

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 II*

# The evaluation of charged particles low energy reaction cross-sections

Alexander Gurbich



Leverhulme Professor

*Surrey University Ion Beam Centre*



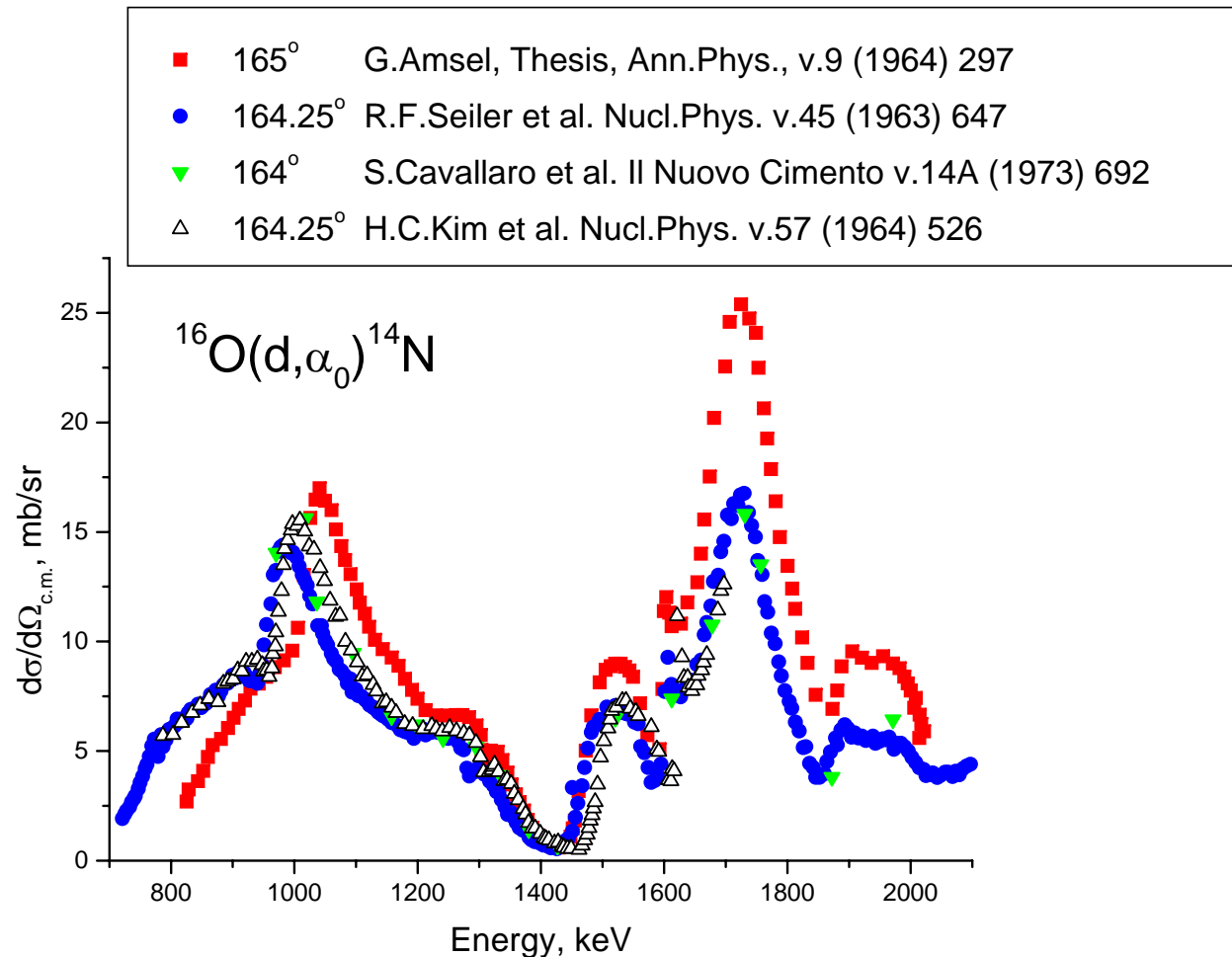
*On leave from the Institute for Physics and Power  
Engineering, Obninsk, Russia*

# Evaluation of nuclear cross-sections

The evaluation of the cross-sections for any particular reaction consists in the elaboration of the most accurate possible cross-sections through incorporation of the all relevant experimental data in the framework of nuclear physics theory

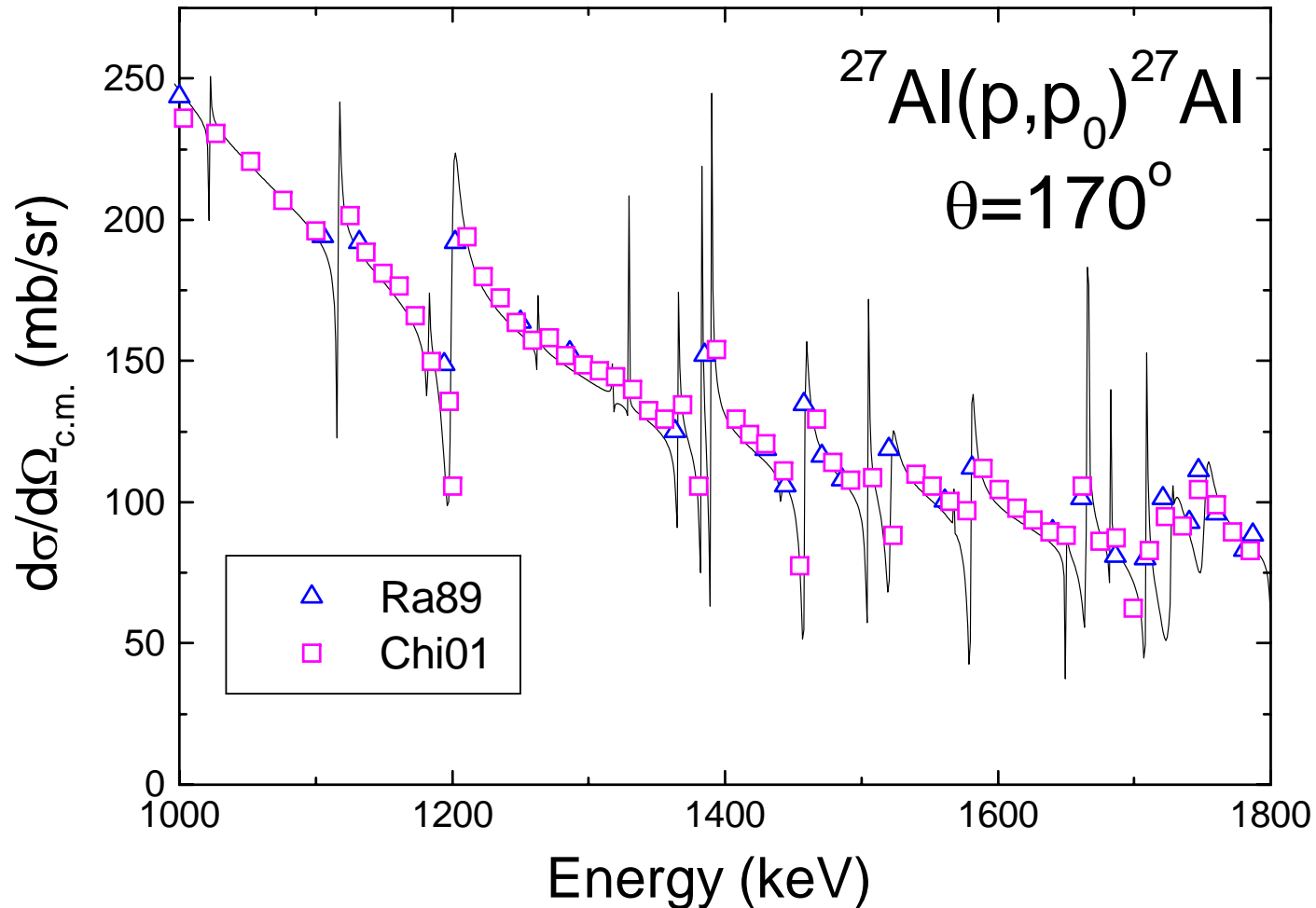
# THE REASONS WHY EVALUATION IS NEEDED

**Reason 1:** because of discrepancies between results of different measurements



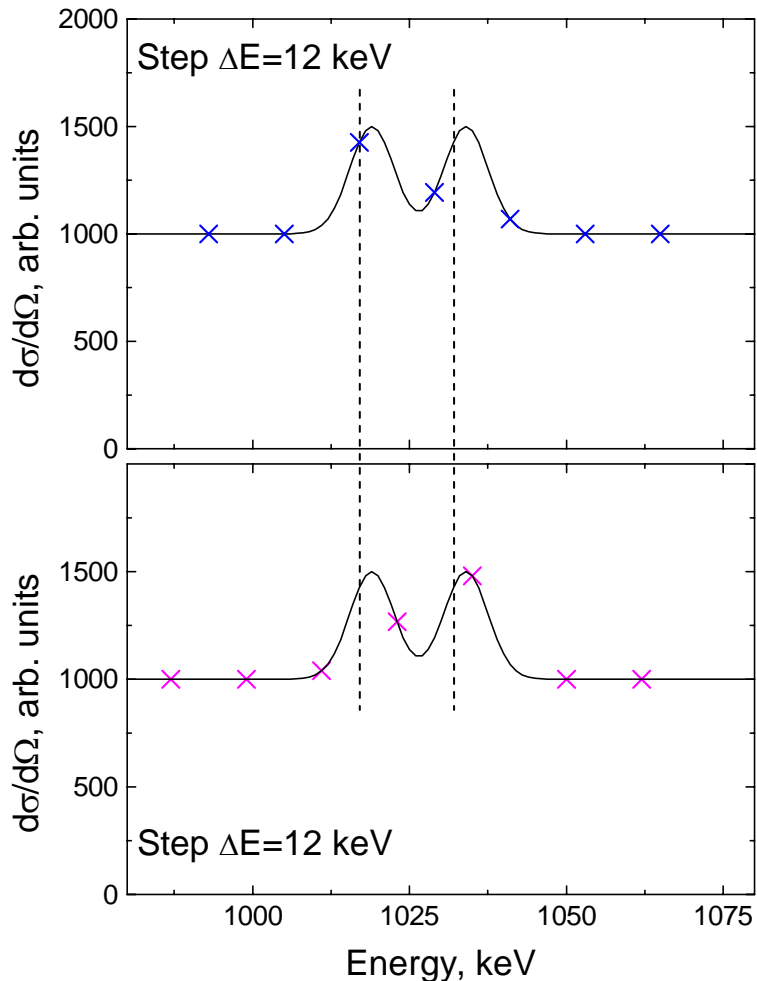
# THE REASONS WHY EVALUATION IS NEEDED

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



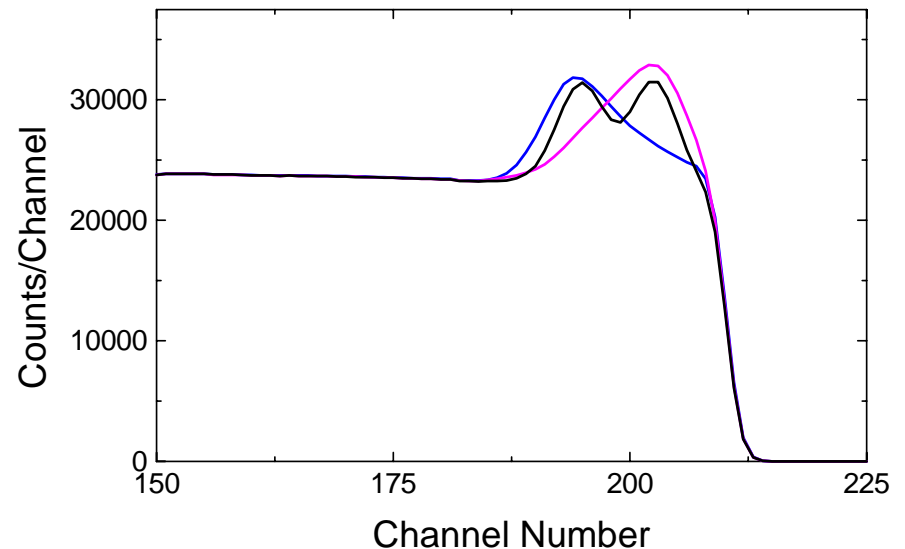
# WHY IS A FINE STRUCTURE ESSENTIAL?

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



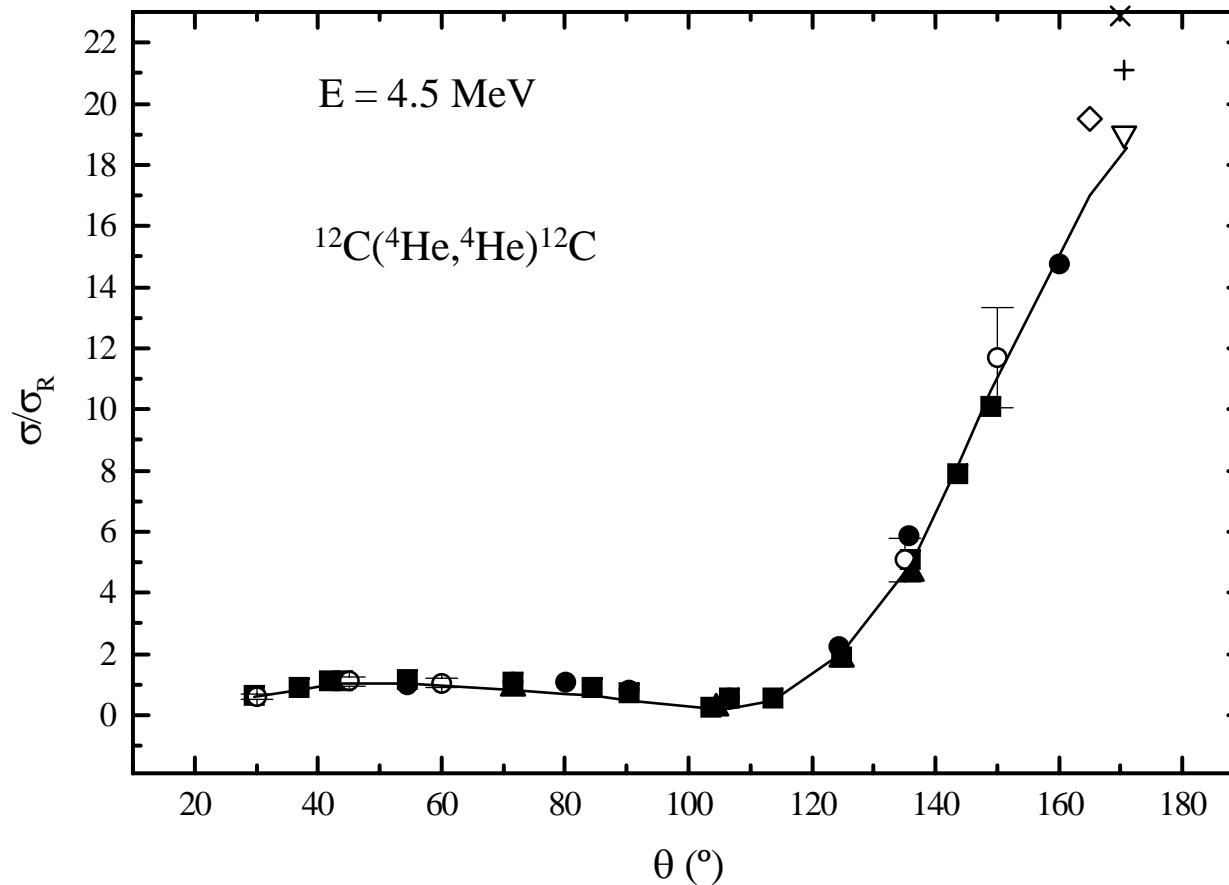
## Simulated EBS spectra

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

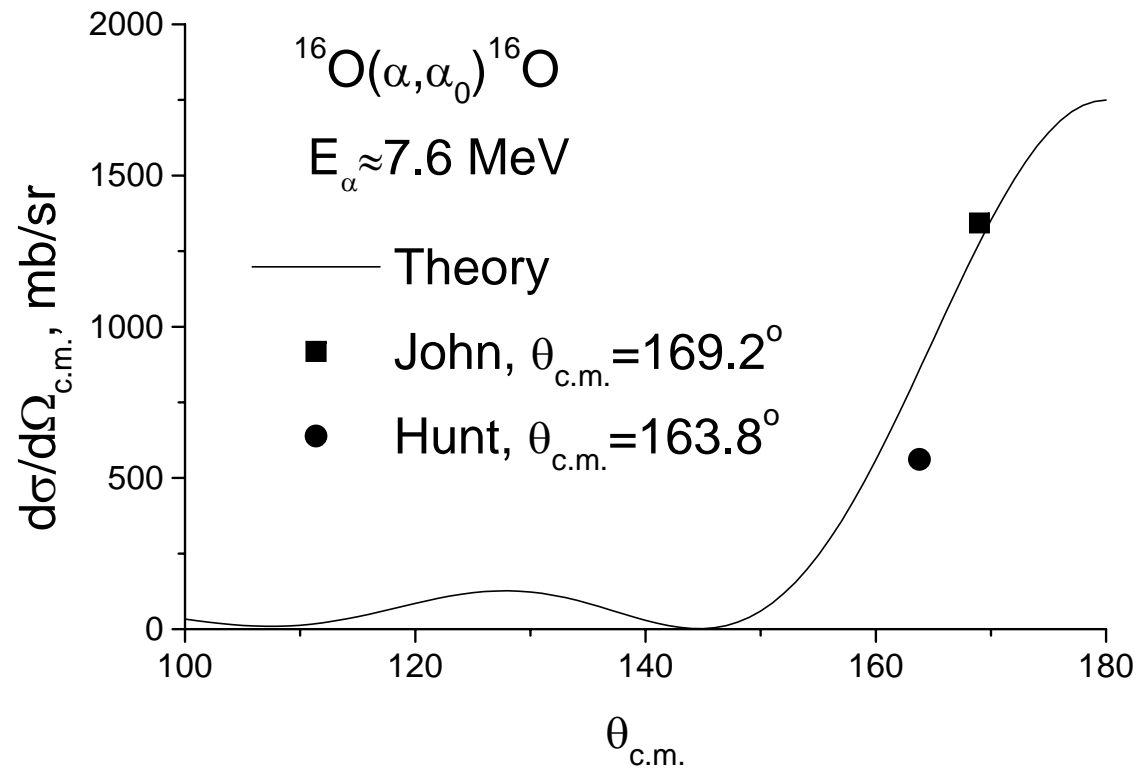


# THE REASONS WHY EVALUATION IS NEEDED

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



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



# 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  $d\sigma/d\Omega(E, \theta)$



# 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.

ENDF: Evaluated Nu...

http://www-nds.iaea.org/exfor/endl.htm

Help » ENDF Format Manual | Plot+ Databases » Medical | NGAtlas | RIPL | FENDL | IRDF-2002 | EXFOR | CINDA

# Evaluated Nuclear Data File (ENDF)

Database Version of February 08, 2011

Software Version of 2011.04.28 Old interface is [\[here\]](#)



## News & History

2011/01 New libraries and software improvements:

- 1) [EAF-2010](#): European Activation File (816 materials/60MeV), UK, issued in 2010
- 2) [TENDL-2010](#): TALYS-based Evaluated Nuclear Data Library, 2010 [\[page\]](#)
- 3) Easy to get full pre-processed material ([PEN](#): temperature=293.16 Kelvin, accuracy=0.1%)

2010/10 Software extensions:

Core nuclear reaction database contain recommended, evaluated cross sections, spectra, angular distributions, fission product yields, photo-atomic and thermal scattering law data, with emphasis on neutron induced reactions. The data were analyzed by experienced nuclear physicists to produce recommended libraries for one of the national nuclear data projects (USA, Europe, Japan, Russia and China). All data are stored in the internationally-adopted ENDF-6 format maintained by CSEWG.

**Standard Request** Examples: [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) Go to: [Advanced Request](#); [ENDF-Explorer](#)

Parameters:

Target

Reaction

Quantity

[More Parameters...](#)

Libraries: ☒ All ☐ Selected

Tip of the day

### Major Libraries

- ☐ 1) ENDF/B-VII.0 (USA,2006)
- ☐ 2) JEFF-3.1.1 (Europe,2005-2009)
- ☐ 3) JENDL-4.0 (Japan,2010)
- ☐ 4) CENDL-3.1 (China,2009)
- ☐ 5) ROSFOND-2010 (Russia,2010)
- ☐ 6) BROND-2.2 (Russia,1992)

### Special Libraries

- ☒ Archival
- ☒ Derived

### Options:

Sort by: ☒ Reactions ☐ Evaluations

### Clone Request:

### Feedback:

### Note:

- all criteria are optional (selected by checking ☒)
- selected criteria are combined for search with logical **AND**
- criteria separated in a field by ";" are combined with logical **OR**
- wildcards and intervals are available
- pointwise libraries contain reconstructed resonances using parameters from MF=2 and applied Doppler broadening at a given temperature.

Original ENDF libraries and files for FTP downloading: [\[ENDF-Archive\]](#)

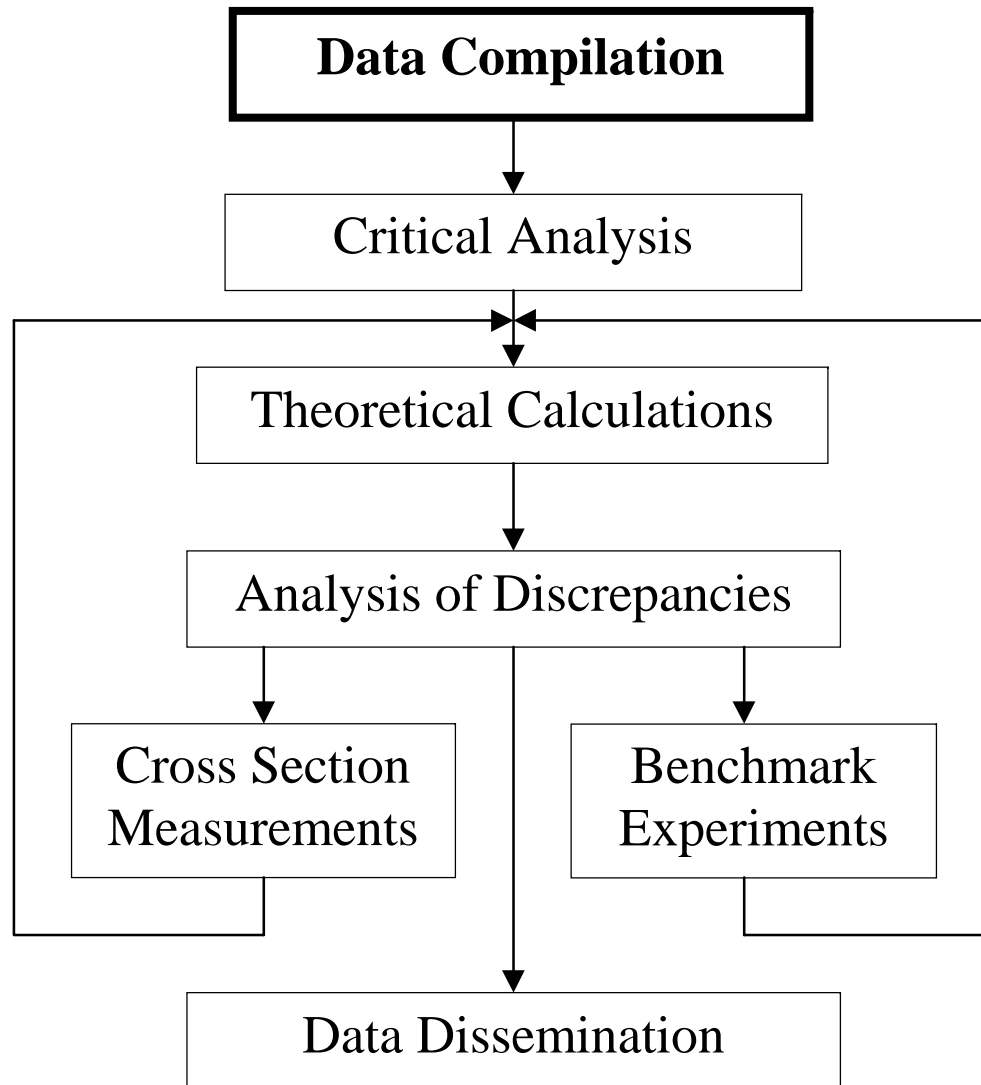
Extensive temperature dependent pointwise libraries: [Point-2009](#) (ENDFB-VII.0)

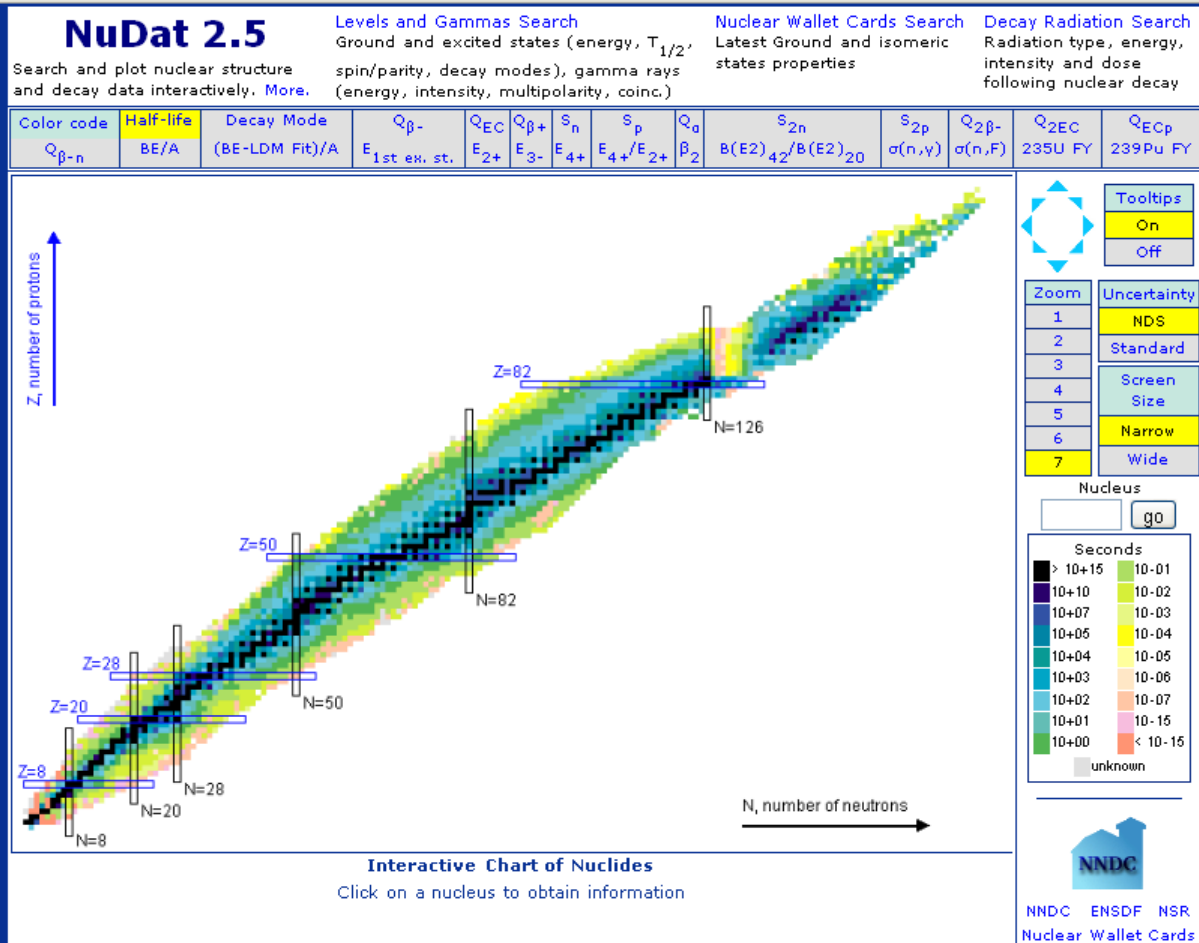
Database Manager: Viktor Zerkov, NDS, International Atomic Energy Agency ([V.Zerkov@iaea.org](mailto:V.Zerkov@iaea.org))

Web and Database Programming: Viktor Zerkov, NDS, International Atomic Energy Agency ([V.Zerkov@iaea.org](mailto:V.Zerkov@iaea.org))

Data Source: Nuclear Energy Agency International Working Party on Evaluation Cooperation (<http://www.nea.fr/html/science/wpec/>) and Cross Section Evaluation Working Group (<http://www.nndc.bnl.gov/csewg/>)

# Evaluation Scheme







## Energy Levels of Light Nuclei, $A = 3 - 20$ Nuclear Data Evaluation Project

### TUNL Nuclear Data Evaluation

Information on mass chains and nuclides available on this website:

3	4
5	6
7	8
9	10
11	12
13	14
15	16
17	18
19	20

Group Info
Publications
HTML
General Tables
Level Diagrams
Tables of EL's
ENSDF
Excitation Functions

- [TUNL Nuclear Data Group](#): Who we are and what we do.

#### Our publications on Energy Levels of Light Nuclei, $A = 5 - 20$ :



- [Publications](#): TUNL evaluations of  $A = 3 - 20$ , and modified versions of Fay Ajzenberg-Selove's publications of  $A = 5 - 20$ , are available here in PDF format. The most recent HTML documents of  $A = 3 - 20$ , and EL diagrams of  $A = 4 - 20$  are also available here. Some reprints and preprints may be requested by mail.
- [HTML for Nuclides](#): HTML documents are available for individual nuclides found within the TUNL or FAS evaluations.

#### Resources relating to our publications:

- [General Tables](#): General Tables in HTML for  $A = 5 - 10$  nuclei.
- [Energy Level Diagrams](#) are available for  $A = 4 - 20$  nuclides.
- [Tables of Energy Levels](#): a brief listing of tables of energy levels from the most recent publication for each nuclide  $A = 4 - 20$ .
- [SiteMap and Complete List of Available TUNL Documents](#): Trying to find a specific TUNL evaluation or preliminary report, HTML document, General Table, Update List or Energy Level Diagram? Click here for a complete list of what's available on our website.

#### Applications and databases relating to the $A = 3 - 20$ nuclides:

- [ENSDF](#): Information for  $A = 2 - 20$  nuclides available through the National Nuclear Data Center (NNDC) site.
- **NEW** [Excitation Functions](#): Compilation of the excitation functions for various  $(p, X)$  and  $(\alpha, X)$  reactions.
- [Thermal Neutron Capture Data](#): Summary of level and branching intensity data measured in Thermal Neutron Capture.
- [Ground-State Decay Data](#): Summary of half-life, branching intensity, and mass excess data measured in ground state beta- and charged-particle-decay.
- [NuDat at BNL](#): Allows to search and plot nuclear structure and nuclear decay data interactively.
- [Palm Pilot Physics Page](#): Links to Palm applications and databases that are of interest to the Nuclear Physics community.

# Table of Isotopes<sup>†</sup>

CD ROM Edition


Version 1.0  
March, 1996


by Richard B. Firestone

Virginia S. Shirley Editor

S.Y. Frank Chu CD-ROM Editor

Coral M. Baglin and Jean Zipkin Assistant Editors

To see brief instructions for Acrobat Reader please click on this green square 

To see README for Table of Isotopes please click on this green square 

<sup>†</sup> This work was supported by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Nuclear Physics Division of the US Department of Energy under contract DE-AC03-76SF00098, subcontract LBL no. 4573810.



Landolt-Börnstein

Numerical Data and Functional Relationships in Science and Technology

*New Series* / Editor in Chief: W. Martienssen

Group I: Elementary Particles, Nuclei and Atoms

Volume 19

# Nuclear States from Charged Particle Reactions

Subvolume A

Tables of Proton and  $\alpha$ -Particle  
Resonance Parameters

Part 1

$Z = 2 - 18$

S.I. Sukhoruchkin

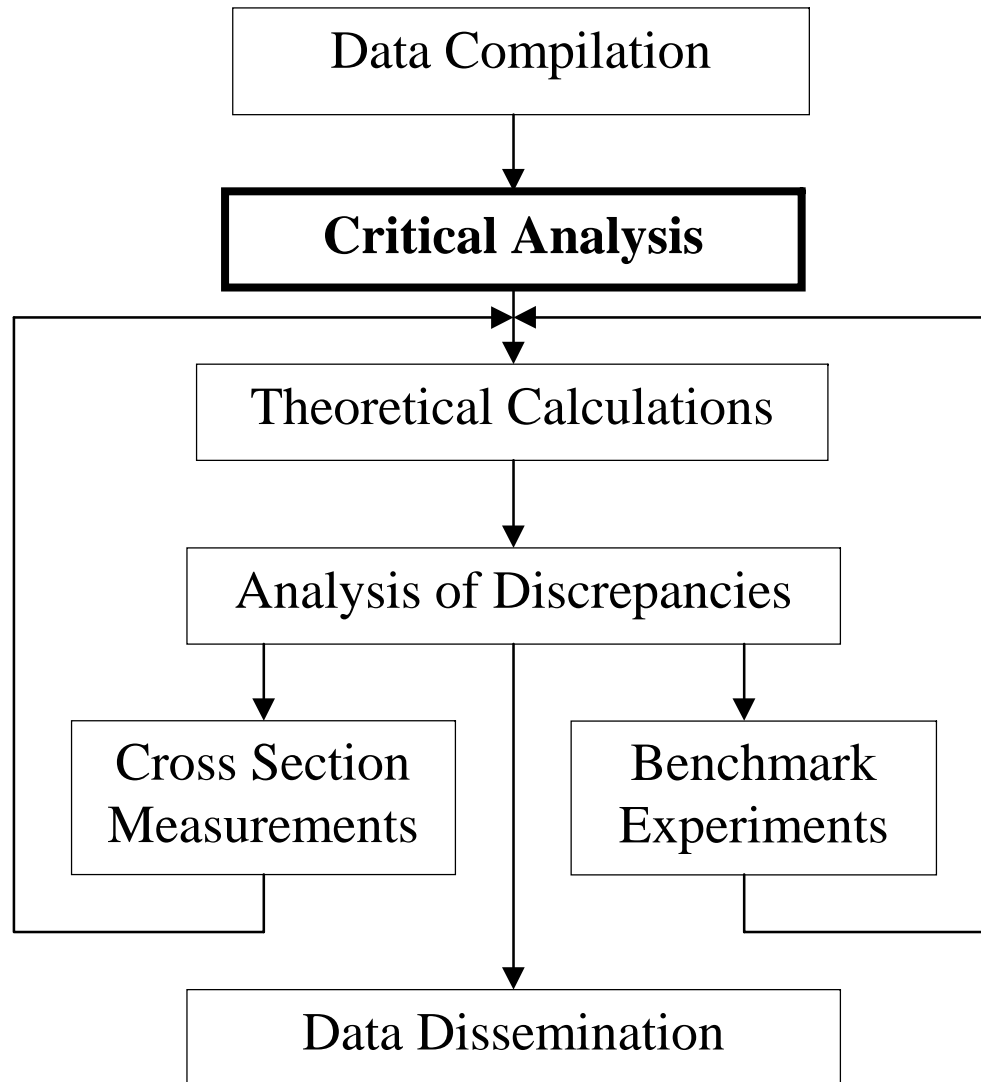
Z.N. Soroko

Edited by H. Schopper



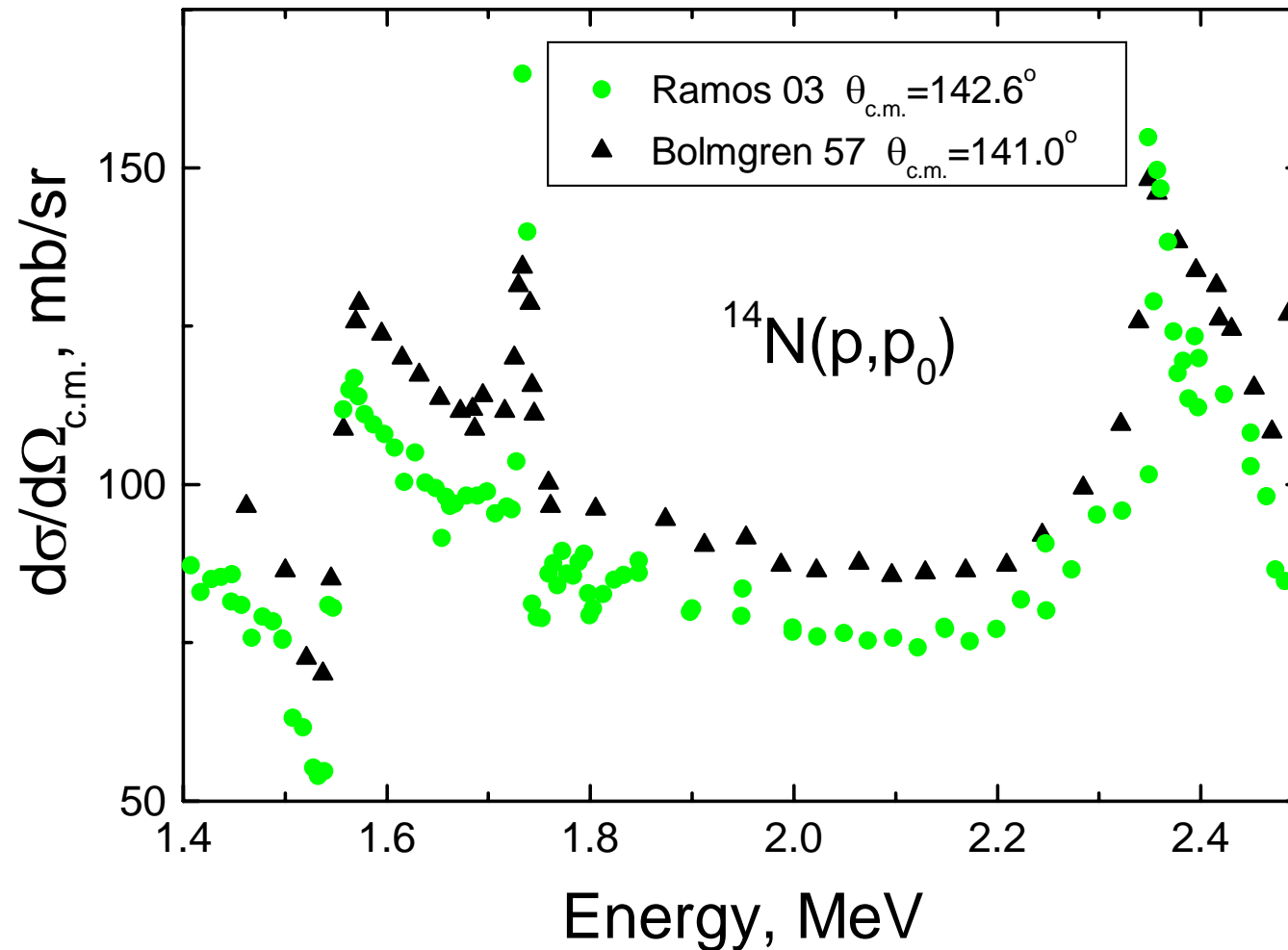
Springer

# Evaluation Scheme

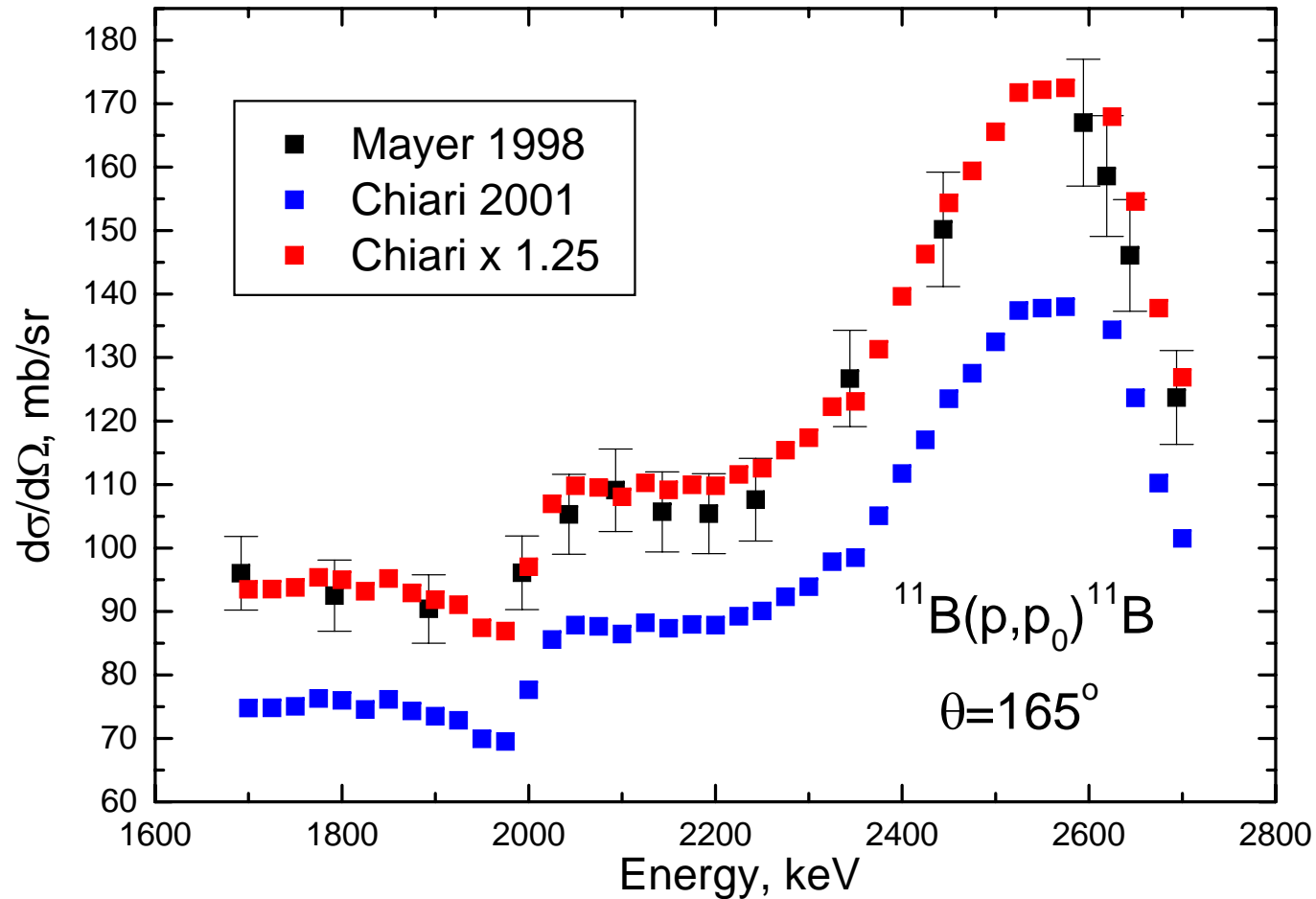




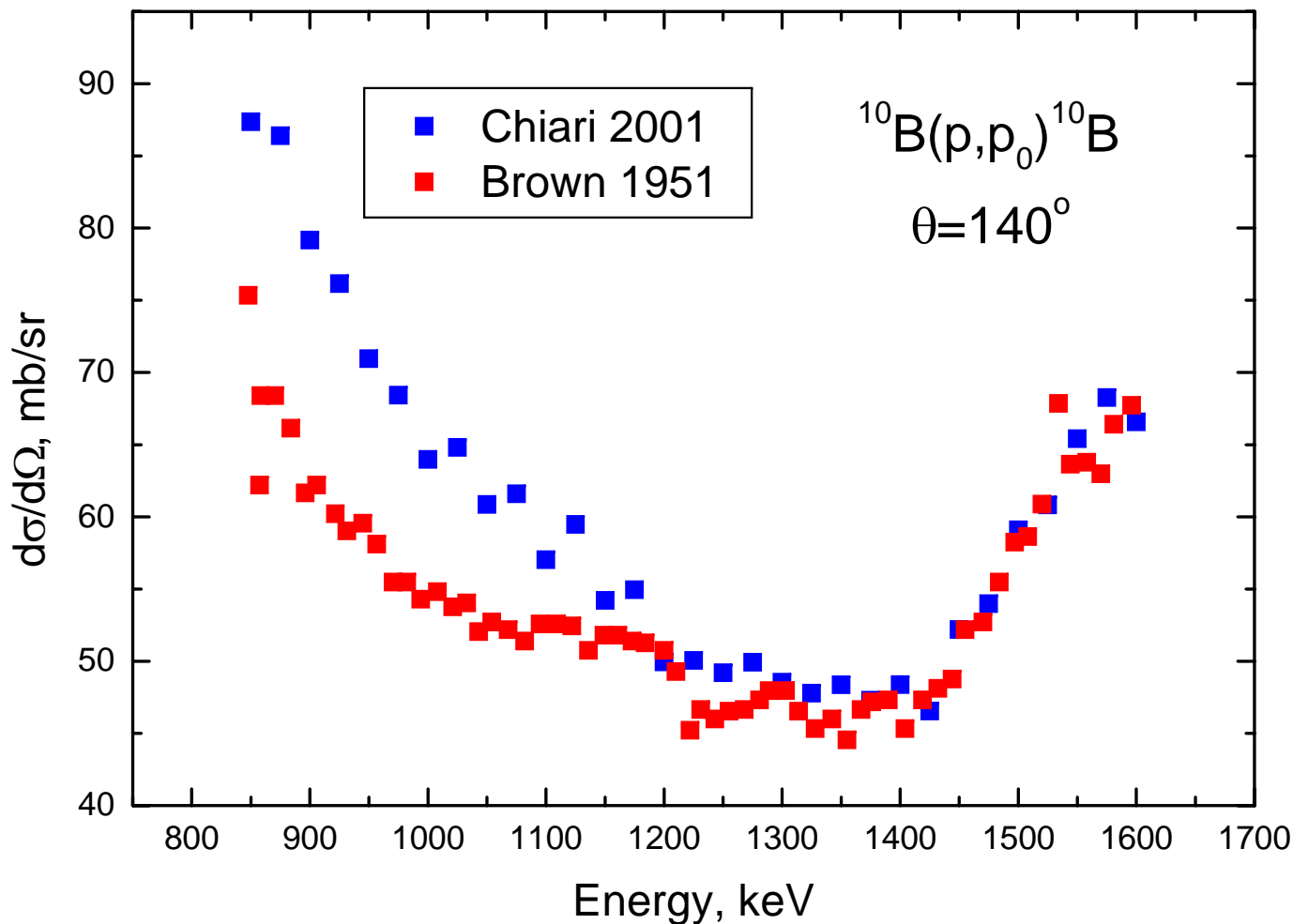
# Comparison of different results for $^{14}\text{N}(p,p_0)^{14}\text{N}$ cross section at the scattering angle of $\sim 140^\circ$



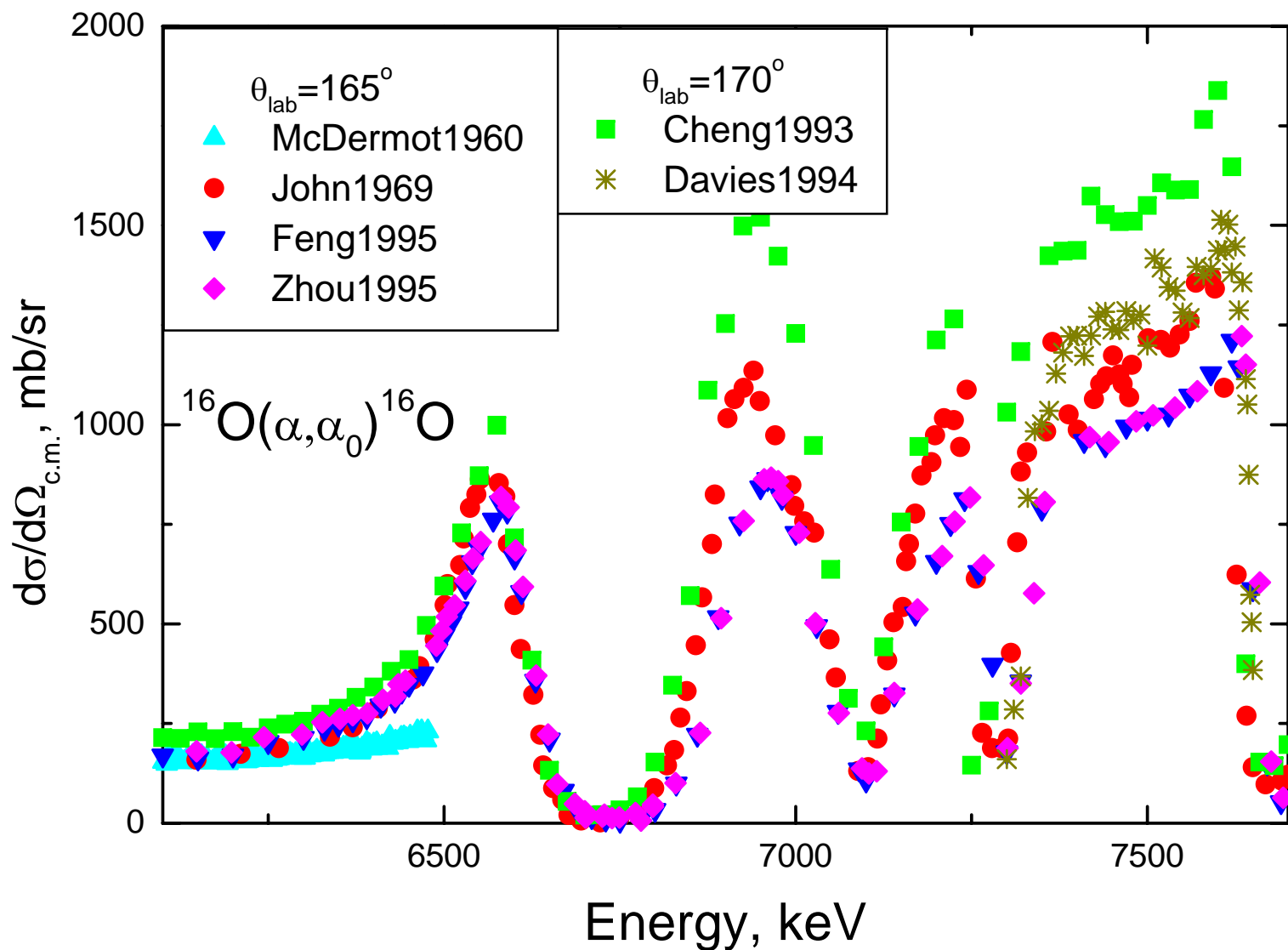
## Comparison of different results for $^{11}\text{B}(p,p_0)^{11}\text{B}$ cross section



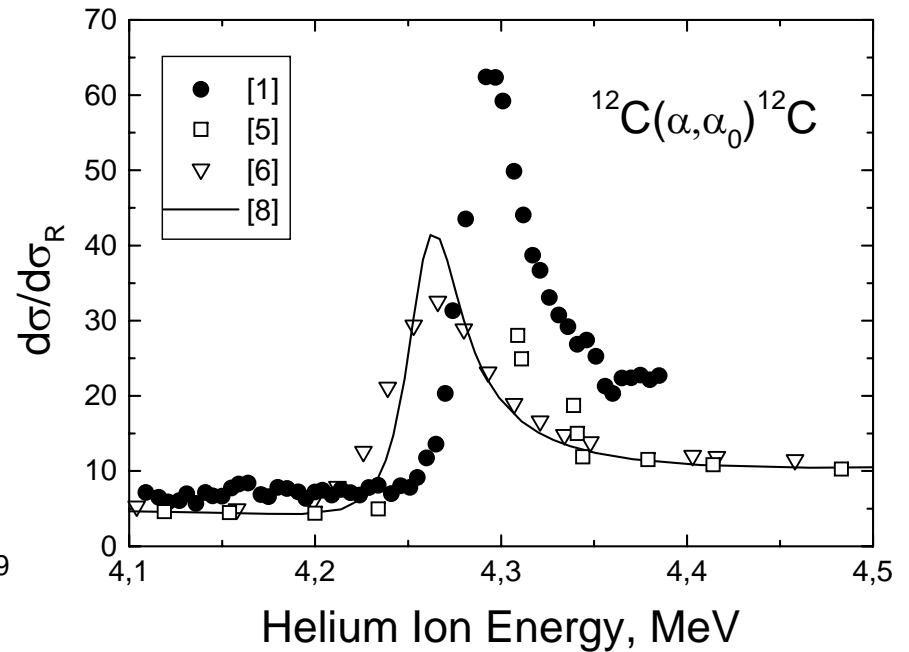
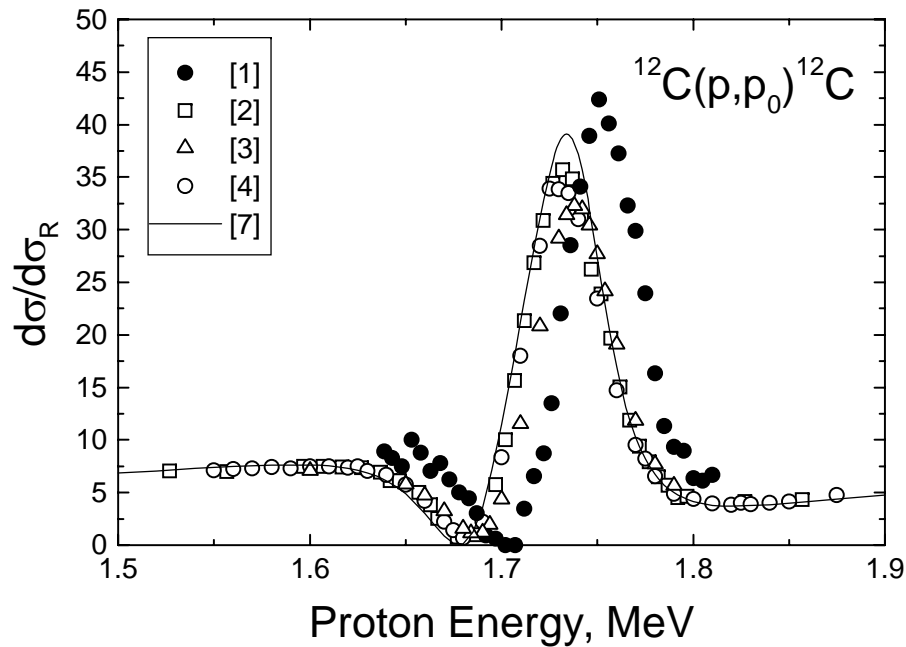
# Comparison of different results for $^{10}\text{B}(p,p_0)^{10}\text{B}$ cross section at the scattering angle of $\sim 140^\circ$



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



# Elimination of apparently erroneous data



# Renormalization of the data set

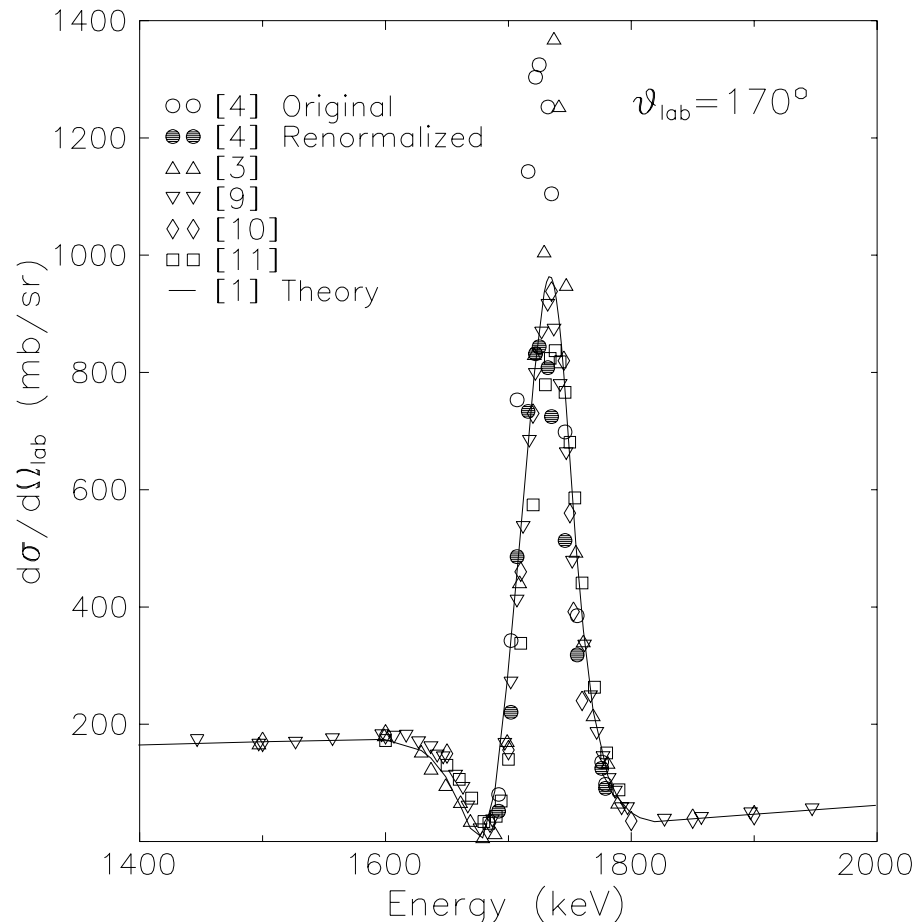
[3] Z. Liu et al. NIM B 74  
(1993) 439

[4] S. Mazzoni et al. NIM B 136-  
138 (1998) 86

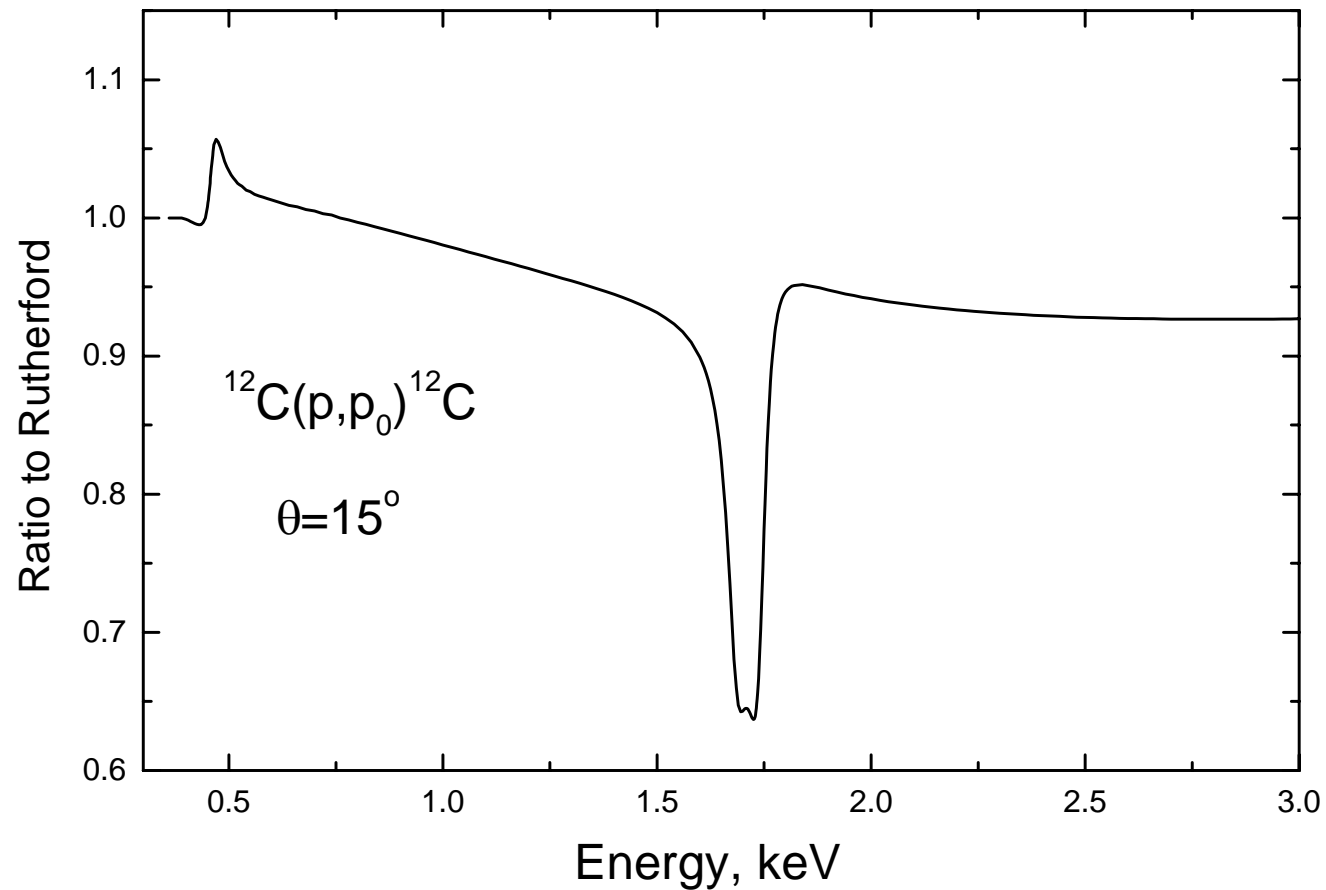
[9] R. Amirikas et al. NIM B 77  
(1993) 110

[10] E. Rauhala NIM B 12 (1985)  
447

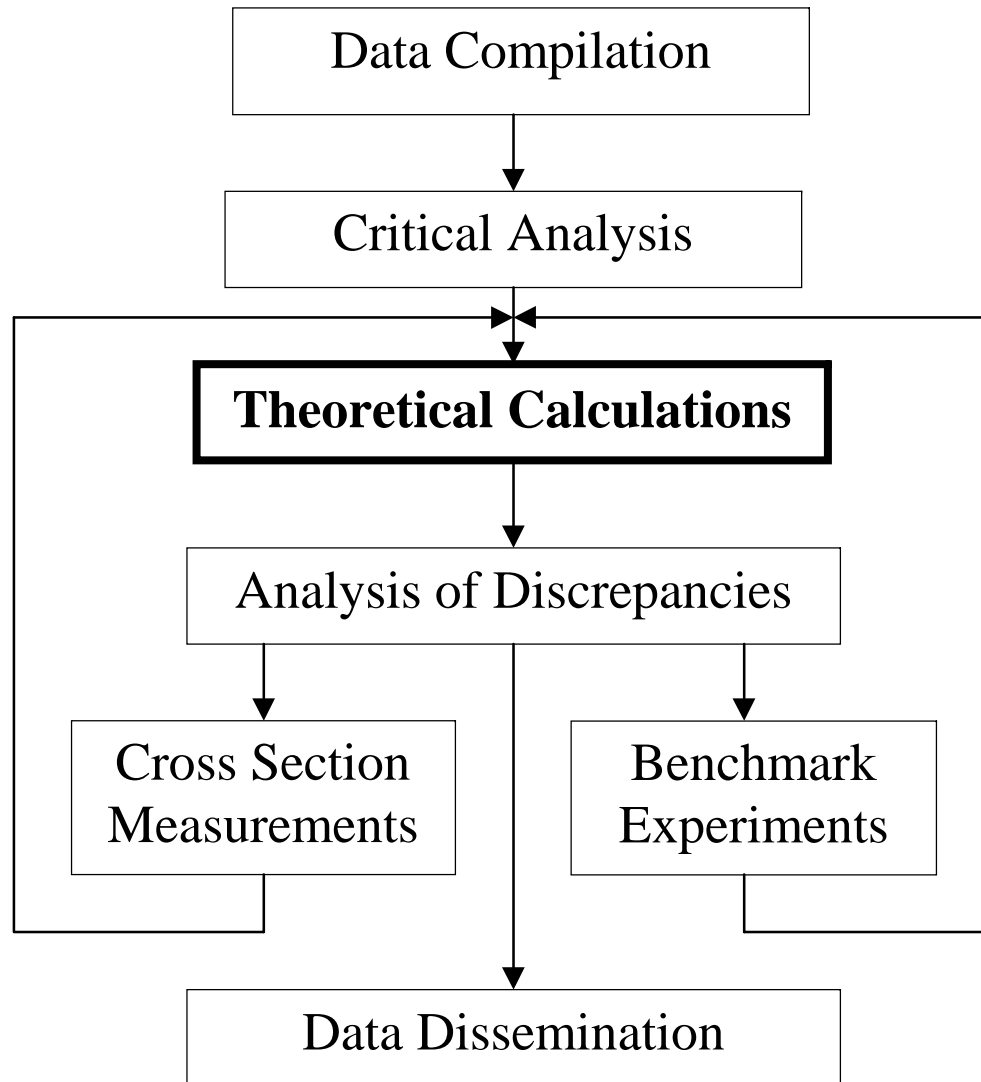
[11] R. Salomonovich NIM B 82  
(1993) 1



# The $^{12}\text{C}(p,p_0)^{12}\text{C}$ cross section at $15^\circ$

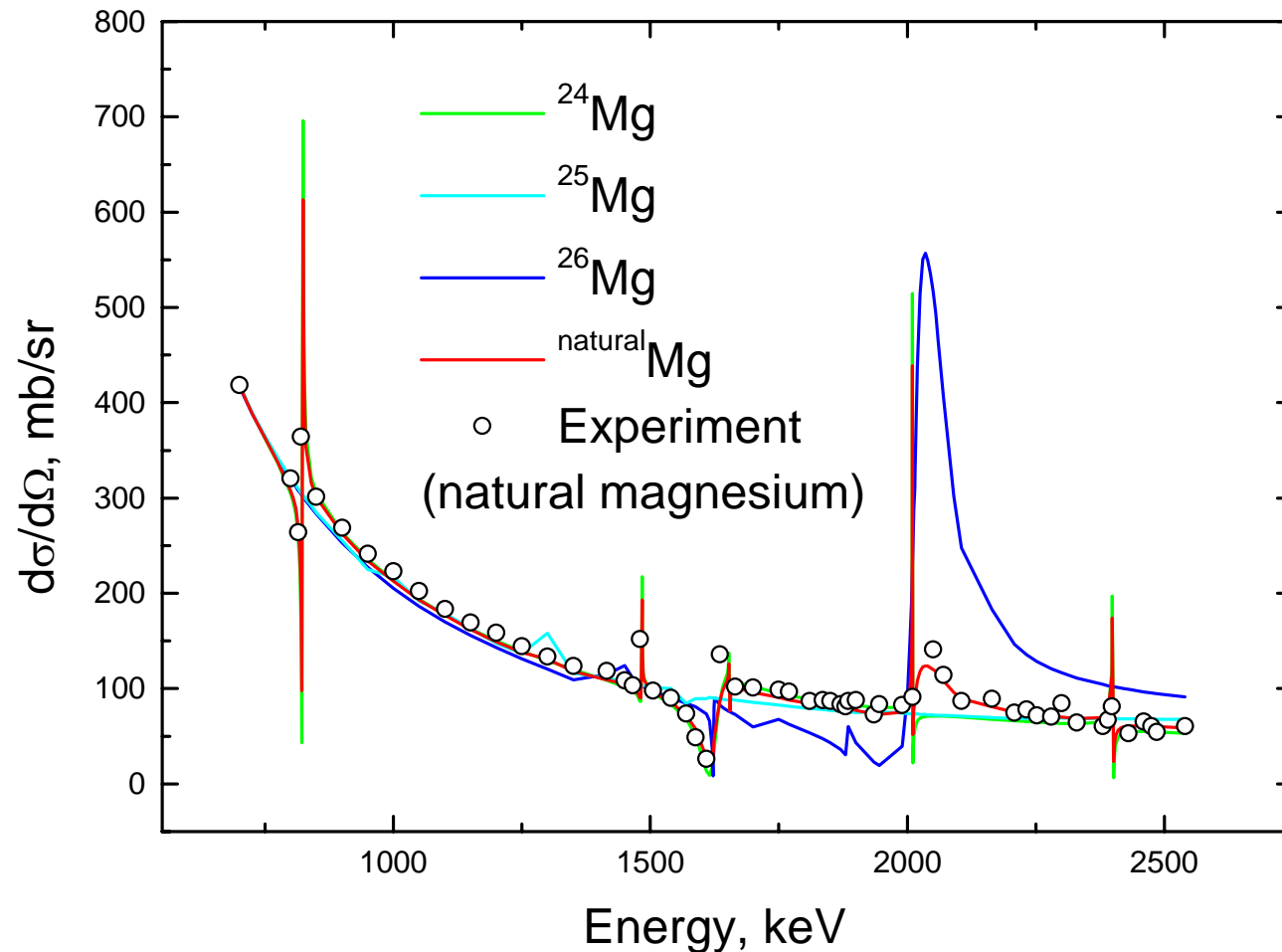


# Evaluation Scheme





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



# R-matrix

(notation by Lane and Thomas)

The R-matrix element is  $R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E}$

with the sum over the compound nuclear levels  $\lambda$ .

The scattering matrix is  $\mathbf{U} = \mathbf{\Omega} \mathbf{W} \mathbf{\Omega}$  where

$$\mathbf{\Omega}_c = \exp[i(\omega_c - \phi_c)], \quad \omega_0 = 0,$$

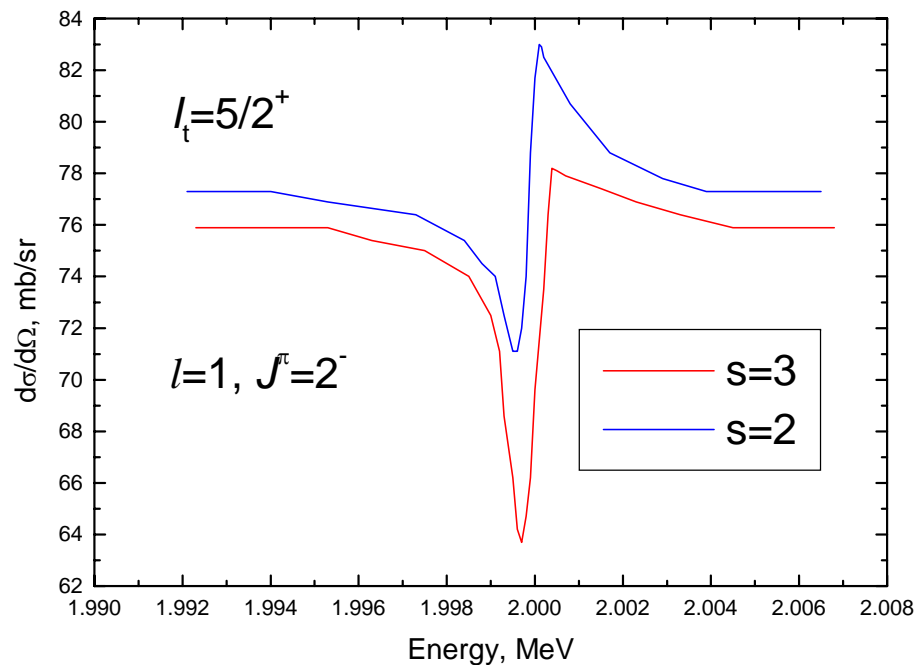
$$\phi_c = \arctan(F_c / G_c), \quad \omega_l = 2 \sum_1^l \arctan(\eta / l), \quad l \geq 1, \quad \eta = Zz / \hbar v$$

$$\mathbf{W} = \mathbf{1} + 2i\mathbf{P}^{1/2}(\mathbf{1} - \mathbf{R}\mathbf{L}_0)^{-1}\mathbf{R}\mathbf{P}^{1/2}$$

The T-matrix element is  $T_{cc'} \equiv T_{\alpha's'l';\alpha,s,l}^{J\pi} = \exp(2i\omega_{\alpha'l'})\delta_{\alpha's'l';\alpha sl} - U_{\alpha's'l';\alpha sl}^{J\pi}$

The cross section is expressed in terms of this T-matrix.

# The effect of channel spin on a resonance shape



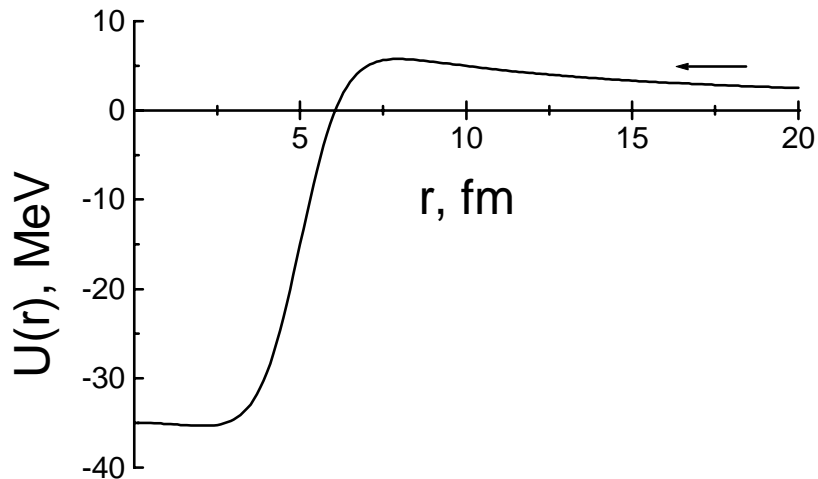
For a target of spin  $I_t$  and projectile of spin  $I_p$  the two spins are coupled to form a channel spin  $s$ . This channel spin is then combined with the relative orbital angular momentum  $l$  to form the spin of the compound nuclear state  $J$ .

Allowed combinations of quantum numbers for elastic proton scattering through the  $J = 2^-$  level of the target with  $I_t^\pi = 5/2^+$

$l$	$s$
1	2
1	3
3	2
3	3

# OPTICAL MODEL

**The standard form of the potential:**



$$U(r) = U_C(r) + U_R(r) + iU_1(r) + U_{so}(r)$$

$$U_R(r) = -V_R f_R(r)$$

$$U_1(r) = 4a_i W_D \frac{df_i(r)}{dr}$$

$$U_{so} = \left( \frac{\hbar}{m_\pi c} \right)^2 V_{so} \frac{1}{r} \frac{df_{so}}{dr} \mathbf{l} \cdot \mathbf{s}$$

$$f_R(r) = \left[ 1 + \exp\left( \frac{r - R_x}{a_x} \right) \right]^{-1}$$

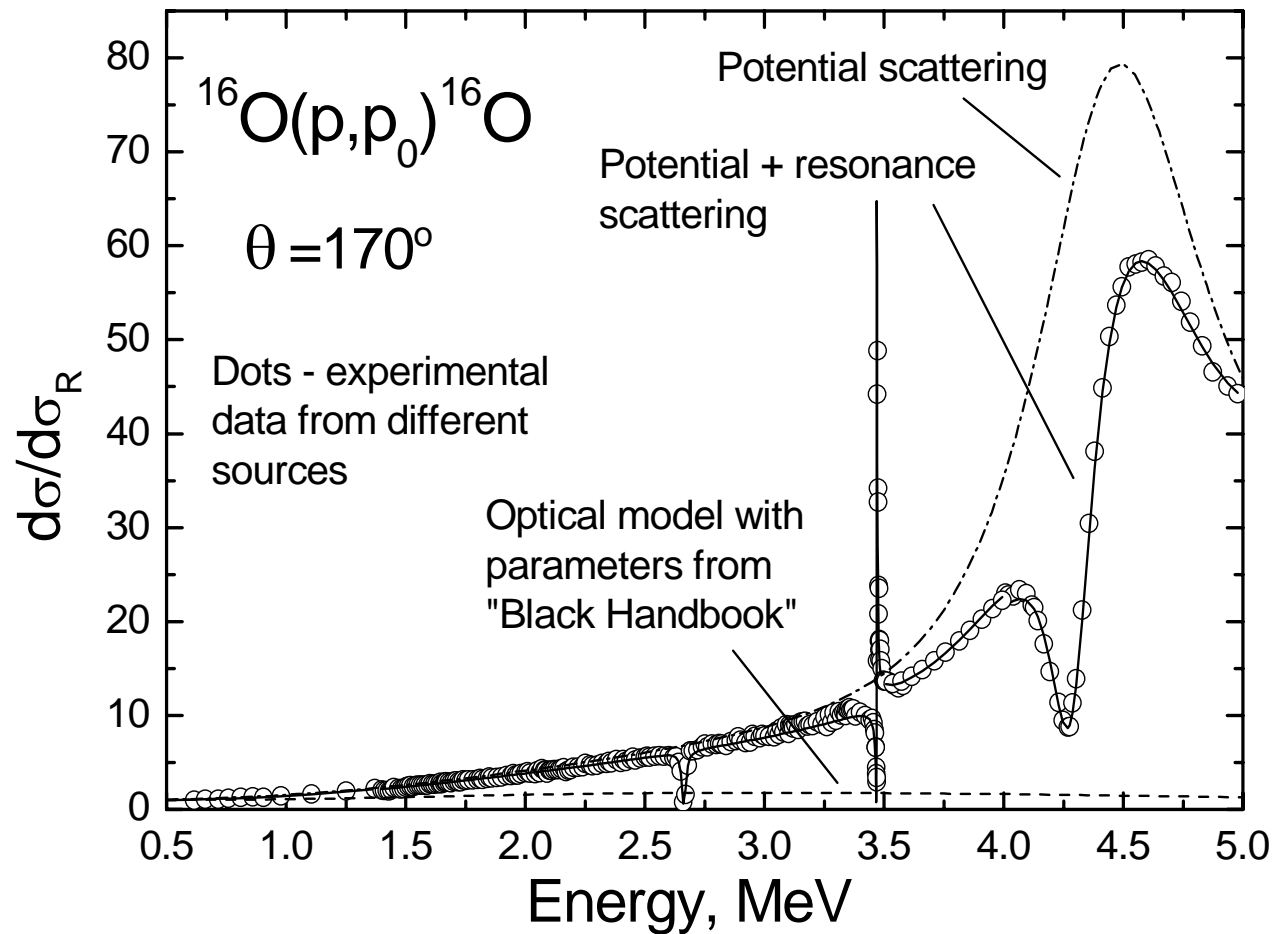
$$R_x = r_x A^{1/3}$$

# OPTICAL MODEL PARAMETERS AT LOW ENERGY

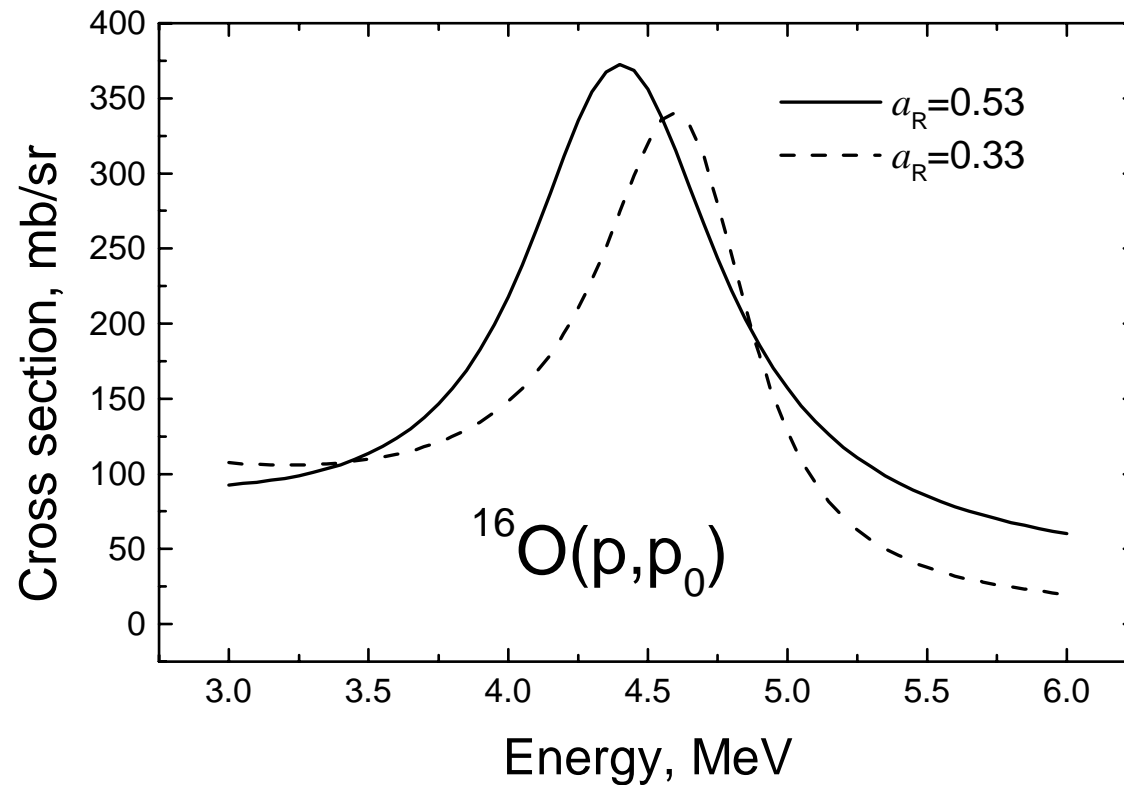
**Global sets are inapplicable at low energy**

- The strength parameters often have strong energy dependence in the vicinity of the Coulomb barrier.
- The real potential radial dependence is of more complicated than Saxon-Woods form.
- The imaginary part of potential reveals non-systematic dependence on nucleus mass number.
- The imaginary part of potential is close to zero for light nuclei.
- Absorption is peaked at the nucleus surface.
- The radius of the imaginary potential diminishes with decreasing energy while its diffuseness increases.

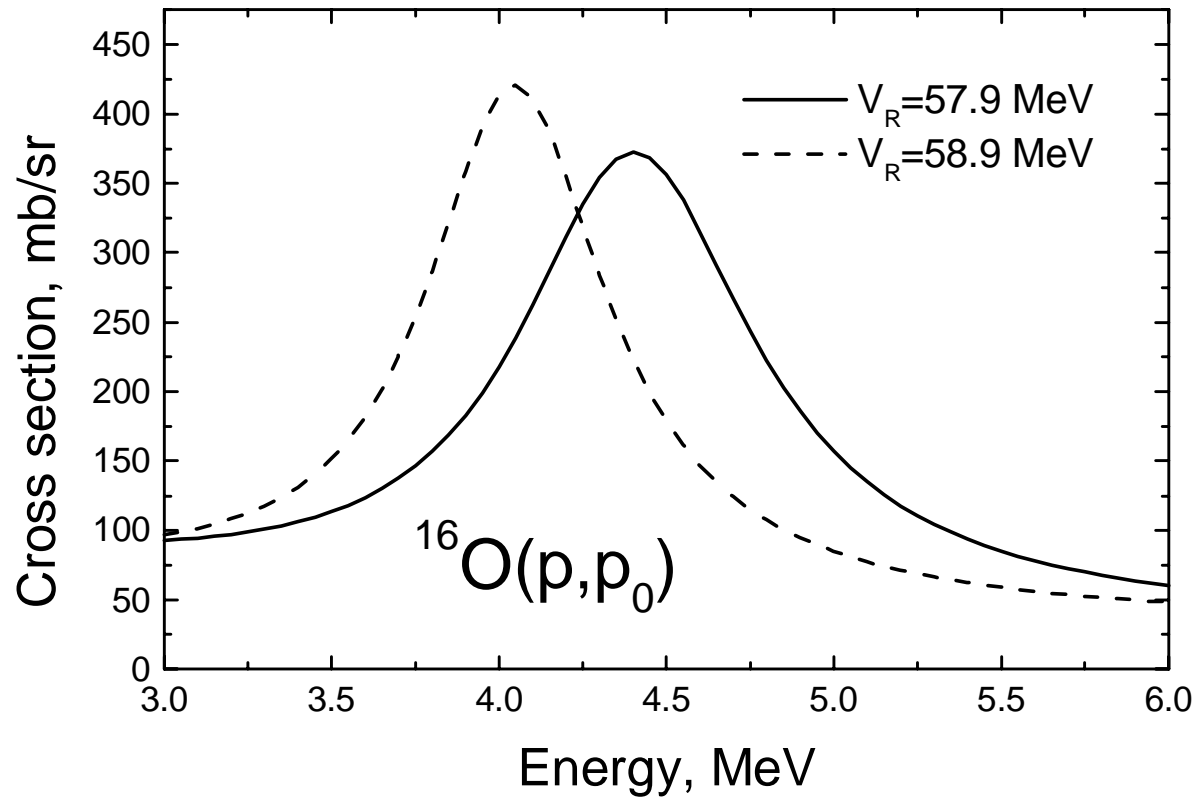
# Shape resonance in $^{16}\text{O}(p,p_0)^{16}\text{O}$



# Shape resonance dependence on $a_R$

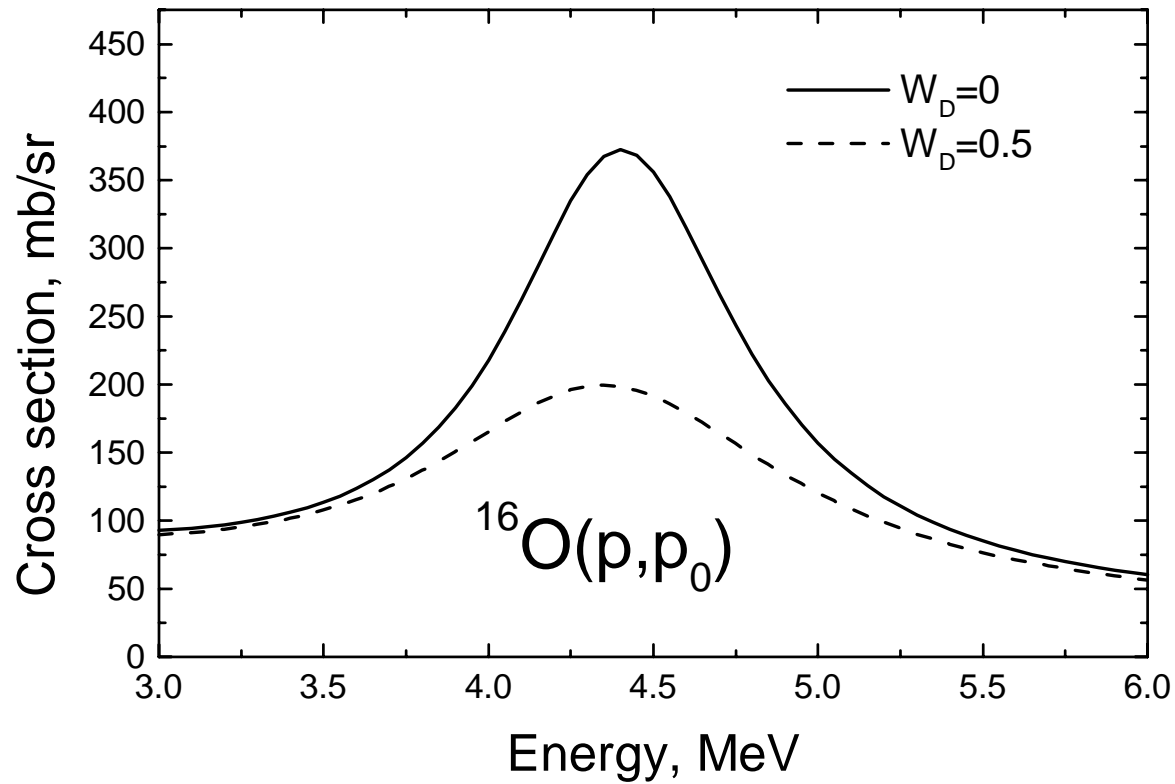


# Shape resonance dependence on $V_R$

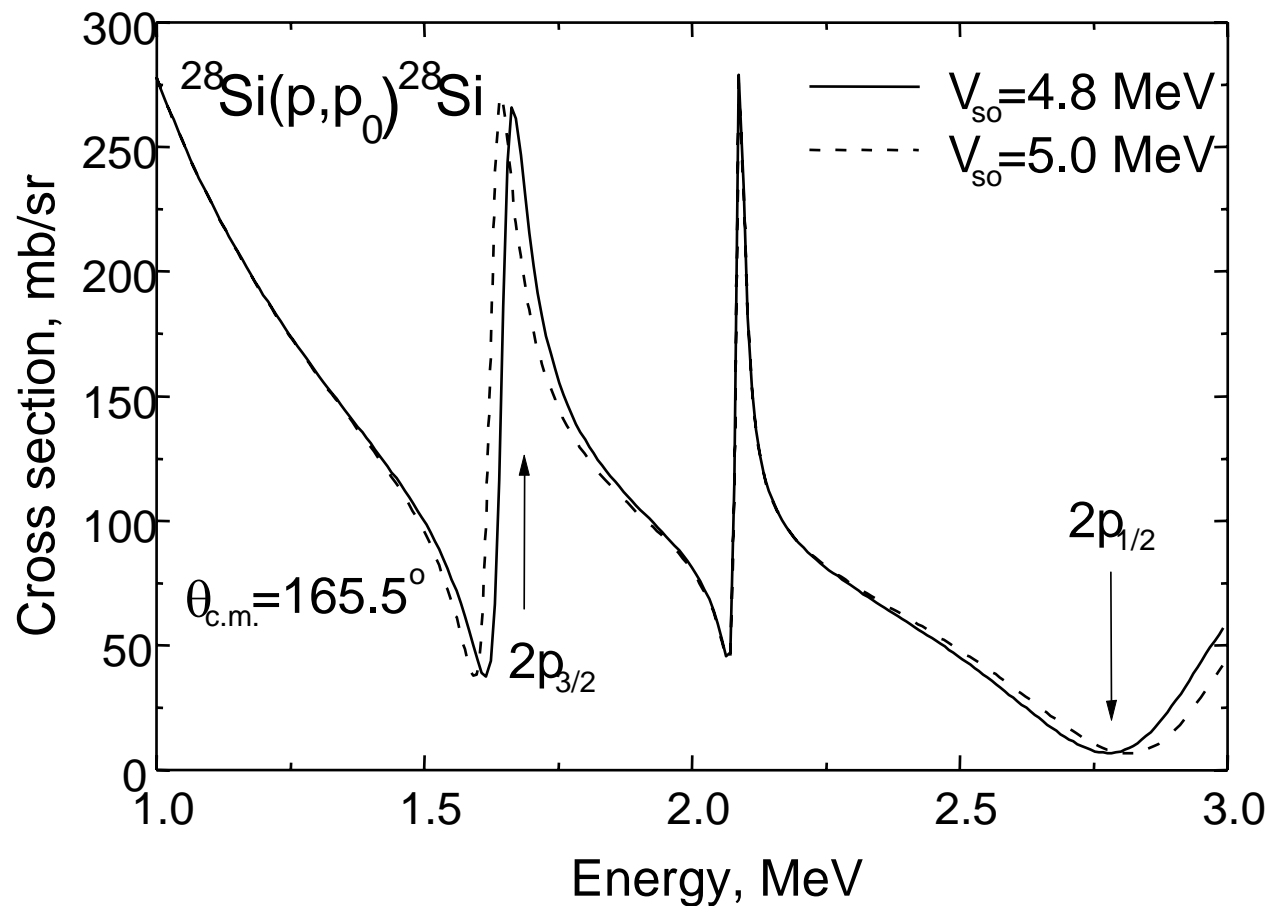




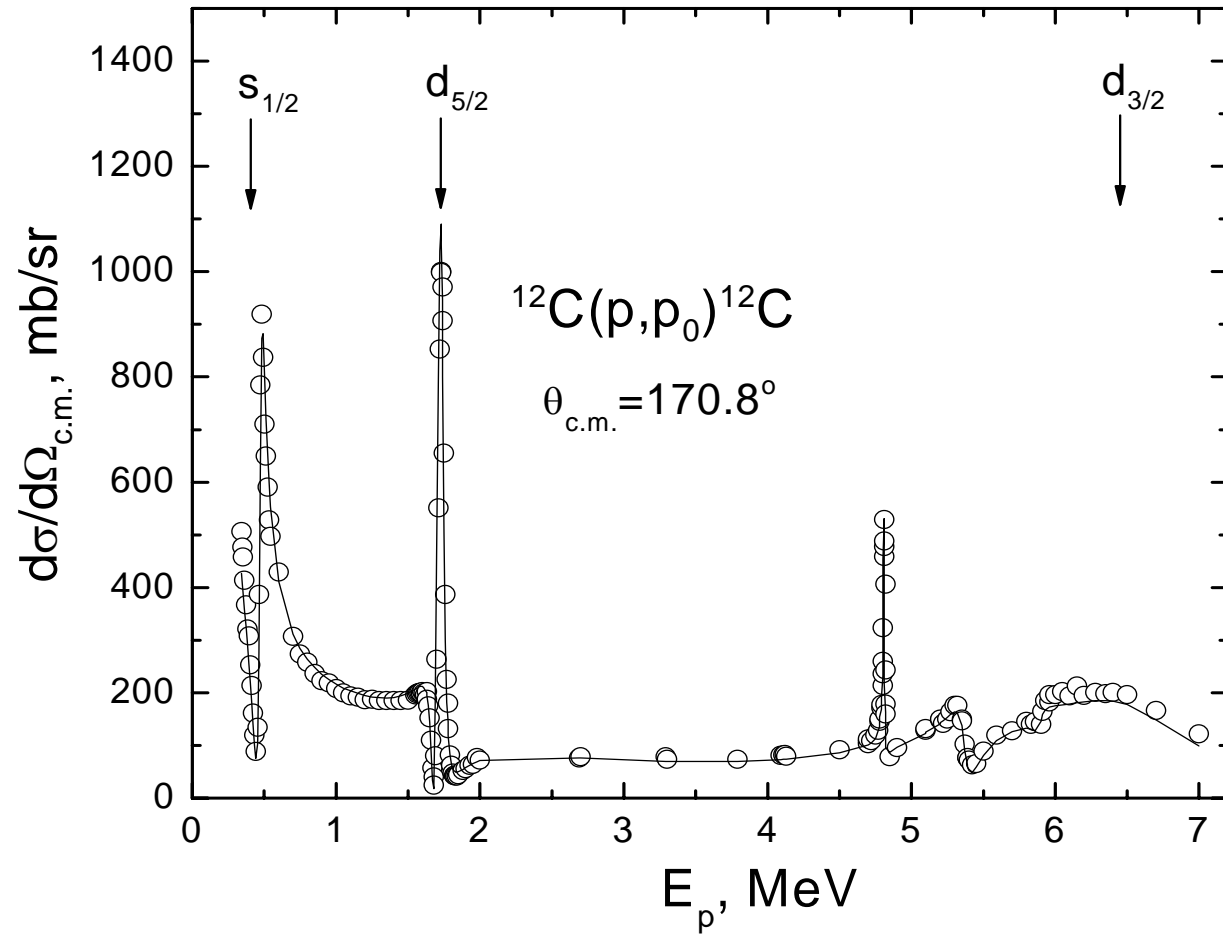
# Shape resonance dependence on $W_D$



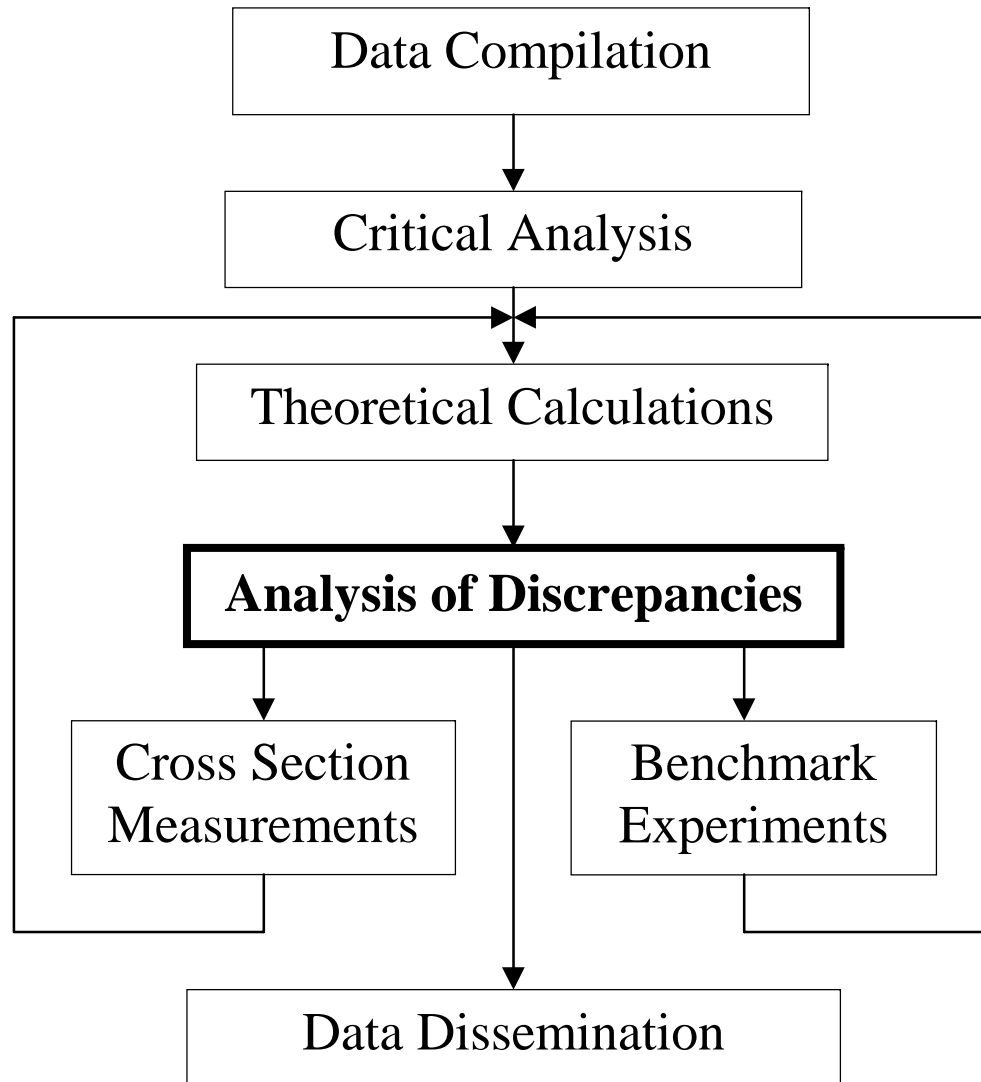
# Splitting of a single particle resonance due to the spin-orbit interaction



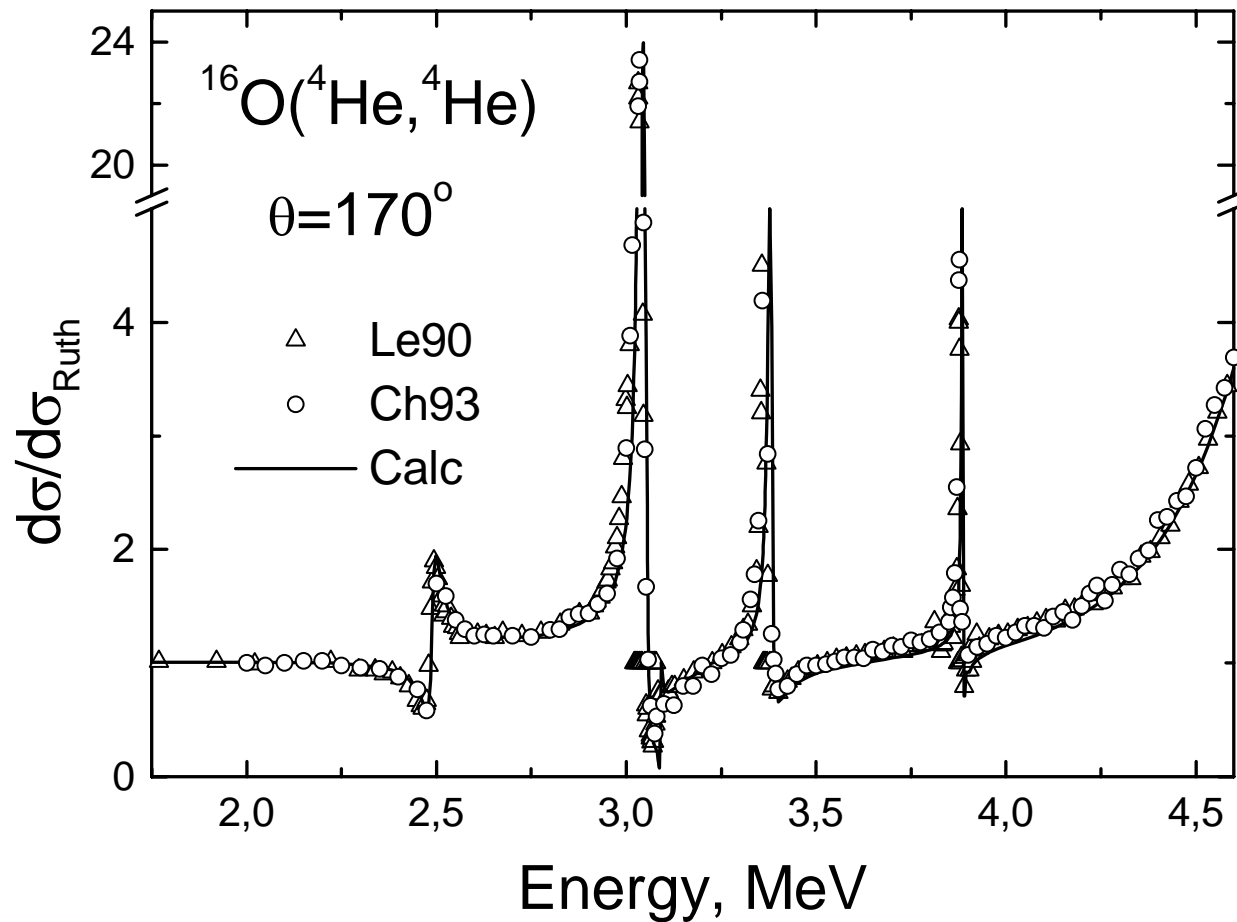
# Shape resonances in $^{12}\text{C}(p,p_0)^{12}\text{C}$



# Evaluation Scheme



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

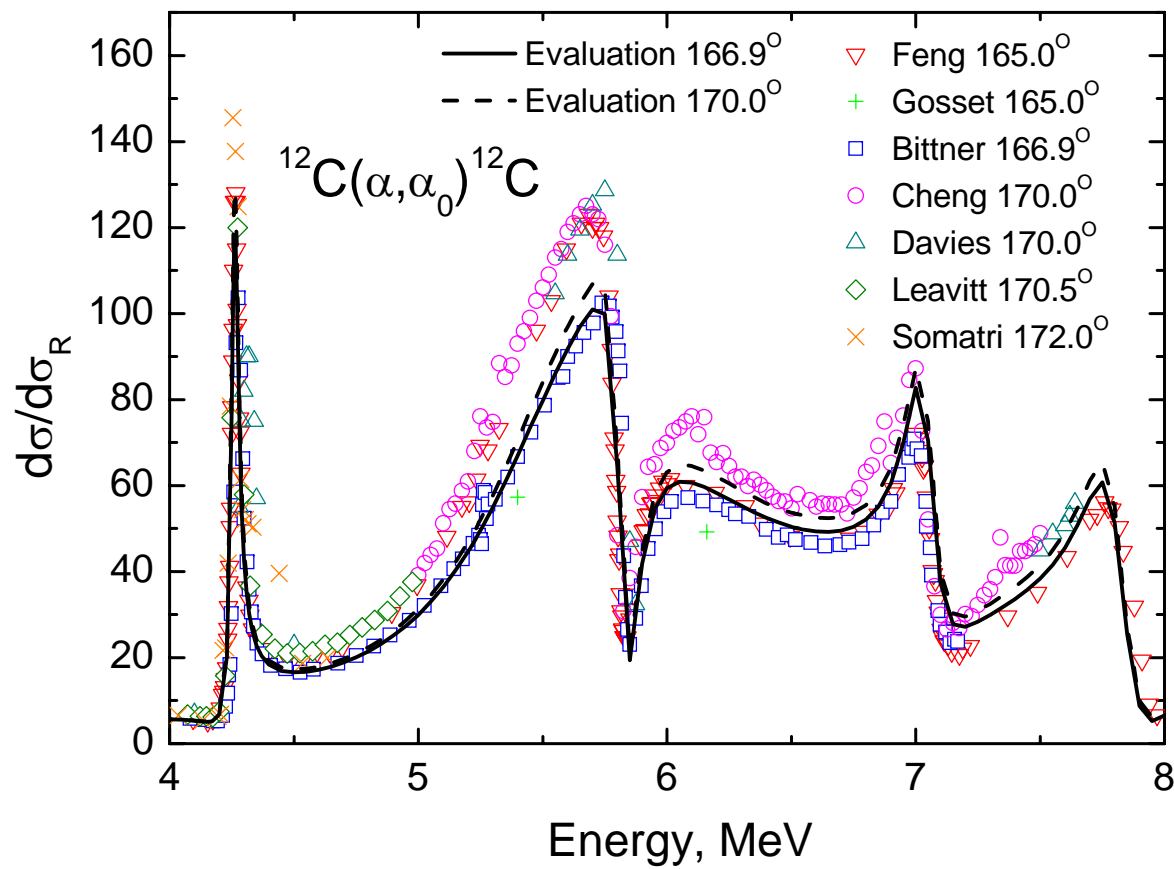




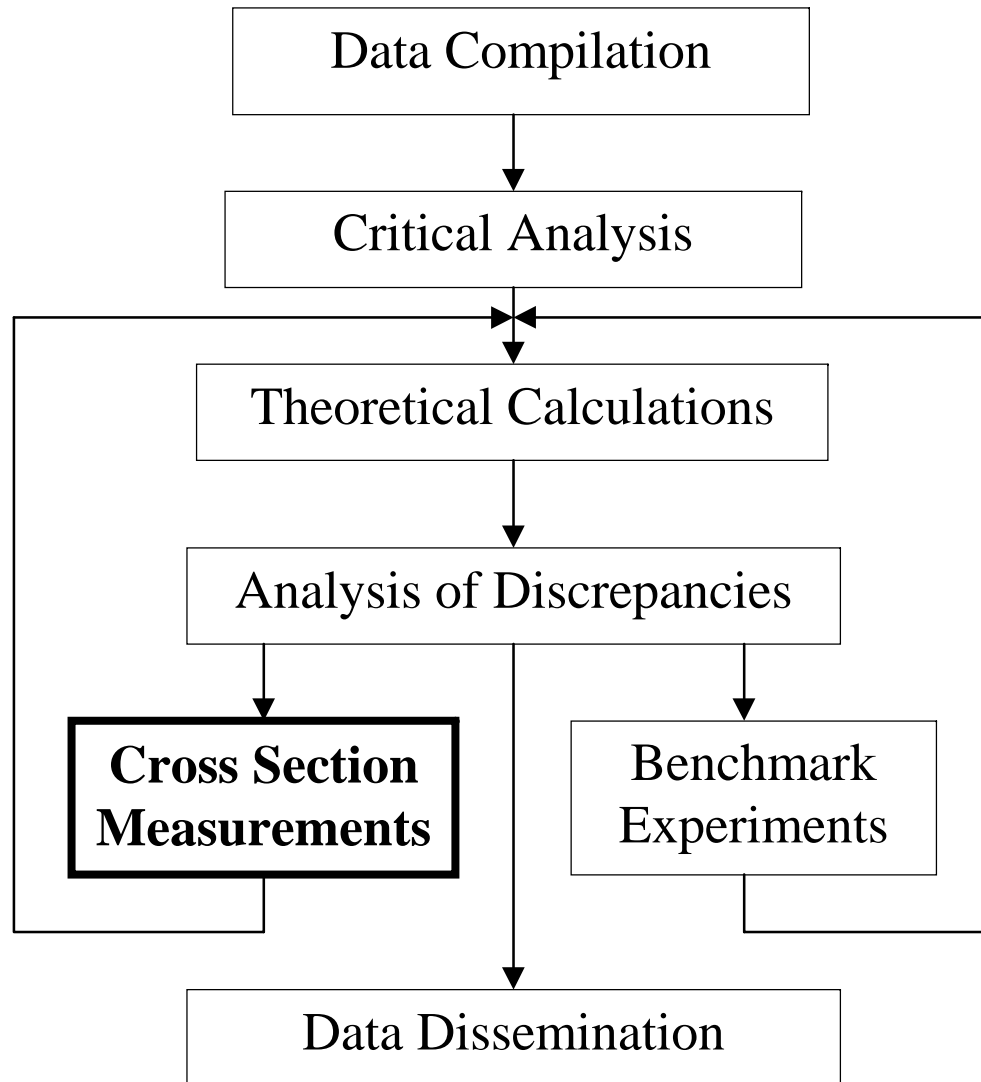
Resonance parameters reported in different works

$E_\alpha$ , keV	$\Gamma_{\text{lab}}$ , keV	Reference
3.0317		Demarche et al. J. Appl. Phys. 100 (2006) 124909
3034 $\pm$ 5		Leavitt, et al. NIM B 44 (1990) 260
3035 $\pm$ 6		Cheng et al., NIM B 83 (1993) 449
3036 $\pm$ 2.3	10.12 $\pm$ 0.37	MacArthur et al., Phys. Rev. C 22 (1980) 356
3038 $\pm$ 5.0	10.0	Soroka et al., NIM B 83 (1993) 311
3042 $\pm$ 3.0	10.26 $\pm$ 0.49	Jarjis, NIM B 12 (1985) 331
3042 $\pm$ 3.0	10.20 $\pm$ 0.40	Wang et al., NIM 211 (1993) 193
3045 $\pm$ 10.0	10.0	Cameron, Phys. Rev. 90 (1953) 839
3038.2 $\pm$ 2	10.1 $\pm$ 0.4	Evaluated (1998, TUNL)

# Analysis of discrepancies

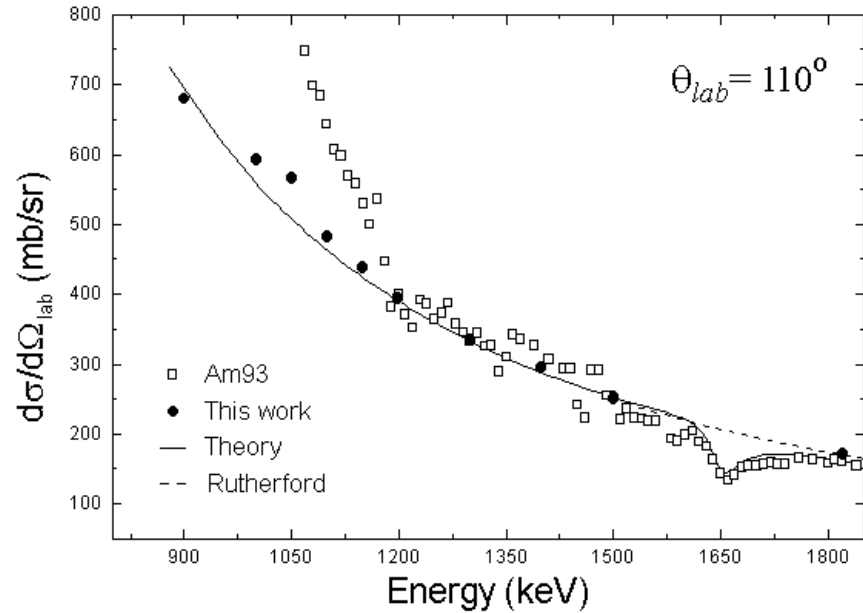
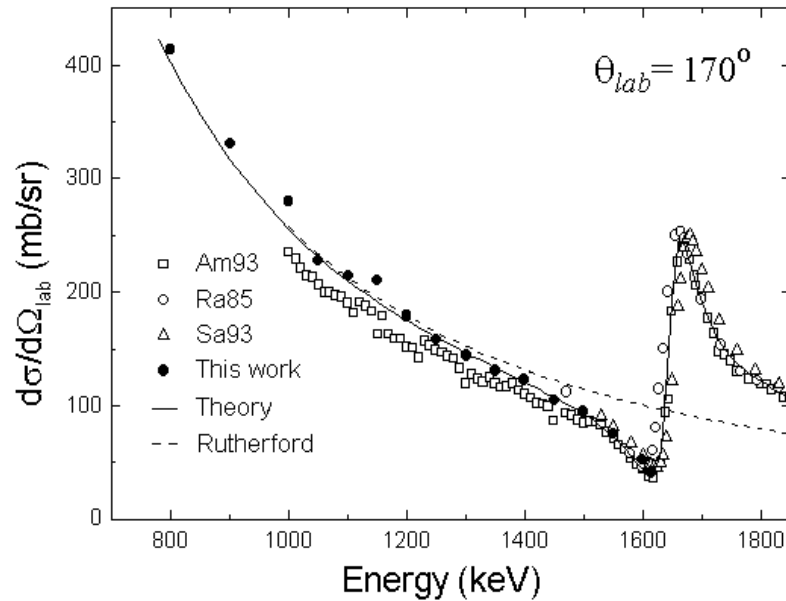


# Evaluation Scheme

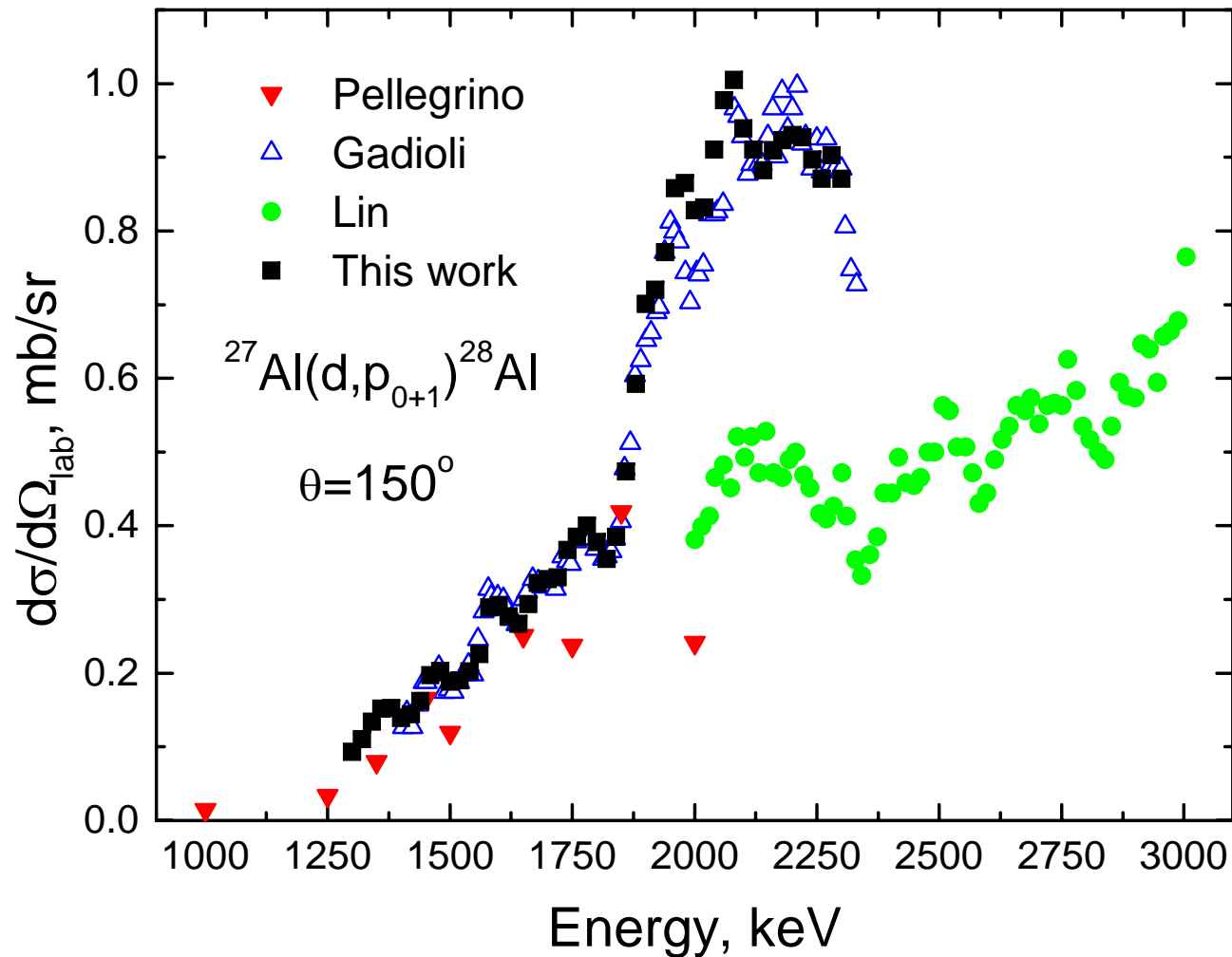




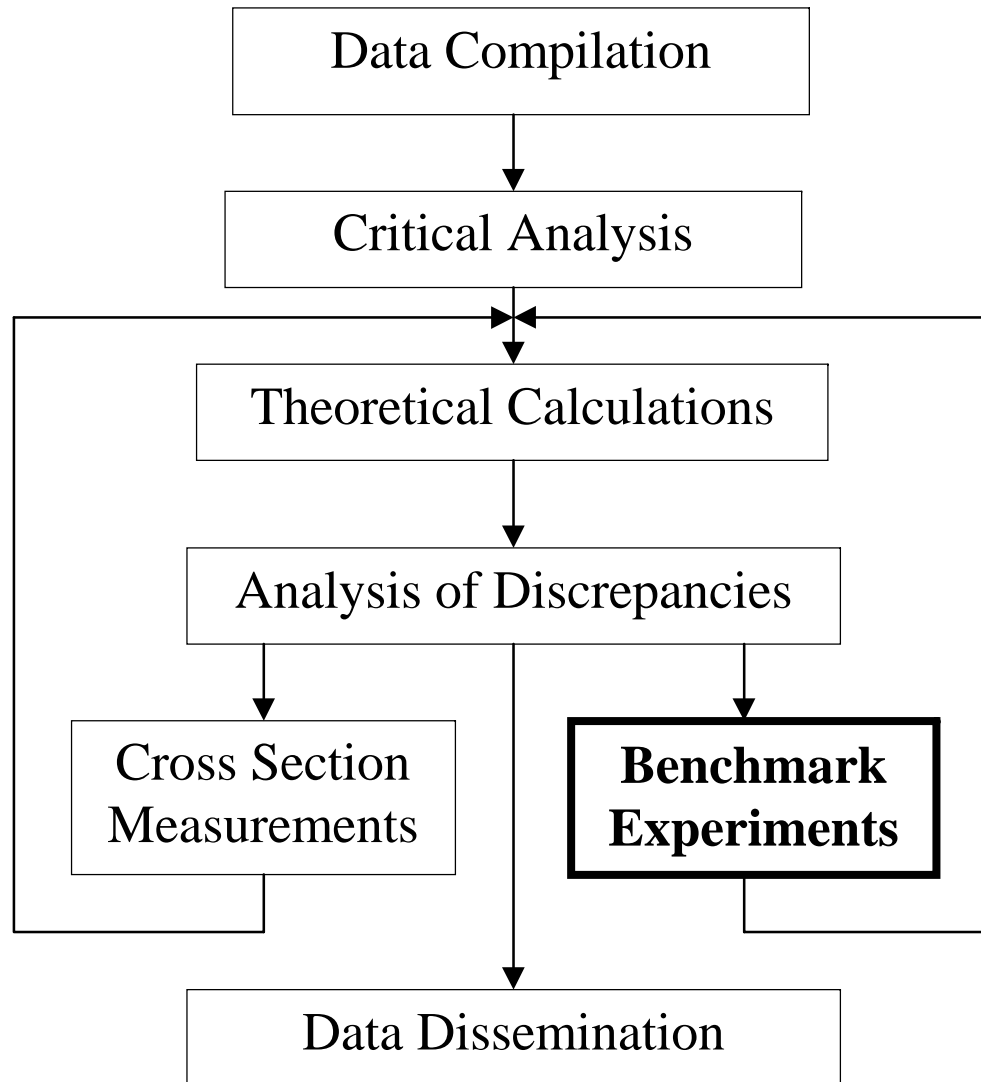
# A measurement to resolve discrepancy



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



# Evaluation Scheme

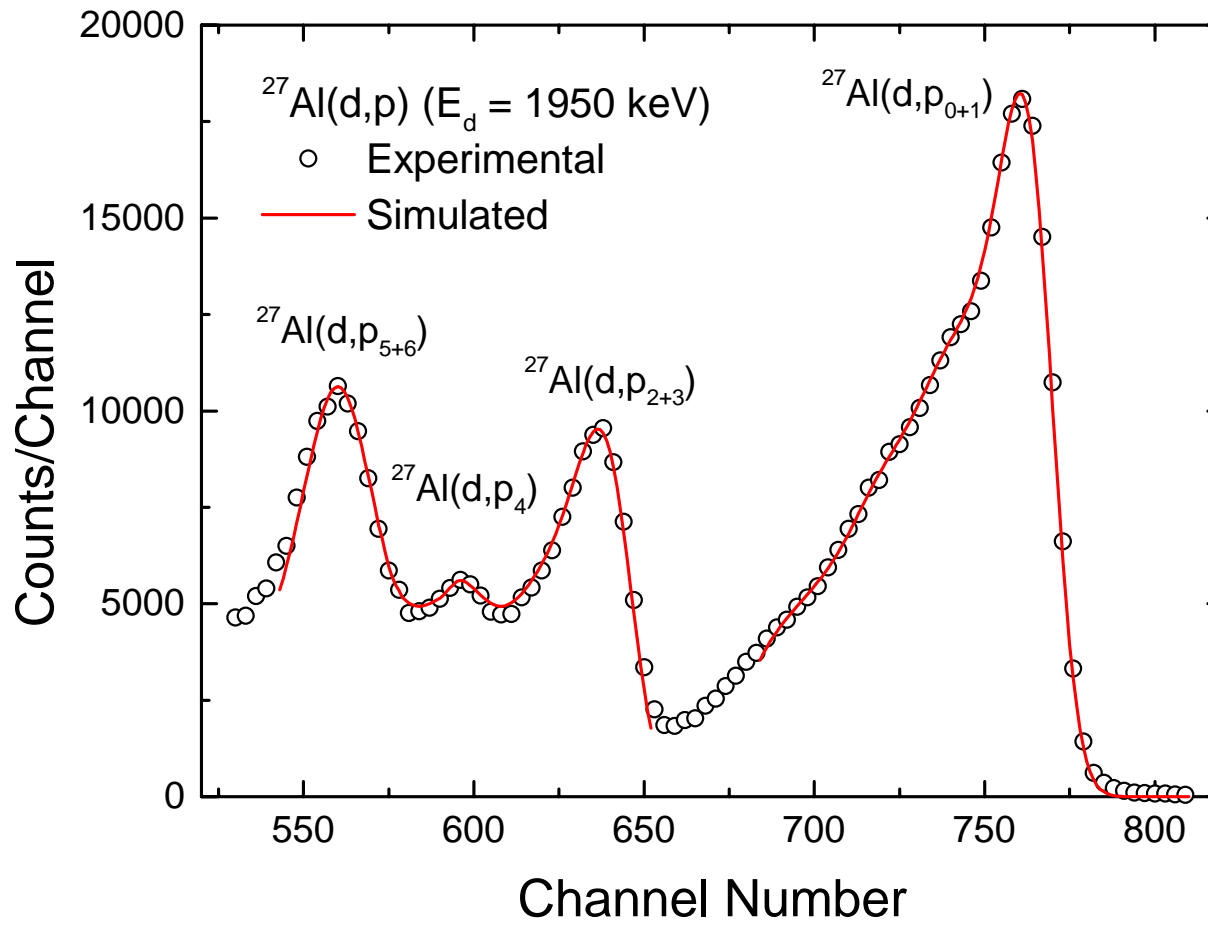


# Benchmarks

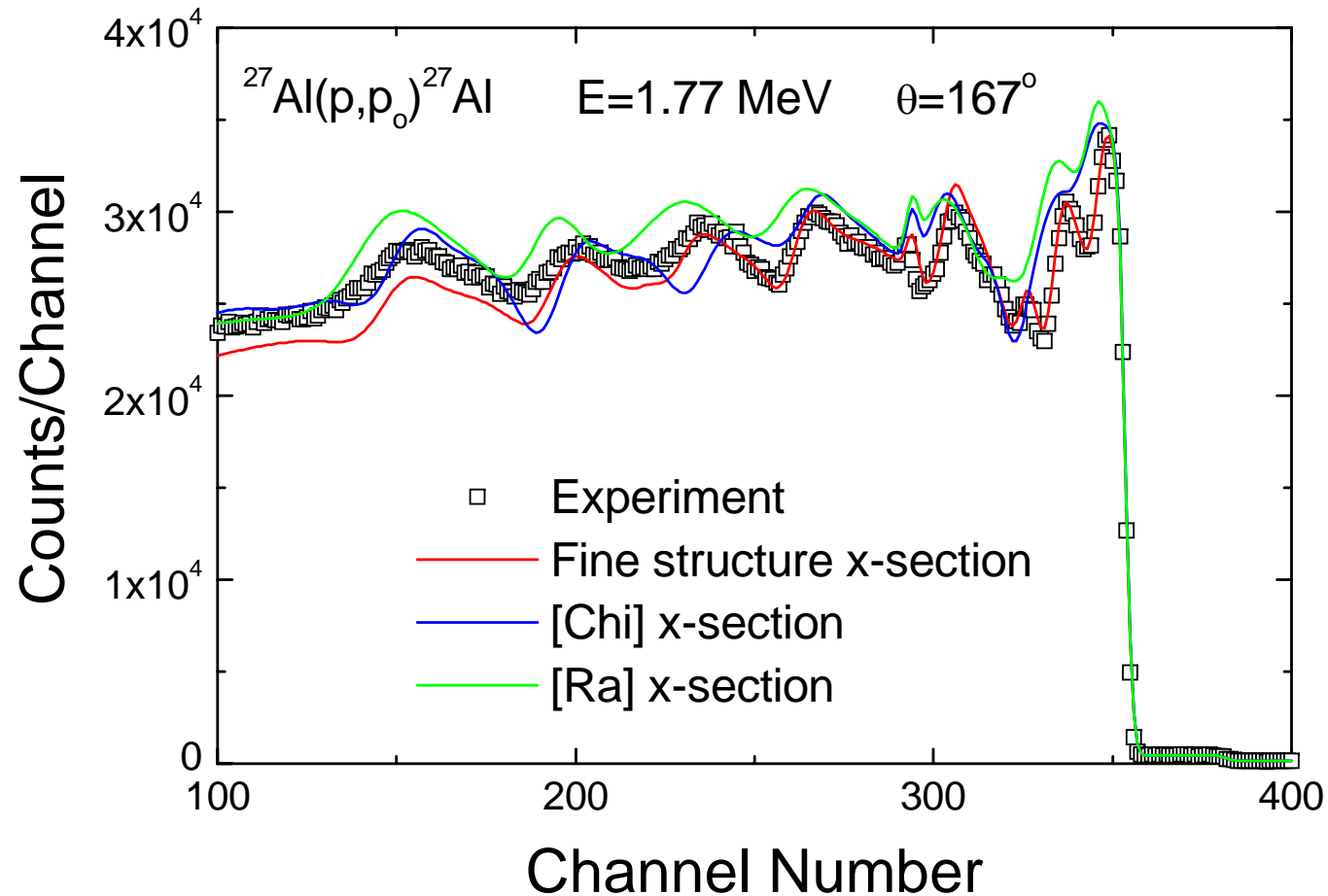
A benchmark is an integral experiment which is compared with a standard direct simulation using microscopic cross-section data in order to verify the data.

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.

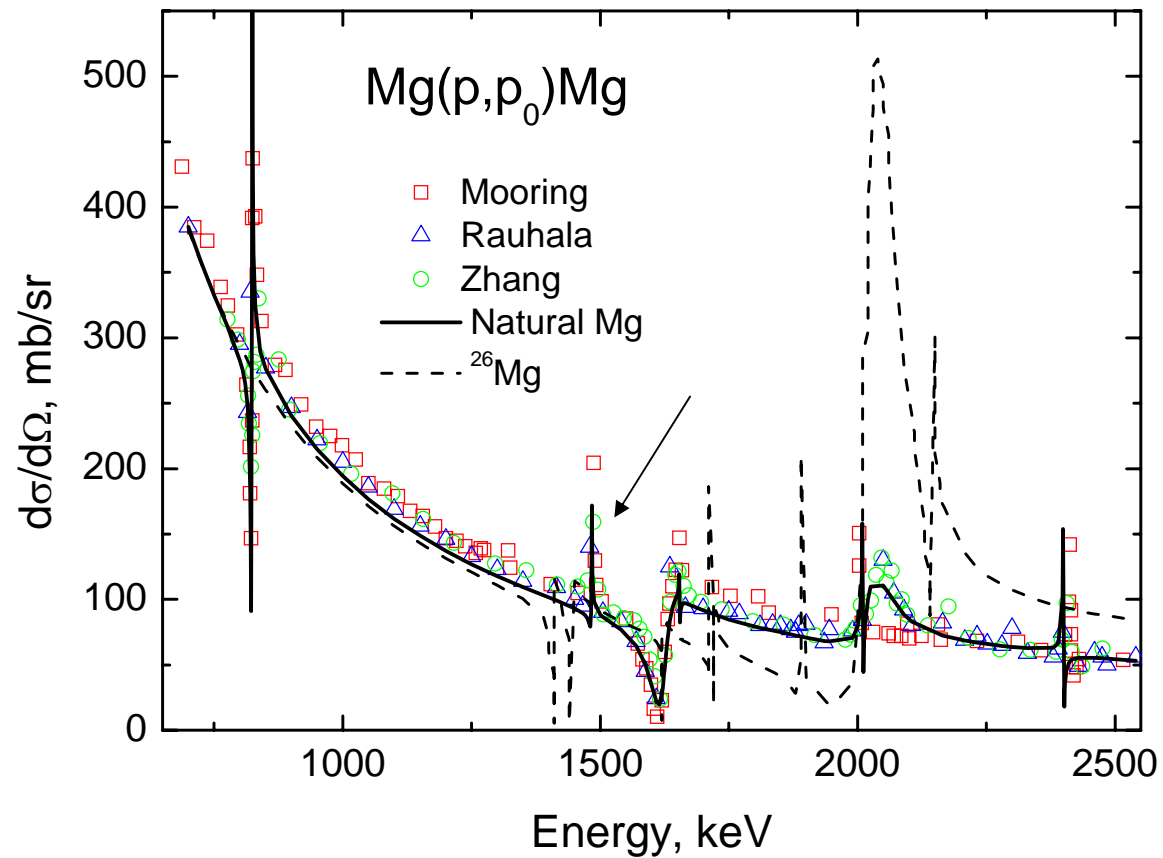
# Benchmark experiment



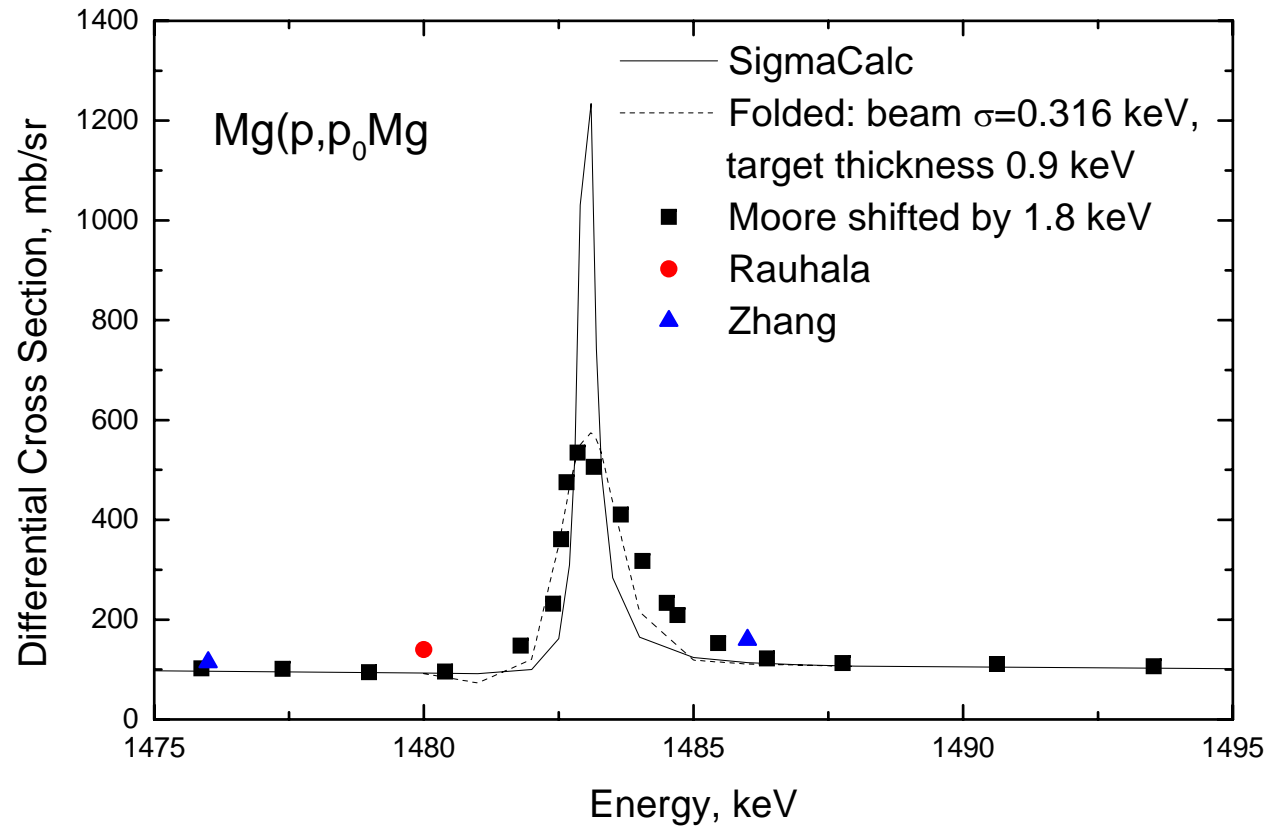
# The benchmark demonstrating the significance of the cross section fine structure



# Mg(p,p<sub>0</sub>)Mg cross-section

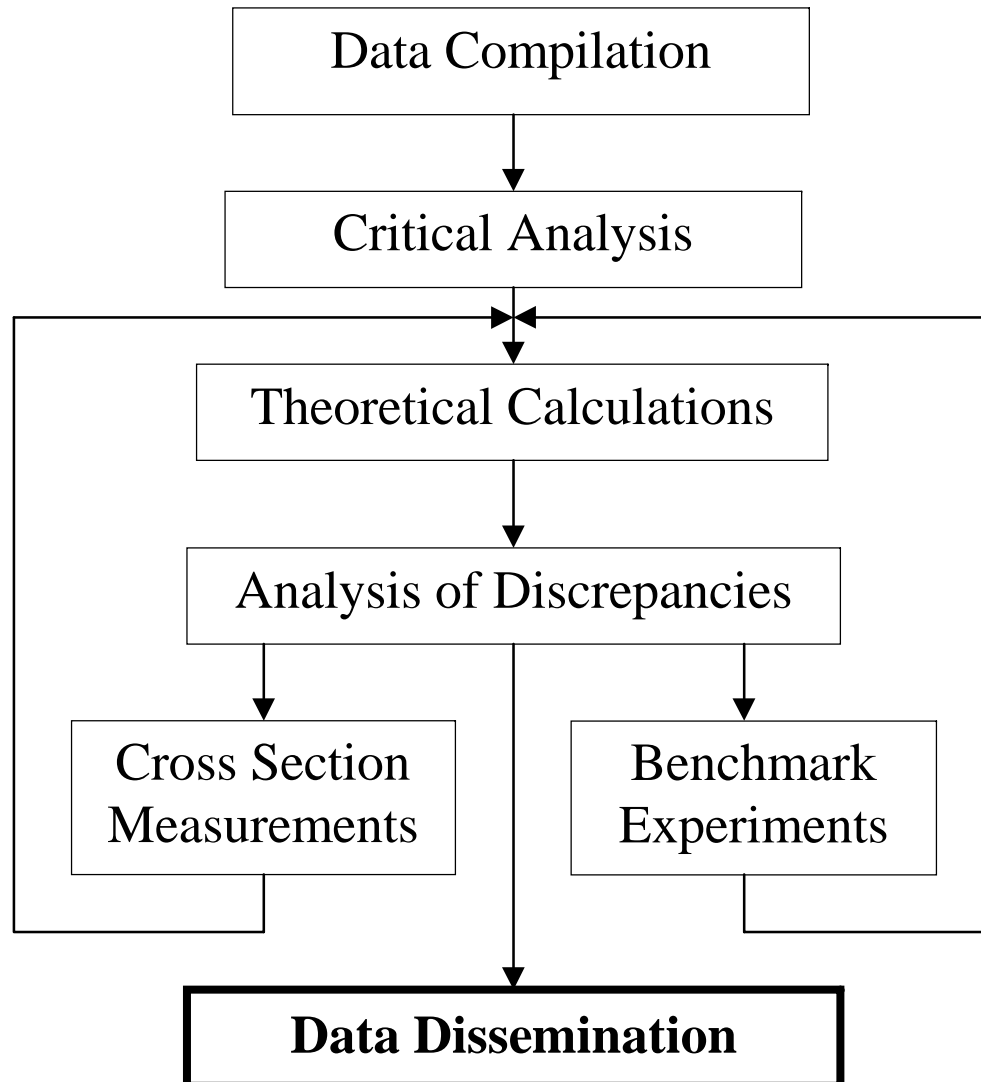


# Narrow resonance problem

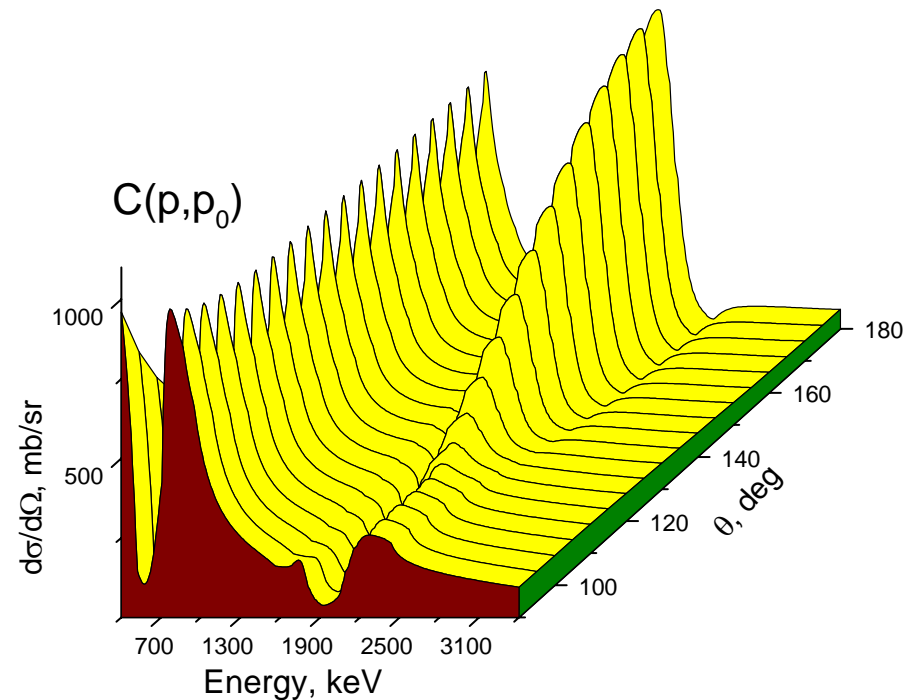
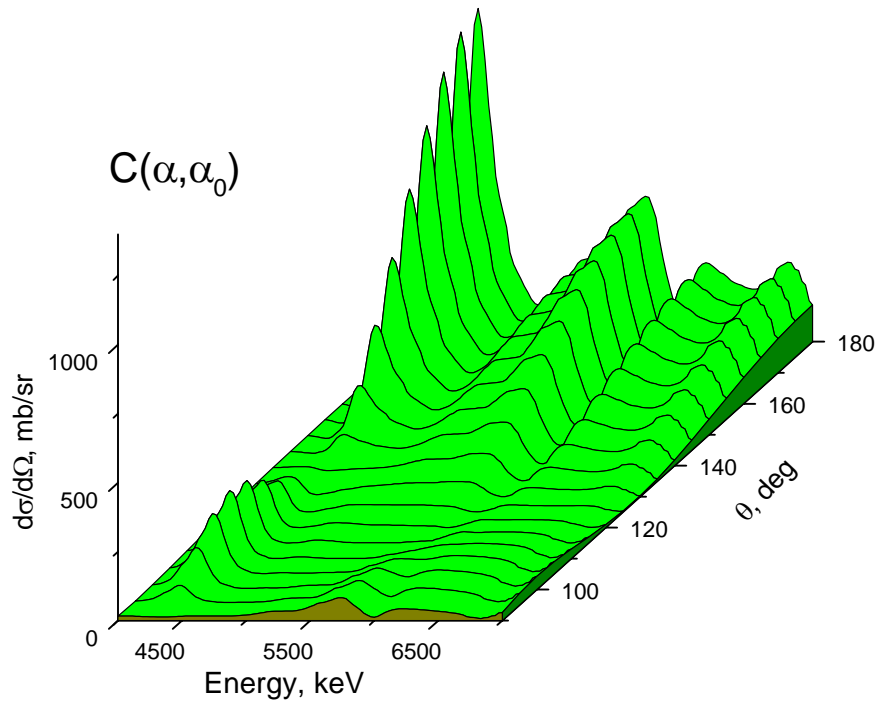




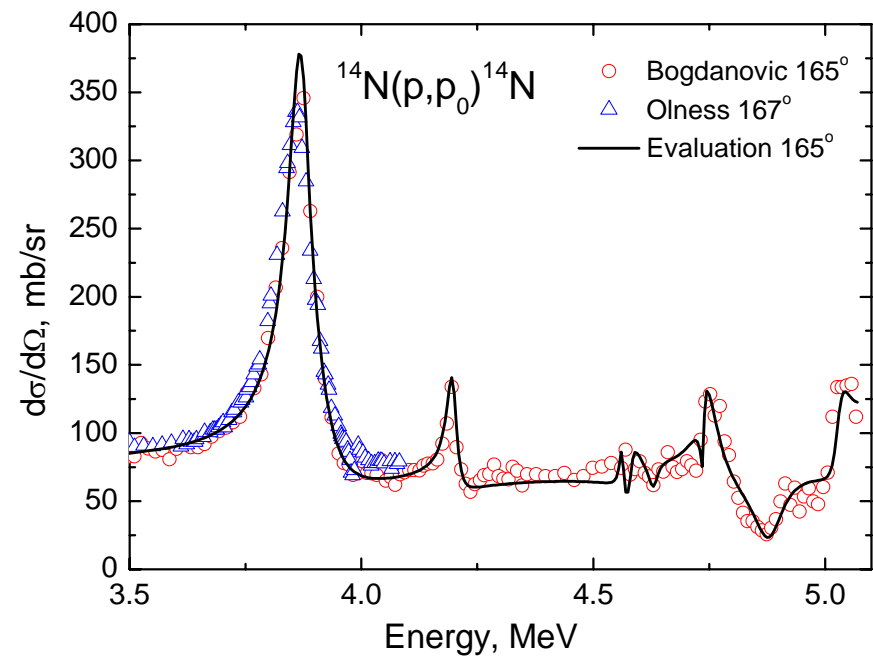
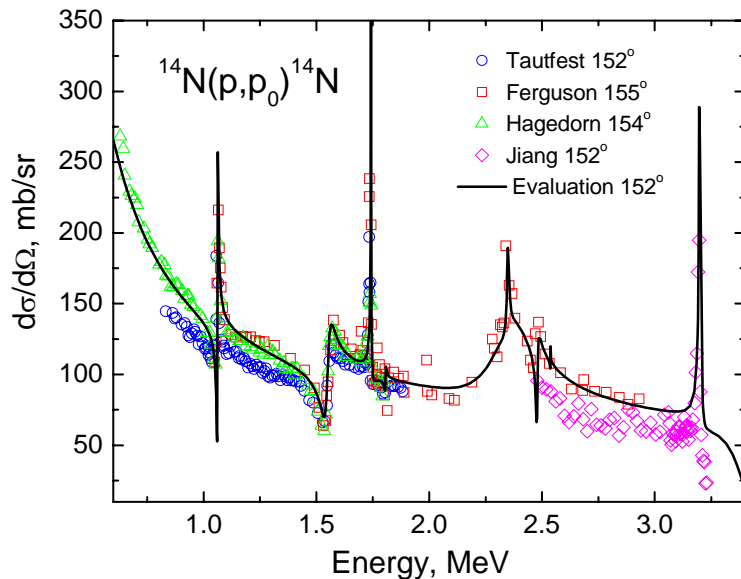
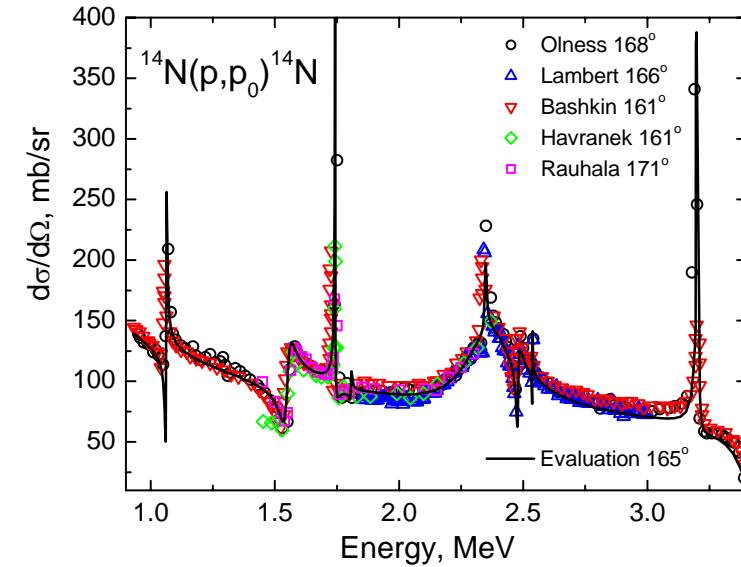
# Evaluation Scheme



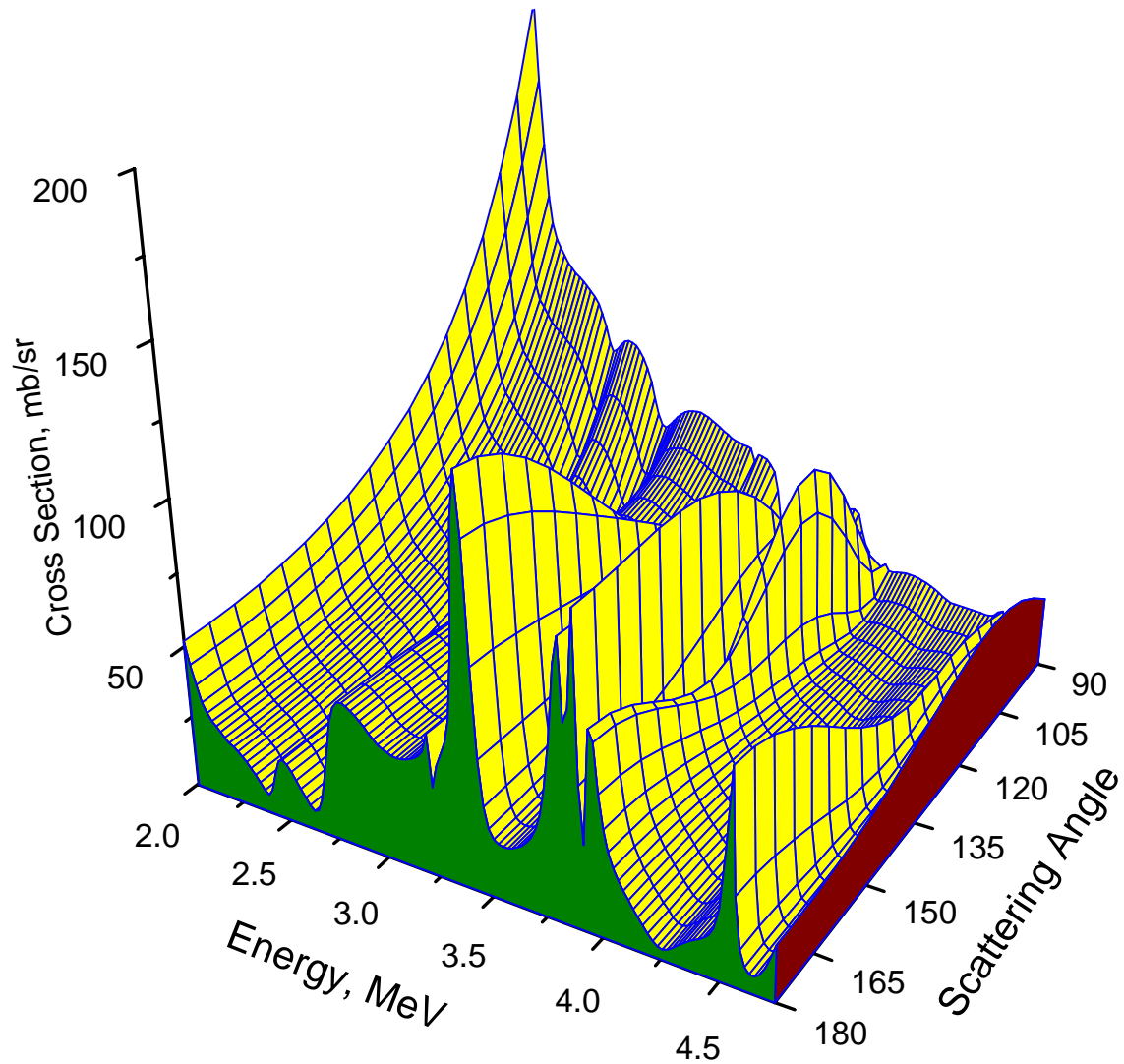
**When cross section has been evaluated it can be calculated for any scattering angle**



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



# Evaluated cross-section $^{14}\text{N}(\alpha, \alpha_0)^{14}\text{N}$





# SigmaCalc

This service provides evaluated (recommended) differential cross sections for Ion Beam Analysis

Format
☐ R33
**Energy**
☒ keV

☐ MeV
**Cross section**
☒ RTR

☐ mb/sr(lab)

☐ mb/sr(c.m.)

☐ b/sr(lab)

☐ b/sr(c.m.)
**Delimiter**
☒ Tab

☐ Space

☐ Comma

☐ Colon

☐ Semicolon
Element
 N-14  
 H-1  
 He-4  
 C-12  
 N-14  
 O-16  
 F-19  
 Ne-20  
 Na-23  
 Mg-24  
 Mg-nat  
 Al-27  
 Si-28  
 Si-nat  
 P-31  
 S-nat  
 Ar-40
Reaction
☐ (p,p)

☐ (α,α)

☐ (α,p)

☐ (d,d)

☐ (d,p<sub>0</sub>)

☐ (d,p<sub>1</sub>)

☐ (d,α<sub>0</sub>)

☐ (d,α<sub>1</sub>)

Calculate

Scattering Angle

155

About

## ►General

## ►Evaluation

## ►Cross sections

<sup>1</sup>H(<sup>4</sup>He,p)

<sup>4</sup>He(p,p)

<sup>12</sup>C(p,p)

<sup>12</sup>C(<sup>4</sup>He,<sup>4</sup>He)

<sup>12</sup>C(d,d)

<sup>14</sup>N(p,p)

<sup>14</sup>N(<sup>4</sup>He,<sup>4</sup>He)

<sup>16</sup>O(p,p)

<sup>16</sup>O(<sup>4</sup>He,<sup>4</sup>He)

<sup>16</sup>O(d,d)

<sup>19</sup>F(p,p)

natMg(p,p)

<sup>23</sup>Na(p,p)

<sup>27</sup>Al(p,p)

natSi(p,p)

natS(p,p)

<sup>40</sup>Ar(p,p)

<sup>40</sup>Ca(p,p)

<sup>48</sup>Ti(p,p)

Nucleus  
N-14

Projectile

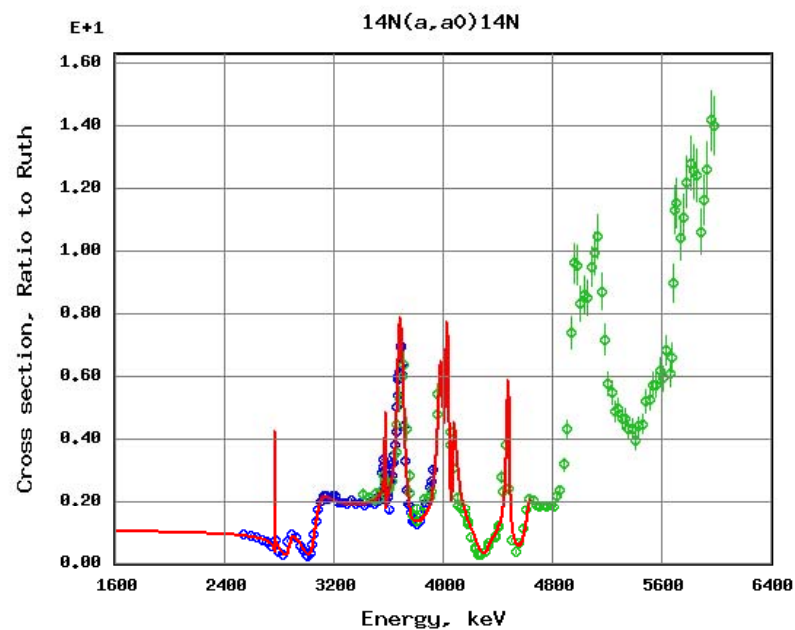
- ☐ p  
☐ d  
☐  $^3\text{He}$   
☒  $\alpha$   
☐  $^6\text{Li}$   
☐  $^7\text{Li}$

Type of data

- ☐ EBS  
☐ NRA  
☐ PIGE  
☒ All

IBANDL

EXFOR

[Home](#)[SigmaCalc](#)[CD version](#)[Upload your data](#)[Updates](#)[Feedback](#)[Nuclear Data Services](#)

Theta=165.0

Theta=165.00

Theta=165.00

SigmaCalc 1.6. File created 17-5-2010

I. Bogdanovic Radovic et al., unpublished

G. Terwagne, G. Genard, M. Yedji and G.G. Ross, J. Appl. Phys.  
104, 084909, 2008

Original

# CONCLUSIONS

- The evaluation of the cross-sections provides the most reliable data.
- Though theory is unable to provide the cross section *a priori* prediction, a particular cross section can be reliably represented by adjusting model parameters.
- There are still many problems in calculations of charged particle cross-sections in the framework of existing theories.



## **Joint ICTP-IAEA Workshop on Nuclear Data for Analytical Applications**

**21-25 October 2013**

*Miramare - Trieste, Italy*

The Abdus Salam International Centre for Theoretical Physics (ICTP), in collaboration with the International Atomic Energy Agency (IAEA) is organizing a workshop on **Nuclear Data for Analytical Applications**, which will be held at ICTP, Trieste, Italy, from 21 to 25 October 2013.

The workshop will continue the series of "Nuclear Data for Science and Technology" workshops initiated in 1999, and held at regular intervals since then. Since the late 20<sup>th</sup> century many new non-energy applications of nuclear techniques have been developed, accompanied by a growing need for new and improved nuclear data. New applications include: nuclear medicine, astrophysics, transmutation, materials analysis, thin layer activation techniques, accelerator-driven technologies, and measurements of nuclear quantities for basic science, all of which frequently require the use and understanding of charged-particle data.

Ion Beam Analysis (IBA) is a powerful analytical technique that makes substantial use of nuclear data for a wide range of applications in materials science, art, archaeology, geology, surface and interface engineering as well as environmental studies. IBA exploits the interactions of rapid charged particles (from ~0.1 to a few MeV) with matter to determine the composition and structure of the surface regions of solids. Considerable effort has been devoted by the IAEA to improve the nuclear data required for this technique, resulting in the creation of the IBANDL database. The efficient application of these IBA techniques requires appropriately trained and dedicated physicists.

### **Topics to be covered:**

- nuclear data and on-line retrieval systems
- fundamentals of energetic particle interaction with matter, atoms and nuclei
- overview of IBA techniques (RBS, ERDA, EBS, NRA, PIGE)
- nuclear data for IBA – IBANDL data library
- nuclear data for Particle Induced Gamma ray Emission (PIGE)
- applications of IBA and PIGE in particular

### **PARTICIPATION**

Scientists and students from all countries which are members of the United Nations, UNESCO or IAEA may attend the School. As it will be conducted in English, participants should have an adequate working knowledge of that language. Although the main purpose of the Centre is to help research workers from developing countries, through a programme of training activities within a framework of international cooperation, a limited number of students and post-doctoral scientists from developed countries are also welcome to attend. As a rule, travel and subsistence expenses of the participants should be borne by the home institution. Every effort should be made by candidates to secure support for their fare (or at least half-fare). However, limited funds are available for some participants who are nationals of, and working in, a developing country. Such support is available only for those who attend the entire activity. **There is no registration fee.**

**IN COLLABORATION WITH**



### **DIRECTORS**

**A. GURBICH**  
*(IPPE, Russia)*

**P. DIMITRIOU**  
*(IAEA, Austria)*

### **LOCAL ORGANISOR**

**C. TUNIZ**  
*(ICTP, Italy)*