



CROSS SECTIONS FOR PARTICLE-REARRANGEMENT IN ION-MOLECULE COLLISIONS 1.

HYDROGEN AND HELIUM SPECIES

November 1994

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編集兼発行 日本原子力研究所印 刷 いばらき印刷㈱

JAERI-Data/Code 94-015

Cross Sections for Particle-rearrangement in Ion-molecule Collisions I.

Hydrogen and Helium Species

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(Received October 17, 1994)

Experimental cross sections for particle-rearrangement in the ion-molecule collisions between primary plasma constituents have been collected for edge plasma studies. Total and partial cross sections are compiled in graphical forms. Brief comments on the cross-section measurements are given for each reaction. The literature has been surveyed through March 1994.

Keywords: Cross Section, Particle-rearrangement, H, D, H₂, HD, D₂, He

This report was prepared as an account of work supported partly by a research contract of JAERI with University of Osaka Prefecture in the fiscal year 1993.

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イオン-分子間衝突での粒子組み替え反応断面積 I 水素及びヘリウム種

日本原子力研究所東海研究所原子炉工学部 市原 晃•早川 滋雄* •左高 正雄 白井 稔三

(1994年10月17日受理)

エッジプラズマのモデリング及び診断に必要なイオンー分子反応の断面積に関する実験データを 収集した。1994年3月までの文献を対象として収集された反応の全および部分断面積を図にまとめ た。

本報は、大阪府立大学への委託調査をふくむ。

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1. Introduction

It has been widely known from recent experiments on tokamak plasmas that conditions of edge plasma affect crucially on the overall plasma performance[1]. The edge plasma is characterized by the temperature range of 1 to 200 eV and the particle densities in the range of $10^{12} - 10^{15}$ cm⁻³. Because of the low temperatures, not only neutral particles but also molecular species exist and a variety of collision processes occur in the edge plasma. This makes the analysis of edge plasma very complex. Accurate knowledge of the cross sections for these collision processes gives the basis of the edge plasma modeling and diagnostics. Sufficient accumulation of reliable atomic and molecular data is, therefore, strongly required for the future development of the fusion reactor.

This report presents a compilation of the experimental total and partial (state-selective) cross sections for particle-rearrangement in the ion-molecule collisions. As a first step, hydrogen and helium species, which are the primary plasma constituents, are selected. All relevant papers published till March 1994 were collected and surveyed using bibliographic information in references [2-4]. Absolute total and partial cross sections are presently available for twenty-one and six collision systems, respectively. They are compiled in graphical forms together with the recommended data in Ref.[3] and analytical fits, when available. We cite the uncertainties of the data as given by the authors. A short review is given on the cross-section measurements.

It is well known in a theoretical description [5] in terms of the Langevin model that cross section for exothermic reaction varies inversely as the square root of the collision energy and its reaction rate constant is independent of the collision energy for reactions of the type X^+ + YH \rightarrow XH $^+$ + Y. The rate coefficients at thermal energies are available in a few comprehensive compilations.[6]

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2. Explanation of Figures

Figures. Cross section vs Energy

Ordinate: Cross section (in cm²)

Abscissa: Collision energy (in eV/amu)

Experimental cross sections are shown by circles, triangles or squares in figures. The analytical curves are indicated by solid or dotted lines.

For the $D_2^+(v=0-3) + H_2 \rightarrow HD_2^+ + H$ reactions (Figs.32-35), collision energies defined in the analytical curves of Barnett ([3] in References for Introduction) are multiplied by a factor of 10 in order to obtain the reasonable agreement with the experimental cross sections. Similarly, the collision energies of Barnett for the $HD^+(v=0-4) + He \rightarrow HeH^+ + D$ (Figs. 42-46) reactions are multiplied by a factor of 3.

- ibid, Nos. 42-47, edited by J. Botero (IAEA, Vienna, 1991-1993).
- [3] C.F. Barnett, Atomic Data for Fusion Volume 1: Collisions of H, H₂, He and Li Atoms and Ions with Atoms and Molecules, edited by H.T. Hunter, M.I. Kirkpatrick, I.Arvarez, C. Cisneros, and P.A. Phaneuf, Oak Ridge Natl. Lab. Rep. ORNL-6086/V1 (1990).
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2. Explanation of Figures

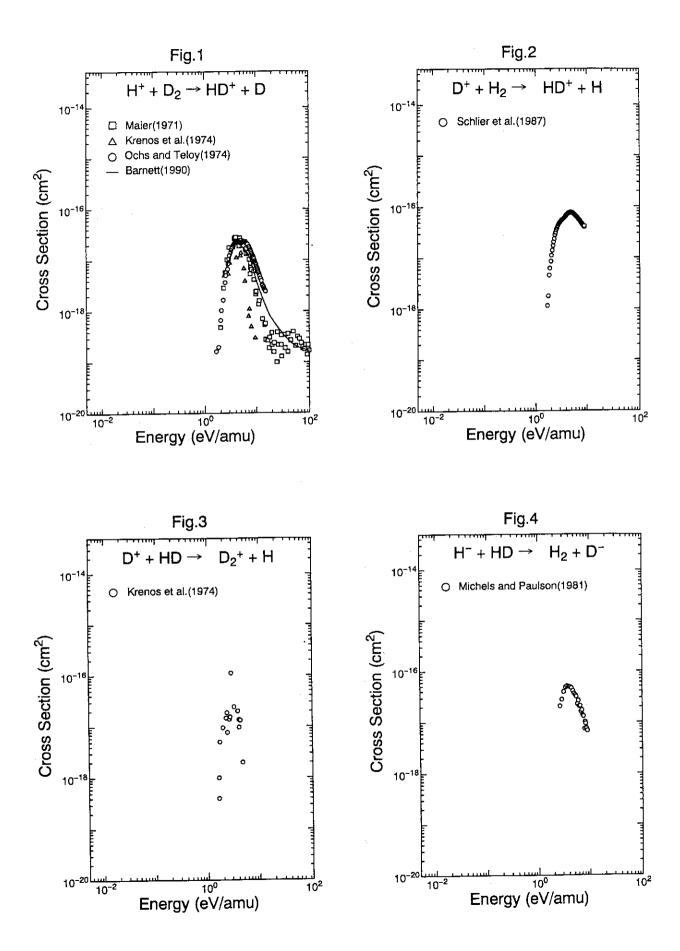
Figures. Cross section vs Energy

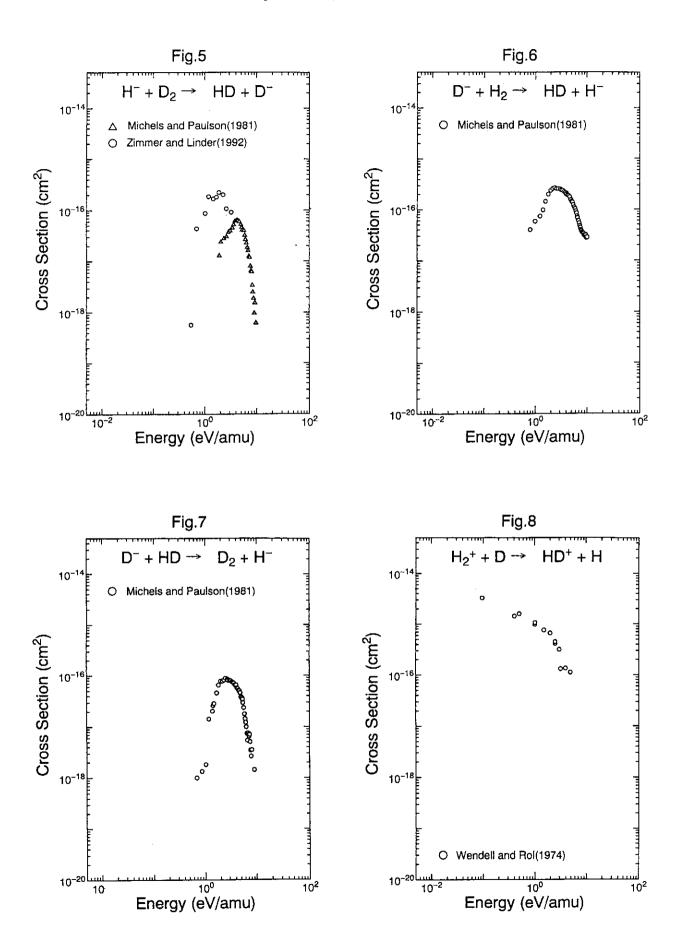
Ordinate: Cross section (in cm²)

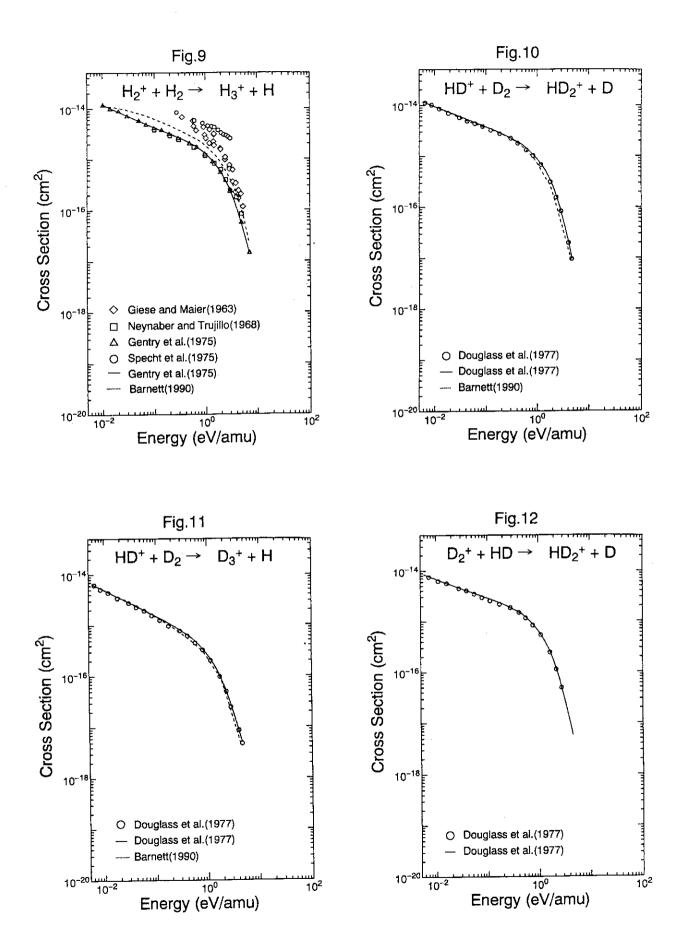
Abscissa: Collision energy (in eV/amu)

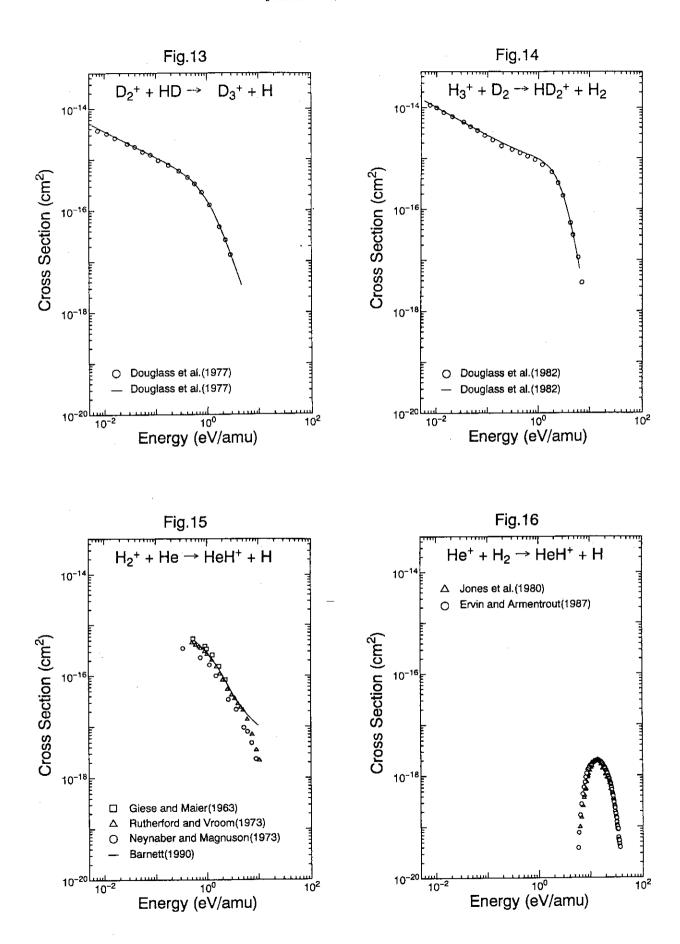
Experimental cross sections are shown by circles, triangles or squares in figures. The analytical curves are indicated by solid or dotted lines.

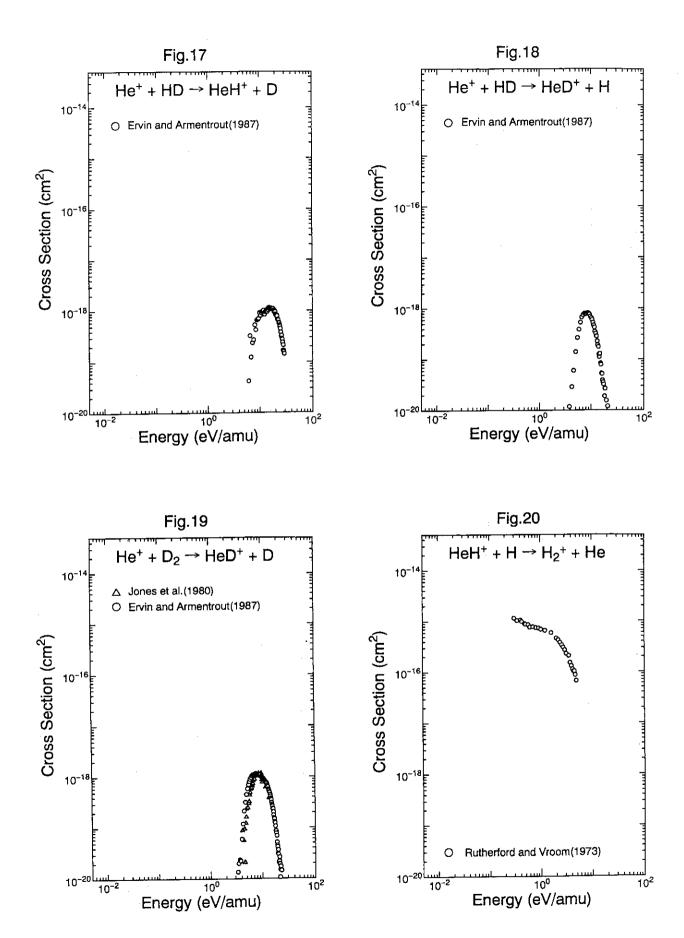
For the $D_2^+(v=0-3) + H_2 \rightarrow HD_2^+ + H$ reactions (Figs.32-35), collision energies defined in the analytical curves of Barnett ([3] in References for Introduction) are multiplied by a factor of 10 in order to obtain the reasonable agreement with the experimental cross sections. Similarly, the collision energies of Barnett for the $HD^+(v=0-4) + He \rightarrow HeH^+ + D$ (Figs. 42-46) reactions are multiplied by a factor of 3.

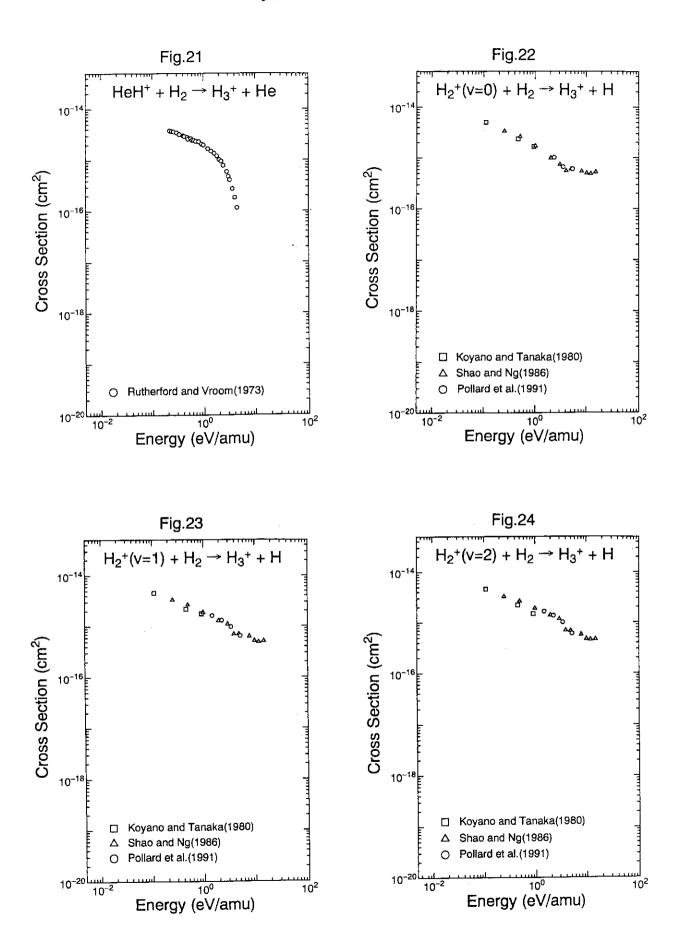


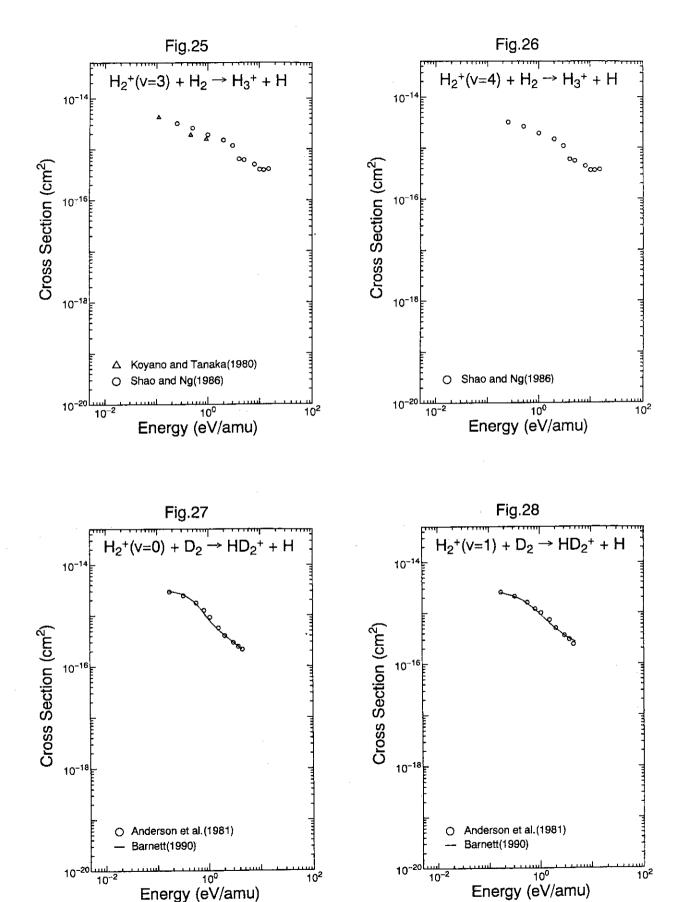


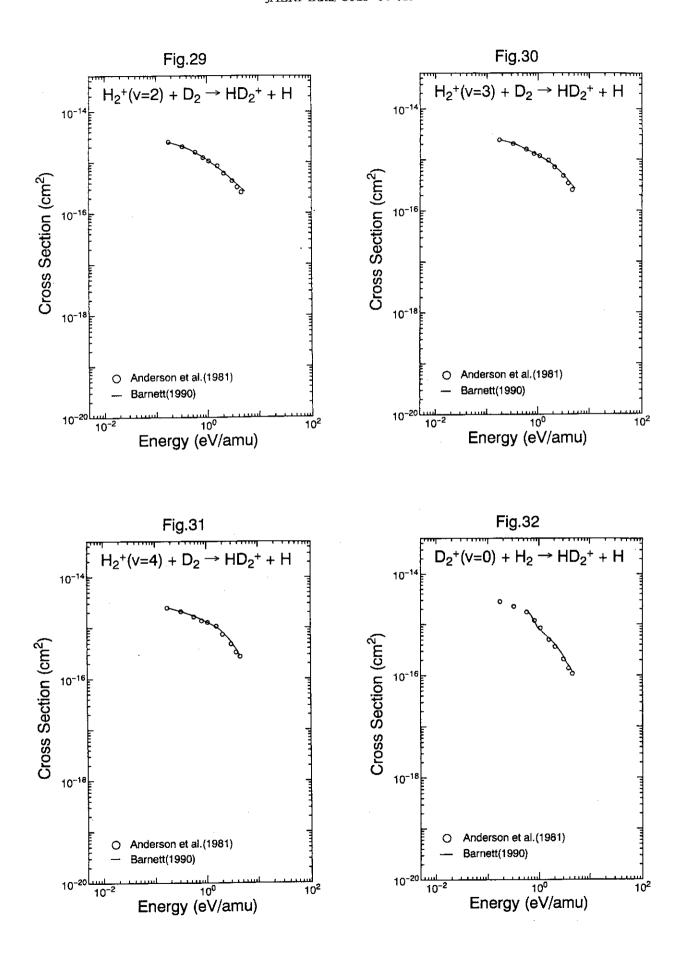


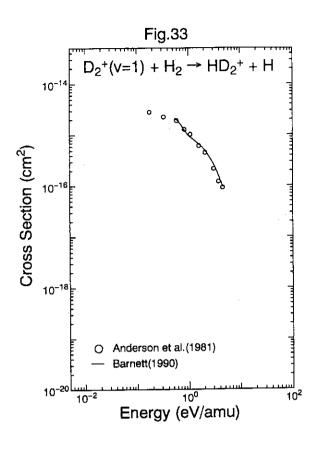


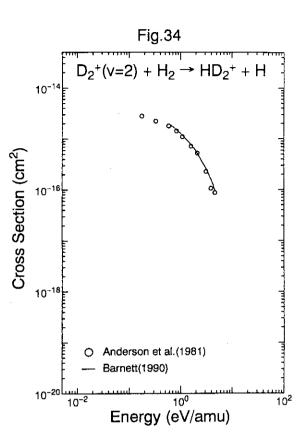


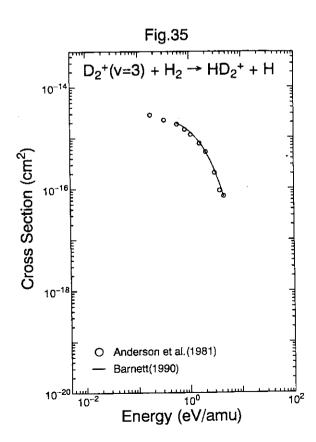


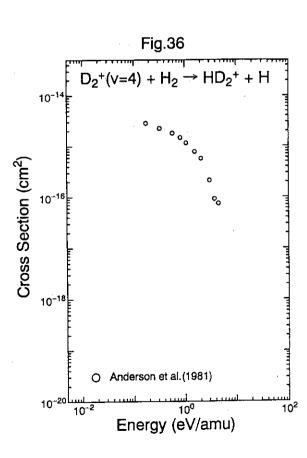


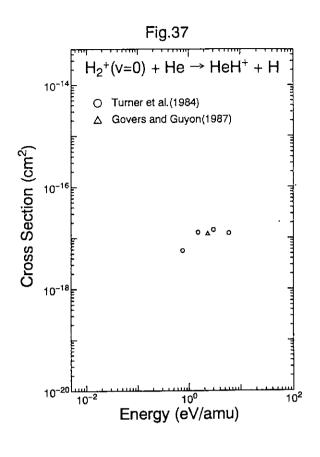


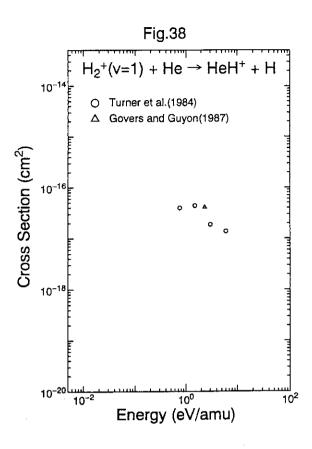


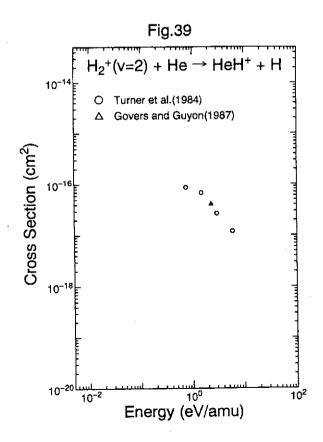


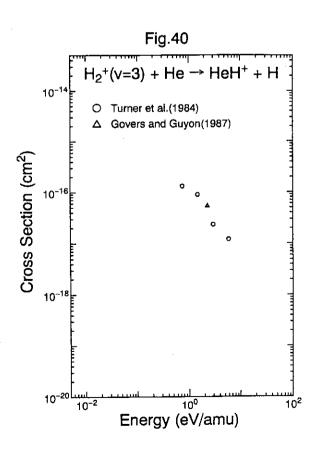


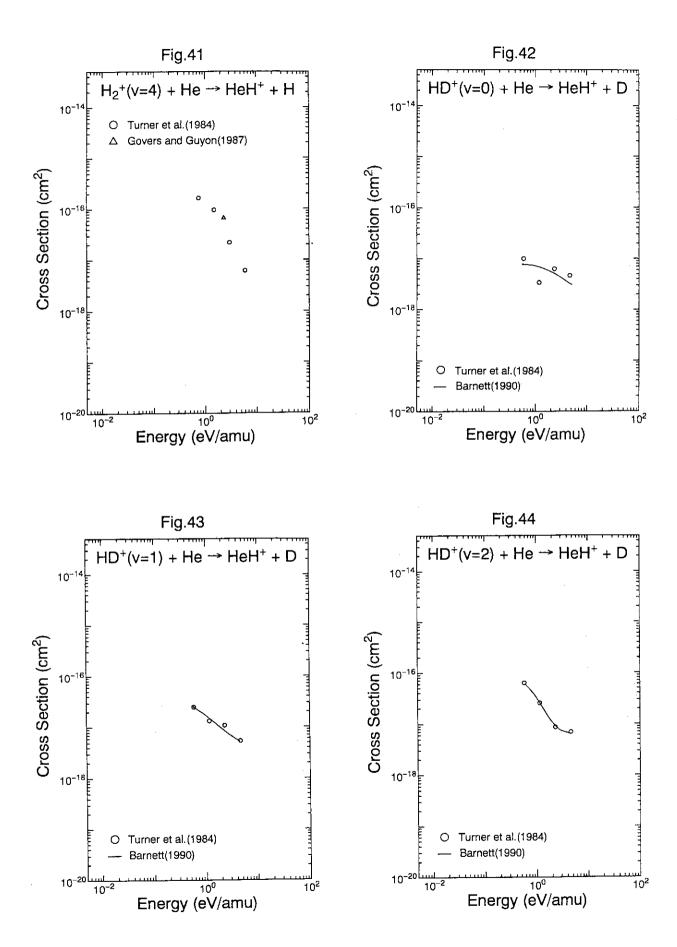


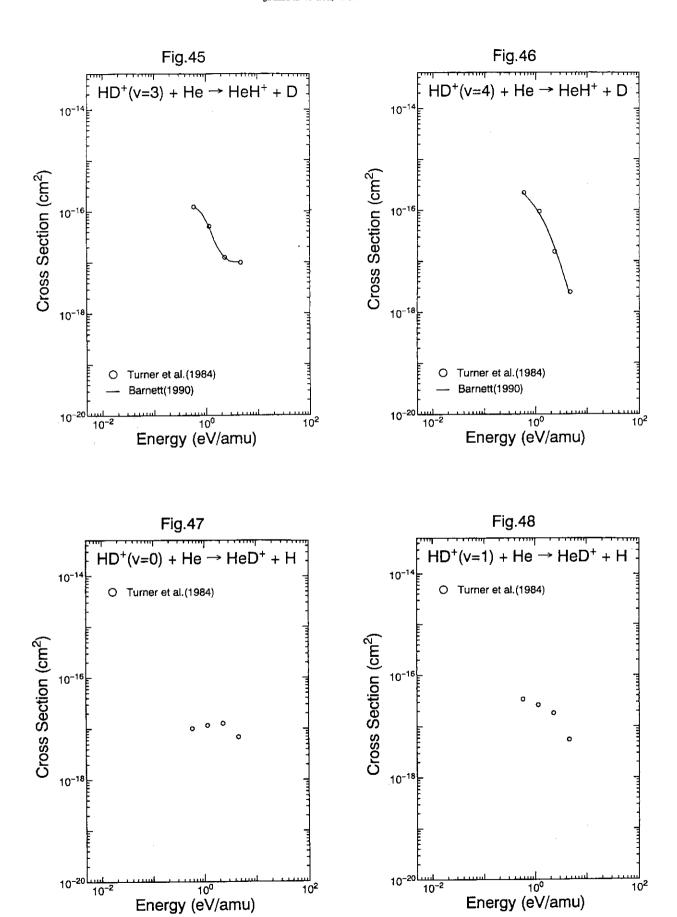


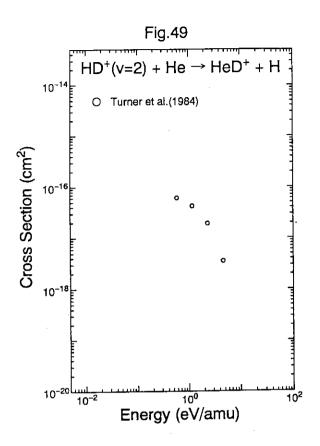


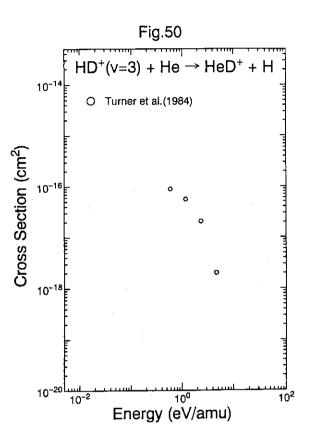


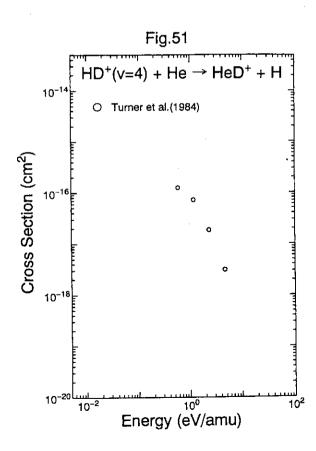












3. Brief Comments on Cross-Section Measurements

The measurements for total and state-selective cross sections are summarized in Tables I and II, respectively. Reaction systems, range of collision energies, experimental methods and range of absolute errors are listed with references.

For the measurements of total cross sections for ion-molecule reactions, widely used techniques are the tandem mass spectrometer (TMS) method and the guided beam (GB) technique. In the TMS method, a beam of mass-selected ions collides with a neutral target gas in a collision chamber, and the ionic products are analyzed in a second mass spectrometer. The GB technique was devised to overcome some disadvantages of the TMS method. A reduction of the number of excited ions in the primary beam and good definition of the kinetic energy are attained by the use of electric field to guide ions. Besides a collection and detection probability for the secondary ions approaches unity for all scattering angles in a broad energy band. Absolute measurement of total cross sections by means of the GB technique is considered to be more reliable than that by the TMS method.

In the merged beam (MB) technique, a fast beam of mass- and energy-selected neutral species, instead of a neutral gas in a collision chamber, is merged with a primary ion beam. This technique enables to determine total cross sections in a wide range of collision energies down to extremely low energies.

In the crossed beam (CB) technique, a target gas beam is crossed with a primary ion beam. The energy and angle distributions of the reaction products are measured using a rotatable detector with energy and mass analysis. It is now possible to carry out measurements down to energies of the order of 0.1 eV. However, absolute measurement is generally difficult, because it is not easy to determine collision volume accurately.

In most of the TMS experiments of total cross sections collected here, the primary ions are produced by electron impact. The beam may contain ions in excited states. In the MB experiments the neutral molecules are formed by means of electron transfer to corresponding ions produced by electron impact. The beam may contain molecules in excited vibrational and rotational states.

For the state-selective measurements collected here, reactants in a specific vibrational state are produced by photoionization of respective parent molecules.

3.1 Total Cross Sections

$$H^+ + D_2 \rightarrow HD^+ + D$$
 (Fig.1)

Absolute cross section was measured by Maier[1] using a TMS apparatus. The values are estimated to be low by a factor of 4 or more, since a correction of secondary-ion-loss to the walls of the reaction chamber was not made. In the CB experiment of Krenos *et al.*[2], the collision volume (path length times number density) of the neutral gas beam was estimated by normalizing it to the experiment of Moran and Roberts[3] for the $H_2^+ + H_2 \rightarrow H_3^+ + H$ reaction. The number density for the D_2 beam was determined using an effusive flow relation. The total cross section was deduced from the measurement at 0° laboratory angle assuming that the angular distribution of the product ions for the $H_1^+ + D_2 \rightarrow HD^+ + D$ reaction is similar to that for the $H_2^+ + H_2 \rightarrow H_3^+ + H$ reaction. The absolute error of the total cross section is estimated to be a factor of 2 or 3. In the GB experiment of Ochs and Teloy[4], a good agreement with trajectory surface hopping calculation[4] is obtained. The estimated error of the absolute cross section is $\pm 20\%$.

$$D^+ + H_2 \rightarrow HD^+ + H$$
 (Fig.2)

The GB experiment was carried out by Schlier et al. [5] with an estimated error of $\pm 10\%$.

$$D^+ + HD \rightarrow D_2^+ + H$$
 (Fig.3)

In the CB experiment of Krenos et al.[2], total cross section was measured with an estimated error of a factor of 2 or 3.

$$H^{-} + HD \rightarrow H_{2} + D^{-}, H^{-} + D_{2} \rightarrow HD + D^{-}$$

 $D^{-} + H_{2} \rightarrow HD + H^{-}, D^{-} + HD \rightarrow D_{2} + H^{-} \text{ (Fig.4-7)}$

Cross sections of these processes were measured by Michels and Paulson[6] using a TMS apparatus with an error of a factor of 2. Negative ions were produced by dissociative attachment of electron to NH_3 and H_2O . The energy spread of the reactant ion beam was 0.5 to 1.0 eV. The cross section for the $H^- + D_2 \rightarrow HD + D^-$ reaction was also measured by Zimmer and Linder[7] using a CB apparatus. The absolute value was determined by comparing the intensity of detected ions for the $H^- + D_2$ reaction with that for the elastic H^- + He scattering, whose absolute cross section is known both experimentally and theoretically. The estimated error is about 20% around the maximum of cross section and increases to about

30% at the higher energies. They determined the threshold energy of 0.42 ± 0.06 eV, in contrast with about 1.3 eV in the TMS experiment[6]. The discrepancy between the CB and TMS cross sections below 3.0 eV is attributed to the transmission and collection efficiency problem of the TMS experiment.

$$H_2^+ + D \rightarrow HD^+ + H$$
 (Fig.8)

The MB experiment was carried out by Wendell and Rol[8]. The D beam was formed by electron transfer to the D⁺ ions produced in the arc source. The absolute values were determined by comparing the HD⁺ count rate with the count rate of NaO⁺ in the measurement of the $O_2^+ + Na \rightarrow NaO^+ + O$ reaction[9], the absolute cross section of which is known. They assumed that the collection efficiency of the HD⁺ ion was the same as of the NaO⁺ ion. The error of their measurement is estimated to be about $\pm 60\%$.

$$H_2^+ + H_2 \rightarrow H_3^+ + H$$
 (Fig.9)

In the TMS experiment of Giese and Maier[10], the primary ion energy was determined with an error of 0.1 eV, and the absolute cross section was measured with an estimated error of ±40%. Neynaber and Trujillo[11] measured the cross section using a MB apparatus. The H₂ beam was formed by electron transfer to the H₂⁺ ion produced by electron impact. The absolute measurement was carried out at 1.0 eV and the cross section of 12x10⁻¹⁶ cm² was obtained with an estimated error of -26 to +37%. The normalization of relative cross sections was made with this absolute value. The error of the relative cross section is estimated to be -11% to +6% at 0.1 eV, and the standard deviation is about ±18% at 3 eV. A similar MB measurement was carried out by Gentry et al.[12]. They determined the absolute cross section of 12.91x10⁻¹⁶ cm² at 1.0 eV with an estimated standard deviation of 4.2%. Both the MB measurements agree well with each other. Specht et al.[13] measured the cross section using a beam-gas-mass-analysis apparatus. Their result is more than a factor of 3 larger than the MB measurements[11,12]. In the measurement of Specht et al. the H₂⁺ ions were formed from the H₂ molecules by the impact of metastable He* atoms. In parallel with this reaction electronically excited neutrals H^* and H_2^* were produced by the $He^* + H_2 \rightarrow H^* + H + He$ and $He^* + H_2 \rightarrow H_2^* + He$ reactions, respectively. The discrepancy is attributed that both reactions $H^* + H_2 \rightarrow H_3^+ + e$ and $H_2^* + H_2 \rightarrow H_3^+ + H_3^+ + H_4^+ + e$ are included in the experiment of Specht et al.

$$HD^{+} + D_{2} \rightarrow HD_{2}^{+} + D, HD^{+} + D_{2} \rightarrow D_{3}^{+} + H$$

 $D_{2}^{+} + HD \rightarrow HD_{2}^{+} + D, D_{2}^{+} + HD \rightarrow D_{3}^{+} + H \text{ (Figs.10-13)}$

Cross sections for these reactions were measured by Douglass *et al.*[14] using a MB apparatus. The neutral D_2 and HD beams were obtained by electron transfer to the D_2^+ and HD⁺ ions, after these D_2^+ and HD⁺ ions were produced by electron impact. The absolute measurement was carried out at 0.1 eV and the relative cross sections were normalized to it. The errors of the absolute cross sections for the HD⁺ + $D_2 \rightarrow$ HD₂⁺ + D and the HD⁺ + $D_2 \rightarrow$ D₃ + H reactions are estimated to be about 15%, and those for the D_2^+ + HD \rightarrow HD₂⁺ + D and D_2^+ + HD \rightarrow D₃⁺ + H reactions to be about 30%.

$$H_3^+ + D_2 \rightarrow HD_2^+ + H_2 \text{ (Fig.14)}$$

The MB experiment was performed by Douglass et al.[15]. The D_2 beam was formed from the parent D_2^+ ions through electron transfer. The absolute cross section was determined at 1.0 eV and the relative cross sections were normalized to it. The error of the absolute cross sections is estimated to be about 13%.

$$H_2^+$$
 + He \rightarrow HeH⁺ + H (Fig.15)

In the TMS experiment of Giese and Maier[10], the primary ion energy was determined with an error of 0.1 eV, and the absolute cross section was measured with an estimated error of $\pm 40\%$. In the CB experiment of Rutherford and Vroom[16], the neutral beam density was determined by using laws for effusion and the absolute cross section was measured with estimated errors of $\pm 20\%$ at high impact energies and of $\pm 30\%$ at the lowest energy. In the MB experiment of Neynaber and Magnuson[17], the absolute cross section of 2.3 x10⁻¹⁶ cm² at 1.0 eV was obtained with an estimated error of +47% to -40%. The normalization of the relative cross sections was made with this absolute value. The errors of the relative cross sections are about $\pm 15\%$ for E ≤ 5 eV and about $\pm 20\%$ for E > 5 eV.

$$He^+ + H_2 \rightarrow HeH^+ + H$$
, $He^+ + HD \rightarrow HeH^+ + D$
 $He^+ + HD \rightarrow HeD^+ + H$, $He^+ + D_2 \rightarrow HeD^+ + D$ (Figs.16–19)

The cross section measurement was carried out by Ervin and Armentrout[18] for those reactions using a GB apparatus with an estimated error of a factor of 2. The He⁺ ions were produced by electron impact ionization with electron energies below the threshold for

formation of metastable Rydberg states. Jones et al.[19] measured the relative cross sections for the $He^+ + H_2 \rightarrow HeH^+ + H$ and $He^+ + D_2 \rightarrow HeD^+ + D$ reactions using a TMS apparatus. Their cross sections were normalized at each peak to the GB measurement of Ervin and Armentrout[18].

$$HeH^+ + H \rightarrow H_2^+ + He$$
 (Fig.20)

In the CB experiment of Rutherford and Vroom[16], the absolute cross section was measured with estimated errors of $\pm 20\%$ at high impact energies and of $\pm 30\%$ at the lowest energy.

$$\text{HeH}^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{He (Fig.21)}$$

The CB measurement was carried out by Rutherford and Vroom[20]. The neutral beam density was determined using laws for effusion. The maximum error of the absolute cross section is estimated to be $\pm 20\%$ at high impact energies and $\pm 30\%$ at the lowest collision energy.

3.2 State-Selective Cross Sections

$$H_2^+(v=0-4) + H_2 \rightarrow H_3^+ + H \text{ (Figs.22-26)}$$

Cross sections were measured by Koyano and Tanaka[21] with a threshold electron-secondary ion coincidence (TESICO)-BG apparatus. The relative cross sections were converted to the absolute values using the thermal rate constant of Theard and Huntress[22] in the case of v=0 at the room temperature ($k(v=0)=2.5x10^{-9}$ cm³ s⁻¹, corresponding to the cross section of $92x10^{-16}$ cm² at average collision energy of 0.033 eV). Shao and Ng[23] measured the absolute cross sections with a state-selective photoionization (SSPI)-GB apparatus. The error of the collision energy is estimated to be 0.1 eV. The standard deviations of the relative cross sections for v=0-4 are \leq 10% and \leq 20% at E=1-5 eV and 6-15 eV, respectively. Pollard *et al.*[24] measured the relative cross section using a resonantly enhanced multi-photon ionization (REMPI)-CB apparatus. The absolute values were determined with the results of Shao and Ng[23]. The error of the collision energy is estimated to be \pm 0.10 eV. A good agreement is obtained among the cross sections in these three measurements.

$$H_2^+(v=0-4) + D_2 \rightarrow HD_2^+ + H, D_2^+(v=0-4) + H_2 \rightarrow HD_2^+ + H$$
(Figs.27-36)

Anderson et al. [25] measured the absolute cross sections for these reaction systems using a SSPI-GB apparatus with an estimated error of $\pm 25\%$.

$$H_2^+(v=0-4)+ \text{ He } \rightarrow \text{HeH}^+ + \text{H, HD}^+(v=0-4)+ \text{ He } \rightarrow \text{HeH}^+ + \text{D}$$

 $+ \text{HD}^+(v=0-4)+ \text{ He } \rightarrow \text{HeD}^+ + \text{H (Figs.37-51)}$

Cross sections for these reactions were measured by Turner et al. [26] using a SSPI-GB apparatus. Govers and Guyon[27] measured the cross sections for the $H_2^+(v=0-6) + He \rightarrow HeH^+ + H$ reactions with a threshold photo-electron photo-ion coincidence (TPEPICO)-CB apparatus. Their measurement was made at the energy of 3.1 eV, and the relative cross sections were normalized to the values of Chupka et al. [28,29]. The estimated error of the cross sections is about $\pm 25\%$.

Table I. Measurements of Total Particle-Rearrangement Cross Sections

Reaction	Collision energy ^a	Method ^b	Absolute error	Reference
${\text{H}^+ + \text{D}_2 \rightarrow \text{HD}^+ + \text{D}}$	1.3 -100	TMS	factor of 4	1
	2.9 - 9.4	СВ	factor of 2-3	2
	2.5 - 15	GB	±20%	4
$D^+ + H_2 \rightarrow HD^+ + H$	0. – 9	GB	±10%	5
$D^+ + HD \rightarrow D_2^+ + H$	1.7 - 4.8	CB	factor of 2-3	2
$H^- + HD \rightarrow H_2 + D^-$	0.7 - 13	TMS	factor of 2	6
$H^- + D_2 \rightarrow HD + D^-$	0.6 - 13	TMS	factor of 2	6
	0.4 - 4	CB	±30%	7
$D^- + H_2 \rightarrow HD + H^-$	0.5 - 10	TMS	factor of 2	6
$D^- + HD \rightarrow D_2 + H^-$	0.4 - 8	TMS	factor of 2	6
$H_2^+ + D \rightarrow HD^+ + H$	0.05 - 5	MB	±60%	8
$H_2^+ + H_2 \rightarrow H_3^+ + H$	0.3 - 5	TMS	±40%	10
	0.1 - 5	MB	-26% to 37% at 1eV	11
	0.01 - 7	MB	-2.2 to 1.8%	12
	0.2 - 3			13
$HD^+ + D_2 \rightarrow HD_2^+ + D$	0.006- 4.7	MB	±15%	14
$\mathrm{HD}^+ + \mathrm{D}_2 \rightarrow \mathrm{D}_3^+ + \mathrm{H}$	0.006- 4.7	MB	±15%	14
$D_2^+ + HD \rightarrow HD_2^+ + D$	0.006- 4.7	MB	±30%	14
$D_2^+ + HD \rightarrow D_3^+ + H$	0.006- 4.7	MB	±30%	14
$H_3^+ + D_2 \rightarrow HD_2^+ + H_2$	0.006- 6.4	MB	±13%	15
$H_2^+ + He \rightarrow HeH^+ + H$	0.53 - 2.3	TMS	±40%	10
	0.5 - 10.5	CB	±30%	16
	0.04 - 9	MB	-40 to 47% at 1 eV	17
$He^+ + H_2 \rightarrow HeH^+ + H$	0.08 - 37	GB	factor of 2	18
	0.08 - 23	TMS		19
$He^+ + HD \rightarrow HeH^+ + D$	0.06 - 29	GB	factor of 2	18
$He^+ + HD \rightarrow HeD^+ + H$	0.06 - 29	GB	factor of 2	18
$He^+ + D_2 \rightarrow HeD^+ + D$	0.05 - 25	GB	factor of 2	18
	0.05 - 13	TMS		19
$HeH^+ + H \rightarrow H_2^+ + He$	0.24 - 4.8	CB	±30%	16
$HeH^+ + H_2 \rightarrow H_3^+ + He$	0.21 - 4.2	CB	±30%	20

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- a) Relative collision energy is given in eV/amu.
- b) Abbreviations are defined as follows:

TMS - tandem mass spectrometer (beam-gas)

CB - crossed beam

GB - guided beam

MB - merged beam

Table II. Measurements of State-Selective Particle-Rearrangement Cross Sections

Reaction	Collision energy ^a	Method ^b	Absolute error	Reference	
$H_2^+(v=0-3) + H_2$					
\rightarrow $H_3^+ + H$	0.11 - 0.93	TESICO-BG		21	
(v=0-4)	0.04 - 15	SSPI-GB	±20%	23	
(v=0-2)	1.5 - 5.3	REMPI-CB		24	
$H_2^+(v=0-4)+ D_2$					
\rightarrow $HD_2^+ + H$	0.17 - 4.6	SSPI-GB	±25%	25	
$D_2^+(v=0-4)+ H_2$					
$\rightarrow HD_2^+ + H$	0.17 - 4.6	SSPI-GB	±25%	25	
$H_2^+(v=0-4)+$ He					
\rightarrow HeH $^+$ + H	0.75 - 6	SSPI-GB		26	
(v=0-6)	2.3	TPEPICO-CB	±25%	27	
HD⁺(v=0-4)+ He					
\rightarrow HeH ⁺ + D	0.6 - 4.7	SSPI-GB		26	
HD ⁺ (v=0-4)+ He					
\rightarrow HeD ⁺ + H	0.6 - 4.7	SSPI-GB		26	

a) Relative collision energy is given in eV/amu.

TESICO - threshold electron-secondary ion coincidence

SSPI - state selective photoionization

REMPI - resonantly enhanced multi-photon ionization

TPEPICO - threshold photo-electron photo-ion coincidence

BG - beam gas

GB - guided beam

CB - crossed beam

b) Abbreviations are defined as follows:

4. Analytical Fits

Empirical analytical fits were carried out by Gentry et al. [12] and Douglass et al. [14,15] to their experimental cross sections. The analytical formula is expressed as

$$log_{10}\sigma = (b_1 + b_2 log_{10}E_0)F(-y) + (b_3 + b_4 log_{10}E_0)F(y),$$
(1)

$$F(y) = e^{y}/(1 + e^{y}),$$

with $y=(\log_{10}E_0-b_5)b_6^2$ and $E_0=b_0E$,

where σ is the cross section in 10^{-16} cm² and E the collision energy in eV/amu. In Table III fit parameters $\{b_i\}$ to be used with Eq.(1) are presented.

Table III. Fit Parameters for Cross Sections

Reaction	b_0	b ₁	b ₂	b ₃	b_4	b ₅	b ₆
$H_2^+ + H_2 \rightarrow H_3^+ + H^a$	1.0	1.07254	- .5	1.43575	-4.41373	.83887	1.5410
$HD^+ + D_2 \rightarrow HD_2^+ + D^b$	1.714	1.2438	4146	-1.6950	-8.1470	1.4972	1.5638
$\mathrm{HD}^+ + \mathrm{D}_2 \rightarrow \mathrm{D}_3^+ + \mathrm{H}^b$	1.714	.7703	5242	2259	-2.8924	.8912	1.6515
D ₂ ⁺ + HD → HD ₂ ⁺ + D ^b	1.714	1.0719	4249	1.0529	-6.1341	1.1622	1.4880
$D_2^+ + HD \rightarrow D_3^+ + H^b$	1.714	.6294	5232	0260	-2.1136	.5060	1.7555
$H_3^+ + D_2 \rightarrow HD_2^+ + H_2^c$	1.714	.99985	56766	3.46514	-5.20255	.86080	1.9482

a) Reference 12.

b) Reference 14.

c) Reference 15.

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