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# Absolute cross section measurements for dissociative capture of $H_2^+$ in Ar

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**Abstract**

Absolute differential and total cross sections for dissociative capture of $H_2^+$ in Ar to produce $H^-$, at projectile energies between 1.0 and 5.0 keV and for scattering angles from $-4^\circ$ to $4^\circ$ were measured. The absolute total cross sections (TCS) for the dissociative capture to produce $H^-$ are of the order of magnitude of $10^{-17}$ cm$^2$ and our measurements appear to merge well with previous experimental results. The measured TCS are one order of magnitude lower than the dissociative capture for the formation of $H^0$ atoms. The angular distributions of the $H^-$ fragment show a monotonic decrease in the differential cross sections with increasing angle and several interesting structures are observed, which give information on the production of $H^-$, i.e., attributed to the predissociative states of $H_2^+$ interacting with the target and with the two electron capture to form the excited state $H_2^-$.


*Keywords:* $H_2^+$; Angular distribution; Absolute cross section; Collision induced dissociation; Fragmentation mechanism; Ion fragmentation energies

## 1. Introduction

Among the many interactions and dynamical processes found in nature, the dissociative capture processes of $H_2^+$ ions in collision with atoms are one the most fundamental ones in "molecular ion-atom" collisions. Therefore, electron capture in collisions of ions with atoms in the low-keV-energy region has been one of the most active research areas for a long time [1–7], experimentally and theoretically, in atomic and molecular physics. This research provides fundamental information in atomic and molecular spectroscopy and many-body collision dynamics. The study of dissociative capture is also important in applications such as astrophysics [8], plasma modeling [9] and fusion research [10]. The dissociation of the $H_2^+$ ion, the simplest molecular ion, has long been investigated but little attention has been paid to the dissociative capture process to produce $H^-$ ions [6,7,11]. Recently we have reported [5] measurements of the absolute total and angular cross sections of the dissociative capture to produce $H^0$ fragments by the collision of $H_2^+$ on Ar atoms at low-keV energies. We suggested that the dissociative capture (DC) strongly favors molecules aligned along their velocity direction ($\Theta = 0$). Very little information is available regarding the cross sections for the dissociation capture of the formation of $H^-$ fragment [6]. In this paper we present absolute total and angular cross sections of the DC to produce $H^-$ ions by the collision of $H_2^+$ on Ar, i.e.,

$$H_2^+ + \mathrm{Ar} \rightarrow H^- + \cdots \quad (1)$$

at the incident energies between 1.0 and 5.0 keV, and for scattering angles from $-4^\circ$ to $4^\circ$.

## 2. Experiment

The experimental apparatus (Fig. 1) and technique were the same as those described in detail elsewhere [5]. The $H_2^+$ molecular ions were produced in a Colutron type ion source containing a mixture of 75% $H_2$ gas (ultra high purity), and 25% Ar to enhance ion production. $H_2^+$ ions were extracted and accelerated from 1.0 to 5.0 keV. Ions were focused by an Einzel lens and directed to a Wien velocity filter in order to obtain an analyzed $H_2^+$ beam at the desired velocity. The ions passed between cylindrical electrostatic defections plates, which were used both

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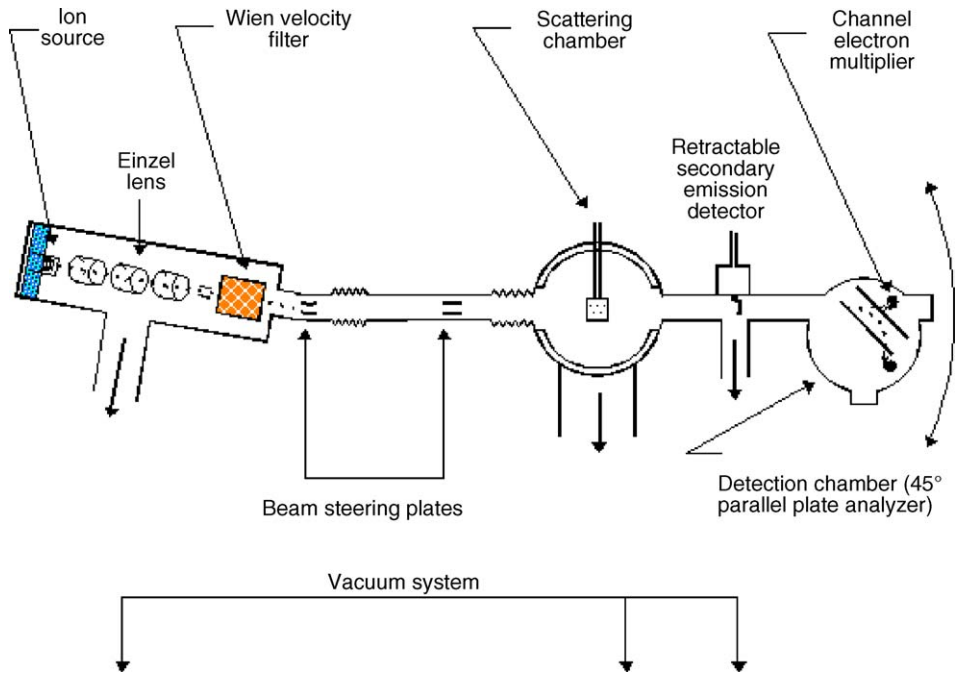


Fig. 1. Schematic diagram of the experimental apparatus.

to steer the beam and to bend it by 10°. The collimated $H_2^+$ beam entered the interaction cell, which housed a gas target cell, where the dissociation phenomena took place to form $H^-$, $H^+$ or $H^0$. The detector assembly rotated about the center of the gas target cell so that angular distributions could be obtained. The $H^-$ dissociation fragments, separated by a 45° parabolic electrostatic analyzer, were counted by channel electron multipliers (CEMs). The measured quantities were $I_0$ is the number of $H_2^+$ ions incident per unit area per second; $n$ the number of argon atoms per unit volume; $L$ the effective length of the scattering chamber; $I(\theta)$ is the number of $H^-$ fragments per unit solid angle ($d\Omega$) per second detected at angle ($\theta$) with respect to the incident beam direction. Thin target conditions were used in this experiment. The absolute differential cross sections (DCS) for the formation of $H^-$ were evaluated from the measured quantities by the expression:

$$\frac{d\sigma}{d\Omega} = \frac{I(\theta)}{nLI_0} \tag{2}$$

The total cross sections (TCS) for the production of the $H^-$ ions were obtained by numerical integration of $d\sigma/d\Omega$ over all measured angles.

The overall uncertainties were 15%, which arise from: the effective length of the target cell (3%); density determination (7%); measurements of the incident ion current (2%); detector calibration (3%). The absolute TCSs were reproducible to within 10%.

## 3. Results and discussion

Five processes can be produced by the dissociative capture of the molecular hydrogen $H_2^+$ in collisions with Ar atoms, which are:

$$H_2^+ + Ar \rightarrow (H_2^0)^* + Ar^+ \rightarrow H^0 + H^0 + Ar^+ \tag{3}$$

$$H_2^+ + Ar \rightarrow (H_2^0)^* + Ar^+ \rightarrow H^+ + H^0 + Ar^+ + e \tag{4}$$

$$H_2^+ + Ar \rightarrow (H_2^0)^* + Ar^+ \rightarrow H^+ + H^+ + Ar^+ + 2e \tag{5}$$

$$H_2^+ + Ar \rightarrow (H_2^0)^* + Ar^+ \rightarrow H^- + H^+ + Ar^+ \tag{6}$$

$$H_2^+ + Ar \rightarrow (H_2^-)^* + Ar^{2+} \rightarrow H^- + H^0 + Ar^{2+} \tag{7}$$

All of the above processes contribute to the measured signals of protons, negative hydrogen and neutral atoms produced in the DC process. The present experimental TCS for the production of the $H^-$ fragment (processes (6) and (7)) are shown in Fig. 2 together with Fedorenko's et al. [6] results for 12 keV. In the present experiment it was only possible to measure the DCSs until $\Theta_{max}$. For $\Theta > \Theta_{max}$ the DCSs drop below the experimental detection limit, and it was therefore necessary to perform a simple power-law extrapolation in order to obtain an upper limit of this contribution for all the energies, this was of $7 \times 10^{-19}$ cm$^2$, which is less than a 10% for energies above 2 keV. The integral cross sections are therefore, for all practical purposes, equal to the absolute TCSs. The absolute TCS for the formation of $H^-$ is of the order of magnitude of $10^{-17}$ cm$^2$. Although the present measurements do not overlap in energy with Fedorenko's et al. [6] results, it is readily apparent that the present absolute TCS for the dissociative capture to produce $H^-$ are consistent with Fedorenko's et al. [6] results. For the molecular $H_2^+$ ions incident on Ar at low energies, process (3) is the dominant dissociative capture mechanism, analogous to the case of an incident atomic beam. On the other hand, processes (6) and (7) require an interaction with the tightly bound target core electrons in order to obtain the necessary energy transfer (>17.32 and >13.39 eV,

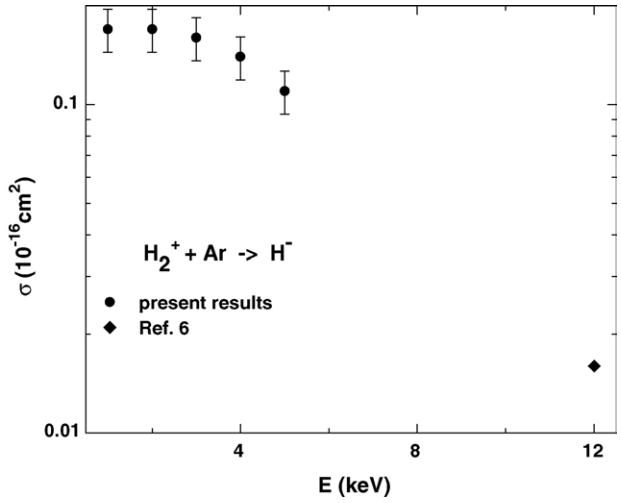


Fig. 2. Absolute total cross section for the production of $H^-$ fragments from collisions of $H_2^+$ on Ar.

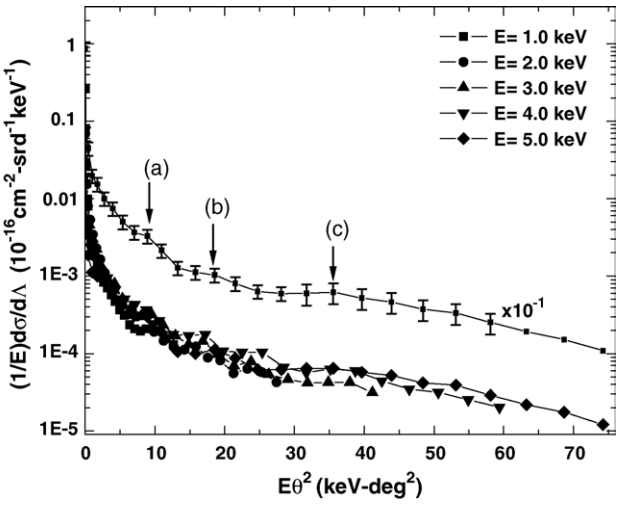


Fig. 4. Scaled angular distribution.

respectively). This fact advises a weaker probability for the production of the $H^-$ fragment, which is consistent with the present results. Previous measurements reported by Martínez and Yousif [5] for the TCS of process (3) indicate an order of magnitude of $10^{-16}$ cm$^2$, which is about ten times bigger than that reported in this paper for the formation of the $H^-$ fragment.

Fig. 3 illustrates typical DCS of the $H^-$ fragment for $H_2^+$ incident on Ar gas target at the collision energy between 1.0 and 5.0 keV. It can be seen that $H^-$ is formed mainly in the forward direction, and several defined structures appear at angles different from $0^0$. It well known that a peak in the angular distribution for a fragment can be interpreted as due to a singularity in the Jacobean of a transformation [7,11]. So, the dissociation energy can be determined from the location of the peak $E_d = E\theta^2_{peak}$. To gain more insight into the collision processes and to derive information about some features of the molecular interaction involved, the measured angular distributions are replotted in terms of the scaled variables $E\theta^2$ and $(1/E)\,d\sigma/d\Omega$ as shown in Fig. 4. The solid line of Fig. 4 is an average of all the measured angular distributions together with the statistical error. As can be seen in the figure, a clear structure (label "a" in Fig. 4) was observed which can be correlated with the value of $E_d$ when the maximum is reached in each structure; that value is 2.71 eV (8.9 keV deg$^2$) and two vestige of structures (labels "b" and "c" in Fig. 4) are notice between 4.05 and 6.56 eV (13.29 and 21.52 keV deg$^2$), and 9.66 and 12.08 eV (31.74 and 39.64 keV deg$^2$). Some of these structures have been observed previously in the dissociation of $H_2^+$ on Mg [11] (4.0, 7.2 and 12.1 eV), and in $H_2^+$ on Kr [7] (4.0 and 7.3 eV). Peterson and Bae [12] observed between 7.0 and 8.0 eV the same type of structures in the $D_2^+ + Cs$ system. They concluded that this peak is caused by the predissociation of the $c^3\Pi_u$ state into the repulsive $b^3\Sigma_u^+$. This in turn was based on the research of de Bruijn et al. [1] who used different gas targets. They found that the structure between 7.2 and 10.0 eV was always present with different intensities according to the characteristics of the gas target; the structure at 4.0 eV appears in Mg and Kr targets and we have found it is also present in an Ar target between 4.05 and 6.56 eV. We feel that the agreement between these released kinetic energies and the *E*d values found, yield to assure that a single electron is transferred from the Ar atom to the molecular ion leading to excited products, that can capture another electron in the way out of the cell producing the $H^-$, i.e.,

$$H_2^+(X^2\Sigma_g^+) + Ar \rightarrow H_2^0(c^3\Pi_u) + Ar^+ \rightarrow H_2^0(b^3\Sigma_u^+) + Ar^+ \rightarrow H^0 + H^0 + Ar^+ \quad (8)$$

followed by

$$H^0 + Ar \rightarrow H^- + Ar^+ \quad (9)$$

This interpretation is the same as that of Peterson and Bae [12] for $D_2^+ + Cs$. For the peak at 2.71 eV, the possible explanation is to consider the double electron capture of the $H_2^+$ ($X^2\Sigma_g^+$) to the repulsive state $H_2^-$ ($b + e^-{}^2\Sigma_g^+$) at the internuclear separation of 1.2 Å,which give a dissociation energy of approximately 2 eV

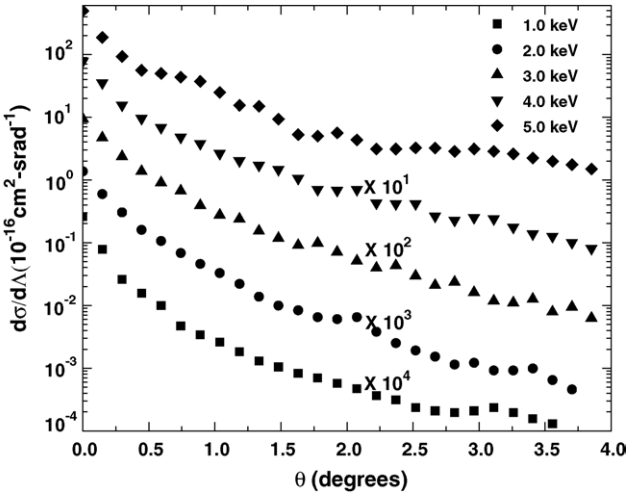


Fig. 3. Angular distributions for the formation of $H^-$ fragment from collisions of $H_2^+$ on Ar.

(see potential energy curves of Ref. [13]), i.e.,

$$H_2{}^+(X^2\Sigma_g{}^+) + Ar \rightarrow H_2{}^-(b + e^{-2}\Sigma_g{}^+) + Ar^{2+} \rightarrow H^- + H^0 + Ar^{2+} \quad (10)$$

Since the DCSs and TCS contain contributions from the two-dissociation channel; those are reactions (8) follows by (9) and (10); from the present work, it was not possible to identify the contributions of them. The contributions of the mechanisms involved in the formation of $H^-$ require a careful study of the molecular potential energy curves of the collision system.

Due to the relevant information contained in the shape of the TCS as a function of the collision energy for charge exchange (CE), we can consider that there are two processes that compete with each other. Knowing that the TCSs for different processes depend strongly on the ionization potential of the target atom and the low-energy behavior in asymmetric charge–transfer collisions, they can be discussed in terms of the energy $E_m$ at which the electron capture cross section reaches a maximum value. Based on simple energy balance arguments it would appear that the TCS should exhibit a near-resonant behavior, i.e., the energy $E_m$ at which the cross sections of the processes (8) follow by (9) is of 33,422.39 eV that agrees with the increasing behavior of the TCSs for reactions (9) and (10) measured by Martínez and Yousif [5] and Martínez et al. [14]. While for reaction (10), the energy $E_m$ is of 700 eV. Although it is not possible to identify the specific processes from the present study the shape of the curve in Fig. 2 suggest that may be due to process (10).

## 4. Conclusions

In conclusion, the total and angular cross-sections of $H^-$ fragments as a result of the interaction of $H_2{}^+$ with Ar gas have been measured. The angular distributions exhibit several structures that fit with those originated from the predissociation of the same molecular ion with different targets. This fact indicates that the reaction $H_2{}^+ + Ar \rightarrow H_2 + Ar^+ \rightarrow H + H + Ar^+$, followed by $H + Ar \rightarrow H^- + Kr^+$ is suitable and can explain the presence of the structures at the same dissociation energy as those due to the predissociation. While the structure at 2.1 eV is attributed to come from the process $H_2{}^+ (X^2\Sigma_g{}^+) + Ar \rightarrow H_2{}^- (b + e^{-2}\Sigma_g{}^+) + Ar^{2+} \rightarrow H^- + H^0 + Ar^{2+}$, which is the cause of the shape of the absolute total cross section. The TCS for the formation of $H^-$ are of the order of magnitude of $10^{-17}$ cm$^2$ and our measurements appear to merge well with previous experimental result.

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