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Single electron capture in slow collisions of H_2^+ ions with H_2, O_2 and N_2 diatomic molecules

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Abstract

Collisions of the slow molecular hydrogen ions, H_2^+ on H_2, O_2 and N_2 diatomic molecules in the energy range 700–2000 eV have been studied experimentally using the time-of-flight technique. The total cross sections for H_2^+ with H_2, O_2 and N_2 are found to be in the range of $(1.79 \pm 0.27–2.78 \pm 0.42)$ Å^2, $(3.43 \pm 0.51–5.15 \pm 0.78)$ Å^2 and $(3.46 \pm 0.52–5.03 \pm 0.75)$ Å^2, respectively. The measured electron capture cross sections show a slowly increasing behavior as a function of the incident energy. The measured cross sections for H_2^+ with H_2 systems are compared with the existing data.

Keywords: Electron capture; By slow H_2^+ ions

1. Introduction

Investigations of charge exchange reactions in ion–atom, ion–molecule and more recently ion–ion collisions are of fundamental interest in detailed understanding of collisions mechanisms involved. Theses reactions are also of great importance in of variety of research fields, such as the description of many astrophysical and terrestrial environments [1] and controlled thermonuclear fusion or ion accelerator technology [2]. Charge transfer with molecular targets has received considerable experimental attention. Numerous measurements have been made with ion beam [3–9], flow tubes [10] and ion traps [11]. Model computations of electron capture in low-energy multiply charged ion–atom collisions have progressed to an advanced state, being successfully able to reproduce the available data on differential and total cross sections, studies of ion–molecule collisions are considered in an early or partially developed stage. Experimental methods combined with theoretical calculations from Landau–Zener model to ab-initio molecular expansion methods within either time-dependent or time-independent collision treatment [12–16], provide a comprehensive study of these reactions.

Single electron capture constitutes the dominant charge transfer process in slow collisions between charged ions and neutral gas molecules. At low impact energies, total capture cross sections are dominated by capture from outermost target shell. However, as the projectile energy increases, capture from inner shells plays the main role until at high energies charge exchange from the K-shell dominates. In general, cross sections for processes in which more than one electron is captured are considerably smaller than single electron capture processes [7].

During a collision between a charged projectile and a target molecule an electron of the target molecule can be captured by the projectile into the ground state or into an excited state:

$$H_2^+ + H_2 \rightarrow H_2 + H_2^+ + \Delta E$$

$$H_2^+ + N_2 \rightarrow H_2 + N_2^+ + \Delta E$$

$$H_2^+ + O_2 \rightarrow H_2 + O_2^+ + \Delta E.$$

The energy defect ΔE is determined by the difference between the recombination energy, which is released after the capture of an electron by the projectile, and the energy needed to ionize the target molecules. At low impact energy, the reaction window of single electron capture favors moderately exothermic reactions over endothermic or strongly exothermic reactions. At this low impact energy regime, electron capture takes place very

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effectively through pseudocrossings of the adiabatic potential energy curves describing the initial and final molecular system.

The lack of extensive total cross-section measurements for the collisions of H_2^+ with atomic and molecular targets has suggested more work is necessary in order to obtain accurate data at low impact energies. Therefore, the main goal of this article is to provide reliable measurements for single electron capture by charged ions in collision with neutral diatomic molecules. We illustrate this by measuring the absolute total cross sections of H_2^+ on H_2, O_2 and N_2 collisions. The energy range covered by the present experimental study is between 0.7 and 2 keV. These total cross sections will be compared with the existing experimental and theoretical data.

2. Experimental set-up and procedure

2.1. General

Details of the experimental arrangement have been given previously [3–7], so the experimental set-up will be described here briefly. H_2^+ ions were produced in the recoil ion source (RIS) in collision of F^{4+} beam with H_2 molecular gas. The recoil H_2^+ ions were extracted, accelerated and passed through the first accelerating unit (Einzel-type lens) by an applied electric field which is transverse to the F^{4+} beam direction. After that, the collimated recoil H_2^+ ions were directed into differentially pumped target cell where capture phenomena took place to form H_2^0. The gas-target cell was a 5.8-cm long cylinder cell with entrance and exit apertures of 1 and 2.5 mm in diameter, respectively. The gas target was kept low enough (typically ∼0.6 mTorr) to ensure single collision conditions. The target cell was field-free to avoid an undesired deflection of slow, highly charged ions. After leaving the gas-target cell, the emergent ions travelled through the second acceleration unit, which is identical to the first acceleration unit, to a position sensitive channel-plate detector via a parallel-plate electrostatic analyzer. The neutral beam of H_2^0 passed straight through the analyzer, where as the separation of charged ions occurred inside the analyzer. The analyzer voltage was set to detect the H_2^+ ions. The ions were analyzed according to their time-of-flight which is proportional $\sqrt{m/q}$ (mass-to-charge ratio). The use of the electrostatic analyzer in conjunction with the TOF technique allows one to identify the various events associated with the charged ions.

2.2. Evaluating of the absolute total cross section

Thin target conditions were used in this experiment, the absolute total single electron capture cross sections for formation of H_2^0 were evaluated by the following expression:

$$\sigma = \frac{H_2^0}{N_t n \varepsilon l}$$

where H_2^0 is the total number of the neutral events, N_t the measured number of incident ions, n the number of gas particles per cm^3 in the collision target cell and is related the measured pressure p in Pa according to $n = 2.45 \times 10^{14} p$ (at 22 °C), ε the detection efficiency of detector and l is the geometric length of the target cell. For the efficiency of the channel-plate detector (32.4%), we used the product of the active area ratio of the first channel-plate from the manufacturer's manual, which is 60%, and the transmission of the grids at the entrance of the detector, which is 54% [17,18].

2.3. Error estimate

The total uncertainties are estimated at 85% confidence level. The total uncertainty corresponds to quadrature sum of the statistical and systematic errors. The errors mainly originated from the fluctuation of the data, the gas target pressure stability in the measurements, the absolute transmission of the meshes and that of the detection efficiency of the microchannel plate. The counts from the background gas were measured without the H_2^+ ions and were usually less than 5%. These counts were subtracted from the data.

3. Results and discussion

Table 1 lists the measured absolute total cross sections and the total uncertainties for single electron capture by H_2^+ ions from H_2, O_2 and N_2 molecular gases as a function of collision energies. The energy dependence of single electron capture cross section is shown in Fig. 1. The total cross sections obtained exhibit a monotonically increasing behavior as a function of the impact energy. This behavior is typical of single electron capture cross sections between singly charged ions and neutral molecules for which capture is usually favored only between atomic ground states. This can be understood from the reaction window, which get boarder with increasing energy.

3.1. H_2^+–H_2

Fig. 2 shows the values for total cross sections measured in this investigation and the results of earlier studies. It can be noted that first, in the energy range 600–2000 eV, the present

Table 1
Lists the measured absolute total cross sections (Å^2) and the total uncertainties (15%) for single electron capture by H_2^+ ions from H_2, O_2 and N_2 molecular gases

E (eV)	$\sigma_{H_2^+,H_2}$	$\sigma_{H_2^+,O_2}$	$\sigma_{H_2^+,N_2}$
700	1.79	3.43	3.46
800	1.91	3.7	3.61
900	2.01	3.89	3.73
1000	2.1	4.01	3.86
1100	2.19	4.14	3.98
1200	2.25	4.26	4.14
1300	2.36	4.41	4.23
1400	2.44	4.51	4.38
1500	2.52	4.63	4.48
1600	2.56	4.75	4.54
1700	2.64	4.88	4.69
1800	2.72	4.97	4.78
1900	2.77	5.06	4.94
2000	2.78	5.15	5.03

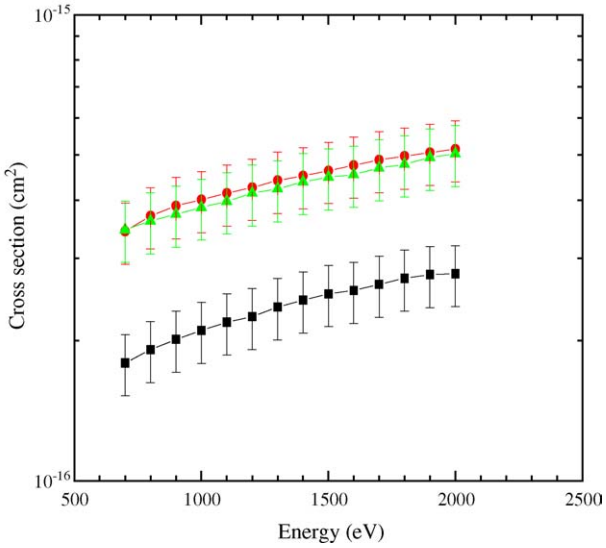

Fig. 1. Total cross sections for one-electron capture by H_2^+ ions from H_2 (■), O_2 (●) and N_2 (▲) molecular gases.

and the previous measured cross sections [19,21,25] increase slowly as the collision energy increases. Second, without exception, it is visible that there are discrepancies in the results with one another. These discrepancies may be due to random experimental errors, the differences in ion source operating conditions and the collection of slow ions. The use of energy sensitive detectors plays a significant role in eliminating this source of error. Third, there are significant deviations between experimental measurements theoretical calculation by Gurnee–Magee [23]. The Gurnee–Magee calculation pertains to the single resonant process:

$$H_2^+(v=0) + H_2(v=0) \rightarrow H_2(v=0) + H_2^+(v=0).$$

This result suggests the inadequacy of collisional wave function employed in this calculation. Leventhal–Moran-Friedman [22] took into account the vibrational states of the incident ions.

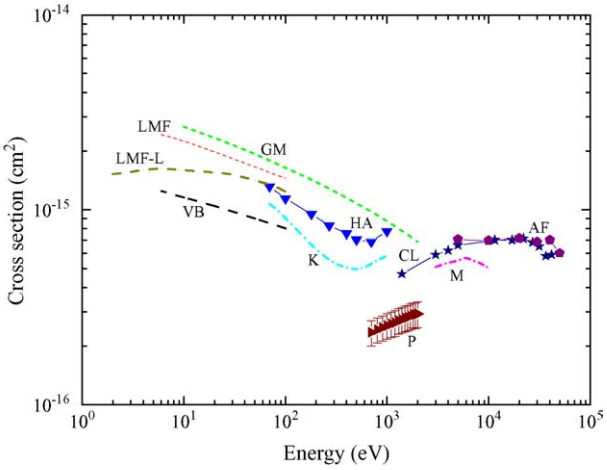

Fig. 2. Plot of total cross sections vs. the ion energy for one-electron capture by H_2^+ ions from H_2. P: present experimental result; K: Koopman [19]; VB: Vance et al. [20]; HA: Howard et al. [21]; LMF-L: calculation corrected for Langevin orbiting cross section (see Ref. [22,23]); LMF: Leventhal et al. [22], GM: Gurnee et al. [23]; M: McClure [24]; CL: Latimer et al. [25]; AF: Afrosimov et al. [26].

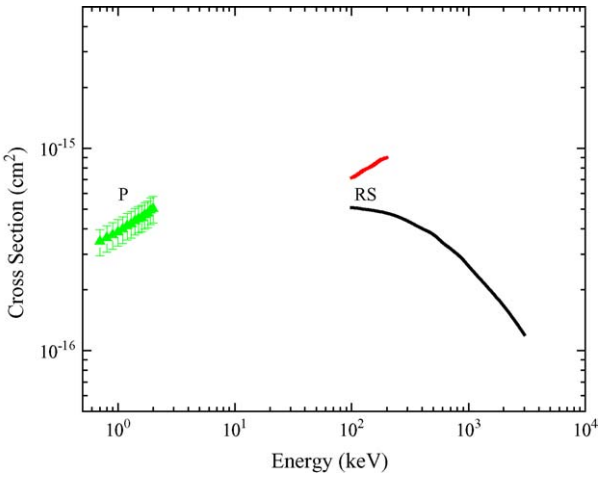

Fig. 3. Plot of total cross sections vs. the ion energy for one-electron capture by H_2^+ ions from N_2. P: present experimental result; RS, Ropke et al. [27].

They considered the initial H_2^+ ions are in Franck-Condon distribution of vibrational states. The final vibrational distribution of the product H_2 molecules produced by charge transfer was then taken simply to be the sum of all translational probabilities from H_2^+ ($v_i' = j$) to H_2 ($v_f'' = j$) which have the same value of j. Theory significantly overestimates the cross section. Last, it is apparent in these values [19,21] that there is a minimum in the cross section around 500 eV. Below this energy, the cross section behaves in a manner characteristic of resonance while at higher energies non-resonant behavior becomes dominant and the cross section increases with increasing energy.

3.2. H_2^+–N_2

The present low-energy data and the high-energy measurements [27] are shown in Fig. 3. It can be seen that; first the present measurements slowly increase with increasing incident energies. Second, the high-energy data are inconsistent with one another.

3.3. H_2^+–O_2

The dependence of the measured cross sections on the collision energy is shown in Fig. 1. These total single electron capture cross sections display slowly increasing behavior with increasing impact energies. Unfortunately, lack of experimental and theoretical data prohibits significant and direct comparison with present data.

4. Conclusion

We have presented the total electron capture cross sections for H_2^+ ions with H_2, O_2 and N_2 reactions at collision energies between 0.7 and 2.0 keV. The results of this investigation can be summarized as follows:

(a) The total cross sections for single electron capture were obtained for H_2^+ with H_2, O_2 and N_2 and found to be in the range of $(1.79 \pm 0.27–2.78 \pm 0.42)$ Å^2, $(3.43 \pm 0.51–$

$5.15 \pm 0.78)$ Å^2 and $(3.46 \pm 0.52–5.03 \pm 0.75)$ Å^2, respectively.

(b) The energy dependence of total cross sections is quite consistent with experimental results of Koopman [19], Howard et al. [21] and Latimer et al. [25].

(c) The literature values for H_2^+–H_2 system are widely scattered and are certainly inconsistent with one another. For this reason, it is quite conceivable that further work will have to be carried out in order to produce reliable data for direct comparison with those shown in Figs. 1–3.

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