Resources in IAEA

H.-K. Chung

Atomic and Molecular Data Unit Nuclear Data Section

2017 Joint ICTP-IAEA School on Atomic Processes in Plasmas

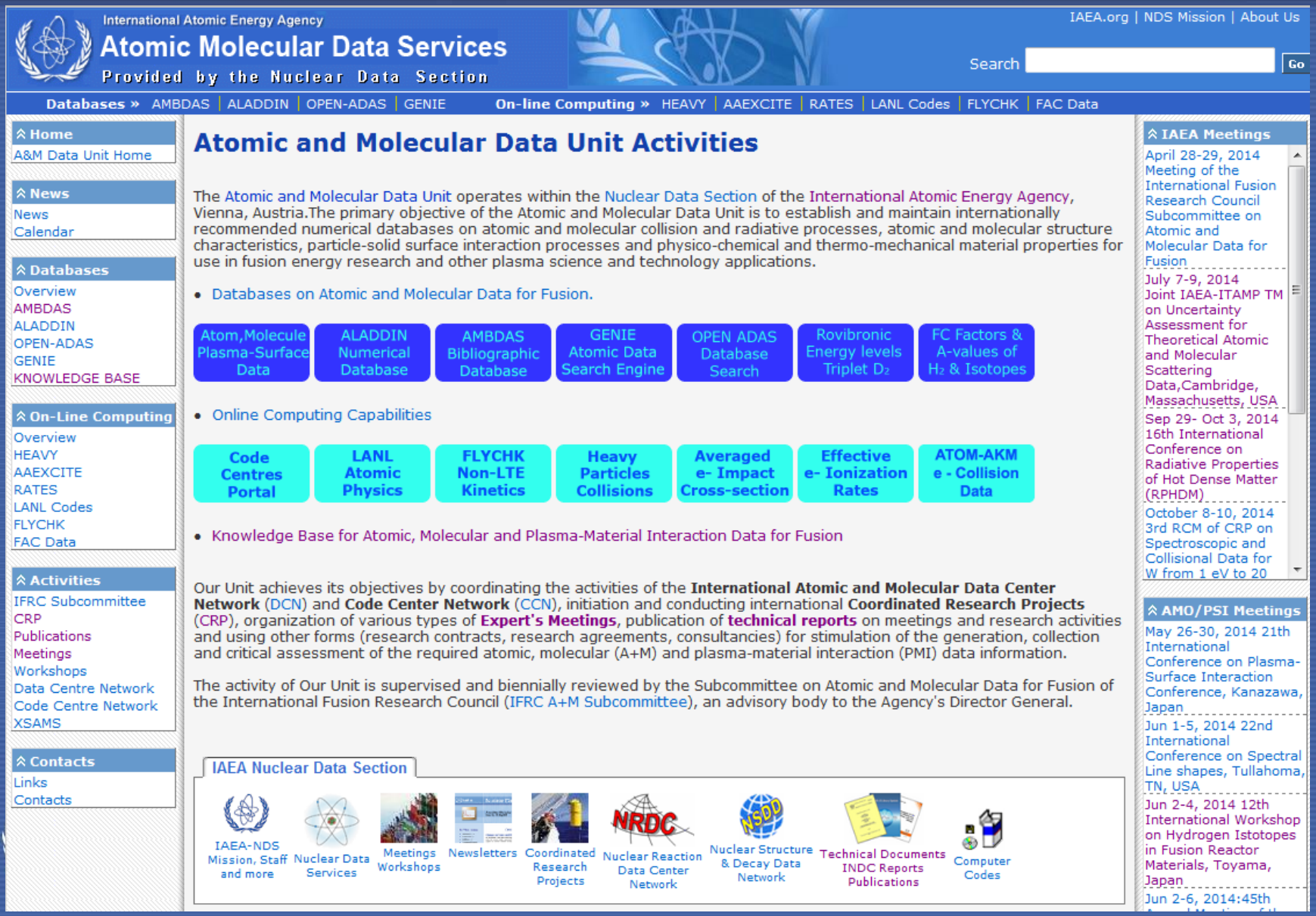
2 March 2017, Trieste, Italy

IAEA

International Atomic Energy Agency

IAEA AMD Unit Home Page (AMDIS)

http://www-amdis.iaea.org



International Atomic Energy Agency
Atomic Molecular Data Services
Provided by the Nuclear Data Section

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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 D_2 | FC Factors & A-values of H_2 & 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), an advisory body to the Agency's Director General.

IAEA Nuclear Data Section

IAEA-NDS Mission, Staff and more | Nuclear Data Services | Meetings Workshops | Newsletters | Coordinated Research Projects | Nuclear Reaction Data Center Network | Nuclear Structure & Decay Data Network | Technical Documents INDC Reports Publications | Computer Codes

IAEA Meetings

April 28-29, 2014 Meeting of the International Fusion Research Council Subcommittee on Atomic and Molecular Data for Fusion

July 7-9, 2014 Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data,Cambridge, Massachusetts, USA

Sep 29- Oct 3, 2014 16th International Conference on Radiative Properties of Hot Dense Matter (RPHDM)

October 8-10, 2014 3rd RCM of CRP on Spectroscopic and Collisional Data for W from 1 eV to 20

AMO/PSI Meetings

May 26-30, 2014 21th International Conference on Plasma-Surface Interaction Conference, Kanazawa, Japan

Jun 1-5, 2014 22nd International Conference on Spectral Line shapes, Tullahoma, TN, USA

Jun 2-4, 2014 12th International Workshop on Hydrogen Istotopes in Fusion Reactor Materials, Toyama, Japan

Jun 2-6, 2014:45th

DATABASES

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Databases : ALADDIN

http://www-amdis.iaea.org/ALADDIN

- Data list: http://www-amdis.iaea.org/ALADDIN/datalist.php
  - Data from 1980-2006 for evaluated / compiled data
  - Data from CRPs recently
  - ~17600 sets for A&M data (~ 8500 rad. rec. APID 16)
  - ~ 6400 data for Surface data
- Database Development
  - TM on “Improving the Database for Physical and Chemical Sputtering”
  - Consultancy by C. Hill (VAMDC) -- Database modernization
    - Database normalization / Data migration
    - VAMDC node / web interface development
- Future Work
  - Review of the data quality
  - Data compilation and evaluation

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ALADDIN: Numerical Database

Data Dissemination http://www-amdis.iaea.org/ALADDIN

- Data list: http://www-amdis.iaea.org/ALADDIN/datalist.php
  - Data from 1980-2006 for evaluated / compiled data
  - Data developed through CRPs, TMs and CMs
  - ~17600 sets for A&M data (~ 8500 rad. rec. APID 16)
  - ~ 6400 data for Surface data
- Atomic and Molecular Collisional Database
  - Heavy Particle Collisions / Electron Collisions / Photon Collisions
  - Search by Reactants, Products, Process, Data Types, Authors, Publication
- Plasma Surface Interaction Database
  - Reflection / Sputtering / Radiation Enhanced Sublimation / Penetration
  - Search by Projectile, Surface, Chemical Component, Data Type, Author, Publication
  - Specification by Predrag Krstic, Fred Meyer, Denis Humbert, June 2007
- Database searchable through GENIE
- ALADDIN system developed by R. Hulse adopted by the A+M Unit in 1988 is now replaced by MySQL database but the name is kept.

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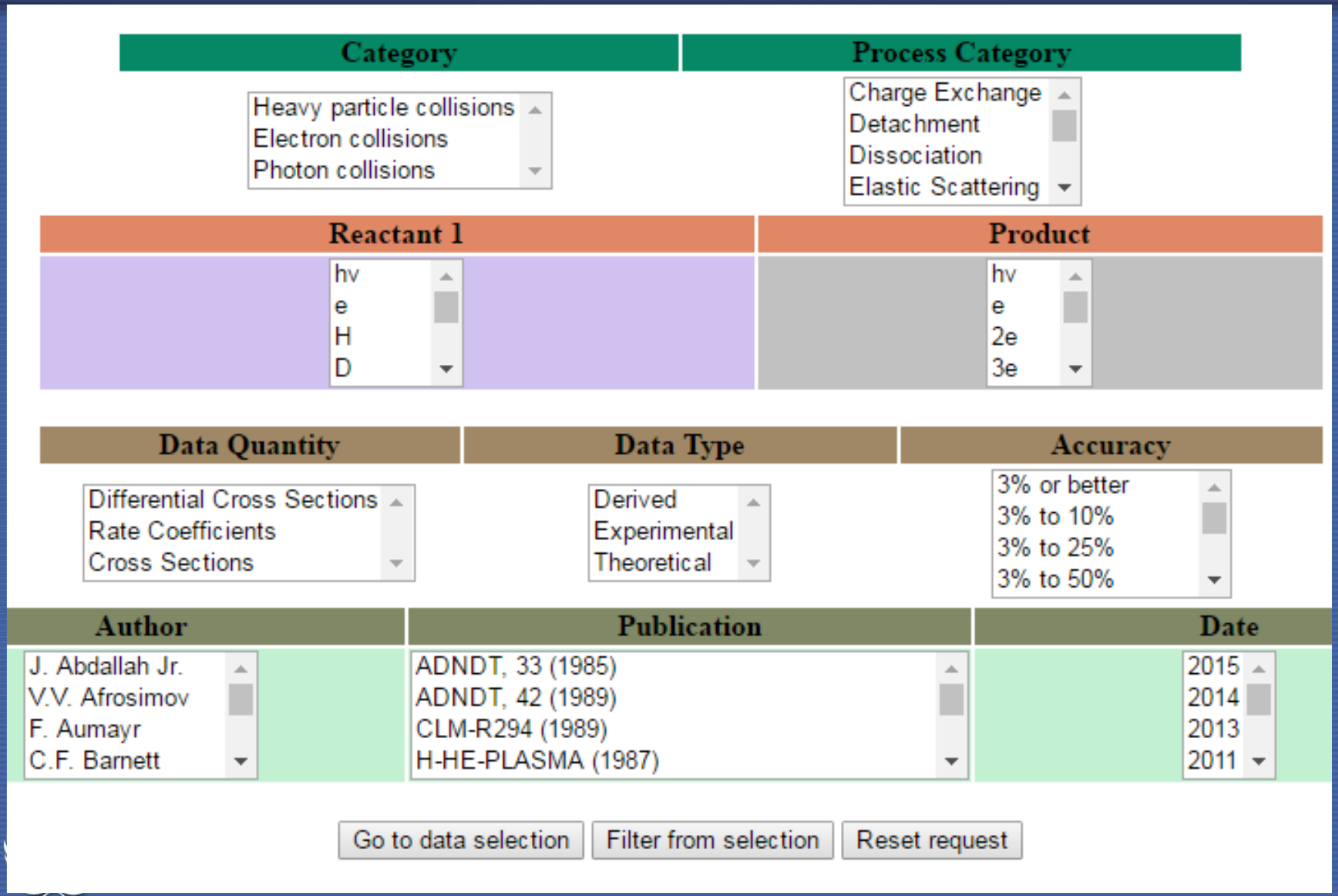
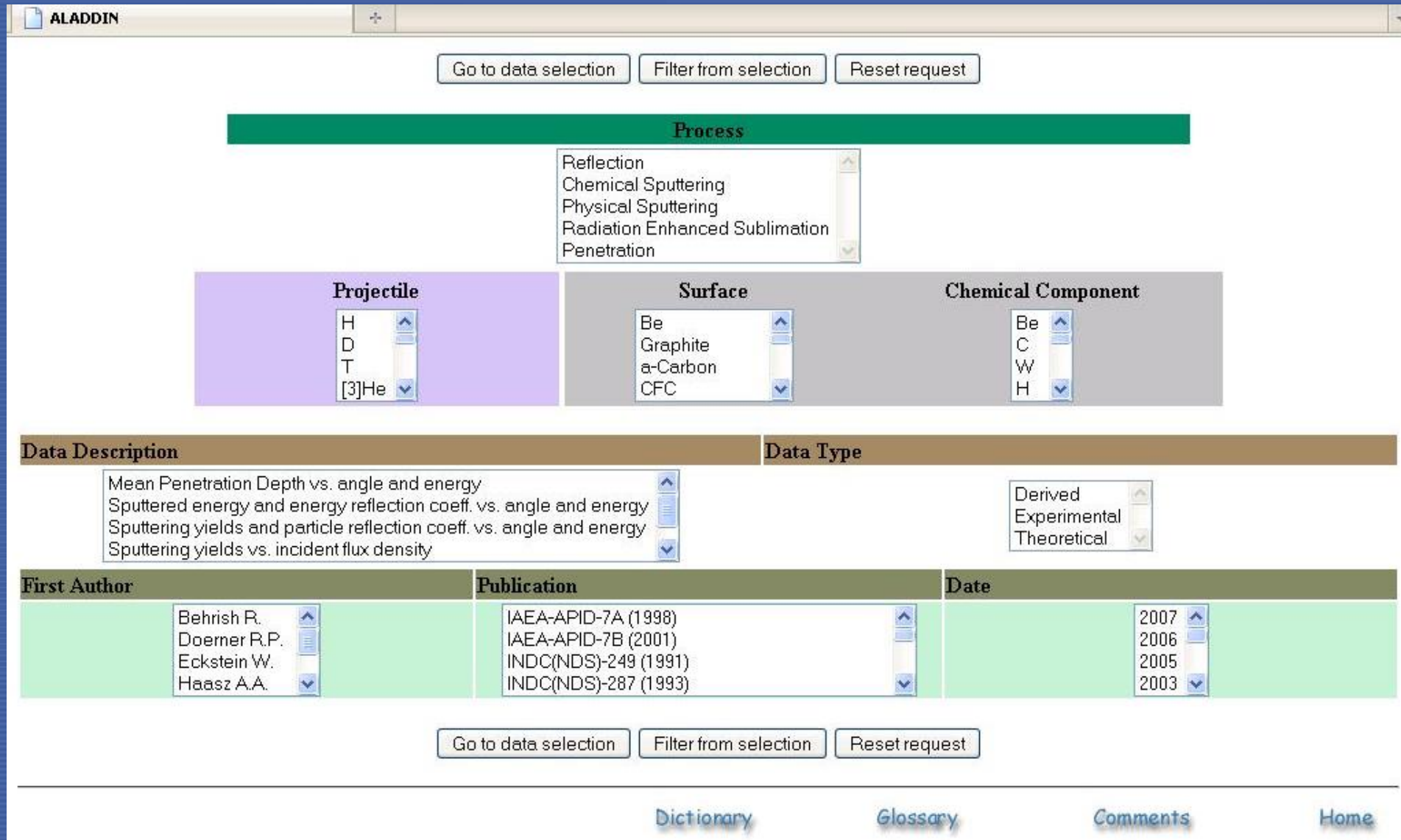
ALADDIN A&M Data



ALADDIN PSI Database



Databases: AMBDAS

http://www-amdis.iaea.org/AMBDAS

- Data Source
  - Spectroscopic data from NIST (A. Kramida & J. Fuhr)
  - Collisional data from ORNL
  - Atomic, Molecular and Plasma-Surface Interaction Data entries relevant to fusion
  - No Bibliographic data for A&M collisions and PSI available since 2010
- Version 3.1 (April 2010)
  - Search by Reactants, Process, Authors, Keywords, Year
  - Results with Author, Title, Reference and DOI (Digital Object Identifier) Link
- All data in the International Bulletin available on Atomic and Molecular Data for Fusion through AMBDAS

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AMBDAS Screen Shot

AMBDAS: Query Output

2 references found. Processing the output...

1. R. Warmbier, R. Schneider, A. R. Sharma, B. J. Braams, J. M. Bowman, P. H. Hauschildt

   Ab initio modeling of molecular IR spectra of astrophysical interest: Application to CH_4.

   Astron. Astrophys. **495**, 655 (2009). doi:10.1051/0004-6361:200810983

Theory | 0-9000 K | Reactant Data

2. G. Czako, B. C. Shepler, B. J. Braams, J. M. Bowman

   Accurate ab initio potential energy surface, dynamics, and thermochemistry of the F + CH_4 -> HF + CH_3 reaction.

   J. Chem. Phys. **130**, 084301 (2009). doi:10.1063/1.3068528

Theory | 630 cm^{-1} | Reactant Data

submit | reset

- [ ] J. M. Bowman
- [ ] B. J. Braams
- [ ] G. Czako
- [ ] P. H. Hauschildt
- [ ] R. Schneider
- [ ] A. R. Sharma
- [ ] B. C. Shepler
- [ ] R. Warmbier

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Knowledge base (wiki style)

http://www-amdis.iaea.org/w

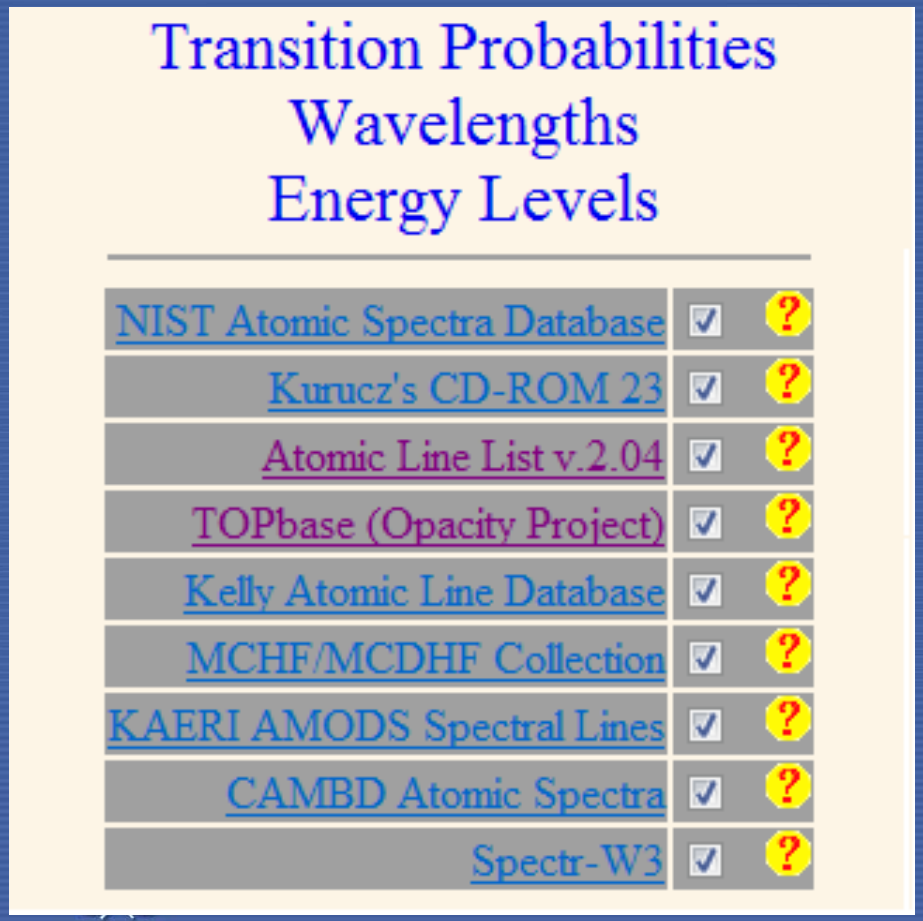
- Introduction
- Data Needs
  - Magnetic Confinement Fusion
  - Inertial Confinement Fusion
  - Atomic Data
  - Molecular Data
  - Plasma-Material Interaction Data
- Data Sources
  - Online Databases
  - Data Centers
  - Code Centers Network
- Data Exchange
  - Data Producers Directory
  - Data Exchange Forum
- Special Topics
  - IAEA Coordinated Research Projects (CRP)
  - IAEA Workshops
  - NLTE Kinetics Code Comparison Workshops
  - ITPA (International Tokamak Physics Activity)
  - European Fusion Development Agreement (EFDA)
- Fusion Research
  - Magnetic Confinement Fusion Research
  - Inertial Confinement Fusion Research

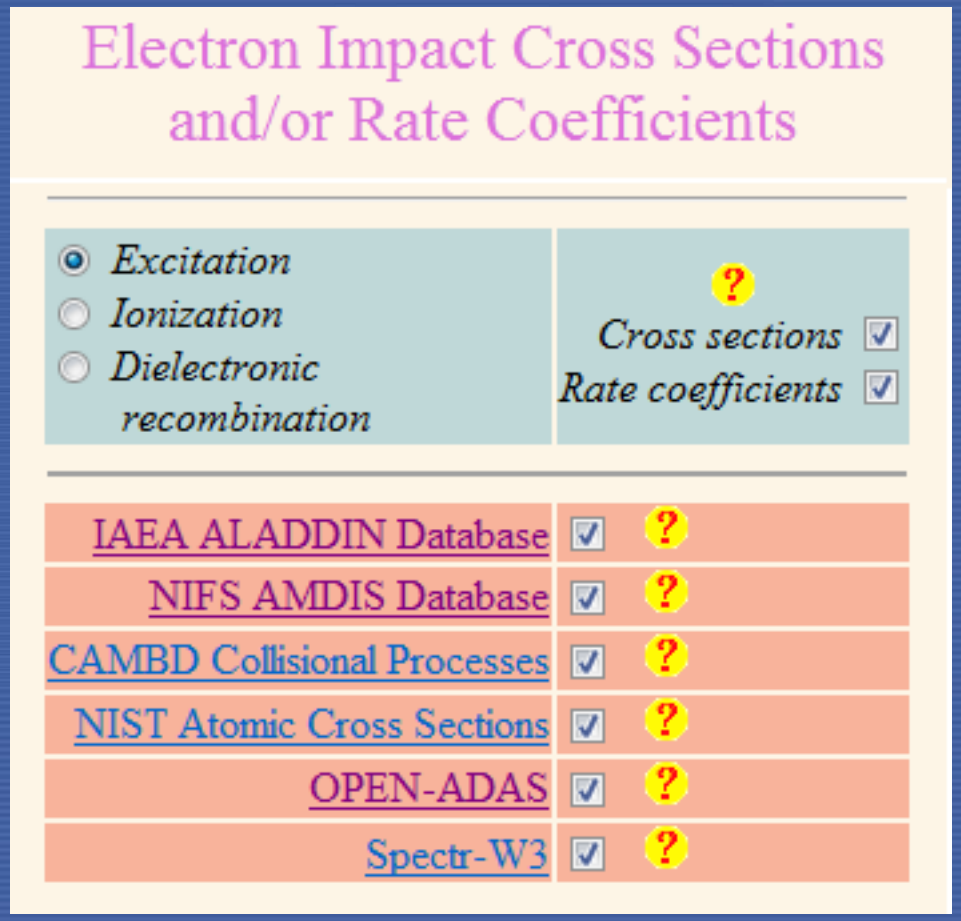
Contents from INDC reports, APID volumes and Presentations. Few changes since 2012

Databases Search Engine: GENIE

http://www-amdis.iaea.org/GENIE

- Resumed only in late 2013
- No statistics available yet – Chianti possibility





IAEA Online Codes and Code Data

- Online Codes
  - Average Approximation http://www-amdis.iaea.org/AAEXCITE/
    - Electron impact excitation cross sections for any ion and configuration
  - Heavy particle collisions http://www-amdis.iaea.org/HEAVY/
    - Excitation, ionization and charge exchange for bare nucleus on hydrogenic target
  - Effective Ionization/Recombination Rates http://www-amdis.iaea.org/RATES/
    - Level population distributions and radiative power rates from CR modeling
- Code Generated Data
  - LANL atomic data from CRP http://www-amdis.iaea.org/LANL/
    - Si, Cl, Ar ions (~ 2 GB)
  - FLYCHK Collisional-Radiative code results http://www-amdis.iaea.org/FLYCHK
    - Charge state distributions and radiative loss rates for Z=1-79 for T_e=0.5 eV- 100 keV
  - ATOM-AKM code results https://int-amdis.iaea.org/Atom_AKM/
    - Electron-impact excitation and ionization cross-sections and rate coefficients (H-Be)
  - FAC atomic physics data http://www-amdis.iaea.org/FAC/
    - He – Si atoms (~ 30 GB)

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Atomic data from FLYCHK

http://www-amdis.iaea.org/FLYCHK

FLYCHK: Generalized Model of Atomic Processes In Plasmas

On-line Capability of NLTE kinetics Code

The FLYCHK code provides a simple and general modeling capability to generate atomic level populations and charge state distributions for low-Z to mid-Z elements under NLTE(Non-Local Thermodynamic Equilibrium) conditions. The code is currently available at the **password-protected NIST website.** For more information on details, validity and limitations of the code, please click **the FLYCHK information page** .

Steady-State Charge State Distributions

Average charge states <Z> of atoms from Z=1 (Hydrogen) to Z=79 (Gold) are calculated by FLYCHK code and plotted over a wide range of plasma conditions. The calculation is done for the steady-state plasmas with electron temperatures from 0.5 eV to 100 keV and electron densities from 10^{12} cm^{-3} to 10^{24} cm^{-3}. Click the element in the periodic table and a page will apear with the information on <Z>, Charge State Distribution and Total Radiative Power Loss Rates of the element.

Rate Coefficients at Coronal Equilibirum for Plasma Modeling Applications

To help plasma modeling applications, Rate coefficients of Direct Ionization, Excitation-Autoionization, Radiative Recombination and Dielectronic Recombination at coronal conditions are generated for a wide range of plasma temperatures from 0.5 eV to 100 keV. Also avaialble are the Radiative Loss rates per Charge State, both Line radiation and Recombination radiation. They are available at the same page as Charge state distributions. The details of the methods are found at **the FLYCHK Rates information page** .

check the section on "About FLYCHK rate coefficients" .

Atomic data from FAC

http://www-amdis.iaea.org/FLYCHK

- FAC (Flexible Atomic Codes, M. Gu, 2008) is widely used in plasma physics community
  - Complete software package to generate atomic energy levels, radiative transition rates, collisional excitation and ionization cross-sections by electron impact, photoionization and autoionization cross-sections.
  - Freely available from http://sprg.ssl.berkeley.edu/~mfgu/fac/
- FAC data generated from Helium to Silicon ions
  - Total of 8 Gigabytes with energy levels up to n=20
  - With a proper post-processing code, a collisional-radiative model can be quickly established.
- FLYFAC project (FLYCHK code + FAC data)
  - Fortran 95 code of post-processing code to establish a CR model using SQL-based cFAC data (E. Stambulchik, Weizmann Institute of Science)

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Hydrogen Molecular Data

Franck-Condon Factors, Transition Probabilities and Radiative Lifetimes for Hydrogen Molecules and their Isotopomeres

U. Fantz, D. Wünderlich (May 2004)

IAEA INDC(NDS)-457 report pdf file (2.7 MB)
Notation and Energy of electronic states in energetic order for each multiplet system

Eigenvalues

Franck-Condon factors

- H2
- D2
- T2
- HD
- HT
- DT

Transition Probabilities

- H2
- D2
- T2
- HD
- HT
- DT

Radiative Lifetimes for vibrational levels

Effective Radiative Lifetimes

Effective Transitions Probabilities

For the complete set of data, please contact us

Rovibronic energy levels for triplet electronic states of molecular deuterium

B. P. Lavrov and I. S. Umrikhin
Faculty of Physics, St.-Petersburg State University
St.-Petersburg, 198904, Russia
J. Phys. B: Atomic, Molecular and Optical Physics, 41 105103 (2008)

Data Presentation, INDC (NDS) report (PDF file)

$a\,^3\Sigma_g^+$ Energy levels	$h\,^3\Sigma_g^+$ Energy levels	$n\,^3\Pi_u^-$ Energy levels	$(5d)\,^3\Sigma_g^+$ Energy levels
$c\,^3\Pi_u^+$ Energy levels	$i\,^3\Pi_g^+$ Energy levels	$p\,^3\Sigma_g^+$ Energy levels	$(6d)\,^3\Sigma_g^+$ Energy levels
$c\,^3\Pi_u^-$ Energy levels	$i\,^3\Pi_g^-$ Energy levels	$r\,^3\Pi_g^+$ Energy levels	$(7d)\,^3\Sigma_g^+$ Energy levels
$d\,^3\Pi_u^+$ Energy levels	$j\,^3\Delta_g^+$ Energy levels	$r\,^3\Pi_g^-$ Energy levels	$(8d)\,^3\Sigma_g^+$ Energy levels
$d\,^3\Pi_u^-$ Energy levels	$j\,^3\Delta_g^-$ Energy levels	$s\,^3\Delta_g^-$ Energy levels	$(9d)\,^3\Sigma_g^+$ Energy levels
$e\,^3\Sigma_u^+$ Energy levels	$k\,^3\Pi_u^+$ Energy levels	$u\,^3\Pi_u^+$ Energy levels	$(7p)\,^3\Pi_u^-$ Energy levels
$f\,^3\Sigma_u^+$ Energy levels	$k\,^3\Pi_u^-$ Energy levels	$u\,^3\Pi_u^-$ Energy levels	$(8p)\,^3\Pi_u^-$ Energy levels
$g\,^3\Sigma_g^+$ Energy levels	$n\,^3\Pi_u^+$ Energy levels		$(9p)\,^3\Pi_u^-$ Energy levels

Code Distributions (2015)

- GRASP2K code distribution https://www-amdis.iaea.org/GRASP2K

  In collaboration with P. Jönsson and J. Ekman (Malmö Univ, Sweden)

  Most used atomic structure and transition probability code package

  Grasp2K relativistic atomic structure package, *Computer Physics Communications, Volume 184, Issue 9, September 2013, 2197-2203*

- FAC/cFAC code distribution https://www-amdis.iaea.org/FAC/

  In collaboration with M. F. Gu (UC-Berkeley, USA) and E. Stambulchik (Weizmann Institute of Science, Israel)

  Most used atomic physics code package

  GitHub repositories for FAC/cFAC codes

  https://github.com/fnevgeny/fac

  https://github.com/fnevgeny/cfac

- FLYFAC(cFACDB) collisional-radiative code development in progress

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