



60 Years

IAEA

Atoms for Peace and Development

Consultants' Meeting on Developments in Data Exchange

Meeting Objectives

B. J. Braams and H.-K. Chung

International Atomic Energy Agency (IAEA) *60 Years* *Atoms for Peace and Development*



60 Years
Atoms for Peace and Development

[ABOUT US](#) ▾[OUR WORK](#)[NEWS CENTRE](#) ▾[PUBLICATIONS](#) ▾[SCIENTIFIC RESOURCES](#)[Home](#) / [Our Work](#)

Our Work

The IAEA works for the safe, secure and peaceful uses of nuclear science and technology. Its key roles contribute to international peace and security, and to the world's Millennium Goals for social, economic and environmental development.

Main Work Areas

Nuclear Technology & Applications



This work involves helping countries use nuclear and isotopic techniques to promote sustainable development objectives in agriculture, human health, water resource management, marine environment and industrial applications.

Nuclear Safety & Security



This work is being carried out mainly to provide a strong, sustainable and visible global nuclear safety and security framework, protecting people and the environment from the harmful effects of ionizing radiation.

Safeguards & Verification



This work is being carried out to fulfill the duties and responsibilities of the IAEA as the world's nuclear inspectorate, performing an indispensable role in global efforts to stop the spread of nuclear weapons.

Nuclear Data Section

Hot Topics » ENDF/B-VII.1 • TENDL-2014 • JENDL-4.0u2 • IBANDL **News** » Damage cross section database extended by SS-316 and Eurofer

NEW

GRUCON - ENDF Data Processing Package [page]

Prepro-2015 - ENDF/B Pre-Processing Codes [page]

IRDF - International Reactor Dosimetry and Fusion File v1.05 [page]

[Main](#) | [All](#) | [Reaction Data](#) | [Structure & Decay](#) | [by Applications](#) | [Doc & Codes](#) | [Index](#) | [Events](#) | [Links](#) | [News](#)



EXFOR

Experimental nuclear reaction data



LiveChart of Nuclides

Interactive Chart of Nuclides



CINDA

Nuclear reaction bibliography



ENDF

Evaluated nuclear reaction libraries



ENSDF

evaluated nuclear structure and decay data (+XUNDL) **



NSR

Nuclear Science References *

NuDat 2.6

selected evaluated nuclear structure data **

RIPL

reference parameters for nuclear model calculations

IBANDL

Ion Beam Analysis Nuclear Data Library

Charged particle reference cross section

Beam monitor reactions

PGAA

Prompt gamma rays from neutron capture

FENDL

Fusion Evaluated Nuclear Data Library

Photonuclear

cross sections and spectra up to 140MeV

IRDF

International Reactor Dosimetry and Fusion File

NAA

Neutron Activation Analysis Portal

Safeguards Data

recommendations, August 2008

Medical Portal

Data for Medical Applications

Standards

- Neutron cross-sections, 2006
- Decay data, 2005

*Database at the IAEA, Vienna

**Database at the US NNDC

IAEA Nuclear Data Section



IAEA-NDS
Mission, Staff
and more



A+M
Atomic
and
Molecular
Data



Meetings
Workshops



Newsletters



Coordinated
Research
Projects



Nuclear Reaction
Data Center
Network



Nuclear Structure
& Decay Data
Network



Technical Documents
INDC Reports
Publications



Computer
Codes

Atomic and Molecular Data Unit

News (2016-05-27): Three relevant professional (P-4) posts are advertised on the [IAEA Employment web pages](#) under Current Vacancies. [Vacancy Notice 2016/0336](#) is for a Unit Head, Atomic and Molecular Data Unit. The Unit Head leads a team of one other physicist and 2 computer professionals to implement the Agency's programme on data for atomic, molecular and plasma-material interaction processes in fusion devices and other plasma applications. [Vacancy Notice 2016/0266](#) is for a Nuclear Fusion Physicist, responsible for supporting international cooperation on fusion research activities and fostering the exchange of scientific results among partners. [Vacancy Notice 2016/0265](#) is for a Nuclear Physicist (Accelerators), who will support international cooperation on the development of accelerator-based techniques and applications thereof, foster exchange of scientific results and support Member States through advice on the role and utilization of accelerators. (Accelerator applications for plasma-material interaction studies, materials science, atomic and molecular physics and neutral beam heating of fusion plasma could all be within the purview of this position.)

News (2015-10-03): [Hyun Chung](#) is a recipient of the 2015 [John Dawson Award for Excellence in Plasma Physics Research](#) of the American Physical Society. The citation reads: "For creative and novel use of the hard x-ray free electron laser to isochorically create high density plasmas and accurately measure the ionization potential depression, and for new theory that addresses discrepancies with long standing models and provides stimulus for continued developments." [More information on the IAEA News Centre page.](#)

Atomic and Molecular Data Unit Activities

The [Atomic and Molecular Data Unit](#) operates within the [Nuclear Data Section](#) of the [International Atomic Energy Agency](#), Vienna, Austria. The primary objective of the Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other plasma science and technology applications.

Databases on Atomic and Molecular Data for Fusion.

Atom, Molecule
Plasma-Surface
Data

ALADDIN
Numerical
Database

AMBDAS
Bibliographic
Database

GENIE
Atomic Data
Search Engine

OPEN ADAS
Database
Search

Rovibronic
Energy levels
Triplet D₂

FC Factors &
A-values of
H₂ & Isotopes

Online Computing Capabilities

Code
Centres
Portal

LANL
Atomic
Physics

FLYCHK
Non-LTE
Kinetics

Heavy
Particles
Collisions

Averaged
e- Impact
Cross-section

Effective
e- Ionization
Rates

ATOM-AKM
e- Collision
Data

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

Our Unit achieves its objectives by coordinating the activities of the [International Atomic and Molecular Data Center Network \(DCN\)](#) and [Code Center Network \(CCN\)](#), initiation and conducting international [Coordinated Research Projects \(CRP\)](#), organization of various types of [Expert's Meetings](#), publication of [technical reports](#) on meetings and research activities and using other forms (research contracts, research agreements, consultancies) for stimulation of the generation, collection and critical assessment of the required atomic, molecular (A+M) and plasma-material interaction (PMI) data information.

The activity of Our Unit is supervised and biennially reviewed by the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC A+M Subcommittee).

Aladdin Numerical Database



ALADDIN

Numerical database maintained by
the IAEA Nuclear Data Section A+M Data Unit

Atomic and Molecular Data

Electron Collisions
Photon Collisions
Heavy Particle Collisions

Particle-Surface Interactions

Erosion, Sputtering, Sublimation
Reflection
Trapping, Penetration

Note

Data presented here are IAEA recommended at their time of compilation. Data are mostly compiled from the [IAEA APID series](#), published results of [Co-ordinated research projects \(CRP\)](#) and from consultancies inside the IAEA Atomic and Molecular Data Unit.

Aladdin Numerical Database

Electron collisions / Be

Reset page

Complete restart

Cross sections

select all data

Go to numerical data

Reset form

Units in Energy origin

eV

Projectile

Apply unit conversion

1	2	3	4	Reactants	Products	7	Comment	Authors	Year	Publication	Validity Limits in eV	
<input type="checkbox"/>	ION	B	DER	e, Be [G]		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	9.30000e+00	----- (E _p)
<input type="checkbox"/>	ION	B	DER	e, Be ⁺ [G]		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	1.82000e+01	----- (E _p)
<input type="checkbox"/>	ION	B	DER	e, Be ²⁺ [G]		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	1.53900e+02	----- (E _p)
<input type="checkbox"/>	ION	B	DER	e, Be ³⁺ [G]		BELI		M.A. Lennon et al.	1988	JPCRD, 17/3 (1988)	2.17700e+02	----- (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s3d 1D]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	1.26670e+00	3.91993e+02 (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s3d 3D]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	1.58235e+00	3.92309e+02 (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s3p 1P]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	1.78508e+00	3.92511e+02 (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s3p 3P]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	1.98237e+00	3.92709e+02 (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s3s 1S]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	2.52932e+00	3.93256e+02 (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s3s 3S]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	2.85994e+00	3.93586e+02 (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s2p 1P]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	3.80826e+00	3.94535e+02 (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s ² 1S]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	9.27371e+00	4.00000e+02 (E _p)
<input type="checkbox"/>	ION	A	THE	e, Be [2s2p 3P]	e, Be ⁺	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	6.51038e+00	3.97237e+02 (E _p)
<input type="checkbox"/>	EXC	A	THE	e, Be [2s3d 1D]	e, Be [2s4f 1F]	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	4.10079e-01	3.91993e+02 (E _p)
<input type="checkbox"/>	EXC	A	THE	e, Be [2s3d 1D]	e, Be [2s4f 3F]	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	4.10079e-01	3.91993e+02 (E _p)
<input type="checkbox"/>	EXC	A	THE	e, Be [2s3d 1D]	e, Be [2s4p 1P]	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	2.86674e-01	3.91993e+02 (E _p)
<input type="checkbox"/>	EXC	A	THE	e, Be [2s3d 1D]	e, Be [2s4d 3D]	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	3.85044e-01	3.91993e+02 (E _p)
<input type="checkbox"/>	EXC	A	THE	e, Be [2s3d 1D]	e, Be [2s4d 1D]	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	5.01374e-01	3.91993e+02 (E _p)
<input type="checkbox"/>	EXC	A	THE	e, Be [2s3d 1D]	e, Be [2s4p 3P]	TAB1D	comment	I. Bray, D. Fursa	2014	Atomic data and collisional radiative model for beryllium and its ions, Physica Scripta, T161, 014007 (2014)	2.44500e-01	3.91993e+02 (E _p)

AMBDAS Bibliographical Database

AMBDAS

Atomic and Molecular Bibliographic Data System

Available Reactant/Surface Codes	Reactant Code	Ion Charge
? Reactant 1	<input type="text"/> H, Na, H2O, HF	<input type="text"/> 2, 26, -1
Reactant 2	<input type="text"/> H, Na, H2O, HF	<input type="text"/>
? Isoelectr. Sequence	<input type="text"/> H, Be, Ca	
? Surface	<input type="text"/> Mg, Ag2O, Metal	

Examples are given in green

Attention: the codes are case-sensitive, i.e., 'HF' is *Hafnium* and 'HF' is *Hydrogen-Fluorine*

Category	Process
<ul style="list-style-type: none"> Structure and Spectra Photon Collisions Electron Collisions Heavy Particles Collisions Surface Interactions Beam Heating and Fueling of Plasmas 	<ul style="list-style-type: none"> --- Structure and Spectra --- Line Shapes and Shifts Structure, Spectra Interatomic Potentials Polarizabilities, Electric moments Energy Levels, Wavelengths

Bibliography

? Author's name	<input type="text"/> Mott, N*Mott, *stein*	2 nd author's name	<input type="text"/>
? Keywords/Patterns	<input type="text"/> res*nance, "electron impact"	Exp vs Theory	<input type="text" value="-----"/> ▾
Years	<input type="text"/> - <input type="text"/> 98, 1998, 02, 2002	Reference Type	<input type="text" value="-----"/> ▾

Sort by Year: | Abstract/Comment: | Search Case Sensitive: The maximal allowed number of references is 200.

GENIE Search Engine

GENIE










A General Internet Search Engine for Atomic Data

Transition Probabilities
Wavelengths
Energy Levels

Ion:

Enter wavelength in Å:

From to


NIST Atomic Spectra Database	<input checked="" type="checkbox"/>	
Kurucz's CD-ROM 23	<input checked="" type="checkbox"/>	
Atomic Line List v.2.04	<input checked="" type="checkbox"/>	
TOPbase (Opacity Project)	<input checked="" type="checkbox"/>	
Kelly Atomic Line Database	<input checked="" type="checkbox"/>	
MCHF/MCDHF Collection	<input checked="" type="checkbox"/>	
KAERI AMODS Spectral Lines	<input checked="" type="checkbox"/>	
CAMBD Atomic Spectra	<input checked="" type="checkbox"/>	
Spectr-W3	<input checked="" type="checkbox"/>	









Electron Impact Cross Sections
and/or Rate Coefficients

Ion:

- Excitation
- Ionization
- Dielectronic recombination


Cross sections
Rate coefficients

IAEA ALADDIN Database	<input checked="" type="checkbox"/>	
NIFS AMDIS Database	<input checked="" type="checkbox"/>	
CAMBD Collisional Processes	<input checked="" type="checkbox"/>	
NIST Atomic Cross Sections	<input checked="" type="checkbox"/>	
OPEN-ADAS	<input checked="" type="checkbox"/>	
Spectr-W3	<input checked="" type="checkbox"/>	

Data Evaluation and Uncertainty Assessment



Joint IAEA-NFRI Technical Meeting on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion

Daejeon, Republic of Korea

4-7 September 2012

Organized by the
International Atomic Energy Agency (IAEA)

In conjunction with the
8th International Symposium on Standard Reference Data

Hosted by the
National Fusion Research Institute, Republic of Korea

Special Issue of Fusion Science and Technology

Data Evaluation and Uncertainty Assessment



Joint IAEA-ITAMP Technical Meeting on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data

Cambridge, Massachusetts, USA

7-9 July 2014

Organized by the International Atomic Energy Agency (IAEA) and
Institute of Theoretical Atomic, Molecular and Optical Physics (ITAMP) at Harvard-Smithsonian Center for Astrophysics

Organizers: H. Sadeghpour, J. F. Babb, K. Bartschat, J. Tennyson, D. R. Schultz, H.-K. Chung, B. J. Braams

The workshop brings together a number of people who are working on electron collisions with atoms, ions, and molecules, heavy-particle collisions, and electronic structure of atoms and molecules (with structure viewed here as a prerequisite for collision calculations). The primary goals are to come up with reasonable uncertainty estimates for calculations using the various methods of collision physics: perturbative, nonperturbative, time-independent, time-dependent, semi-classical, etc. Generally, the workshop focus will be on theoretical atomic and molecular data relevant to fusion and astrophysical plasmas, where modeling codes mostly use theoretical atomic and molecular data for which assessments of their accuracy are necessary. There will also be data users at the meeting, as well as some who manage databases.

[Abstracts and ITAMP workshop information](#)

[Background information on IAEA data evaluation activities](#)

Presentations

Monday, July 7, 2014

8:30AM Registration

Session I - Chair: Jim Babb

9:00AM 9:05AM Welcome (ITAMP)

9:05AM 9:20AM **Hyun-Kyung Chung (IAEA)**, "Meeting Objective"

9:20AM 10:00AM **Gordon Drake**, "Uncertainty Estimates: A new Editorial Standard"

Data Evaluation and Uncertainty Assessment



Joint IAEA-NFRI Technical Meeting on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion

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Hosted by the
National Fusion Research Institute, Republic of Korea

Special Issue of Fusion Science and Technology

Data Evaluation and Uncertainty Assessment



IAEA Technical Meeting on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications

19-21 December 2016, IAEA Headquarters, Vienna, Austria

Meeting reference: **IAEA-A9-TM-52452**.

- View [Meeting Information Sheet](#) (PDF file)
- Download [Abstract Template](#) (MS Word file)
- Download [IAEA Participation Form A](#) (MS Word file)
- Download [IAEA Abstract Submission Form B](#) (MS Word file)
- Download [IAEA Grant Application Form C](#) (MS Word file)

Background

Computer simulations play a critical role in understanding physical and chemical systems. In the last decades verification, validation and uncertainty quantification (VVUQ) of computer simulations has become an important research topic in the physical and chemical sciences and engineering. In support of optimization-based design of a fusion reactor and high precision diagnostics of plasmas in fusion devices the IAEA Atomic and Molecular (A+M) Data Unit has been pursuing VVUQ activities for theoretical A+M data. Our objective is to encourage and support the data development community to provide data users with reasonable uncertainty estimates for calculated A+M data and especially for calculated cross sections. After a series of meetings and discussions with theoretical atomic physicists organized by the Unit it has become clear that the VVUQ methods for theoretical data should develop in collaboration with experimental physicists and benchmark experiments.

Meeting Objectives

The meeting is meant to advance data-oriented research on A+M processes and properties that are important for plasma simulations and plasma diagnostics for fusion energy development and other plasma applications. Leading theoretical and experimental A+M physicists are invited along with plasma physicists using A+M data to discuss uncertainty assessments and benchmark experiments for A+M data for fusion and other plasma applications. The discussion topics are as follows:

- Prioritization of A+M data needs for fusion applications.
- Experimental methods and systems to benchmark theoretical A+M collision data.
- Target uncertainties of A+M collision data for fusion applications.
- Uncertainty quantification methods for theoretical A+M data.
- Network of A+M physicists doing benchmark experiments and computations.

Among other things the meeting will identify the most important data needs for fusion applications, decide what can be done to benchmark those data and formulate a plan of action among experimental and theoretical A+M physicists to carry out this benchmarking and perform the associated uncertainty assessment. Questions to be addressed include:

Developments in Data Exchange

Brainstorming meeting on the topics of

- Large data
- Heterogeneous data
- Data development, machine learning
- Correlated uncertainties, covariances
- Uncertainty propagation
- ...

Where possible in the context of plasma modelling.

Objective: inspiration for activities, areas of emphasis, by A+M Data Unit over the next 7 years or so.