Nuclear Cross Sections Analysis and R-matrix Tools - Minischool
Surrey Ion Beam Centre and Department of Physics
University of Surrey, Thursday May 9th – Friday May 10th 2013

Leverhulme Lecture I

Nuclear Data for Ion Beam Analysis

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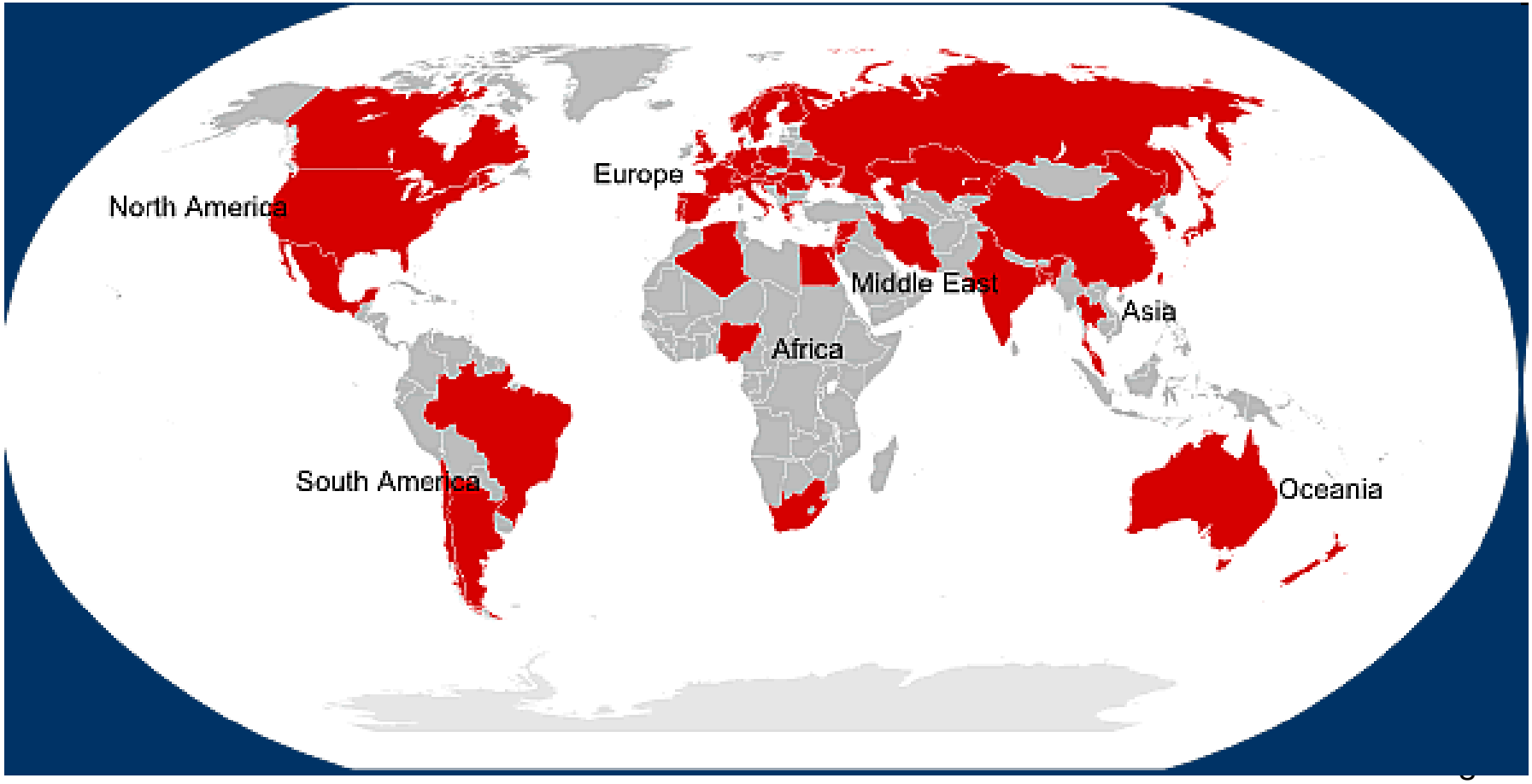
Ion Beam Analysis
(from Wikipedia)

- Ion beam analysis ("IBA") is an important family of modern analytical techniques involving the use of MeV ion beams to probe the composition and obtain elemental depth profiles in the near-surface layer of solids.

- IBA is an area of active research.

IAEA Physics Section database contains 163 low-energy electrostatic accelerators. Most of them are used for IBA.



What is “nuclear data”?

- *Quantitative* results of any scientific investigation of the nuclear properties of matter: nuclear physics data, or “nuclear constants”.
- ***Examples:*** cross sections, γ-rays, nuclear spectroscopy information on the positions, spin and parity of the nuclear energy levels

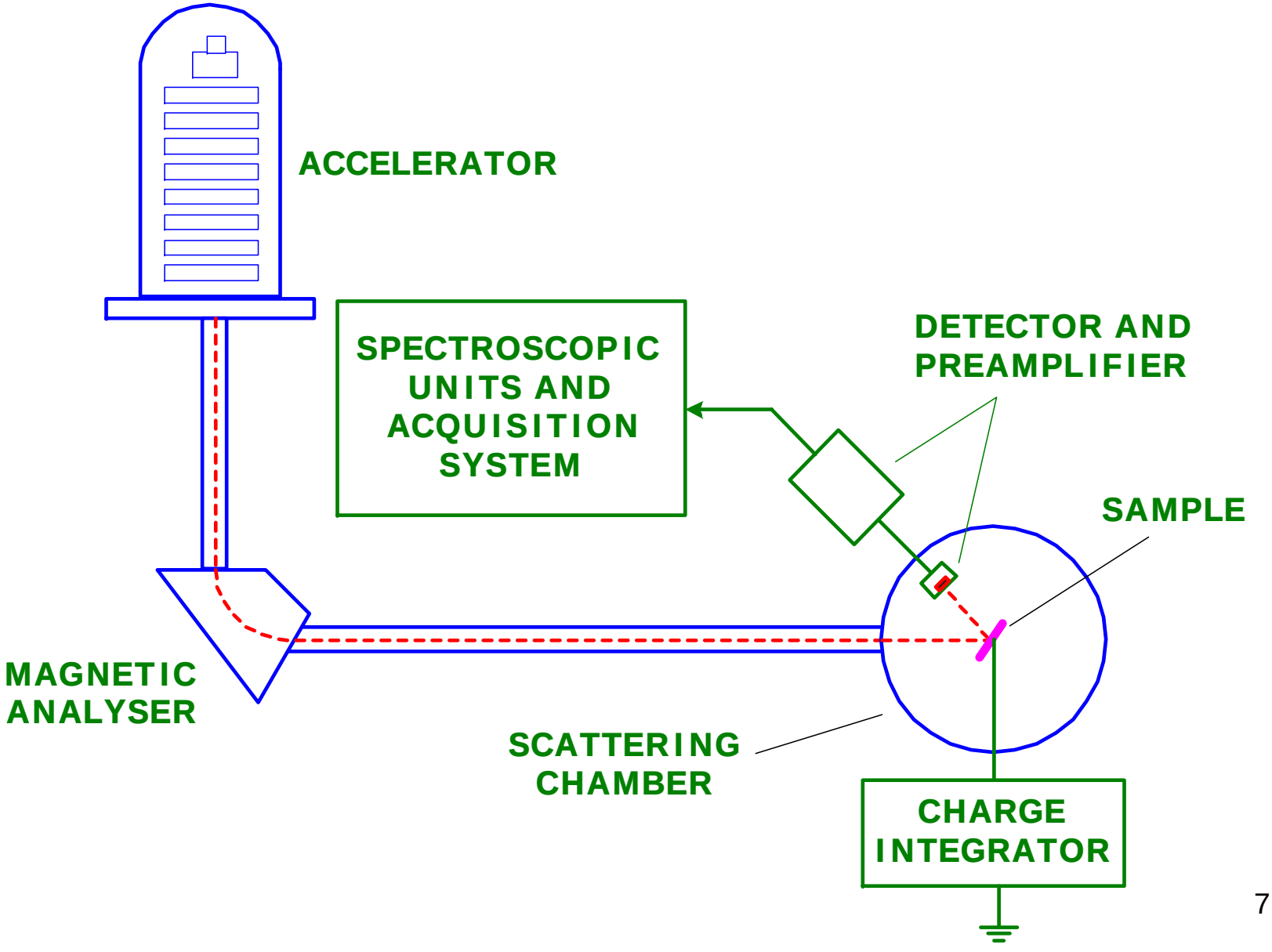
IBA METHODS

Method	Acronym	Interaction
Particle-Induced X-ray Emission	PIXE	Characteristic X-ray emission following ionization by the primary beam
Rutherford Backscattering Spectrometry	RBS	Elastic scattering at backward angles
Nuclear (non-Rutherford) Backscattering Spectrometry	NBS	Elastic scattering at backward angles
Elastic Recoil Detection Analysis	ERDA	Elastic recoil at forward angles, not necessarily Rutherford
Nuclear Reaction Analysis	NRA	Nuclear reaction between incident beam and nuclei in the target, producing a light charged particle
Particle Induced Gamma Emission	PIGE	Prompt gamma emission during ion beam irradiation

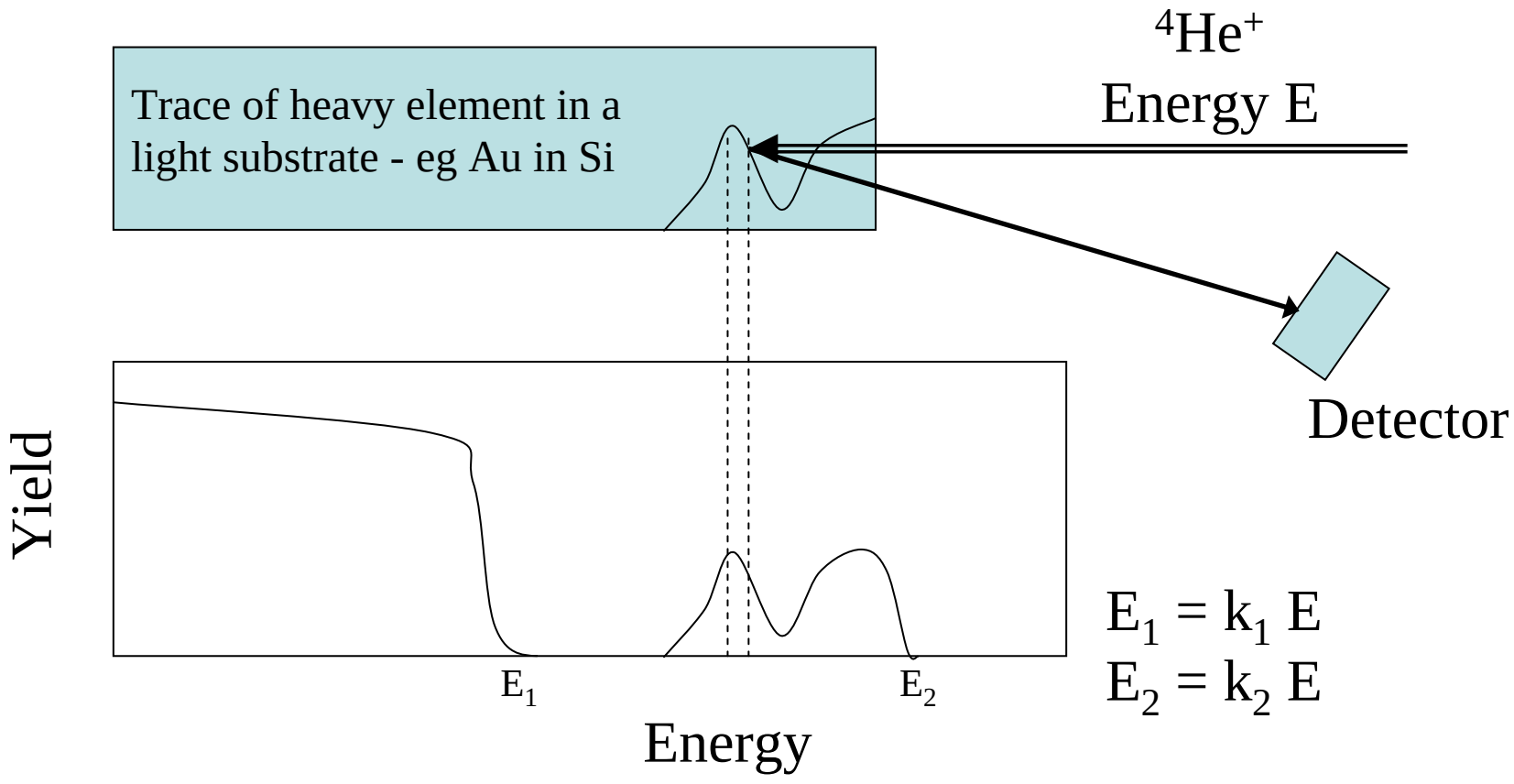
Ion Beam Analysis features

- All IBA methods are highly sensitive and allow the detection of elements in the sub-monolayer range.
- The depth resolution is typically in the range of a few nanometers to a few ten nanometers.
- The analyzed depth ranges from a few ten nanometers to a few ten micrometers.
- IBA methods are always quantitative with an accuracy of a few percent.

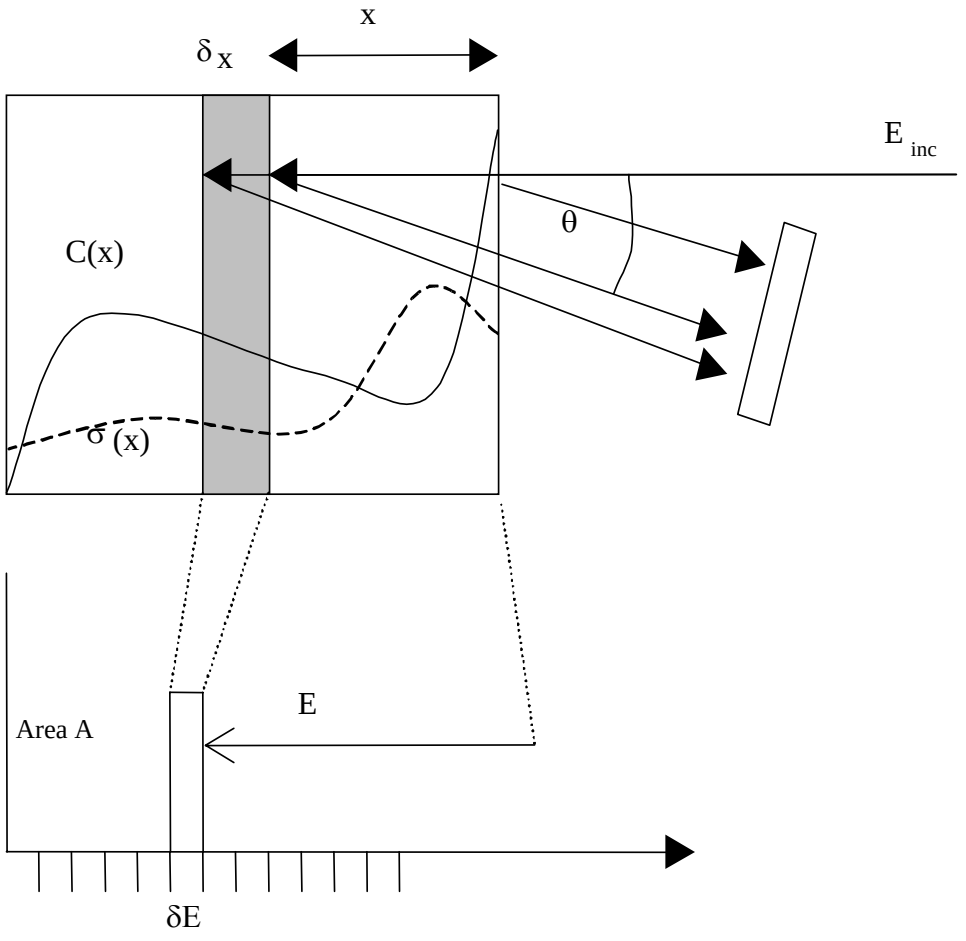
IBA experimental layout



RBS - principle



NRA Depth Profiling : Principle

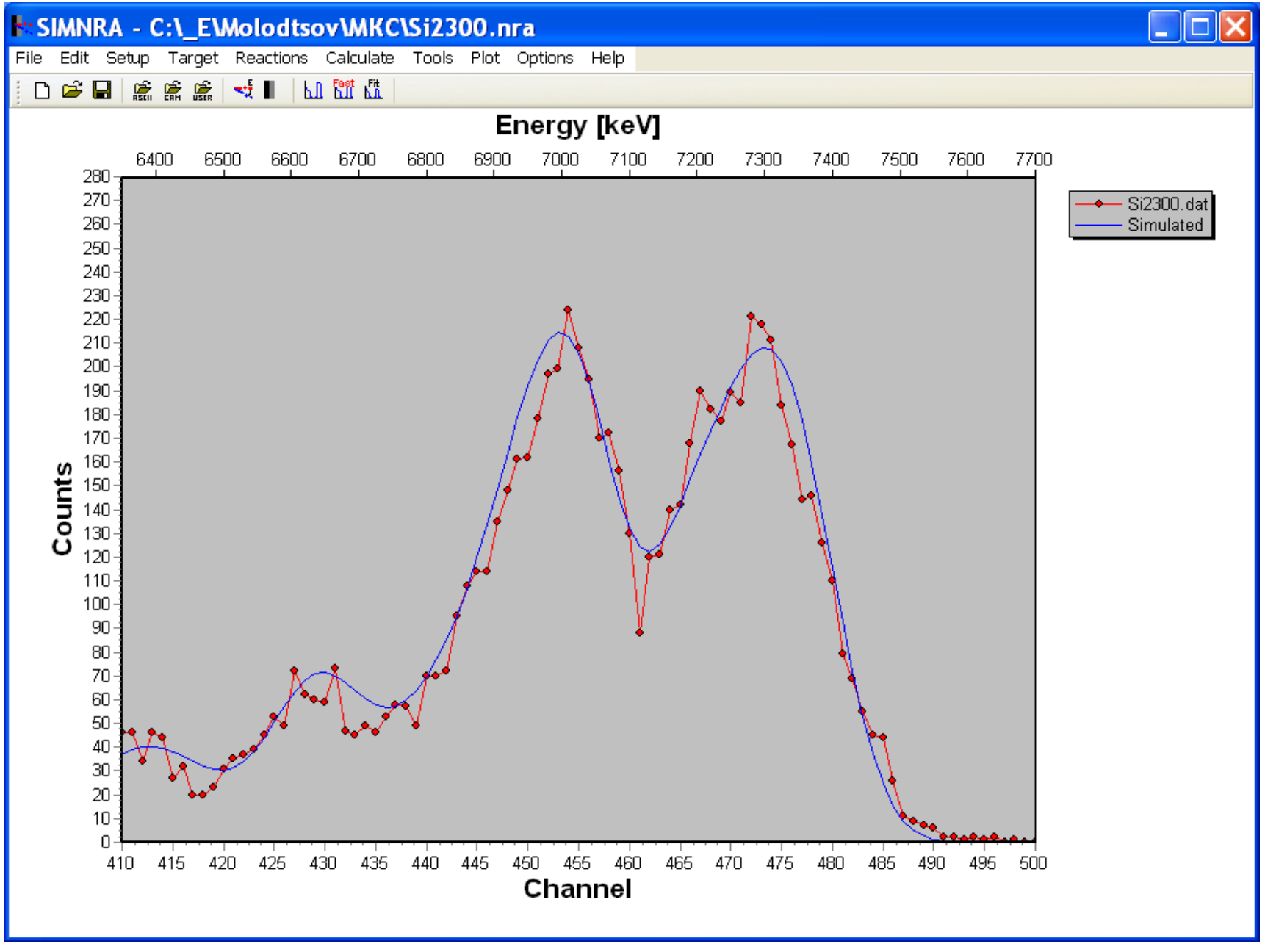


$$Y_i(E) = \int_0^{\infty} \frac{N_0 c(x)\sigma(\theta, E_1)\delta\Omega}{S(E')\left[\frac{-1}{\cos\theta} + \frac{kS(E_1)}{S(kE_1)}\right]} \; G(E' - E, \Gamma(x)) \; dE'$$

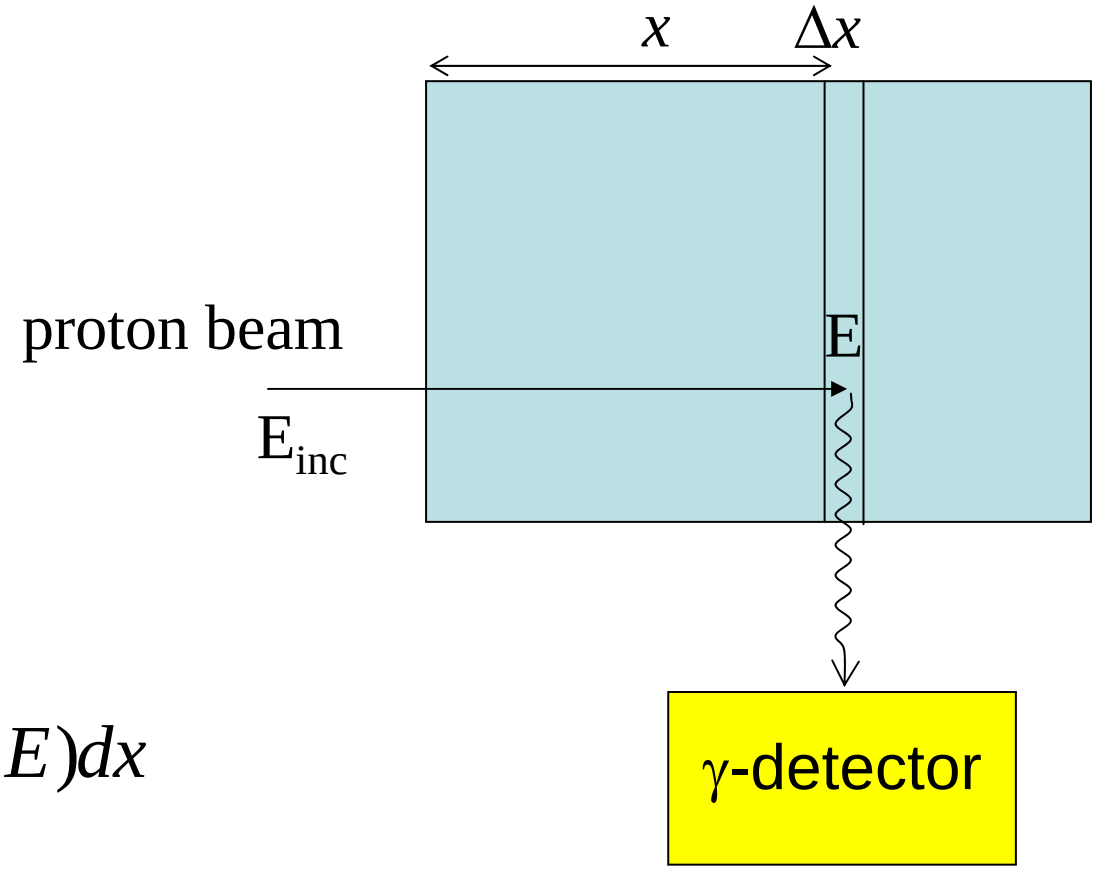
A channel of width δE_c at energy E_c in the spectrum corresponds to a slice of width δx at depth x in the sample, with Ec and δEc being inversely related to x and δx through a linear combination of the stopping powers for the incident and outgoing particle

The number of particles accumulated into that histogram bin is proportional to c(x), δx, and $\sigma(E_x)$, where E_x is the energy of the incident beam when it gets to depth x

Simulation of the IBA spectrum to derive depth profile



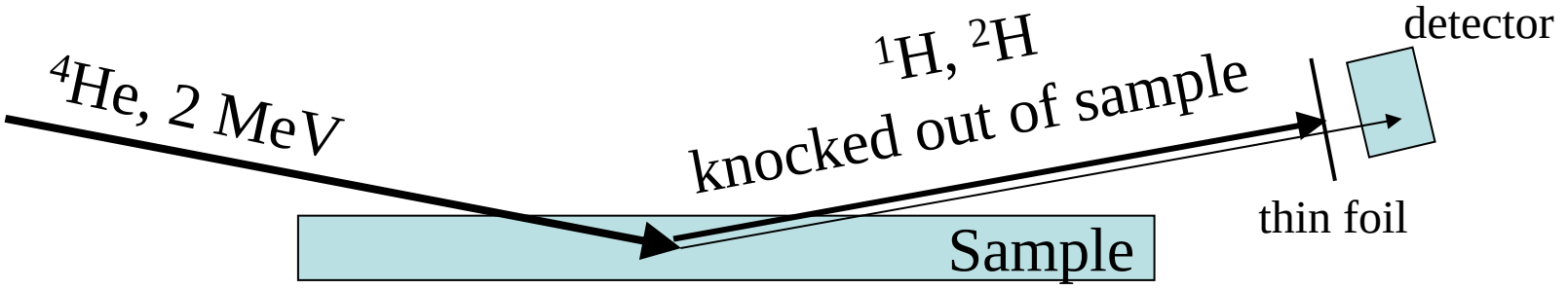
PIGE – principle



$$Y_{\Delta x} = K\int_{\Delta x} C(x)\sigma(E)dx$$

$$Y = \mathrm{K}\int_{0}^{R} C(x)\sigma(E)dx = K\int_{E_{inc}}^{0} C(x)\frac{\sigma(E)}{S(E)}dE$$

Elastic Recoil Detection Analysis



What nuclear data are needed for IBA?

Differential cross sections $d\sigma(E)/d\Omega$ for:

- elastic scattering of light ions (p, d, ^{4}He, ^{7}Li,…)
- nuclear reactions induced by p, d, ^{4}He, ^{3}He in the energy range of 0.5÷15 MeV

Distinctive feature of the nuclear data for IBA (as compared with other applications)

- IBA uses differential cross sections rather than total ones – data for different angles are needed
- IBA employs data mainly for elements of natural abundance rather than for separated isotopes – data acquired in nuclear physics studies are often not sufficient

Coordinated Research Projects organized by the IAEA Nuclear Data Section

- Development of a Reference Database for Ion Beam Analysis (2005 – 2009)

- Development of a Reference Database for Particle-Induced Gamma-ray Emission (PIGE) Spectroscopy (2011 – 2015)

Nucleus

H-1

Projectile

- p
- d
- ^{3}He
- α
- ^{6}Li
- ^{7}Li

Type of data

- EBS
- NRA
- PIGE
- All

IBANDL

EXFOR

Home

SigmaCalc

CD version

Upload your data

Updates

Feedback

Nuclear Data Services

Nuclear Data Service

IBANDL

This is the Ion Beam Analysis Nuclear Data Library produced according to the recommendations of the IAEA Technical Meeting held at the IAEA Headquarters in Vienna (29 to 30 October 2003). This data collection is a result of merging SigmaBase and NRABASE. It contains most of the available experimental nuclear cross-sections relevant to Ion Beam Analysis. Excitation functions are presented both as graphs and data files. The numerical data are in the R33 format. All the entries are supplied with a reference to the data source. The data published only in a graphical form were digitized using a precise technique. Where all efforts were made to ensure that the most accurate information was adopted, no guarantee can be given concerning the full validity of the data, and the IAEA accepts no responsibility for usage of IBANDL.

Maintaining IBANDL as a dynamically developing collection of the IBA nuclear data significantly depends on the activity of all members of the IBA community. Contributions to IBANDL are welcome. If you have new experimental results upload your data now.

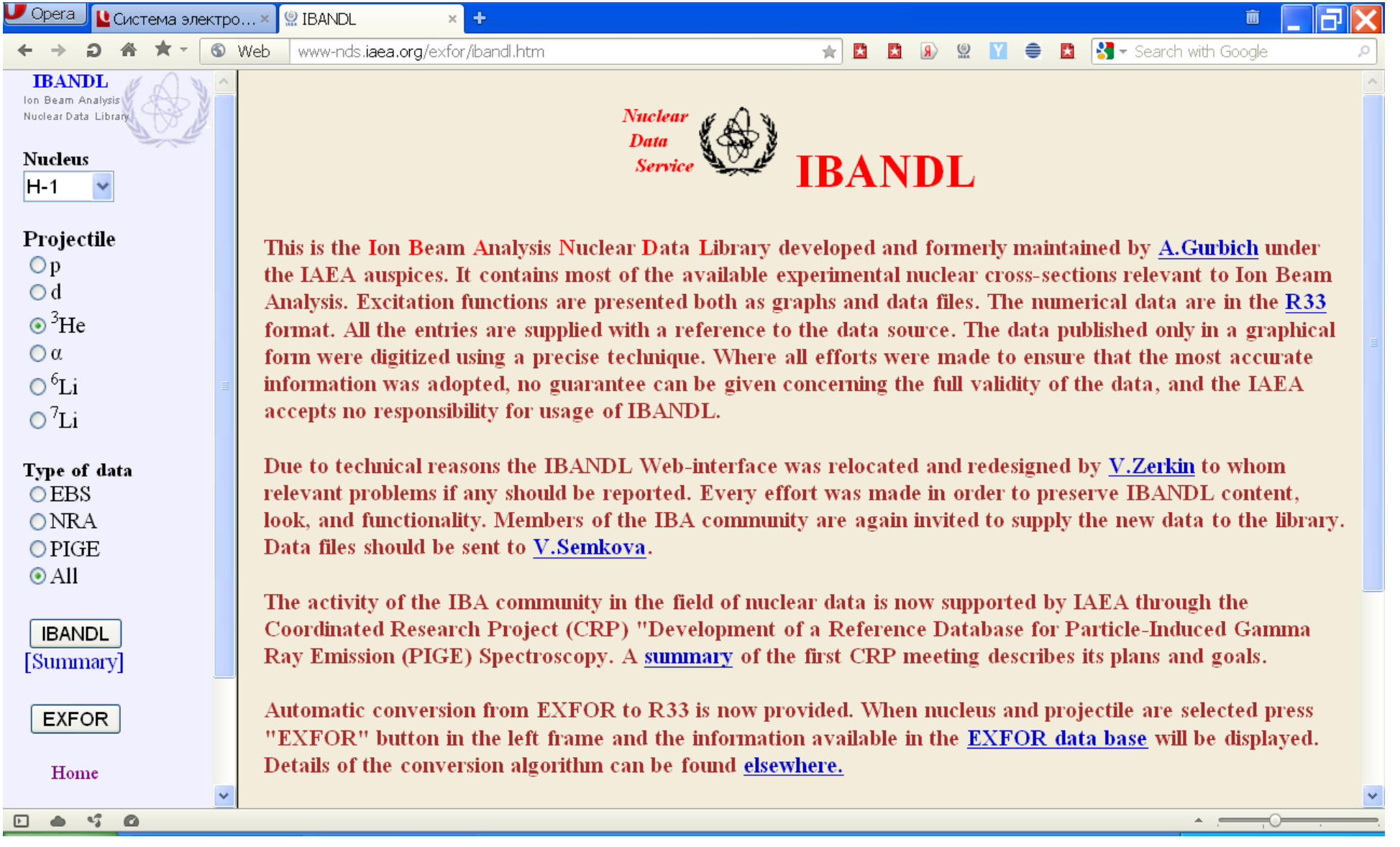
The activity of the IBA community in the field of nuclear data is now supported by IAEA through the Coordinated Research Project (CRP). A summary of the first CRP meeting describes its plans and goals. The second Research Coordination Meeting (see the RCM summary) was held on 18 - 21 June 2007 at IAEA headquarters in Vienna.

Automatic conversion from EXFOR to R33 is now provided. When nucleus and projectile are selected press "EXFOR" button in the left frame and the information available in the EXFOR data base will be displayed. Details of the conversion algorithm can be found elsewhere.

A complete CD version of IBANDL updated in December, 2010 is available on request.

When citing data retrieved from IBANDL both the original article and the database should be referenced.
Example:
A. Scientist et al., Journal..., data retrieved from the IBANDL database, http://www-nds.iaea.org/ibandl/

Last update: 15.09.2011 A. Gurbich


Opera
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Ion Beam Analysis
Nuclear Data Library
Nucleus
H-1
Projectile
p
d
3He
α
6Li
7Li
Type of data
EBS
NRA
PIGE
All
IBANDL
[Summary]
EXFOR
Home
Nuclear Data Service
IBANDL
This is the Ion Beam Analysis Nuclear Data Library developed and formerly maintained by A.Gurbich under the IAEA auspices. It contains most of the available experimental nuclear cross-sections relevant to Ion Beam Analysis. Excitation functions are presented both as graphs and data files. The numerical data are in the R33 format. All the entries are supplied with a reference to the data source. The data published only in a graphical form were digitized using a precise technique. Where all efforts were made to ensure that the most accurate information was adopted, no guarantee can be given concerning the full validity of the data, and the IAEA accepts no responsibility for usage of IBANDL.
Due to technical reasons the IBANDL Web-interface was relocated and redesigned by V.Zerkin to whom relevant problems if any should be reported. Every effort was made in order to preserve IBANDL content, look, and functionality. Members of the IBA community are again invited to supply the new data to the library. Data files should be sent to V.Semkova.
The activity of the IBA community in the field of nuclear data is now supported by IAEA through the Coordinated Research Project (CRP) "Development of a Reference Database for Particle-Induced Gamma Ray Emission (PIGE) Spectroscopy. A summary of the first CRP meeting describes its plans and goals.
Automatic conversion from EXFOR to R33 is now provided. When nucleus and projectile are selected press "EXFOR" button in the left frame and the information available in the EXFOR data base will be displayed. Details of the conversion algorithm can be found elsewhere.

R33 Format for Communication of Reaction Cross Sections in the IBA Community

```
Comment: The thick film method was employed at different incident beam energies
and the results were combined into a single  cross section. The values agree with
our thin film results, which generally exceed those of Saad et al (1966) by a factor of 2.
File created by R33 Manager version 0.21

Version: R33
Source: M.J.F.Healy and D.W.Lane. Nucl. Instr & Meth B 136-138 (1998) 66-71
Name: Healy, M.J.F.
Address1: Cranfield University.
Address2: RMCS Shrivenham
Address3: Swindon. SN6 8LA.
Address4: United Kingdom.
Address5: Tel +44 1793 785736 Fax: +44 1793 785774
Address6: email m.j.f.healy@rmcs.cranfield.ac.uk
Serial Number:
SubFile: 32sdp.r33
X4Number:
Reaction: 32S(d,p0)33S
Distribution: Energy
Composition:
Masses:    2.000,   32.000,    1.000,   33.000
Zeds: 1, 16, 1, 16
Qvalue:   6418.00,      0.00,      0.00,      0.00,      0.00
Theta:    150.00
Sigfactors: 1.00, 0.00
Enfactors: 1.00, 0.00, 0.00, 0.00
Units: mb
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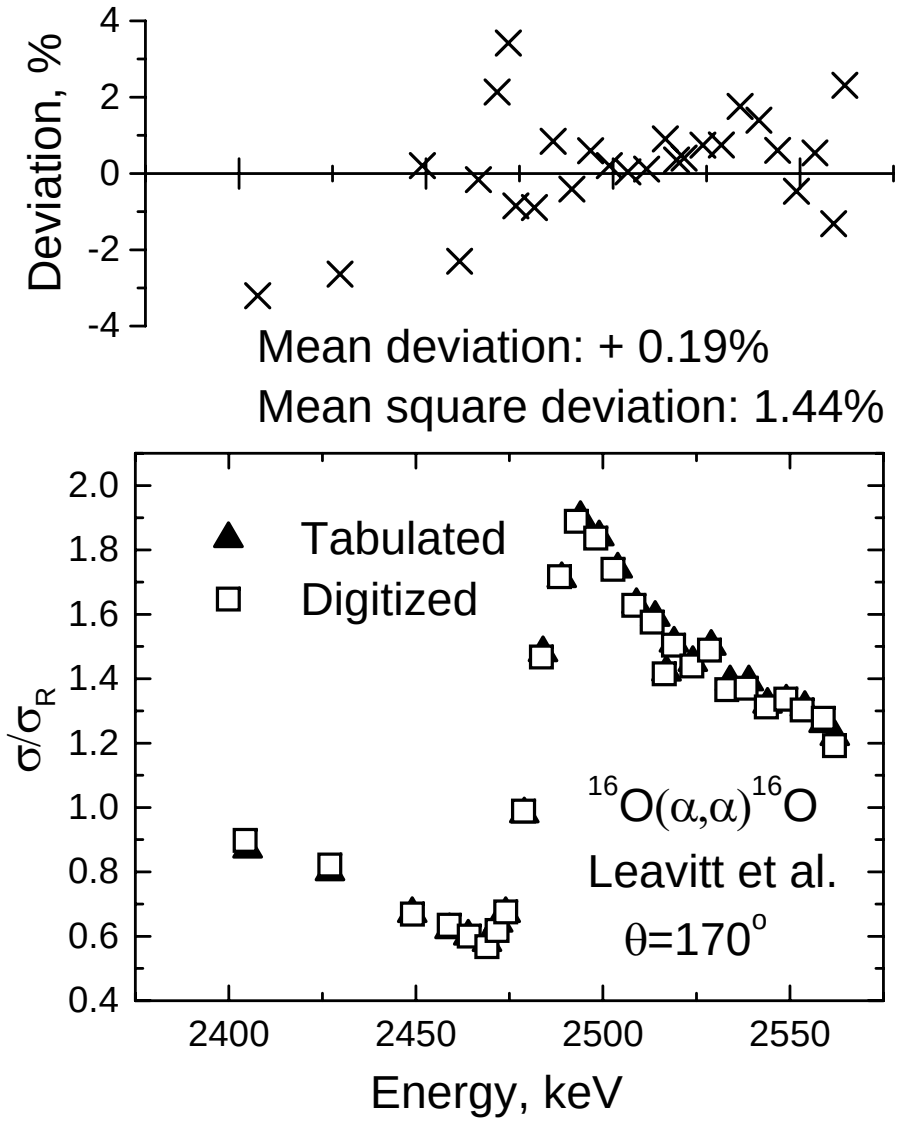
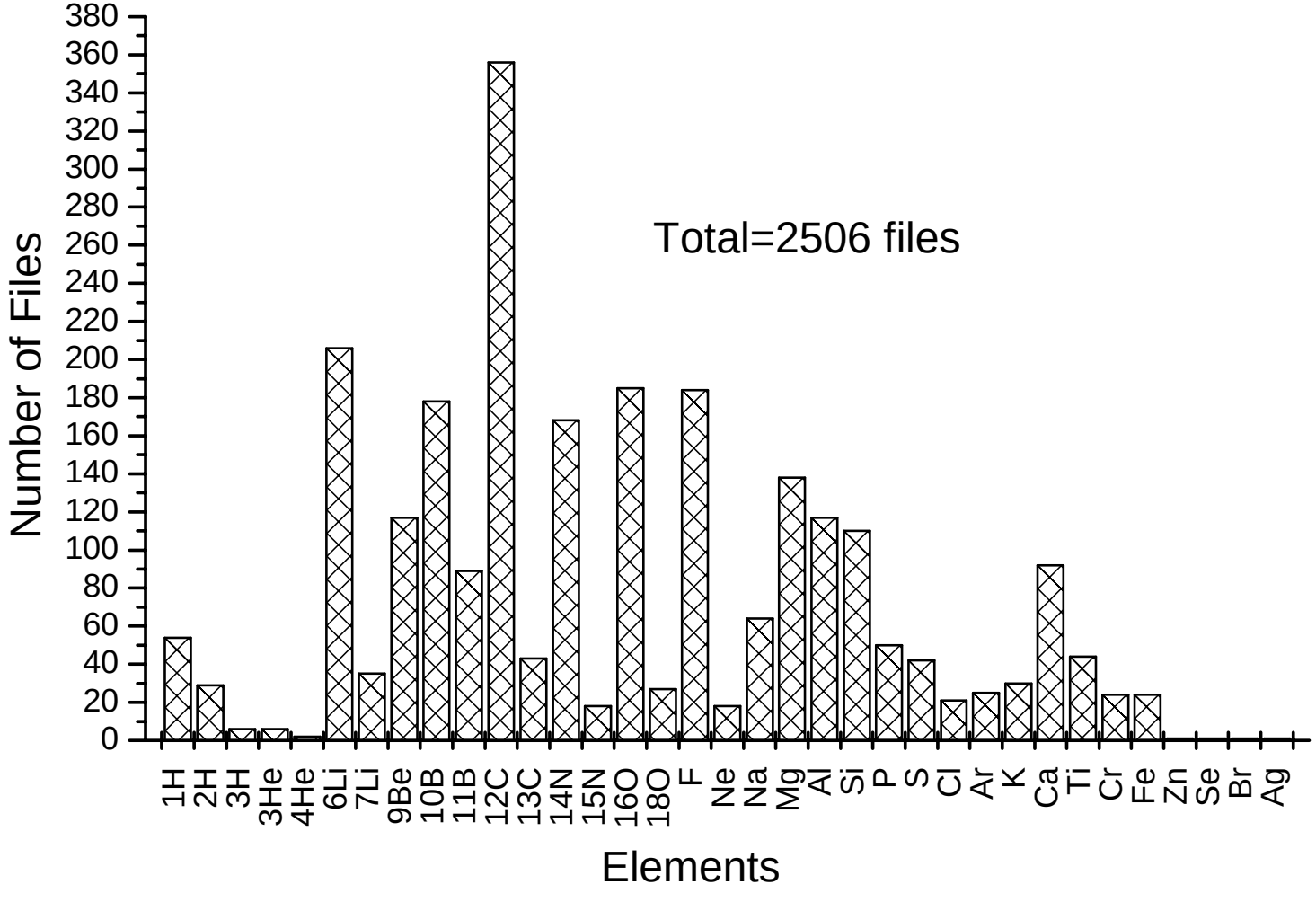
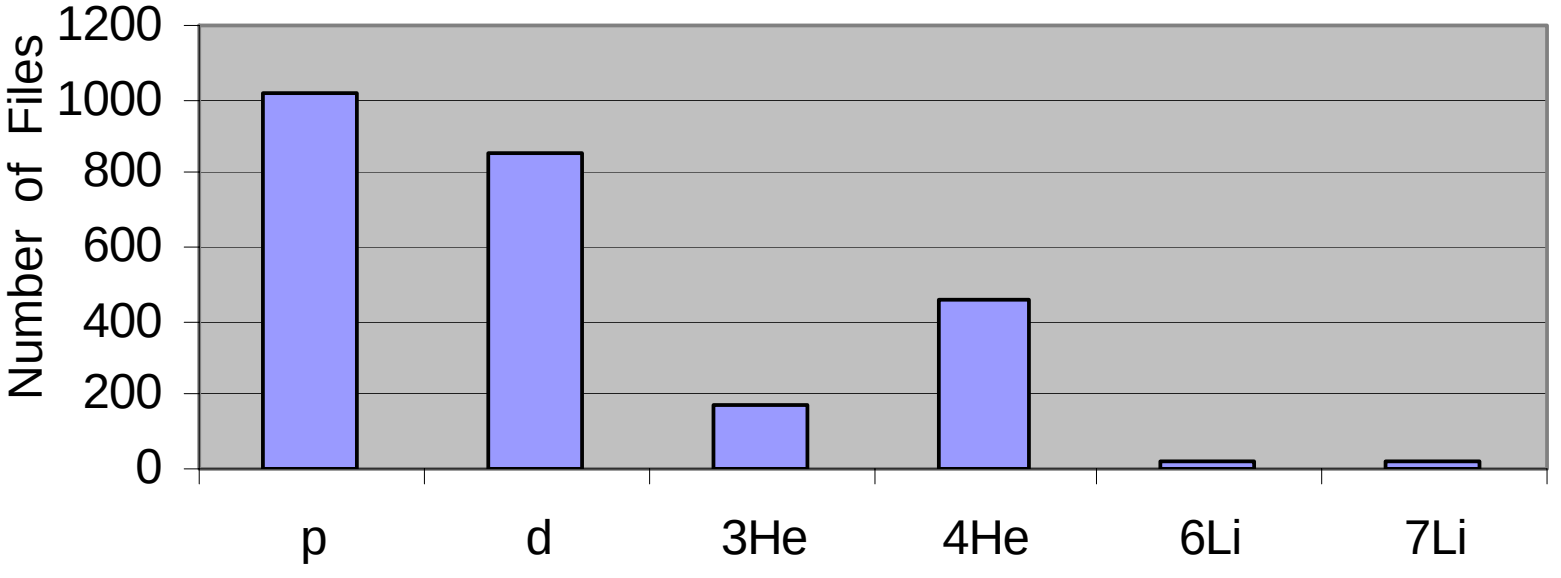
How accurate is digitizing?



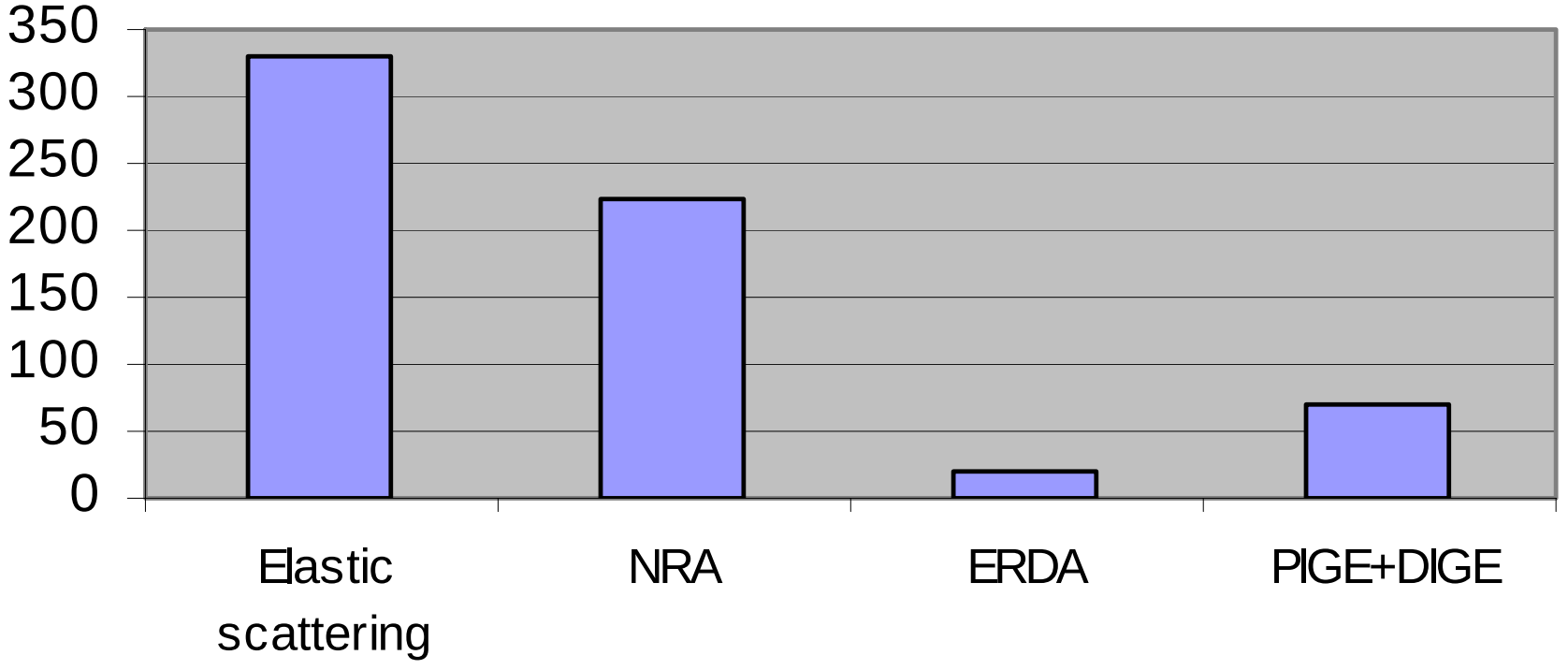
Content of IBANDL (by element)



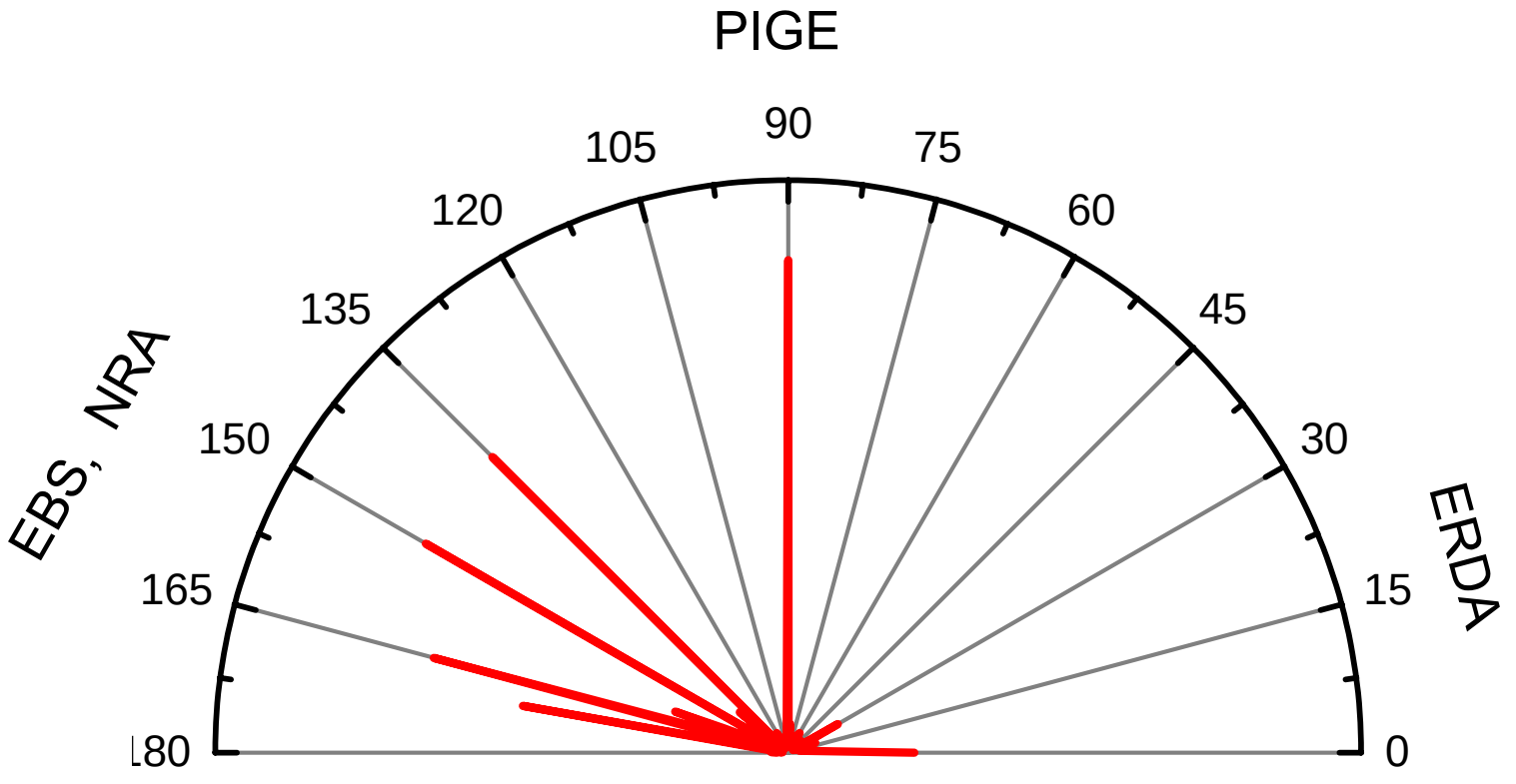
Content of IBANDL (by projectile)



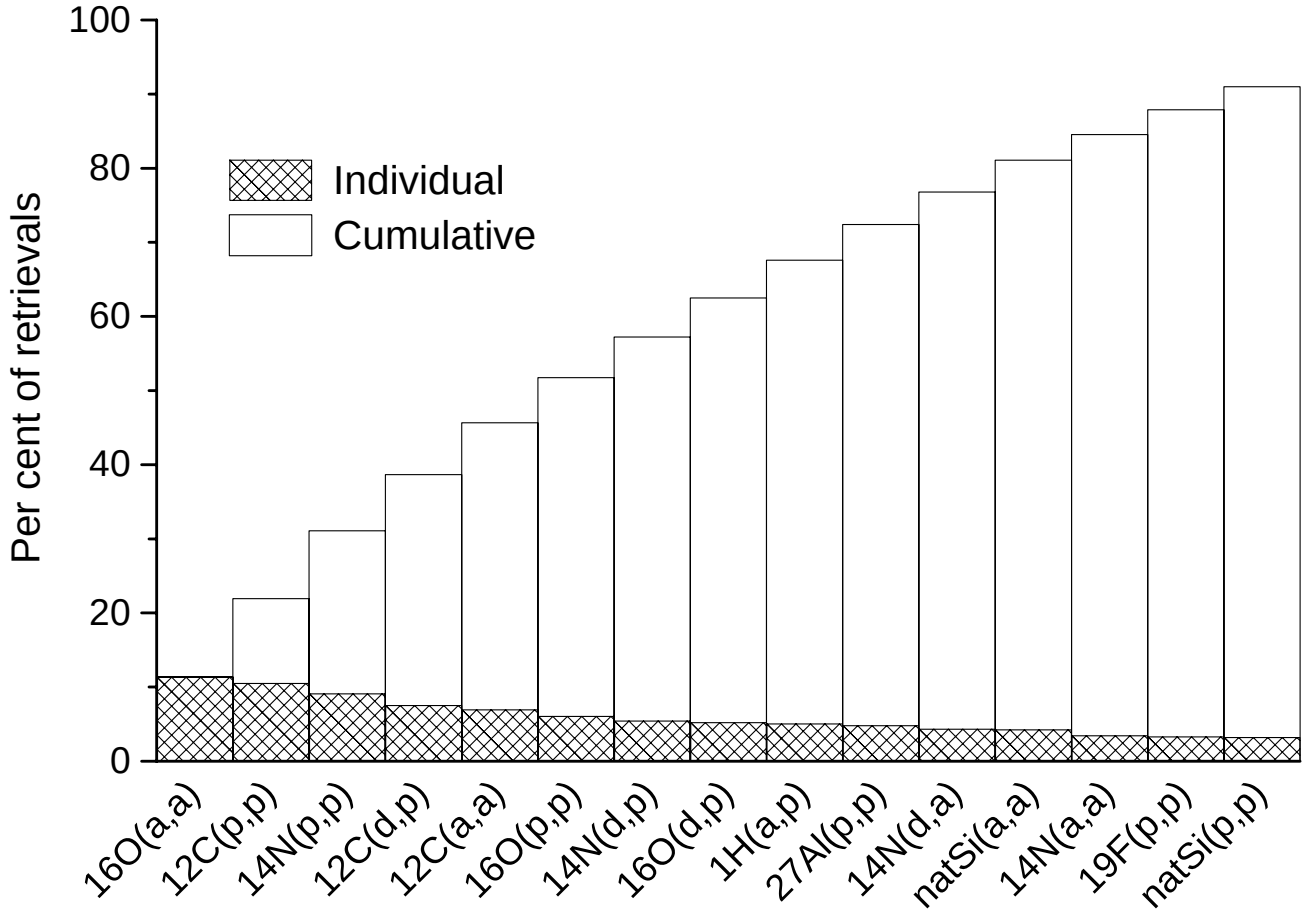
Content of IBANDL by reaction



The distribution of the compiled data on angle

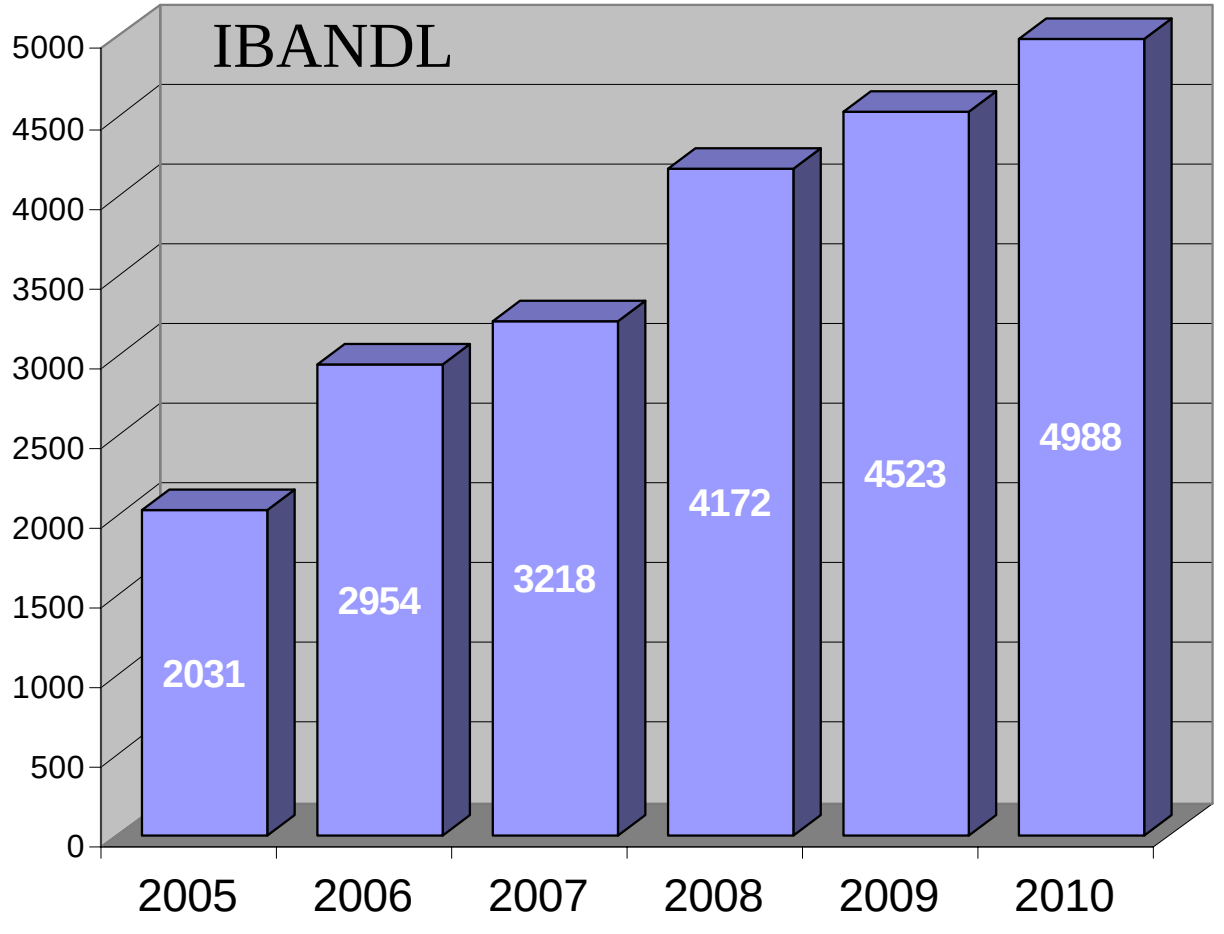


The IBANDL statistics showing most popular retrievals



>90% of retrievals are for 7 elements / 15 cross sections

Number of hits per year



Conclusions

- IBANDL has become a main source of the cross section data for IBA
- There are a lot of discrepancies in the compiled data
- New measurements and benchmarks are under way to resolve the problems
- Some of the most wanted cross sections have been evaluated and the work on evaluation is in progress
- The recommended cross sections will be elaborated in result of the CRP activity
- The CRP results will serve to the IBA community in establishing a firm basis for analytical work