# Data Evaluation of Helium and its Isotopes

# Evaluation of Cross Section for Electron Impact with hydrogen /helium and their Combination Molecules in Fusion Plasma

(1) Based on previous research for $H_2$, $D_2$, HD (experimental data)

- Cross sections for electron collisions with hydrogen molecules

  Journal of Physical and Chemical Reference Data, 37 (2), 913 (2008)

- Electron impact cross sections for deuterated hydrogen and deuterium molecules

  Report on Progress in Physics, 73, 116401 (2010)

+ Electron impact cross sections of vibrationally and electronically excited diatomic molecules
+ Theoretical and experimental data survey
+ Evaluation(only experimental data)

(2) Making general data evaluation procedures

- organized several evaluation meeting → how to evaluate data
- Still working

TM on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion (2012)

TM on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data (2014)

**TM on Uncertainty Assessment and Benchmark Experiments For Atomic and Molecular Data for Fusion Applications (2016)**

IAEA
International Atomic Energy Agency

INDC(NDS)- 0627
Distr. LP,NE,SK

**INDC International Nuclear Data Committee**

**Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion**

**Summary Report of a Joint IAEA-NFRI Technical Meeting**

Daejeon Convention Center, Daejeon, Republic of Korea

4–7 September 2012

Prepared by

Hyun-Kyung Chung

November 2012

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

## ➔ Roadmap to the Establishment of Internationally Agreed Standard Data Library for AM/PSI Data Relevant to Fusion Applications

**Phase 0:** Inventorise the AM/PSI Data Collection used by Fusion/Plasma Community

**Phase 1:** Establishment of infrastructure towards evaluated data library

**Phase 2:** Establishment of evaluated data library

**Phase 3:** Establishment and maintenance of standard data library

## ➔ Developing an Evaluators Network

## ➔ Guidelines for Uncertainty Assessment of Theoretical Data (how to proceed)

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# Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion

## Summary Report of a Joint IAEA-NFRI Technical Meeting

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November 2012

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

## ➔Which Systems are the Priorities for Evaluation :

- Electron scattering on **CH4.**
- For electron-molecule collisions we considered hydrogenic systems but decided that so many data are available that CH4 would be easier (and also relevant

## ➔ Action Items

NFRI to organize a **data evaluation group for demonstration**

- The group will demonstrate the evaluation procedure by the editorial board.
- **The group will establish general guidelines for evaluation criteria, evaluation process**
- The group will demonstrate the evaluation process from the scratch to the final product as discussed in the meeting

# A+M data evaluation for fusion and other plasma applications

Mi-Young Song, Jung-Sik Yoon

*National Fusion Research Institute, Plasma Technology Research Center,*

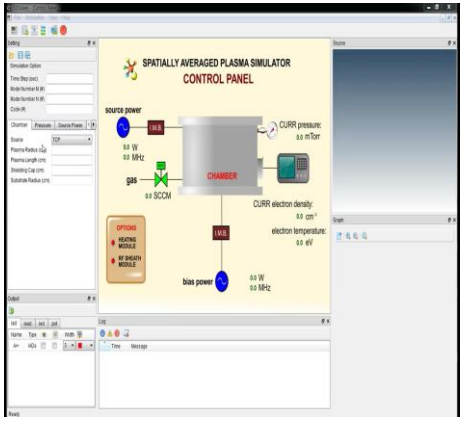
➔ Group Members:
Y. Itikawa (Japan),
G. P. Karwasz (Nicolaus Copernicus University),
J. Tennyson (University College London),
V. Kokoouline(University of Central Florida),
H. Cho(Chung-Nam National University),
Y. Nakamura (Tokyo Denki University),

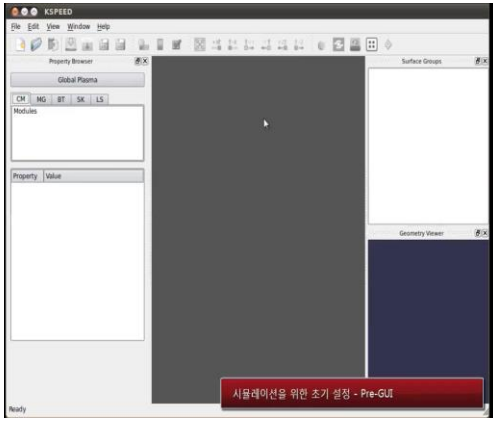
# A+M Data need for Plasma Applications (Simulation)

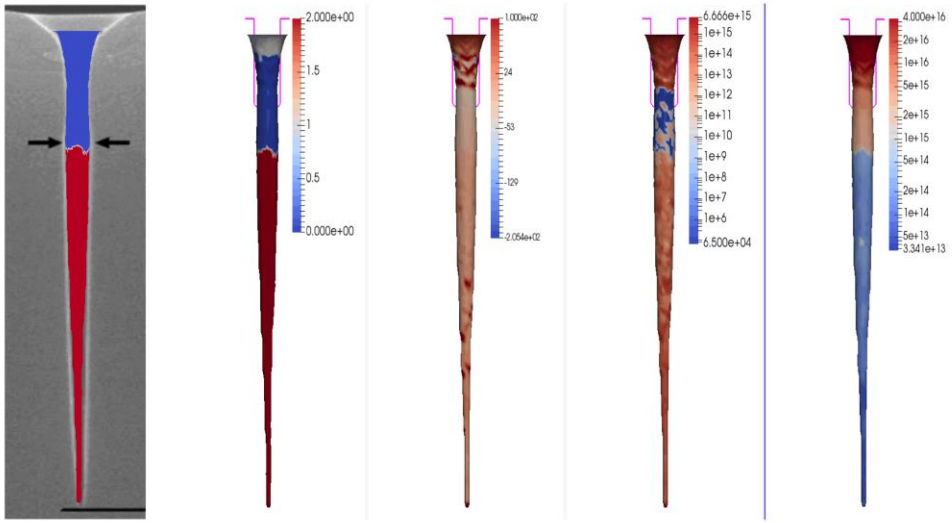
**Our achievements toward a realistic plasma process simulation**

K-SPEED 2016

Zero-D Bulk plasma simulator + 3D Feature profile simulator

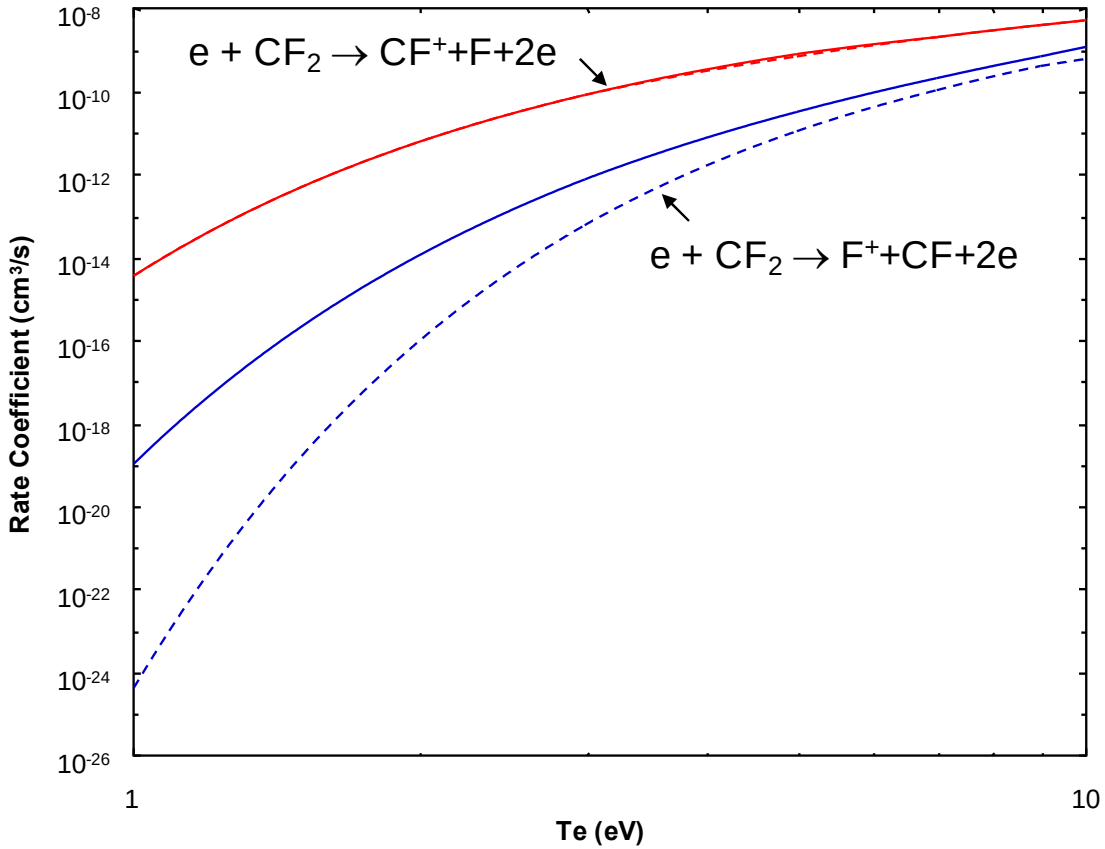


# Motivation – Same cross section, but different coefficient

Reaction rate coefficient for
$e+SiH_4 \rightarrow SiH^+_3 + 2e$ ~ $10^{-2}$ $cm^3/s$ (from article A)
~ $10^{-9}$ $cm^3/s$ (from article B)
~ $10^{-11}$ $cm^3/s$ (from article C)



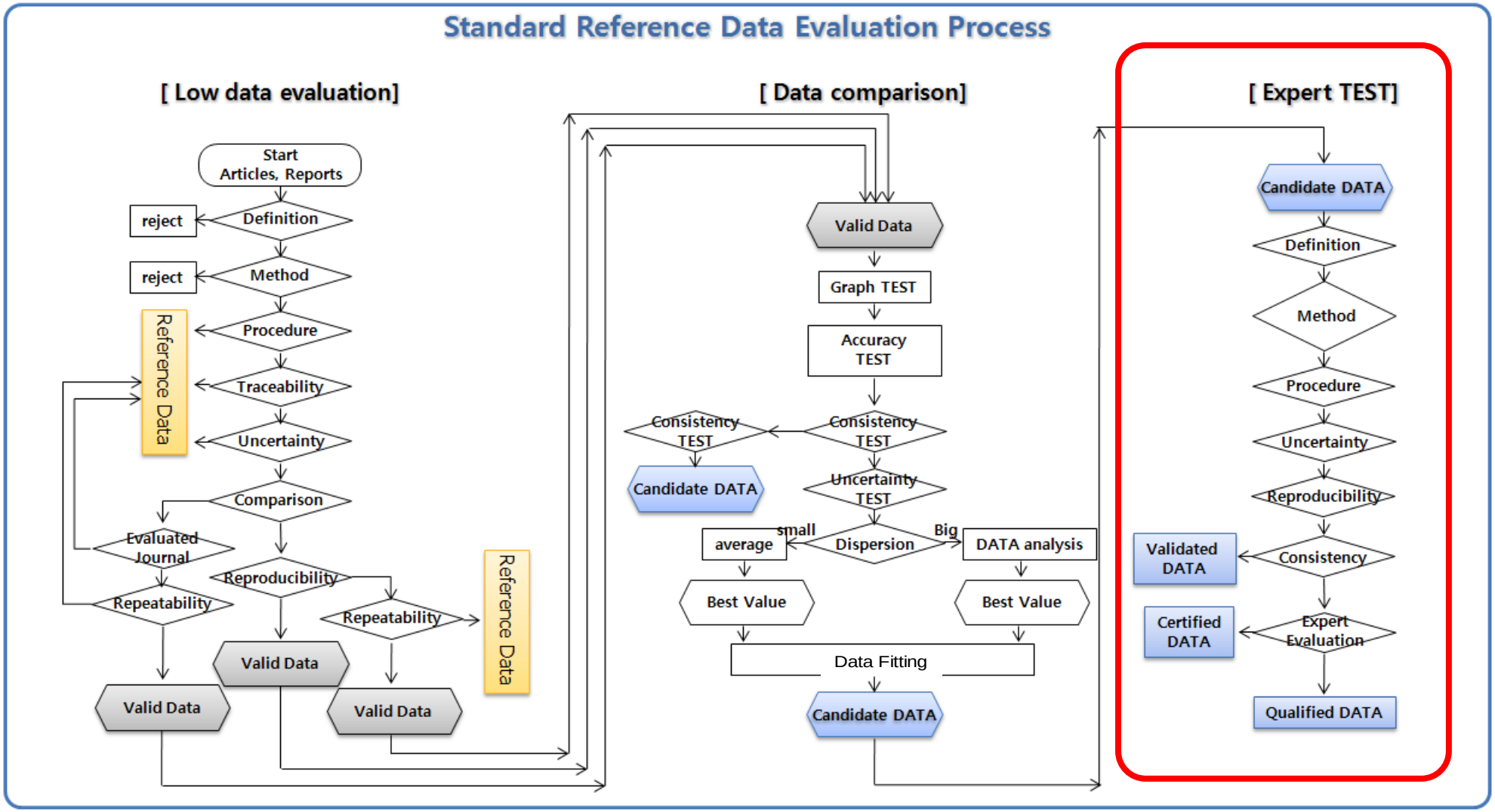

Reaction rate coefficient from Tarnovsky (cross section)

Solid line : DCPP
Dashed line : Ho, Chemkin


• P. Ho, J. E. Johannes, and R. J. Buss, and E. Meeks, J. Vac. Sci. Technol. A **19**(5), 2344 (2001).
• http://www.sandia.gov/chemkin/
• V. Tarnovsky, P. Kurunczi, D. Rogozhinikov, and K. Becker, Int. J. Mass Spectrom. Ion Processes 128, 181 (1993).

# Data Evaluation (Domestic project before IAEA TM @ Daejeon, 2012)

Supported by National Standard Reference Data (SRD) Project from Ministry of Industry

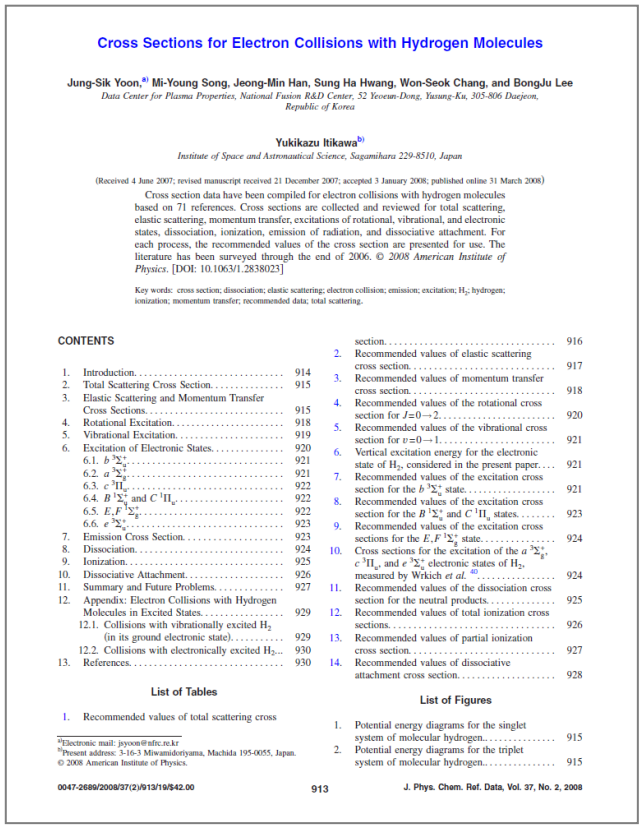


# Data Evaluation (Domestic project before IAEA TM @ Daejeon, 2012)

① Cross sections for electron collisions with hydrogen molecules
*Journal of Physical and Chemical Reference Data, 37 (2), 913 (2008)* ***-Prof. Itikawa***

② Elastic cross sections for electron collisions with molecules relevant to plasma processing
*Journal of Physical and Chemical Reference Data, 39 (3), 913 (2010)*
***-Prof. Cho, Prof. Tanaka, Prof. Buckman etc***

③ Electron-impact cross sections for deuterated hydrogen and deuterium molecules
*Report on Progress in Physics, 73, 116401 (2010)* ***-Prof. Kumar***



Cross Sections for Electron Collisions with Hydrogen Molecules

Jung-Sik Yoon,[a)] Mi-Young Song, Jeong-Min Han, Sung Ha Hwang, Won-Seok Chang, and BongJu Lee
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Yukikazu Itikawa[b)]
*Institute of Space and Astronautical Science, Sagamihara 229-8510, Japan*

(Received 4 June 2007; revised manuscript received 21 December 2007; accepted 3 January 2008; published online 31 March 2008)

Cross section data have been compiled for electron collisions with hydrogen molecules based on 71 references. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, excitations of rotational, vibrational, and electronic states, dissociation, ionization, emission of radiation, and dissociative attachment. For each process, the recommended values of the cross section are presented for use. The literature has been surveyed through the end of 2006. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2838023]

Key words: cross section; dissociation; elastic scattering; electron collision; emission; excitation; $H_2$; hydrogen; ionization; momentum transfer; recommended data; total scattering.

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Elastic Cross Sections for Electron Collisions with Molecules Relevant to Plasma Processing

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(Received 26 May 2010; revised manuscript received 16 July 2010; published online 1 September 2010)

Absolute electron-impact cross sections for molecular targets, including their radicals, are important in developing plasma reactors and testing various plasma processing gases. Low-energy electron collision data for these gases are sparse and only the limited cross section data are available. In this report, elastic cross sections for electron-polyatomic molecule collisions are compiled and reviewed for 17 molecules relevant to plasma processing. Elastic cross sections are essential for the absolute scale conversion of inelastic cross sections, as well as for testing computational methods. Data are collected and reviewed for elastic differential, integral, and momentum transfer cross sections and, for each molecule, the recommended values of the cross section are presented. The literature has been surveyed through early 2010. © *2010 American Institute of Physics*. [doi:10.1063/1.3475647]

Key words: differential cross sections; electron collisions; integrated elastic scattering cross sections; momentum transfer cross sections.

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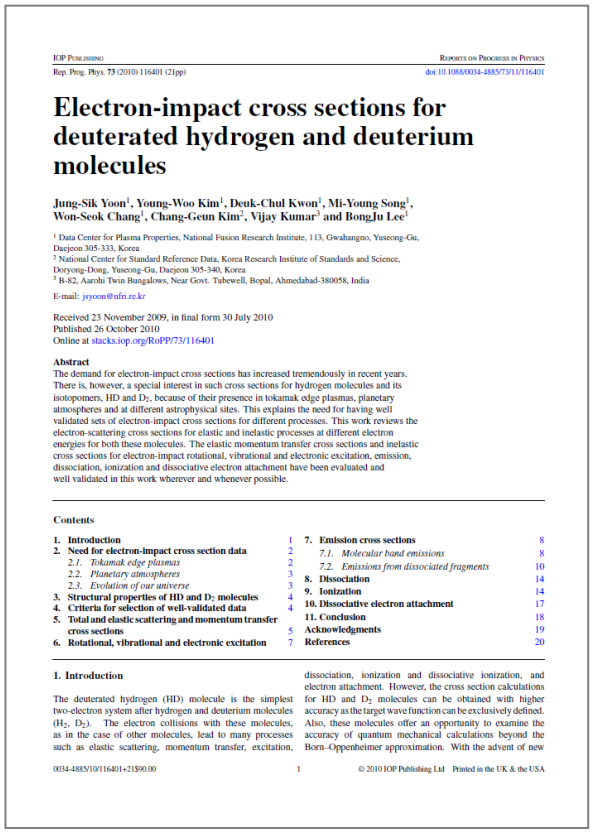

IOP Publishing
Reports on Progress in Physics
Rep. Prog. Phys. **73** (2010) 116401 (21pp)
doi:10.1088/0034-4885/73/11/116401

Electron-impact cross sections for deuterated hydrogen and deuterium molecules

Jung-Sik Yoon[1], Young-Woo Kim[1], Deuk-Chul Kwon[1], Mi-Young Song[1], Won-Seok Chang[1], Chang-Geun Kim[2], Vijay Kumar[3] and BongJu Lee[1]

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Received 23 November 2009, in final form 30 July 2010
Published 26 October 2010
Online at stacks.iop.org/RoPP/73/116401

**Abstract**
The demand for electron-impact cross sections has increased tremendously in recent years. There is, however, a special interest in such cross sections for hydrogen molecules and its isotopomers, HD and $D_2$, because of their presence in tokamak edge plasmas, planetary atmospheres and at different astrophysical sites. This explains the need for having well validated sets of electron-impact cross sections for different processes. This work reviews the electron-scattering cross sections for elastic and inelastic processes at different electron energies for both these molecules. The elastic momentum transfer cross sections and inelastic cross sections for electron-impact rotational, vibrational and electronic excitation, emission, dissociation, ionization and dissociative electron attachment have been evaluated and well validated in this work wherever and whenever possible.

Contents



## 1. Introduction

The deuterated hydrogen (HD) molecule is the simplest two-electron system after hydrogen and deuterium molecules ($H_2$, $D_2$). The electron collisions with these molecules, as in the case of other molecules, lead to many processes such as elastic scattering, momentum transfer, excitation, dissociation, ionization and dissociative ionization, and electron attachment. However, the cross section calculations for HD and $D_2$ molecules can be obtained with higher accuracy as the target wave function can be exclusively defined. Also, these molecules offer an opportunity to examine the accuracy of quantum mechanical calculations beyond the Born–Oppenheimer approximation. With the advent of new

# Lessons learned (from Prof. Itikawa and other experts)

- **Process of data evaluation (or compilation)**

  Literature survey → Collection of numerical data → Evaluation of the collected data → Recommendation of the best values

**➔"Data evaluation" is the important but difficult part**

**➔ We have no standard method of it**

- **For data evaluation, the following points should be taken into account**

➔Quoted uncertainty

➔Agreement among the data obtained by different authors/methods

➔How the absolute values were determined

➔Physics involved

➔Consistency between related but different quantities

➔Reliability of authors : Judged from their previous works

# Lessons learned

➔ **There is no standard method of data evaluation.**

➔ The result of evaluation (i.e., the recommended data) **may be different depending on who evaluates them.**

➔ Prof. Itikawa suggest : evaluation of the evaluated data

(1) Consistency of the total scattering cross section
(2) Swarm parameters
(3) Modelling result

**Still…**
**we are thinking**

➔ Find and train **“evaluators”** (scientists who are engaged in data evaluation)

→ **Organize network of evaluators**

# TM on Data Evaluation (2012)

# Coordination Meetings for Evaluation

http://www-amdis.iaea.org/DCN/Evaluation/ H. Chung @ DCN meeting (2015)

| | |
|---|---|
| Feb 12 | • CM on Procedures for Evaluation of AM/PMI Data for Fusion: Current status & future coordination (Japan) |
| Jun 12 | • CM on Data Evaluation & Establishment of a Standard Library of AM/PMI Data for Fusion (IAEA) |
| Sep 12 | • TM on Data Evaluation for AM/PSI Processes in Fusion (Korea) |
| May 13 | • TM (CCN) on General Guidelines for Uncertainty Assessments of Theoretical Data |
| Dec 13 | • CM on Evaluation of Data for Collisions of Electrons with Nitrogen Molecule and Nitrogen Molecular Ion |
| Jul 14 | • Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic Molecular Scattering Data |
| Jun 15 | • CM on Guidelines for Uncertainty Quantification of Theoretical Atomic and Molecular Data |
| Jul 15 | • CM on Evaluation & Uncertainty Assessment for Be, C, Ne<br>• TM (CCN) on Simulation of PMI Experiments |
| Sep 15 | • CM on Recommended Data for Processes of Tungsten (Korea) |

# TM on Data Evaluation 2012

http://www-amdis.iaea.org/meetings/NFRI2012/

- More than 20 Participants from 11 countries
- Proceeding papers published at Fusion Science and Technology (2013)
- Community Consensus needed to produce evaluated/recommended data
  - Disseminate standard definitions of *TERMINOLOGIES* adopted internationally
  - Disseminate materials with the *CRITICAL ANALYSIS SKILLS* → NRC report
  - Involve *COMMUNITY* in data evaluation → eMOL, Group evaluation
- Technical Issues
  - Assessment for THEORETICAL data → **UNCERTAINTY ESTIMATES**
  - Assessment of EXPERIMENTAL data → Self-consistency checks
  - ERROR PROPAGATION and SENSITIVITY ANALYSIS → Uncertainties in "Data" & "Data Processing Toolbox"

IAEA

**H. Chung @ DCN meeting (2015)**

# Group Evaluation (start from 2013)

**Purpose :**

**➔ To establish the internationally agree standard reference data library**

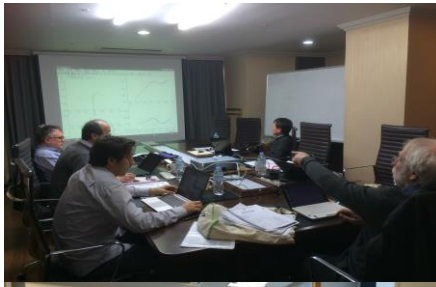
➔ Participants recommended group members and molecule($CH_4$)

➔ Group Members:

Y. Itikawa (Japan),
G. P. Karwasz (Nicolaus Copernicus University),
J. Tennyson (University College London),
V. Kokoouline(University of Central Florida),
H. Cho(Chung-Nam National University),
Y. Nakamura (Tokyo Denki University),
M.-Y. Song (National Fusion Research Institute)

# Group Evaluation

- 1st GM : 23~25, January 2013, @Gunsan, Korea
- 2nd GM : 25~27 June 2013, @Daejeon, Korea
- 3rd GM : 23~24 September 2013, @OU, UK
- 4th GM : 8~9 January 2014, @Seoul, Korea
- 5th GM : 4~5 July 2014, @Cumberland Lodge, UK
- 6th GM : 14 December 2014, @Daejeon, Korea
- 7th GM : 14~15 May 2015, @UCL, UK
- 8th GM : 17~19 November 2015, @Seoul, Korea
- 9th GM : 13~16 May 2016, @UCL, UK
- 10th GM : 27 September 2016 @NFRI, Korea








# Group Evaluation - ($CH_4$)

## Cross Sections for Electron Collisions with Methane

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*Plasma Technology Research Center, National Fusion Research Institute, 814-2 Osikdo-dong, Gunsan, Jeollabuk-do 573-540, South Korea*

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(Received 18 December 2014; accepted 8 April 2015; published online 28 May 2015)

Cross section data are compiled from the literature for electron collisions with methane ($CH_4$) molecules. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, excitations of rotational and vibrational states, dissociation, ionization, and dissociative attachment. The data derived from swarm experiments are also considered. For each of these processes, the recommended values of the cross sections are presented. The literature has been surveyed through early 2014. © *2015 AIP Publishing LLC.* [http://dx.doi.org/10.1063/1.4918630]

Key words: attachment; dissociation; electron collisions; evaluation; ionization; total cross sections.

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[a]Author to whom correspondence should be addressed; electronic mail. mysong@nfri.re.kr.






## JPCRD vol. 44, No2, 023101 (2015)

- ➔ present a systematic review of the published cross sections for processes resulting from electron collisions with methane up to early 2014.
- ➔ Both measurements and theoretical predictions are considered, although priority is given to high quality measurements with published uncertainties where available

# Group Evaluation - ($CH_4$)

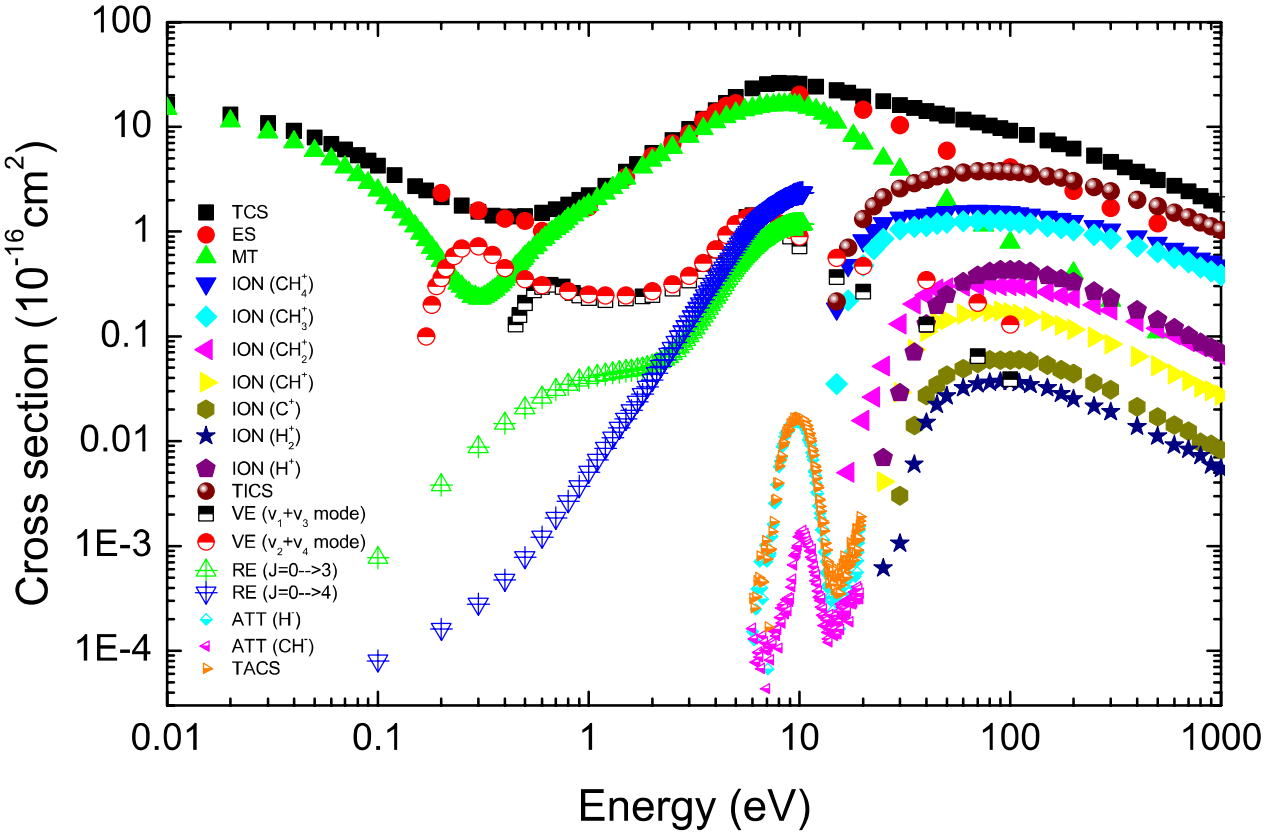


FIG. 23. The summary of cross section for electron collisions with methane. TCS - total scattering, ES - elastic scattering, MT - momentum transfer, ION - partial ionization, TICS - total ionization, VE - vibrational excitation, RE - rotational excitation, ATT - dissociative attachment, and TACS - total dissociative attachment.

# Group Evaluation - ($C_2H_2$) – under review (JPCRD, 2016)

## Cross Sections for Electron Collisions with Acetylene

Mi-Young Song[a),1] Jung-Sik Yoon,[1] Hyuck Cho,[2] Grzegorz P. Karwasz,[3] Viatcheslav Kokoouline,[4] Yoshiharu Nakamura,[5] and Jonathan Tennyson[6]

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[5)] 6-1-5-201 Miyazaki, Miyamae, Kawasaki, 216-0033, Japan

[6)] Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

(Revised 18 November 2016)

Cross section data are compiled from the literature for electron collisions with the acetylene (HCCH) molecule. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, excitations of rotational and vibrational states, dissociation, ionization, and dissociative attachment. The data derived from swarm experiments are also considered. For each of these processes, the recommended values of the cross sections are presented. The literature has been surveyed through early 2016.

PACS numbers: 34.80.Bm, 52.20.Fs
Keywords: electron collisions, total cross sections, ionization, dissociation, attachment, evaluation

### I. INTRODUCTION

Acetylene (HCCH) is the simplest triply-bonded hydrocarbon molecule and has particular importance in a variety of different plasma processes. For example plasma can be used to make HCCH from coal[1], natural gas[2] and methane[3,4]. Conversely acetylene plasmas are used for a variety of chemistries[5]; they are used to make $C_2$[6], CH*[7], fullerenes[8], diamonds[9], carbon nanoparticles[10], hydrocarbon nanoparticle[11], nanotubes[12,13] and polymers[14], as well as other chemical processes[15,16]. Acetylene plasmas are used to provide a variety of different coatings[17,18]. The role of acetylene in fusion plasmas has also been considered[19,20]. Acetylene is well-known from combustion, where oxy-acetylene flames provide particularly hot (~3000 K) flames which are in routine everyday use. Acetylene is also an important component of cool carbon-rich stars Matsuura et al. [21] whose spectra require considerable data to model[22].

This work uses the same methodology as our recent review of electron – methane collision data[23]. However there have been significantly fewer experimental studies of electron – acetylene collisions. This means that the accuracy for many of the cross sections we recommend is less satisfactory. Measured cross sections for processes involving ground state acetylene have been previously compiled and assessed[24,25]. In this paper, we compile and review data reported up to early 2016 for the various cross sections involving electron scattering from acetylene. We suggest recommended cross sections for the different scattering processes and identify processes which would benefit from further study.

[a)] Electronic mail: corresponding author at mysong@nfri.re.kr

### II. TOTAL SCATTERING CROSS SECTION

The total cross section (TCS) in acetylene, compared to methane, have been measured in relatively few experiments. The TCS in the low energy region is dominated by a $^2\Pi_g$ resonant state, centered around 2.5 eV[26], with a TCS exceeding $40\times10^{-16}$ cm$^2$. At 6 eV another, $^2\Sigma_g^+$ resonant state was observed[26]. In the TCS this latter resonance appears as broad maximum, with a somewhat similar amplitude (about $27\times10^{-16}$ cm$^2$) and position (about 8 eV) to that in $CH_4$, see Song et al.[23]

A number of theoretical studies have also characterized these resonances[27–31] generally via consideration of elastic scattering. These studies will be considered as appropriate below.

In the region of the $^2\Pi_g$ resonance we analysed four experiments:

- absolute measurements by Brüche[32] who used a Ramsauer-type apparatus at 1-50 eV energy range;
- absolute measurements with use of an electrostatic analyzer[33] by the group of Szmytkowski et al.;[33] at 0.6-270 eV;
- absolute measurements with magnetically guided electron (and positron) beam at 1-400 eV by Sueuko and Mori[34];
- normalized transmission current in the dissociative attachment experiment by Dressler and Allan[35].

➔ present a systematic review of the published cross sections for processes resulting from electron collisions with acetylene up to early 2016.

➔ Both measurements and theoretical predictions are considered, although priority is given to high quality measurements with published uncertainties where available.

➔ There is considerable variation in the reliability of the available data.

# Group Evaluation – on going projects

## ➔ Cross sections for electron collisions with $NF_3$
## ➔ Cross sections for electron collisions with $NO_2$, $N_2O$

### Cross Sections for Electron Collisions with $NF_3$

Mi-Young Song[a),1] Jung-Sik Yoon,[1] Hyuck Cho,[2] Grzegorz P. Karwasz,[3] Viatcheslav Kokoouline,[4] Yoshiharu Nakamura,[5] and Jonathan Tennyson[6]
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(Revised 15 October 2016)

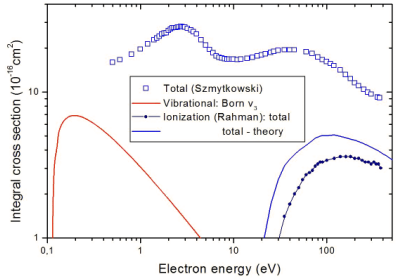
Cross section data are compiled from the literature for electron collisions with nitrogen trifluoride ($NF_3$) molecules. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, excitations of rotational and vibrational states, dissociation, ionization, and dissociative attachment. The data derived from swarm experiments are also considered. For each of these processes, the recommended values of the cross sections are presented. The literature has been surveyed through mid 2016.

PACS numbers: 34.80.Bm, 52.20.Fs
Keywords: electron collisions, total cross sections, ionization, dissociation, attachment, evaluation

#### I. INTRODUCTION

Nitrogen trifluoride or trifluoramine ($NF_3$) gas is widely used in plasma processing technology. A discussion on the use in thin-film and solar cell production, chemical laser, environmental impact, etc.

In the ground electronic state $^1A'$ the molecule has a shape of a pyramid of the $C_{3v}$ group with fluorine atoms forming an equilateral triangle. Due to its symmetry, the dipole moment of the molecule is aligned along the $C_3$ symmetry axis. Geometry, electric dipole moment, and rotational constants are specified in Table I.



# Lessons Learned from Group Evaluation (2013~2016)

➔ Group evaluation can make data collection more widely.
- consider the unpublished or research data using network

➔ Data generation (theoretically)
- if there are no data, but important data for evaluation!

➔ Various expert knowledge is including in Group evaluation
- although there are no standard method, we found effective and reasonable method → Group Evaluation

➔ Most important lesson is **leave the all comments on paper** for community

# Summary - Data Evaluation

➔ **Final Goal : Standard Data Library for AM/PSI data for fusion and other plasma application**

- establis valuation process

➔ **Evaluati**

(1) Consi

- $Q_T$ ( ocess)

(2) Swarr

(3) Model

- Chem

# Recommended Data of Helium(experiment)

# coming soon!