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Report on Cross Section Data Compilation for  
Electron and Ion Collisions with Molecules of Hydrogen,  
Hydrogen Isotopes, Nitrogen, Oxygen, Hydrocarbons,  
Water and Carbon Oxide

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# Report on Cross Section Data Compilation for Electron and Ion Collisions with Molecules of Hydrogen, Hydrogen Isotopes, Nitrogen, Oxygen, Hydrocarbons, Water and Carbon Oxide

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## Abstract

A working group searched and reviewed literatures relevant to cross section data for various processes of electron and ion collisions with molecules of hydrogen, hydrogen isotope, hydrocarbon, nitrogen, oxygen, carbon oxide, and water. New data collected by this working group were added to the NIFS (National Institute for Fusion Science) database (<https://dbshino.nifs.ac.jp>) for molecular target, i. e. AMOL (electron collision) and CMOL (ion collision). A new online bibliography database for electron-molecule scattering (<http://crdb.nifs.ac.jp/bib/iti/top.php>) was developed. This is a summary report of this work done by the working group in 2003-2004.

Keywords: electron-molecule collision, ion-molecule collision, cross section, database

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# 1. Introduction

During our '03-'04 activity, we have concentrated our effort on specifically aiming at molecular targets in fusion plasma. We have collected new data and evaluate them for a variety of molecules from hydrogen molecules to hydrocarbons both by electron and ionic impacts. There is a large volume of data collected from previous activities in NIFS for H<sub>2</sub> and D<sub>2</sub> targets. However, for these molecules in hydrogen family, we have found quite a few new experimental as well as theoretical data for various processes by electron and proton impacts and hence, have undertaken an effort of collecting and critically evaluating them and finally have updated our data base in NIFS. We were also concerned with fragmentation processes of molecules after ionization and charge transfer and collected a few new data for fragmentation and fragmented species, while from different perspective, we looked into water molecule since it is relevant to medical purpose as well. As a recent trend, coupled with rapid development of plasma-processing, vigorous experimental and theoretical studies have been performed for hydrocarbons by electron and ion impacts and as a consequence, a large volume of data have been found and collected. Even those molecules where no data is available for hydrocarbon molecules, our experimental members have carried out research to determine collision dynamics and provide accurate cross section data for as a wide energy range as possible. This aspect, that we are able to carry out own research for providing cross section data if necessary, is a part of our strengths and uniqueness of this working group.

The members of this working group are:

- Mineo Kimura (Ion collision: Kyushu University),
- Yukikazu Itikawa (Electron collision: Institute of Space and Astronautical Science, professor emeritus),
- Makoto Imai (Ion collision: Kyoto University),
- Toshio Kusakabe (Ion collision: Kinki University),
- Kenji Motohashi (Ion fragmentation: Tokyo University of Agriculture and Technology),
- Lukas Pichl (Ion collision: International Christian University),
- Reiko Suzuki (Ion collision: Hitotsubashi University),
- Akinori Igarashi (Electron collision: Miyazaki University),
- Daiji Kato (Electron collision: National Institute for Fusion Science),

- Masashi Kitajima (Electron collision: Sophia University),
- Kengo Moribayashi (Electron collision: Japan Atomic Energy Agency),
- Toru Morishita (Electron collision: University of Electro-Communications),
- Takako Kato (Coordinator: National Institute for Fusion Science),
- Izumi Murakami (Coordinator: National Institute for Fusion Science).

Below, each report from individual member is presented.

M. Kimura

## 2. Electron collisions

Electron collisions for molecules of  $\text{H}_2, \text{D}_2, \text{HD}, \text{H}_3^+, \text{D}_3^+, \text{C}_m\text{H}_n, \text{O}_2, \text{H}_2\text{O}$  and  $\text{CO}$  were considered in this work. There were several relevant data books published already. A list of the data books was prepared by Itikawa. Members of this subgroup reviewed the data books on the list. In addition, they searched new publications also which were not considered in the data books. Integrated cross sections of all fundamental processes by electron collision were collected in this work. The collected data were added to the AMOL database.

### 2.1 $\text{H}_2, \text{HD}$ and $\text{D}_2$ (A. Igarashi)

We have added  $e^- + \text{H}_2$  scattering cross sections to AMOL for total, elastic, momentum transfer, excitation, ionization, attachment, and photo emission. Data for other targets:  $\text{H}_2^+, \text{H}_3^+, \text{HD}, \text{HD}^+, \text{D}_2, \text{D}_2^+, \text{D}_3^+$  were also included. The literatures are found in Refs. [1]-[12], and summarized in Table I.

TABLE I: Reference table for hydrogen molecule

Process	References
Total	[1], [13]-[24]
Elastic	[4, 9, 25-33]
Momentum transfer	[1, 3, 4, 8, 26, 27, 31-35]
Rotational excitation	[8, 9, 12, 28, 34, 36-39]
Vibrational excitation	[3, 8, 10, 12, 27, 28, 32-36],[40]-[48]
Electronic excitation	[9, 12, 31, 43], [49]-[63]
Ionization	[2, 5, 7, 9, 64-69]
Stopping	[8, 11]
Dissociation	[2, 5, 9]
Photo emission	[5, 9]

## 2.2 $C_mH_n$ (M. Kitajima)

Electron collisions with hydro-carbons are known to play an important role in the edge of the fusion plasmas. In order to understand the plasmas and construct the modeling of the plasmas, a complete cross section database is necessary and, a number of experimental and theoretical cross section data have been reported. Compilation of these cross section data has been carried out periodically [70–72]. Analytic fit curves of the recommended electron impact cross sections for small hydro-carbons by Janev *et al.* [71] and Shirai *et al.* [72] have been stored into the new version of the cross section database, AMOL. Most of the cross section data reported up to 2004 other than compiled by Janev *et al.* [71] and Shirai *et al.* [72] have also been stored into the database. Molecules and processes for the stored cross section data sets are shown in Table II-IV.

TABLE II: Reference table for electron impact cross section data of  $C_mH_n$  ( $m = 1$ ).

Molecule	Process	References
CH <sub>4</sub>	total	V [72], E [73], T [74]
	elastic scattering	V [72]
	momentum transfer	V [72]
	total ionization	V [71], V [72], T [75], T [76], T [77], E [78], E [79], E [80], E [81]
	ionization	
	$CH_4 + e \rightarrow CH_4^+ + 2e$	V [71], V [72], E [80], E [81], E [82]
	dissociative ionization	
	$CH_4 + e \rightarrow CH_3^+$	V [71], V [72], E [80], E [81], E [82]
	$CH_4 + e \rightarrow CH_2^+$	V [71], V [72], E [80], E [81], E [82]
	$CH_4 + e \rightarrow CH^+$	V [71], V [72], E [80], E [81], E [82]
	$CH_4 + e \rightarrow C^+$	V [71], V [72], E [80], E [81], E [82]
	$CH_4 + e \rightarrow H_2^+$	V [71], V [72], E [81], E [82]
	$CH_4 + e \rightarrow H^+$	V [71], V [72], E [81], E [82]
	$CH_4 + e \rightarrow CH_2^+ + H^+$	E [83]
	$CH_4 + e \rightarrow CH^+ + H^+$	E [83]
	$CH_4 + e \rightarrow C^+ + H^+$	E [83]
	11 channels of ionic fragment pair production at 200eV	E [82]
	total dissociation	V [72]
	attachment	
	$CH_4 + e \rightarrow CH_4^-$	V [72]
CH <sub>3</sub>	total	T [74]
	total ionization	V [71], T [84]
	ionization	
	$CH_3 + e \rightarrow CH_3^+ + 2e$	V [71]
	dissociative ionization	
	$CH_3 + e \rightarrow CH_2^+$	V [71]
	$CH_3 + e \rightarrow CH^+$	V [71]
$CH_3 + e \rightarrow C^+$	V [71]	
$CH_3 + e \rightarrow H_2^+$	V [71]	
$CH_3 + e \rightarrow H^+$	V [71]	
CH <sub>2</sub>	total	T [74]
	total ionization	V [71], T [84]
	ionization	
	$CH_2 + e \rightarrow CH_2^+ + 2e$	V [71]
dissociative ionization		
$CH_2 + e \rightarrow CH^+$	V [71]	
$CH_2 + e \rightarrow C^+$	V [71]	

(continued.)

Molecule	Process	References
	$\text{CH}_2 + e \rightarrow \text{H}_2^+$	V [71]
	$\text{CH}_2 + e \rightarrow \text{H}^+$	V [71]
CH	total	T [74]
	total ionization	V [71], T [86]
	ionization	
	$\text{CH} + e \rightarrow \text{CH}^+ + 2e$	V [71]
	dissociative ionization	
	$\text{CH} + e \rightarrow \text{C}^+$	V [71]
	$\text{CH} + e \rightarrow \text{H}^+$	V [71]
	excitation	
	$\text{CH}(X \ ^2\Pi) + e \rightarrow \text{CH}(A \ ^2\Delta)$	T [85]
	$\text{CH}(X \ ^2\Pi) + e \rightarrow \text{CH}(B \ ^2\Sigma^-)$	T [85]
	$\text{CH}(X \ ^2\Pi) + e \rightarrow \text{CH}(C \ ^2\Sigma^+)$	T [85]
	$\text{CH}(X \ ^2\Pi) + e \rightarrow \text{CH}(a \ ^4\Sigma^-)$	T [85]

TABLE III: Reference table for electron impact cross section data of  $C_mH_n$  ( $m = 2$ ).

Molecule	Process	References
$\text{C}_2\text{H}_6$	total	V [72], E [73]
	elastic scattering	V [72]
	momentum transfer	V [72]
	total ionization	V [71], V [72], E [79], E [81]
	ionization	
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2\text{H}_6^+ + 2e$	V [71], V [72], E [81], E [82], E [87]
	dissociative ionization	
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2\text{H}_5^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2\text{H}_4^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2\text{H}_3^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2\text{H}_2^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2\text{H}^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{CH}_3^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{CH}_2^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{CH}^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}^+$	V [71], V [72], E [81], E [82], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{H}_3^+$	V [72], E [82]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{H}_2^+$	V [72], E [82]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{H}^+$	V [72], E [82]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2\text{H}_5^{2+}$	V [71], E [87]
	$\text{C}_2\text{H}_6 + e \rightarrow \text{C}_2\text{H}_3^{2+}$	E [87]
	42 channels of ionic fragment	
	pair production at 200eV	E [82]
	total dissociation	V [72]
$\text{C}_2\text{H}_5$	total ionization	V [71]
	ionization	
	$\text{C}_2\text{H}_5 + e \rightarrow \text{C}_2\text{H}_5^+ + 2e$	V [71]
	dissociative ionization	
	$\text{C}_2\text{H}_5 + e \rightarrow \text{C}_2\text{H}_4^+$	V [71]
	$\text{C}_2\text{H}_5 + e \rightarrow \text{C}_2\text{H}_3^+$	V [71]
	$\text{C}_2\text{H}_5 + e \rightarrow \text{C}_2\text{H}_2^+$	V [71]
	$\text{C}_2\text{H}_5 + e \rightarrow \text{C}_2\text{H}^+$	V [71]
	$\text{C}_2\text{H}_5 + e \rightarrow \text{CH}_3^+$	V [71]
	$\text{C}_2\text{H}_5 + e \rightarrow \text{CH}_2^+$	V [71]
	$\text{C}_2\text{H}_5 + e \rightarrow \text{CH}^+$	V [71]
	$\text{C}_2\text{H}_5 + e \rightarrow \text{C}^+$	V [71]
$\text{C}_2\text{H}_4$	total	V [72], E [73], E [88]
	elastic scattering	E [89]
	momentum transfer	V [72], E [89]
	total ionization	V [71], V [72], E [84]



(continued.)

Molecule	Process	References
	ionization	
	$C_2H_4 + e \rightarrow C_2H_4^+ + 2e$	V [71], V [72]
	dissociative ionization	
	$C_2H_4 + e \rightarrow C_2H_3^+$	V [71], V [72]
	$C_2H_4 + e \rightarrow C_2H_2^+$	V [71], V [72]
	$C_2H_4 + e \rightarrow C_2H^+$	V [71], V [72]
	$C_2H_4 + e \rightarrow C_2^+$	V [71], V [72]
	$C_2H_4 + e \rightarrow CH_3^+$	V [71], V [72]
	$C_2H_4 + e \rightarrow CH_2^+$	V [71], V [72]
	$C_2H_4 + e \rightarrow CH^+$	V [71], V [72]
	$C_2H_4 + e \rightarrow C^+$	V [71], V [72]
	$C_2H_4 + e \rightarrow H_2^+$	V [72]
$C_2H_4 + e \rightarrow H^+$	V [72]	
$C_2H_3$	total ionization	V [71]
	ionization	
	$C_2H_3 + e \rightarrow C_2H_3^+ + 2e$	V [71]
	dissociative ionization	
	$C_2H_3 + e \rightarrow C_2H_2^+$	V [71]
	$C_2H_3 + e \rightarrow C_2H^+$	V [71]
	$C_2H_3 + e \rightarrow C_2^+$	V [71]
	$C_2H_3 + e \rightarrow CH_2^+$	V [71]
	$C_2H_3 + e \rightarrow CH^+$	V [71]
$C_2H_3 + e \rightarrow C^+$	V [71]	
$C_2H_3 + e \rightarrow H^+$	V [71]	
$C_2H_2$	total	V [72], E [73], E [90]
	elastic scattering	V [72]
	momentum transfer	V [72]
	total ionization	V [71], V [72], T [86]
	ionization	
	$C_2H_2 + e \rightarrow C_2H_2^+ + 2e$	V [71], V [72]
	dissociative ionization	
$C_2H_2 + e \rightarrow CH^+$	V [71], V [72]	
$C_2H_2 + e \rightarrow C_2H^+$	V [71], V [72]	
$C_2H_2 + e \rightarrow C_2H_2^{2+}$	V [71]	
$C_2H$	total ionization	V [71]
	ionization	
	$C_2H + e \rightarrow C_2H^+ + 2e$	V [71]
	dissociative ionization	
	$C_2H + e \rightarrow C_2^+$	V [71]
	$C_2H + e \rightarrow CH^+$	V [71]
$C_2H + e \rightarrow C^+$	V [71]	
$C_2H + e \rightarrow H^+$	V [71]	

TABLE IV: Reference table for electron impact cross section data of  $C_mH_n$  ( $m = 3$ ).

Molecule	Process	References	
$C_3H_8$	total	V [72], E [91]	
	elastic scattering	V [72]	
	momentum transfer	V [72]	
	total ionization	V [71], V [72], E [79]	
	ionization		
	$C_3H_8 + e \rightarrow C_3H_8^+ + 2e$	V [71], V [72], E [92], E [82], E [93]	
	dissociative ionization		
	$C_3H_8 + e \rightarrow C_3H_7^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_6^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_5^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_4^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_3^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_2^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_2H_5^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_2H_4^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_2H_3^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_2H_2^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_2H^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_2^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow CH_3^+$	V [71], V [72], E [92], E [82], E [93]	
	$C_3H_8 + e \rightarrow CH_2^+$	V [71], V [72], E [92], E [82], E [93]	
	$C_3H_8 + e \rightarrow CH^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C^+$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow H_3^+$	E [82], E [93]	
	$C_3H_8 + e \rightarrow H_2^+$	E [82], E [93]	
	$C_3H_8 + e \rightarrow H^+$	E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_5^{2+}$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_4^{2+}$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_3^{2+}$	V [71], V [72], E [82], E [93]	
	$C_3H_8 + e \rightarrow C_3H_2^{2+}$	V [71], V [72], E [82], E [93]	
	89 channels of ionic fragment pair production at 200eV	E [82], E [93]	
	$C_3H_7$	total ionization	V [71]
	$C_3H_6$ (propene)	total	V [72], E [94]
		total ionization	V [71], V [72]
	$C_3H_6$ (cyclopropane)	total	V [72], E [94]
		total ionization	V [72]
	$C_3H_5$	total ionization	V [71]
$C_3H_4$ (allene)	total	E [91], E [95]	
	elastic scattering	E [95], T [96]	
	momentum transfer	E [95], T [96]	
$C_3H_4$ (propyne)	total	E [91], E [95]	
	total ionization	V [71]	
	elastic scattering	E [95], T [96]	
	momentum transfer	E [95], T [96]	
$C_3H_4$ (cyclopropene)	elastic scattering	T [96]	
	momentum transfer	T [96]	
$C_3H_3$	total ionization	V [71]	
$C_3H_2$	total ionization	V [71]	
$C_3H$	total ionization	V [71]	

### 2.3 O<sub>2</sub> (D. Kato)

Cross section data were found in previous data compilations listed below.

- Hayashi (1981) [1] presented recommended values of integral and momentum-transfer cross sections for elastic collision and total scattering cross section by electron impact for energies of  $10^{-3}$ eV to keV range. Estimated error of the momentum-transfer cross section was up to 20 %.
- Trajmar (1983) [3] compiled experimental cross section data for various processes which had become available since 1970.
- Tawara and Kato (1987) [7] compiled experimental cross section data for electron impact ionization. To that end, they surveyed relevant literatures up to mid-1986. Those numerical data are stored as one of our databases (AMDIS:Atomic and Molecular Data Interactive System).
- A comprehensive data compilation was reported by Itikawa *et al.* (1989) [97], which included total scattering, elastic scattering, momentum transfer, excitation of rotational, vibrational, and electronic states, dissociation, ionization, and attachment. Later, Itikawa (1994) [98] presented a set of cross section data updated.
- Kanik *et al.* (1993) [99] critically reviewed experimental cross section data for total and elastic scattering, excitation and ionization, and deduced a set of recommended cross sections.
- Zecca *et al.* (1996) [10] reviewed updated experimental data and presented available data for elastic and total scattering, vibrational and electronic excitation, dissociation and ionization cross sections at energies from 0.74 upto 1000 eV.
- Majeed and Strickland (1997) [100] surveyed cross section measurements in the late 1980s and early 1990s, and presented a recommended data set for total ionization and vibrational and electronic excitations.
- Brunger and Buckman (2002) [12] reported a data compilation at low to intermediate energies ( $10^{-3}$ eV-100eV) with the intention to update the data compilation by Trajmar *et al.* [3] in 1983.

The cross section data of the above compilations are summarized in Table V. Note this report presents experimental and recommended data only. In some cases, the same data of the identical

paper were included in different compilations. Measurement of ionization cross section by Tian and Vidal (1998) [101] is included in Table V. The data were added to the AMOL database.

Total cross sections and (gross) ionization cross sections are fairly accurate within 5-10 %. Elastic cross sections have uncertainty of 20 % due to lack of reliable differential cross sections. Electronic excitation cross section for vibrationally excited targets is scarce. In measurements of dissociation cross sections, fraction of fragment ion in a particular excited state is unknown. The total, elastic and excitation cross sections show broad maxima at electron energies of about 10 eV, while the ionization cross sections and the emission cross sections of dissociation fragments have maxima at about 100 eV.

TABLE V: Cross section data collection for electron collision with O<sub>2</sub>. (E) stands for experimental data and (V) for recommended data.

Process	Electron Energy (eV)
Grand total	0.15-100(E) [12], 1-2000(V) [1], 0.5-1600(E) [3], 1-1000(V) [99], 0.1-1000(V) [97], 0.74-1000(E) [10]
Elastic	1-100(E) [12], 1-1000(V) [1], 2-500(E) [3], 1-1000(V) [99], 0.6-1000(V) [97], 0.74-1000(E) [10]
Elastic momentum transfer	1-100(E) [12], 0-1000(V) [1], 2-200(E) [3], 0.6-1000(V) [97]
Vibrational excitation sum of $v'=1-12$ $v'=1,2,3,4$ total	4-45(E) [97] 5-15, 20(E) [12] 1-30(V) [100], 0.74-15(E) [10]
Electronic excitation total	15-1000(E+V) [10]
$a^1\Delta_g$	2.6-28.6(E) [12], 1.5-200(E) [3, 97], 2-200(V) [100]
$b^1\Sigma_g^+$	5-20(E) [12], 2-150(E) [3, 97], 2-100(V) [100]
$A^3\Sigma_u^+ + C^3\Delta_u + c^1\Sigma_u^-$	20-500(E) [3], 9-20(E) [12], 10-500(E) [97], 6-200(V) [100]
Schumann-Runge continuum ( $I^3\Pi_g + B^3\Sigma_u^- + \text{unknown}$ )	20-500(E) [3, 97]
$B^3\Sigma_u^-$	15-50(E) [12], 9-1000(V) [100]
$I^3\Pi_g$	15-50(E) [12], 8-200(V) [100]
$W=8.9$ eV	9-1000(V) [100]
longest band ( $W=9.97$ eV)	15-50(E) [12], 11-1000(V) [100]
second band ( $W=10.29$ eV)	15-50(E) [12], 12-500(V) [100]
$W=9.7-12.1$ eV	20-100(E) [3, 97]
Rydberg	17-1000(V) [100]
Inelastic (elec. + rovib.)	4-1000(V) [99]
<u>Ionization</u>	

(continued.)

Process	Electron Energy (eV)
gross ionization	13-1000(E) [98], 13-1000(E) [100], 20-1000(E) [10]
total single-ionization	12.5-20000(E) [7], 15-1000(V) [99], 17.5-600(E) [101]
total double-ionization	45-600(E) [101]
total dissociative ionization	19-1000(V) [97]
O <sub>2</sub> <sup>+</sup>	13-500(E) [7], 17.5-600(E) [101], 13-170(V) [97]
	13-1000(V) [98]
O <sub>2</sub> <sup>2+</sup>	42-167(E) [7]
O <sup>+</sup>	42-167(E) [7], 25-600(E) [101]
O <sup>+</sup> +O	25-600(E) [101]
O <sup>+</sup> +O <sup>+</sup>	45-600(E) [101]
O <sup>2+</sup>	70-600(E) [101], 55-1000(E) [98]
O <sup>2+</sup> +O	100-600(E) [101]
O <sup>2+</sup> +O <sup>+</sup>	100-600(E) [101]
sum of O <sup>+</sup> and O <sub>2</sub> <sup>2+</sup>	18-1000(E) [98]
ionization excitation: O <sub>2</sub> <sup>+</sup> (b <sup>4</sup> Σ <sub>g</sub> <sup>-</sup> )	20-5000(V) [97]
Emission cross section	
O(2p <sup>3</sup> 3s <sup>3</sup> S → 2p <sup>4</sup> <sup>3</sup> P, 130.4 nm)	20-4000(E) [97]
O(2p <sup>3</sup> 3s <sup>3</sup> D → 2p <sup>4</sup> <sup>3</sup> P, 98.9 nm)	25-400(E) [97]
O(2p <sup>3</sup> 3d <sup>3</sup> D → 2p <sup>4</sup> <sup>3</sup> P, 102.7 nm)	25-400(E) [97]
O(2p <sup>3</sup> 3p <sup>3</sup> P → 2p <sup>3</sup> 3s <sup>3</sup> S, 844.7 nm)	20-1000(E) [97]
O <sub>2</sub> <sup>+</sup> (b <sup>4</sup> Σ <sub>g</sub> <sup>-</sup> → a <sup>4</sup> Π <sub>u</sub> )	20-5000(E) [97]
O <sup>+</sup> (2s2p <sup>4</sup> <sup>4</sup> P → 2s <sup>2</sup> 2p <sup>3</sup> <sup>4</sup> S, 83.3 nm)	40-2000(E) [97]
Dissociation	
neutral products only	15-150(E) [10]
Dissociative attachment	
O <sup>-</sup> +O	5-12(E) [97]

## 2.4 H<sub>2</sub>O (K. Moribayashi)

There are a lot of data of electron impact cross sections of H<sub>2</sub>O in Ref. [8, 102]. In addition to the papers cited in Ref. [8, 102], we have found 19 papers which the cross sections for the processes of elastic scattering [103–107], dissociation and emission [108–111], ionization and dissociation [84, 112–117], and vibrational excitation [118, 119] were shown. It is noted that a data compilation updated by Itikawa and Mason [120] has been published after the present work. They assessed the data carefully and provided recommended data for all major processes. These cross sections are useful for the analysis of the radiation irradiation on the biological materials.

## 2.5 CO (T. Morishita)


Recently, Brunger and Buckman [12] reported a comprehensive study of experimental cross sections of electron collision with diatomic molecular targets at low to intermediate energies ( $10^{-3}$ eV-100eV). The author (TM) got cross section data of CO molecules on their report for elastic, rotational excitation, vibrational excitation and electronic excitation, and input the data into the AMOL database.

## 2.6 New bibliography databases (L. Pichl)


Upon suggestion of Professor Y. Itikawa, member of the data update working group, we have also developed a new bibliography database for electron-molecule scattering which is available online at the Coordination Research Center of NIFS [121, 122]. The online interface and sample data are shown in Fig. 1.

To this aim, the group of the University of Aizu set up a small database server for experimental purposes in cooperation with Dr. Daiji Kato. The bibliography database is novel by allowing the users to search for *target molecule* and *collision process* entries. The server also hosts other online databases and tools for cooperative projects with other database working groups, especially Dr. Akira Sasaki, JAEA and Dr. Lukáš Pichl, University of Aizu.

アドレス http://crdb.nifs.ac.jp/bib/iti/top.php



# Bibliography Database



Author

Year

Journal

Title

Category

Molecule/Process

[ [Prof. Itikawa's list](#) | [Joint Search](#) | [Evolutionary Database](#) ]

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アドレス http://crdb.nifs.ac.jp/bib/iti/search.php

68 RESULTS [1-10]

author	year	journal	volume	page	title	category	molecule/process
R. A. Bonham	1994	Jpn. J. App. Phys.	33	4157	Electron impact cross section data for carbon tetrafluoride	B	CF4/elas, CF4/mom, CF4/vib, CF4/att, CF4/ion, CF4/diss
M. C. Bordage, P. Segur, A. Chouki	1996	J. Appl. Phys.	80	1325	Determination of a set of electron impact cross sections in tetrafluoromethane consistent with experimental determination of swarm parameters	D	CF4/rot, CF4/mom, CF4/vib, CF4/att, CF4/diss, CF4/ion
M. J. Brunger, S. J. Buckman	2002	Phys. Rep.	357	215	Electron-molecule scattering cross-sections. I. Experimental techniques and data for diatomic molecules	A	H2/tot, H2/elas, H2/mom, H2/rot, H2/vib, H2/e-exc, N2/tot, N2/elas, N2/mom, N2/rot, N2/vib, N2/e-exc, O2/tot, O2/elas, O2/mom, O2/vib, O2/e-exc, CO/tot, CO/elas, CO/mom, CO/rot, CO/vib, CO/e-exc, NO/tot, NO/elas, NO/mom, NO/vib, NO/e-exc, Cl2/tot, Cl2/elas, HF/elas, HF/rot, HF/vib, HCl/elas, HCl/rot, HCl/vib
M. Capitelli, C. M. Ferreira, B. F. Gordiets, A. I. Osipov	2000	Plasma Kinetics in Atmospheric Gases	0	0		C	N2/elas, N2/e-exc, N2/ion, O2/elas, O2/e-exc, O2/ion

FIG. 1: Bibliography database for electron-molecule scattering with search capabilities for target molecules and collisional processes. Data by courtesy of Prof. Y. Itikawa. Available online at [121].

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### 3. Ion collisions

Following sections concern ion-molecule collision. Cross section data compilation for target molecules of H<sub>2</sub>, HD, D<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, C<sub>m</sub>H<sub>n</sub>, CO and CO<sub>2</sub> is presented. The data were added to the CMOL database.

#### 3.1 H - Ne projectiles colliding with H<sub>2</sub>, D<sub>2</sub>, N<sub>2</sub> and O<sub>2</sub> (M. Imai)

In the present work, new data were added for collision systems of atoms and ions of H - Ne projectiles colliding with molecules of hydrogen, deuterium, nitrogen and oxygen with intention to update Table 13 of the previous report (NIFS-DATA-70 [1]). Data for state-selective collisions are also included [3],[8]. Note that Dmitriev *et al.* [7] have studied single electron capture by helium-like projectiles of Li, Be and N ions at the ground and metastable(1s2s) states from N<sub>2</sub> molecules.

Projectile ionic species	Target molecular species	References
H <sup>0</sup> , H <sup>+</sup> , D <sup>+</sup>	H <sub>2</sub> , HD, D <sub>2</sub>	[4, 6, 10]
N <sup>5+</sup>	H <sub>2</sub>	[3, 8]
O <sup>q+</sup> (q=0,2-6)	H <sub>2</sub>	[5, 9]
He <sup>2+</sup>	O <sub>2</sub>	[2]
Li <sup>+</sup>	N <sub>2</sub>	[7]
Be <sup>2+</sup>	N <sub>2</sub>	[7]
N <sup>5+</sup>	N <sub>2</sub>	[7]
O <sup>0</sup>	N <sub>2</sub> , O <sub>2</sub>	[9]

#### 3.2 Dissociative charge exchange of H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CO, CO<sub>2</sub> and C<sub>n</sub>H<sub>m</sub> (K. Motohashi)

Data of ion-production cross sections, emission cross sections and branching ratios for dissociative charge exchange in ion-molecule collisions in the impact-energy range from 1 eV to 100 keV were compiled and analyzed. Papers on cross sections, branching ratios and the kinetic energy release (KER) of fragment ions in "Journal of Physics B", "Physical Review A", "Physical Review Letters" and "The Journal of Chemical Physics" in 1969 to 1999 were collected.

Fragmentation or dissociation of molecule is one of the most fundamental processes among chemical reactions. Dissociation via the charge exchange of ion-molecule collisions is especially important

in the plasma of ionosphere and nuclear fusion because of their large cross sections. There have been very scarce, however, of quantitative studies on dissociative ion-molecule collisions in low energy (from 1 eV to 100 keV). In this report, the data on cross sections, branching ratios of ion production, and KERs of fragment ions in dissociative charge exchange processes of ion-molecule collisions are compiled and summarized.

Studies on dissociative charge exchange of ion-molecule collisions reported in 1969 to 1999 were found in "Journal of Physics B", "Physical Review A", "Physical Review Letters" and "The Journal of Chemical Physics". In the present research, incident ions of  $H^+$ ,  $C^{q+}$ ,  $N^{q+}$ ,  $O^{q+}$ , and rare gas ions were considered. Target molecules were  $H_2$ ,  $N_2$ ,  $O_2$ ,  $CO$ ,  $CO_2$  and the simple hydrocarbon molecules. Collision energy is in the range from 1 eV to 100 keV. Charge exchange process is dominant in this energy range.

The cross-section measurements of dissociative charge transfer in ion-molecule collisions are listed in Table VI. Five papers in keV energy range and four papers in eV energy range are included. All of them are experimental studies. Detected particles are fragment ions except for the study of reference [16]. Absolute cross sections of secondary ion formation from many kinds of simple molecules were measured by Gilbody's group [11–13]. The cross sections were obtained by normalizing the values of total cross sections of secondary ion formation to ones measured by de Heer *et al.* [20]. Errors of their cross sections were estimated to be less than 20%. This value includes reading error of about 7% associated with relative measurements and uncertainty of 10% in normalization procedure. Lindsay *et al.* [14] measured relative differential cross sections for the production of secondary protons from the specific states of  $H_2^+*$  in 5-25 keV  $H^+$ - $H_2$  collisions by coincidence technique with a time-of-flight mass separator and a parallel plate energy analyzer. Inouye *et al.* [16] measured relative optical emission cross sections of excited  $CH^*$  and  $CH^+$  radicals produced in collisions of  $He^+$  and  $Ar^+$  with acetylene. Only relative cross sections were measured because absolute values of detection efficiency of their optical system were unknown. Absolute state-selected cross sections for abstraction-charge transfer reactions were measured by a group of Iowa State University [17–19]. The state-selected measurements were carried out by use of reactant ions ( $C^+$  and  $O^+$ ) produced by a high-pressure ion source or a VUV photoionization ion source.

In general, measured cross sections for production of secondary particles have relatively large errors because of large uncertainties of detection efficiencies. The detection efficiency generally depends on energies and angles of particles to be detected. It is also difficult to determine absolute values because normalization procedures have uncertainties.

TABLE VI: Cross section measurements of dissociative charge transfer in ion-molecule collisions.

Incident ions	Target molecules	Species	Collision energy	Partial cross sections of	Ref.
H <sup>+</sup>	O <sub>2</sub> , N <sub>2</sub> , CO, and CH <sub>4</sub>	O <sup>+</sup> , O <sup>2+</sup> , N <sup>+</sup> , N <sup>2+</sup> , C <sup>+</sup> , C <sup>2+</sup> , CH <sup>+</sup> , CH <sub>2</sub> <sup>+</sup> , CH <sub>3</sub> <sup>+</sup> , H <sup>+</sup> , H <sub>2</sub> <sup>+</sup>	5-45 keV	Secondary ion formation	[11]
He <sup>+</sup>	H <sub>2</sub> , N <sub>2</sub> , O <sub>2</sub> , CO, CO <sub>2</sub> , and CH <sub>4</sub>	H <sup>+</sup> , N <sup>+</sup> , N <sup>2+</sup> , O <sup>+</sup> , O <sup>2+</sup> , C <sup>+</sup> , C <sup>2+</sup> , CO <sup>+</sup> , CH <sup>+</sup> , CH <sub>2</sub> <sup>+</sup> , CH <sub>3</sub> <sup>+</sup> , and H <sub>2</sub> <sup>+</sup>	5-45 keV (LAB)	Secondary ion formation	[12]
Ne <sup>+</sup> and Na <sup>+</sup>	H <sub>2</sub> , N <sub>2</sub> , O <sub>2</sub> , and CO	H <sup>+</sup> , N <sup>+</sup> , N <sup>2+</sup> , O <sup>+</sup> , O <sup>2+</sup> , C <sup>+</sup> , and C <sup>2+</sup>	5-45 keV (LAB)	Secondary ion formation	[13]
H <sup>+</sup>	H <sub>2</sub>	H <sup>+</sup>	5-25 keV (LAB)	State-selected fragmentation	[14]
H <sup>+</sup>	N <sub>2</sub>	N <sup>+</sup>	5-25 keV	Ion-pair formation	[15]
He <sup>+</sup> and Ar <sup>+</sup>	C <sub>2</sub> H <sub>2</sub>	CH <sup>+</sup> (A-X), (B-X), and CH <sup>+</sup> *(B-A)	30-300 eV (LAB)	Optical emission	[16]
C <sup>+</sup>	N <sub>2</sub>	N <sup>+</sup> and CN <sup>+</sup>	4-8 eV (CM)	Abstraction-charge transfer	[17]
O <sup>+</sup>	H <sub>2</sub> and D <sub>2</sub>	H <sup>+</sup> , D <sup>+</sup> , OH <sup>+</sup> and OD <sup>+</sup>	0.02-12 eV (CM)	Abstraction-charge transfer	[18]
O <sup>+</sup>	N <sub>2</sub>	N <sup>+</sup> and NO <sup>+</sup>	0.06-40 eV (CM)	Abstraction-charge transfer	[19]

### 3.3 Charge transfer of C<sub>m</sub>H<sub>n</sub> (T. Kusakabe)

Collision processes between ions and molecules are important in basic research and in a number of applications such as astrophysics, plasma science and material science. However, the present knowledge of collisions processes involving molecular targets is limited and the amount of collision data is very scarce. Collision data of charge transfer processes by slow ions from molecular targets are urgently required in many applied fields because charge transfer makes a dominant contribution at energies below 100 keV/u. Among many types of molecules, various hydrocarbons, such as CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and so forth, have been observed near the divertor edge. Hence, charge transfer processes for these large hydrocarbons (C<sub>m</sub>H<sub>n</sub>, where  $m = 1 - 4$ ) are also important which provide essential ingredients for the modeling of plasma and carbon behavior. Here we attempt to review cases of some selective hydrocarbons as shown in the following Table.

We searched not only some research journals, but also consulted some data books [21–23]. For hydrocarbons, very few investigations have been carried out. We found only 4 publications [24–27]. Therefore, we undertook the effort to carry out a joint experimental and theoretical study of charge transfer from these hydrocarbons by H<sup>+</sup>, He<sup>2+</sup>, C<sup>q+</sup> ( $q = 1-3$ ), Ne<sup>q+</sup> ( $q = 2-6$ ) and Ar<sup>q+</sup> ( $q = 2-9$ )

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Projectile ionic species:	All species of atomic ions
Target molecular species:	Hydrocarbon molecules ( $C_mH_n$ , where $m = 1 - 4$ )
Energy region:	a few eV - a few MeV
Search of papers published:	Primarily before 2003, but recent interval (2000 - 2003) for light ions ( $H^+ - Ne^{q+}$ ).
References:	[21]-[27]

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ion impacts below 10 keV. We have also carried out a careful study on the effect of vibrational states and isomer of the target. Results will be published elsewhere.

### 3.4 Charge transfer in collisions of $O^{q+}$ ions with $H_2(1s^2X^1\Sigma_g^+)$ (L. Pichl)

There have been two theoretical papers on electron capture in  $O^{q+}$  collisions with the  $H_2$  molecule published in 2004 [28, 41]. Pichl *et al.* [28] calculated the state-resolved and total cross sections with  $q = 1$  for the ground-state  $O^+(^4S)/H_2$  collision using the electronic-state molecular orbital approximation (quantal and semiclassical) with the projectile energy ranging between 50 eV/u and 10 keV/u. They also extrapolated the theoretical method beyond this interval. The results in [28] agree well with different sets of experimental data below and above the projectile energy of 100 eV/u as shown in Fig. 2.

Wang *et al.* [41] calculated the state-resolved and total cross section for the ground-state  $O^{3+}(^2P)/H_2$  collision including target vibrations to some extent while neglecting the possibility of multiple electron capture and Coulomb explosion of the target. The results for fixed  $H_2$  internuclear distance including a comparison to semiclassical results by L. Pichl and M. Kimura are shown in Fig. 3. Final geometry-averaged data including state-resolved cross-section and comparison of various theoretical approaches were also published [41]. Note the agreement of the full-quantal cross sections computed in Stancil's group in University of Georgia with the semiclassical results by Pichl *et al.* in the energy range of 0.1 to 1.0 keV, where both methods apply (cf. Fig. 3).

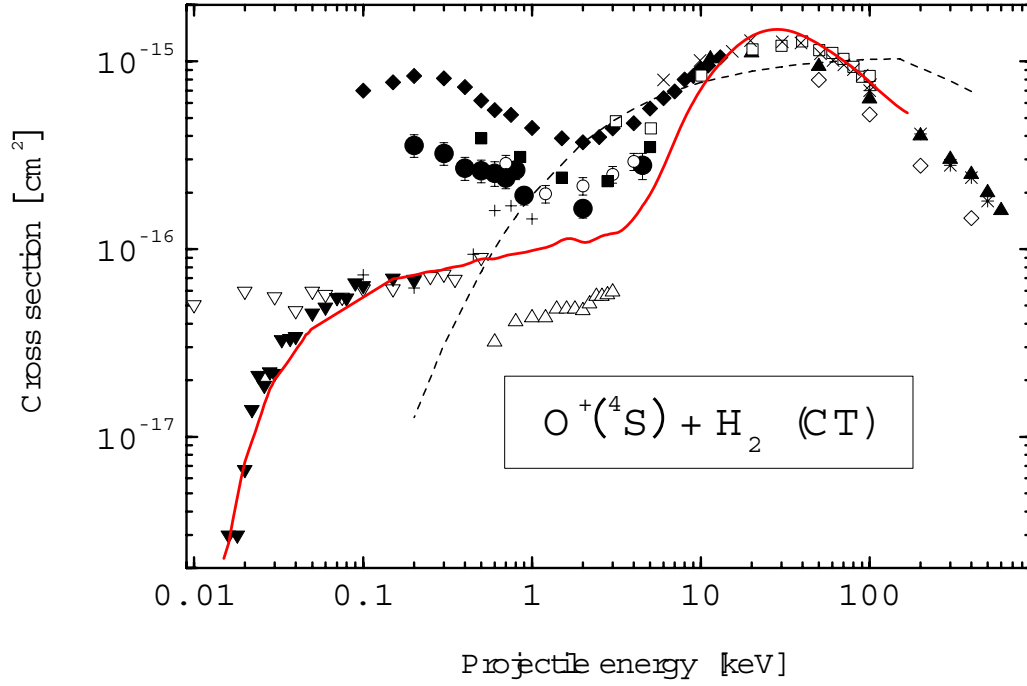


FIG. 2: Total charge transfer cross section for collisions of  $O^+(^4S)$  with the ground-state  $H_2$  (full line) and various experimental data. Solid circle: Kusakabe *et al.* [29], open circle: Kusakabe *et al.* [30], solid square: Sieglaff *et al.* [31], +: Irvine and Latimer [32], solid down triangle: Flesch and Ng [39], open down triangle: Xu *et al.* [33], open square: Hoffman *et al.* [34], solid diamond: Nutt *et al.* [35], solid triangle: Phaneuf *et al.* [36],  $\times$ : Lockwood *et al.* [37], and open triangle: Moran and Wilcox [38]. Dashed line: Olson formula [40] and solid line: our calculation [28].

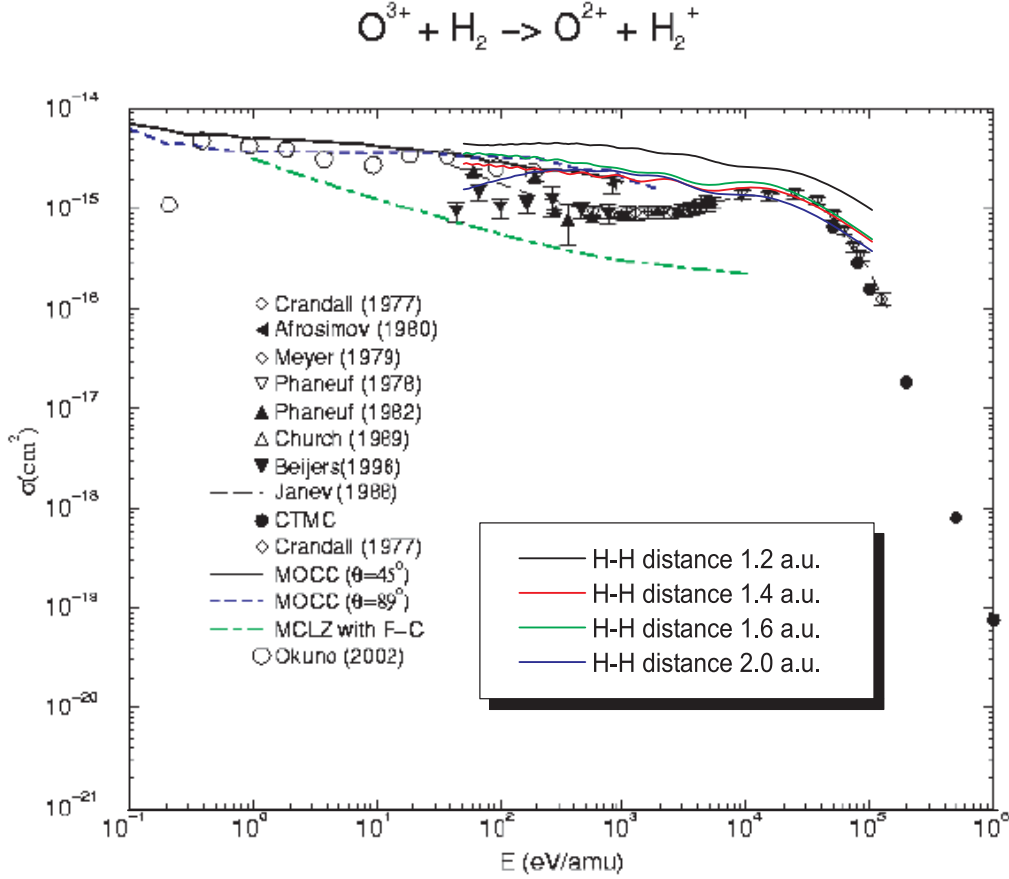


FIG. 3: Single electron capture in collisions of  $\text{O}^{3+}(^2P)$  with ground-state  $\text{H}_2$  for various target internuclear separation and collision angles. The lines show semiclassical approximation by L. Pichl and M. Kimura. The final data for averaged geometries are given in [41].

### 3.5 Evaluation and fitting formulas for $\text{H}^+, \text{O}^+/\text{H}, \text{O}, \text{N}_2, \text{O}_2$ charge-transfer cross sections (L. Pichl)

As a part of our data evaluation effort, we have compiled the evaluation of charge transfer cross sections in collisions of  $\text{H}^+, \text{O}^+/\text{H}, \text{O}, \text{N}_2, \text{O}_2$  (including data resolved with respect to the ground-state  $\text{O}^+(^4S)$  and the metastable  $\text{O}^+(^2D, ^2P)$  ions) in the energy range of 1 eV to 200 keV, which was recently published by Lindsay and Stebbings [42]. Table VII shows the fitting formulas [42] of the Rice University group. The values of the parameters and the applicable energy ranges are listed in Table VIII.

In addition, the integral cross sections for direct scattering of ground-state  $O^+$  ions on He,  $H_2$ ,  $O_2$  and  $N_2$  measured in the same group are shown in Table IX. The cross sections include contributions from all elastic and inelastic processes resulting in a fast  $O^+$  ion. These data complement the charge-transfer cross sections included in the NIFS database. The experimental conditions for the direct scattering measurements [43] were as follows. For  $H_2$ ,  $N_2$ , and  $O_2$  at energies of 0.5 - 5 keV, the angular range is 0.18 - 4.82 degs. The corresponding angular range for He is 0.22 - 4.82 degs. The angular range for the 0.1 keV data is 1.0 - 20 degs.

TABLE VII: Functional form of the charge transfer cross sections in  $10^{-16} \text{cm}^2$ .  $E$  is projectile energy in keV.

Process	$f(E)$
$H^+$ -H	$(a_1 - a_2 \ln E)^2 (1 - e^{-a_3/E})^{4.5}$
$H^+$ -O	$(a_1 - a_2 \ln E)^2 (1 - e^{-a_3/E})^2 + (a_4 - a_5 \ln E)(1 - e^{-a_6/E})^2$
$O^+$ -H	$(a_1 - a_2 \ln E)^2 (1 - e^{-a_3/E})^{0.8}$
$O^+$ ( $^4S$ )-H	$(a_1 - a_2 \ln E)^2$
$O^+$ -O	$(a_1 - a_2 \ln E)^2 (1 - e^{-a_3/E})^{0.8}$
$O^+$ ( $^4S$ )-O	$(a_1 - a_2 \ln E)^2$
$O^+$ ( $^2D, ^2P$ )-O	$(a_1 - a_2 \ln E)^2$
$H^+$ - $N_2$	$a_1 e^{-(\ln E - a_2)^2/a_3} (1 - e^{-E/a_4})^2 + (a_5 - a_6 \ln E)^2 (1 - e^{-a_7/E})^2$
$H^+$ - $O_2$	$(a_1 - a_2 \ln E)^2 (1 - e^{-a_3/E})^{1.5} + (a_4 - a_5 \ln E)^2 (1 - e^{-a_6/E})$
$O^+$ ( $^4S$ )- $N_2$	$(a_1 - a_2 \ln E)(1 - e^{-a_3/E})^{1.7} + a_4(1 - e^{-a_5/E})^4(1 - e^{-E/a_6})^3$
$O^+$ ( $^2D, ^2P$ )- $N_2$	$(a_1 - a_2 \ln E)^2 (1 - e^{-a_3/E})^{0.5} + (a_4 - a_5 \ln E)^2 (1 - e^{-a_6/E})^{1.5}$
$O^+$ ( $^4S$ )- $O_2$	$a_1(1 - e^{-a_2/E})^2 + (a_3 - a_4 \ln E)^2 (1 - e^{-E/a_5})^4$
$O^+$ ( $^2D, ^2P$ )- $O_2$	$(a_1 - a_2 \ln E)^2$

TABLE VIII: Fitting parameters and the applicable energy range for Table VII

Process	Parameters ( $a_1, a_2, \dots$ )	Range (keV)
H <sup>+</sup> -H	4.15, 0.531, 67.3	0.005 - 250
H <sup>+</sup> -O	2.91, 0.0886, 50.9, 4.73, -0.862, 0.0306	0.002 - 100
O <sup>+</sup> -H	3.13, 0.170, 87.5	0.025 - 600
O <sup>+</sup> ( <sup>4</sup> <i>S</i> )	3.74, 0.143	0.004 - 0.4
O <sup>+</sup> -O	4.07, 0.269, 415	0.04 - 380
O <sup>+</sup> ( <sup>4</sup> <i>S</i> )-O	4.75, 0.601	0.5 - 5
O <sup>+</sup> ( <sup>2</sup> <i>D</i> , <sup>2</sup> <i>P</i> )-O	3.92, 0.392	0.5 - 5
H <sup>+</sup> -N <sub>2</sub>	12.5, 1.52, 3.97, 0.360, -1.20, 0.208, 0.741	0.1 - 100
H <sup>+</sup> -O <sub>2</sub>	1.83, -0.545, 15.8, 6.35, -0.801, 0.240	0.05 - 100
O <sup>+</sup> ( <sup>4</sup> <i>S</i> )-N <sub>2</sub>	0.800, -1.60, 20.4, 0.453, 0.400, 0.00833	0.01 - 185
O <sup>+</sup> ( <sup>2</sup> <i>D</i> , <sup>2</sup> <i>P</i> )-N <sub>2</sub>	8.46, -1.07, 0.155, 0.919, -1.08, 12.2	0.01 - 185
O <sup>+</sup> ( <sup>4</sup> <i>S</i> )-O <sub>2</sub>	2.16, 0.250, 2.85, -0.103, 0.144	0.01 - 5
O <sup>+</sup> ( <sup>2</sup> <i>D</i> , <sup>2</sup> <i>P</i> )-O <sub>2</sub>	4.19, 0.0315	0.005 - 5

 TABLE IX: Integral cross sections of O<sup>+</sup>(<sup>4</sup>*S*) direct scattering

$E(\text{keV})$	He ( $10^{-16}\text{cm}^2$ )	H <sub>2</sub> ( $10^{-16}\text{cm}^2$ )	N <sub>2</sub> ( $10^{-16}\text{cm}^2$ )	O <sub>2</sub> ( $10^{-16}\text{cm}^2$ )
0.1	5.2	-	5.9	7.6
0.5	$4.81 \pm 0.48$	$3.09 \pm 0.77$	$5.63 \pm 1.24$	$6.41 \pm 0.96$
1.5	$4.40 \pm 0.44$	$2.73 \pm 0.41$	$3.72 \pm 0.45$	$5.30 \pm 0.53$
5.0	$2.31 \pm 0.28$	$1.68 \pm 0.42$	$2.64 \pm 0.45$	$3.75 \pm 0.38$

### 3.6 Charge transfer in collisions of H<sup>+</sup> with C<sub>*m*</sub>H<sub>*n*</sub> (R. Suzuki)

As a part of our ongoing study on various physical phenomena in collisions of positively charged heavy ions with molecules [6, 44–47], here we report our results on the total charge transfer cross sections in collisions of protons with hydrocarbons. In particular, we review our charge transfer cross sections for the C<sub>2</sub>H<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> targets, and the overall qualitative trend in the capture cross sections as a function of the number of carbon atoms in the target C<sub>*m*</sub>H<sub>*n*</sub> molecule.

First, we have studied the electron capture and direct elastic scattering in collisions of H<sup>+</sup> ions with C<sub>2</sub>H<sub>4</sub> below 10 keV [48]. Within the molecular representation, both the semiclassical as well



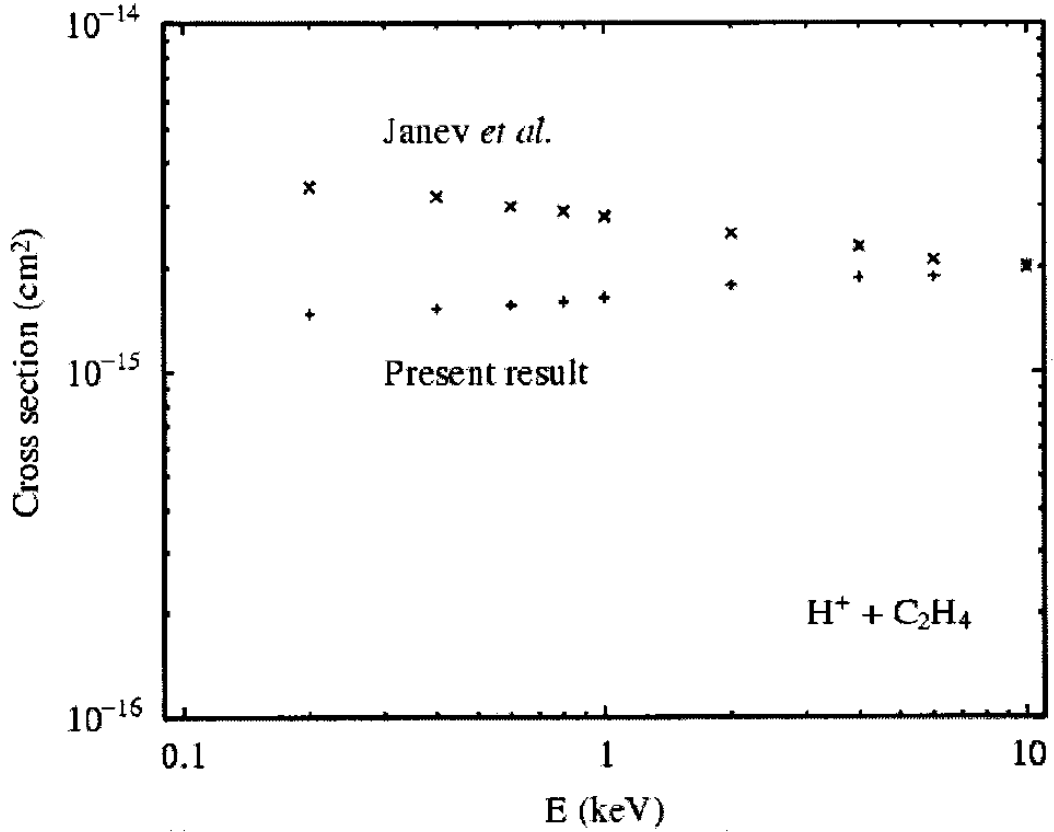


FIG. 4: Total charge transfer cross section for the collision of  $H^+$  with  $C_2H_4$ .

as fully quantum-mechanical approaches were used. In order to account for the steric effect, the calculations were carried out at three different molecular configurations, in which  $H^+$  approaches (i) parallel and (ii) perpendicular to the C=C axis in the molecular plane, and (iii) perpendicular to this plane. We find that electron capture in the (iii) configuration takes place preferentially over that in the (i) and (ii) configurations at scattering angles above 15 degs, while the results for (i) and (ii) are comparable in magnitude below 10 degs, although (ii) dominates slightly at still smaller angles. The total capture cross sections for the (iii) and (ii) configurations differ by a factor of 4 above 500 eV, while those for (i) lie between these values. Below 500 eV, the results for (i) and (iii) are similar in magnitude, while that for the (ii) configuration sharply decreases. The total capture cross section is shown in Fig. 4

As the next target system with larger number of hydrogen atoms, we theoretically studied charge-transfer processes in the collisions of  $H^+$  ions with  $C_2H_6$  molecules below 10-keV collision energies, and obtained the converged total as well as differential cross sections in this energy range. The present collision system suggests that the combination of the Demkov-type and Landau-Zener type

mechanisms primarily governs the scattering dynamics for the flux exit from the initial channel. The charge-transfer cross sections were found to agree very well with all available experimental data below a few keV, but begin to deviate above 3 keV, in which case the present results slowly decrease, while the measurements stay nearly constant. From the study of the electronic state calculation, we have also provided some information on the fragmented species, which elucidates the fragmentation mechanism of the  $C_2H_6^+$  ions produced by the charge transfer. The vibrational effect of the initial target to charge transfer has also been qualitatively examined. The total charge transfer cross section as a function of energy is plotted in Fig. 5.

For the sake of applications including the modeling of energy balance in the fusion edge plasmas, it is important to assess the trends in the electron capture cross sections over a wide range of hydrocarbons. Fig. 6 summarizes our results for various hydrocarbons molecules at the collision energy below 10 keV. Further details are given in References [48, 49].

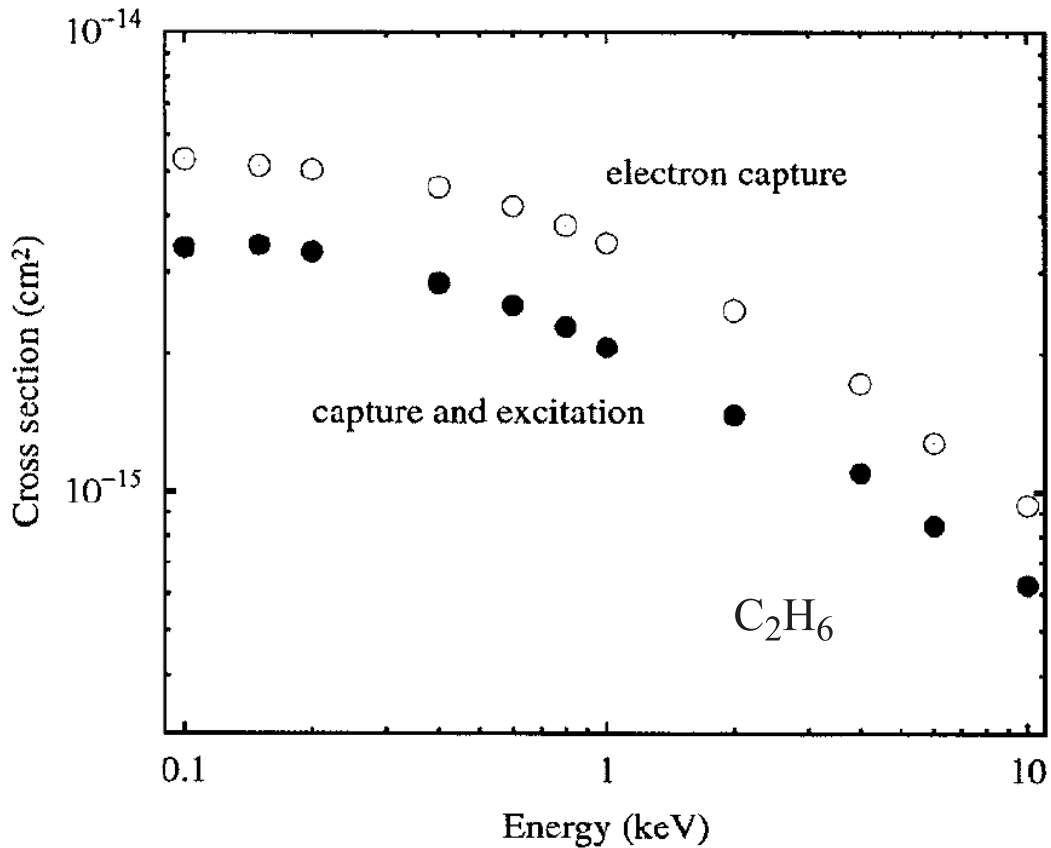


FIG. 5: Total electron capture and simultaneous target excitation cross sections for the collision of  $H^+$  with  $C_2H_6$ .

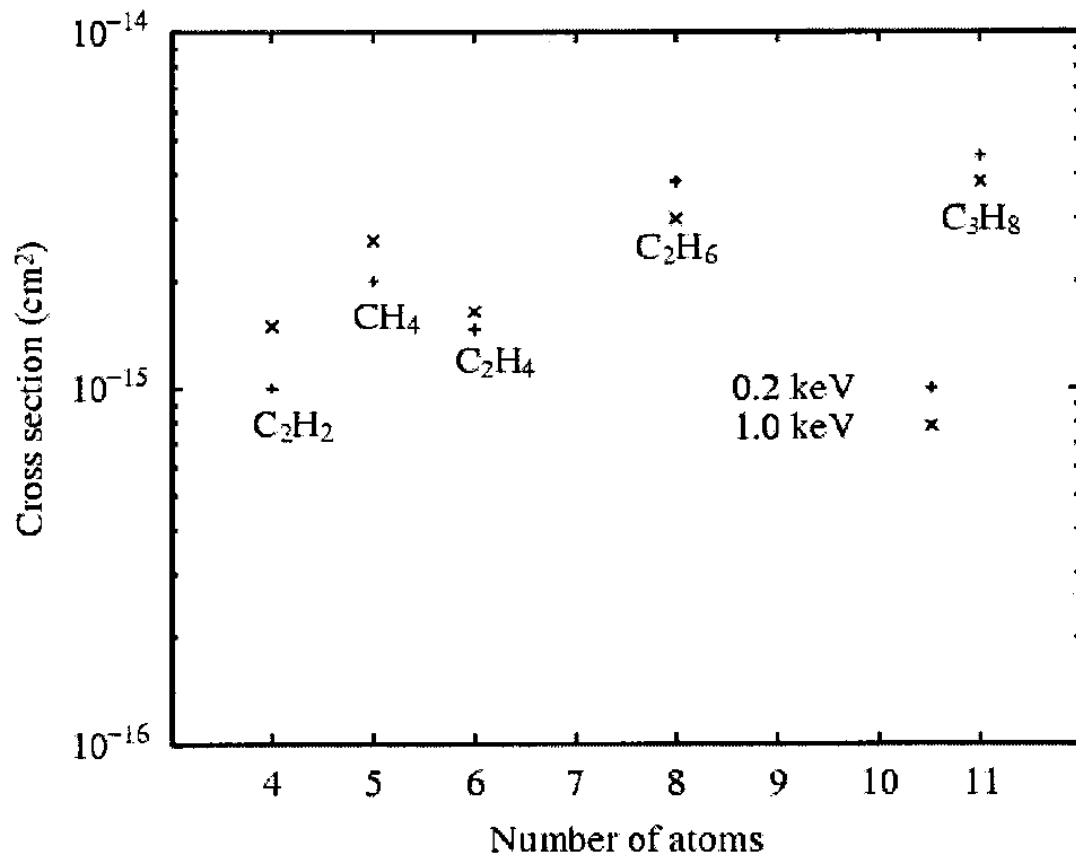


FIG. 6: Trends in the total charge transfer cross sections for collisions of  $H^+$  with hydrocarbons at specific energies as shown.

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