the authors interests, targets availability, etc. rather than is initiated by actual needs. An urgent task is to make a complete inventory of the cross sections of the first importance to IBA. The most comprehensive facility for the cross section measurement was reported by Florence group which uses a scattering chamber equipped with an array of detectors located in the angle interval from 100 to 170 degrees. Measurement of the charged particle cross sections is a good task for application of a growing interest in nuclear physics from the side of developing countries.

Contribution by E. Rauhala

**Database of Evaluated Cross-Sections for Ion
Beam Applications**

*IAEA technical meeting
Vienna, 29-30 October 2003*

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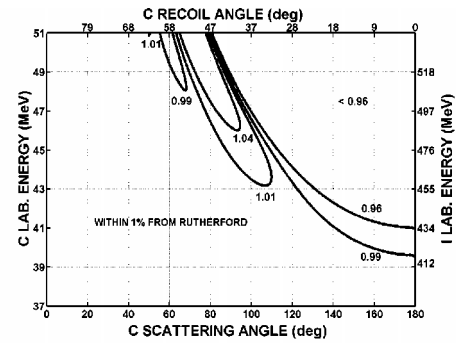
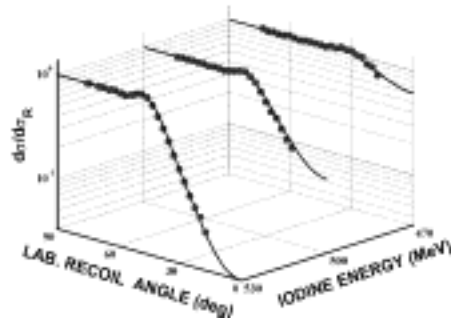
*Petteri Pusa
Tommy Ahlgren
Alexander Gurbich
Jyrki Räisänen
Tommy Alanko*

Recent studies on scattering of ions in Helsinki

- Backscattering or elastic recoil cross section energy and angular distributions were measured
- Nuclear models were applied to fit and analyze the data
- The models were used to predict cross sections for extended angular intervals

- Novel Monte – Carlo calculations for multiple scattering were investigated

The iodine – carbon system



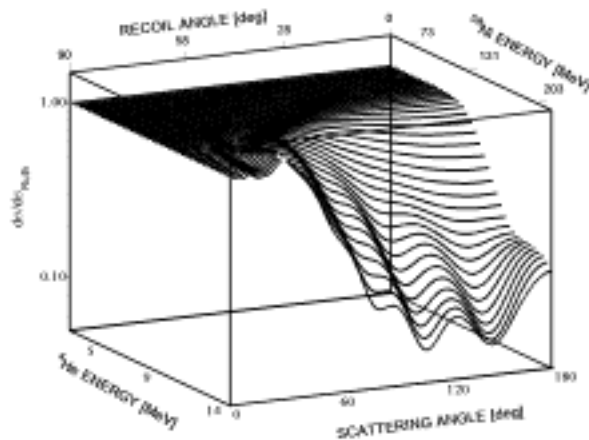
Experimental C(I, C) elastic recoil scattering cross sections at different energies and Optical Model fits. The OM was used to obtain Rutherford scattering threshold contours for the C + I scattering system. The iodine beams can probe μm ranges.

P. Pusa, E. Rauhala, T. Alanko and J. Räsänen, J. Appl. Phys. 93 (2003) 6370.

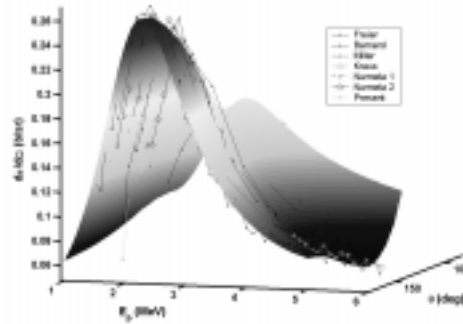
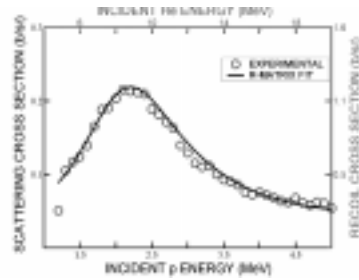
The helium – nickel system

He + Ni elastic scattering in the energy – angle – plane, calculated by the optical model.

A. Nurmela, P. Pusa, E. Rauhala and J. Räsänen, J. Appl. Phys. 91 (2002) 2438



The hydrogen – helium system



Elastic scattering cross sections for the p + He system and the R-matrix fit. Data at a backscattering angle of 129° corresponding to a recoil angle of 20° are shown. The cross section at the resonance is ~ 250 times Rutherford.

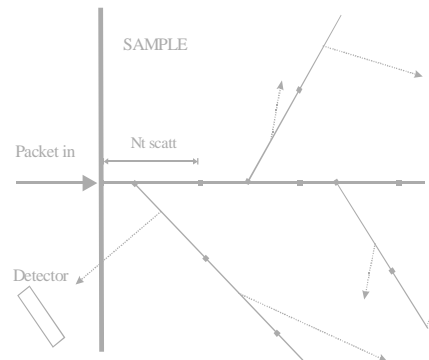
P. Pusa, E. Rauhala, A. Gurbich and A. Nurmela, unpublished

Ion fraction - Monte Carlo – a method for elastic backscattering simulations

Problems due to multiple scattering are encountered in deep probing RBS and low energy RBS.

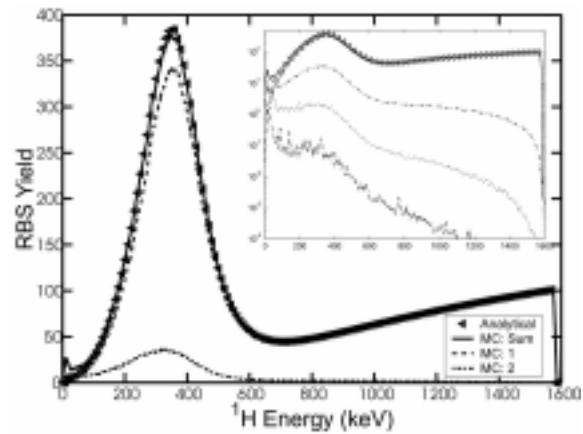
Introduction of ion packets in Monte-Carlo simulations increases the simulation speed by several orders of magnitude compared to conventional MC.

Non-RBS cross sections are easily implemented.



Simulated non-Rutherford backscattering spectra for 2.3 MeV protons incident on carbon. Comparison between single (GISA) and multiple scattering is shown.

Optical model calculation with parameters for p + C from Gurbich (1998).



P. Pusa, T. Ahlgren and E. Rauhala, submitted to NIM B (IBA 2003)

This meeting

- A need exists to maintain the nuclear data bases by an established organization – IAEA/NDS together with the IBA community?
- Experimental “raw” cross section data, suggested evaluated data, theoretical models, calculated cross sections, etc. could be included
- Format readable by computers but also by humans
- The long term aim could be to develop program packets for nuclear model calculations to be incorporated into IBA data analysis programs

Contribution by G. Battistig

SIGMABASE

Created by I. Vickridge and G. Vizkelethy in New Zealand and USA Idaho
The web site is mirrored, maintained and hosted at MFA, Budapest, Hungary
by G. Battistig

Cross section data

nuclear reactions:

d, ^3He , ^6Li , ^7Li , ^9Be , ^{10}B , ^{11}B , ^{12}C , ^{13}C , ^{14}N , ^{15}N , ^{16}O , ^{18}O , ^{19}F , ^{32}S

(p,p) elastic cross sections:

H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, Ca, Ti

 (α,α) elastic cross sections:

Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, Cl, Ar, K, Ca

Elastic recoil cross sections:

$^1\text{H}(\alpha,p)^4\text{He}$, $^1\text{H}(^3\text{He},p)^3\text{He}$, $^2\text{H}(\alpha,d)^4\text{He}$



Research Institute for Technical Physics and Materials Science
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Vienna, 2003

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Demo versions of commercial programs:

- * **OM_DAQ** An MCA (Multichannel Analyzer) program by Oxford Microbeams Ltd.
- * **MPAWIN** MPA/PC Multiparameter system software for Windows and DOS by FAST ComTec, Communication Technology GmbH
- * **SPAN** Software for Analyzing MCA Spectra by W.N.Lennard

PC programs

- * **ALEGRIA 1.2** Conversion of ERD and NRA spectra to depth profile by F. Schiettekatte and G. Ross
- * **DEPTH** Depth resolution and cross section calculations by E. Szilagyi.
- * **GISA 3.3** RBS simulation and evaluation by J. Saarilahti
- * **RUMP ERD** A modification of RUMP to handle ERD better by L.J.M. Jaegers and J.L.J. van IJzendoorn.
- * **SENTRAS** Simulation and evaluation of NRA by G. Vizkelethy
- * **SIMNRA** Version 5.0, Simulation of RBS with emphasis on Non-Rutherford Scattering by M. Mayer
- * **SPACES (DOS)** Calculation of energy straggling and excitation curves by I. Vickridge.
- * **SPACES for Windows** Windows version of I. Vickridge's SPACES
- * **Nuclear Reaction Database** A nuclear reaction database program by A. Gurbich.



Research Institute for Technical Physics and Materials Science
Budapest, Hungary

Vienna, 2003

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Documents:

- * **DSIR Physical Sciences Report 33**, Proposed ACSII Format For Communication of Reaction Cross Section in the IBA Community by I. C. Vickridge, Nuclear Science Group, DSIR, New Zealand
- * **SRIM** (formerly TRIM) manuals January 9, 1996
 - o HTML format (not completely ready yet)
 - o Postscript format
 1. Part I.
 2. Part II.

Other Nuclear Data Servers and Home pages

Further needs:

- * more and remeasured cross section data
- * well defined experimental parameters, target materials, geometries
- * data evaluation, analysis



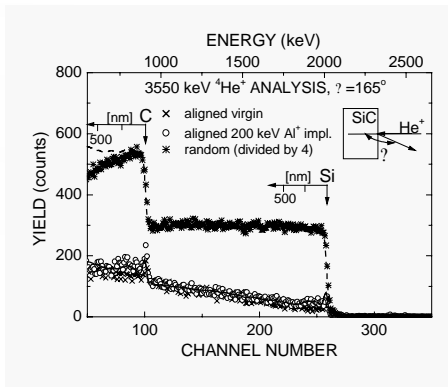
Research Institute for Technical Physics and Materials Science
Budapest, Hungary

Vienna, 2003

3

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Budapest, Hungary

- * 5 MV van de Graaff accelerator with different chambers, microbeam
- * RBS + channeling, NRA, resonances, ERD, PIXE
- * semiconductors, thin films, implanted layers, oxidation and nitridation, etc.



α - RBS, channeling
Enhanced cross section for carbon above 3.5 MeV



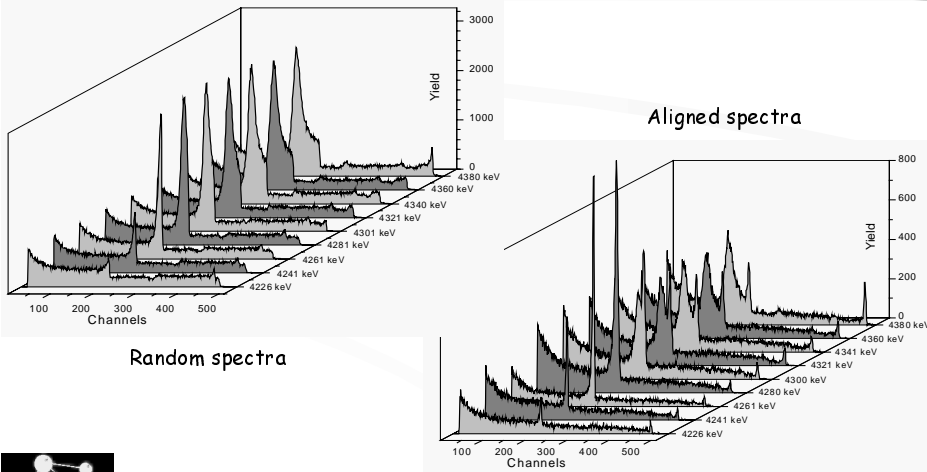
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Enhancing the sensitivity: $^{12}\text{C}(\alpha,\alpha)^{12}\text{C}$ resonance at 4.26 MeV

He⁺ beam
Energy varies between 4226 keV and 4380 keV
IBM geometry, Detection angle: 165°, $\chi_{\text{min}} \approx 8\%$
non-implanted 6H-SiC samples

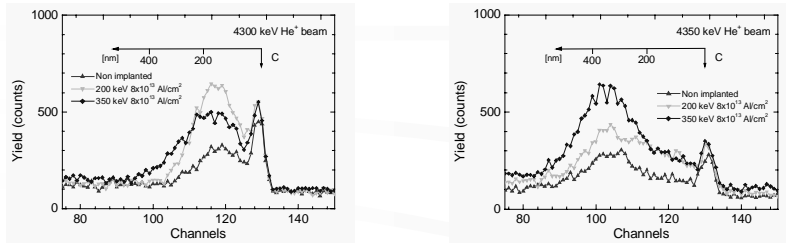


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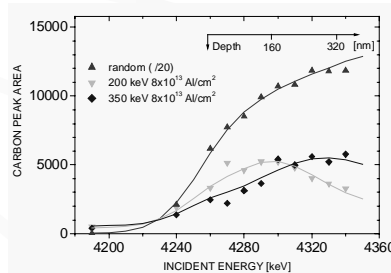
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5

6H-SiC samples were implanted with Al ions at 200 keV and 350 keV with the dose of $8 \times 10^{13} \text{ cm}^{-2}$ at room temperature. Random and aligned spectra were recorded at different He⁺ beam energies around the 4.26 MeV resonance in the non-Rutherford cross section of ^{12}C . Varying the beam energy the number of displaced carbon atoms are measured at various depth and an excitation curve can be derived.



The shape of the excitation curve resembles the concentration of the displaced carbon atom. In the case of lower energy implantation the maximum damage appears at about 150 nm below the surface while at 350 keV implantation this depth is about 280 nm. The distribution of displaced carbons are wider for the higher energy implantation. For comparison the excitation curve for random case is also shown. Solid lines represent DEPTH calculations. To eliminate the background the corresponding aligned virgin spectra were subtracted.



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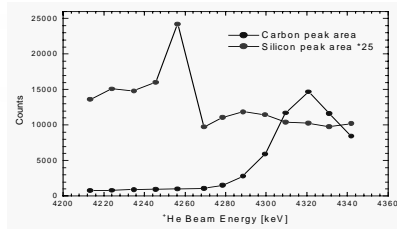
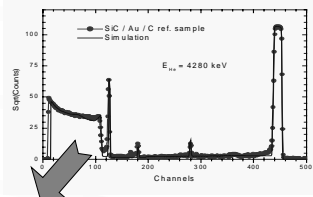
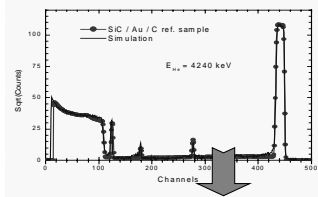
Vienna, 2003

6

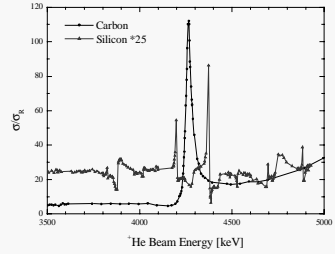
Cross sections for He on C and Si around 4.26 MeV

In order to verify the cross sections of C and Si, thin layer of SiC was deposited onto a $8.4 \times 10^{17} \text{ cm}^{-2}$ Gold layer on vitreous Carbon substrate. BS spectra were taken in the energy range of 4.2 MeV to 4.5 MeV using the energy scanning system of the tandem accelerator of CNA.

From the C and Si peak areas the cross section curves can be created. We found out that the resonance peak in C cross section at 4.26 MeV is **smaller** by about **12.5%** than the value given [Feng et al. 1994]. Also the cross section of Si [Leung et al. 1972] should be **shifted** by **13 keV**.



C and Si peak area



The corrected C and Si cross sections

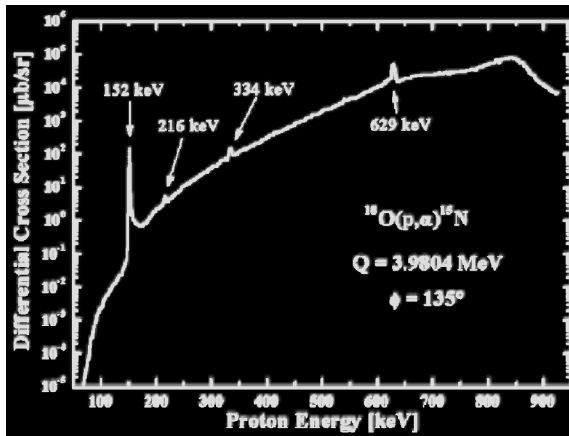


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Cross Section for $^{18}\text{O}(p,\alpha)^{15}\text{N}$ nuclear reaction



Resonances:

- 152 keV, $\Gamma \approx 100 \text{ eV}$, medium
- 216 keV, $\Gamma \leq 1 \text{ keV}$, weak
- 334 keV, $\Gamma \leq 1 \text{ keV}$, weak
- 629 keV, $\Gamma \approx 2.1 \text{ keV}$, strong



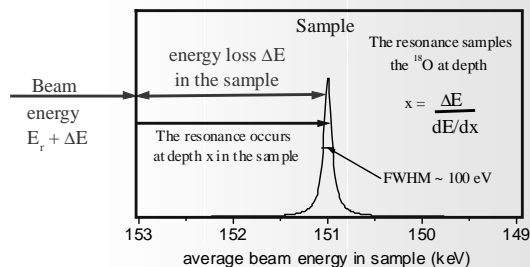
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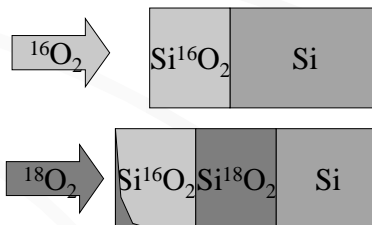
8

Narrow Nuclear Resonance profiling of ^{18}O

The alpha particle yield as a function of beam energy is an image of the concentration profiles of ^{18}O



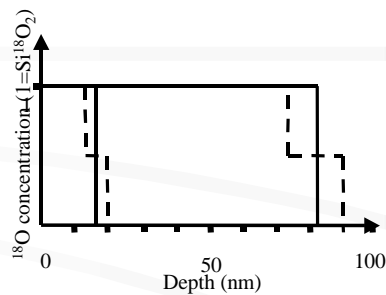
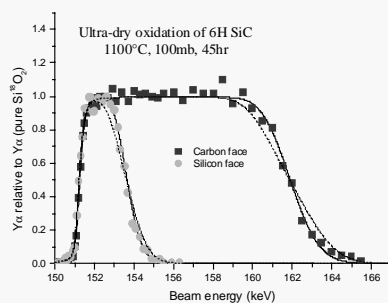
Stable isotopic tracing



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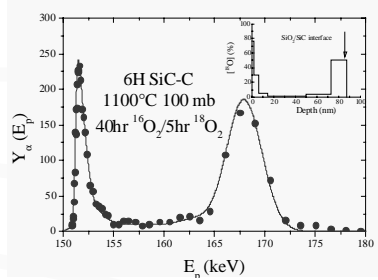
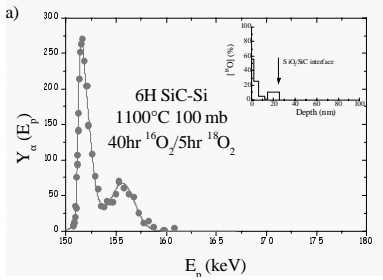
Oxidation in pure $^{18}\text{O}_2$ followed by resonance profiling shows that the oxide is stoichiometric. The solid lines are calculated best fit excitation curves for pure SiO_2 of thickness 79nm (SiC-C) and 16nm (SiC-Si). The dotted lines are calculated excitation curves for depth distributions containing the same total amount of ^{18}O , distributed as shown on the right.



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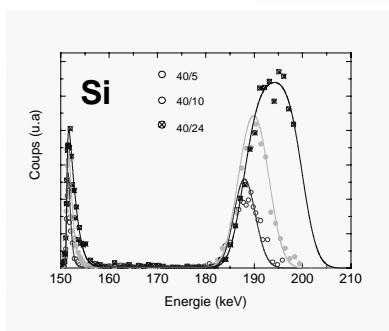
10



In contrast to the case of dry thermal oxidation of silicon, we observe on SiC that the isotopic enrichment of the oxide that grows at the interface is less than 100%. We believe that this could mean that silicon atoms are injected into the oxide during growth.

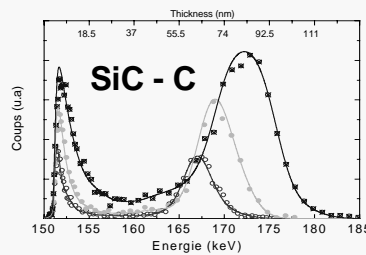
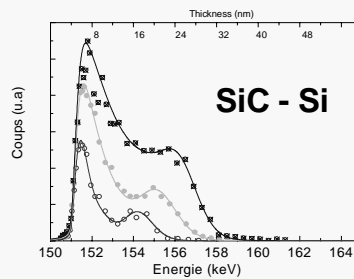


Excitation curves
¹⁶O₂ 40 h + ¹⁸O₂ 5h, 10h, 25h
100 mbar, 1100°C



Deal-Grove model describes the oxidation kinetics for Si

Similar shapes for SiC, but different oxidation rate and ratio

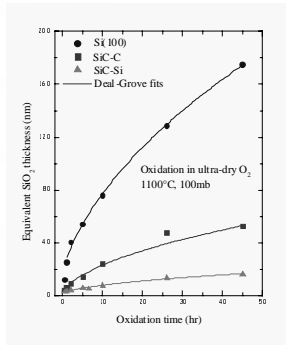


Kinetics and pressure dependence

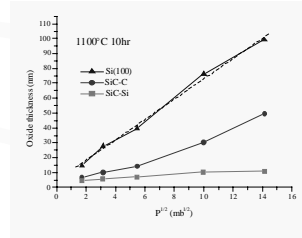
^{18}O areal density by NRA

$^{18}\text{O}(p,\alpha)^{15}\text{N}$ at 730 keV

The material studied here is n-type 6H SiC, double-polished, on-axis from CREE Research inc. The UHV furnace allows ultra-dry ($[\text{H}_2\text{O}] < 1\text{ppm}$) oxidation.



The growth rates are sub-linear for both faces of 6H SiC. This cannot be caused by a simple interfacial limitation of the reaction rates.



Pressure dependence in the parabolic regime. Thickness $\sim p$ for 6H SiC-C and $\sim p^{1/4}$ for 6H SiC-Si, suggesting the establishment of different chemical equilibria in the interfacial region.



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Budapest, Hungary

Vienna, 2003

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Contribution by G. Vizkelethy

SIGMABASE
Past, Present, Future

György Vizkelethy
Sandia National Laboratories



Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.



Outline

- **The beginnings**
- **Present state (demo)**
- **Problems we are facing**
- **Future (solutions to our problems)**



The beginnings

- 1974-77 : The Catania Handbook
- 1988-89 : Paris, NRA, working with Georges Amsel and Ian Vickridge (SENRAS 1988)
- 1990-95 : Handbook of Modern Ion Beam Materials Analysis
- 1991 : Namur conference, R33 format
- 1992 : Denton, Workshop on Resources for Ion Beam Analysis
- 1993 : FTP server, IBA-11 workshop (Balatonfured)
- 1995 : Web server, introduction of SIGMABASE to the IBA community at IBA-12 (Tempe)
- 1997 : IBA-13 (Lisbon) workshop, SIMNRA
- 2000 : Workshop on long terms needs for nuclear data, IAEA, Vienna, late November (Ian Vickridge, Alexander Gurbich)



What can SIGMABASE offer?

- Nuclear and elastic scattering cross sections
 - NRA (D to ^{32}S) - G.Vizkelethy, G. Giorginis, G.Terwagne
 - ERD - V. Quillet, G.Terwagne
 - (p,p), (α,α) - J. Leavitt and L. McIntyre
- IBA programs (OM_DAQ, MPAWIN, SPAN, ALEGRIA, DEPTH, SIMNRA, SPACES, SENRAS, etc.)
- Links to useful IBA sites



How to access the SIGMABASE

- Main Website (ISU)
 - <http://ibaserver.physics.isu.edu/sigmabase>
- European mirror (MFA)
 - <http://www.mfa.kfki.hu/sigmabase>
- **Sandia Ion Beam Analysis Table of the Elements**
 - <http://www.sandia.gov/1100/1111/Elements/table.htm>



The problems we are facing

- Our data is not considered as evaluated cross sections ([see disclaimer](#))
- People like more taking than giving
- SIGMABASE should not rely on a person, it should be supported by an institution



Selected Low Energy Nuclear Reaction Data

4 Selected Low Energy Nuclear Reaction Data

Edited by L. C. Fildeman and S. T. Pirovka
 International Atomic Energy Agency, Vienna, 1971
 IAEA Library Catalogue No. ST-100/100

1.1. Introduction	1
1.2. Generalized cross-sections	11
1.3. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.4. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.5. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.6. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.7. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.8. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.9. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.10. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.11. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.12. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.13. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.14. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.15. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.16. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.17. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.18. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.19. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11
1.20. Generalized cross-sections for the reaction $^{100}\text{Mo}(p, n)^{100}\text{Tc}$	11

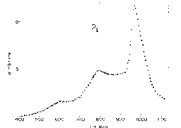
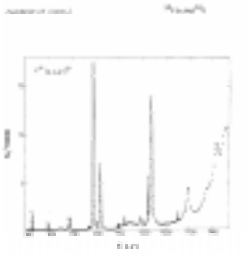
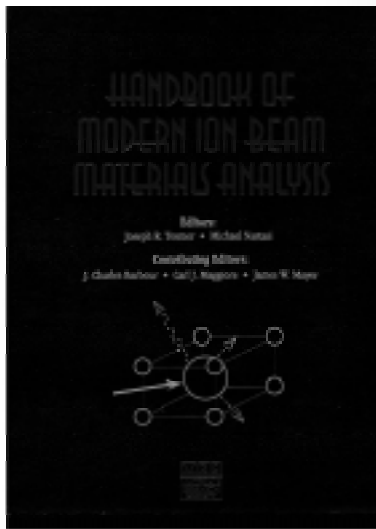


FIG. 4.37. Cross section vs. incident energy at $\theta_{LAB} = 150^\circ$ for $^{100}\text{Mo}(p, n)^{100}\text{Tc}$ reaction. From Proc. 5th Int. Acad. and N. Serov, Anal. Chem. 22, 2489 (1973).



The New Ion Beam Handbook (1991/1995)



Data in the Appendices I

APPENDIX
I

NON-RUTHERFORD ELASTIC BACKSCATTERING CROSS SECTIONS

Compiled by

R. P. Cox, T. A. Leavitt, and L. C. McIntyre, Jr.

University of Arizona, Tucson, Arizona

This appendix contains non-Rutherford elastic backscattering cross-section data for a variety of target nuclei. The data are presented in a format similar to that of the Rutherford cross-section data in Appendix II. The data are presented in a format similar to that of the Rutherford cross-section data in Appendix II. The data are presented in a format similar to that of the Rutherford cross-section data in Appendix II.

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The procedure used to digitize the cross-section plots is described in the notes on the back cover of this appendix.

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The procedure used to digitize the cross-section plots is described in the notes on the back cover of this appendix.

Non-Rutherford Elastic Backscattering Cross Sections

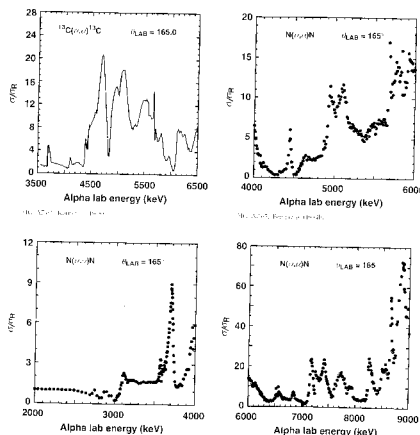


Fig. 1.1. $^{12}\text{C}(\alpha, \alpha)^{12}\text{C}$

Fig. 1.2. $\text{N}(\alpha, \alpha)\text{N}$

Fig. 1.3. $\text{N}(\alpha, \alpha)\text{N}$

Fig. 1.4. $\text{N}(\alpha, \alpha)\text{N}$



U

Data in the Appendices II

APPENDIX
II

PARTICLE-PARTICLE NUCLEAR REACTION CROSS SECTIONS

Compiled by

L. J. Foster

Los Alamos National Laboratory, Los Alamos, New Mexico

G. V. Kikigthy

Mississippi State University, Forestville, Idaho

M. Lee, J. R. Tesmer, and M. Nastasi

Los Alamos National Laboratory, Los Alamos, New Mexico

This appendix contains particle-particle nuclear reaction cross-section data for a variety of target nuclei. The data are presented in a format similar to that of the Rutherford cross-section data in Appendix I. The data are presented in a format similar to that of the Rutherford cross-section data in Appendix I.

The particle-particle nuclear reaction cross-section data are presented in a format similar to that of the Rutherford cross-section data in Appendix I. The data are presented in a format similar to that of the Rutherford cross-section data in Appendix I. The data are presented in a format similar to that of the Rutherford cross-section data in Appendix I.

Particle-Particle Nuclear Reaction Cross Sections

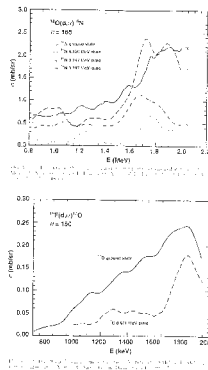




Fig. 2.1. $^{10}\text{B}(\alpha, n)^{13}\text{C}$

Fig. 2.2. $^{10}\text{B}(\alpha, p)^{11}\text{B}$





Contribution by M. Mayer

Cross Section Data in SIMNRA 5.0

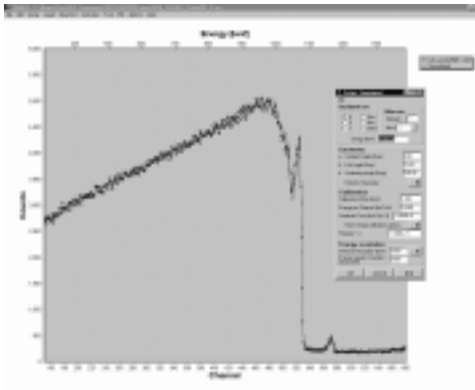
M. Mayer
Max-Planck-Institut für Plasmaphysik, EURATOM Association, 85748 Garching, Germany

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What is SIMNRA?

- **RUMP-like program** for simulation of MeV ion beam analysis spectra
 - RBS including RBS with Non-Rutherford cross sections
 - ERDA including ERDA with Non-Rutherford cross sections
 - NRA
- **Windows program** with fully graphical user interface
- **300 cross sections** included
 - for RBS, ERDA, NRA
 - for incident H, ^3He , ^4He , ^6Li , ^7Li



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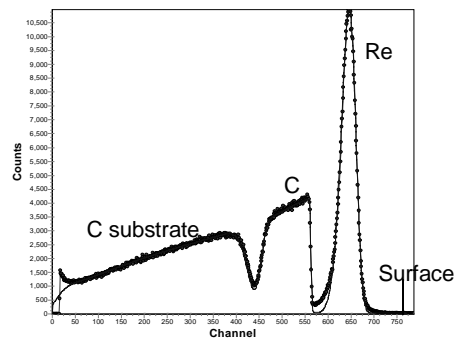
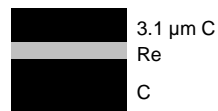


Why non-Rutherford RBS?



- **Increased interest** in RBS with non-Rutherford cross sections during the last years
 - Better sensitivity for light elements: 10 – 50 x Rutherford
 - Larger analysed depth (protons, high energy ^4He)
 - Simulation programs easily available (RUMP, SIMNRA)
 - Many cross section data available

RBS with 1.6 MeV H^+ . $\theta = 165^\circ$



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Cross section data in SIMNRA



Cross section data in SIMNRA originate from

- **SigmaBase**
 - Tesmer/Nastasi, Handbook of Modern Ion Beam Materials Analysis, 1995
 - Error corrected (incorrect Q values, ...): Vickridge/Mayer 2002
- **Added by author**
 - About 90 data files
 - Digitised from original publication or correspondence with authors
 - Most data submitted to SigmaBase

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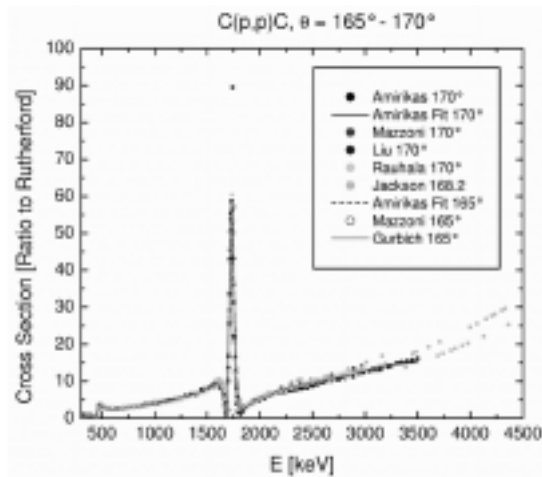


Cross section data in SIMNRA (2)



Comparison and recommendation of proton cross section data available at SIMNRA HomePage: <http://www.rzg.mpg.de/~mam>

- D
- C
- N
- O
- Al
- Si



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Cross section data needs



- **Evaluated** cross section data (backscattering, reactions) are absolutely necessary
 - Large number of data available
 - Large scatter of experimental data
 - Sometimes large inaccuracies of individual data
- Theory based **extrapolation** of data to intermediate angles/energies
 - SigmaCalc
- **Long term** availability and storage of cross section data
- **Free** (uncensored) availability of cross section data
- **Easy readable** format for humans and computers
 - Current format: R33 (ASCII)

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Update to the R33 cross section file format

By I. C. Vickridge

SAFIR

Groupe de Physique des Solides, UMR 7588 du CNRS

Tour 23, Universités de Paris 7 et 6

2, Place Jussieu

75251 Paris

Introduction

In September 1991, in response to the workshop on cross sections for Ion Beam Analysis (IBA) held in Namur (July 1991, *Nuclear Instruments and Methods* B66(1992)), a simple ascii format was proposed to facilitate transfer and collation of nuclear reaction cross section data for Ion Beam Analysis (IBA) and especially for Nuclear Reaction Analysis (NRA). Although intended only as a discussion document, the ascii format - referred to as the R33 (Report 33) format - has become a de facto standard. In the decade since this first proposal there have been spectacular advances in computing power and in software usability, however the cross-platform compatibility of the ascii character set has ensured that the need for an ascii format remains.

Nuclear reaction cross section data for Nuclear Reaction analysis has been collected and archived on internet websites over the last decade. This data has largely been entered in the R33 format, although there is a series of elastic cross sections that are expressed as the ratio to the corresponding Rutherford cross sections that have been entered in a format referred to as RTR (ratio to Rutherford). During this time the R33 format has been modified and added to - firstly to take into account angular distributions, which were not catered for in the first proposal, and more recently to cater for elastic cross sections expressed as the ratio-to-Rutherford, which it is useful to have for some elastic scattering programs. It is thus timely to formally update the R33 format.

There also exists the large nuclear cross section data collections of the Nuclear Data Network - of which the core centres are the OECD NEA Nuclear Data Bank, the IAEA Nuclear Data Section, the Brookhaven National Laboratory National Nuclear Data Centre and CJD IPPE Obninsk, Russia. The R33 format is now proposed to become a legal computational format for the NDN. It is thus also necessary to provide an updated formal definition of the R33 format in order to provide the necessary specification for adoption of R33 as an accepted computational format.

Guiding considerations.

In defining the updated R33 format I have required that previous valid R33 files should also conform to the updated format. This is so that R33 reading programs that conform to the updated specification will be able to read the existing R33 files - providing backward compatibility. There is also some redundancy in the format. This is partly from intellectual laziness, but also provides some checking of internal consistency to weed out errors.

The new R33 Format definition.

An R33 data file contains one cross section either as a function of (laboratory) incident energy, or as a function of (laboratory) detection angle. The file is made up of entries, and the data section. Each entry consists of a legal keyword followed by a colon followed by a space, followed by data in Ascii format. The keyword may be in any mixture of upper and lower case characters. Legal separators for numerical data are space, comma, colon, and semi-colon characters. Decimal points are represented only by full stops, and not by commas (as can be the case in some European countries). The legal ascii character set for the purposes of R33 files is ascii 0 to ascii FF. Apart from the 'Comment' entry and the optional 'Version' entry, entries may be in any order. Each entry ends with a carriage-return line-feed sequence. Some entries are optional [O], most are required [R], and some are mutually exclusive [Mx] where all entries for which the value of x is the same are mutually exclusive. See below for special conditions that apply to the keywords 'Comment', 'Nvalues', 'Data', and 'EndData'. Default values are suggested for R33 reading routines, so that if an optional entry is omitted, or if a required entry is unreadable or missing illegally, the value of the corresponding variable in the reader is well-defined. All energies are expressed for the laboratory frame in keV and all angles in the laboratory frame in degrees. English is the preferred language.

Syntax of an R33 Entry

The syntax for the list of legal keywords and the associated data is :

Keyword: [Mx, O/R] (Default) <data type>

*Note: Additional notes and guidelines concerning use of the entry.
Data type may be:*

string (an arbitrary series of ascii characters)

*n (integer) a series of ascii characters without decimal point
representing a signed integer number*

*r (real) a series of ascii characters that represent a signed real
number. Format is fairly flexible - but only decimal points (and NOT
decimal commas) are accepted. Any format that can be read in a
Borland Pascal readln(r) statement is acceptable.*

List of legal entries

Comment: [R] ('None') <String>

*Note: An unlimited number of ascii characters, including single CR
LF sequences, but terminating by a double CR LF sequence. There is
no requirement to embed CR LF sequences within the Comment,
however it is recommended to place CR LF sequences at convenient
places at least every 80 characters so that if the file is printed, the
comment field is printed on successive lines that are not longer than
80 characters. The double CR LF sequence that signals the end of the*

comment is simply a blank line. It is not felt necessary to specify an upper limit to the size of the comment, however it is expected that a useful comment would not be longer than a few tens of lines - or a few thousand characters. Note that unix systems place only a LF character to signal an end-of-line. This is illegal for R33 files. There are freeware and shareware utilities that can add the necessary CR characters if R33 files are generated under Unix.

Version: [O] ('DSIR R33') <String>

Note: Allowed values are (case-insensitive) 'DSIR R33' and 'DSIR R33a'. This entry can be used to signal that the file conforms to the special subset of R33 files proposed by M. O. Thompson for elastic scattering cross sections for use in RUMP. Sigabase files will always be DSIR R33, but the 'R33a' variant is detailed here for completeness. All R33a files are legal R33 files, but R33a files have the following additional conditions:

- 1) The Version entry is required, and must be the first entry after the Comment.*
- 2) Only elastic cross sections can be in valid R33a files*
- 3) Nvalues must either not be present, or have a value of less-than-or-equal-to zero.*

Source: [R]('Unknown')<String>

Note: A concise bibliographic source (preferable) or another indication of where the data has come from (avoid if possible). This field should contain the most authoritative original source for the data. This will usually be the original publication, or thesis reference. In some cases data has been input by experimenters before or without publication. In this case this entry should contain something like 'Measured and input by D. Withrington'. It should be kept small - an upper limit of 256 characters is suggested, but not required. It would be expected that further details pertaining to Mrs Withrington would be found in the Comment.

Name: [R]('unknown')<String>

Note: The name of person or institution responsible for creating the R33 file. For R33 files automatically created from Exfor files, this would be IAEA, or NNDC, or International Nuclear Data Network or whatever. No provision is made here for including update histories, however this may be accommodated in the Comment field.

Address1: [O] (') <String>

...

Address9: [O] (') <String>

Note: The address of the person or institution responsible for creating the R33 file. Up to nine lines of address information may be included. This can include telephone numbers, emails and so on.

Serial Number: [R] (0) <n>

Note: The serial number will be a number providing a unique link

back to the Exfor dataset from which the R33 file was generated. The default value of zero means that this number has not been assigned.

Reaction: [R] (' ') <String>

Note: the reaction string is written in a standard format that can be parsed without too much difficulty. It conforms to the usual notation of:

target nucleus(incident ion, light product)product nucleus

Nuclei are specified by their chemical symbol preceded by A : eg 28Si, or 6Li. The mass number is required. Some common light species may also be represented by shorthand notation, with lower case being required.

n=neutron

p=proton

d=deuterium

t=triton

a=alpha particle

h=3He

x=x-ray

g=gamma

The light product may correspond to a particular energy level of the product nucleus. This is signalled by a 'postfix' on the light product. For example, 16O(d,p1)17O is the (d,p) reaction which leaves the residual 17 oxygen in the 1st excited state. Some cross sections may be sums of several particle groups corresponding to different excited states of the compound or product nucleus. Usually such a cross section would be used when the particle groups are not resolved by the detection method employed. In this case, the postfix lists the states concerned, separated by plus signs. E.g. 14N(d,p5+6)15N. Some elastic cross sections correspond to targets having several isotopes. In this case, it is necessary to use the 'target' keyword.

Masses: [R] (1,1,1,1) <n,n,n,n>

Note: Four values of A corresponding to the four nuclei specified in the reaction string, separated by legal separators. In principle the masses could be deduced directly from the reaction string, however in the interests of simplicity it seems worthwhile adding them to the R33 file to avoid having to write a reaction string parser in R33 readers. In the special case where the 'target' keyword is used, the values there override those contained in the 'Masses' entry.

Zeds: [R] (1,1,1,1) <n,n,n,n>

Note: Four integers representing the atomic number of the four nuclei specified in the reaction string. The Zs could also be deduced directly from the reaction string, but see the comment in the Masses entry.

Target: [O] ('Natural') <string, r, string, r, ...>

Note: This entry caters for elastic cross sections measured from targets that contain a mixture of isotopes from which the elastically scattered particles are not resolved. It consists of a list of isotopes and atom-proportions, or the value 'natural' (case insensitive) which means that a target of naturally occurring isotopic composition has been used. Isotopes are specified as for the reaction string, without shorthand notation. Example :

Target: 12C, 23.0, 13C, 26.0

If the proportions do not sum to 100, then it is assumed that they are relative amounts. In the example given, 23/49 of the atoms are 12C, and 26/49 are 13C.

Qvalue: [R] (0.0) <r, r, r, r, r>

Note: A list of up to five Q values, expressed in keV, separated by legal separators. As explained in the Reaction entry, some cross sections are for multiple particle groups, for example when the groups are not resolved experimentally. In this case a Q value is required for each particle contributing to the cross section.

Distribution: [R] ('Energy') <String>

Note: Allowed values are 'Energy', 'Angle' or 'Total'. This entry says whether the data contained in this file are for a cross-section as a function of laboratory energy ('Energy') or laboratory angle ('Angle'). The value 'Total' signals that the cross section is a function of laboratory energy, integrated over all detection angles. Values are case insensitive.

Theta: [M1, R] (0.0) <r>

Energy: [M1,R] (1.0) <r>

Note: Theta gives the laboratory angle with respect to the incident beam, so that backscattering would be 180°. Energy gives the laboratory energy of the incident beam. If both entries are present (an illegal condition ...) then only the entry corresponding to the keyword in the 'Distribution' entry will be used.

Sigfactors: [O] (1.0, 0.0) <r,r>

Note: Scale conversion factor and its associated error common to all the cross section data. See original R33 publication in Appendix 1 for discussion.

Units: [O] ('mb') <String>

Note: Valid values are 'mb' and 'rr'. R33 files are always in mb/sr, or units proportional to mb/sr for differential cross sections, and mb for total cross sections. The constant of proportionality given in the enfactors entry is independent of energy. Some users find it preferable to have elastic scattering cross sections relative to the Rutherford cross section. Since the conversion factor is no longer energy-

independent, the enfactors entry can no longer cater for this. In this case, the units entry should specify 'rr' for ratio to Rutherford. Nevertheless, it is recommended that elastic cross sections be stored as cross sections just like the inelastic scattering cross sections - i.e. in mb/sr.

Enfactors: [O] (1.0, 0.0, 0.0, 0.0) <r,r,r,r>

Note: Scale conversion factors and associated errors common to all the energy or angle data. See original R33 publication in Appendix 1 for discussion.

Nvalues: [M2,R] (0)<n>

Data: [M2,R]

Enddata: [O]

Note: two methods are allowed for representing the data. The first corresponds to the original R33 specification. The data immediately follow the 'Nvalues' entry consists of the cross section data, one point per line, and each point represented by four values (X, dX, Y, dY):

*energy(or angle), energy(or angle) random error, sigma, sigma
random error*

The data ends after Nvalues lines of data, and any subsequent lines are ignored.

Alternatively (and recommended), the data may be bracketed by 'Data' and 'Enddata' entries. An entry of 'Nvalues: 0' is equivalent to a 'Data' entry. The data immediately follow the Data entry, one point per line as for the Nvalues option, and the file terminates with the end of the file, or with the optional EndData entry. Nvalues is maintained for backward compatibility, but in practice most routines will simply read and count the number of lines read until the end of the file or an EndData entry is reached, so this is the preferred option. The use of the Enddata entry simply allows a check that all of the data values are contained in the file and have been read.

Data entries must be arranged in order of increasing energy or angle. Duplicate energy or angle values are not allowed (the cross section must be single-valued).

The R33 Manager©

A small, user-friendly Windows program has been written to help manage R33 files. This program

- Allows graphical visualisation of R33 files
- Allows modification of all parameters in an R33 file
- Allows creation of new valid R33 files

- Creates an ascii file containing CSV entries of the main details of all R33 files in a directory. This file may readily be imported into common spreadsheet or database programs.

The R33 Manager© is freely available from the Sigmabase websites. The most up to date version may be obtained directly from the author: vickridge@gps.jussieu.fr.

Appendix 1.

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DSIR Physical Sciences Report 33

Proposed ASCII Format for Communication of Reaction Cross Sections in the IBA Community

by I.C. Vickridge
Nuclear Sciences Group

Note: This document differs from report 33 as archived by Geological and Nuclear Sciences Ltd (the successor to DSIR Physical Sciences, Nuclear Sciences Group) by inclusion of the 'DISTRIBUTION' field. This field may have the value 'Energy' or 'Angle'. If DISTRIBUTION is 'Energy' then there must be a 'THETA' field; if DISTRIBUTION is 'Theta' then there must be an 'ENERGY' field. The use of a 'negative' energy to indicate angular distributions was not a good idea!

Abstract This report describes an ASCII data format for the communication of Ion Beam Analysis (IBA) cross-section data. It is proposed that the IBA community adopt this format to simplify setting up an IBA cross-section database at a later date.

Keywords Nuclear cross sections; ion beams; computers; data storage; data transmission

Introduction

At the Third International Conference on Chemical Analysis, (Namur, July 8-12 1991) a workshop was held on the establishment of a database of cross-section data of interest to the IBA community and a summary of the discussions is likely to be published in the proceedings [1]. Although no firm followup action (apart from writing the report [1]) was proposed at the workshop, the general utility of such a database was widely endorsed, and a consensus was arrived at for a number of issues. As an interim measure until a centralised database is set up, it is proposed that the IBA community adopt a standardised way of transmitting measured cross-section data. This report proposes such a standard.

Scope

This standard is intended to apply to charged incident particle prompt IBA cross-sections giving rise to nuclear interactions (i.e. excluding PIXE, but including PIGME) in the energy range from 0 to say 50MeV. Although the detection of neutrons as products of nuclear reactions is included, the use of incident neutron beams for prompt NRA is not included for the time being. The file format is intended to be sufficiently flexible that these cross sections may be tabulated if the need arises. This statement of scope is not intended to be definitive - the scope of the database to be set up will be decided by the operating organisation. For example the 50MeV limit would not exclude tabulations of the cross-sections of reactions of interest for hydrogen depth profiling in the laboratory frame in which hydrogen is the stationary target, however it is not suggested that all of the (d,p) cross-sections need to be measured up to 50MeV for IBA!

The special case of resonant nuclear reactions may need specification of further fields, but at present they may be accommodated as experimentally measured thin target excitation curves and prospective authors may be invited to include as much information as possible about target thickness, uniformity etc, and deduced resonance parameters in the COMMENT field of the proposed file format. The total number of resonances of interest to the IBA community is not likely to be more than a few hundred, and inclusion of this data either as a special subsidiary database or as special records in the main cross-section database should not be of great technical difficulty.

The choice of ASCII

Whilst it is recognised that ASCII representation will take up a lot more space than binary representation, the transportability of ASCII between virtually all computing platforms probably far outweighs the space disadvantage. Furthermore ASCII files are readily transmittable via even very rudimentary E-mail systems, and communications programs. Local binary formats, for example for use in RUMP [2] or SENRAS [3], or for producing local hardcopy (e.g. with GENPLOT [4]) of cross-sections of interest, will undoubtedly be adopted at each site.

Nevertheless, the ASCII format has been designed in such a way that inclusion into PC based databases or spreadsheets should be relatively straightforward. In the event that a centralised database is set up, collection, collation and archival of the data will be very much easier for data that is already in a standard format. The format has also been designed to be flexible, especially with respect to the addition of further fields.

Inclusion of errors/absolute versus relative cross-sections.

As far as tabulation of cross-section data is concerned these two issues are intimately related. We assume that the tabulated cross-sections and energies are estimates of the physical value they represent. The tabulated errors (where present) are estimates of the standard deviation of the spread in values if the measurement of that energy or cross-section were repeated under identical experimental conditions. These estimates reflect the precision, or repeatability, of individual data values.

Normally the physical value sought (cross section or energy) is inferred from the actual value measured in an experiment (e.g. number of counts, or NMR probe magnetic field value) by application of knowledge of the experimental parameters (e.g. solid angle and detector efficiency, or ion mass, charge state, and trajectory radius in the analysing magnet). These experimental parameters are also imperfectly known, although in well designed experiments there should not be significant random fluctuations in their values! They may be assumed to be the same for all the data values in a given experimental run, and often vary insignificantly between experimental runs. We assume a simple linear relationship between the measured parameter and the inferred physical quantity. This is a simplification, since systematic errors may change in a non-random way during an experiment - temperature dependence of gains in electronic equipment; target instability under the beam; and so on. However we assume that a good experimenter keeps these effects much smaller than the random errors associated with each data point. The uncertainty in our knowledge of the constant relating the physical quantity to the measured quantity is a measure of the systematic error in the experiment. The smaller this uncertainty the greater the accuracy of the measurement.

Assume that the tabulated cross-section values are called T_S^k (indexed from $k=1$ to $k=NVALUES$) and the corresponding real absolute cross-section values S^k . Then we define F_S by

$$S^k = F_S T_S^k \quad \text{for each value of } k.$$

The conversion factor F_S and its associated error dF_S are included in the file as a field. Now it is clear that if $F_S=1$, then the tabulated values are simply the absolute cross section. However if the tabulated data are numbers of counts or some other units then F_S converts the tabulated data into absolute cross-sections. By definition values of F_S and $dF_S=0$ are taken to mean that the conversion factor and absolute accuracy respectively are unknown.

Similar considerations will apply to the energy values for each data point, with an additional possibility of a shift error in the energy scale. Assume that the tabulated energy values are T_E^k and that the real corresponding energy values are E^k . Then the factors F_{0E} , F_{1E} , and the associated errors dF_{0E} and dF_{1E} are defined by:

$$E^k = F_{0E} T_E^k + F_{1E}.$$

Obviously, although F_{0E} is dimensionless, F_{1E} has the same dimensions as the T_E^k . These will be keV.

The 'random' errors may be listed after each data point in the file. The error values will be understood to mean that the author estimates that there is a 68.2% probability that the average value of an infinite number of measurements would lie between the tabulated value plus the tabulated error and the tabulated value minus the tabulated error. This means that if the random errors in the data follow a normal distribution the tabulated error is just the standard deviation. For normal counting statistics in which more than about 10 counts are recorded, the tabulated error would then just be the square root of the number of counts (multiplied by whatever factor was necessary to convert the counts into the tabulated units). If these error values are not given or are set to zero, then it is assumed that no estimate of the data precision has been furnished by the author. At the moment no provision is made for asymmetrical error estimates.

The ASCII file format:

COMMENT: Arbitrary length, may contain embedded spaces, tabs, carriage returns (CR), linefeeds (LF). Must contain at least 1 CRLF sequence every 80 characters.

Contains comments on the reliability of the data, the experimental arrangement, target thickness etc. Would also normally include the publication details if the data has been published, or an indication of how the author wishes to be cited in work which makes use of this data. (e.g. "please cite A.G. Physicist, pers. comm." or "please cite Another Physicist (2015), IBA Data Archives vol 1 (1) pp.107-118".

The author may also include here any details of semi-empirical fits that he or she may propose for the data - equations, and values of coefficients. Comment ends with "CR LF CR LF" i.e. a blank line.

NAME:

ADDRESS1:

ADDRESS2:

ADDRESS3:

ADDRESS4:

ADDRESS5:

ADDRESS6:

SERIAL NUMBER:

REACTION:

DISTRIBUTION:

MASSES:

QVALUE:

THETA:

SIGMA FACTORS:

ENERGY FACTORS:

NVALUES:

energy, sigma, energy error, sigma error, CR LF

energy, sigma, energy error, sigma error, CR LF

(continue until NVALS values is reached)

Example

COMMENT: A. Good Physicist. Institute for Fantastic Physics, 200 Nevernever street, Richton, Peoples Democratic Kingdom of Nirvana. Telephone (+123) 456789, fax 987654, E-mail AGP@FANPHYS.NIRVANA. This data is completely bogus. It was measured by a totally thick student and I've only sent it to the database so that some poor soul can try to evaluate it because I couldn't.

NAME: Physicist, A. G.
ADDRESS1: Inst. for Fantastic Physics,
ADDRESS2: 200 Nevernever street,
ADDRESS3: Richton 75005,
ADDRESS4: People's Democratic Kingdom of Nirvana.
ADDRESS5:
ADDRESS6:
SERIAL NUMBER: 123456
REACTION: 2H(d,t)p
DISTRIBUTION: Energy
MASSES: 2, 2, 3, 1
QVALUE: 8956
THETA: 35
SIGFACTORS: 1.0 0.0
ENFACTORS: 1.0, 0.0, 0.0, 0.0
NVALUES: 10
100 7.334e-1.1 .03e-14
200 7.334e-1.1 .03e-14
300 7.334e-1.1 .03e-14
400 7.334e-1.1 .03e-14
500 7.334e-1.1 .03e-14
600 7.334e-1.1 .03e-14
700 7.334e-1.1 .03e-14
800 7.334e-1.1 .03e-14
900 7.334e-1.1 .03e-14
1000 7.334e-1.1 .03e-14

Notes:

- 1) The ASCII file is broken up into fields.
- 2) Each field ends with a CR LF (Hexadecimal Od OA), except for the special case COMMENT field, which ends with CR LF CR LF (which means a blank line when the file is printed out). The comment field is the first field.
- 3) No field except the COMMENT field is longer than 80 characters (excluding the CR and LF characters *but including the comment name and colon*). The reason for this (and also for the CR LF every 80 or less characters in the comment) is so that the cross section file may be readily printed out in simple ASCII to any device that can print up to 80 characters on one line. There is no limit on the length of the comment, which may contain any of the ASCII character set (up to Hexadecimal FF) in any order, except the double CR LF sequence anywhere other than at the end i.e. it may not contain blank lines). The comment is preferably to be in English.
- 4) Each field except the data begins with its name, in capitals, followed immediately by a colon and a space (HEX 20).
- 5) The serial number is at present irrelevant, but would be assigned by a hypothetical database management organisation.

A double standard is proposed for the specification of nuclear reaction species. The most robust would be the complete chemical symbol to denote the atomic number, with the mass number prefixed (e.g. an alpha particle would be 4HE, and RBS on Si would be 28SI(4HE,4HE)28SI), and suffixed particle group numbers (e.g. 16O(2H,1H0)17O and 16O(2H,1H1)17O for $^{16}\text{O}(d,p_0)$ and $^{16}\text{O}(d,p_1)$ respectively. Neutrons would be 1N. Gamma rays would be represented by G or g, and X-rays (although it is not at present intended to include PIXE data in the cross-section data-base) by X or x. An optional notation is to use lowercase letters to specify the various light projectiles and products that are features of IBA:

p for proton
d for deuteron
t for triton

a for alpha
g for gamma
x for X-ray
n for neutron

A fairly free numerical format is suggested for the data values. Valid separators would include space, comma, semicolon, colon, and tab. The numeric data may be specified using exponential notation (e.g. 1000 could 0.1e4, or 1e3, or 10e2) or simple decimal notation (1000, 1000.0 etc) to an arbitrary number of digits. 7 digits is suggested as a reasonable maximum.

Units

All quantities are referred to the laboratory frame of reference. Energies will be specified in keV, angles in degrees, and absolute differential cross-sections in mb/sr. If cross-sections are specified in other units (e.g. counts per uC per mg/cm²) then this should be clearly stated in the COMMENT field, and F_S set to the appropriate value.

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usernames: ANONYMOUS for FTP file transfer;
FENDL2 for FTP file transfer of FENDL-2.0;
RIPL for FTP file transfer of RIPL.
NDSOHL for FTP access to files sent to NDIS "open" area.

Web: <http://www-nds.iaea.org>
