

# Atomic and Molecular Data in Argentina

Raul Barrachina

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**COMISIÓN NACIONAL DE ENERGÍA ATÓMICA**  
ARGENTINA





## MILESTONES



CNEA Creation.

1950

Firts 50 Kg Sodium  
Diuranate.

1952

Physics Institute  
in Bariloche is  
created.

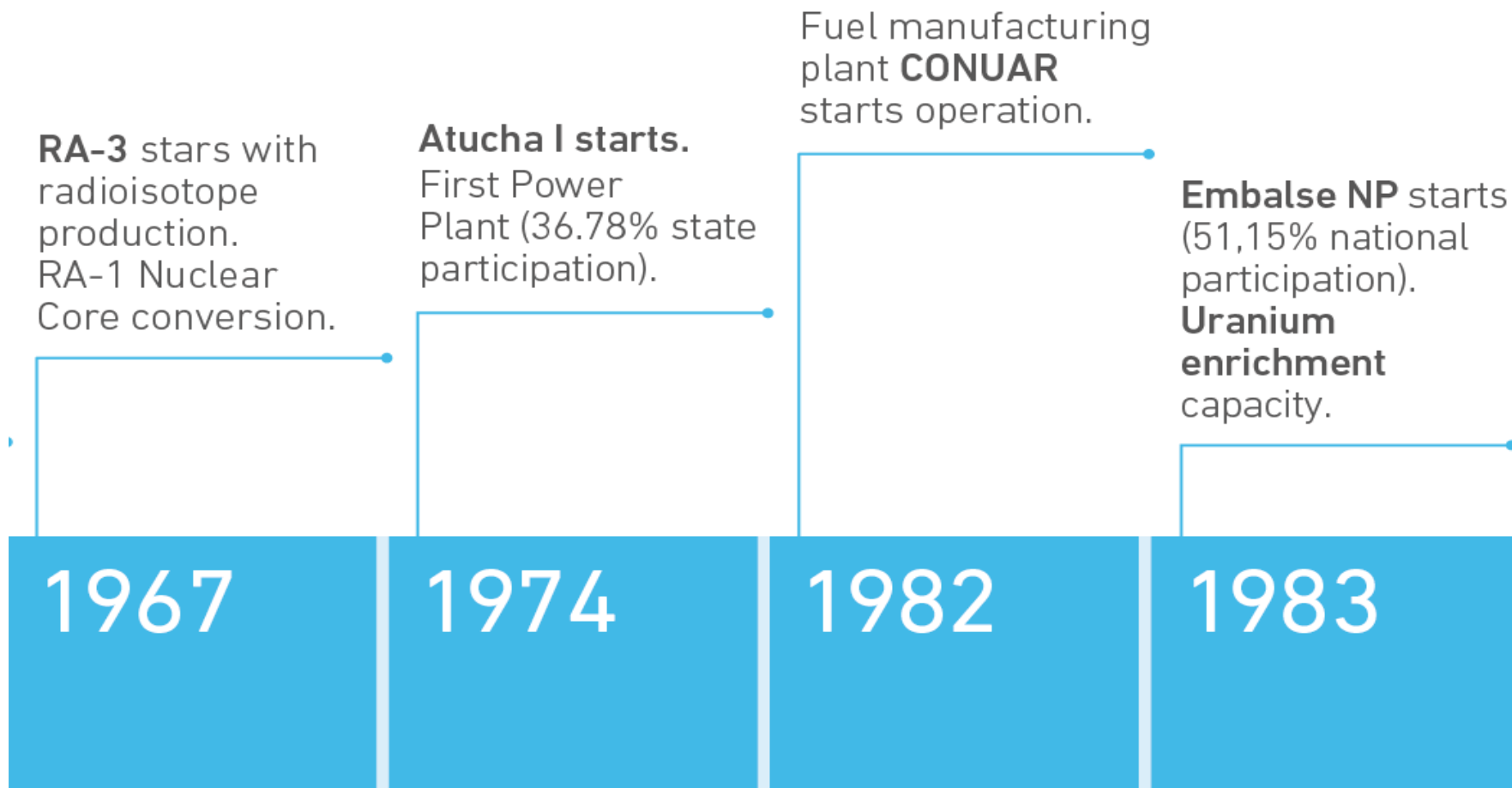
1955

CNEA starts **RA-1**,  
first research  
reactor.

1958

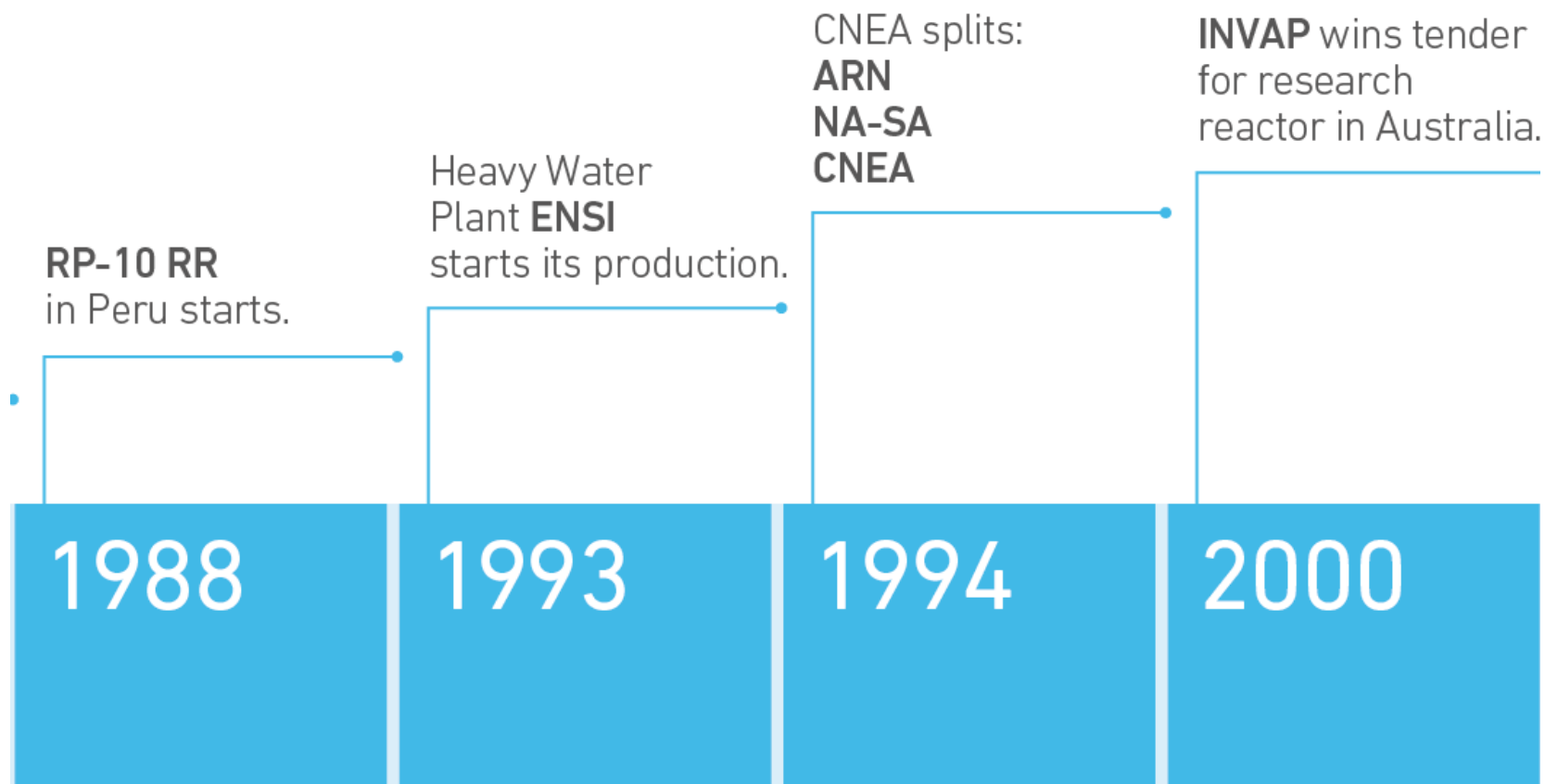


## MILESTONES





## MILESTONES

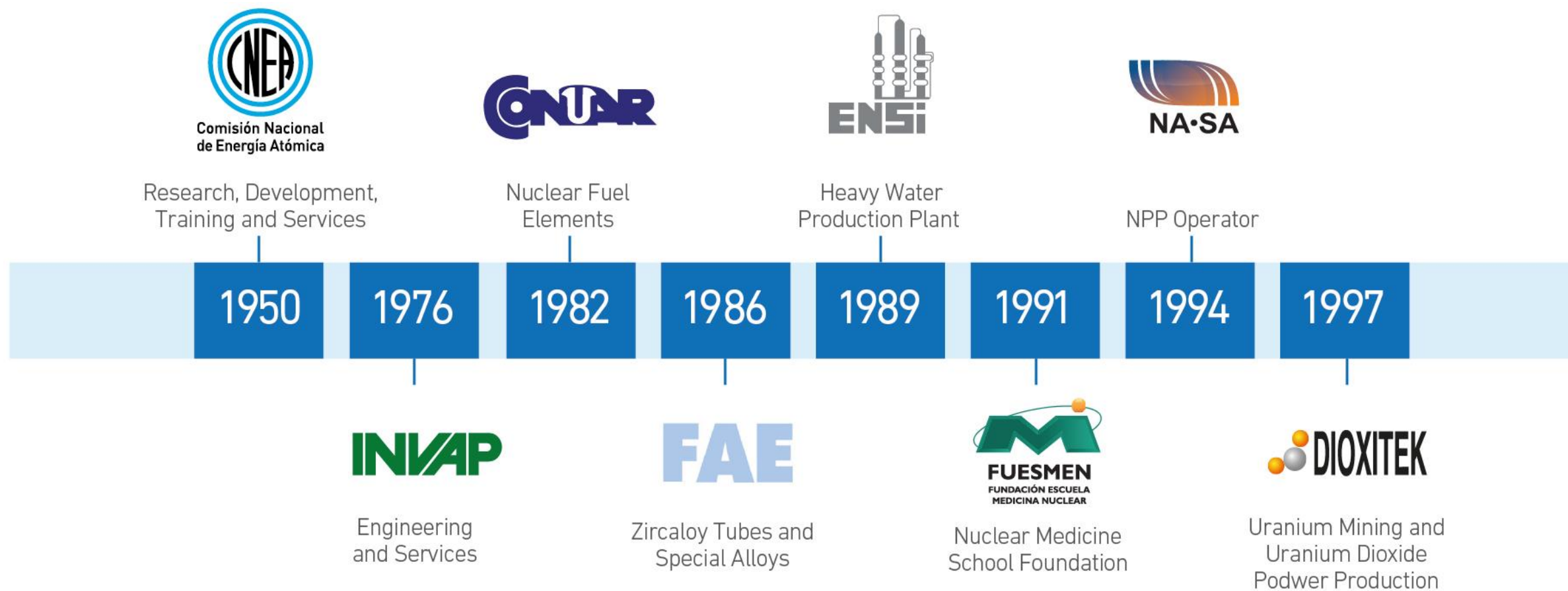








## START-UPS AND SPIN-OFFS





## NUCLEAR REACTORS AND OTHER FACILITIES

NPPs						CNA I 357 Mwe		CNE 648 Mwe					CNA2 692 Mwe	CAREM 25 Mwe			
Research Reactors	RA1 40 Kw	RA0 1 Mw	RA2	RA3 10 Mw	RA4 1 Mw			RA 6 1 Mw			RA 8 10-100 W						
ARGENTINA	1957	1965	1966	1968	1972	1974		1982	1984		1997		2014	2017			
ABROAD							1978			1988	1989	1995		1998	2006	2013	
Research Reactors									PERU RP10 10 Mw	ALGERIA NUR 1 Mw			EGYPT ETRR 22 Mw	AUSTRALIA OPAL 20 Mw			
Fuel Elements Manufacturing Plant										ALGERIA FEMP			EGYPT FEMP				
Radioisotopes Production Plant											CUBA RPP			AUSTRALIA RPP	EGYPT RPP		





# COMISIÓN NACIONAL DE ENERGÍA ATÓMICA

## ARGENTINA



 **3** ATOMIC CENTERS

 **6** RESEARCH REACTORS

 **2** NPPS UNDER CONSTRUCTION

 **4** REGIONALS: CUYO, NORTHWEST, PATAGONIA AND CENTRAL

 **2** OPERATING NPPS

 **1** TECHNOLOGY CENTER

 **4** NUCLEAR MEDICINE CENTERS

 **4** RADIATION PLANTS FOR INDUSTRIAL USE

 **1** HEAVY WATER INDUSTRIAL PLANT

 **5** RESEARCH PARTICLE ACCELERATOR

 **1** INDUSTRIAL MINING COMPLEX

 **1** URANIUM PURIFICATION PLANT

 **1** URANIUM ENRICHMENT PLANT

 **9** MINING SITES

 **5** PARTICLE ACCELERATOR FOR RADIOISOTOPES PRODUCTION

 **4** ENVIRONMENTAL RESTITUTION AREAS

 **3** EDUCATIONAL INSTITUTIONS

 **339** INDUSTRIAL FACILITIES

 **1** NUCLEAR FUEL FABRICATION FACILITIES

 **2** NUCLEAR MEDICINE CENTERS UNDER CONSTRUCTION

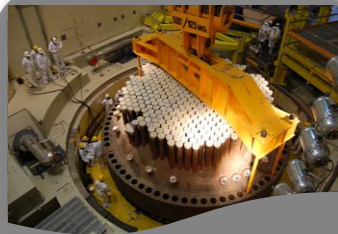


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ARGENTINA



**CAREM  
Reactor**



**life extension  
CNE**



**4<sup>th</sup> and 5<sup>th</sup>  
NPP**



**Heavy Water  
Plant**



**Uranium  
Enrichment**



**RA – 10 RR**



**Nuclear  
Medicine**



**Radioisotopes**



**Uranium  
dioxide**



**Uranium  
mining**



# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA







# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA

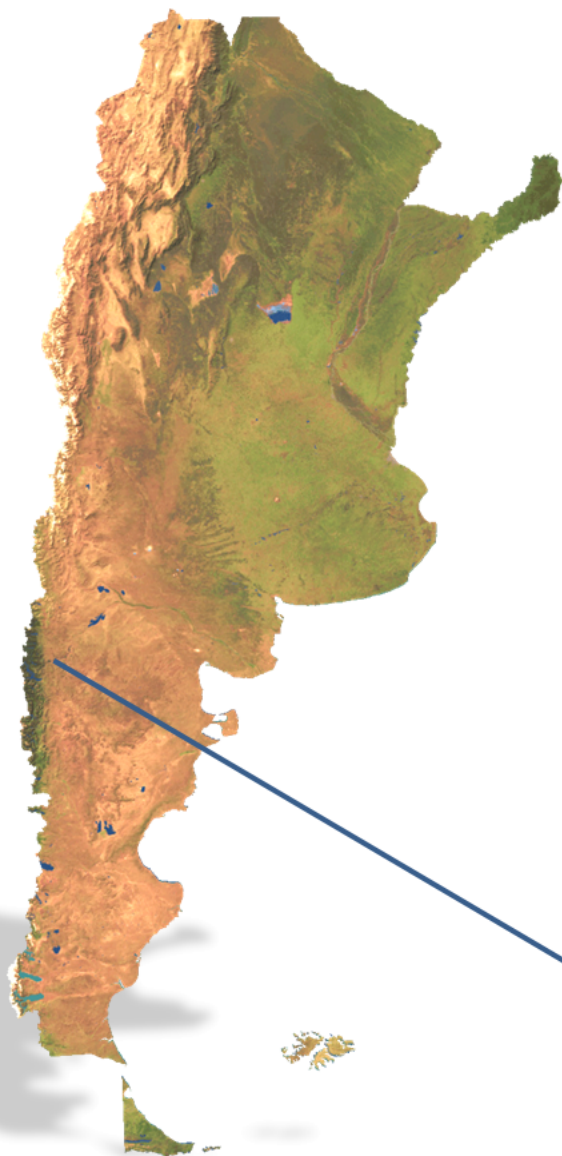






# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA



BARILOCHE  
ATOMIC CENTRE



# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA



- 1.7 MeV Tandem, 300 keV and 100 keV accelerators
- TOF-ISS and XPS, UPS, AES, SIMS spectroscopy
- STM and AFM microscopes
- COLTRIMS

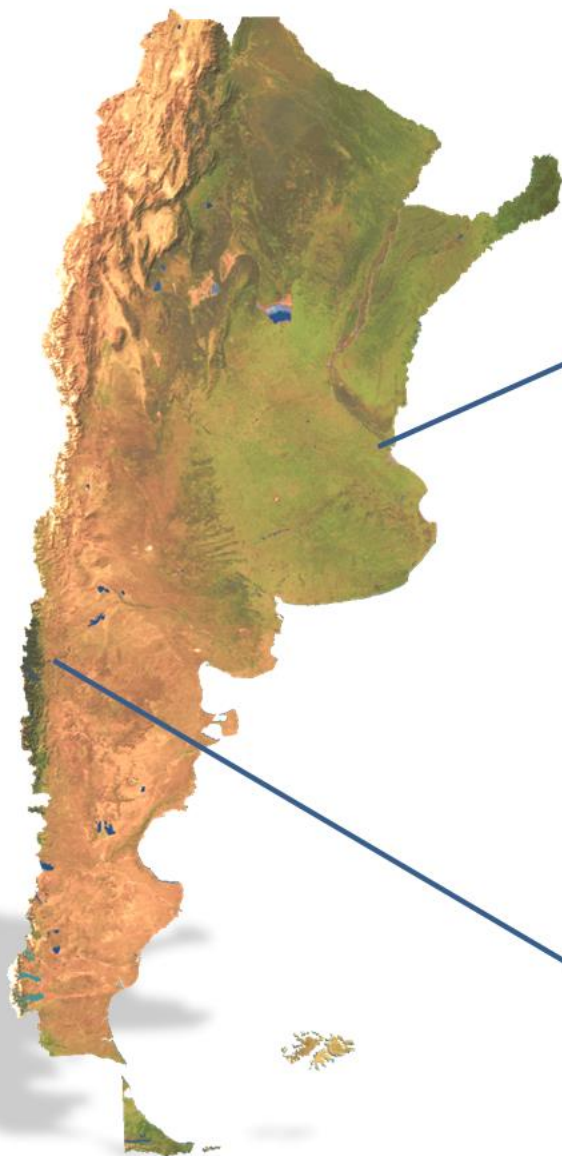


BARILOCHE  
ATOMIC CENTRE



# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA



CONICET



IAFE Buenos Aires



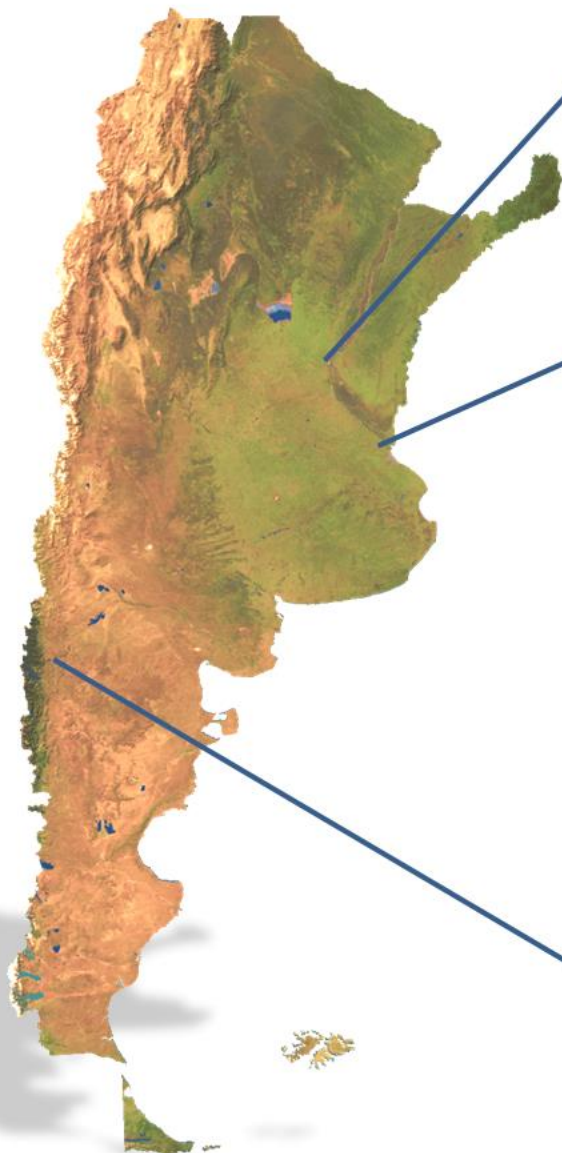
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CONICET



IFIR Rosario



CONICET



IAFE Buenos Aires



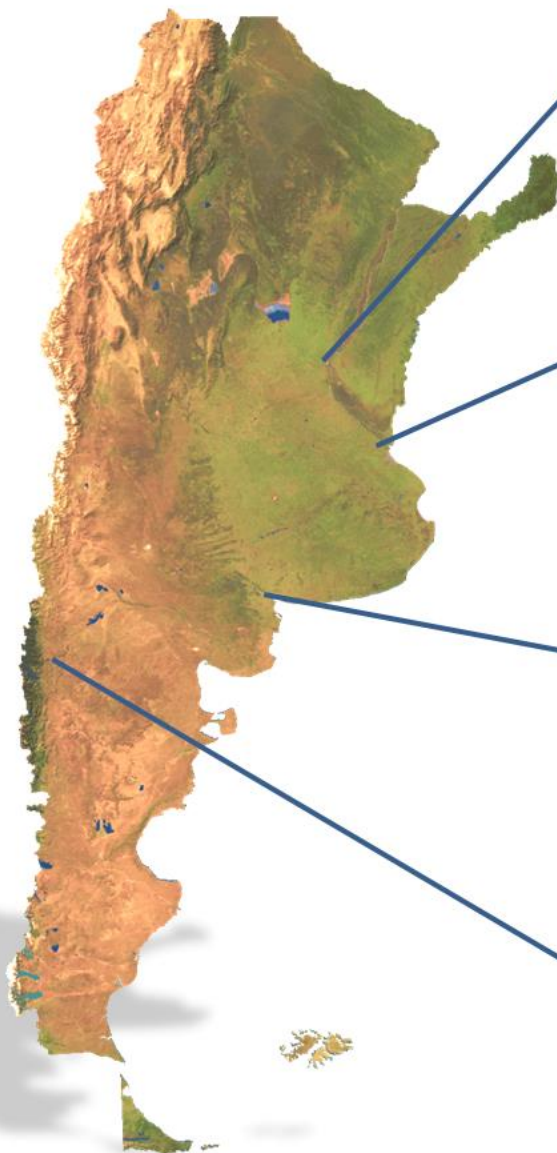
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IFISUR Bahía Blanca



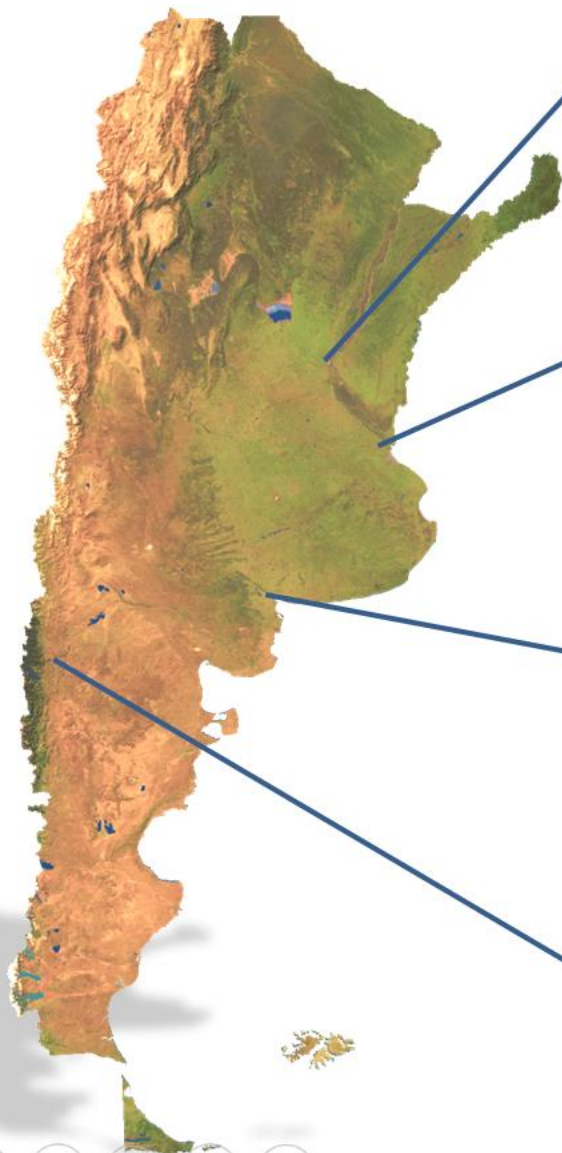
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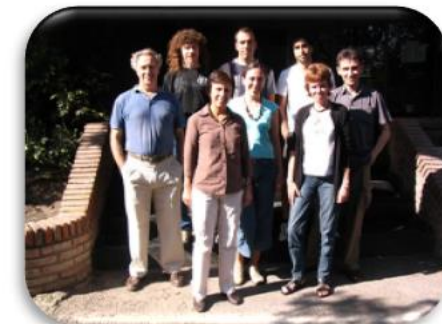
Roberto Rivarola



CONICET



IAFE Buenos Aires



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IFISUR Bahía Blanca



Carlos Roberto Garibotti

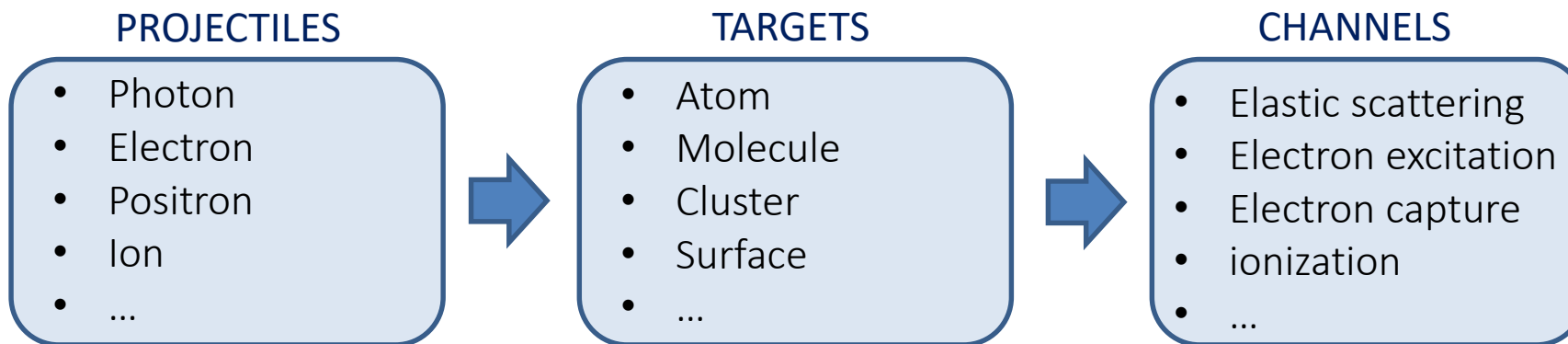


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# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

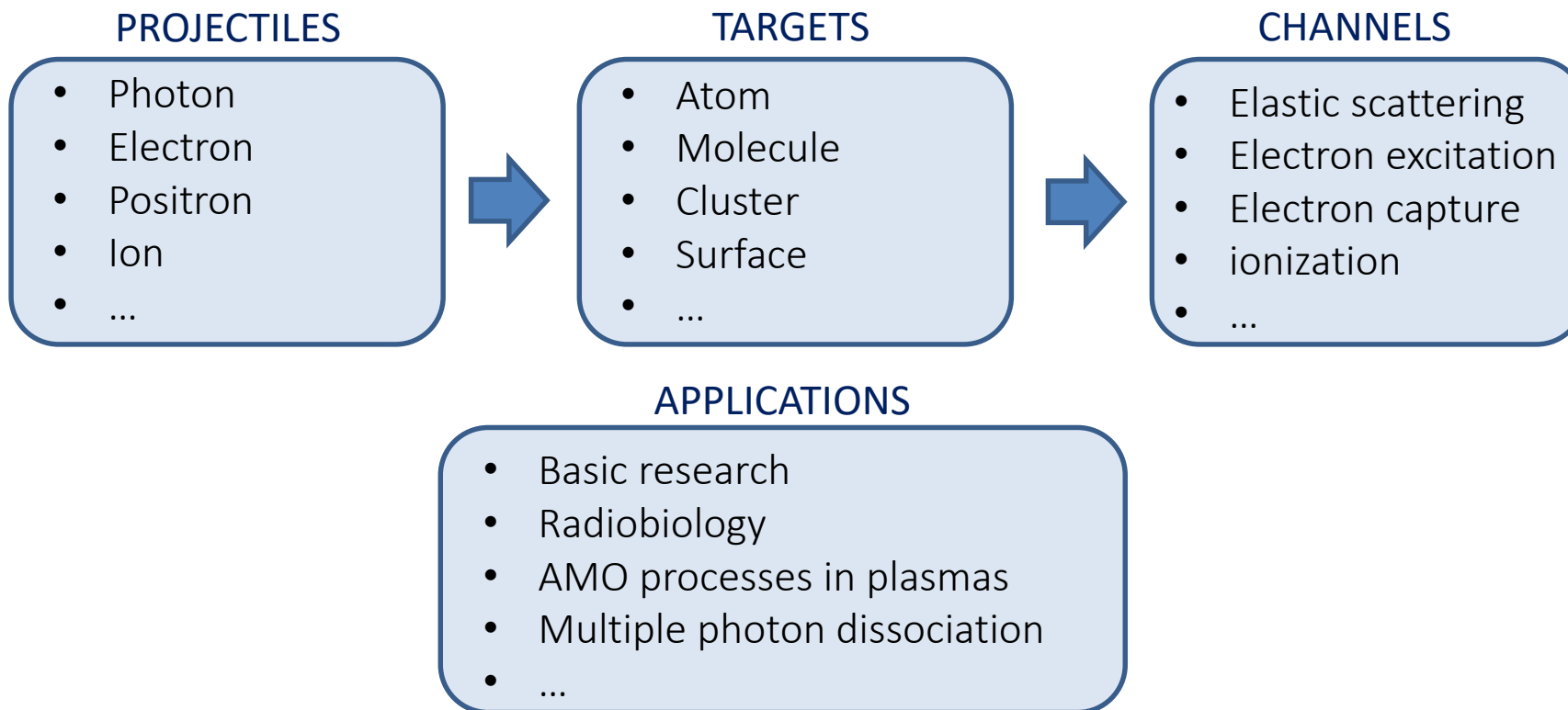
## ARGENTINA





# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA







# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA

### PROJECTILES

- Photon
- Electron
- Positron
- Ion
- ...



### TARGETS

- Atom
- Molecule
- Cluster
- Surface
- ...

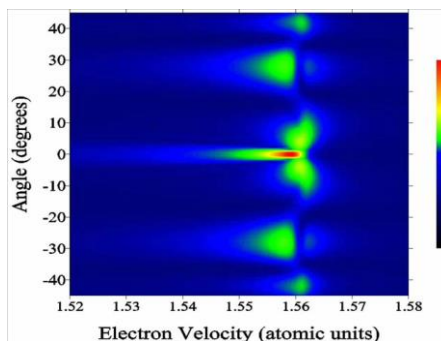


### CHANNELS

- Elastic scattering
- Electron excitation
- Electron capture
- ionization
- ...

### APPLICATIONS

- Basic research
- Radiobiology
- AMO processes in plasmas
- Multiple photon dissociation
- ...



### THEORETICAL TECHNIQUES

- Continuum Distorted Wave
- Classical Trajectory Montecarlo
- Generalized Sturmian Functions
- Time-Dependent Close-Coupling
- ...



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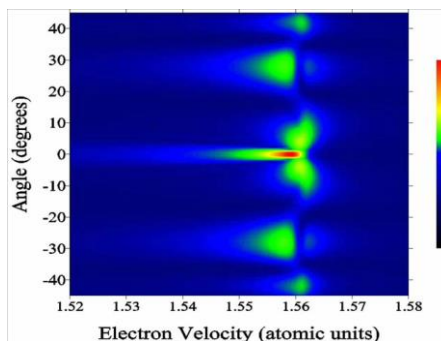
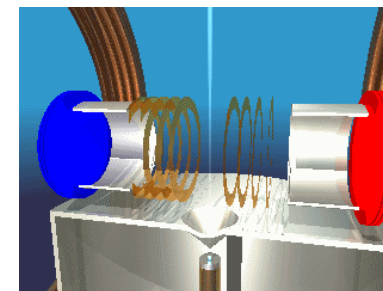


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- Continuum Distorted Wave
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- Generalized Sturmian Functions
- Time-Dependent Close-Coupling
- ...

### EXPERIMENTAL TECHNIQUES

- Electron spectroscopy
- COLTRIMS
- PIXE, RBS, ERDA
- XPS, UPS, AES, SIMS
- STM, AFM



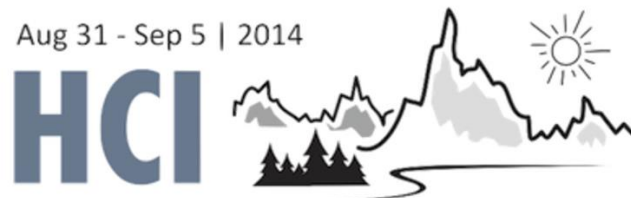
# ATOMIC, MOLECULAR AND OPTICAL PHYSICS ARGENTINA



XXIV International Conference on  
Photonic, Electronic and Atomic Collisions

Rosario, Argentina, July 20 - 26, 2005

Aug 31 - Sep 5 | 2014



San Carlos de Bariloche





ATOMIC, MOLECULAR AND OPTICAL PHYSICS  
ARGENTINA



# Dinamo

**D**ATOS Y CÓDIGOS **I**NFORMÁTICOS **N**UCLEARES, **A**TÓMICOS,  
**M**OLECULARES Y **Ó**PTICOS





ATOMIC, MOLECULAR AND OPTICAL PHYSICS  
ARGENTINA



# Dinamo

**D**ATOS Y CÓDIGOS **I**NFORMÁTICOS **N**UCLEARES, **A**TÓMICOS,  
**M**OLECULARES Y **Ó**PTICOS

- It is responsible for providing fundamental NAMO data for CNEA's nuclear and non-nuclear science and technological projects.
- It coordinates the generation, collection and critical assessment of the required data by NAMO groups in Argentina.

# Data Bank

An international reference centre for computer codes, nuclear and thermochemical data

## Computer Program Services



The Data Bank **collects, tests and distributes computer programs**. It also preserves and distributes integral experiment data, databases, processed libraries, benchmark and NEA safety joint projects. Over 2 000 documented packages are available.

[More »](#)



## Nuclear Data Services

The Data Bank is an international reference centre for **nuclear data compilation and dissemination**, with strong activities in the development of specialised tools for visualising and analysing differential, experimental, evaluated and integral data.

[More »](#)

## Thermochemical database



The Thermochemical Database (TDB) Project develops a **comprehensive chemical thermodynamic database** of selected chemical elements for safety assessments of radioactive waste disposal systems.

[More »](#)



## Training courses

The Data Bank **organises training courses and workshops** on the widely used computer programs for particle transport and interactions, nuclear data processing and thermodynamic data collection and assessment.

[More »](#)

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# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA



## Stopping Power of Matter for Ions

### Graphs, Data, Comments and Programs

Last update: 20 July, 2017 ([see Updates](#))



This site was created in 1990 by **Prof. Helmut Paul** (1929-2015), from the University of Linz. For 25 years he collected the published stopping power data, including the first measurements performed in the 30s. He made his exhaustive collection of **stopping power data, graphs, and programs** available to the entire scientific community through this online database. Since then, this database has been extensively employed in theoretical and experimental research and in applied sciences. For details on Helmut Paul's work on stopping power see the following **publications**.

This collection considers **all ions and targets**: solids (amorphous or polycrystalline), gases, elements and compounds, including new materials such as polymers, oxides and silicates. It treats the **"electronic"** stopping power assuming that "nuclear" stopping has been subtracted.

Detailed information on the content and organization of the database is provided in the **Introduction** page available also on the left-hand menu bar. Graphs and data files for **Hydrogen Ions**, **Helium Ions**, and **Heavier Ions** can also be found by following the links on the left-hand menu bar.

In 2015, the collection was taken over by the **Nuclear Data Section** of the **International Atomic Energy Agency**. Since December 2015, **Dr Claudia Montanari**, from the Instituto de Astronomía y Física del Espacio, CONICET and Universidad de Buenos Aires, Argentina, is collaborating with the IAEA on the updating and development of the database.

Sadly, Helmut passed away on 21 December 2015. He will be dearly missed, but he will always be remembered through his legacy: the stopping power database. A personal account of life as a physicist by Helmut Paul can be found [here](#).

**Please send your questions, comments and suggestions regarding...**

...methods, graphs and data to:

Dr Claudia Montanari / Instituto de Astronomía y Física del Espacio  
Email: [mclaudia@iafe.uba.ar](mailto:mclaudia@iafe.uba.ar)

...this site to:

International Atomic Energy Agency / Nuclear Data Section  
Email: [nds.contact-point@iaea.org](mailto:nds.contact-point@iaea.org)





## The IAEA stopping power database, following the trends in stopping power of ions in matter

C.C. Montanari<sup>a,\*</sup>, P. Dimitriou<sup>b</sup>

<sup>a</sup> Instituto de Astronomía y Física del Espacio, CONICET and Universidad de Buenos Aires, Buenos Aires, Argentina

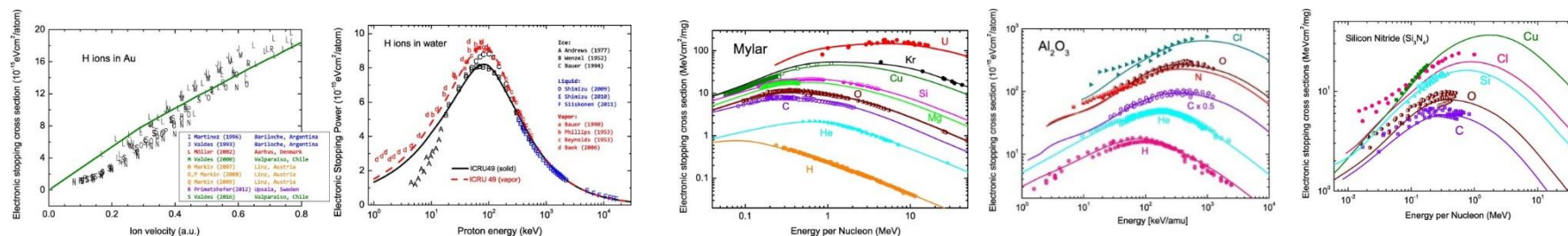
<sup>b</sup> Division of Physical and Chemical Sciences, International Atomic Energy Agency, Vienna, Austria



### ABSTRACT

The aim of this work is to present an overview of the state of art of the energy loss of ions in matter, based on the new developments in the stopping power database of the International Atomic Energy Agency (IAEA). This exhaustive collection of experimental data, graphs, programs and comparisons, is the legacy of Helmut Paul, who made it accessible to the global scientific community, and has been extensively employed in theoretical and experimental research during the last 25 years. The field of stopping power in matter is evolving, with new trends in materials of interest, including oxides, nitrides, polymers, and biological targets. Our goal is to identify areas of interest and emerging data needs to meet the requirements of a continuously developing user community.

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# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA

<https://www-amdis.iaea.org/HEAVY/>

### Heavy Particle collisions

This is your gateway to the calculation of cross sections for excitation, ionization and charge transfer in heavy particle collisions, using codes developed by A. Dubois, J.P. Hansen and P. Fainstein. [Click here](#) for a description of the method and references for the excitation and charge exchange code of Dubois and Hansen. [Click here](#) for a description of the method and references for the ionization code of Fainstein.

Use of the interface to run the code is restricted to registered users. If you wish to run the code, please contact us with your request, including your name, institution and brief reason for wishing to run the code. [Click here](#) to submit your request.

**WARNING - In order to successfully navigate you must use the radio buttons to go to and from different pages. Using your browser buttons may cause incorrect information to be passed to a new page.**

**PLEASE USE THE EXIT BUTTON TO END THE CALCULATIONS, SO THAT TEMPORARY FILES WILL BE DELETED.**

[Click here to proceed with the bound state transitions \(charge exchange and excitation\)](#)

[Click here to proceed with ionization cross sections](#)

[Click here to go to IAEA Atomic and Molecular Data Unit home page.](#)





# ATOMIC, MOLECULAR AND OPTICAL PHYSICS ARGENTINA



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## Main Page

### Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data For Fusion

#### knowledge base

- [Main Page](#)
- [Data Needs](#)
- [Data Sources](#)
- [Data Exchange](#)
- [Special Topics](#)
- [Fusion Research](#)

#### navigation

- [IAEA AMD WEB](#)
- [IAEA CRP](#)
- [Community Forum](#)
- [Current events](#)
- [Recent changes](#)
- [Random page](#)
- [Help](#)

#### search

#### toolbox

- [What links here](#)
- [Related changes](#)

## Code Centers Network

- [Curtin University, Australia](#) I. Bray
- [Kitasato University, Japan](#) F. Koike
- [Universidad Autonoma de Madrid, Spain](#) I. Rabadan
- [University P. & M. Curie, Paris, France](#) A. Dubois
- [University of Bari, Italy](#) M. Capitelli
- [Kurchatov Institute, Russian Federation](#) A. Kukushkin
- [Lebedev Institute, Russian Federation](#) L. Vainshtein
- [Forschungszentrum Juelich Germany](#) D. Reiter
- [National Institute for Standards and Technology, USA](#) Y. Ralchenko
- [Princeton Plasma Physics Laboratory, USA](#) D. Stotler
- [Los Alamos National Laboratory, USA](#) J. Abdallah Jr.
- [International Atomic Energy Agency](#) B. J. Braams
- [University of Toronto, Canada](#) D. Elder
- [Ernst-Moritz-Arndt University, Griefswald, Germany](#) R. Schneider
- [HULLAC](#) M. Klapisch
- [Comision Nacional de Energia Atomica, Argentina](#) P.D. Fainstein ←

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- 1 Introduction
- 2 Data Needs
  - 2.1 Magnetic Confinement Fusion
  - 2.2 Atomic Data
  - 2.3 Molecular Data
  - 2.4 Plasma-Material Interaction Data
- 3 Data Sources
  - 3.1 Researchers and research groups
  - 3.2 Online Databases
  - 3.3 Data Centers
  - 3.4 Code Centers Network
- 4 Data Exchange
  - 4.1 Data Exchange Forum
- 5 Special Topics
  - 5.1 IAEA Coordinated Research Projects (CRP)
  - 5.2 IAEA Workshops
  - 5.3 NLTE Kinetics Code Comparison Workshops
  - 5.4 Meetings on A+M+PMI/PSI Processes and Data
  - 5.5 ITPA (International Tokamak Physics Activity)
  - 5.6 European Fusion Development Agreement (EFDA)





## THEORETICAL TECHNIQUES

- CDW codes
  - Projectiles: light ion (nude and neutral), electrons, positrons
  - Targets: Atoms, Simple and Complex (biological) Molecules
  - Channels: single and multiple ionization, charge exchange, transfer ionization
- CTMC
- Generalized Sturmian Functions
- Time-Dependent Close-Coupling



# ATOMIC, MOLECULAR AND OPTICAL PHYSICS

## ARGENTINA

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### EXPERIMENTAL TECHNIQUES

- Projectiles: H/D/T , He, Li beams.
- Targets: Atoms, Molecules, Surfaces
- Energies:  $\approx 30$  keV – 3 MeV



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- Numerical and Bibliographic database
- Direct contact for any expertise





# AN EASY PIECE OF THEORY

**Q: IS IT VALID TO CALCULATE CROSS SECTIONS IN PLASMAS USING  
PURE COULOMB POTENTIALS?**



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PURE COULOMB POTENTIALS?**

**IOP** Publishing

Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. **49** (2016) 235702 (11pp)

[doi:10.1088/0953-4075/49/23/235702](https://doi.org/10.1088/0953-4075/49/23/235702)

## **Zero-energy resonance effects in atomic processes within a plasma environment**

**C F Clauser and R O Barrachina**

Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica and Universidad Nacional de Cuyo, Av. Bustillo 9500, 8400 Bariloche, Argentina



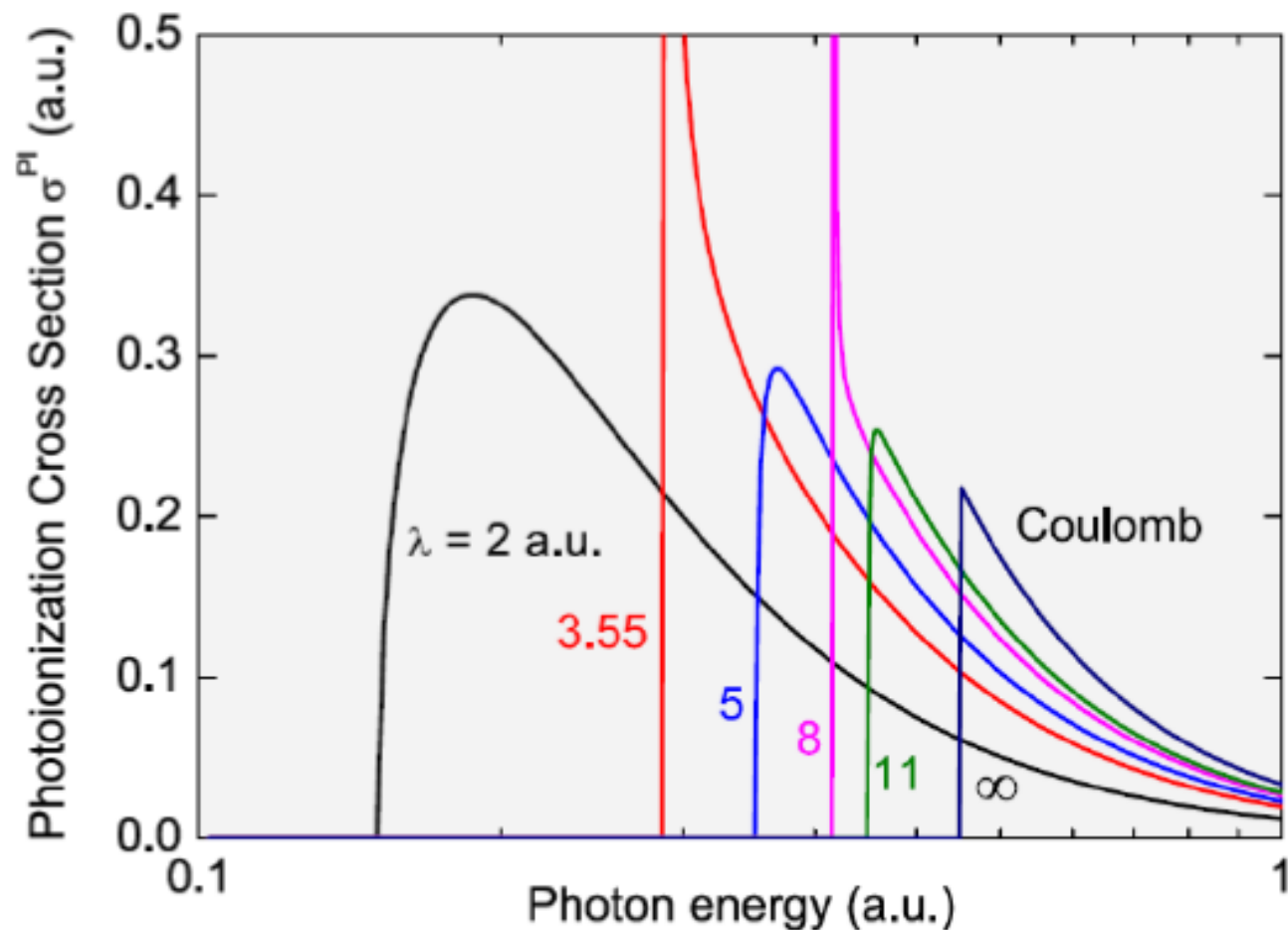
# AN EASY PIECE OF THEORY

Q: IS IT VALID TO CALCULATE CROSS SECTIONS IN PLASMAS USING PURE COULOMB POTENTIALS?

## Example: Photoionization

$$V_{\lambda}^Y(r) = \frac{Z}{r} e^{-r/\lambda}$$

$\lambda = 3.55, 8, \dots \Rightarrow$  Zero-energy resonance

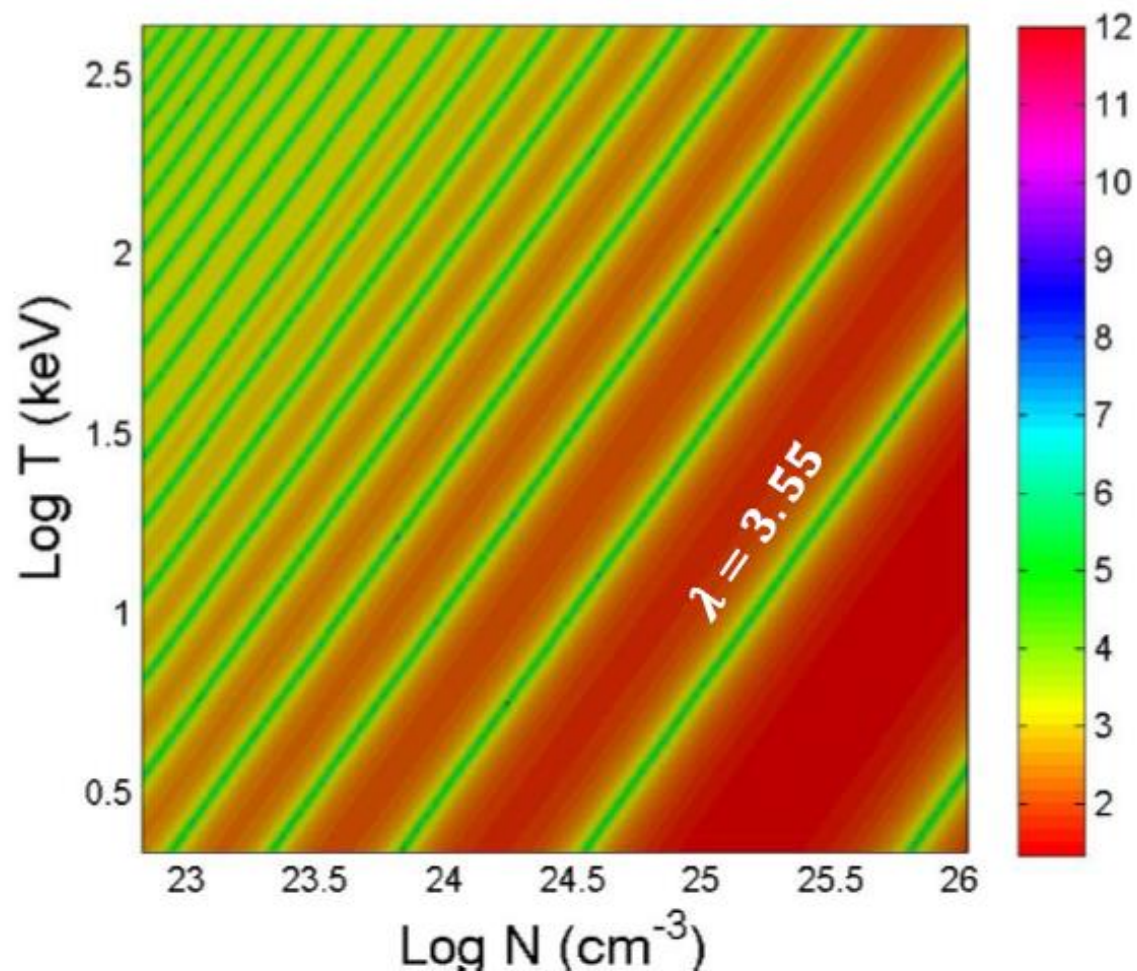






# AN EASY PIECE OF THEORY

Q: IS IT VALID TO CALCULATE CROSS SECTIONS IN PLASMAS USING PURE COULOMB POTENTIALS?



A: YES

In **dilute plasmas**, even a small variation of  $N$  and  $T$  might encompass many zero-energy resonant conditions. The averaged cross section mimics that of a pure Coulomb potential

A: NO

In **high density plasmas**, zero-resonances have to be taken into account. Using pure Coulomb potentials is not valid.



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Based on a 50-year experience on AMO physics, CNEA and its fellow institutes are willing to contribute with the international atomic and molecular data center network.



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**THANK YOU FOR  
YOUR ATTENTION**

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