The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

2172-6

Joint ICTP-IAEA Workshop on Nuclear Data for Science and Technology: Analytical Applications

8 - 12 November 2010

Differential cross sections for ion beam analysis

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Obninsk
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The Abdus Salam International Centre for Theoretical Physics

FRIDAY, 12 NOVEMBER 2010
11.00 - 12.30
The GIAMBIAGI Lecture Hall

Workshop on Nuclear Data for Science and Technology: Analytical Applications

DIFFERENTIAL CROSS SECTIONS FOR ION BEAM ANALYSIS

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Institute of Physics and Power Engineering
Obninsk, Russia

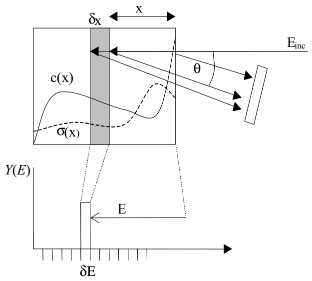
PLAN OF THE LECTURE

- **Needs of IBA in nuclear data**
- **Ion Beam Analysis Nuclear Data Library (IBANDL)**
- **EXFOR data base**
- **Evaluation of nuclear data**

What nuclear data are needed for IBA?

Sort of data	Projectiles	Targets	Type of interaction	Energy range
Differential cross sections $d\sigma(E)/d\Omega$, γ–ray yields	p, d, ^{3}He, ^{4}He, heavy ions	All elements	Elastic scattering, nuclear reactions	0.5÷10 MeV

NRA Depth Profiling



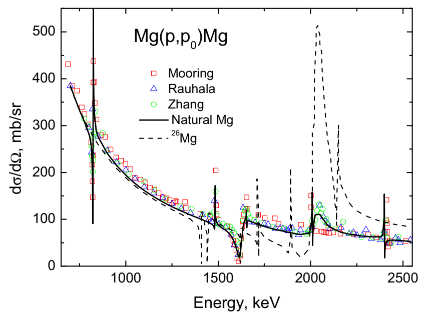
- A channel of width δE at energy E in the spectrum corresponds to a slice of width dx at depth x in the sample, with E and δE being inversely related to x and δx through a linear combination of the stopping powers for the incident and outgoing particle
- The number of particles accumulated into that 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.

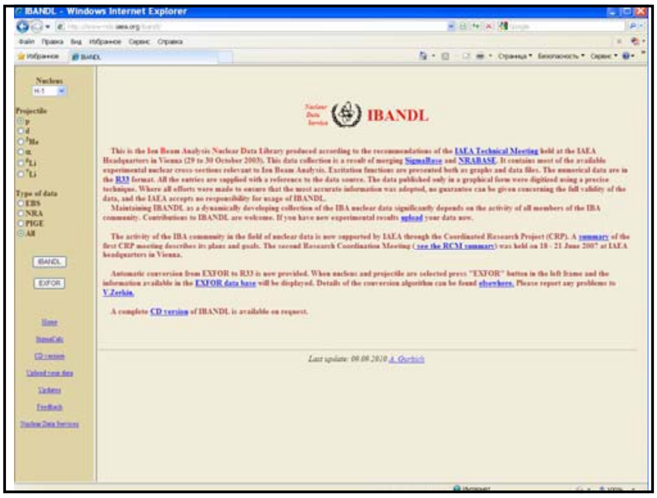
$$Y_i(E)=\int_0^\infty \frac{N_0 c(x)\sigma(\varphi,E_1)\delta\Omega}{S(E')\left[\frac{-1}{\cos(\varphi+\theta)}+\frac{1}{\cos(\theta)}\frac{kS(E_1)}{S(kE_1)}\right]}\frac{1}{1.06\Gamma(x)}\exp\left(-\frac{(E'-E)^2}{0.36\Gamma^2(x)}\right)dE'$$

Distinctive feature of the nuclear data for IBA

- 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

The difference between cross sections for separate isotopes and for an element of natural abundance




IBANDL - Windows Internet Explorer
Nucleus
Projectile
Type of data
IBANDL
Nuclear Data Service
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).
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.
A complete CD version of IBANDL is available on request.
IBANDL
EXFOR
Home
SigmaCalc
CD version
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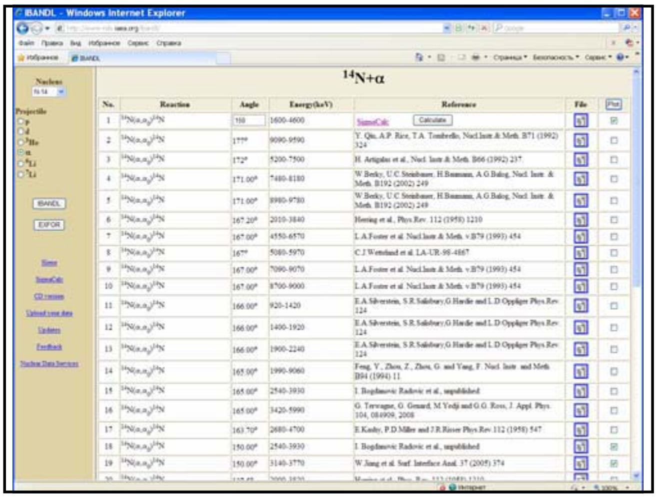
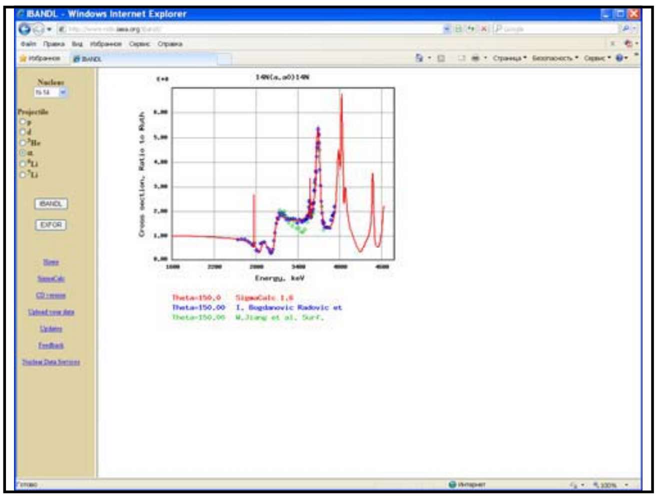

IBANDL - Windows Internet Explorer
Nucleus
Projectile
IBANDL
EXFOR
14N+α
No.
Reaction
Angle
Energy(keV)
Reference
File
Plot
1 14N(α,α0)14N 150 1600-4600 SigmaCalc Calculate
2 14N(α,α0)14N 177° 9090-9590 Y. Qiu, A.P. Rice, T.A. Tombrello, Nucl.Instr.& Meth. B71 (1992) 324
3 14N(α,α0)14N 172° 5200-7500 H. Artigalas et al., Nucl. Instr. & Meth. B66 (1992) 237
4 14N(α,α0)14N 171.00° 7480-8180 W.Berky, U.C.Steinbauer, H.Baumann, A.G.Balog, Nucl. Instr. & Meth. B192 (2002) 249
5 14N(α,α0)14N 171.00° 8980-9780 W.Berky, U.C.Steinbauer, H.Baumann, A.G.Balog, Nucl. Instr. & Meth. B192 (2002) 249
6 14N(α,α0)14N 167.20° 2010-3840 Herring et al., Phys.Rev. 112 (1958) 1210
7 14N(α,α0)14N 167.00° 4550-6570 L.A.Foster et al. Nucl.Instr.& Meth. v.B79 (1993) 454
8 14N(α,α0)14N 167° 5080-5970 C.J.Westerdaal et al. LA-UR-98-4867
9 14N(α,α0)14N 167.00° 7090-9070 L.A.Foster et al. Nucl.Instr.& Meth. v.B79 (1993) 454
10 14N(α,α0)14N 167.00° 8700-9000 L.A.Foster et al. Nucl.Instr.& Meth. v.B79 (1993) 454
11 14N(α,α0)14N 166.00° 920-1420 E.A.Silverstein, S.R.Salisbury, G.Hardie and L.D.Oppliger Phys.Rev. 124
12 14N(α,α0)14N 166.00° 1400-1920 E.A.Silverstein, S.R.Salisbury, G.Hardie and L.D.Oppliger Phys.Rev. 124
13 14N(α,α0)14N 166.00° 1900-2240 E.A.Silverstein, S.R.Salisbury, G.Hardie and L.D.Oppliger Phys.Rev. 124
14 14N(α,α0)14N 165.00° 1990-9060 Feng, Y., Zhou, Z., Zhou, G. and Yang, F. Nucl. Instr. and Meth. B94 (1994) 11
15 14N(α,α0)14N 165.00° 2540-3930 I. Bogdanovic Radovic et al., unpublished
16 14N(α,α0)14N 165.00° 3420-5990 G. Terwagne, G. Genard, M.Yedji and G.G. Ross, J. Appl. Phys. 104, 084909, 2008
17 14N(α,α0)14N 163.70° 2680-4700 E.Kashy, P.D.Miller and J.R.Risser Phys.Rev.112 (1958) 547
18 14N(α,α0)14N 150.00° 2540-3930 I. Bogdanovic Radovic et al., unpublished
19 14N(α,α0)14N 150.00° 3140-3770 W.Jiang et al. Surf. Interface Anal. 37 (2005) 374


IBANDL - Windows Internet Explorer
Nucleus
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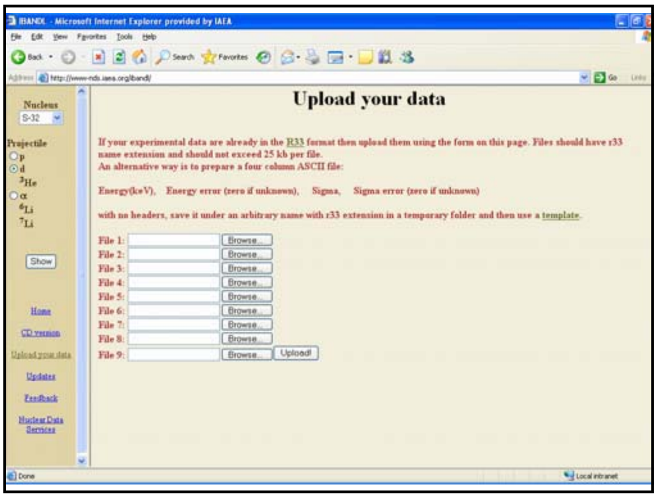
Updates
Feedback
Nuclear Data Services
14N(a,a0)14N
Cross section, Ratio to Ruth
Energy, keV
Theta=150.0 SigmaCalc 1.6
Theta=150.00 I. Bogdanovic Radovic et
Theta=150.00 W.Jiang et al. Surf.



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
Data:
 1005.000,  0.000,   0.011, 0.000
 1010.000,  0.000,   0.012, 0.000
 1015.000,  0.000,   0.016, 0.000
 1020.000,  0.000,   0.019, 0.000
 1025.000,  0.000,   0.020, 0.000
 1030.000,  0.000,   0.019, 0.000
 1035.000,  0.000,   0.017, 0.000
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 1045.000,  0.000,   0.015, 0.000
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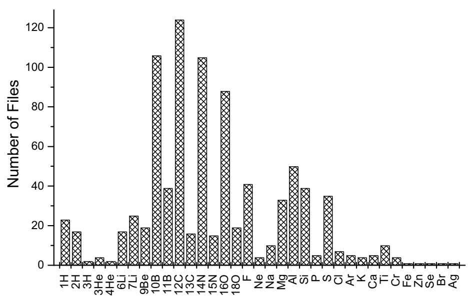
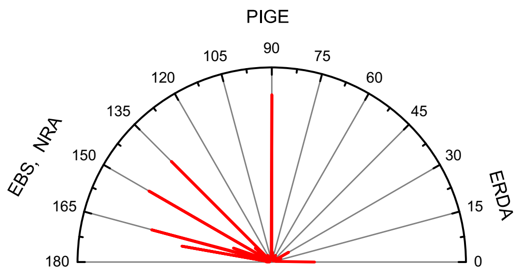
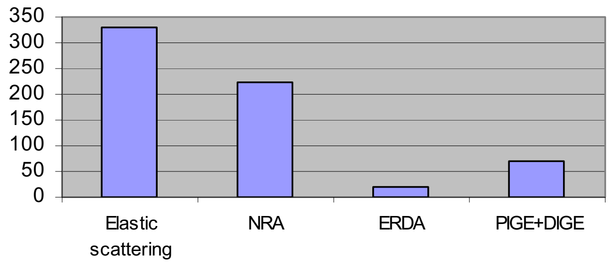
The IBANDL content by element



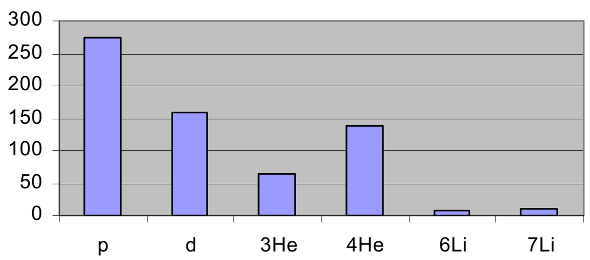
The distribution of the available data on angle



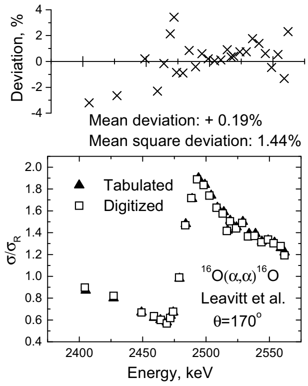
Content of IBANDL (by reaction)

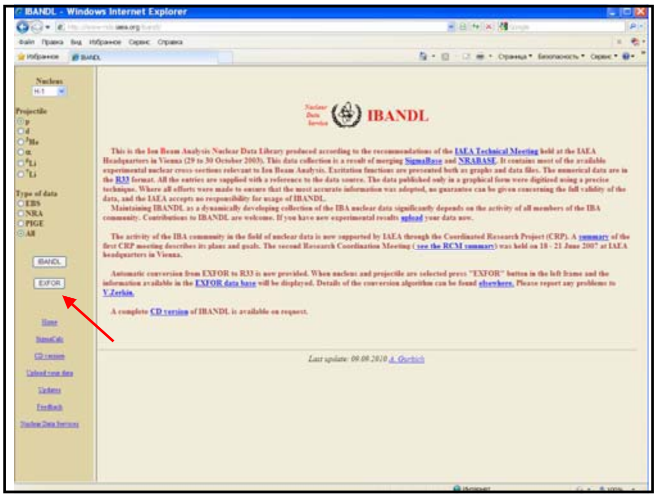


Content of IBANDL (by projectile)



How accurate is digitizing?





What is EXFOR

Database for all experimental nuclear reaction data, such as all total and differential cross section types, resonance parameters, fission and other product yields, production cross sections, spectra, polarization data, etc. etc.

Started in 1970 for neutron data, later extended to charged-particle and photonuclear data

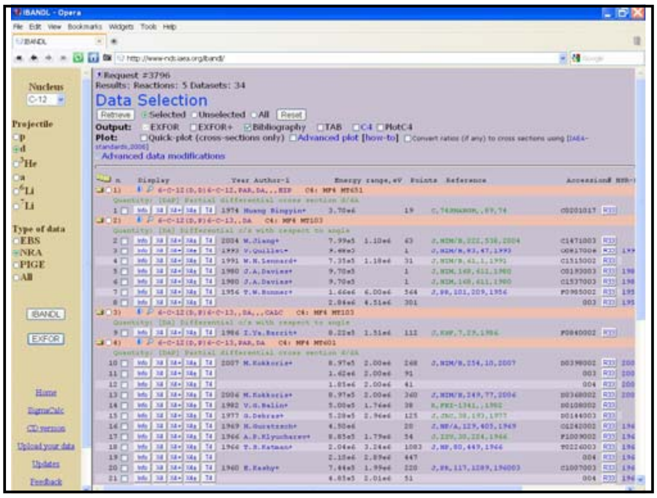
Includes also structured abstract of experimental method and bibliographic information

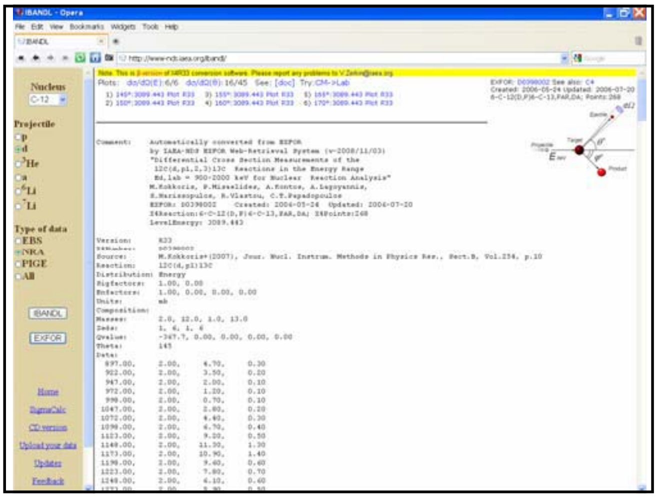
EXFOR format

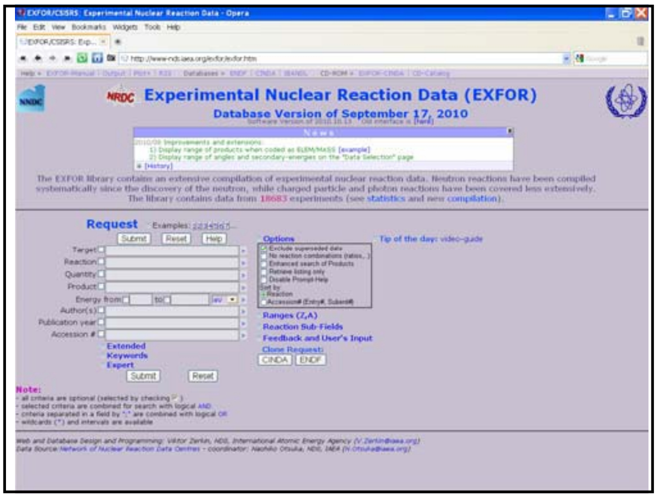
Data exchanged in 80-character ASCII files, managed with relational database system with sophisticated retrieval possibilities see http://www-nds.iaea.org/exfor/)

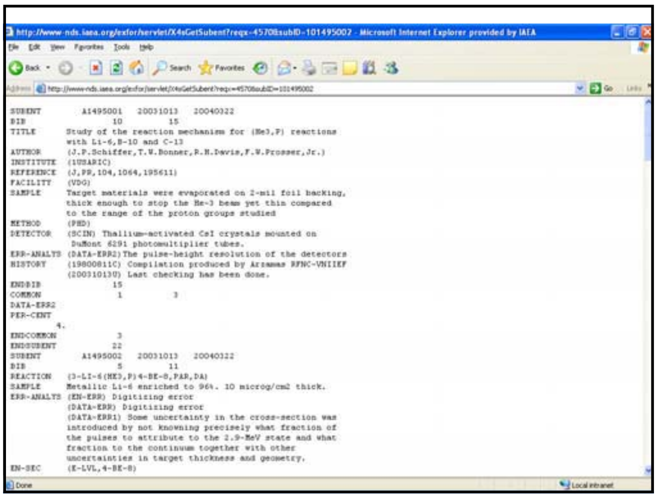
Data presentation very flexible (close to authors' presentation in publication): different units, varying number of data columns, etc.

Several "computational" output formats for processing and plotting; not yet working for differential data (but coming soon)









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BIB                 10         15
TITLE       Study of the reaction mechanism for (He3,P) reactions
            with Li-6,B-10 and C-13
AUTHOR      (J.P.Schiffer,T.W.Bonner,R.H.Davis,F.W.Prosser,Jr.)
INSTITUTE   (1USARIC)
REFERENCE   (J,PR,104,1064,195611)
FACILITY    (VDG)
SAMPLE      Target materials were evaporated on 2-mil foil backing,
            thick enough to stop the He-3 beam yet thin compared
            to the range of the proton groups studied
METHOD      (PHD)
DETECTOR    (SCIN) Thallium-activated CsI crystals mounted on
             DuMont 6291 photomultiplier tubes.
ERR-ANALYS  (DATA-ERR2)The pulse-height resolution of the detectors
HISTORY     (19800811C) Compilation produced by Arzamas RFNC-VNIIEF
            (20031013U) Last checking has been done.
ENDBIB              15
COMMON               1          3
DATA-ERR2
PER-CENT
        4.
ENDCOMMON            3
ENDSUBENT           22
SUBENT        A1495002   20031013   20040322
BIB                  5         11
REACTION    (3-LI-6(HE3,P)4-BE-8,PAR,DA)
SAMPLE      Metallic Li-6 enriched to 96%. 10 microg/cm2 thick.
ERR-ANALYS  (EN-ERR) Digitizing error
            (DATA-ERR) Digitizing error
            (DATA-ERR1) Some uncertainty in the cross-section was
            introduced by not knowning precisely what fraction of
            the pulses to attribute to the 2.9-MeV state and what
            fraction to the continuum together with other
            uncertainties in target thickness and geometry.
EN-SEC      (E-LVL,4-BE-8)
```
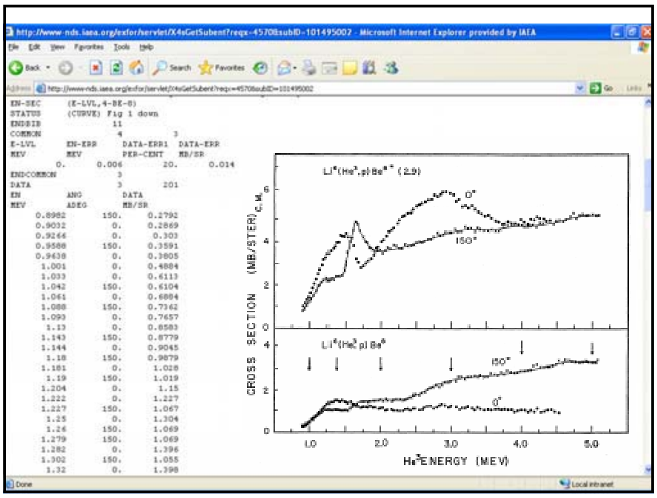
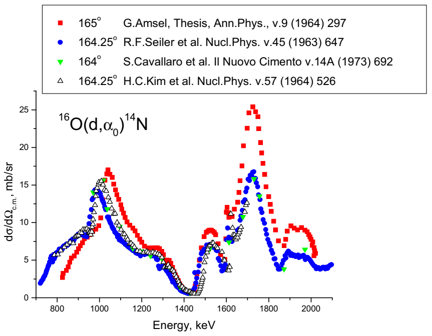



```
EN-SEC      (E-LVL,4-BE-8)
STATUS      (CURVE) Fig 1 down
ENDBIB              11
COMMON               4          3
E-LVL       EN-ERR     DATA-ERR1  DATA-ERR
MEV         MEV        PER-CENT   MB/SR
        0.      0.006       20.      0.014
ENDCOMMON            3
DATA                 3        201
EN          ANG        DATA
MEV         ADEG       MB/SR
    0.8982       150.     0.2792
    0.9032         0.     0.2869
    0.9264         0.      0.303
    0.9588       150.     0.3591
    0.9638         0.     0.3805
     1.001         0.     0.4884
     1.033         0.     0.6113
     1.042       150.     0.6104
     1.061         0.     0.6884
     1.088       150.     0.7362
     1.093         0.     0.7657
      1.13         0.     0.8583
     1.143       150.     0.8779
     1.144         0.     0.9045
      1.18       150.     0.9879
     1.181         0.      1.028
      1.19       150.      1.019
     1.204         0.       1.15
     1.222         0.      1.227
     1.227       150.      1.067
      1.25         0.      1.304
      1.26       150.      1.069
     1.279       150.      1.069
     1.282         0.      1.396
     1.302       150.      1.055
      1.32         0.      1.398
```

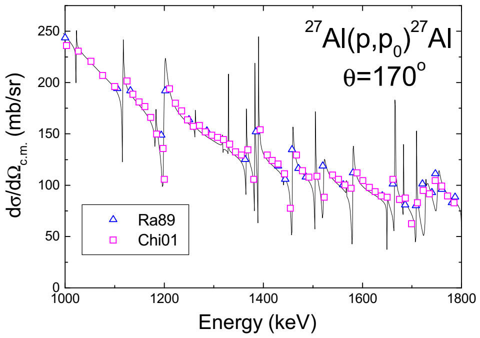
THE REASONS WHY EVALUATION IS NEEDED

Reason 1: because of discrepancies between results of different measurements



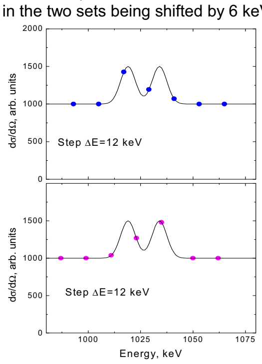
THE REASONS WHY EVALUATION IS NEEDED

Reason 2: because cross section may has a fine structure missed in some measurements



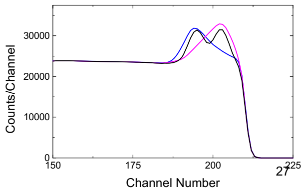
WHY IS A FINE STRUCTURE ESSENTIAL?

Suppose "true" cross section is as shown by a solid line and two measurements with 12 keV step are made, the measured points in the two sets being shifted by 6 keV



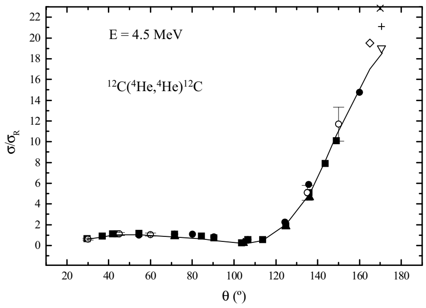
Simulated EBS spectra

Black line – simulation with "true" cross section, blue and magenta – simulation with sparse point cross section measurements

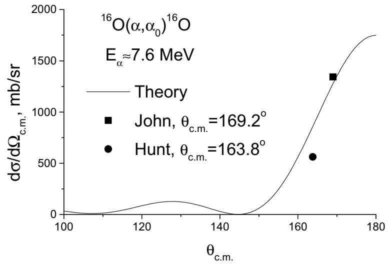


THE REASONS WHY EVALUATION IS NEEDED

Reason 3: because cross section may have a strong dependence on angle.



Comparison of different results for $^{16}O(\alpha,\alpha_0)^{16}O$ cross section



The comparison of the results obtained by «thin» and «thick» target methods for Si(α,α) cross section

K.-M. Kallman, Z. Phys. A 356 (1996) 287

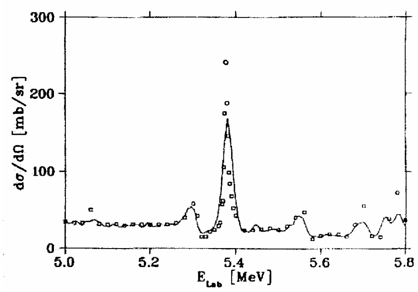


Fig. 2. The excitation function obtained with the thick-target method (full line) compared to the excitation function from [4] (dots)

Evaluation Problem

Given:

Different sets of (generally inconsistent) experimental data measured at sparse points on energy and angle

Find:

The most accurate possible smooth curves of $d\sigma/d\Omega(E,\theta)$

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Solution

Step 1: search in the literature and nuclear data bases to find all relevant experimental data.

Step 2: digitize data published only as graphs.

Step 3: compare data from different sources.

Step 4: examine reported experimental conditions and errors assigned to the data.

Step 5: select the apparently reliable experimental points.

Step 6: identify nuclear physics processes corresponding to the case.

Step 7: fit free parameters of the theoretical model.

Step 8: produce the optimal theoretical differential cross-section.

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The Essence of Evaluation

To produce evaluated cross-section through incorporation of the data measured under different experimental conditions at different scattering angles into the frameworks of the unified theoretical approach.

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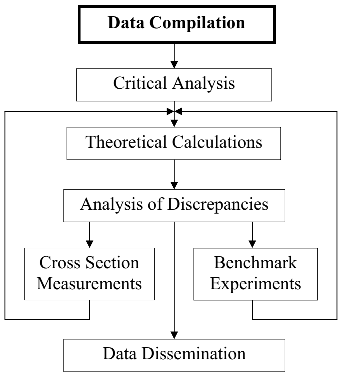
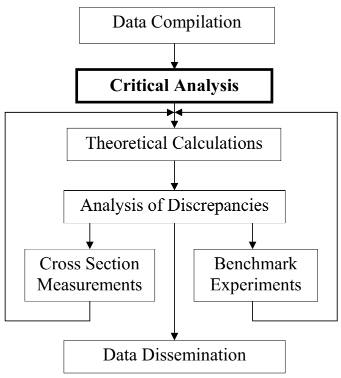
Evaluation Scheme



34

Evaluation Scheme



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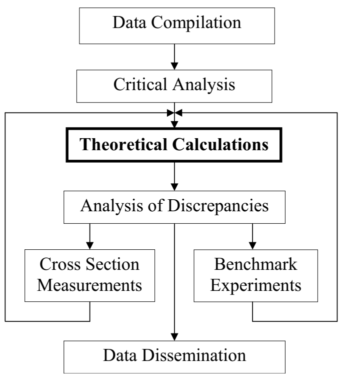
Evaluation Scheme



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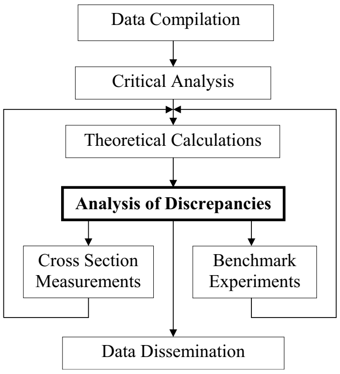
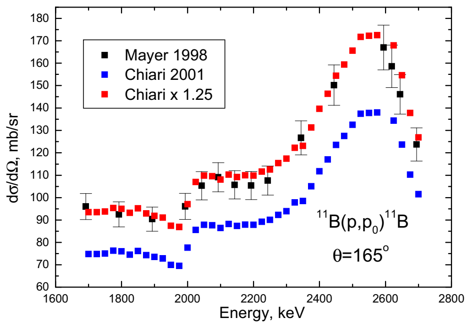
Evaluation Scheme



Comparison of different results for $^{11}B(p,p_0)^{11}B$ cross section



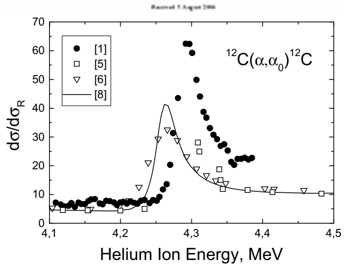
Comparison of different results for $^{12}C(\alpha,\alpha_0)^{12}C$ cross section


Available online at www.sciencedirect.com
ELSEVIER
NIM B Beam Interactions with Materials & Atoms

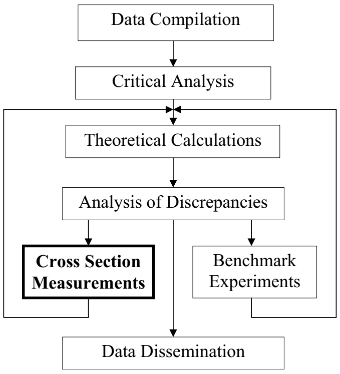
Discussion

Comment on "Carbon analysis using energetic ion beams" [Nucl. Instr. and Meth. B 222 (2004) 538–546]

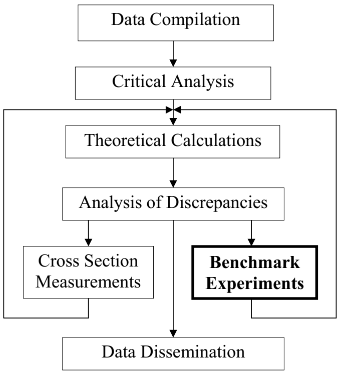
A.F. Gurbich *



Evaluation Scheme



Evaluation Scheme

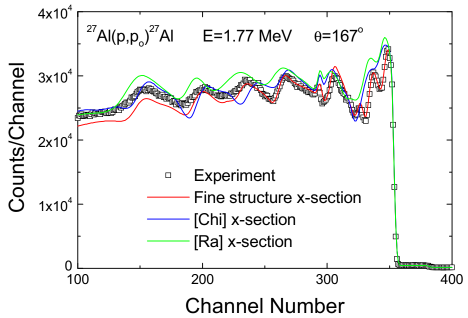


Benchmarks

A benchmark is an integral experiment which is compared with a standard direct simulation using microscopic cross-section data in order to verify the data.

This is an extension of the definition taken from reactor physics where microscopic neutron data are verified by comparison of calculated integral reactor characteristics such as e.g. neutron flux with results of direct measurements.

The benchmark demonstrated the significance of the cross section fine structure



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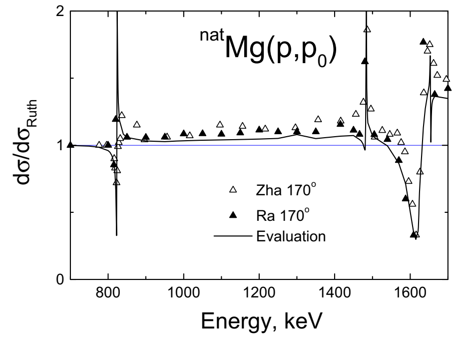
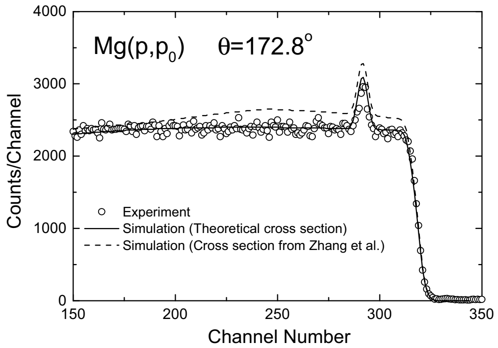
The deviation of the cross section for $Mg(p,p_0)$ from Rutherford above 800 keV



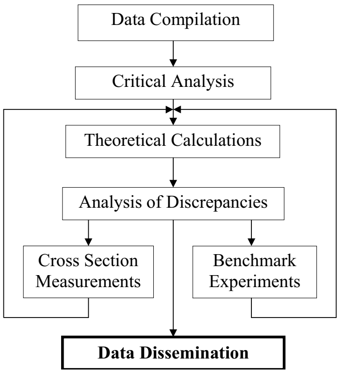
44

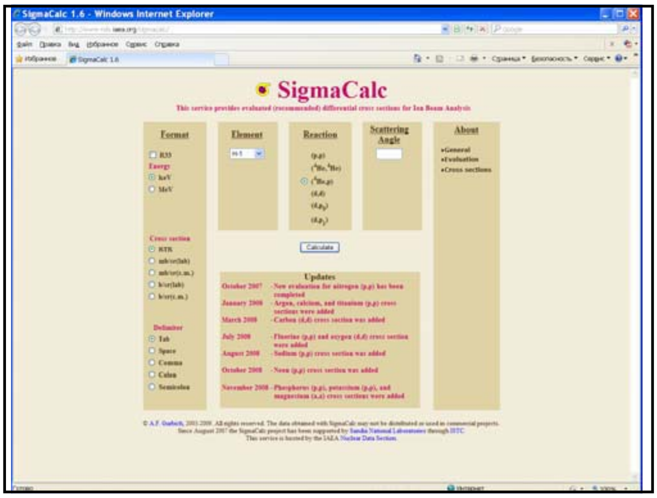
The benchmark for $Mg(p,p_0)$

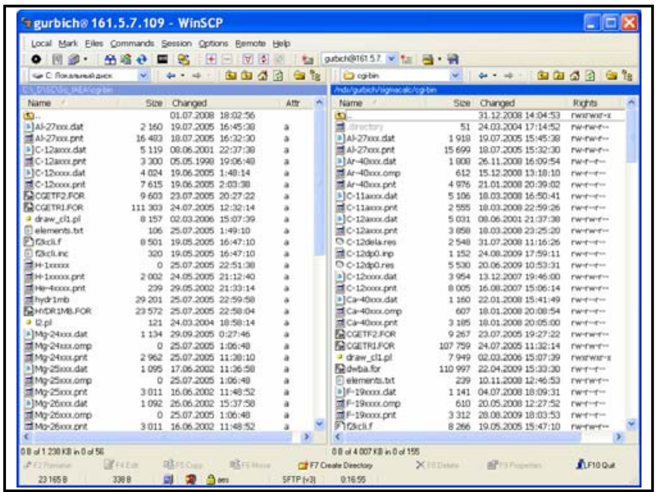


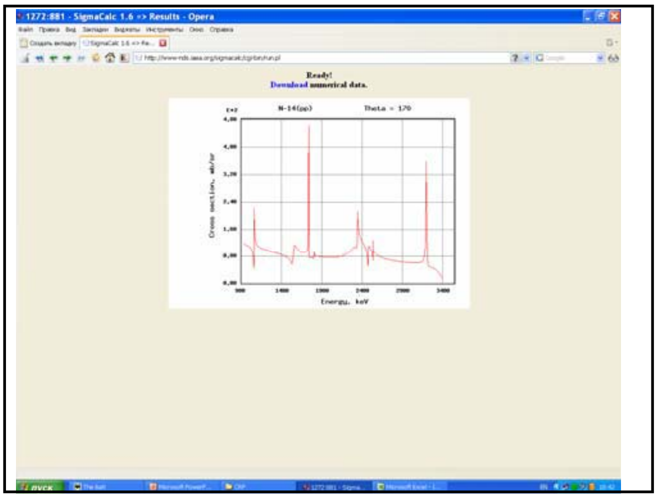
45

Evaluation Scheme

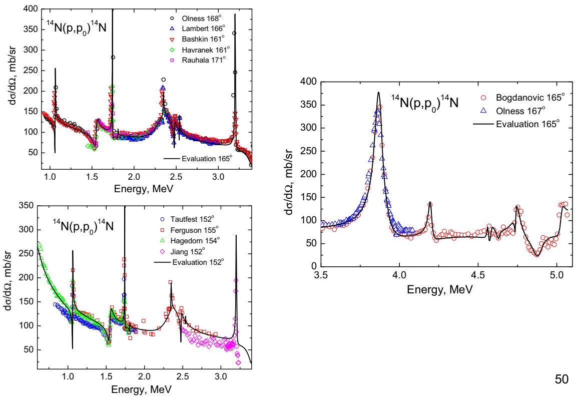




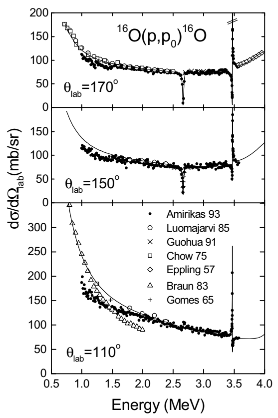




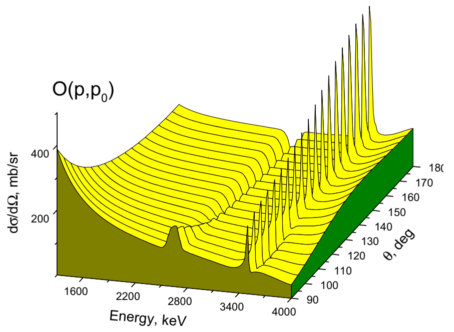
Evaluation of the $^{14}N(p,p_0)^{14}N$ cross-section



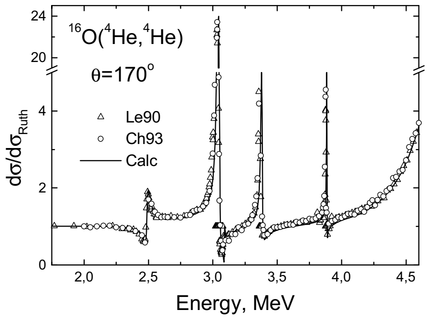
Evaluation of the proton elastic scattering from oxygen



The evaluated cross section for proton elastic scattering from oxygen



Comparison of different results for $^{16}O(\alpha,\alpha_0)^{16}O$ cross section

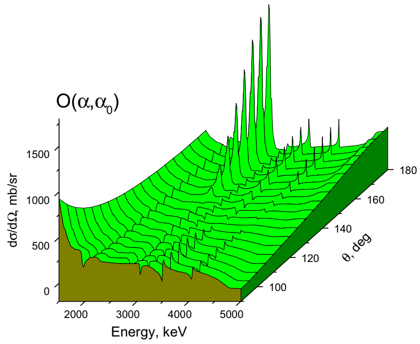


$^{16}O(\alpha,\alpha_0)^{16}O$

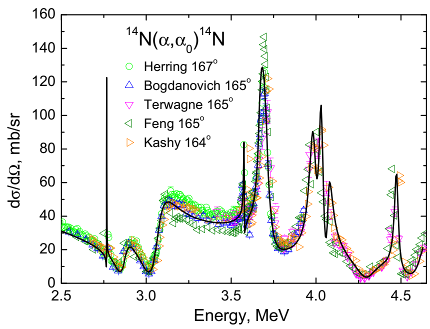
Resonance parameters reported in different works

E_α, keV	Γ_{lab}, keV	Reference
3.0317		Demarche et al. J. Appl. Phys. 100 (20060) 124909
3034±5		Leavitt, et al. NIM B 44 (1990) 260
3035±6		Cheng et al., NIM B 83 (1993) 449
3036±2.3	10.12+0.37	MacArthur et al., Phys. Rev. C 22 (1980) 356
3038±5.0	10.0	Soroka et al., NIM B 83 (1993) 311
3042±3.0	10.26±0.49	Jarjis, NIM B 12 (1985) 331
3042±3.0	10.20±0.40	Wang et al., NIM 211 (1993) 193
3045±10.0	10.0	Cameron, Phys. Rev. 90 (1953) 839
3038.2±2	10.1±0.4	Evaluated (1998, TUNL)

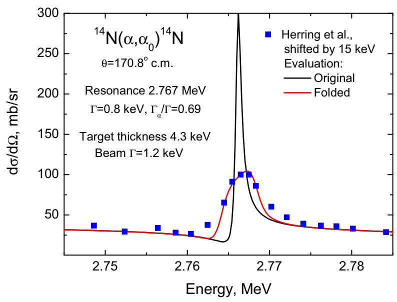
The evaluated cross section for alpha elastic scattering from oxygen



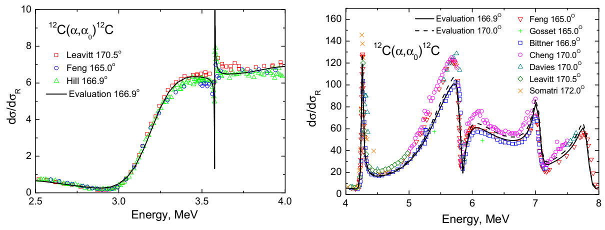
Evaluation of the $^{14}N(\alpha,\alpha_0)^{14}N$ cross-section



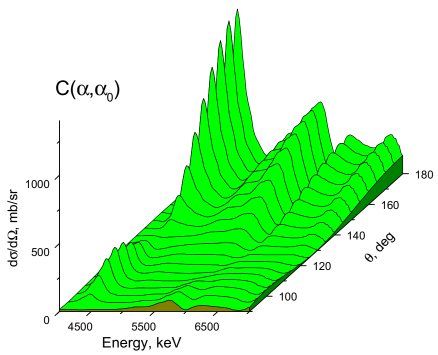
$^{14}N(\alpha,\alpha_0)^{14}N$ narrow resonance



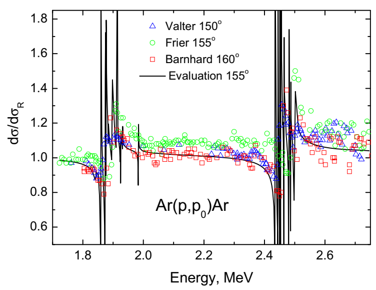
Evaluation of the $^{12}C(\alpha,\alpha_0)^{12}C$ cross-section



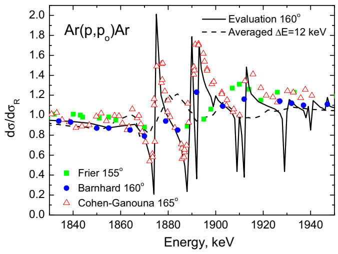
The evaluated cross section for alpha elastic scattering from carbon



Evaluation of the $Ar(p,p_0)Ar$ cross-section



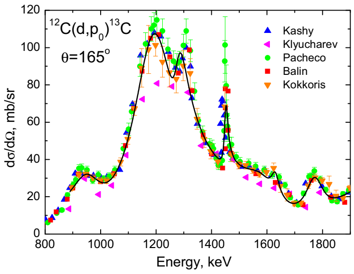
Ar(p,p$_0$)Ar fine structure



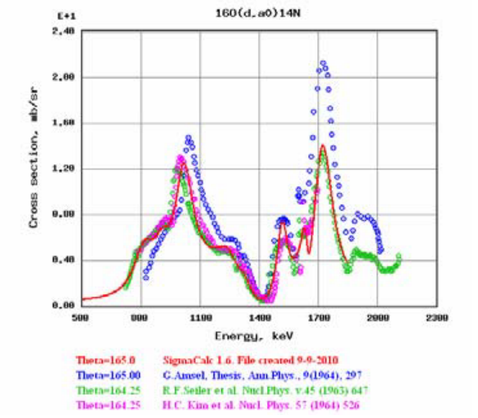
Most useful reactions with deuterons

$^{2}H(d,p)^{3}H$	Q = 4.03 MeV
$^{12}C(d,p)^{13}C$	Q = 2.72 MeV
$^{14}N(d,p)^{15}N$	Q = 8.62 MeV (p$_0$)
$^{14}N(d,\alpha)^{12}C$	Q = 13.57 MeV (α_0)
$^{16}O(d,p)^{17}O$	Q = 1.92 MeV (p$_0$)
$^{16}O(d,\alpha)^{14}N$	Q = 3.11 MeV
$^{27}Al(d,p)^{28}Al$	Q = 5.50 MeV (p$_0$)
$^{27}Al(d,\alpha)^{25}Mg$	Q = 6.71 MeV (α_0)
$^{28}Si(d,p)^{29}Si$	Q = 6.25 MeV

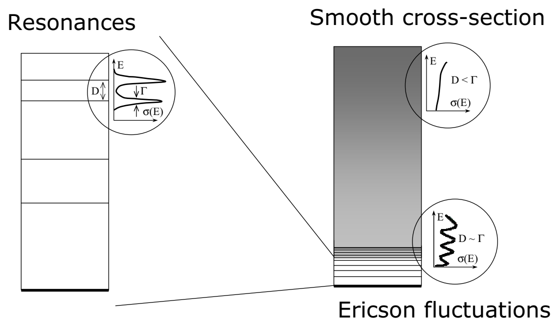
Evaluation of the $^{12}C(d,p_0)^{13}C$ cross-section



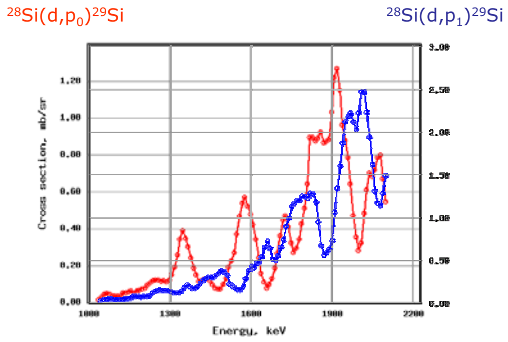
$^{16}O(d,\alpha_0)^{14}N$ cross-section at 165°



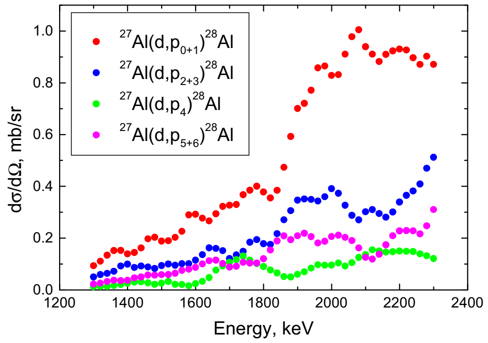
Three regions in the compound nucleus excitation and corresponding cross-section behavior



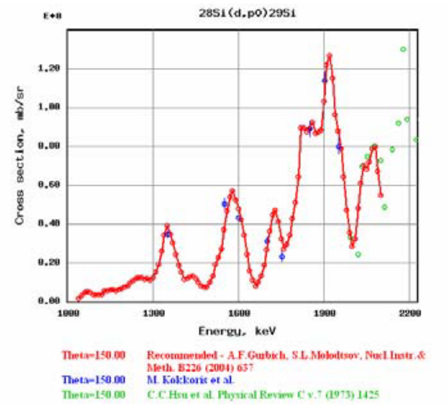
Ericson fluctuations in the $^{28}Si(d,p)^{29}Si$ reaction



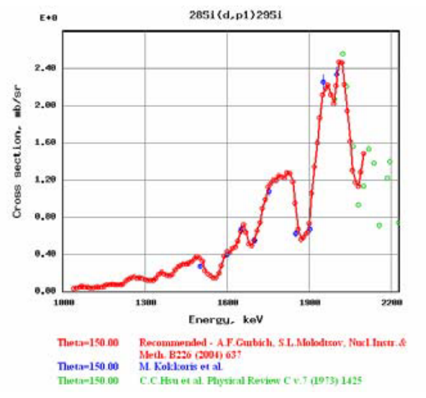
Ericson fluctuations in the $^{27}Al(d,p)^{28}Al$ reaction



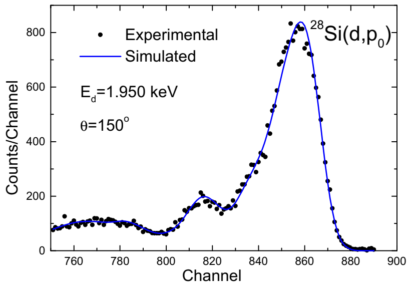
"Recommended" cross-section for $^{28}Si(d,p_0)^{29}Si$ at 150°



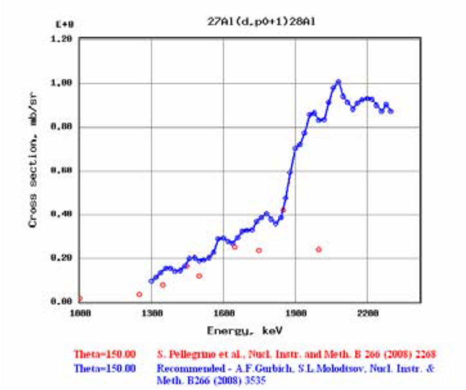
"Recommended" cross-section for $^{28}Si(d,p_1)^{29}Si$ at 150°



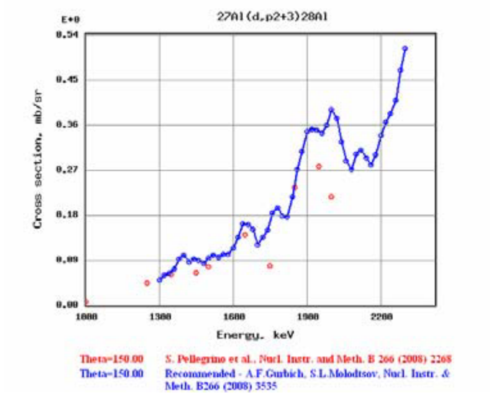
Benchmark for the $^{28}Si(d,p_0)^{29}Si$ cross-section



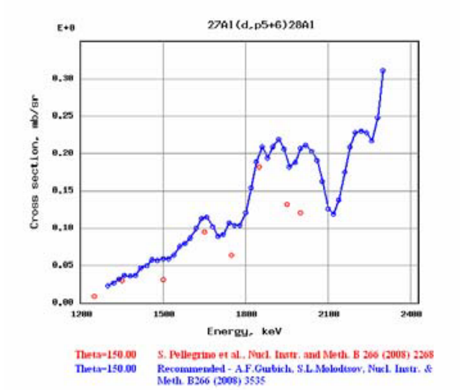
"Recommended" cross-section for $^{27}Al(d,p_{0+1})^{28}Al$ at 150°



"Recommended" cross-section for $^{27}Al(d,p_{2+3})^{28}Al$ at 150°



“Recommended” cross-section for $^{27}Al(d,p_{5+6})^{28}Al$ at 150°



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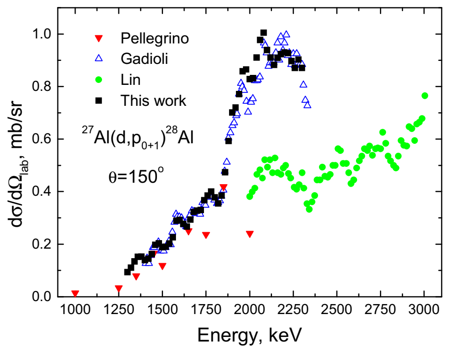
The comparison of the results of a new measurement with other data for $^{27}Al(d,p_{0+1})^{28}Al$



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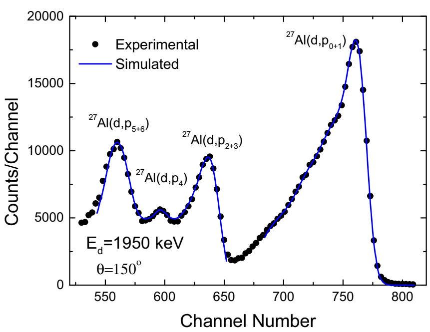
Benchmark for the $^{27}Al(d,p)^{28}Al$ cross-section



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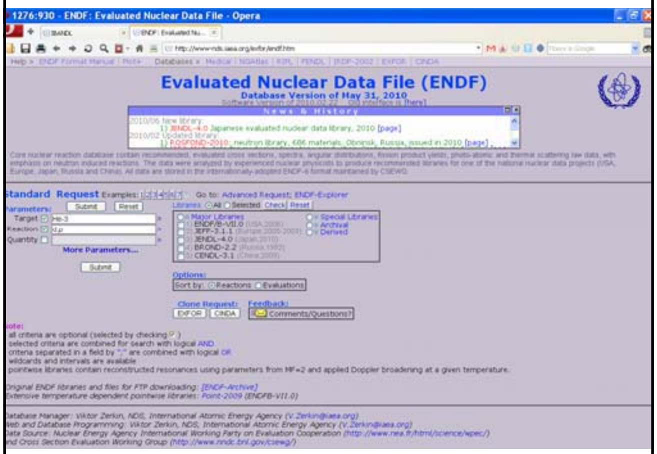
Most useful reactions with ^3He

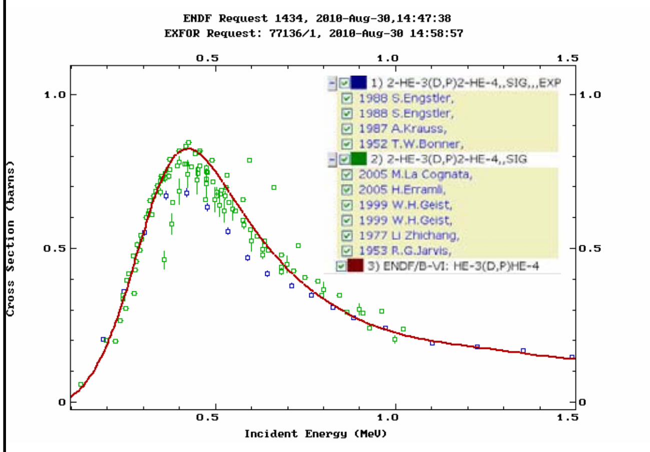
$^2H(^3He,p)^4He$	Q = 18.35 MeV
$^2H(^3He,\alpha)^1H$	Q = 18.35 MeV
$^9Be(^3He,p_0)^{11}B$	Q = 10.32 MeV (p_0)
$^{12}C(^3He,p)^{14}N$	Q = 4.78 MeV (p_0)



ENDF Section Summary

Evaluation		
Library	ENDF/B-VI	
Material	MAT=225 ZA=2003 2-HE-3	
Sub-Library	NSUB=10020 (D)	
Lab	LLNL	
Author(s)	R. M. WHITE & D. A. RESLER	
Date(s)	ENDATE=19910613 RDATE= DDATE=DIST-SEP91 EDATE=EVAL-MAY91	
Sections	2	
Section		
File	MF3	Cross sections
Section	MT103 (D, P)	Production of a proton, plus a residual. Sum of MT=600-649, if they are present.
Reaction-code	HE-3(D,P)HE-4,SIG	
Lines	287	
Parameters	QM=1.83532e+7 QI=1.83532e+7 LR=0	
Product(s)	H-1, HE-4	

Tabulated Data:		
Points: 847		
Energy (eV)		
Min 1187.5	Max 3e+07	Reset
From 1187.5	To 3e+07	Get data: Submit
Calculation of Cross Section for a Single Energy:		
Energy (eV) = 1.8e+6		Calculate
Cross Section (b) = 0.11587687		



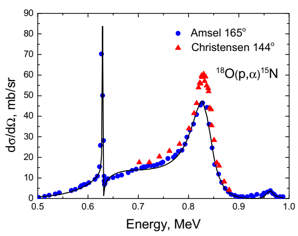
Most useful reactions with protons

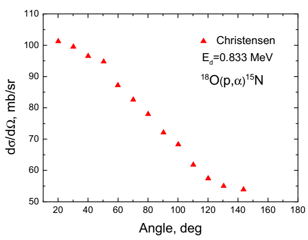
$^{7}Li(p,\alpha)^{4}He$ Q = 17.3 MeV

$^{11}B(p,\alpha)^{8}Be$ Q = 8.5 MeV

$^{18}O(p,\alpha)^{15}N$ Q = 4.0 MeV

$^{18}O(p,\alpha)^{15}N$ cross-section





COORDINATED RESEARCH PROJECT ON NUCLEAR DATA FOR IBA

IAEA
International Atomic Energy Agency

INDC (NDS)-0481
Distr. G, NC

INDC International Nuclear Data Committee

Development of a Reference Database for Ion Beam Analysis

Summary Report of the First Research Coordination Meeting

IAEA Headquarters
Vienna, Austria
21 – 23 November 2005

Prepared by
I. Vickridge* and O. Schwerer

IAEA Nuclear Data Section, Vienna, Austria
*Institut des NanoSciences de Paris, Université de Paris 6 et 7, France

IAEA Headquarters, Vienna, Austria
January 2006

Conclusions

- IBANDL is a main source of the cross section data for IBA
- There are a lot of discrepancies in the compiled data
- The evaluation of the IBA cross sections provides the most reliable 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