

Evaluated Theoretical Cross Section Data for Charge Exchange of Multiply Charged Ions with Atoms. II. Hydrogen Atom-Partially Stripped Ion Systems

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The existing theoretical cross section data for charge exchange of partially stripped ions on atomic hydrogen are evaluated in the energy range from ~ 10 eV/u to $\sim 10^3$ keV/u. The evaluation has been carried out by using both pure theoretical arguments and comparison with the most accurate experimental data. Ions with atomic numbers $Z = 3-8, 10, 12, 13, 14, 16, 18, 22, 26, 30, 36, 41, 42, 48, 54, 73,$ and 74 , in charge states q between $q = 2$ and $q = (Z - 1)$, have been examined. A brief discussion of the evaluation criteria is also given.

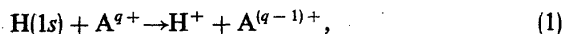
Key words: charge exchange; cross section; ions; multiply charged ions; partially stripped ions.

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1. Introduction

This paper continues the presentation of evaluated theoretical cross section data for charge exchange of multiply charged ions on atoms. In the previous paper,¹ we evaluated the cross section data for hydrogen atom-fully stripped ion systems, as well as the validity regions and accuracies provided by different theoretical methods employed in the calculations. In the present paper, we shall evaluate and present cross section data for the reactions



where q is the charge of an incompletely stripped ion, ranging from $q = 2$ to $q = Z - 1$ (Z being the corresponding nuclear charge). The energies in this paper are quoted in the form of the laboratory energy of the ion (E) in eV (or keV or MeV) divided by the mass of ion (M) expressed in atomic mass units (u). The energy range covered in the present study is from ~ 10 eV/u to ~ 1 MeV/u in which the overwhelming majority of the calculations have been done. However, in the presentation of the data sources, we shall go beyond the above energy limits for reasons of completeness.

Since most of the theoretical methods for treating reaction (1) are the same as those for the hydrogen atom-fully stripped ion charge exchange reactions, and since a detailed

discussion of their main features and validity regions has been given in Ref. 1, in their presentation here we shall be very brief, emphasizing only those differences which are specific for their application to the incompletely stripped ion case. Nevertheless, we shall keep the presentation self-consistent and give all the necessary information for the use of evaluated data contained in this article. Unlike Ref. 1, this paper analyzes only the total cross sections. There exist very few partial cross section calculations, and they will be identified when discussing the data sources.

2. Theoretical Methods

In contrast to the hydrogen atom-fully stripped ion system, in the case studied here more than one electron is involved in the system. This circumstance has the following important implications for the collision dynamics.

(i) The high intrinsic symmetry of the $\text{H} + \text{Z}$ system is broken in the case of many-electron systems. As a consequence the Wigner-von Neuman noncrossing rule becomes less restrictive and the number of the quasimolecular states interacting via a radial coupling mechanism at low collision energies is substantially increased. Methods which explicitly utilize the symmetry properties of the $\text{H} + \text{Z}$ system [like the multichannel Landau-Zener model with rotational coupling (M-LZ-RC) or the classical analytical model (Cl M-An) discussed in Ref. 1] cannot be applied to the case of $\text{H} + \text{A}^{q+}$ collision system.

(ii) The molecular-orbital expansion methods meet much more serious difficulties in dealing with the electronic structure calculations (i.e., determination of the basis wave functions, potentials and coupling matrix elements) in the $\text{H} + \text{A}^{q+}$ system than in the case of the $\text{H} + \text{A}^{Z+}$ system.

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(iii) At sufficiently high collision energies, the electron capture process becomes strongly coupled with processes involving transitions of the ion electrons, and the whole collision dynamics becomes extremely complex.

Below we shall discuss how the above mentioned features of the $H + A^{q+}$ system influence the accuracy of the cross section results obtained by different methods. In this section, we shall use atomic units ($e = \hbar = m_e = 1$). The laboratory collision energy per nucleon is related to the collision velocity v by $E/M = 25 (v/v_0)^2$ (keV/u), where $v_0 = e^2/\hbar = 2.19 \times 10^8$ cm/s.

2.1. Low-Energy Methods

In the low-energy region ($E \lesssim 25$ keV/u, $v \lesssim v_0$), only the perturbed stationary state (PSS) method, the Landau-Zener (LZ) model and the absorbing sphere model (ASM) have been used for cross section calculations in the hydrogen atom-partially stripped ion collision systems. The decay models (DM) and the multichannel Landau-Zener (M-LZ) model can in principle also be used for charge transfer calculations in this energy region, but so far they have not been applied to the $H + A^{q+}$ collisions. The PSS method has been widely used in the thermal energy region and for low charged ions in connection with the astrophysical applications.²⁻⁵ In this energy region, the impact parameter version of the PSS method is not applicable and the full quantal scattering equations have to be solved numerically. (The quantal version of the PSS method we designate as PSS-Q.) The electronic structure part of the calculations has been carried out either using the laborious configuration interaction (CI) method^{3,4} or by applying the pseudopotential method.^{2,5} Translational factors in the basis functions are not essential in this energy region. The results of the calculations are frequently presented in form of reaction rate coefficients k_T .

In the energy region above ~ 10 eV/u, PSS calculations in the impact parameter version of the method have also been performed for B^{3+} , C^{4+} , C^{5+} , N^{5+} , and O^{6+} ions.^{6,7}

The accuracy of the PSS cross section calculations crucially depends on the size of the molecular basis used and, for the higher energies, on the treatment of the electron momentum transfer effects. Assuming a high accuracy in solving the electronic structure part of the problem, all the conclusions concerning the accuracy of the PSS method discussed in Ref. 1 remain valid for the $H + A^{q+}$ system.

Regarding the accuracy of the data provided by the decay model (DM) or the absorbing sphere model (ASM), one can expect that it is higher for the $H + A^{q+}$ case than in the $H + Z$ system. The larger number of interacting states in the $H + A^{q+}$ system (or, equivalently, the larger number of open reaction channels) provides a better fulfillment of the basic assumptions of these models. Using the weak energy dependence of the cross section predicted by decay models and the existing experimental data, the following scaling rule can be established:

$$\sigma \simeq 7.0 \times 10^{-16} q^{1.1} \text{ cm}^2, \quad q > 4, \quad 0.1 < E q^{-1/2} < 20, \quad (2)$$

where E is expressed in keV/u. In most cases, the accuracy provided by the scaling rule (2) is better than $\pm 50\%$.

2.2. Intermediate-Energy Methods

Only two methods have been applied so far for cross section calculations in the $H + A^{q+}$ system in the intermediate energy range (between ~ 10 keV/u and ~ 300 keV/u): the Vainshtein-Presnyakov-Sobel'man (VPS) method^{8,9} and the classical trajectory Monte Carlo (CTMC) method.¹⁰ The VPS method is essentially a two-state method. Its application to the $H + A^{q+}$ multichannel electron transfer problem is based on a separate treatment of the interaction of the initial state with each particular final state. This permits the calculation of the partial cross sections $\sigma_{n\ell}$ and $\sigma_n = \sum_{\ell} \sigma_{n\ell}$. The total cross section is obtained by summing σ_n over n for all significantly populated states. The VPS transition probability behaves correctly in both the adiabatic and high energy limits (to the first approximation). However, since the first-order approximation for charge exchange (the Brinkman-Kramers approximation) is by itself incorrect, and empirical factor of 1/3 is introduced in the calculated cross sections^{8,9} to account for the higher order effects. While for the $1s \rightarrow 1s$ transition this factor is close to the proper value ($= 0.295$), for other transitions ($1s \rightarrow n\ell$ where $n \neq 1$, $\ell \neq 0$) it may be substantially different.¹¹ Therefore, the accuracy of this method (referred to below as VPS-emp) is rather uncertain.

The CTMC method is based on numerical solution of the classical equations for the three-body problem. Its application to the $H + A^{q+}$ collision system assumes that the ion is a structureless particle with an effective charge q_{eff} . There is some uncertainty in the determination of q_{eff} which is directly reflected in the accuracy of the cross section results. In any case, the CTMC method is based on a classical treatment of the three-body system and cannot be applied to the $H + A^{q+}$ multielectron system at energies where the ionic structure cannot be adequately represented within the effective charge concept.

2.3. High-Energy Methods

Except for the extension of the VPS-emp method in the region of high energies ($E \gtrsim 300$ keV/u), the eikonal extension of the Brinkman-Kramers approximation¹² (further referred to as BK-Eik) and the continuum distorted wave (CDW) method¹³ have been used for charge exchange calculations in the $H + A^{q+}$ collision systems. The application of the BK-Eik theory to this system is based on the fact that the factor $\alpha(q, v)$ which comes from the eikonal phase in the cross section formula (see Ref. 1),

$$\sigma_{\text{BK-Eik}} = \alpha(q, v) \sigma_{\text{BK}}, \quad (3)$$

depends very weakly on the ionic charge q . This result, obtained for the hydrogen atom-fully stripped ion systems, is also extended to the case of incompletely stripped ions, the many-electron structure of which is taken into account by using an effective charge q_{eff} .¹⁴ The CDW method has been used only for the $H + \text{Li}^{2+}$ collision system.¹³

3. Review of Data Sources

The theoretical studies of charge exchange processes in hydrogen atom-incompletely stripped ion systems are less

extensive than in the hydrogen atom-fully stripped ion case due to the multielectron structure of the collision system and its implications on the complexity of collision dynamics. The available data sources are compiled in Table 1. For each atom-ion pair, the energy region, the computational method, and the character of the data (total or partial cross section, or reaction rate coefficient) are indicated in the table. The data sources for the thermal energy region are also included in this table, but the data contained in them will not be further analyzed.

4. Evaluation Criteria

The evaluation criteria for the accuracy of the charge exchange cross section data are the same as in Ref. 1:

(1) degree of sophistication of the calculations (i.e., size of the basis, inclusion and character of translational factors, way of representation of the ion electronic structure);

(2) degree of the intrinsic accuracy of the method itself (as specified in Table 1 of Ref. 1);

(3) agreement with the most accurate experimental data.

Contrary to the case of the $H + Z$ systems, experimental data are much more available for $H + A^{+q}$ systems, and the agreement with them is used as the main evaluation criterion for the accuracy of the theoretical data. In the cases when no experimental data exist, the accuracy of the data has been assessed on the basis of the criteria (1) and (2). All methods, by themselves, have the same validity region and intrinsic strengths as given in Table 1 of Ref. 1. However, for the multielectron $H + A^{q+}$ system, to achieve a high degree of sophistication of the calculations [criterion (1)], much more laborious calculations must be performed than in the $H + Z$ case. The use of the effective charge concept in the CTMC and BK-Eik calculations introduces an uncontrollable uncertainty which may reduce the accuracy of these methods by $\sim 20\%$ – 30% . In general, the accuracy of the cross section data for the $H + A^{q+}$ system is significantly lower than in the case of the $H + Z$ system.

5. Evaluated Cross Section Data

We have applied the criteria discussed in the preceding section to evaluate the total cross section data listed in Table 1 and belonging to the energy interval 10 eV/u – 1 MeV/u . The data having an accuracy within a factor of two (or better) are presented in Table 2, with example cases shown in Figs. 1–12. The numbers in the figure legend give the references from which the data were taken. Experimental data, where available, are also given in these figures, and the reference number is followed by a letter E. Only the experimental data at the end points of the investigated energy range are shown. Other experimental points are represented by a broken line obtained by using a fitting procedure. In such cases, the comparison of theoretical results with the experimental data can provide more precise information about the accuracy of the theoretical predictions. When experimental data do not exist, the accuracy of the theoretical cross sections can be assessed on the basis of the accuracy provided by the method itself (Table 1 of Ref. 1) and the information on the sophistication of the calculations contained in Table 1 of the present paper.

In presenting the theoretical data in Table 2 and Figs. 1–12, we have adopted the following criteria:

From all the available calculations using the same method, only those with highest accuracy are presented;

If the calculations are also extended outside the region of validity of the applied method, only the part which conforms with the validity region is presented;

The data provided by the VPS-emp method are presented in their entirety, since no reasonable assessment of their accuracy can be made on the basis of theoretical arguments. In cases where experimental data exist, the accuracy of these calculations can be estimated by comparing them with such data. Using these cases, one can conclude that the accuracy of the VPS-emp results is within a factor of two.

Table 1. Theoretical data for charge exchange of atomic hydrogen with partially stripped ions

Reference	Energy Range	LMH ^a	Method ^b	Comments	Data
<u>H-Li²⁺</u>					
9	0.25-625 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ_t, σ_{nl}
14	40-600 keV/u	(M)H	BK-Eik	σ_{BK} multiplied by eikonal factor; Effective charge	σ_t
13	6.25-1225 keV/u	(L)(M)H	CDW		σ_t
<u>H-B²⁺</u>					
21	0.03-9 keV/u	L(M)	CC-MO	2 states; Exponential model	σ_t
<u>H-B³⁺</u>					
6	0.053-5.3 keV/u	L	PSS	8 molecular states;	σ_t
10	37.5-130 keV/u	M	CTMC	Effective charge	σ_t
<u>H-B⁴⁺</u>					
10	37.5-130 keV/u	M	CTMC	Effective charge	σ_t
<u>H-C²⁺</u>					
3	0.5-5 eV	(T)L	PSS-0	Full quantum treatment	k_T
14	40-700 keV/u	(M)H	BK-Eik	CI-basis; Effective charge	$\sigma_t, \sigma_t, \sigma_t$
<u>H-C³⁺</u>					
15	0.1-1.75 eV	(T)L	PSS-0	2 states	σ_t, k_T
19	0.001-4 eV	(T)L	PSS-0	2 states	σ_t, k_T
3	0.5-5 eV	(T)L	PSS-0	CI - basis; Full quantum treatment	k_T
23	0.27-8.1 eV	(T)L	PSS-0	CI - basis;	σ_t
10	37.5-150 keV/u	M	CTMC	Effective charge	σ_t
14	40-1000 keV/u	(M)H	BK-Eik	Effective charge	σ_t
<u>H-C⁴⁺</u>					
5	0.01-100 eV	(T)L	PSS-Q	5 coupled states	σ_t, k_T
6	0.053-5.26 keV/u	L	PSS	7 coupled states	σ_t
20	0.1-2.7 eV	(T)	LZ		k_T
16	2.58 keV/u	L	AS	Accuracy ~40%	σ_t
10	37.5-150 keV/u	M	CTMC	Effective charge	σ_t
22	25-2500 keV/u	(L)M	VPS-emp	1/3 empirical factor	σ_t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ_t

Table 1. Theoretical data for charge exchange of atomic hydrogen with partially stripped ions--Continued

Reference	Energy Range	LMH ^a	Method ^b	Comments	Data
<u>H-C⁵⁺</u>					
7	0.0132-7.58 keV/u	(T)L	PSS	5 coupled states	σ_t
16	2.58 keV/u	L	ASM	Accuracy $\sim \pm 40\%$	σ_t
10	37-150 keV/u	M	CTMC	Effective charge	σ_t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ_t
<u>H-N²⁺</u>					
3	0.5-5 eV	(T)L	PSS-0	CI - basis	k_T
23	$2.7 \times 10^{-4} - 8.1$	(T)L	PSS-Q	CI - basis	σ_t
14	40-800 keV/u	(M)H	BK-Eik	Effective charge	σ_t
<u>H-N³⁺</u>					
19	0.001-4 eV	(T)L	PSS-Q	2 states	σ_t, k_T
3	0.5-5 eV	(T)L	PSS-0	CI - basis	k_T
5	10^{-4} -100 eV	(T)L	PSS-0	4 states	σ_t, σ_n, k_T
10	37.5-150 keV/u	M	CTMC	Effective charge	σ_t
14	40-1000 keV/u	(M)H	BK-Eik	Effective charge	σ_t
<u>H-N⁴⁺</u>					
20	0.1-2.7 eV	(T)L	LZ		k_T
16	2.58 keV/u	L	ASM	Accuracy $\sim \pm 40\%$	σ_t
10	37.5-150 keV/u	M	CTMC	Effective charge	σ_t
22	0.25-2500 keV/u	M(H)	VPS-emp	1/3 empirical factor	σ_t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ_t
<u>H-N⁵⁺</u>					
7	0.0132-7.58 keV/u	(T)L	PSS	5 molecular states	σ_t
16	2.58 keV/u	L	ASM	Accuracy $\sim \pm 40\%$	σ_t
10	37.5-150 keV/u	M	CTMC	Effective charge	σ_t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ_t
<u>H-N⁶⁺</u>					
16	2.58 keV/u	L	ASM	Accuracy $\sim \pm 40\%$	σ_t
10	37.5-150	M	CTMC	Effective charge	σ_t
22	0.25-2500	M(H)	VPS-emp	1/3 empirical factor	σ_t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ_t
<u>H-O²⁺</u>					
3	0.5-5 eV	(T)L	PSS-Q	Full quantal treatment	k_T
14	40-800 keV/u	(M)H	BK-Eik	Effective charge	σ_t

Table 1. Theoretical data for charge exchange of atomic hydrogen with partially stripped ions--Continued

Reference	Energy Range	LMH ^a	Method ^b	Comments	Data
<u>H-O³⁺</u>					
3	0.5-5 eV	(T)L	PSS-Q		k _T
4	0.5-5 eV	(T)L	PSS-Q	Production of (0 ²⁺)*	k _T
10	37.5-100 keV/u	M	CTMC	Effective charge	σ _t
14	40-1000 keV/u	(M)H	BK-Eik	Effective charge	σ _t
<u>H-O⁴⁺</u>					
20	0.1-2.7 eV	(T)L	LZ		k _T
16	2.58 keV/u	L	ASM	Accuracy ~±40%	σ _t
10	37.5-125 keV/u	M	CTMC	Effective charge	σ _t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ _t
<u>H-O⁵⁺</u>					
16	2.58 keV/u	L	ASM	Accuracy ~±40%	σ _t
10	37.5-125 keV/u	M	CTMC	Effective charge	σ _t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ _t
<u>H-O⁶⁺</u>					
7	0.013-7.6 keV/u	(T)L	PSS	8-state molecular CC	σ _t
16	2.58 keV/u	L	ASM	Accuracy ~±40%	σ _t
10	37.5-125 keV/u	M	CTMC	Effective charge	σ _t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ _t
<u>H-O⁷⁺</u>					
16	2.58 keV/u	L	ASM	Accuracy ~±40%	σ _t
10	37.5-150 keV/u	M	CTMC	Effective charge	σ _t
14	50;100;145;1000 keV/u	(M)H	BK-Eik	Effective charge	σ _t
<u>H-Ne²⁺</u>					
3	0.5-5 eV	(T)L	PSS-Q		k _T
<u>H-Ne³⁺</u>					
3	0.5-5 eV	(T)L	PSS-Q		k _T
<u>H-Ne⁴⁺</u>					
20	0.1-2.7 eV	(T)L	LZ		k _T
22	0.25-2500 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ _t
<u>H-Ne⁶⁺</u>					
22	0.25-2500 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ _t
<u>H-Ne⁸⁺</u>					
22	0.25-2500 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ _t

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Table 1. Theoretical data for charge exchange of atomic hydrogen with partially stripped ions--Continued

Reference	Energy Range	LMH ^a	Method ^b	Comments	Data
<u>H-Mg²⁺</u>					
20	0.1-2.7 eV	(T)L	LZ		k _T
21	10-10,000 keV/u	(L)(M)(H)	CC-MO	2 states; Exponential model	σ _t
<u>H-Mg^{q+}; q = 3,4</u>					
20	0.1-2.7 eV	(T)L	LZ		k _T
<u>H-Al^{q+}; q = 4,6,8,10</u>					
22	0.25-2500 keV/u	(L)(M)(H)	VPS-emp	1/3 empirical factor	σ _t
<u>H-Si²⁺</u>					
2	10 ⁻⁴ - 2.5 eV	(T)L	PSS-Q		σ _t , k _T
<u>H-Si³⁺</u>					
20	0.1-2.7 eV	(T)L	LZ		k _T
<u>H-Si⁴⁺</u>					
20	0.1-2.7 eV	(T)L	LZ		k _T
22	0.25-2500 keV/u	(L)(M)(H)	VPS-emp	1/3 empirical factor	σ _t
<u>H-Si^{q+}; q = 6,8,10</u>					
22	0.25-2500 keV/u	(L)(M)(H)	VPS-emp	1/3 empirical factor	σ _t
<u>H-S^{q+}; q = 2,3,4</u>					
20	0.1-2.7 eV	(T)L	LZ		k _T
<u>H-Ar^{q+}; q = 2,3</u>					
20	0.1-2.7 eV	(T)L	LZ		k _T
<u>H-Ar⁴⁺</u>					
29	0.1-2.7 eV	(T)L	LZ		k _T
8	0.2-2000 keV/u	(L)(M)	VPS-emp	1/3 empirical factor	σ _t
<u>H-Ar^{q+}; q = 6,8,10</u>					
8	0.2-2000 keV/u	(L)(M)	VPS-emp	1/3 empirical factor	σ _t
<u>H-Ti^{q+}; q = 4,6,8,10</u>					
22	0.25-2500 keV/u	(L)(M)(H)	VPS-emp	1/3 empirical factor	σ _t
<u>H-Fe^{q+}; q = 4,6,8</u>					
8	0.2-2000 keV/u	(L)(M)(H)	VPS-emp	1/3 empirical factor	σ _t
<u>H-Fe¹⁰⁺</u>					
18	47.3-340 keV/u	M	CTMC		σ _t
17	50-300	M	CTMC		σ _t
8	0.2-2000 keV/u	(L)(M)(H)	VPS-emp	1/3 empirical factor	σ _t

Table 1. Theoretical data for charge exchange of atomic hydrogen with partially stripped ions--Continued

Reference ^a	Energy Range	LMH ^b	Method ^c	Comments	Data
<u>H-Fe¹⁵⁺</u>					
18	47.3-340 keV/u	M	CTMC		σ_t
17	50-300	M	CTMC		σ_t
<u>H-Fe²⁰⁺</u>					
17	50-300	M	CTMC		σ_t
<u>H-Fe²⁴⁺</u>					
24	40-200	(M)H	BK-Eik		$\sigma_t, \sigma_n, \sigma_{n2}$
<u>H-Fe²⁵⁺</u>					
17	50-400	M	CTMC		σ_t
<u>H-Zn²⁺</u>					
21	0.01-4 keV/u	L	CC-MO	2-state exponential model	σ_t
<u>H-Kr^{q+}; q = 4, 6, 8, 10</u>					
8	0.2-2000 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ_t
<u>H-Nb^{q+}; q = 4, 6, 8, 10</u>					
22	0.25-2500 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ_t
<u>H-Mo^{q+}; q = 4, 6, 8, 10</u>					
8	0.2-2000 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ_t
<u>H-Mo¹⁴⁺</u>					
18	47.3-340 keV/u	M	CTMC		σ_t
<u>H-Cd²⁺</u>					
21	0.0025-9 keV/u	L	CC-MO	2-state exponential model	σ_t
<u>H-Xe^{q+}</u>					
8	0.2-2000 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ_t
<u>H-Ta^{q+}; q = 3-5, 7, 9, 11-15</u>					
14	102 keV/u	(M)H	BK-Eik		σ_t
<u>H-Ta^{q+}</u>					
22	0.25-2500 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ_t
14	102 keV/u	(M)H	BK-Eik		σ_t
<u>H-W^{q+}; q = 4, 6, 8, 10</u>					
8	0.2-2000 keV/u	(L)M(H)	VPS-emp	1/3 empirical factor	σ_t

^aT, L, M, H stand for the thermal-, low-, medium-, and high-energy regions, respectively. These letters in parentheses indicate regions in which the methods were applied, although with a restricted validity.

^bDefinition of abbreviations for methods used in Table 1:

CC-MO Close coupling - molecular orbital method
PSS-Q Perturbed stationary state method - quantal version
PSS Perturbed stationary state method - impact parameter version
LZ Landau-Zener model
ASM Absorbing sphere model
CTMC Classical trajectory Monte Carlo method
VPS-emp Vainstein-Presnyakov-Sobelman approximation, empirical
BK-Eik Brinkmann-Kramers - Eikonal theory
CDW Continuum distorted wave approximation

Table 2. Evaluated theoretical total charge exchange cross sections (σ_c) for the process $A^{q+} + H \rightarrow A^{(q-1)+} + H^+$ as a function of E/M, the laboratory energy of the ion divided by the mass of the ion.

E/M (keV/u)	σ_c (10^{-16} cm^2)	E/M (keV/u)	σ_c (10^{-16} cm^2)	E/M (keV/u)	σ_c (10^{-16} cm^2)	E/M (keV/u)	σ_c (10^{-16} cm^2)
H-Li²⁺							
23.9	17.6	0.215	2.43	37.5	15.9	0.117	33.2
47.3	6.51	0.264	3.03	50.0	14.0	0.161	33.2
64.4	2.56	0.326	3.34	75.0	9.47	0.210	36.9
84.2	1.07	0.367	3.35	100.	4.85	0.266	36.6
107.	0.47	0.401	3.26	125.	1.24	0.323	38.2
132.	0.22	0.433	2.98	150.	1.81	0.398	39.3
159.	0.10	0.473	2.89	Ref [10]			
Ref [13]							
40.	10.1	0.519	3.27	Ref [10]			
44.4	7.79	0.559	3.70	Ref [10]			
50.2	5.64	0.648	4.04	Ref [10]			
58.9	3.61	0.756	4.21	Ref [10]			
66.9	2.42	0.792	4.55	Ref [10]			
74.0	1.73	0.842	4.92	Ref [10]			
89.3	0.962	0.893	5.23	Ref [10]			
105.	0.53	0.946	5.43	Ref [10]			
122.	0.30	1.01	5.44	Ref [10]			
142.	0.18	1.07	5.37	Ref [10]			
Ref [21]							
H-B²⁺							
14.7	5.07	1.77	4.91	37.5	8.59	3.37	34.0
18.3	4.85	1.93	4.85	50.0	6.40	3.80	37.3
21.5	4.53	2.06	4.91	75.0	3.12	4.26	40.5
28.2	3.77	2.23	5.24	100.	0.91	4.75	41.0
34.3	3.12	2.58	6.13	125.	0.60	5.26	42.4
39.6	2.47	2.97	6.99	150.	0.61	Ref [6]	
44.2	1.94	3.40	7.58	Ref [10]			
50.7	1.42	3.82	8.03	Ref [10]			
54.5	1.13	4.26	8.18	Ref [10]			
Ref [21]							
37.5	11.9	78.0	4.75	37.5	11.9	37.5	11.9
50.0	9.64	96.3	2.45	50.0	9.64	50.0	9.64
75.0	5.00	117.	1.25	75.0	5.00	75.0	5.00
100.	3.87	136.	0.71	100.	3.87	100.	3.87
125.	1.20	164.	0.36	125.	1.20	125.	1.20
Ref [10]							
13.3	17.5	208.	0.15	13.3	17.5	13.3	17.5
26.0	12.9	Ref [14]		26.0	12.9	26.0	12.9
55.5	8.20	Ref [14]		55.5	8.20	55.5	8.20
105.	4.03	Ref [14]		105.	4.03	105.	4.03
161.	1.72	Ref [14]		161.	1.72	161.	1.72
211.	0.71	Ref [14]		211.	0.71	211.	0.71
Ref [22]							

Table 2. Evaluated theoretical total charge exchange cross sections (σ_t) for the process $A^{q+} + H \rightarrow A^{(q-1)+} + H^+$ as a function of E/M, the laboratory energy of the ion divided by the mass of the ion (continued).

E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)
H-O³⁺							
2.58	66.0	2.58	30.0	0.427	0.145	0.406	51.8
Ref [16]		Ref [16]		0.552	0.356	1.00	47.7
37.5	17.7	37.5	30.7	0.774	0.840	2.02	43.2
50.0	14.8	50.0	29.3	0.975	1.30	10.0	27.3
75.0	9.68	75.0	24.0	1.42	2.27	20.2	19.9
100.	6.43	100.	15.2	2.11	3.46	101.	6.21
125.	1.95	125.	6.40	3.20	4.75	205.	2.40
Ref [10]		150.	5.22	5.08	5.70	279.	1.15
H-O⁴⁺							
0.111	40.6	11.5	6.59	11.5	6.59	Ref [22]	
0.202	42.1	15.5	6.66	15.5	6.66		
0.478	44.8	20.5	6.57	20.5	6.57		
0.857	48.6	30.6	6.22	30.6	6.22		
1.30	47.9	44.8	5.73	44.8	5.73		
1.76	44.5	73.0	5.01	73.0	5.01		
2.50	42.6	122.	4.05	122.	4.05		
3.37	42.8	195.	3.05	195.	3.05		
4.40	43.5	262.	2.48	262.	2.48		
5.65	44.0	373.	1.93	373.	1.93		
7.02	42.5	411.	1.80	411.	1.80		
Ref [7]		Ref [22]		Ref [21]			
H-Ne⁶⁺							
2.58	53.0	5.15	39.3	0.402	14.2	0.343	17.0
Ref [16]		11.5	34.6	0.996	12.3	1.20	17.4
37.5	20.4	41.6	18.5	2.01	10.5	7.96	12.2
50.0	18.6	94.5	7.65	10.1	6.05	19.1	8.43
75.0	12.8	160.	3.11	20.0	4.21	57.9	4.23
100.	7.01	246.	0.96	100.	1.20	104.	2.30
125.	4.26	410.	0.12	203.	0.45	153.	1.33
Ref [10]		Ref [22]		280.	0.20	213.	0.693
H-Ne⁸⁺							
5.11	57.5	0.402	14.2	0.402	14.2	0.343	17.0
11.5	48.7	0.996	12.3	0.996	12.3	1.20	17.4
41.6	28.6	2.01	10.5	2.01	10.5	7.96	12.2
94.4	13.2	10.1	6.05	10.1	6.05	19.1	8.43
159.	6.18	20.0	4.21	20.0	4.21	57.9	4.23
245.	2.54	100.	1.20	100.	1.20	104.	2.30
416.	0.43	203.	0.45	203.	0.45	153.	1.33
Ref [22]		280.	0.20	280.	0.20	213.	0.693
H-Al⁶⁺							
0.405	32.0	0.405	32.0	0.405	32.0	0.343	17.0
0.995	29.3	0.995	29.3	0.995	29.3	1.20	17.4
2.00	25.8	2.00	25.8	2.00	25.8	7.96	12.2
10.1	15.7	10.1	15.7	10.1	15.7	19.1	8.43
20.1	11.2	20.1	11.2	20.1	11.2	57.9	4.23
101.	3.17	101.	3.17	101.	3.17	104.	2.30
204.	1.18	204.	1.18	204.	1.18	153.	1.33
280.	0.54	280.	0.54	280.	0.54	213.	0.693
Ref [22]		Ref [22]		Ref [22]		315.	0.207
H-Si⁴⁺							

Table 2. Evaluated theoretical total charge exchange cross sections (σ_t) for the process $A^{q+} + H \rightarrow A^{(q-1)+} + H^+$ as a function of E/M, the laboratory energy of the ion divided by the mass of the ion (continued).

E/M (keV/u)	σ_t (10^{-15} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)
H-Si⁶⁺							
0.305	35.3	0.353	19.2	0.422	101.	0.294	56.7
1.13	34.4	1.45	19.0	1.96	92.6	0.995	56.5
5.10	28.2	6.69	15.4	8.06	63.3	1.97	53.5
13.1	20.5	16.0	12.1	26.4	37.7	10.0	37.5
35.5	12.6	40.3	7.08	81.4	16.7	19.8	29.3
80.1	6.85	65.9	4.24	144.	9.06	100.	10.6
131.	3.93	115.	2.05	232.	4.13	201.	4.84
201.	2.09	179.	0.79	365.	1.42	252.	3.38
282.	0.95	231.	0.32	618.	0.14	Ref [22]	
352.	0.38	Ref [8]		Ref [8]			
H-Si⁸⁺							
0.321	59.0	0.370	41.0	0.295	16.4	0.295	99.5
1.49	55.2	1.08	41.4	0.996	16.6	0.994	96.3
6.49	41.8	8.15	30.0	1.97	15.4	1.98	89.7
16.0	30.1	18.5	21.0	10.1	10.8	10.1	62.9
41.7	17.9	36.3	13.7	20.0	8.10	20.0	47.7
93.4	9.13	65.0	8.30	101.	2.48	101.	16.4
168.	4.39	115.	4.25	200.	0.85	202.	7.90
234.	2.46	177.	1.82	255.	0.47	252.	5.71
301.	1.26	244.	0.85	Ref [22]		Ref [22]	
376.	0.46	316.	0.26	Ref [22]		Ref [22]	
H-Ti¹⁰⁺							
0.298	94.2	0.389	58.4	0.294	34.9	0.371	17.2
1.45	84.1	2.49	52.4	0.996	36.4	3.41	17.3
7.50	60.6	16.5	31.8	1.98	35.2	14.4	13.7
32.0	31.5	38.3	19.9	10.1	26.3	36.3	10.6
96.5	13.6	87.8	9.76	20.1	20.4	59.1	7.85
153.	7.63	167.	4.21	101.	7.37	92.3	5.62
245.	3.45	240.	2.17	202.	3.14	124.	3.89
313.	1.77	358.	0.69	254.	2.14	154.	2.45
397.	0.65	Ref [8]		Ref [22]		245.	0.36
492.	0.22	Ref [8]		Ref [22]		Ref [8]	
H-Fe⁴⁺							
H-Ti⁴⁺							
H-Ti⁶⁺							
H-Ti⁸⁺							

Table 2. Evaluated theoretical total charge exchange cross sections (σ_t) for the process $A^{q+} + H \rightarrow A^{(q-1)+} + H^+$ as a function of E/M , the laboratory energy of the ion divided by the mass of the ion (continued).

E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)
H-Fe⁶⁺							
0.36	35.6	55.	38.0	0.14	23.9	0.4	55.0
3.13	34.9	75.	33.7	0.17	24.5	1.0	54.1
15.5	24.1	100.	22.3	0.23	24.4	2.0	51.9
47.3	14.7	122.	15.1	0.31	24.1	10.	41.1
94.4	9.34	150.	8.37	0.46	23.3	20.	33.2
130.	6.53	175.	3.84	0.66	21.8	100.	13.4
157.	4.56	200.	2.60	0.96	20.0	200.	4.35
185.	3.13	225.	1.64	1.30	18.5	318.	0.82
233.	1.20	CTMC from Ref [18]		1.72	17.1	Ref [22]	
	Ref [8]			2.21	15.7		
H-Fe⁸⁺							
0.36	55.5	0.36	110.	2.96	14.0	0.4	98.6
3.07	50.3	1.37	101.	3.63	12.9	1.0	92.4
29.7	26.2	10.9	66.4	4.77	11.5	2.0	87.0
72.7	15.7	42.9	34.5	Ref [21]		10.	65.8
110.	11.5	86.8	20.3			20.	53.5
138.	8.57	141.	12.1			100.	21.8
172.	5.88	194.	7.50			200.	8.2
219.	2.80	243.	4.41			317.	2.0
299.	0.72	376.	0.75			Ref [22]	
	Ref [8]	Ref [8]					
H-Fe¹⁰⁺							
		50.0	66.7	0.40	20.0	0.35	16.3
		80.0	61.8	1.0	20.1	2.28	13.6
		103.	51.7	2.0	19.4	19.1	7.15
		127.	38.4	10.	15.7	62.7	3.34
		150.	23.5	20.	12.2	148.	1.36
		175.	14.7	100.	4.12	229.	0.66
		205.	8.36	200.	1.33	261.	0.46
		254.	3.75	318.	0.21	325.	0.18
		300.	1.91	Ref [22]		Ref [22]	
		CTMC from Ref [18]					
H-Kr⁴⁺							
		0.40	38.6	0.40	38.6		
		1.0	38.8	2.0	38.0		
		10.	30.2	10.	30.2		
		20.	25.0	100.	8.20		
		100.	2.36	200.	0.37		
		318.	0.37	Ref [22]			
H-Kr⁶⁺							
		0.40	38.6	0.40	38.6		
		1.0	38.8	2.0	38.0		
		10.	30.2	10.	30.2		
		20.	25.0	100.	8.20		
		100.	2.36	200.	0.37		
		318.	0.37	Ref [22]			
H-Nb⁴⁺							
		0.35	16.3	0.35	16.3		
		2.28	13.6	2.28	13.6		
		19.1	7.15	19.1	7.15		
		62.7	3.34	62.7	3.34		
		148.	1.36	148.	1.36		
		229.	0.66	229.	0.66		
		261.	0.46	261.	0.46		
		325.	0.18	325.	0.18		
		Ref [22]		Ref [22]			

Table 2. Evaluated theoretical total charge exchange cross sections (σ_t) for the process $A^{q+} + H \rightarrow A^{(q-1)+} + H^+$ as a function of E/M , the laboratory energy of the ion divided by the mass of the ion (continued).

E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)
H-Nb 6+							
0.36	33.9	0.54	31.7	50.	57.8	0.67	17.2
2.27	29.6	3.89	31.4	80.	52.0	5.24	16.4
18.8	17.9	27.8	19.9	103.	45.2	26.0	11.5
62.3	9.84	99.1	8.65	127.	29.9	54.7	8.28
148.	3.99	146.	5.30	150.	19.8	100.	5.14
228.	1.98	197.	2.93	175.	10.2	153.	3.03
258.	1.53	322.	0.34	205.	7.40	195.	1.98
321.	0.80	Ref [8]		225.	5.00	240.	0.88
	Ref [22]			254.	4.87	Ref [8]	
				275.	2.81		
				300.	1.22		
				CTMC from Ref [18]			
H-Nb 8+							
0.36	53.5	0.55	54.7				
2.29	47.7	2.81	50.0				
18.9	29.3	22.7	34.8				
62.9	16.2	66.0	21.6				
148.	7.82	127.	12.4				
230.	3.83	182.	7.28				
259.	2.96	255.	2.90				
323.	1.71	502.	0.14				
	Ref [22]	Ref [8]					
H-Nb 10+							
0.36	89.5	0.56	107.				
2.29	70.8	5.00	93.0				
18.8	41.8	21.9	68.9				
62.6	24.1	61.9	44.2				
147.	12.7	112.	28.2				
228.	7.79	153.	19.5				
258.	6.41	198.	13.3				
324.	3.84	241.	9.02				
	Ref [22]	290.	4.18				
		416.	0.76				
		Ref [8]					
H-Mo 4+							
0.44	18.1						
2.32	18.6						
12.7	14.3						
36.0	9.54						
83.4	5.20						
135.	3.16						
191.	1.63						
257.	0.63						
	Ref [8]						
H-Mo 6+							
0.63	34.0						
3.34	32.9						
26.0	23.2						
53.6	16.9						
88.0	11.6						
139.	6.74						
173.	4.42						
218.	2.81						
256.	1.41						
385.	0.20						
	Ref [8]						
H-Xe 6+							
0.67	59.6						
5.24	54.5						
26.0	35.7						
54.7	20.8						
100.	12.3						
153.	8.55						
195.	4.64						
240.	2.39						
	Ref [8]						
H-Xe 8+							
0.67	59.6						
4.90	54.5						
29.8	35.7						
78.5	20.8						
140.	12.3						
177.	8.55						
227.	4.64						
276.	2.39						
419.	0.34						
	Ref [8]						

Table 2. Evaluated theoretical total charge exchange cross sections (σ) for the process $Aq^+ + H \rightarrow A(q-1)^+ + H^+$ as a function of E/M , the laboratory energy of the ion divided by the mass of the ion (continued).

E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)	E/M (keV/u)	σ_t (10^{-16} cm^2)
<u>H-Xe 10+</u>							
0.53	96.2	0.40	34.9	0.38	88.0	0.77	57.0
4.30	84.5	2.15	29.1	2.49	71.2	3.57	53.0
20.0	59.3	18.0	16.8	35.4	35.8	19.5	32.7
58.2	36.4	53.6	9.07	123.	16.2	61.9	17.2
115.	22.0	111.	4.47	195.	9.51	147.	8.96
170.	14.8	188.	1.71	256.	6.20	240.	4.77
222.	9.15	285.	0.35	324.	3.28	292.	3.11
288.	4.60			434.	1.15	348.	1.51
374.	1.06			719.	0.11	580.	0.15
							Ref [8]
<u>H-Ta 6+</u>							
							Ref [22]
<u>H-Ta 7+</u>							
							Ref [8]
							Ref [22]
<u>H-Ta 8+</u>							
							Ref [8]
							Ref [22]
<u>H-Ta 9+</u>							
							Ref [8]
							Ref [22]
<u>H-Ta 10+</u>							
							Ref [8]
							Ref [22]

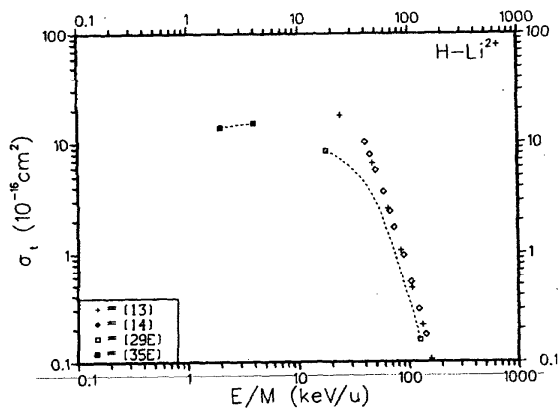


FIGURE 1. Evaluated total charge exchange cross sections for $H + Li^{2+} \rightarrow H^+ + Li^+$.

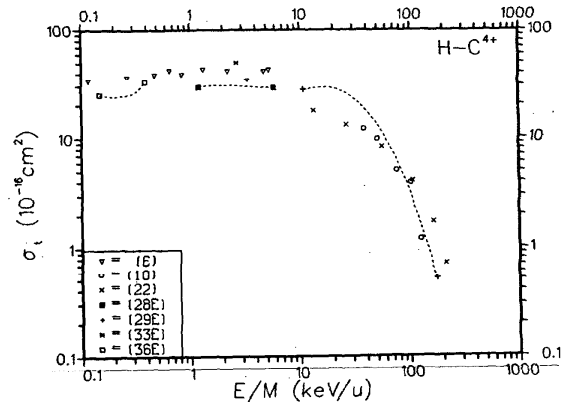


FIGURE 4. Evaluated total charge exchange cross sections for $H + C^{4+} \rightarrow H^+ + C^{3+}$.

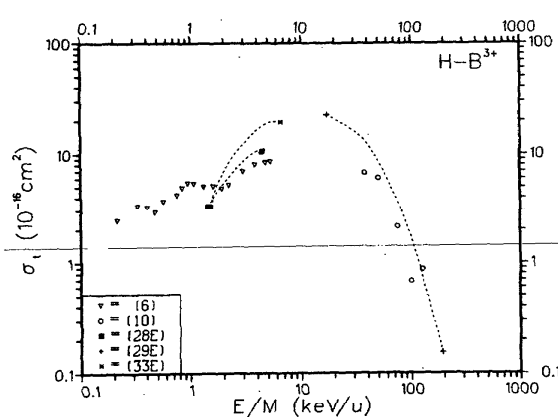


FIGURE 2. Evaluated total charge exchange cross sections for $H + B^{3+} \rightarrow H^+ + B^{2+}$.

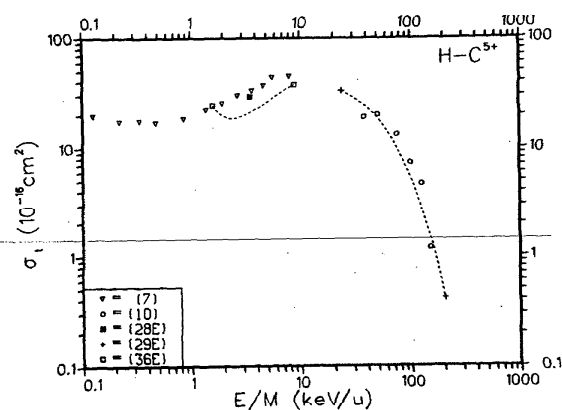


FIGURE 5. Evaluated total charge exchange cross sections for $H + C^{5+} \rightarrow H^+ + C^{4+}$.

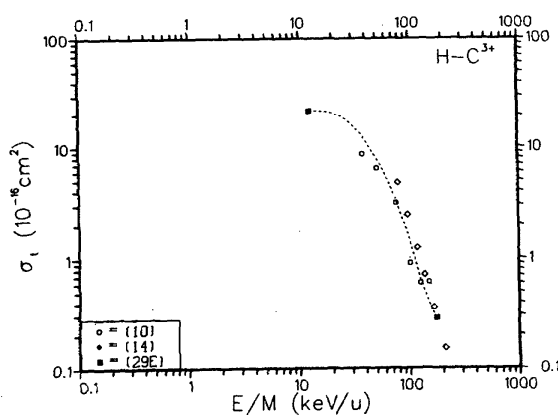


FIGURE 3. Evaluated total charge exchange cross sections for $H + C^{3+} \rightarrow H^+ + C^{2+}$.

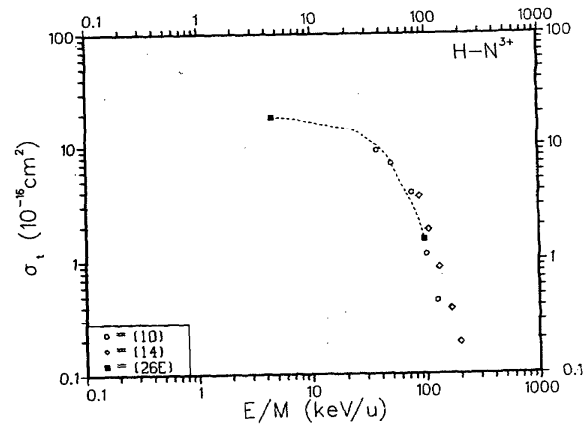


FIGURE 6. Evaluated total charge exchange cross sections for $H + N^{3+} \rightarrow H^+ + N^{2+}$.

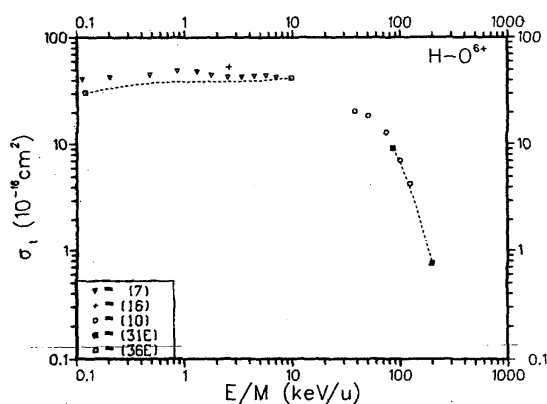


FIGURE 7. Evaluated total charge exchange cross sections for $H + O^{6+} \rightarrow H^{+} + O^{5+}$.

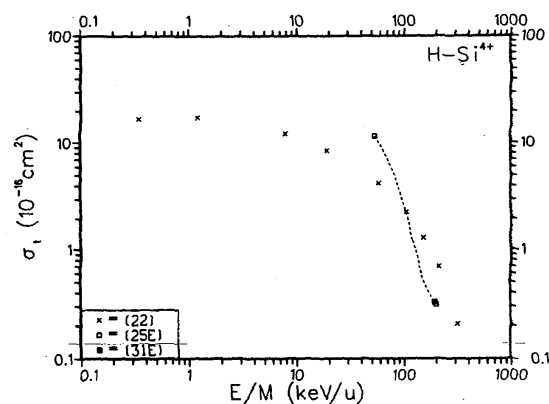


FIGURE 10. Evaluated total charge exchange cross sections for $H + Si^{14+} \rightarrow H^{+} + Si^{13+}$.

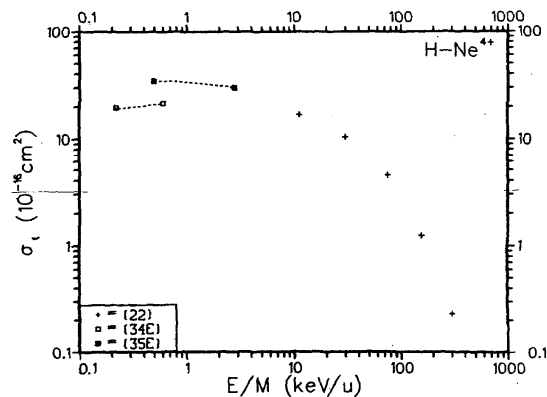


FIGURE 8. Evaluated total charge exchange cross sections for $H + Ne^{4+} \rightarrow H^{+} + Ne^{3+}$.

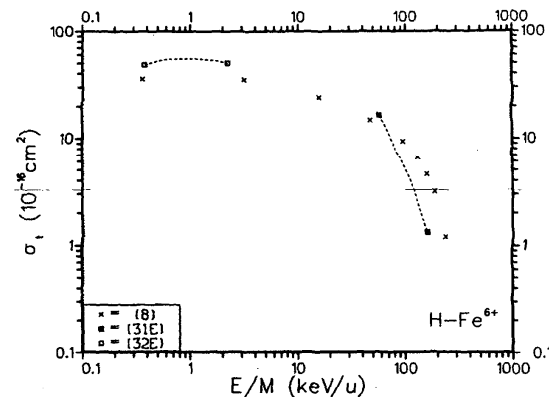


FIGURE 11. Evaluated total charge exchange cross sections for $H + Fe^{6+} \rightarrow H^{+} + Fe^{5+}$.

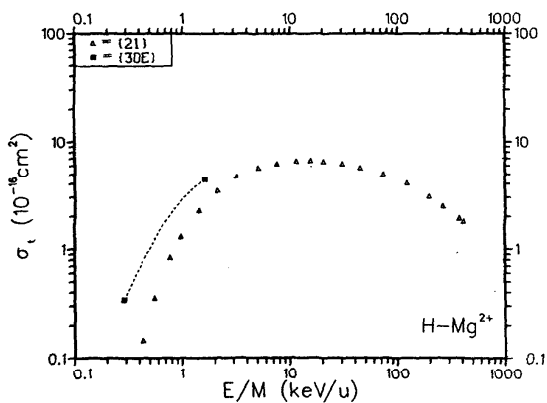


FIGURE 9. Evaluated total charge exchange cross sections for $H + Mg^{2+} \rightarrow H^{+} + Mg^{+}$.

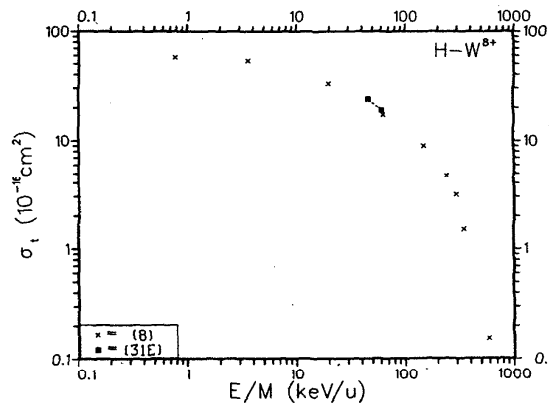


FIGURE 12. Evaluated total charge exchange cross sections for $H + W^{8+} \rightarrow H^{+} + W^{7+}$.

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